



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 11:10 am GMT

PDB ID : 6QLE  
EMDB ID : EMD-4580  
Title : Structure of inner kinetochore CCAN complex  
Authors : Yan, K.; Yang, J.; Zhang, Z.; McLaughlin, S.H.; Chang, L.; Fasci, D.; Heck, A.J.R.; Barford, D.  
Deposited on : 2019-01-31  
Resolution : 3.55 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.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) : 2.31.3

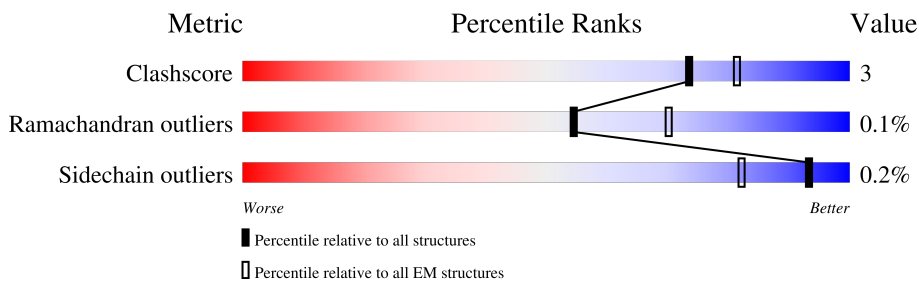
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.55 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.



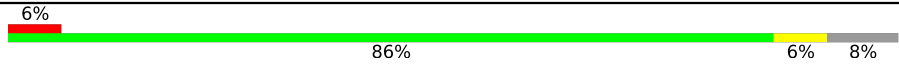

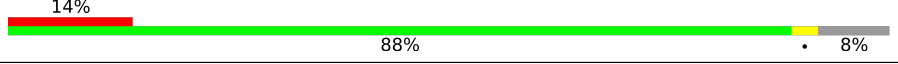
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	181	33% (Upper red bar) 63% (Green), 7% (Yellow), 30% (Grey)
2	I	412	22% (Upper red bar) 78% (Green), 11% (Yellow), 11% (Grey)
3	K	204	18% (Upper red bar) 48% (Green), 48% (Grey)
4	L	245	11% (Upper red bar) 86% (Green), 12% (Yellow), 2% (Grey)
5	N	458	75% (Green), 6% (Yellow), 19% (Grey)
6	O	368	53% (Green), 44% (Grey)
7	P	369	60% (Green), 6% (Yellow), 34% (Grey)
8	Q	261	18% (Upper red bar) 80% (Green), 6% (Yellow), 14% (Grey)

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Mol	Chain	Length	Quality of chain
9	U	186	 6% 86% 6% 8%
10	Y	238	 16% 85% 8% 6%
11	Z	153	 14% 88% 8%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 18162 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 Central kinetochore subunit MCM16,Central kinetochore subunit MCM16,Inner kinetochore subunit MCM16,Mcm16p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	126	952	610	174	167	1	0	0

- Molecule 2 is a protein called Central kinetochore subunit CTF3,Inner kinetochore subunit CTF3,Central kinetochore subunit CTF3,Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	365	2699	1759	449	472	19	0	0

- Molecule 3 is a protein called Inner kinetochore subunit MCM22,Inner kinetochore subunit MCM22,Inner kinetochore subunit MCM22,Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	106	774	491	138	142	3	0	0

- Molecule 4 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	241	1941	1244	320	366	11	0	0

- Molecule 5 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	371	2922	1903	504	503	12	0	0

- Molecule 6 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	205	1658	1078	271	305	4	0	0

- Molecule 7 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	242	1865	1208	323	322	12	0	0

- Molecule 8 is a protein called Inner kinetochore subunit OKP1,Inner kinetochore subunit OKP1,Inner kinetochore subunit OKP1,Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Q	224	1584	996	285	298	5	0	0

- Molecule 9 is a protein called Inner kinetochore subunit AME1,Inner kinetochore subunit AME1,Inner kinetochore subunit AME1,Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	U	172	1231	769	226	233	3	0	0

- Molecule 10 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Y	223	1541	965	275	296	5	0	0

- Molecule 11 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Z	140	995	632	181	181	1	0	0

