



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 02:05 PM JST

PDB ID : 5X0X
EMDB ID : EMD-6699
Title : Complex of Snf2-Nucleosome complex with Snf2 bound to position +6 of the nucleosome
Authors : Li, M.; Liu, X.; Xia, X.; Chen, Z.; Li, X.
Deposited on : 2017-01-23
Resolution : 3.97 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.dev43
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) : 2.31.2

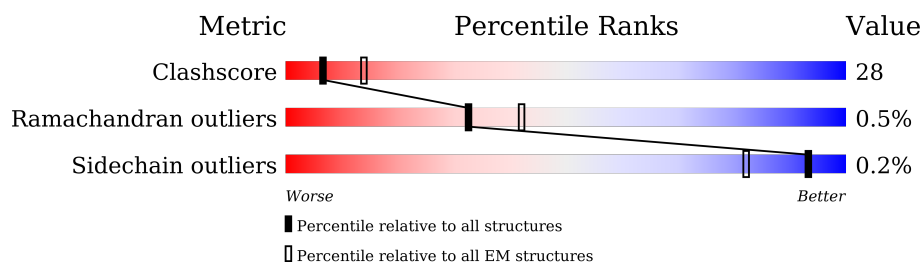
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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.



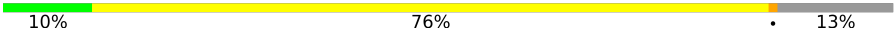
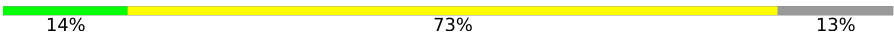

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	125	
4	H	125	

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Mol	Chain	Length	Quality of chain
5	I	167	
6	J	167	
7	O	735	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16748 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	98	Total	C	N	O	S	0	0
			800	505	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			778	491	148	136	3		

- 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	413	127	112	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total	C	N	O		0	0
			811	510	158	143			
3	G	107	Total	C	N	O		0	0
			815	513	159	143			

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	see sequence details	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	see sequence details	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called Transcription regulatory protein SNF2.

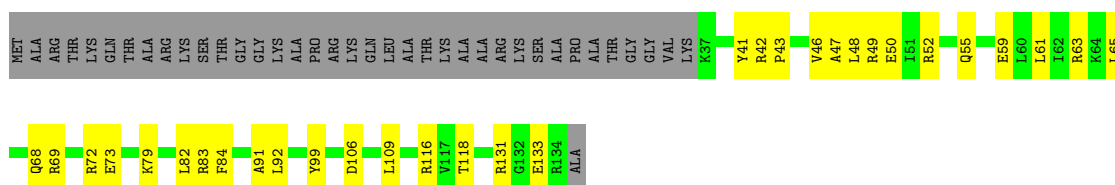
Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	583	Total	C	N	O	S	0	0
			4789	3045	846	881	17		

3 Residue-property plots

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.

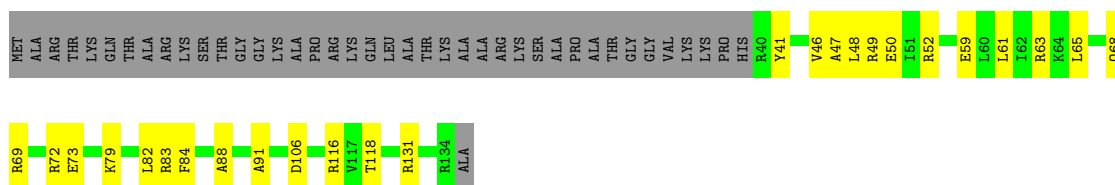
• Molecule 1: Histone H3.2

Chain A: 



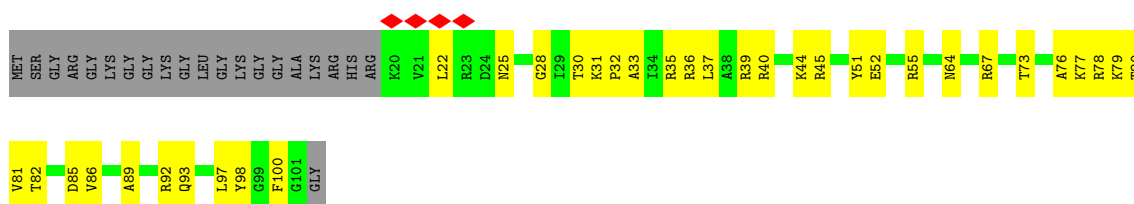
• Molecule 1: Histone H3.2

Chain E: 



• Molecule 2: Histone H4

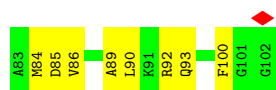
Chain B: 



