wwPDB EM Validation Summary Report

Oct 13, 2024 – 02:27 am BST

PDB ID	:	6T90
EMDB ID	:	EMD-10406
Title	:	OCT4-SOX2-bound nucleosome - SHL-6
Authors	:	Michael, A.K.; Kempf, G.; Cavadini, S.; Bunker, R.D.; Thoma, N.H.
Deposited on	:	2019-10-25
Resolution	:	3.05 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:

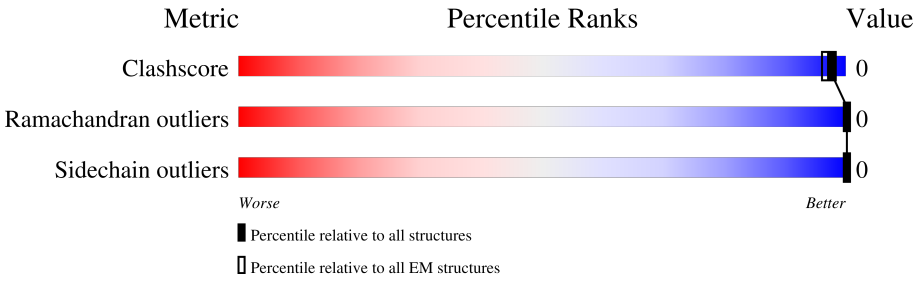
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.05 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	63% 5% 32%
2	B	106	66% 11% 23%
2	F	106	62% 14% 24%
3	C	133	74% 8% 18%
3	G	133	78% 18%
4	D	128	69% 27%
4	H	128	68% 5% 27%
5	E	137	63% 7% 31%

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Mol	Chain	Length	Quality of chain
6	I	153	
7	J	147	
8	K	643	
9	L	105	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13031 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	94	Total	C	N	O	S	0	0
			773	488	147	134	4		

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	C	N	O	S	0	0
			653	412	127	113	1		
2	F	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			837	526	166	145		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	109	Total 840	C 529	N 166	O 145	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 725	C 456	N 130	O 137	S 2	0	0
4	H	93	Total 725	C 456	N 130	O 137	S 2	0	0

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 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
E	-2	GLY	-	expression tag	UNP P68431

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

- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	141	Total	C	N	O	P	0	0
			2870	1368	516	846	140		

- Molecule 7 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	141	Total	C	N	O	P	0	0
			2905	1379	544	842	140		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	73	Total	C	N	O	S	0	0
			593	387	100	103	3		

There are 49 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
K	-255	ASN	-	expression tag	UNP P42212
K	-254	LEU	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
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
K	361	LEU	-	expression tag	UNP Q01860
K	362	PRO	-	expression tag	UNP Q01860
K	363	GLU	-	expression tag	UNP Q01860
K	364	THR	-	expression tag	UNP Q01860
K	365	GLY	-	expression tag	UNP Q01860
K	366	GLY	-	expression tag	UNP Q01860
K	367	HIS	-	expression tag	UNP Q01860
K	368	HIS	-	expression tag	UNP Q01860
K	369	HIS	-	expression tag	UNP Q01860
K	370	HIS	-	expression tag	UNP Q01860
K	371	HIS	-	expression tag	UNP Q01860
K	372	HIS	-	expression tag	UNP Q01860

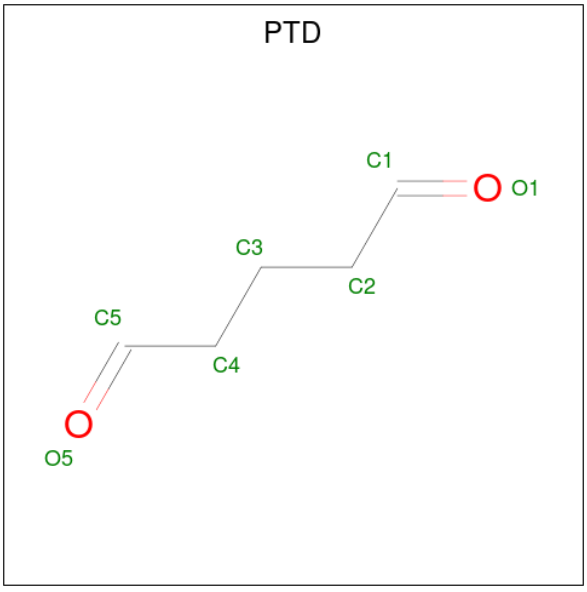
- Molecule 9 is a protein called Transcription factor SOX-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	74	Total	C	N	O	S	0	0
			636	398	129	104	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
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: $C_5H_8O_2$).



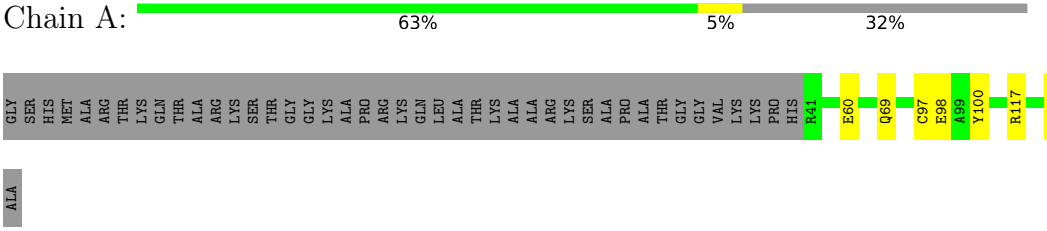
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 5 5	0
10	A	1	Total C 5 5	0
10	C	1	Total C 5 5	0
10	D	1	Total C 5 5	0
10	E	1	Total C 5 5	0
10	E	1	Total C 5 5	0
10	G	1	Total C 5 5	0
10	H	1	Total C 5 5	0
10	K	1	Total C 5 5	0

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.