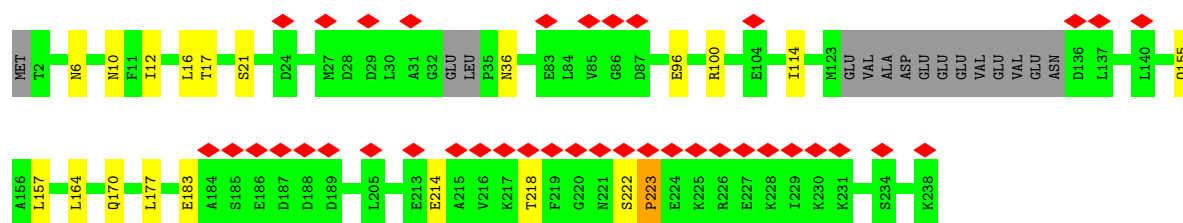






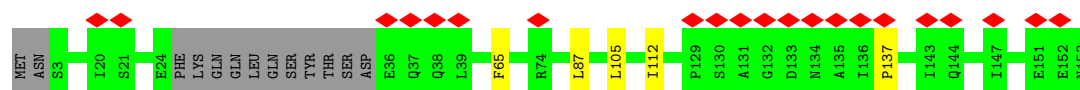


Chain Y: 16% 85% 8% 6%



- Molecule 11: Inner kinetochore subunit NKP2

Chain Z: 14% 88% 8%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	465029, 465029	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32.00	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.221	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.026	Depositor
Map size ( $\text{\AA}$ )	348.80002, 348.80002, 348.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.09, 1.09, 1.09	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	H	0.27	0/960	0.51	2/1297 (0.2%)
2	I	0.31	0/2630	0.54	1/3573 (0.0%)
3	K	0.27	0/780	0.46	0/1055
4	L	0.30	0/1981	0.52	0/2684
5	N	0.31	0/2987	0.52	0/4038
6	O	0.32	0/1689	0.52	0/2275
7	P	0.28	0/1891	0.51	1/2552 (0.0%)
8	Q	0.26	0/1522	0.50	1/2062 (0.0%)
9	U	0.26	0/1109	0.46	0/1501
10	Y	0.27	0/1550	0.53	1/2102 (0.0%)
11	Z	0.28	0/1005	0.50	1/1367 (0.1%)
All	All	0.29	0/18104	0.51	7/24506 (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
4	L	0	1
7	P	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	Q	296	LEU	CA-CB-CG	7.15	131.75	115.30
2	I	478	LEU	CA-CB-CG	6.66	130.62	115.30
7	P	131	LEU	CA-CB-CG	6.44	130.12	115.30
1	H	82	LEU	CA-CB-CG	6.32	129.83	115.30
1	H	136	PRO	N-CA-CB	5.81	110.28	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	40	VAL	Peptide
7	P	274	MET	Peptide

## 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	H	952	0	932	11	0
2	I	2699	0	2538	29	0
3	K	774	0	748	6	0
4	L	1941	0	1946	19	0
5	N	2922	0	2950	19	0
6	O	1658	0	1665	7	0
7	P	1865	0	1855	12	0
8	Q	1584	0	1414	11	0
9	U	1231	0	1083	11	0
10	Y	1541	0	1425	12	0
11	Z	995	0	911	3	0
All	All	18162	0	17467	116	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 3.

The worst 5 of 116 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)
8:Q:343:THR:HG21	10:Y:155:GLN:HE21	1.63	0.63
4:L:13:GLN:NE2	4:L:85:MET:SD	2.75	0.60
7:P:186:ASN:HB3	7:P:200:GLN:HG3	1.84	0.58
10:Y:114:ILE:HD11	10:Y:157:LEU:HD23	1.85	0.58
2:I:416:VAL:HG13	2:I:420:ILE:HD12	1.85	0.58

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	H	120/181 (66%)	119 (99%)	1 (1%)	0	100	100
2	I	328/412 (80%)	301 (92%)	27 (8%)	0	100	100
3	K	100/204 (49%)	100 (100%)	0	0	100	100
4	L	239/245 (98%)	226 (95%)	13 (5%)	0	100	100
5	N	359/458 (78%)	336 (94%)	23 (6%)	0	100	100
6	O	201/368 (55%)	192 (96%)	9 (4%)	0	100	100
7	P	232/369 (63%)	212 (91%)	20 (9%)	0	100	100
8	Q	205/261 (78%)	197 (96%)	8 (4%)	0	100	100
9	U	142/186 (76%)	140 (99%)	2 (1%)	0	100	100
10	Y	217/238 (91%)	200 (92%)	15 (7%)	2 (1%)	17	57
11	Z	136/153 (89%)	131 (96%)	5 (4%)	0	100	100
All	All	2279/3075 (74%)	2154 (94%)	123 (5%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	Y	223	PRO
10	Y	222	SER

### 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	H	93/131 (71%)	93 (100%)	0	100	100
2	I	266/342 (78%)	266 (100%)	0	100	100
3	K	78/124 (63%)	78 (100%)	0	100	100
4	L	217/221 (98%)	217 (100%)	0	100	100
5	N	314/416 (76%)	313 (100%)	1 (0%)	92	97
6	O	185/347 (53%)	185 (100%)	0	100	100
7	P	193/344 (56%)	193 (100%)	0	100	100
8	Q	139/236 (59%)	138 (99%)	1 (1%)	84	93
9	U	110/151 (73%)	110 (100%)	0	100	100
10	Y	140/219 (64%)	140 (100%)	0	100	100
11	Z	87/143 (61%)	86 (99%)	1 (1%)	73	88
All	All	1822/2674 (68%)	1819 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	N	375	ARG
8	Q	274	LYS
11	Z	87	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
9	U	196	ASN
11	Z	102	GLN
10	Y	170	GLN
6	O	238	HIS
8	Q	245	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](#)