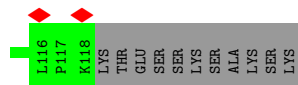
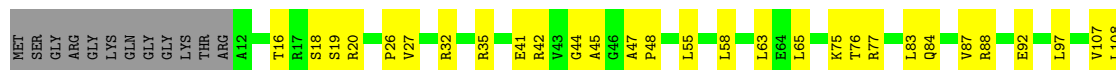
• Molecule 2: Histone H4

Chain F: 

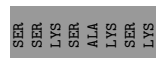




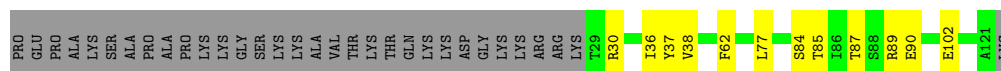
• Molecule 3: Histone H2A



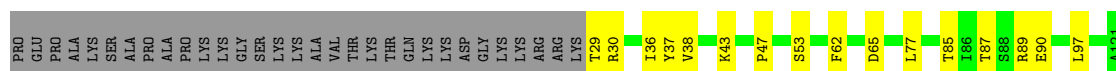
• Molecule 3: Histone H2A



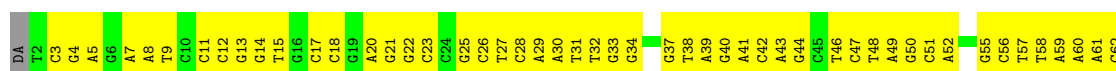
• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



• Molecule 5: DNA (167-MER)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0274	Depositor
Map size (\AA)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/812	0.57	0/1091
1	E	0.58	0/788	0.58	0/1057
2	B	0.67	0/660	0.62	0/885
2	F	0.67	0/680	0.62	0/912
3	C	0.56	0/821	0.59	0/1112
3	G	0.56	0/825	0.59	0/1116
4	D	0.63	0/729	0.59	0/985
4	H	0.63	0/737	0.59	0/993
5	I	1.16	0/3333	1.02	2/5137 (0.0%)
6	J	1.14	0/3381	0.99	1/5221 (0.0%)
7	O	0.36	0/4864	0.56	2/6536 (0.0%)
All	All	0.82	0/17630	0.79	5/25045 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	O	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	132	DG	O4'-C4'-C3'	-6.02	102.09	104.50
7	O	959	PRO	N-CA-CB	5.92	110.40	103.30
7	O	1253	LEU	CA-CB-CG	-5.76	102.04	115.30
5	I	131	DA	O4'-C4'-C3'	-5.14	102.44	104.50
6	J	36	DA	O4'-C4'-C3'	-5.07	102.47	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	O	915	HIS	Peptide
7	O	926	PRO	Peptide
7	O	931	LEU	Peptide

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	800	0	829	33	0
1	E	778	0	813	27	0
2	B	653	0	695	34	0
2	F	672	0	698	32	0
3	C	811	0	849	30	0
3	G	815	0	860	22	0
4	D	718	0	725	11	0
4	H	726	0	747	16	0
5	I	2975	0	1639	201	0
6	J	3011	0	1639	191	0
7	O	4789	0	4882	380	0
All	All	16748	0	14376	854	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 28.

The worst 5 of 854 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)
7:O:1301:ASP:O	7:O:1305:SER:HB2	1.54	1.08
7:O:749:HIS:HB3	7:O:752:LYS:HD3	1.53	0.90
5:I:74:DC:N3	6:J:74:DG:N1	2.19	0.90
5:I:11:DC:O2	6:J:137:DG:N2	2.05	0.89
5:I:110:DC:O2	6:J:38:DG:N2	2.06	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	96/136 (71%)	87 (91%)	9 (9%)	0	100	100
1	E	93/136 (68%)	84 (90%)	9 (10%)	0	100	100
2	B	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
2	F	84/103 (82%)	81 (96%)	3 (4%)	0	100	100
3	C	105/130 (81%)	100 (95%)	4 (4%)	1 (1%)	15	52
3	G	105/130 (81%)	100 (95%)	4 (4%)	1 (1%)	15	52
4	D	91/125 (73%)	83 (91%)	8 (9%)	0	100	100
4	H	91/125 (73%)	83 (91%)	8 (9%)	0	100	100
7	O	569/735 (77%)	494 (87%)	71 (12%)	4 (1%)	22	60
All	All	1314/1723 (76%)	1189 (90%)	119 (9%)	6 (0%)	32	66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	O	954	GLU
7	O	1021	ILE
7	O	1163	THR
7	O	1049	ASN
3	C	87	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/111 (76%)	84 (100%)	0	100	100
1	E	82/111 (74%)	82 (100%)	0	100	100
2	B	67/79 (85%)	67 (100%)	0	100	100
2	F	67/79 (85%)	67 (100%)	0	100	100
3	C	81/102 (79%)	81 (100%)	0	100	100
3	G	82/102 (80%)	82 (100%)	0	100	100
4	D	77/105 (73%)	77 (100%)	0	100	100
4	H	79/105 (75%)	79 (100%)	0	100	100
7	O	526/667 (79%)	524 (100%)	2 (0%)	91	94
All	All	1145/1461 (78%)	1143 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	820	LEU
7	O	1278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
7	O	1025	GLN
7	O	1204	ASN
7	O	1347	ASN
7	O	1202	GLN
4	H	81	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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](#)

There are no chain breaks in this entry.

