



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:34 PM EST

PDB ID : 3JC6
EMDB ID : EMD-6534
Title : Structure of the eukaryotic replicative CMG helicase and pumpjack motion
Authors : Li, H.; Bai, L.; Yuan, Z.; Sun, J.; Georgescu, R.E.; Liu, J.; O'Donnell, M.E.
Deposited on : 2015-11-24
Resolution : 3.70 Å (reported)
Based on initial model : 2Q9Q

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:

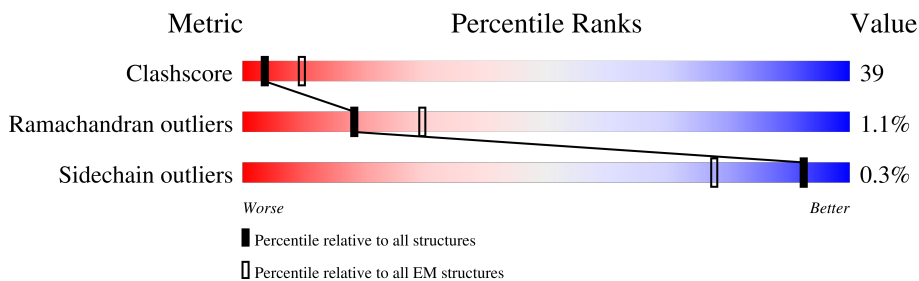
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.70 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.



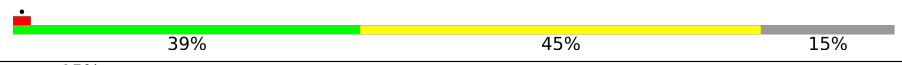


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2	868	
2	3	971	
3	4	933	
4	5	775	
5	6	1017	
6	7	845	
7	E	672	
8	D	294	

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Mol	Chain	Length	Quality of chain
9	B	213	
10	A	208	
11	C	194	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 23732 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	241	1911	1214	338	354	5	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	269	2130	1354	368	404	4	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	275	2203	1391	382	413	17	0	0

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	254	2028	1284	347	388	9	0	0

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	267	2049	1296	366	381	6	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	325	2611	1653	455	491	12	0	0

- Molecule 7 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	553	4482	2862	763	844	13	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	651	ASP	-	EXPRESSION TAG	UNP Q08032
E	652	TYR	-	EXPRESSION TAG	UNP Q08032
E	653	LYS	-	EXPRESSION TAG	UNP Q08032
E	654	ASP	-	EXPRESSION TAG	UNP Q08032
E	655	HIS	-	EXPRESSION TAG	UNP Q08032
E	656	ASP	-	EXPRESSION TAG	UNP Q08032
E	657	GLY	-	EXPRESSION TAG	UNP Q08032
E	658	ASP	-	EXPRESSION TAG	UNP Q08032
E	659	TYR	-	EXPRESSION TAG	UNP Q08032
E	660	LYS	-	EXPRESSION TAG	UNP Q08032
E	661	ASP	-	EXPRESSION TAG	UNP Q08032
E	662	HIS	-	EXPRESSION TAG	UNP Q08032
E	663	ASP	-	EXPRESSION TAG	UNP Q08032
E	664	ILE	-	EXPRESSION TAG	UNP Q08032
E	665	ASP	-	EXPRESSION TAG	UNP Q08032
E	666	TYR	-	EXPRESSION TAG	UNP Q08032
E	667	LYS	-	EXPRESSION TAG	UNP Q08032
E	668	ASP	-	EXPRESSION TAG	UNP Q08032
E	669	ASP	-	EXPRESSION TAG	UNP Q08032
E	670	ASP	-	EXPRESSION TAG	UNP Q08032
E	671	ASP	-	EXPRESSION TAG	UNP Q08032
E	672	LYS	-	EXPRESSION TAG	UNP Q08032

- Molecule 8 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	221	1820	1159	300	348	13	0	0

- Molecule 9 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	181	1513	978	261	270	4	0	0

- Molecule 10 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	208	1696	1065	290	331	10	0	0

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	159	1288	843	207	232	6	0	0

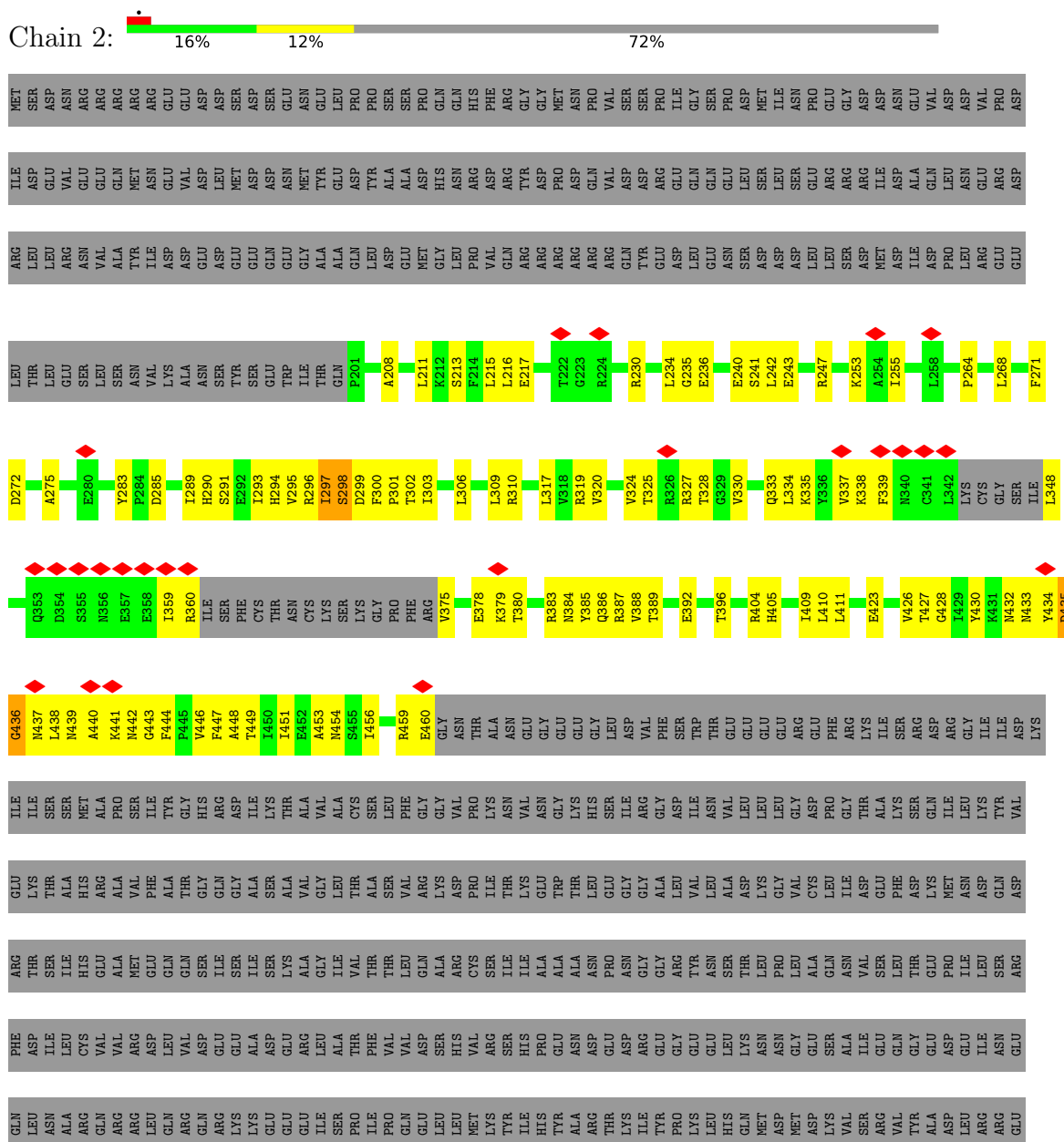
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