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

## 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
2	I	2
8	Q	1
9	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	330:UNK	C	334:UNK	N	15.68
1	Q	139:UNK	C	160:SER	N	14.55
1	U	156:UNK	C	166:PHE	N	13.56
1	I	676:UNK	C	690:VAL	N	12.97

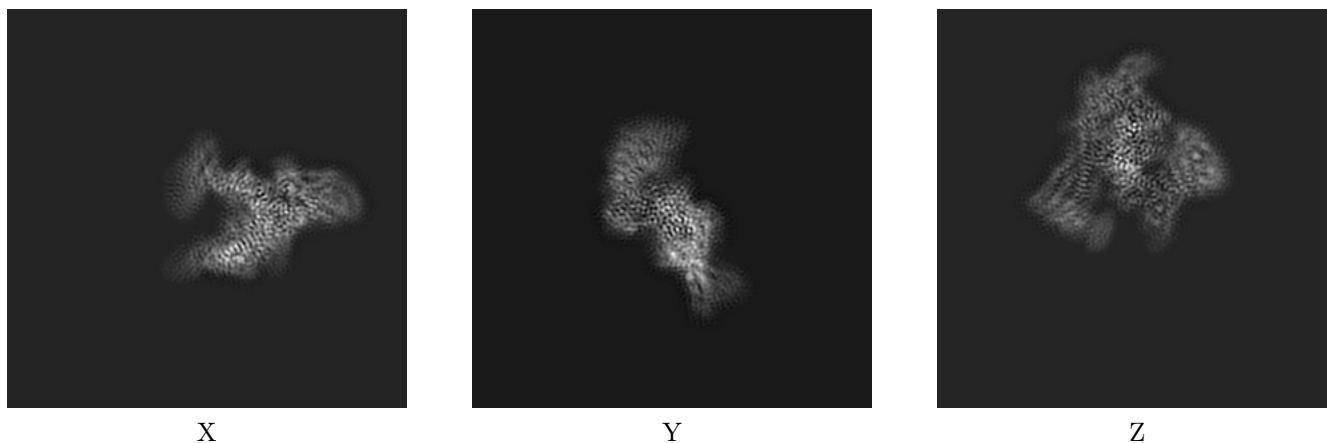
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4580. 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](#)

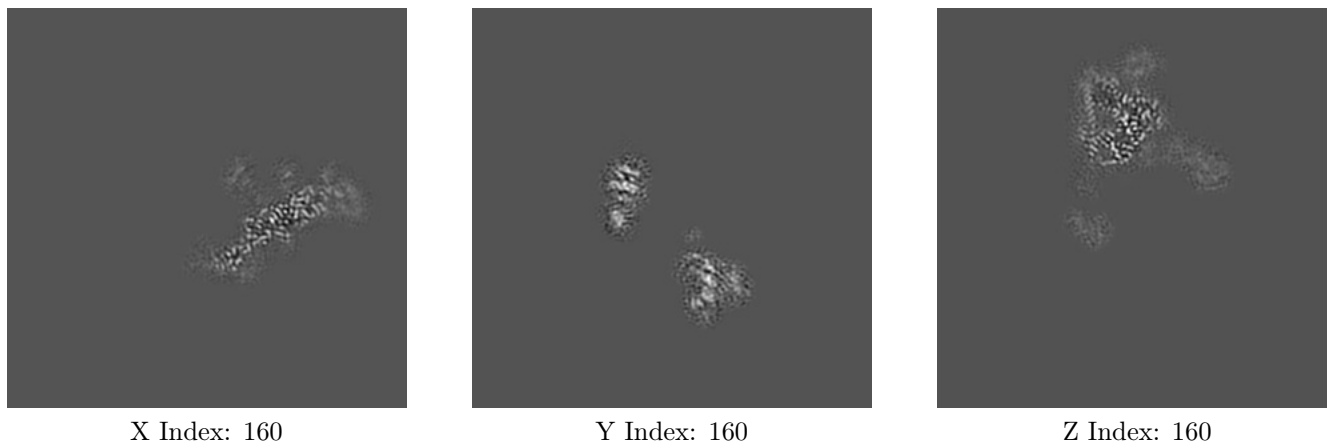
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