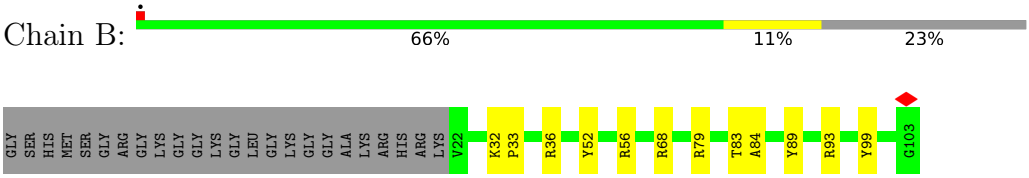
• Molecule 1: Histone H3.1

Chain A:



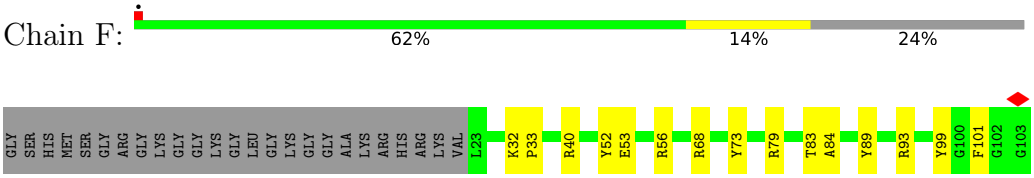
• Molecule 2: Histone H4

Chain B:



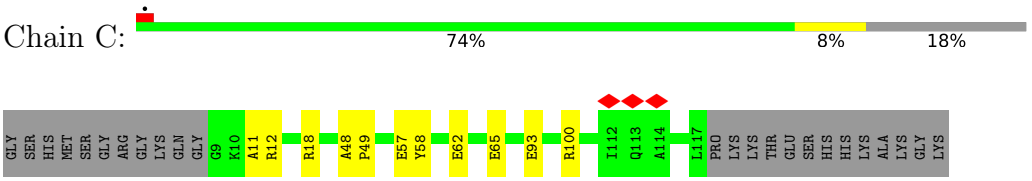
• Molecule 2: Histone H4

Chain F:



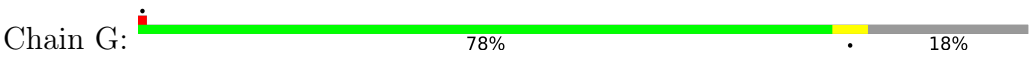
• Molecule 3: Histone H2A type 1-B/E

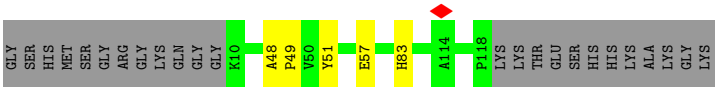
Chain C:



• Molecule 3: Histone H2A type 1-B/E

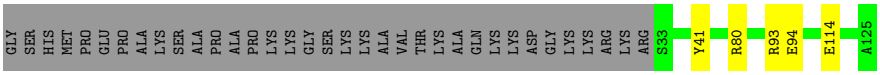
Chain G:





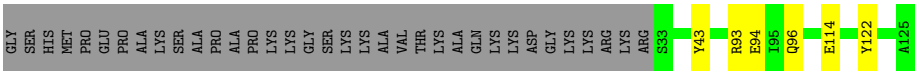
• Molecule 4: Histone H2B type 1-J

Chain D:



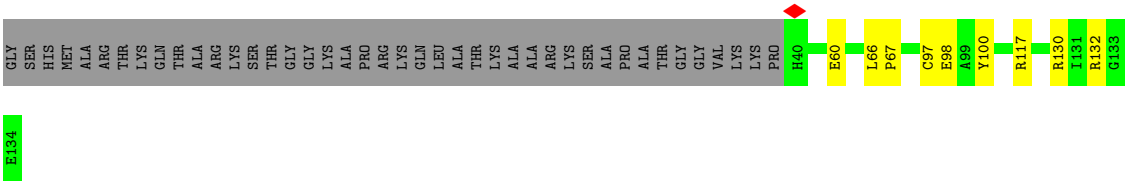
• Molecule 4: Histone H2B type 1-J

Chain H:



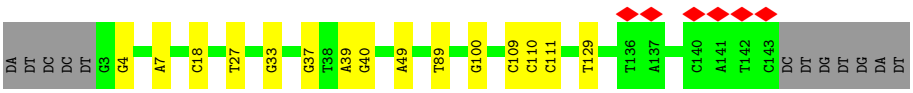
• Molecule 5: Histone H3.1

Chain E:



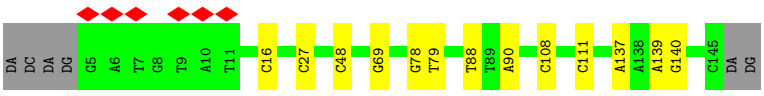
• Molecule 6: DNA (146-MER)

Chain I:



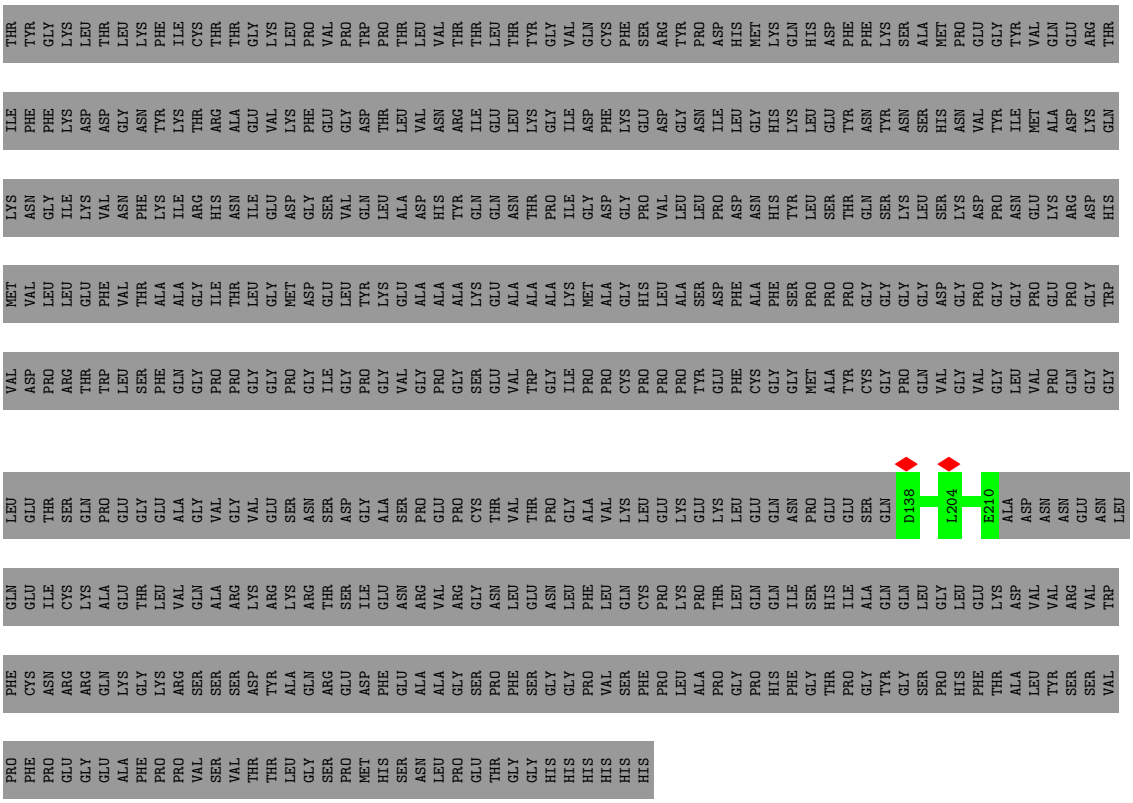
• Molecule 7: DNA (146-MER)

Chain J:



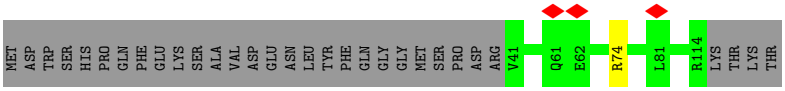
• Molecule 8: Green fluorescent protein,POU domain, class 5, transcription factor 1

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, C1	Depositor
Number of particles used	94282	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	1.087	Depositor
Minimum map value	-0.441	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.15	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	1.60	8/783 (1.0%)	0.90	1/1050 (0.1%)
2	B	1.76	7/660 (1.1%)	0.96	3/883 (0.3%)
2	F	1.73	10/653 (1.5%)	0.99	3/873 (0.3%)
3	C	1.46	12/846 (1.4%)	0.91	1/1139 (0.1%)
3	G	1.35	4/850 (0.5%)	0.85	0/1146
4	D	1.40	4/736 (0.5%)	0.91	4/990 (0.4%)
4	H	1.40	6/736 (0.8%)	0.92	2/990 (0.2%)
5	E	1.57	8/794 (1.0%)	0.91	1/1065 (0.1%)
6	I	1.20	4/3215 (0.1%)	1.39	17/4956 (0.3%)
7	J	1.20	0/3263	1.36	14/5039 (0.3%)
8	K	0.90	0/601	0.76	0/804
9	L	0.97	0/651	0.81	1/866 (0.1%)
All	All	1.34	63/13788 (0.5%)	1.16	47/19801 (0.2%)

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	94	GLU	CG-CD	-8.25	1.39	1.51
1	A	97	CYS	CB-SG	-7.82	1.69	1.82
2	B	93	ARG	CD-NE	-7.65	1.33	1.46
5	E	97	CYS	CB-SG	-7.06	1.70	1.82
6	I	49	DA	C5-C4	-7.01	1.33	1.38

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	93	ARG	NE-CZ-NH2	-9.87	115.36	120.30
4	D	93	ARG	NE-CZ-NH2	-9.66	115.47	120.30
6	I	89	DT	P-O3'-C3'	9.23	130.77	119.70
6	I	4	DG	P-O3'-C3'	8.49	129.89	119.70
5	E	117	ARG	NE-CZ-NH1	8.26	124.43	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	773	0	803	0	0
2	B	653	0	694	2	0
2	F	646	0	685	2	0
3	C	837	0	896	3	0
3	G	840	0	900	1	0
4	D	725	0	736	0	0
4	H	725	0	738	0	0
5	E	783	0	809	1	0
6	I	2870	0	1588	0	0
7	J	2905	0	1586	0	0
8	K	593	0	632	0	0
9	L	636	0	651	0	0
10	A	10	0	12	0	0
10	C	5	0	6	0	0
10	D	5	0	6	0	0
10	E	10	0	12	0	0
10	G	5	0	6	0	0
10	H	5	0	6	0	0
10	K	5	0	6	0	0
All	All	13031	0	10772	9	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 9 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)
3:C:11:ALA:O	3:C:12:ARG:HG3	1.98	0.63
3:C:11:ALA:O	3:C:12:ARG:CG	2.49	0.60
2:F:83:THR:OG1	2:F:84:ALA:N	2.46	0.48
2:B:83:THR:OG1	2:B:84:ALA:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:HB2	2:B:33:PRO:HD3	1.99	0.44

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	92/139 (66%)	92 (100%)	0	0	100	100
2	B	80/106 (76%)	80 (100%)	0	0	100	100
2	F	79/106 (74%)	78 (99%)	1 (1%)	0	100	100
3	C	107/133 (80%)	106 (99%)	1 (1%)	0	100	100
3	G	107/133 (80%)	106 (99%)	1 (1%)	0	100	100
4	D	91/128 (71%)	91 (100%)	0	0	100	100
4	H	91/128 (71%)	91 (100%)	0	0	100	100
5	E	93/137 (68%)	93 (100%)	0	0	100	100
8	K	71/643 (11%)	71 (100%)	0	0	100	100
9	L	72/105 (69%)	72 (100%)	0	0	100	100
All	All	883/1758 (50%)	880 (100%)	3 (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	82/113 (73%)	82 (100%)	0	100	100
2	B	67/81 (83%)	67 (100%)	0	100	100
2	F	66/81 (82%)	66 (100%)	0	100	100
3	C	84/102 (82%)	84 (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	79/106 (74%)	79 (100%)	0	100	100
5	E	83/112 (74%)	83 (100%)	0	100	100
8	K	65/536 (12%)	65 (100%)	0	100	100
9	L	67/95 (70%)	67 (100%)	0	100	100
All	All	757/1434 (53%)	757 (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)