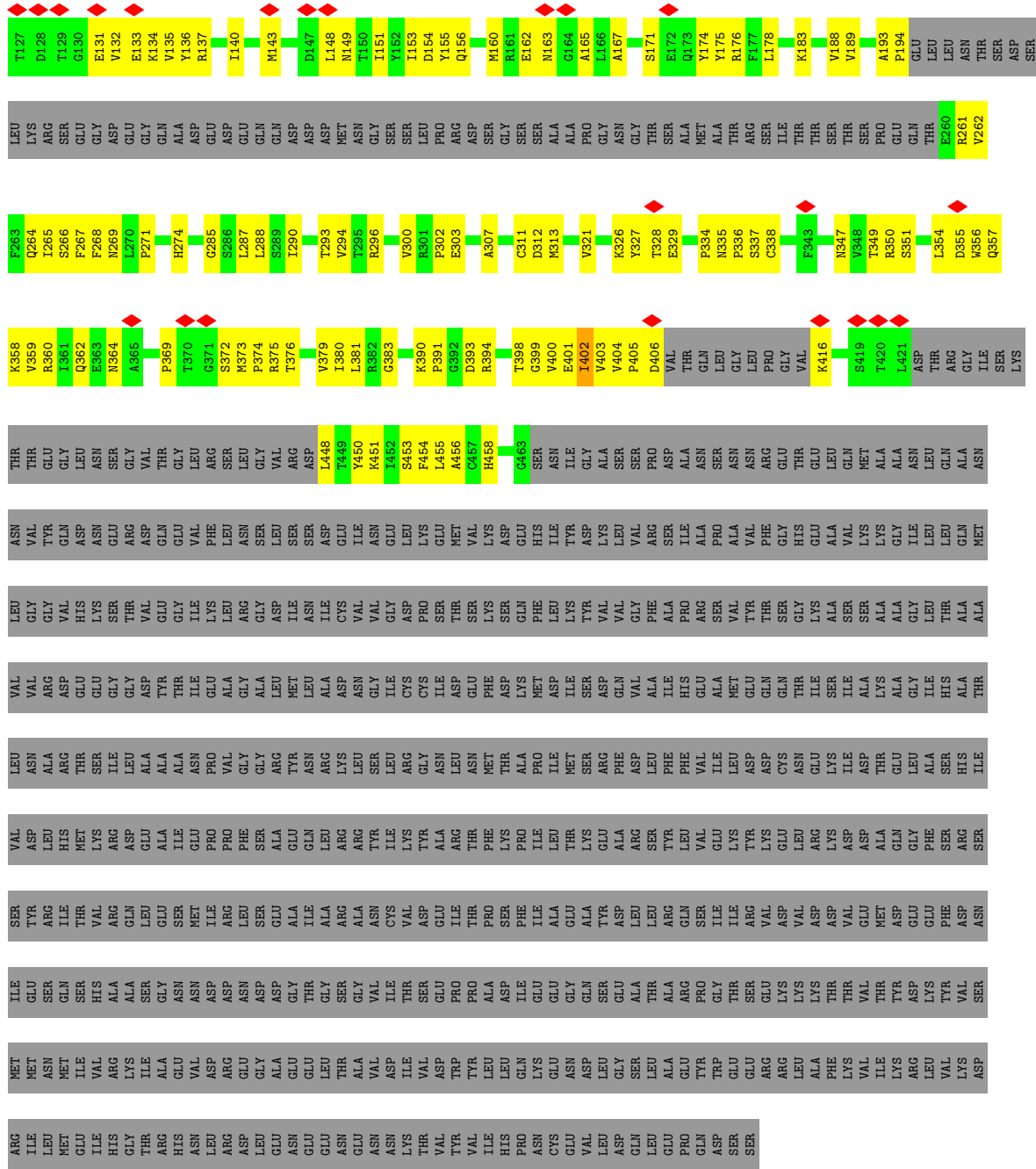
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
12	7	1	1	1	0

3 Residue-property plots

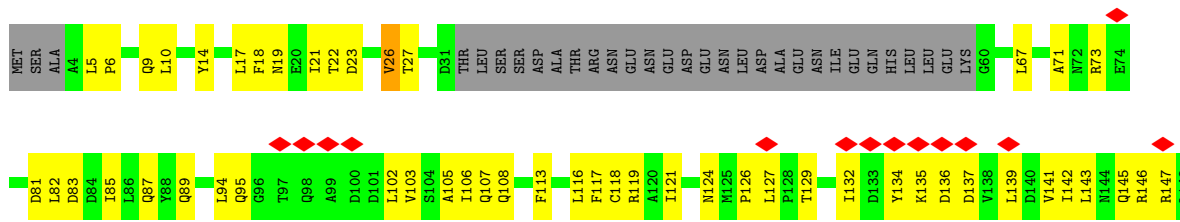
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

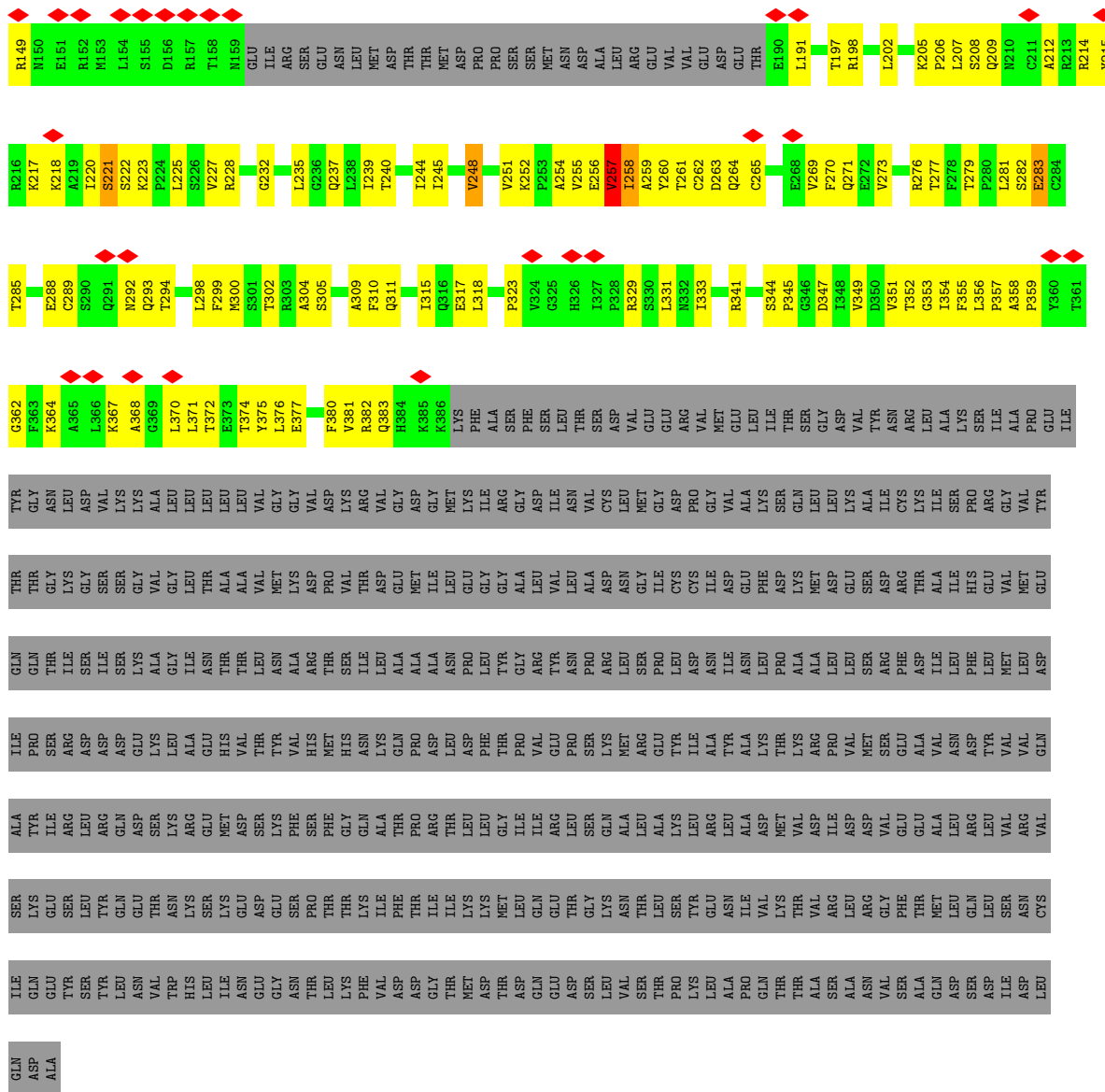
- Molecule 1: DNA replication licensing factor MCM2