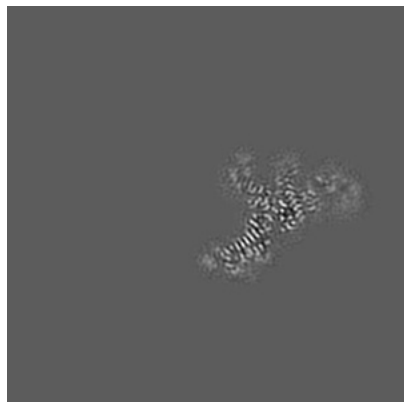




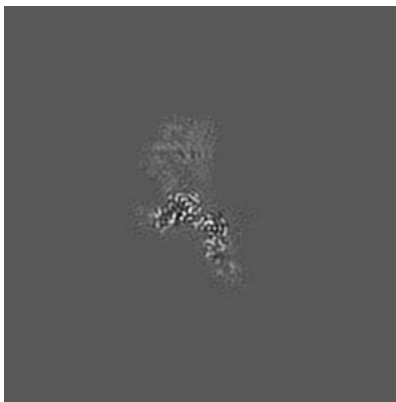
The images above show central slices of the map in three orthogonal directions.

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

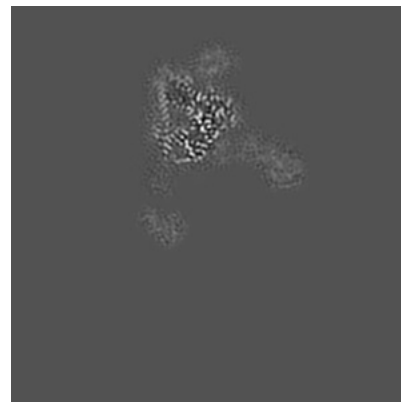
### 6.3.1 Primary map



X Index: 152



Y Index: 200



Z Index: 160

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

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

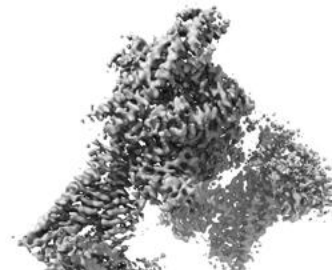
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

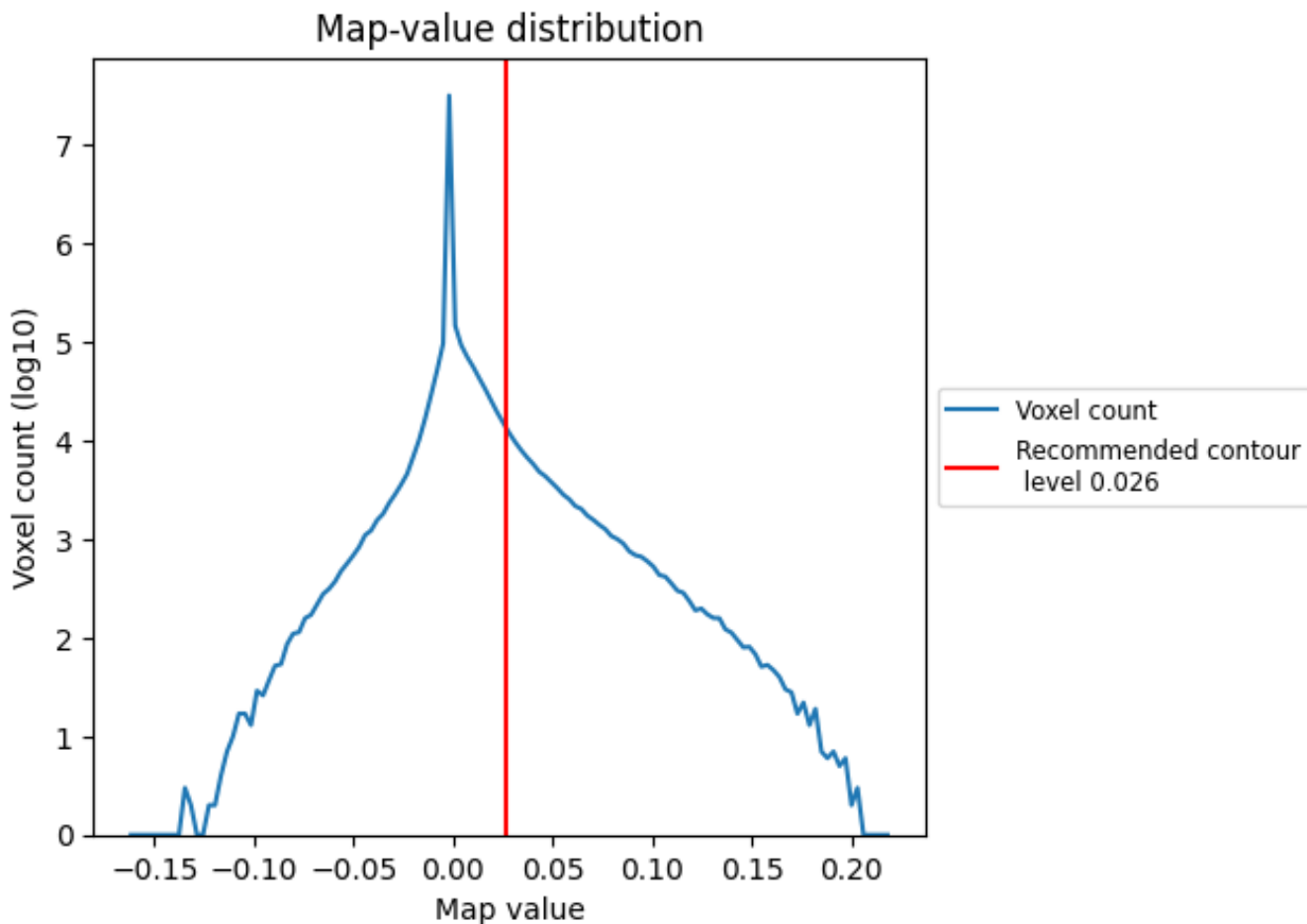
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