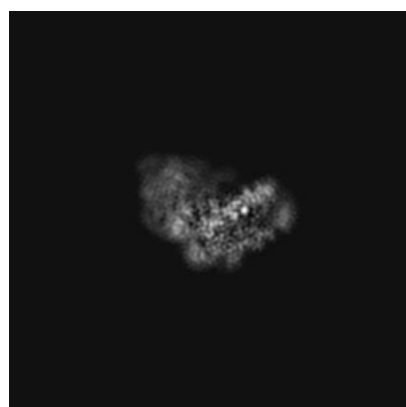
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6699. These allow visual inspection of the internal detail of the map and identification of artifacts.

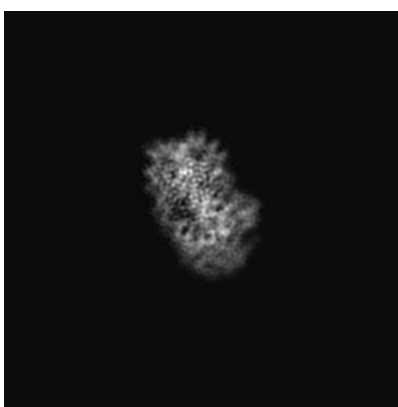
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

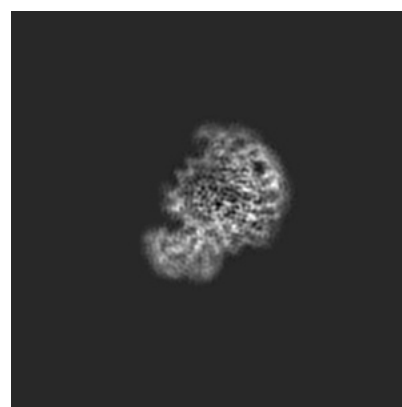
6.1.1 Primary map



X



Y

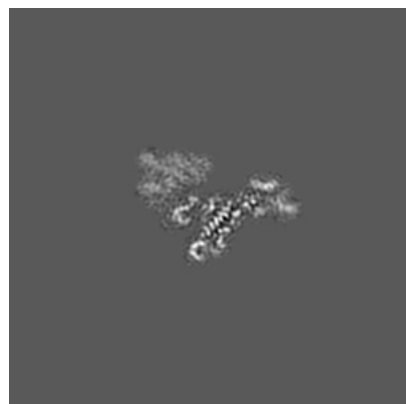


Z

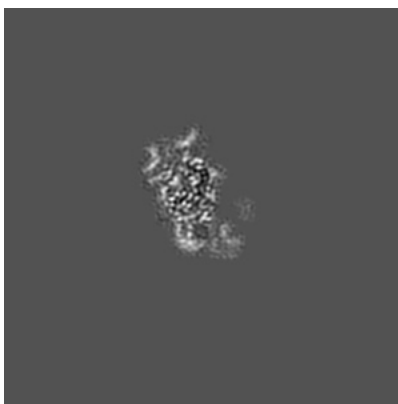
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

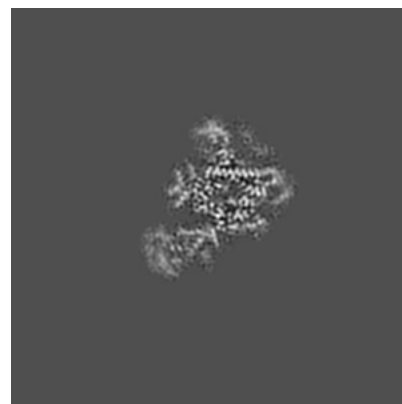
6.2.1 Primary map



X Index: 128



Y Index: 128

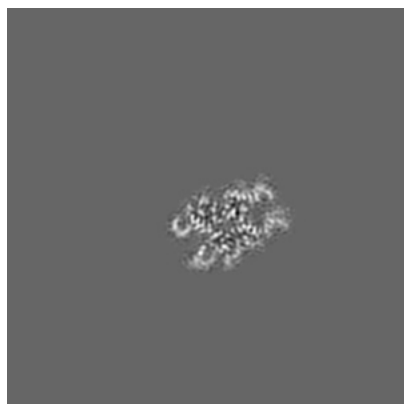


Z Index: 128

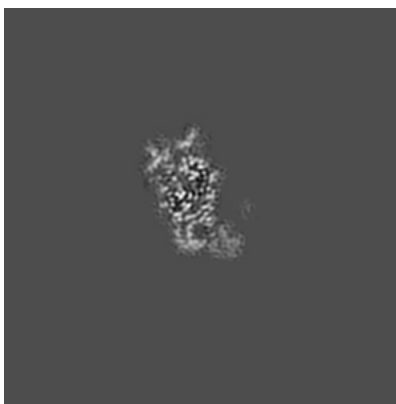
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