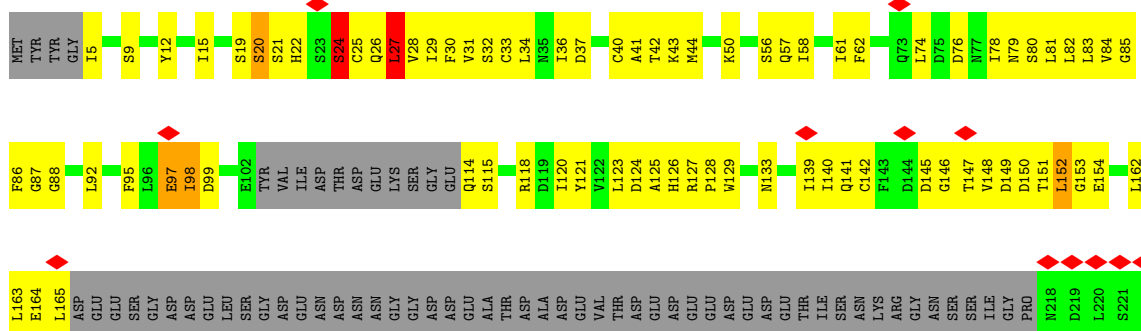
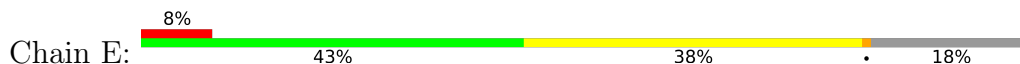


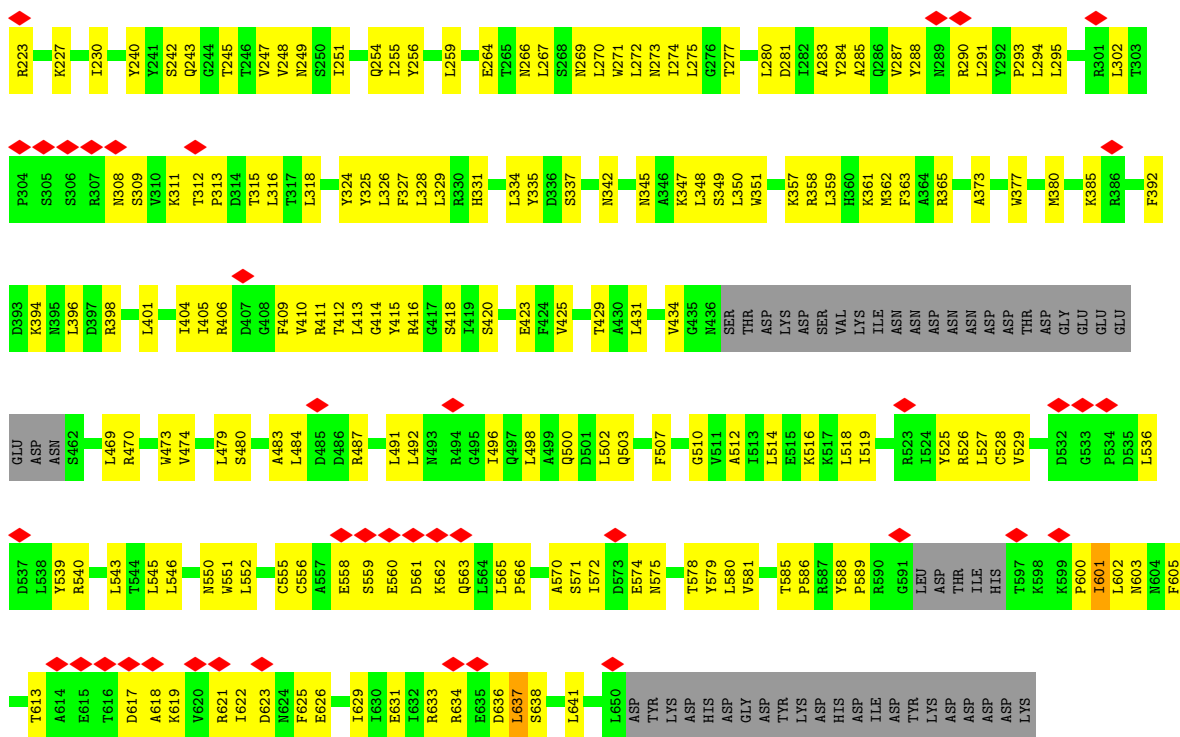
● Molecule 6: DNA replication licensing factor MCM7