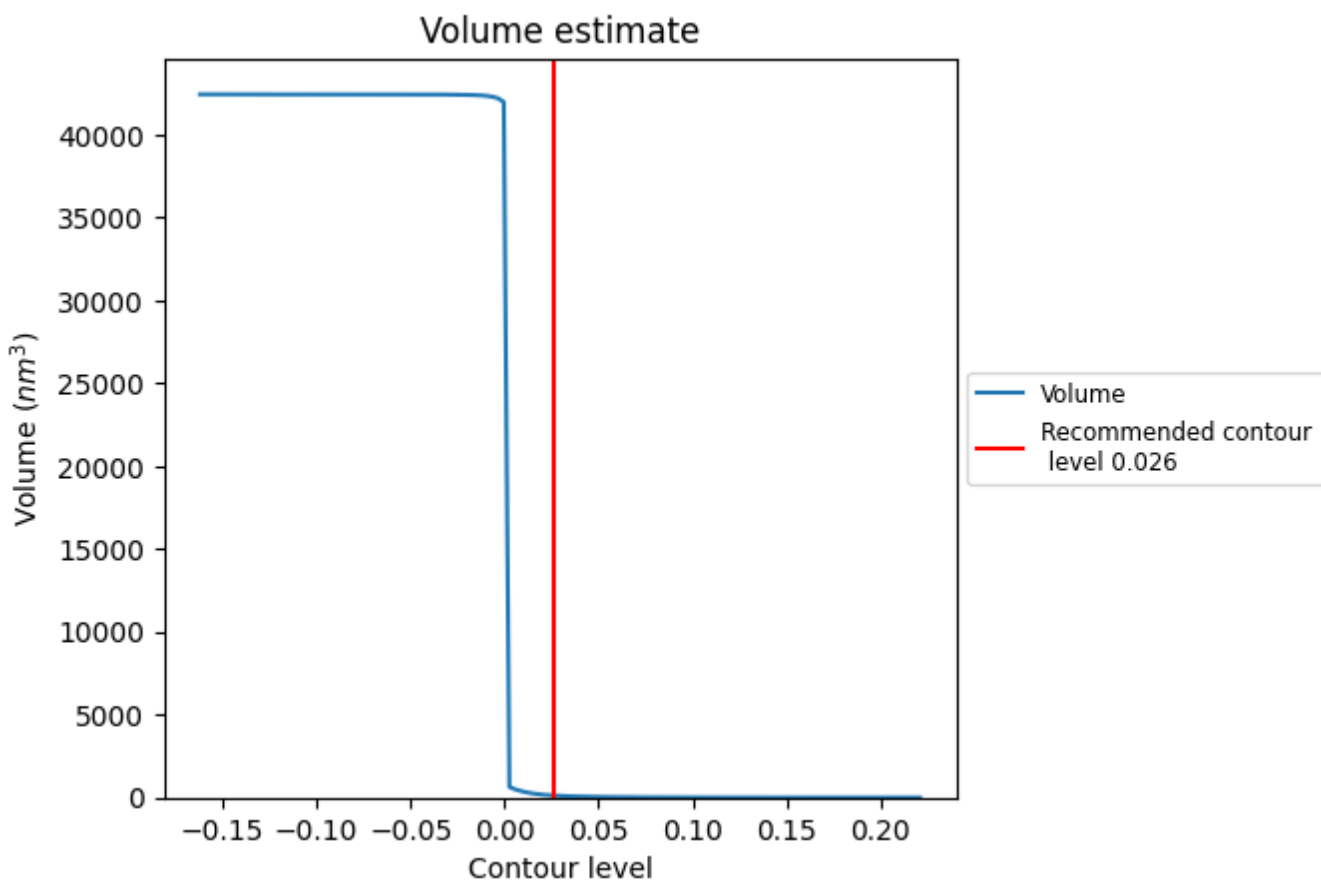
This section contains the results of statistical analysis of the map.

