



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 02:37 PM EST

PDB ID : 7STI
EMDB ID : EMD-25429
Title : Full-length insulin receptor bound with unsaturated insulin WT (1 insulin bound) asymmetric conformation
Authors : Bai, X.C.; Choi, E.
Deposited on : 2021-11-13
Resolution : 4.90 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
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

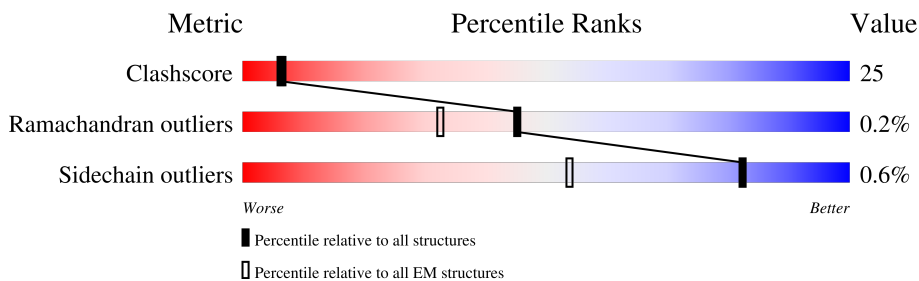
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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 $\leq 5\%$. 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	1372	
1	B	1372	
2	C	110	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13531 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	816	Total	C	N	O	S	0	0
			6585	4179	1134	1220	52		
1	B	814	Total	C	N	O	S	0	0
			6570	4170	1131	1217	52		

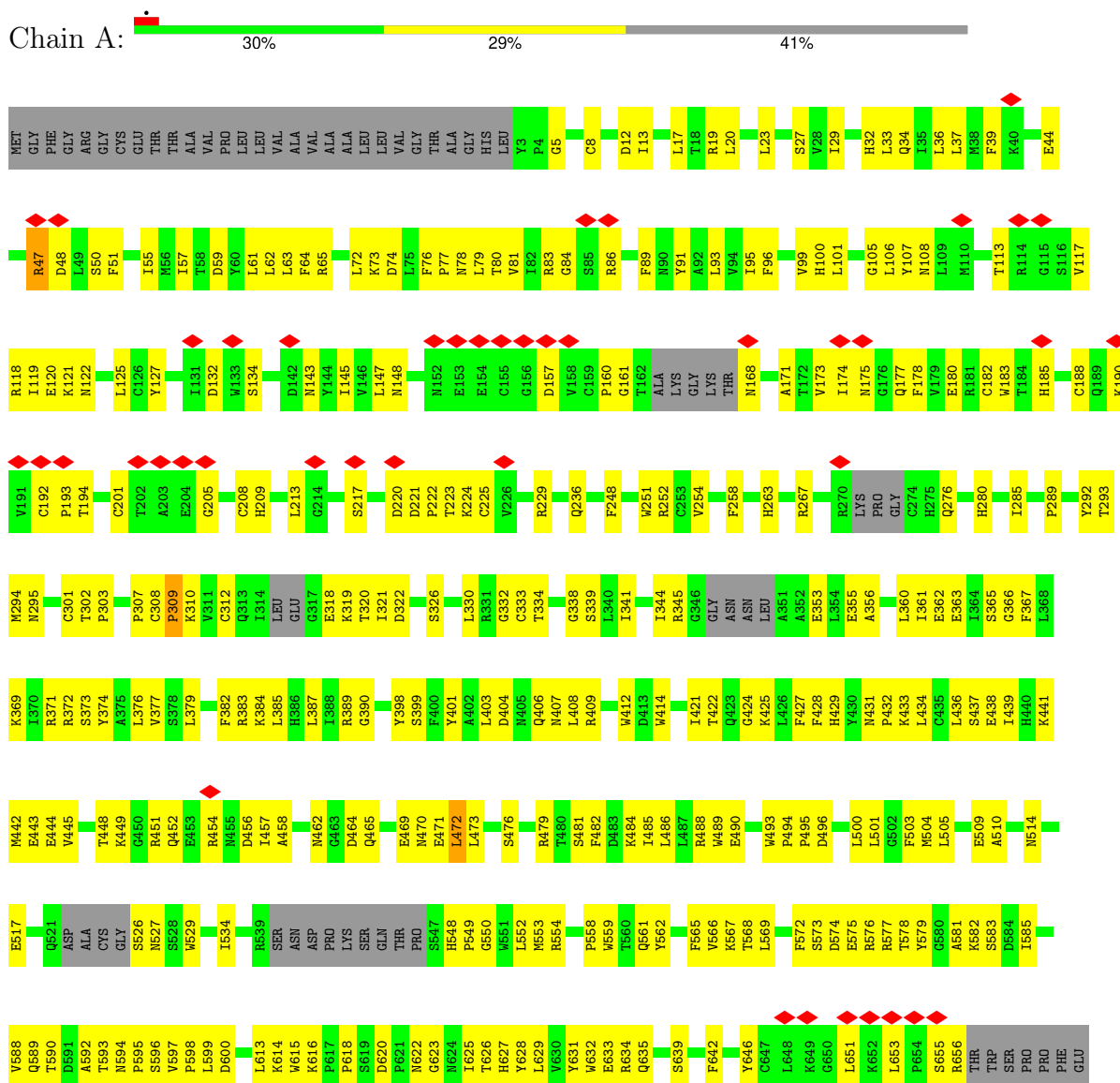
- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	48	Total	C	N	O	S	0	0
			376	238	61	71	6		