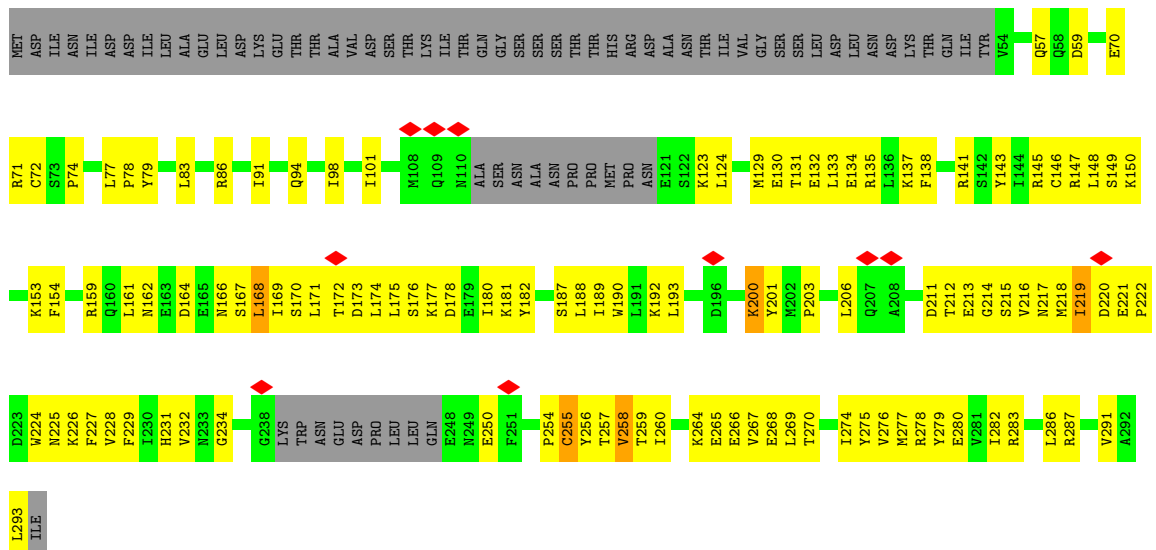


● Molecule 7: Cell division control protein 45



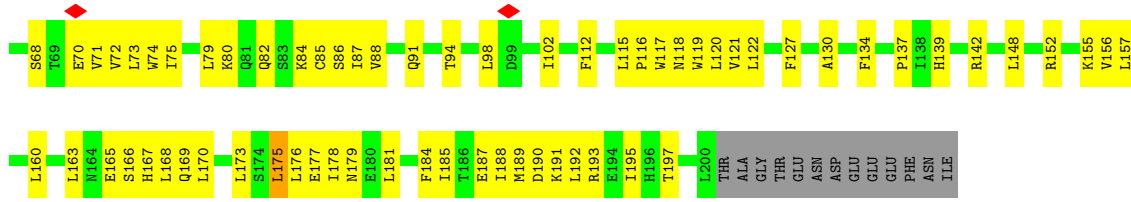


• Molecule 8: DNA replication complex GINS protein SLD5

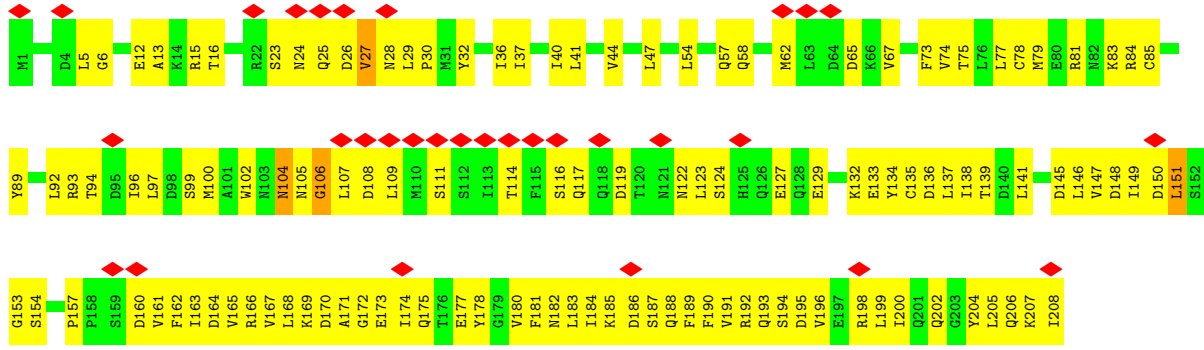


• Molecule 9: DNA replication complex GINS protein PSF2

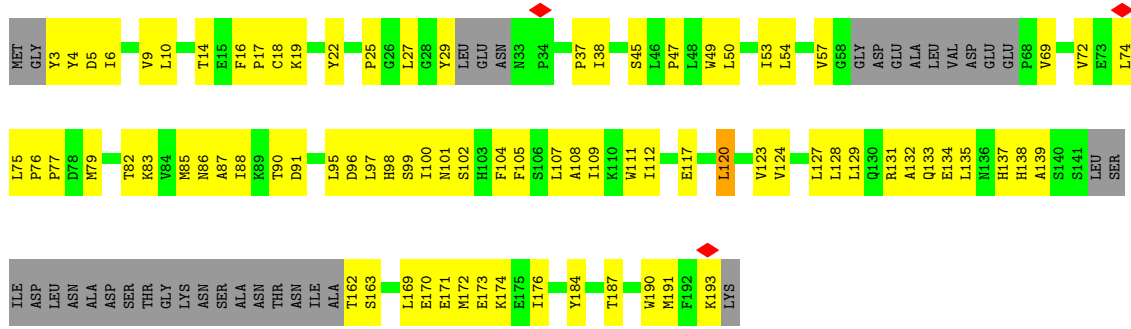




• Molecule 10: DNA replication complex GINS protein PSF1



• Molecule 11: DNA replication complex GINS protein PSF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	469818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	49505	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.01, 1.01, 1.01	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2	0.41	0/1946	0.66	1/2633 (0.0%)
2	3	0.46	0/2179	0.70	1/2963 (0.0%)
3	4	0.38	0/2240	0.67	0/3029
4	5	0.50	0/2057	0.73	2/2781 (0.1%)
5	6	0.39	0/2081	0.66	1/2813 (0.0%)
6	7	0.41	0/2657	0.66	1/3592 (0.0%)
7	E	0.39	0/4563	0.63	2/6173 (0.0%)
8	D	0.43	0/1853	0.64	0/2500
9	B	0.44	0/1545	0.69	0/2092
10	A	0.39	0/1718	0.65	0/2314
11	C	0.46	0/1320	0.64	1/1784 (0.1%)
All	All	0.42	0/24159	0.66	9/32674 (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
2	3	0	2
3	4	0	5
5	6	0	3
6	7	0	4
7	E	0	1
8	D	0	2
10	A	0	4
All	All	0	21

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	27	LEU	CA-CB-CG	7.97	133.63	115.30
4	5	258	LEU	CA-CB-CG	7.60	132.78	115.30
2	3	171	LEU	CA-CB-CG	7.21	131.88	115.30
5	6	105	ASP	CB-CG-OD1	6.55	124.20	118.30
1	2	436	GLY	N-CA-C	5.96	128.01	113.10

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	3	163	ALA	Peptide
2	3	165	ALA	Peptide
3	4	202	LYS	Peptide
3	4	245	ALA	Peptide
3	4	372	GLU	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	2	1911	0	1908	126	0
2	3	2130	0	2105	172	0
3	4	2203	0	2188	198	0
4	5	2028	0	2055	177	0
5	6	2049	0	1959	132	0
6	7	2611	0	2623	165	0
7	E	4482	0	4497	322	0
8	D	1820	0	1823	214	0
9	B	1513	0	1558	150	0
10	A	1696	0	1698	310	0
11	C	1288	0	1298	104	0
12	7	1	0	0	0	0
All	All	23732	0	23712	1852	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 39.