### 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.

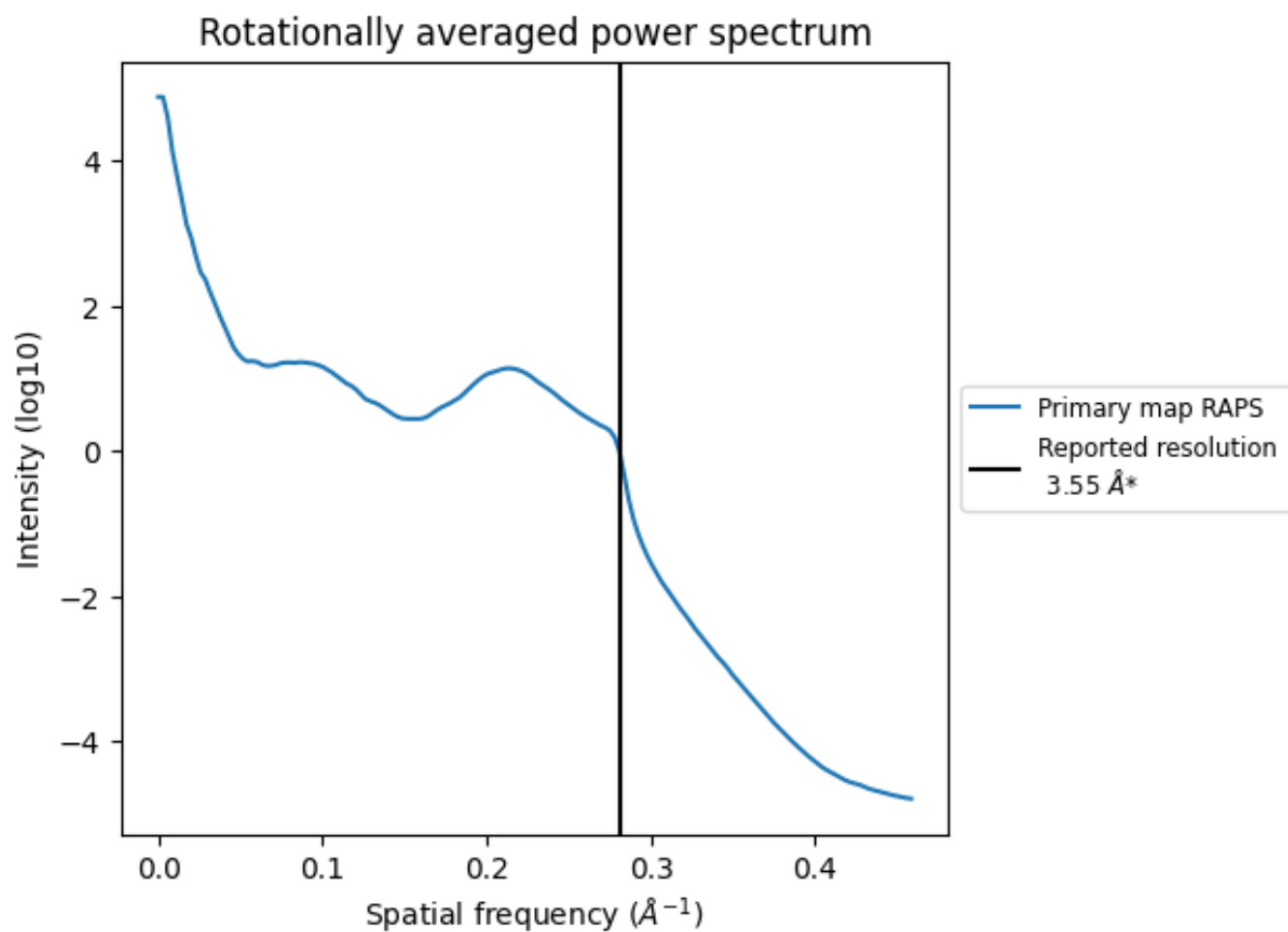
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm<sup>3</sup>; this corresponds to an approximate mass of 110 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  $0.282 \text{\AA}^{-1}$