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: Insulin receptor





MET	GLY	F39	M10	C182	R270
	GLY	K40	M11	W183	LYS
	PHE	T41	M12	C188	PRO
	GLY	R42	M13	C188	GLY
	ARG	P43	M14	P193	C274
	GLY	E44	M15	T194	H275
	CYS	D45	M16	I195	C276
	GLU	F46	M17	C196	Y277
	THR	S50	M18	C196	
	THR	F51	M19	H199	N281
VAL	P52	M20	C208	N282	
PRO	K53	M21	H209	K283	
LEU	M56	M22	C208	P286	
LEU	I57	M23	H209		
VAL	T58	M24	K210	S290	
ALA	D59	M25	C212	G291	
VAL	L62	M26	L213	Y292	
ALA	L63	M27	C216	T293	
ALA	L63	M28	S217	F303	
LEU	F64	M29	E218	C304	
VAL	R65	M30	P219	L305	
GLY	V66	M31	D220	G306	
THR	Y67	M32	D221	P307	
ALA	E70	M33	P222	C308	
GLY	S71	M34	T223	P309	
H1	L72	M35	K224	K310	
L2	C73	M36	C225	V311	
Y3	D74	M37	V226		
P4	L75	M38	A227	T334	
G5	F76	M39	C228	V335	
	P77	M40	N230		
C8	N78	M41	Q236	S339	
P9	L79	M42	C237	L340	
M1	T80	M43	V238	I341	
D12	V81	M44	E239	R345	
I13	R82	M45	T240		
R14	R83	M46	C241	N349	
	G84	M47	Y245	L350	
L17	S85	M48	Y246		
T18	R86	M49	H247	C353	
R19	L87	M50	F248	L354	
L20	Y91	M51	Q249	E355	
	A92	M52	L250	G359	
W25	L93	M53	M251	L360	
C26	V94	M54	R252	I361	
S27	I95	M55	C253	E362	
V28	M100	M56	F258	E363	
I29	L101	M57		I364	
E30	K102	M58	D261	S365	
G31	L106	M59	L262	G366	
H32	I107	M60	H263	F367	
L33	M108	M61	F264	L368	
Q34	L109	M62	K265	K369	
I35		M63		I370	
L36		M64		R371	
L37		M65		R372	
L38		M66			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6130	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	A	0.28	0/6745	0.51	0/9139
1	B	0.29	0/6731	0.51	0/9122
2	C	0.33	0/383	0.48	0/518
All	All	0.29	0/13859	0.51	0/18779

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	6585	0	6384	319	0
1	B	6570	0	6380	353	0
2	C	376	0	346	19	0
All	All	13531	0	13110	674	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 25.