9 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	C	201	4,3	4,4,6	0.45	0	3,3,5	0.41	0
10	PTD	A	202	1,2	4,4,6	0.39	0	3,3,5	0.50	0
10	PTD	H	201	4	4,4,6	0.49	0	3,3,5	0.32	0
10	PTD	D	201	4	4,4,6	0.48	0	3,3,5	0.37	0
10	PTD	E	202	1,5	4,4,6	0.44	0	3,3,5	0.43	0
10	PTD	A	201	1,5	4,4,6	0.40	0	3,3,5	0.45	0
10	PTD	G	201	4,3	4,4,6	0.41	0	3,3,5	0.44	0
10	PTD	E	201	5,2	4,4,6	0.37	0	3,3,5	0.49	0
10	PTD	K	401	9,8	4,4,6	0.43	0	3,3,5	0.41	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	C	201	4,3	-	1/2/2/4	-
10	PTD	A	202	1,2	-	0/2/2/4	-
10	PTD	H	201	4	-	2/2/2/4	-
10	PTD	D	201	4	-	2/2/2/4	-
10	PTD	E	202	1,5	-	0/2/2/4	-
10	PTD	A	201	1,5	-	0/2/2/4	-
10	PTD	G	201	4,3	-	1/2/2/4	-
10	PTD	E	201	5,2	-	0/2/2/4	-
10	PTD	K	401	9,8	-	1/2/2/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	201	PTD	C2-C3-C4-C5
10	H	201	PTD	C1-C2-C3-C4
10	H	201	PTD	C2-C3-C4-C5
10	G	201	PTD	C2-C3-C4-C5
10	C	201	PTD	C1-C2-C3-C4

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.

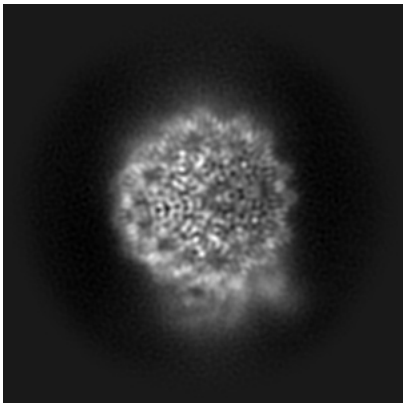
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10406. These allow visual inspection of the internal detail of the map and identification of artifacts.

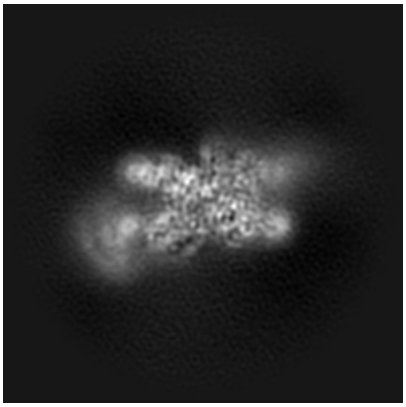
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

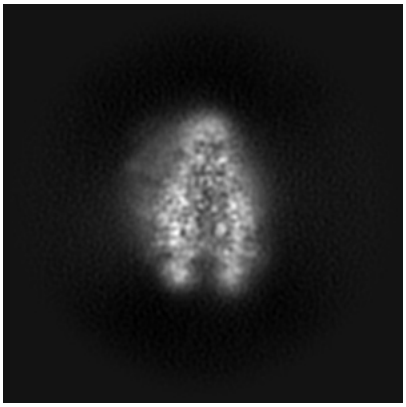
6.1.1 Primary map



X



Y

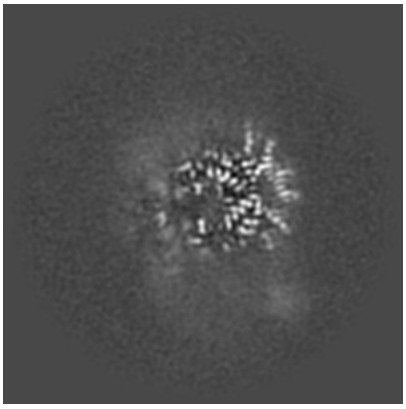


Z

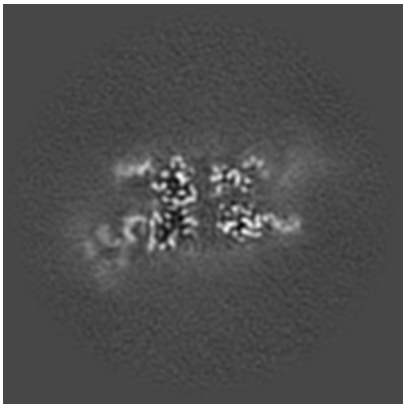
The images above show the map projected in three orthogonal directions.

6.2 Central slices

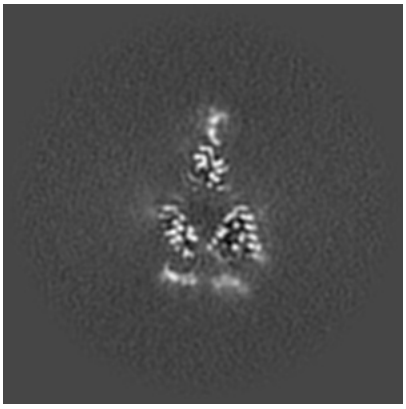
6.2.1 Primary map



X Index: 128



Y Index: 128

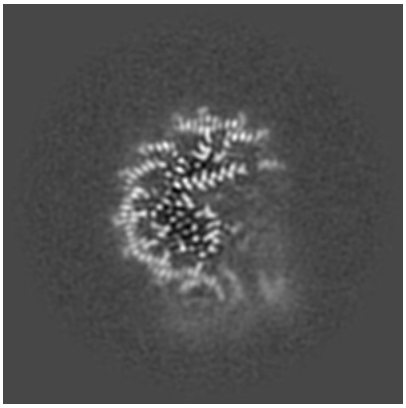


Z Index: 128

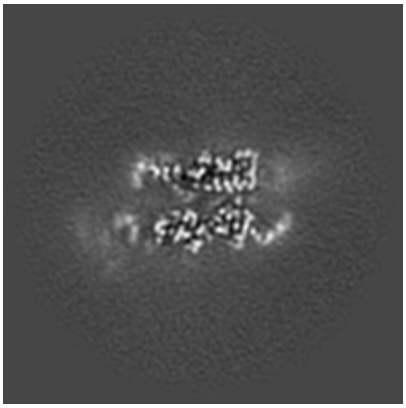
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