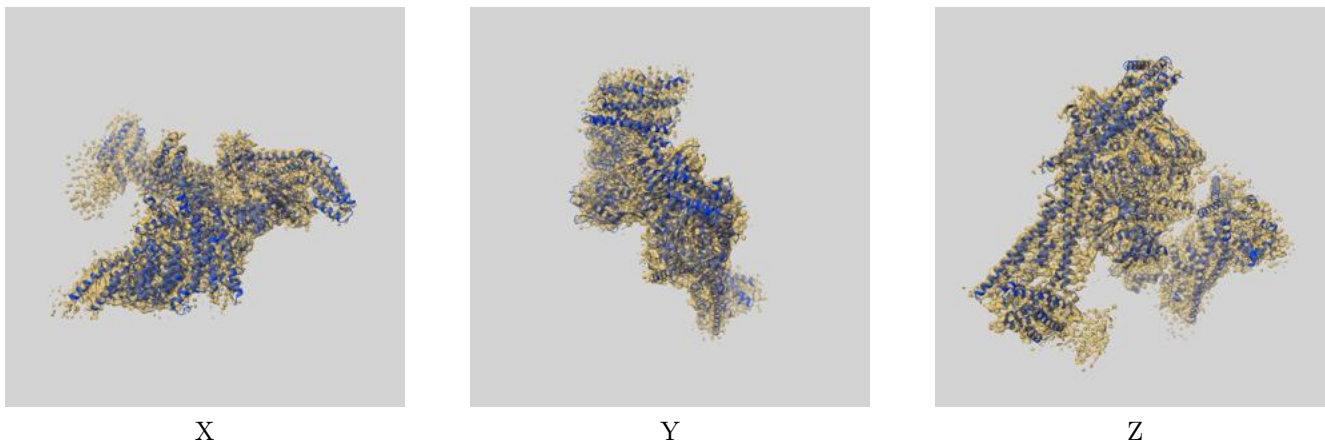
## 8 Fourier-Shell correlation

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

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

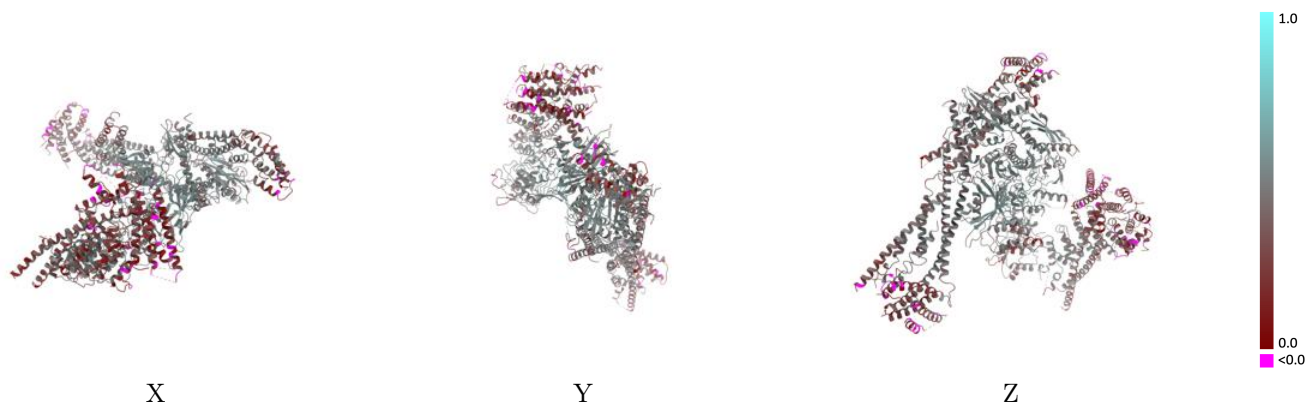
This section contains information regarding the fit between EMDB map EMD-4580 and PDB model 6QLE. Per-residue inclusion information can be found in section 3 on page 6.

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



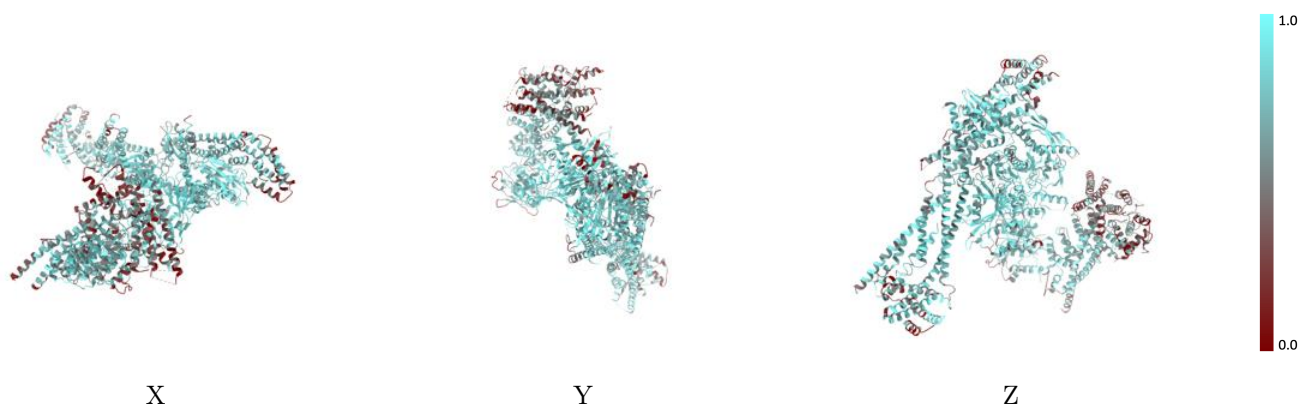
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