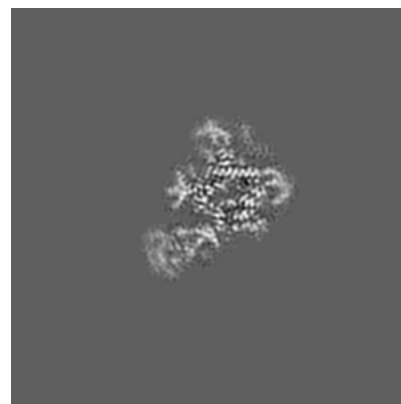
6.3.1 Primary map



X Index: 152



Y Index: 129

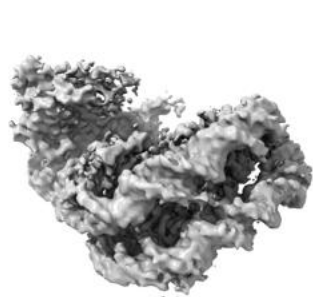


Z Index: 127

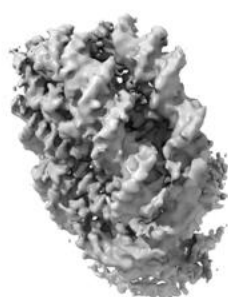
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

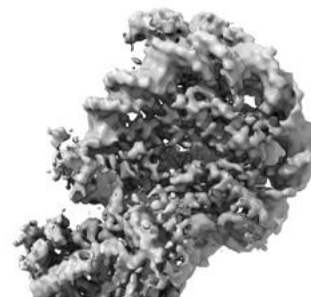
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0274. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