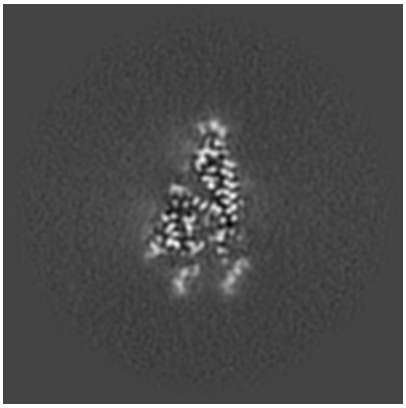
6.3.1 Primary map



X Index: 114



Y Index: 114

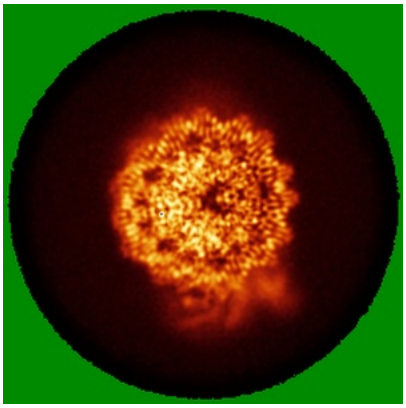


Z Index: 116

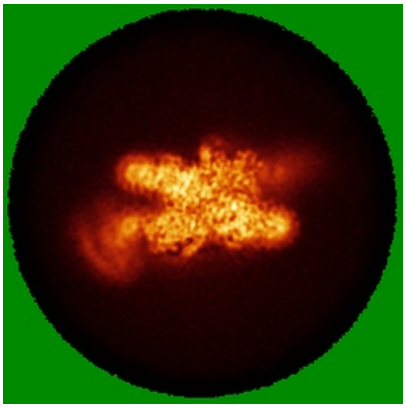
The images above show the largest variance slices of the map in three orthogonal directions.

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

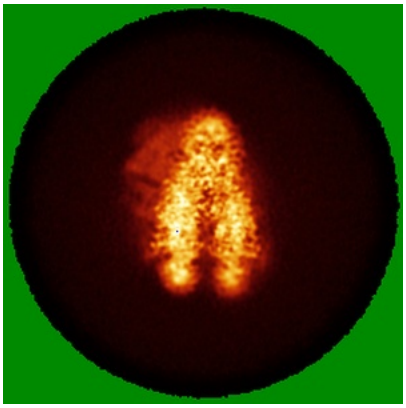
6.4.1 Primary map



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

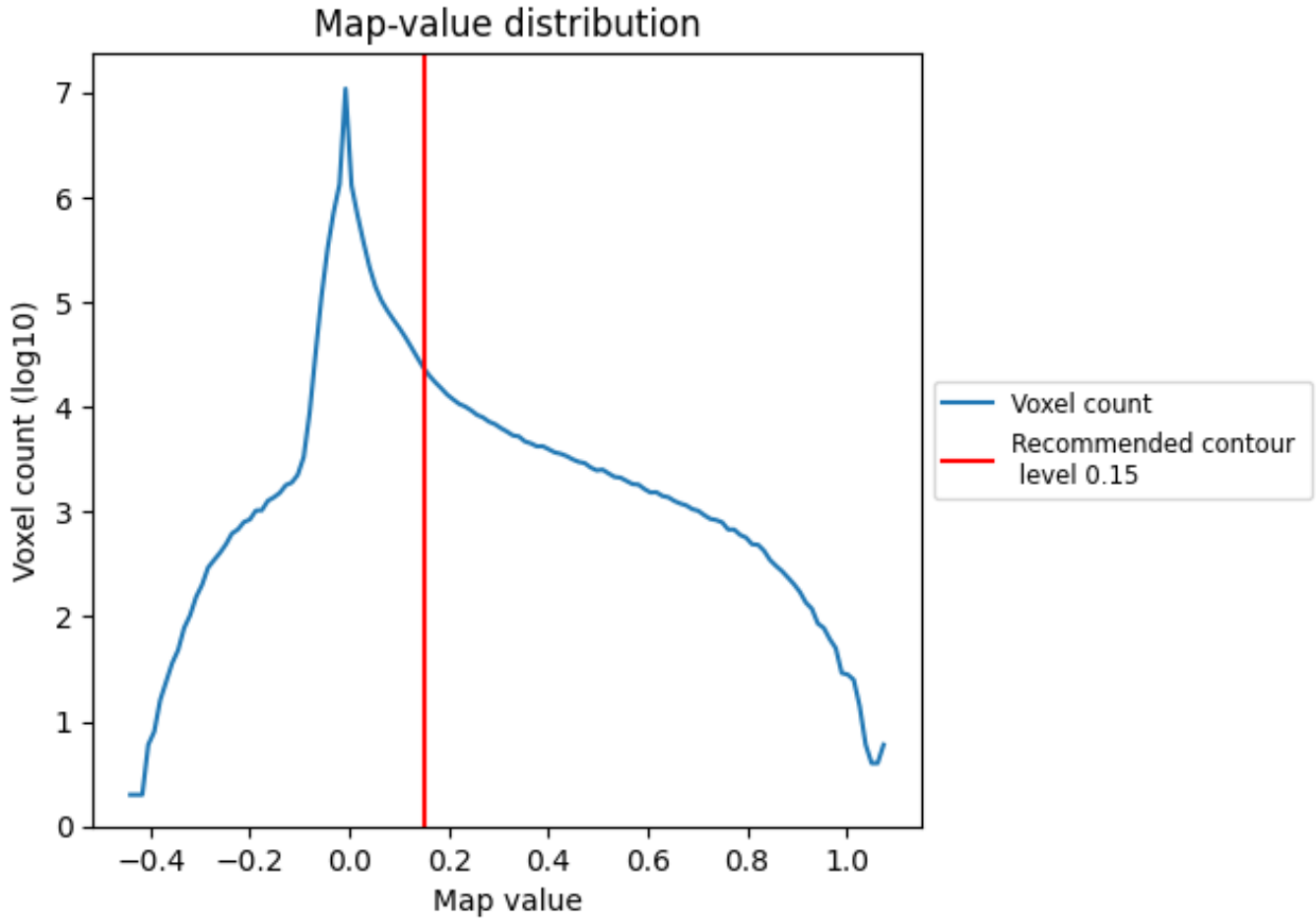
6.6 Mask visualisation (i)