The worst 5 of 1852 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)
4:5:197:PHE:CE2	4:5:329:LYS:HG2	1.19	1.65
6:7:17:LEU:HD11	6:7:102:LEU:CD2	1.37	1.55
5:6:290:ILE:HD13	5:6:454:PHE:CZ	1.40	1.51
3:4:342:MET:HB3	3:4:360:ILE:CD1	1.45	1.46
9:B:187:GLU:OE2	11:C:176:ILE:CG2	1.65	1.43

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	2	235/868 (27%)	205 (87%)	25 (11%)	5 (2%)	7	38
2	3	263/971 (27%)	236 (90%)	22 (8%)	5 (2%)	8	40
3	4	271/933 (29%)	230 (85%)	36 (13%)	5 (2%)	8	41
4	5	244/775 (32%)	222 (91%)	19 (8%)	3 (1%)	13	48
5	6	259/1017 (26%)	229 (88%)	27 (10%)	3 (1%)	13	48
6	7	319/845 (38%)	270 (85%)	45 (14%)	4 (1%)	12	47
7	E	543/672 (81%)	491 (90%)	47 (9%)	5 (1%)	17	54
8	D	215/294 (73%)	197 (92%)	16 (7%)	2 (1%)	17	54
9	B	177/213 (83%)	163 (92%)	14 (8%)	0	100	100
10	A	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	29	66
11	C	151/194 (78%)	144 (95%)	7 (5%)	0	100	100
All	All	2883/6990 (41%)	2567 (89%)	283 (10%)	33 (1%)	18	50

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	291	SER
3	4	450	GLN

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Mol	Chain	Res	Type
6	7	26	VAL
7	E	601	ILE
3	4	419	VAL

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	2	206/770 (27%)	206 (100%)	0	100	100
2	3	236/835 (28%)	236 (100%)	0	100	100
3	4	249/848 (29%)	249 (100%)	0	100	100
4	5	241/688 (35%)	241 (100%)	0	100	100
5	6	207/886 (23%)	207 (100%)	0	100	100
6	7	295/753 (39%)	295 (100%)	0	100	100
7	E	499/607 (82%)	495 (99%)	4 (1%)	81	89
8	D	213/279 (76%)	212 (100%)	1 (0%)	88	94
9	B	171/198 (86%)	170 (99%)	1 (1%)	86	93
10	A	193/193 (100%)	192 (100%)	1 (0%)	88	94
11	C	144/173 (83%)	144 (100%)	0	100	100
All	All	2654/6230 (43%)	2647 (100%)	7 (0%)	92	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	E	152	LEU
8	D	168	LEU
10	A	151	LEU
9	B	175	LEU
7	E	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
6	7	145	GLN
10	A	104	ASN
7	E	26	GLN
10	A	202	GLN
9	B	146	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

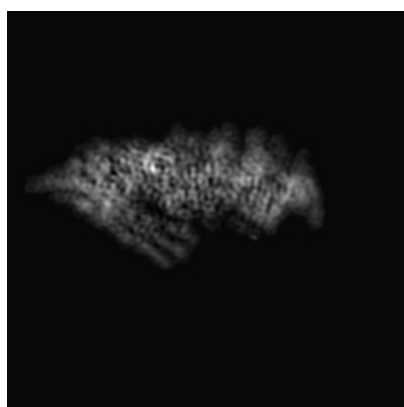
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6534. These allow visual inspection of the internal detail of the map and identification of artifacts.

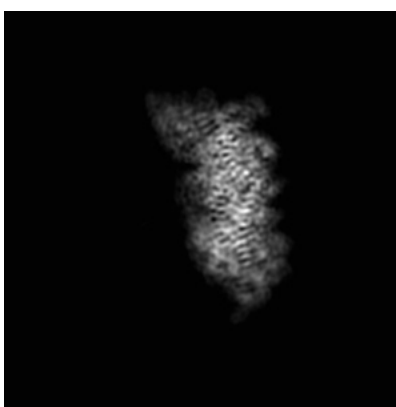
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

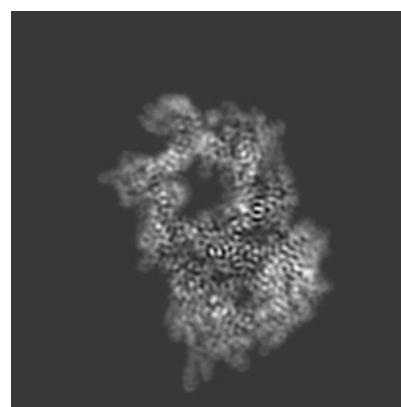
6.1.1 Primary map



X



Y

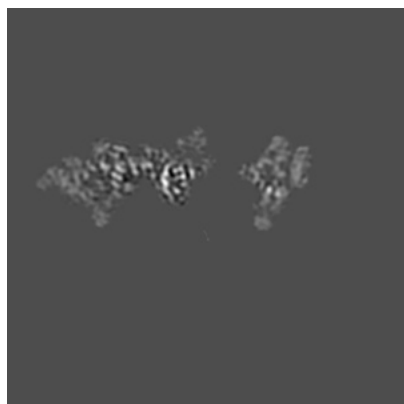


Z

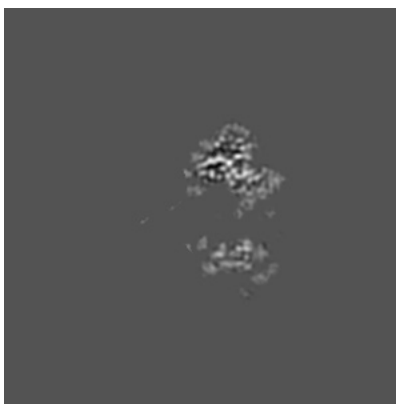
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

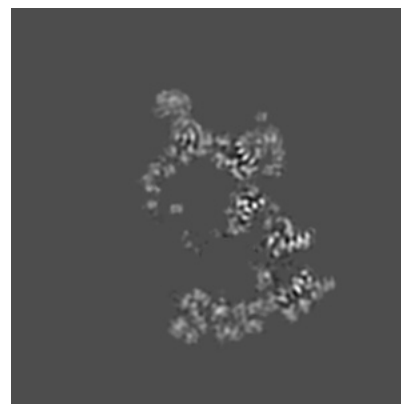
6.2.1 Primary map



X Index: 128



Y Index: 128

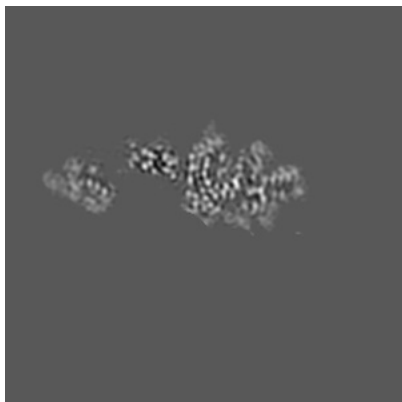


Z Index: 128

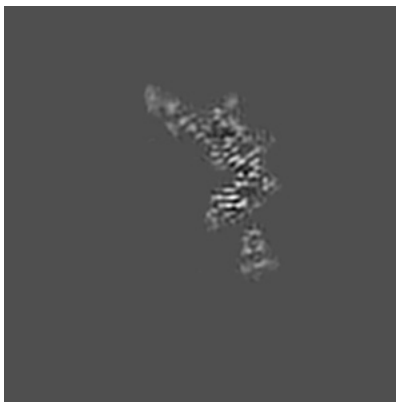
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

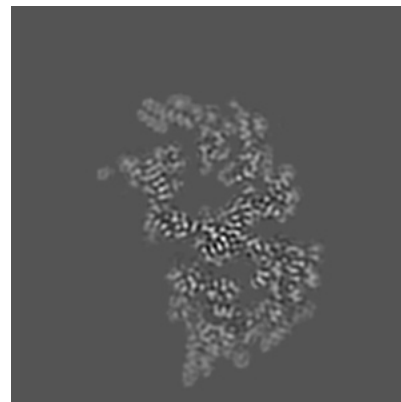
6.3.1 Primary map



X Index: 149



Y Index: 101

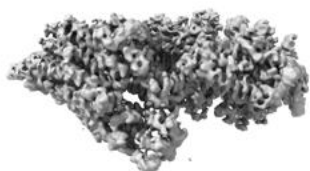


Z Index: 147

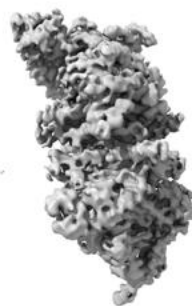
The images above show the largest variance slices of the map in three orthogonal directions.