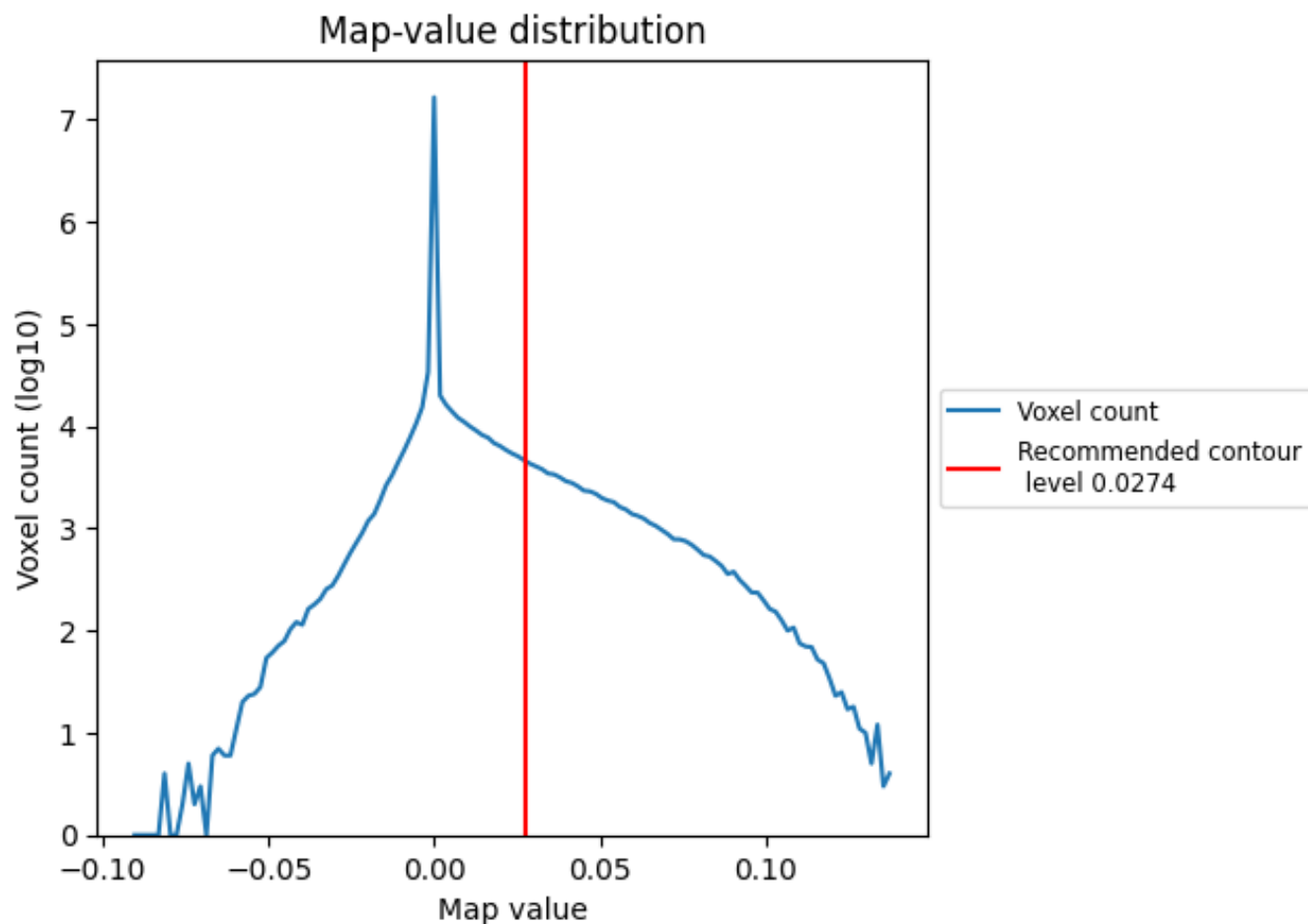
6.5 Mask visualisation

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

7 Map analysis [i](#)

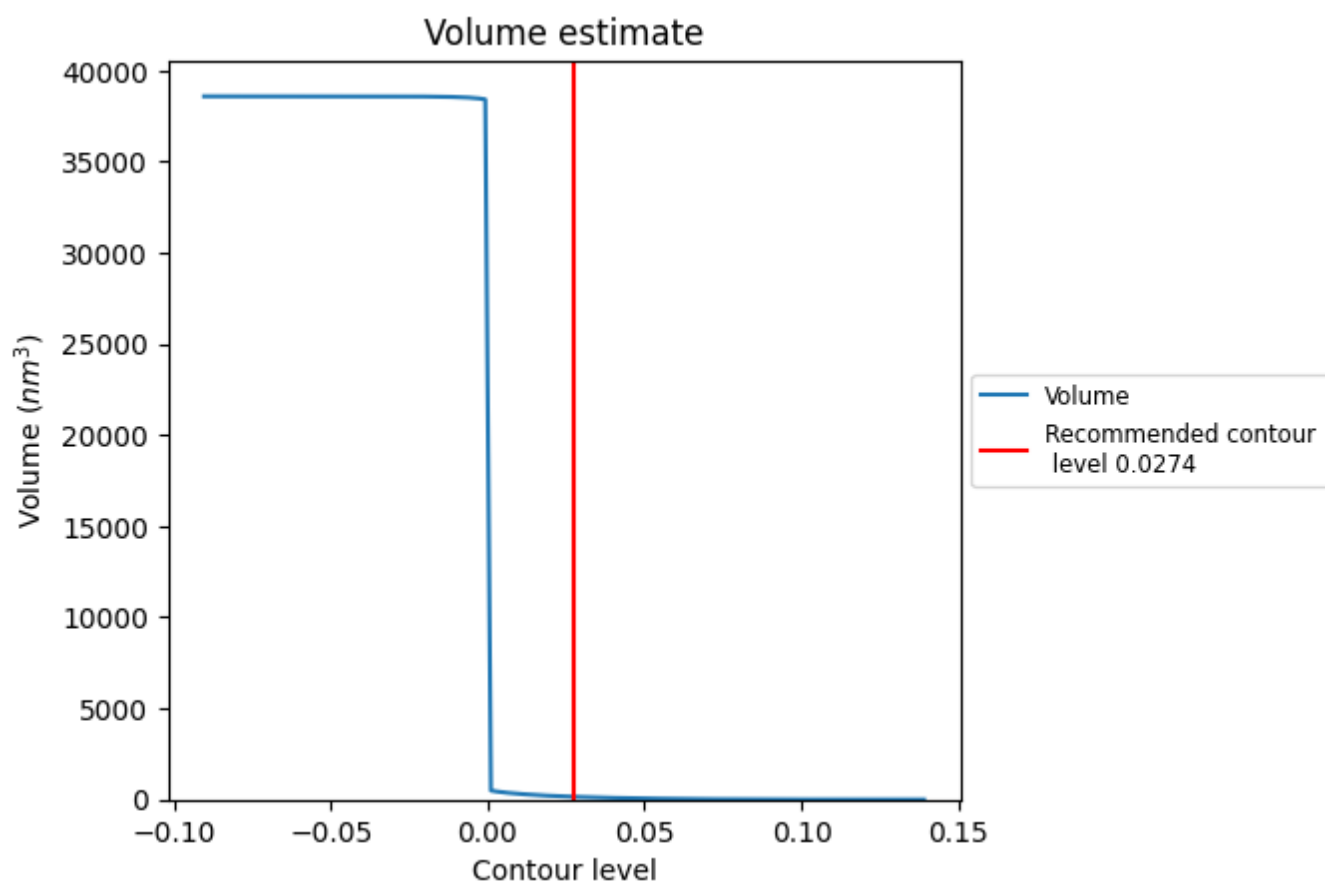
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