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

7 Map analysis

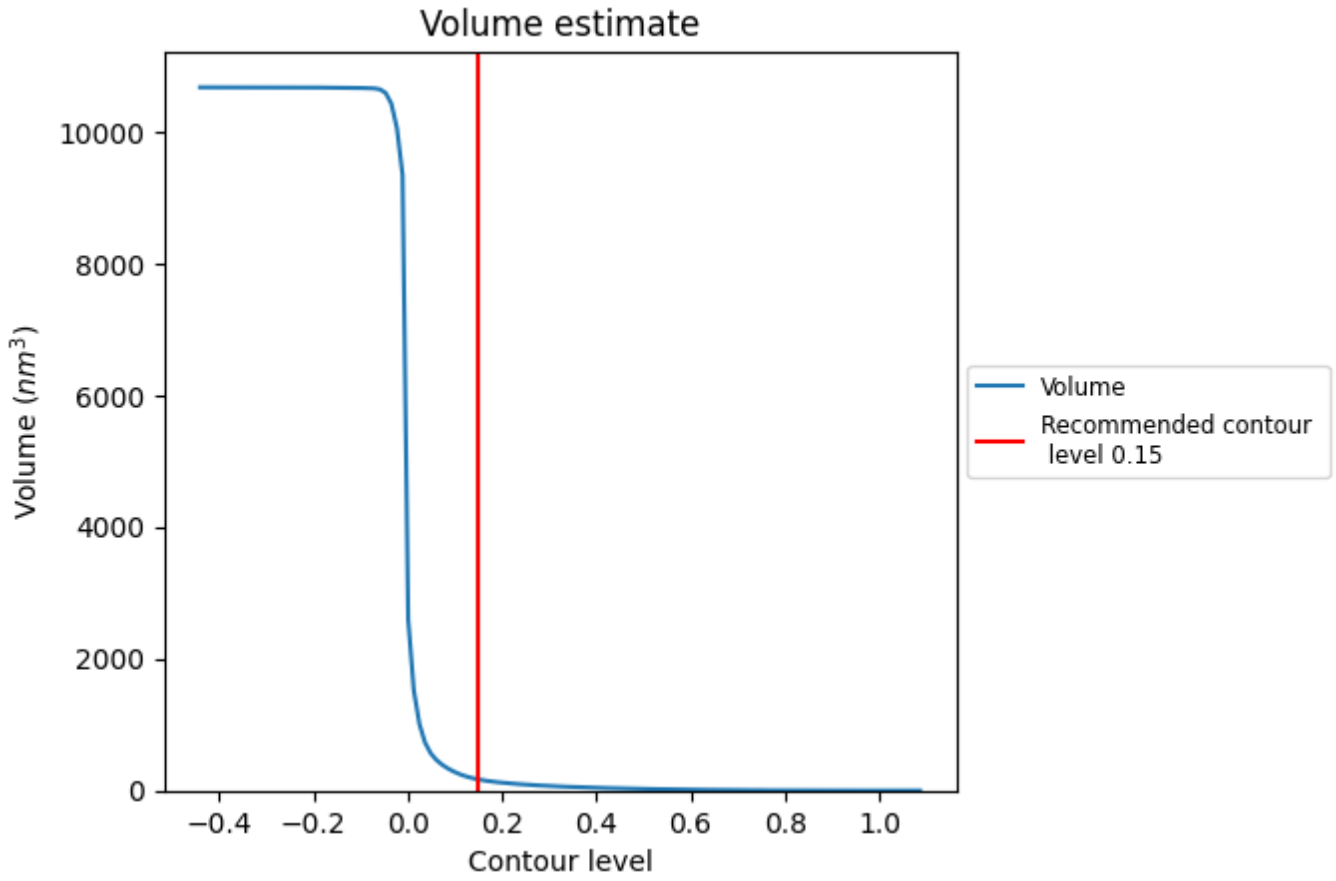
This section contains the results of statistical analysis of the map.

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.