The worst 5 of 674 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)
2:C:7:CYS:HA	2:C:11:LEU:HD23	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:PHE:HB3	1:B:488:ARG:HB2	1.58	0.86
1:A:122:ASN:HB3	1:A:125:LEU:HD23	1.62	0.81
1:B:508:LYS:HD3	1:B:529:TRP:H	1.45	0.81
1:B:341:ILE:HG22	1:B:369:LYS:HB3	1.61	0.80

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	798/1372 (58%)	735 (92%)	60 (8%)	3 (0%)	30	68
1	B	800/1372 (58%)	732 (92%)	68 (8%)	0	100	100
2	C	44/110 (40%)	44 (100%)	0	0	100	100
All	All	1642/2854 (58%)	1511 (92%)	128 (8%)	3 (0%)	45	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	CYS
1	A	309	PRO
1	A	470	ASN

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	743/1228 (60%)	738 (99%)	5 (1%)	81	87
1	B	741/1228 (60%)	737 (100%)	4 (0%)	86	89
2	C	43/88 (49%)	43 (100%)	0	100	100
All	All	1527/2544 (60%)	1518 (99%)	9 (1%)	82	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	850	ARG
1	B	875	ARG
1	A	454	ARG
1	A	472	LEU
1	B	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	295	ASN
1	A	343	ASN
1	A	423	GLN
1	A	431	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

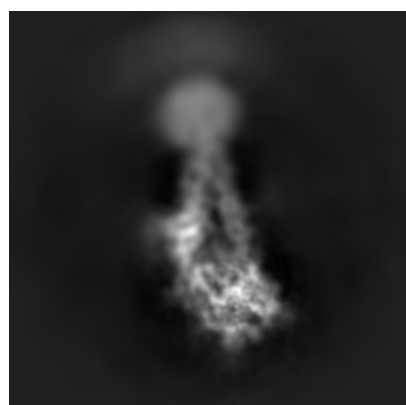
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25429. These allow visual inspection of the internal detail of the map and identification of artifacts.

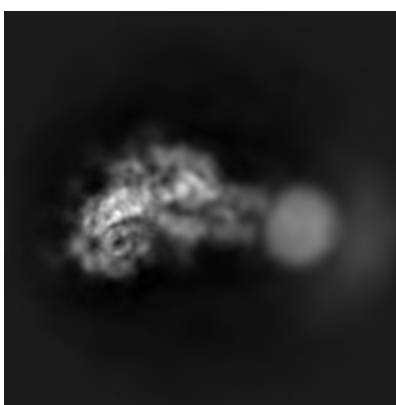
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

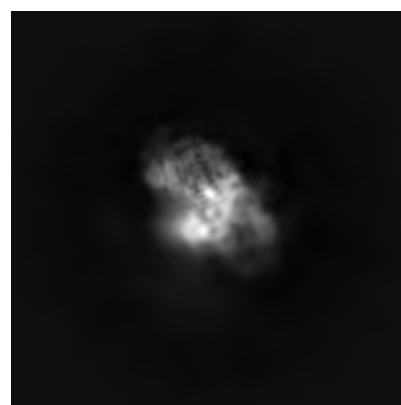
6.1.1 Primary map



X



Y

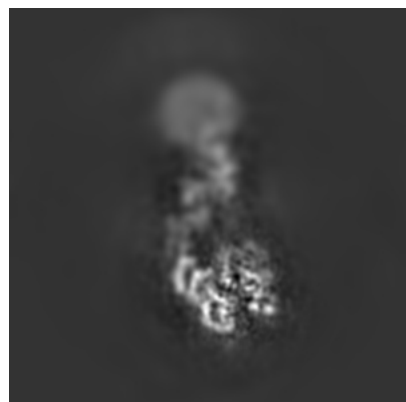


Z

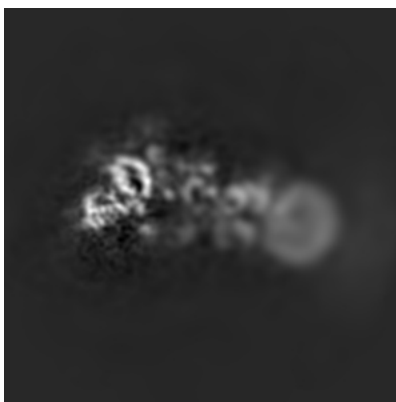
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