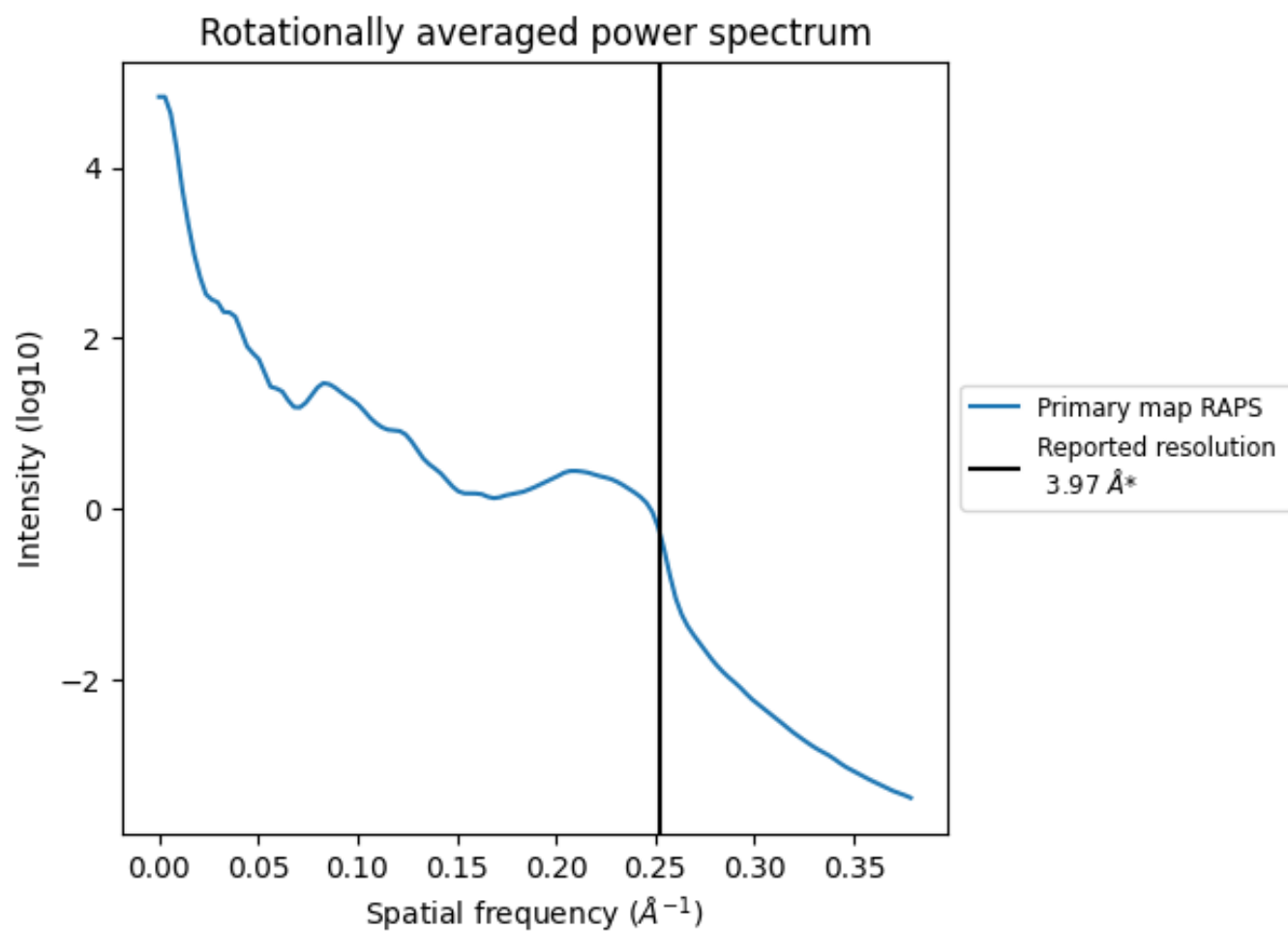
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm^3 ; this corresponds to an approximate mass of 138 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.252 Å⁻¹