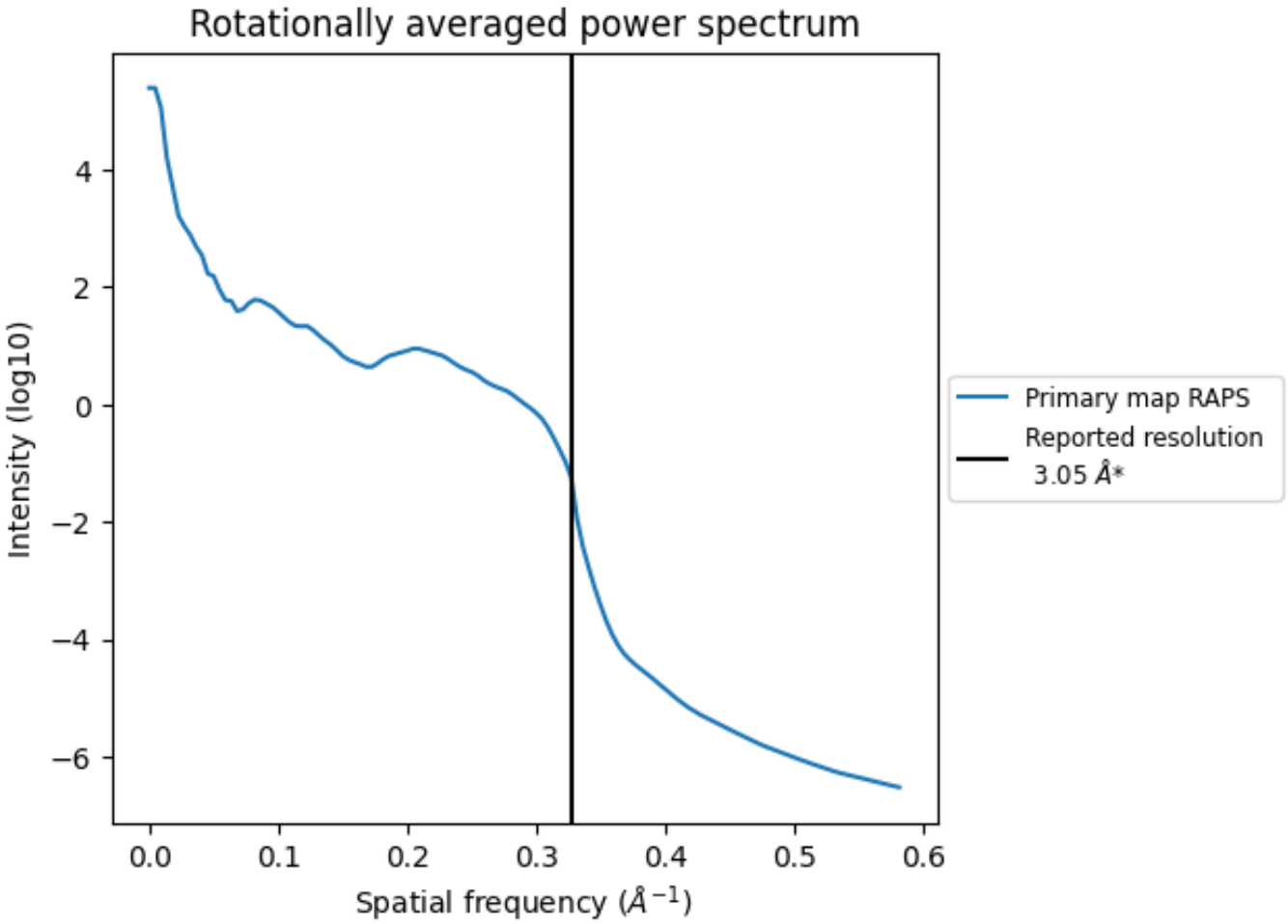
7.2 Volume estimate (i)



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 153 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 0.328 Å^{-1}

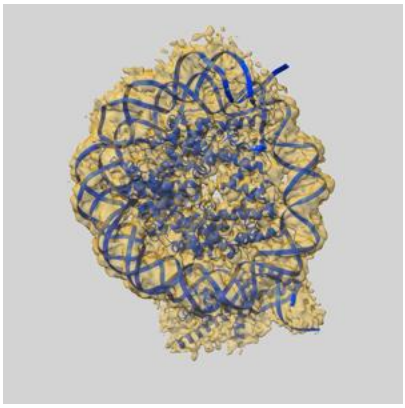
8 Fourier-Shell correlation (i)

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

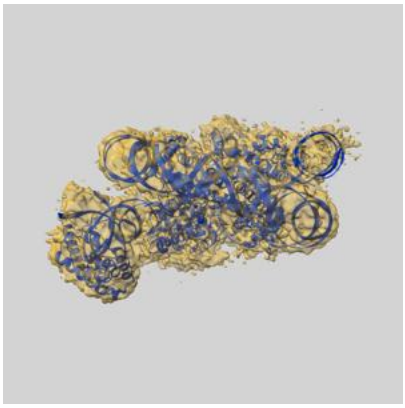
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10406 and PDB model 6T90. Per-residue inclusion information can be found in section 3 on page 10.

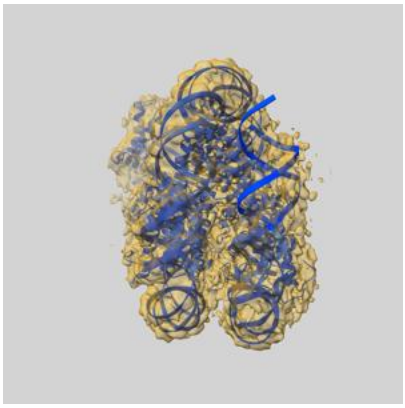
9.1 Map-model overlay



X



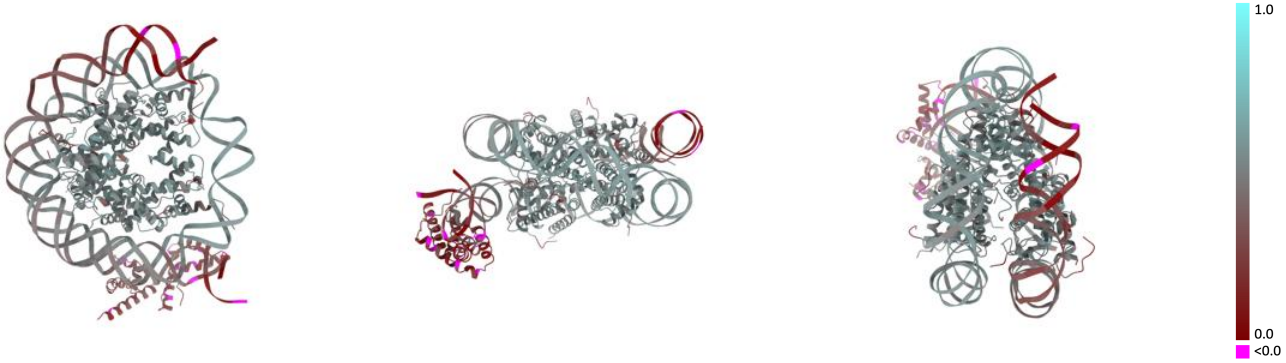
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