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

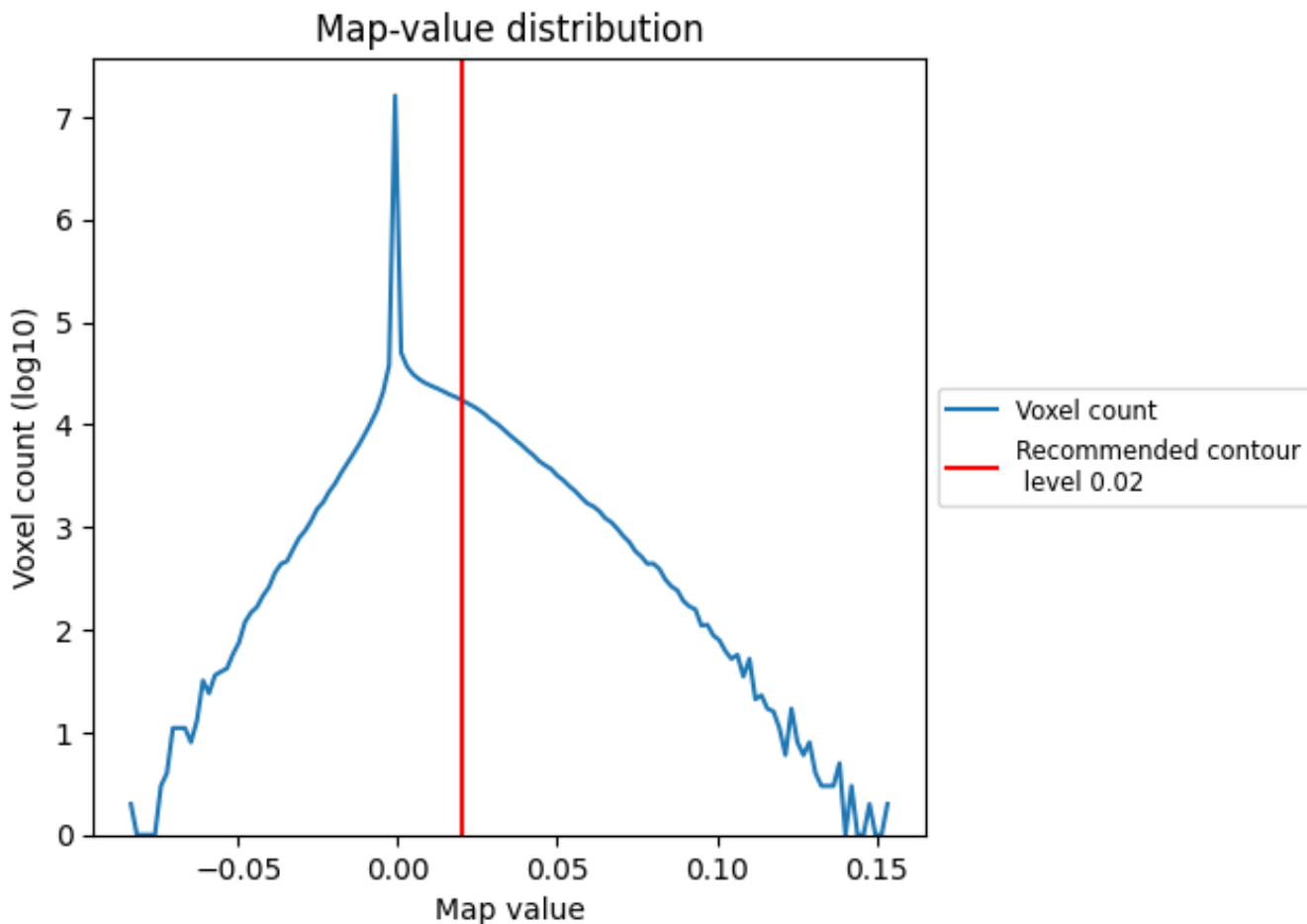
6.5 Mask visualisation

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

7 Map analysis [i](#)

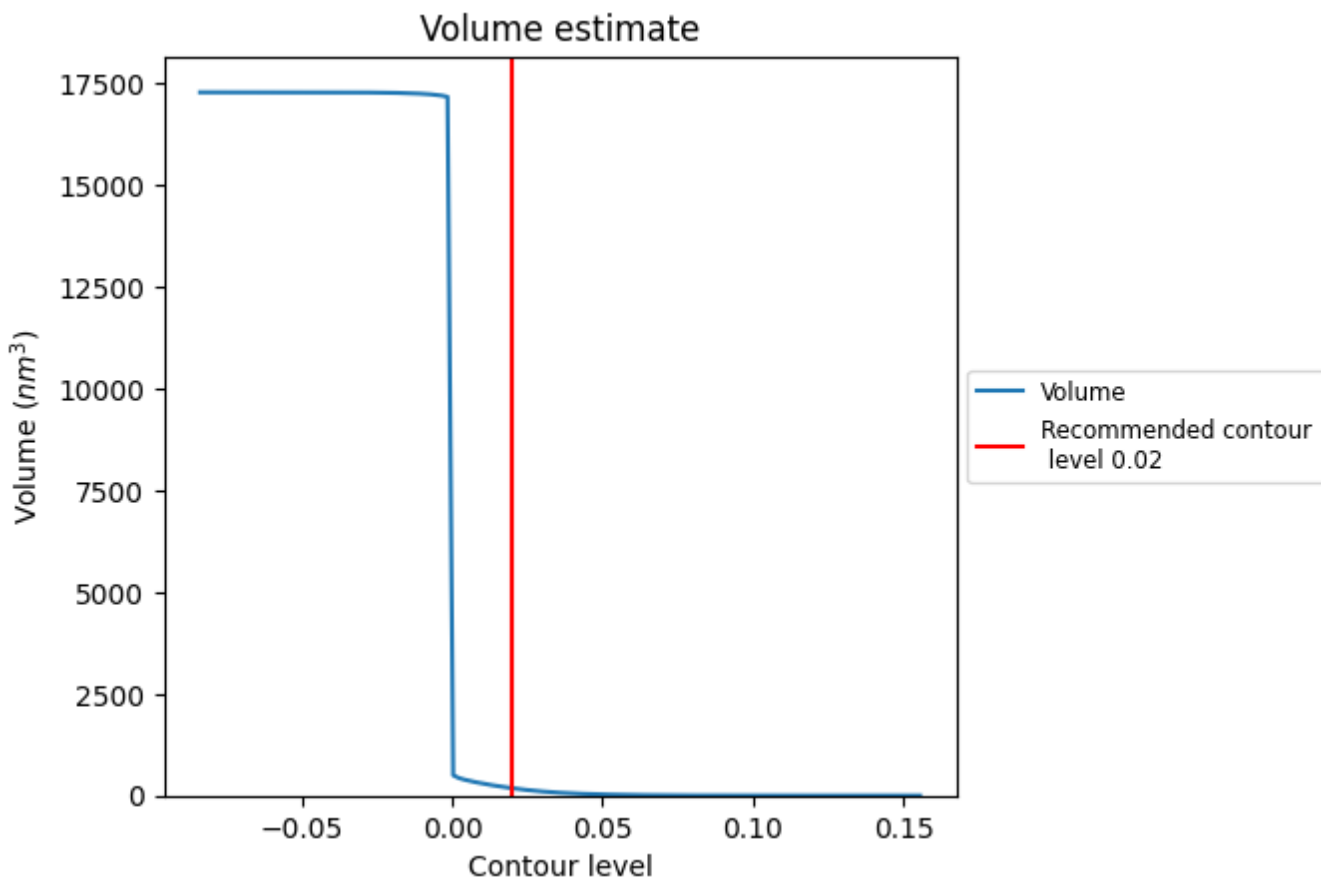
This section contains the results of statistical analysis of the map.