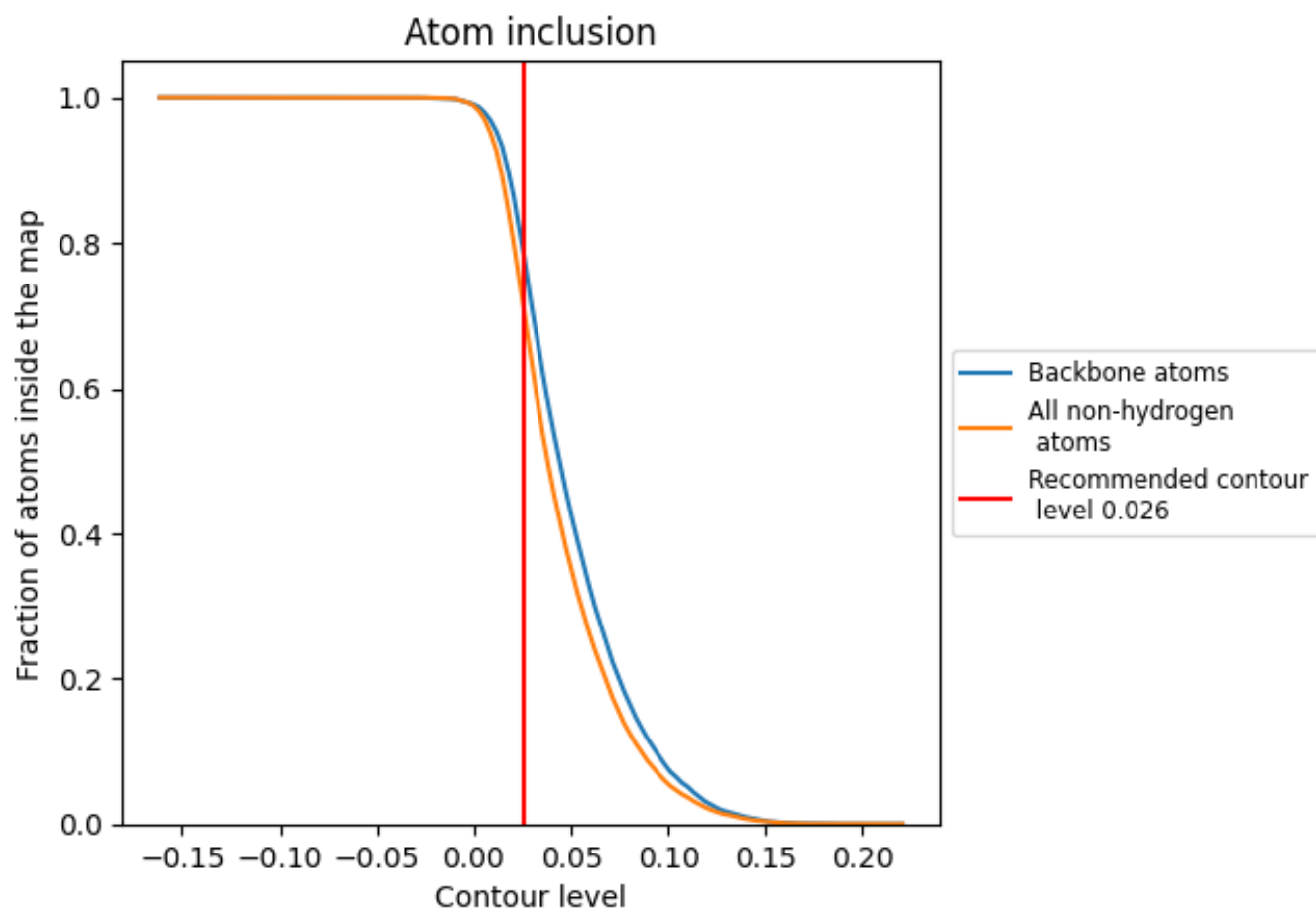
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (0.026).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7022	 0.4150
H	 0.4668	 0.2490
I	 0.6235	 0.3490
K	 0.5007	 0.2630
L	 0.7321	 0.4470
N	 0.8186	 0.5000
O	 0.7897	 0.5070
P	 0.7953	 0.4880
Q	 0.6430	 0.3710
U	 0.7383	 0.4130
Y	 0.6702	 0.3930
Z	 0.6786	 0.3740