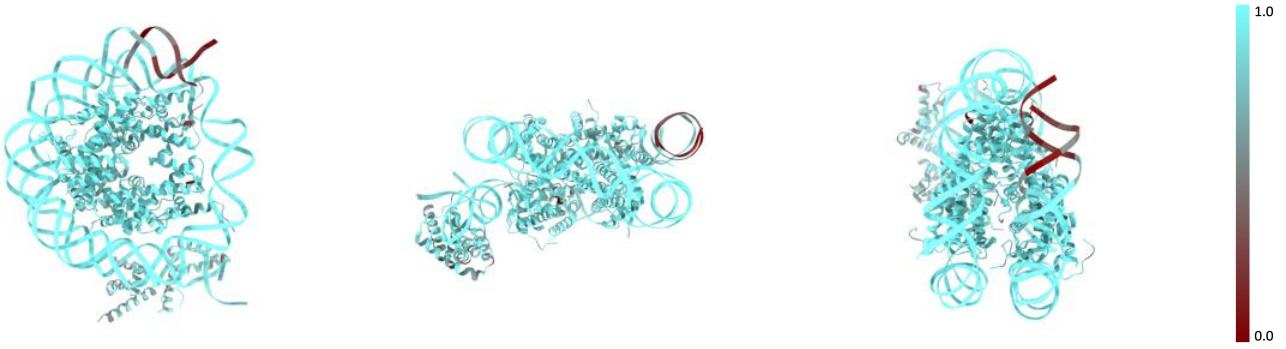
9.2 Q-score mapped to coordinate model



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.

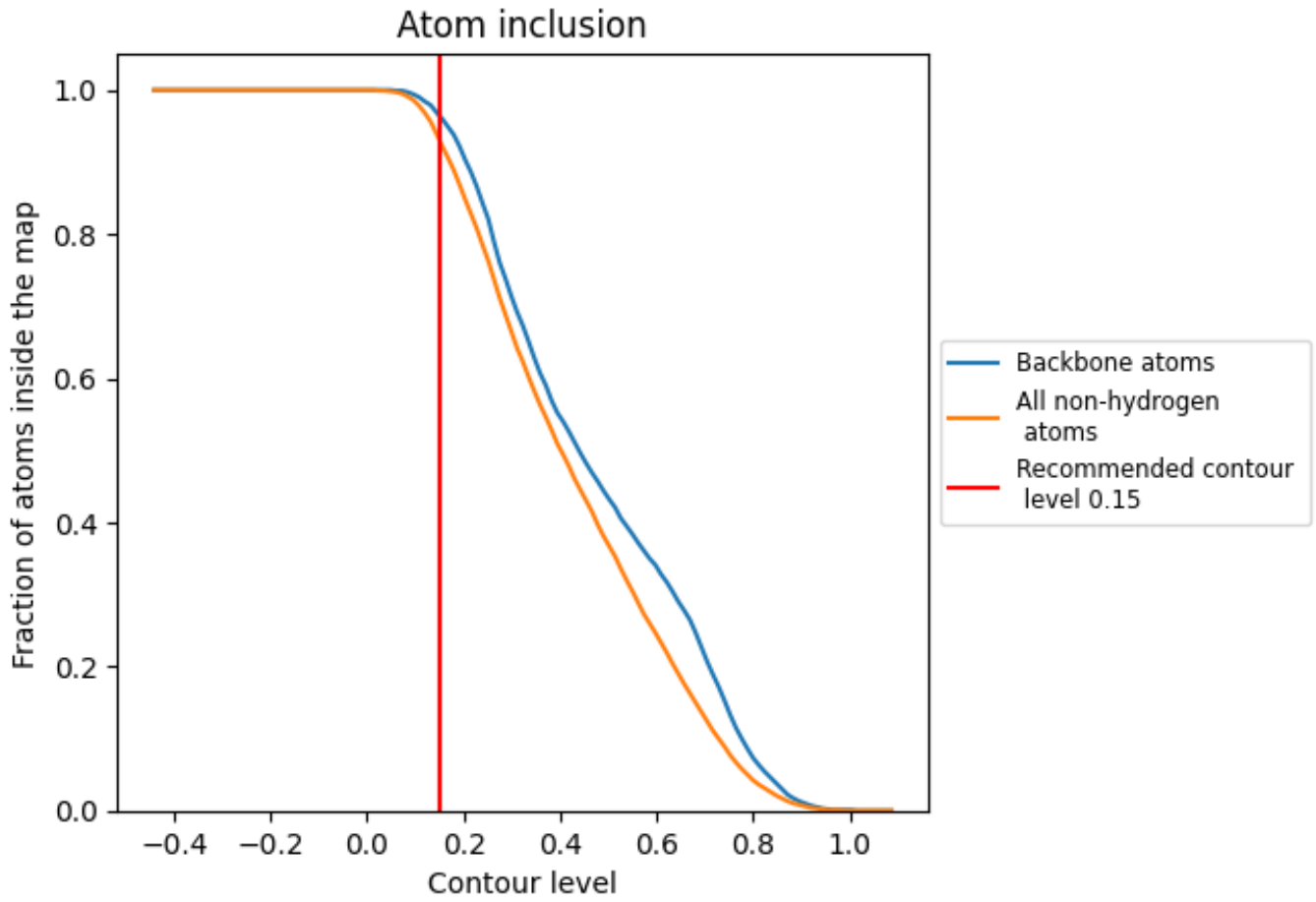
9.3 Atom inclusion mapped to coordinate model



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.4510
A	0.9590	0.5340
B	0.9680	0.5430
C	0.9210	0.5090
D	0.9690	0.5270
E	0.9500	0.5270
F	0.9600	0.5400
G	0.9230	0.4960
H	0.9710	0.5100
I	0.9380	0.4350
J	0.9440	0.4350
K	0.7420	0.2170
L	0.8130	0.1410