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.

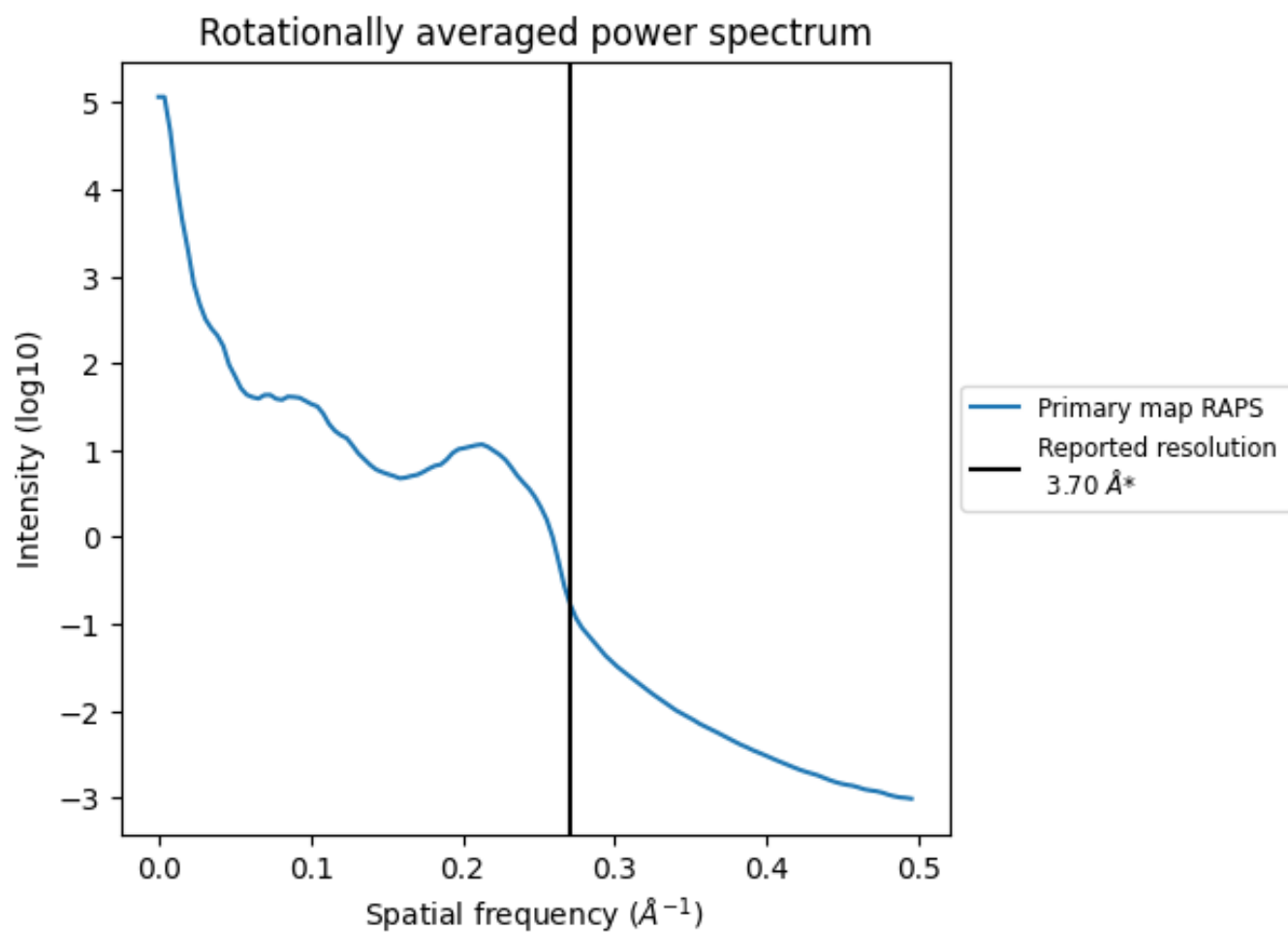
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 164 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 0.270\AA^{-1}

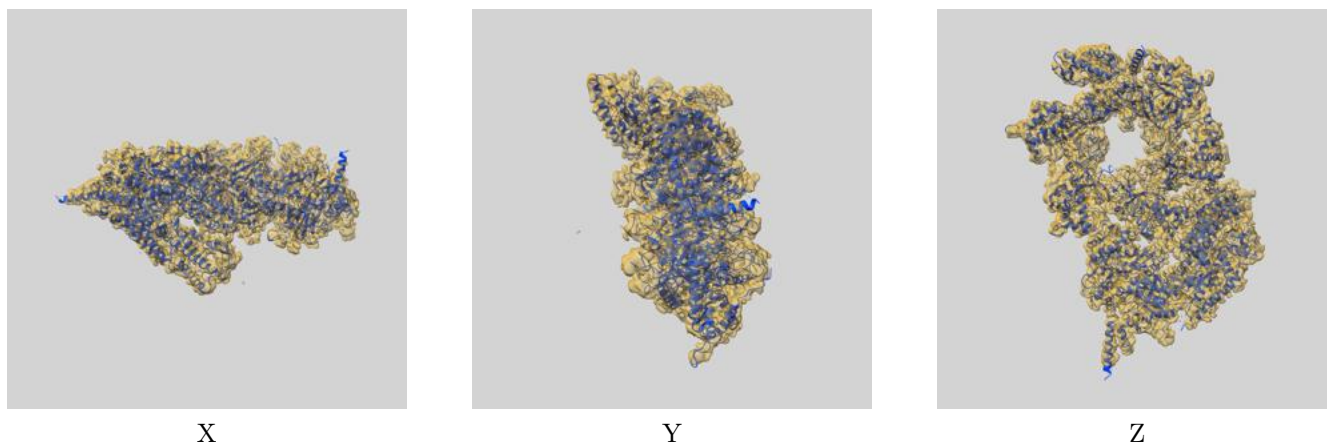
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