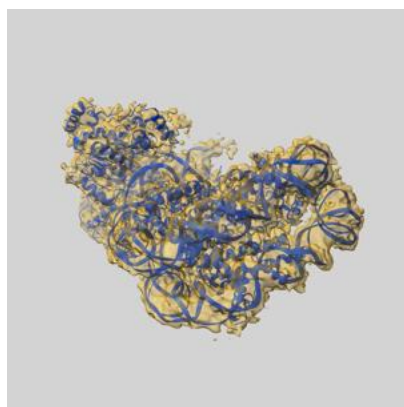
8 Fourier-Shell correlation

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

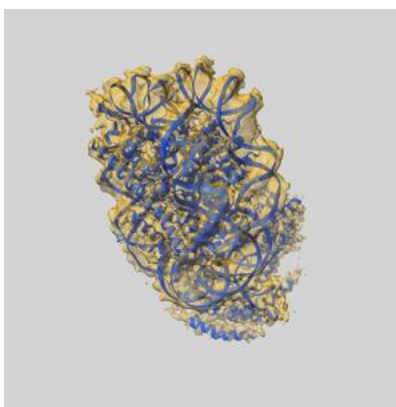
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6699 and PDB model 5X0X. Per-residue inclusion information can be found in section [3](#) on page [6](#).

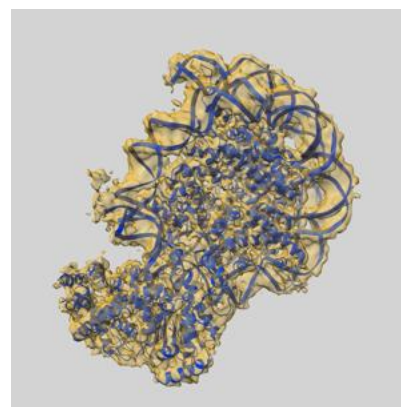
9.1 Map-model overlay [i](#)



X



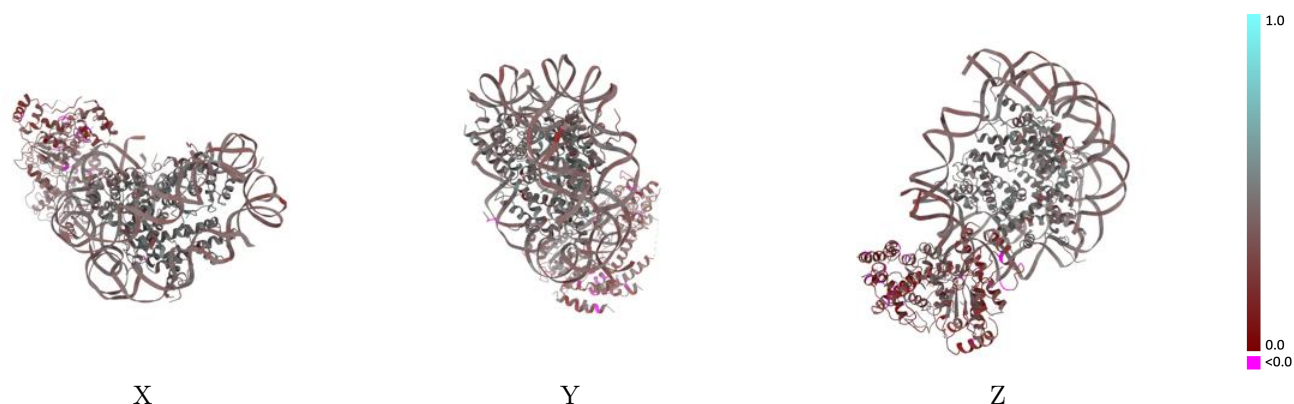
Y



Z

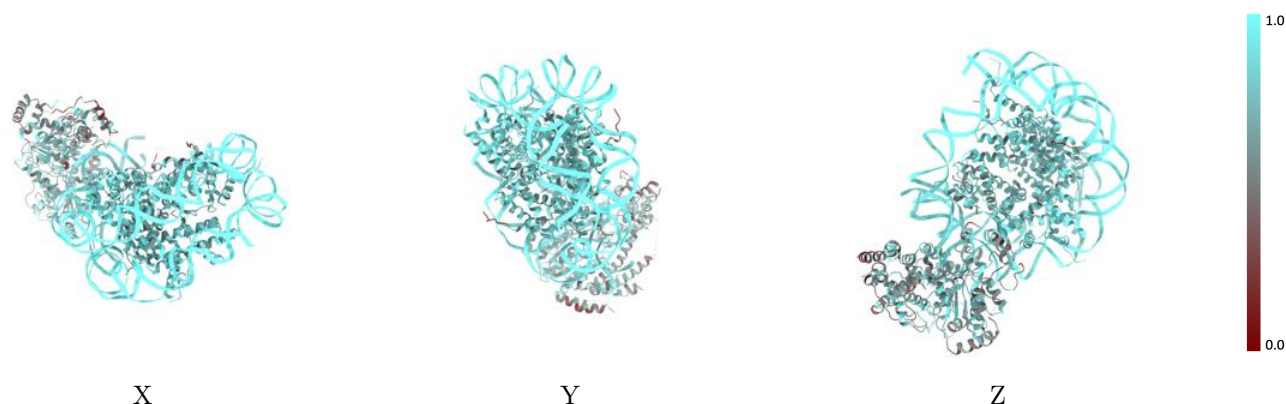
The images above show the 3D surface view of the map at the recommended contour level 0.0274 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