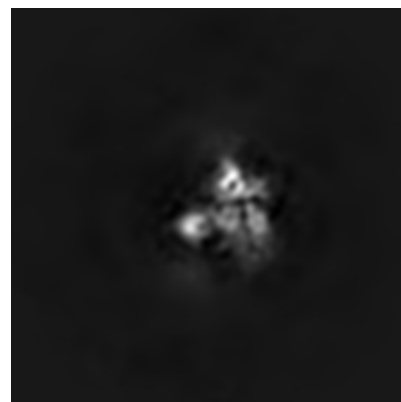
6.2.1 Primary map



X Index: 150



Y Index: 150

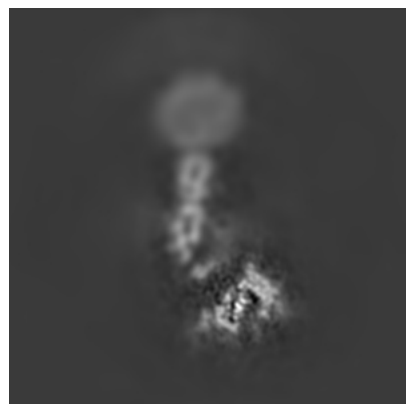


Z Index: 150

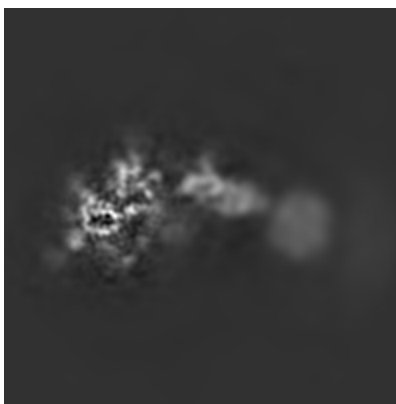
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 135



Y Index: 163

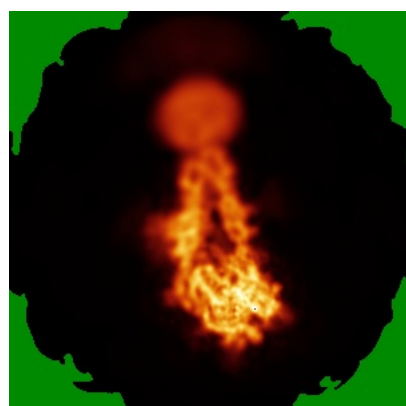


Z Index: 89

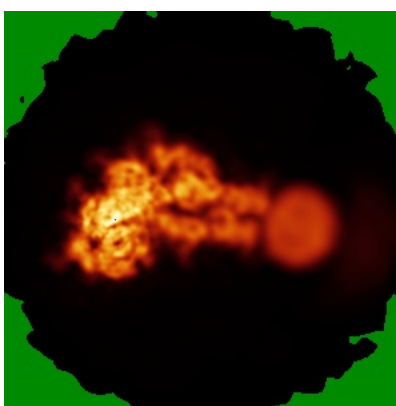
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

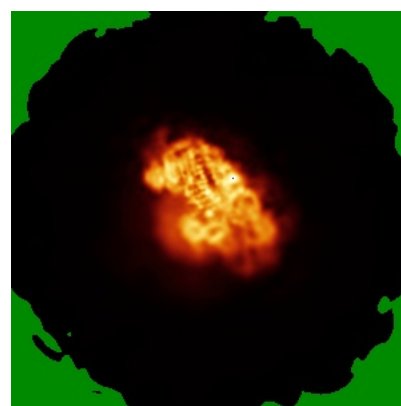
6.4.1 Primary map



X



Y

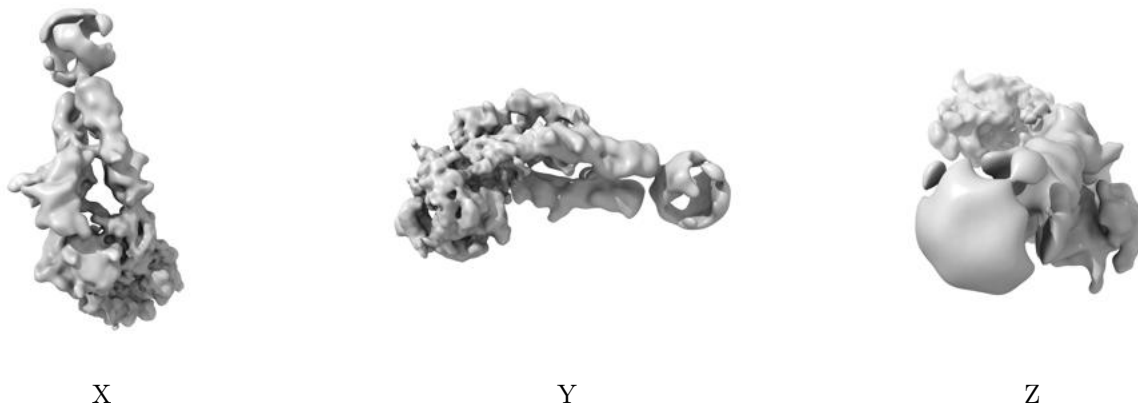


Z

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



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.