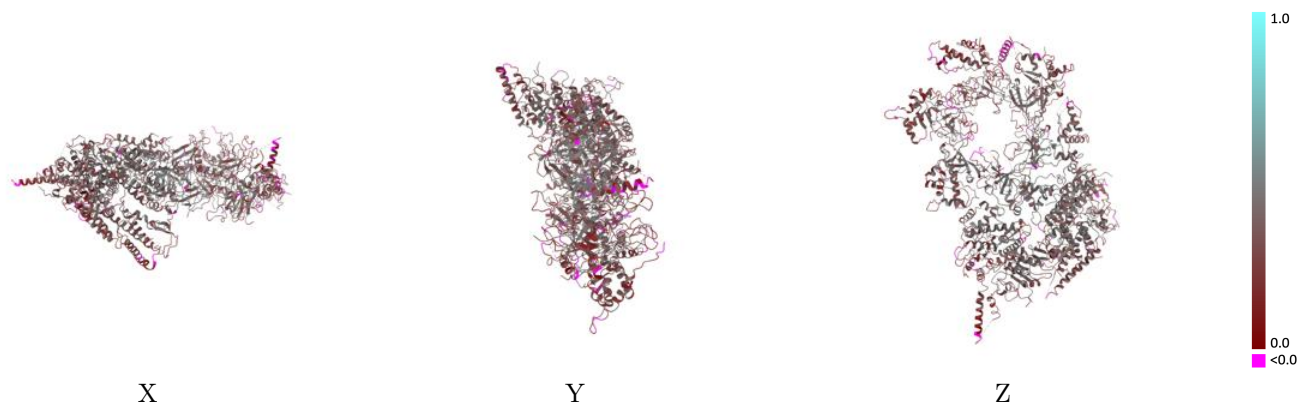
This section contains information regarding the fit between EMDB map EMD-6534 and PDB model 3JC6. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



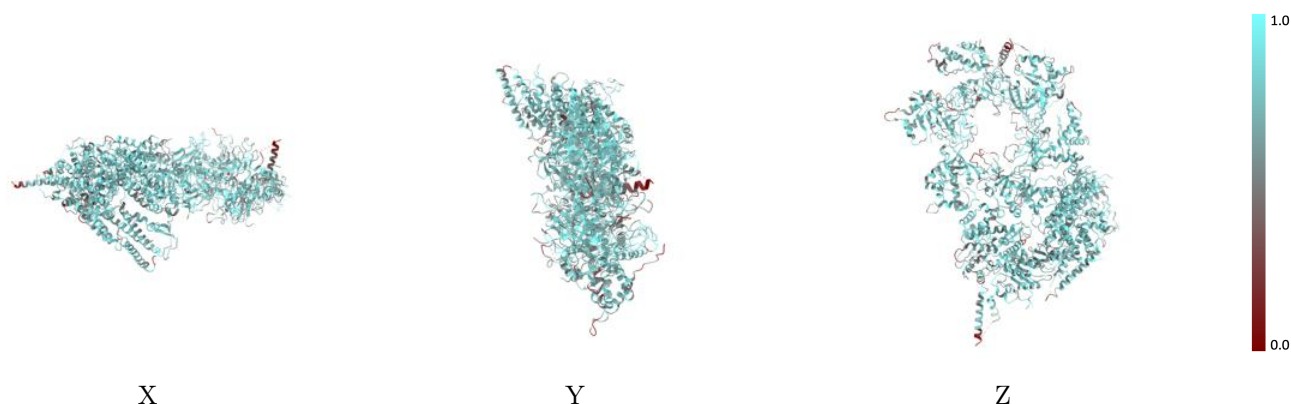
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



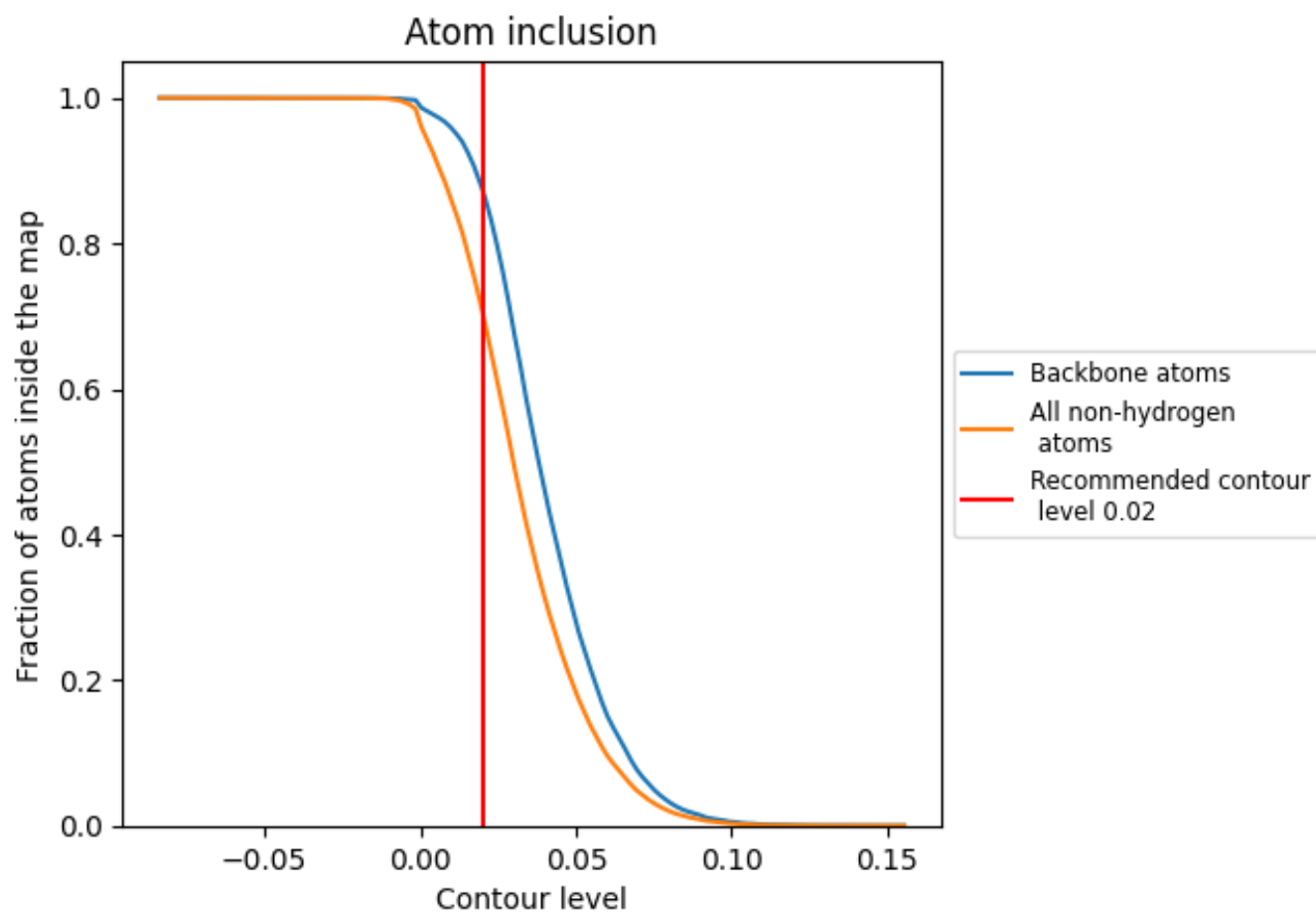
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7055	 0.3290
2	 0.7000	 0.3380
3	 0.7451	 0.3680
4	 0.6763	 0.2630
5	 0.7681	 0.4160
6	 0.6793	 0.2950
7	 0.6517	 0.2910
A	 0.6494	 0.2820
B	 0.7470	 0.3740
C	 0.7679	 0.3830
D	 0.7241	 0.3260
E	 0.6999	 0.3270