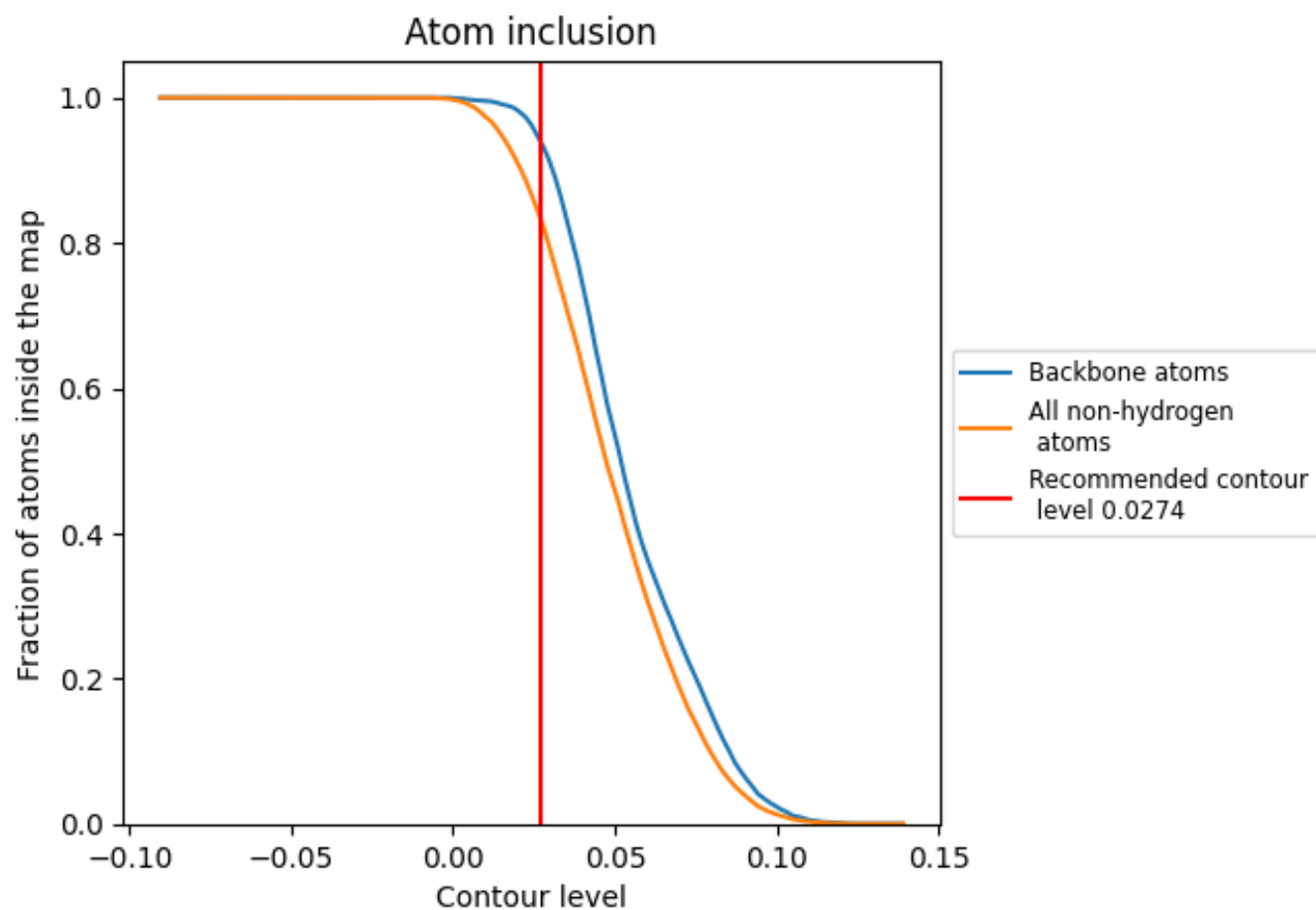
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0274).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 83% 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 (0.0274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8293	 0.3720
A	 0.8301	 0.4390
B	 0.8325	 0.4390
C	 0.8321	 0.4480
D	 0.8573	 0.4260
E	 0.8104	 0.4420
F	 0.7932	 0.4260
G	 0.8506	 0.4390
H	 0.8731	 0.4400
I	 0.9792	 0.3900
J	 0.9814	 0.3890
O	 0.6287	 0.2690