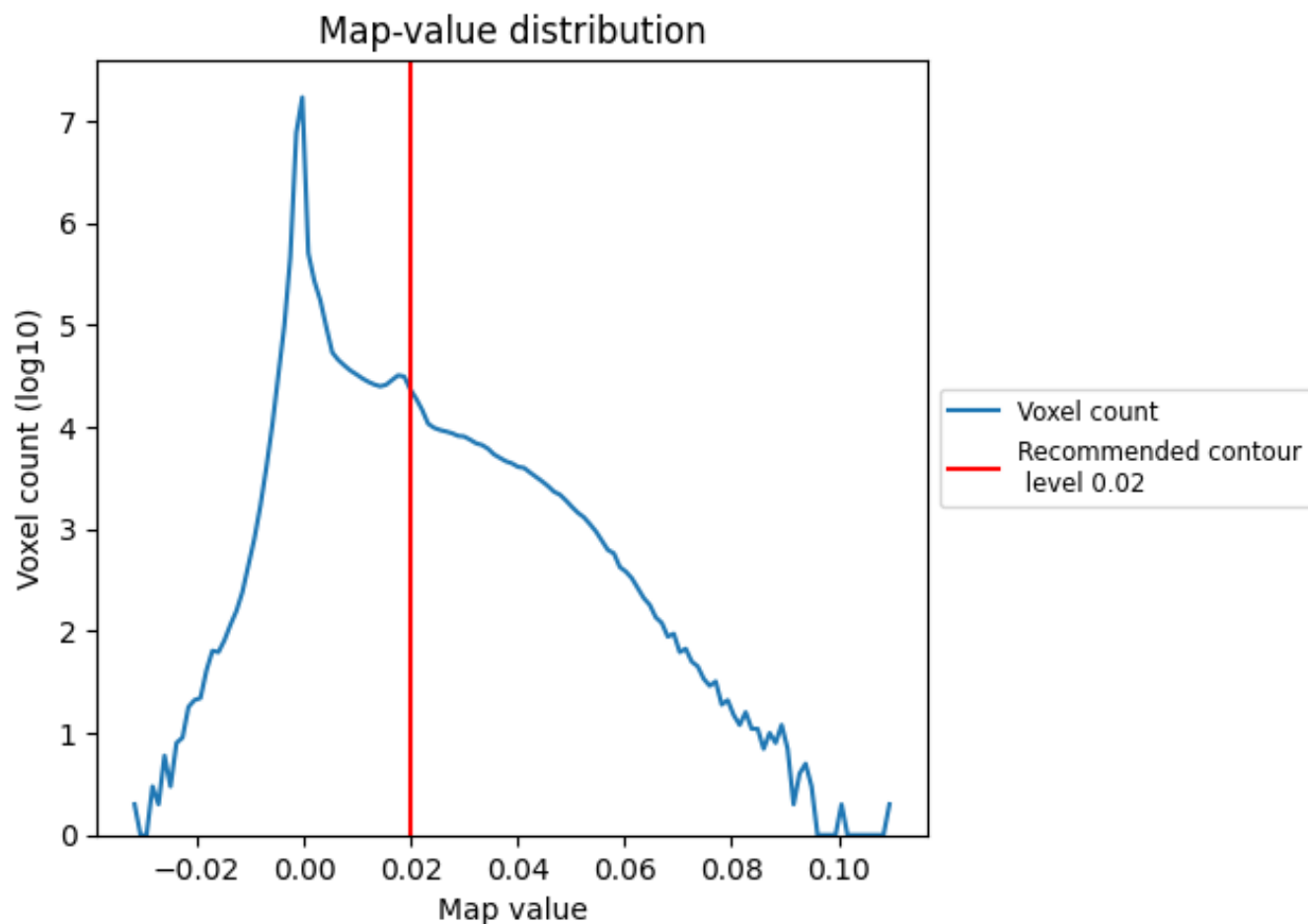
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

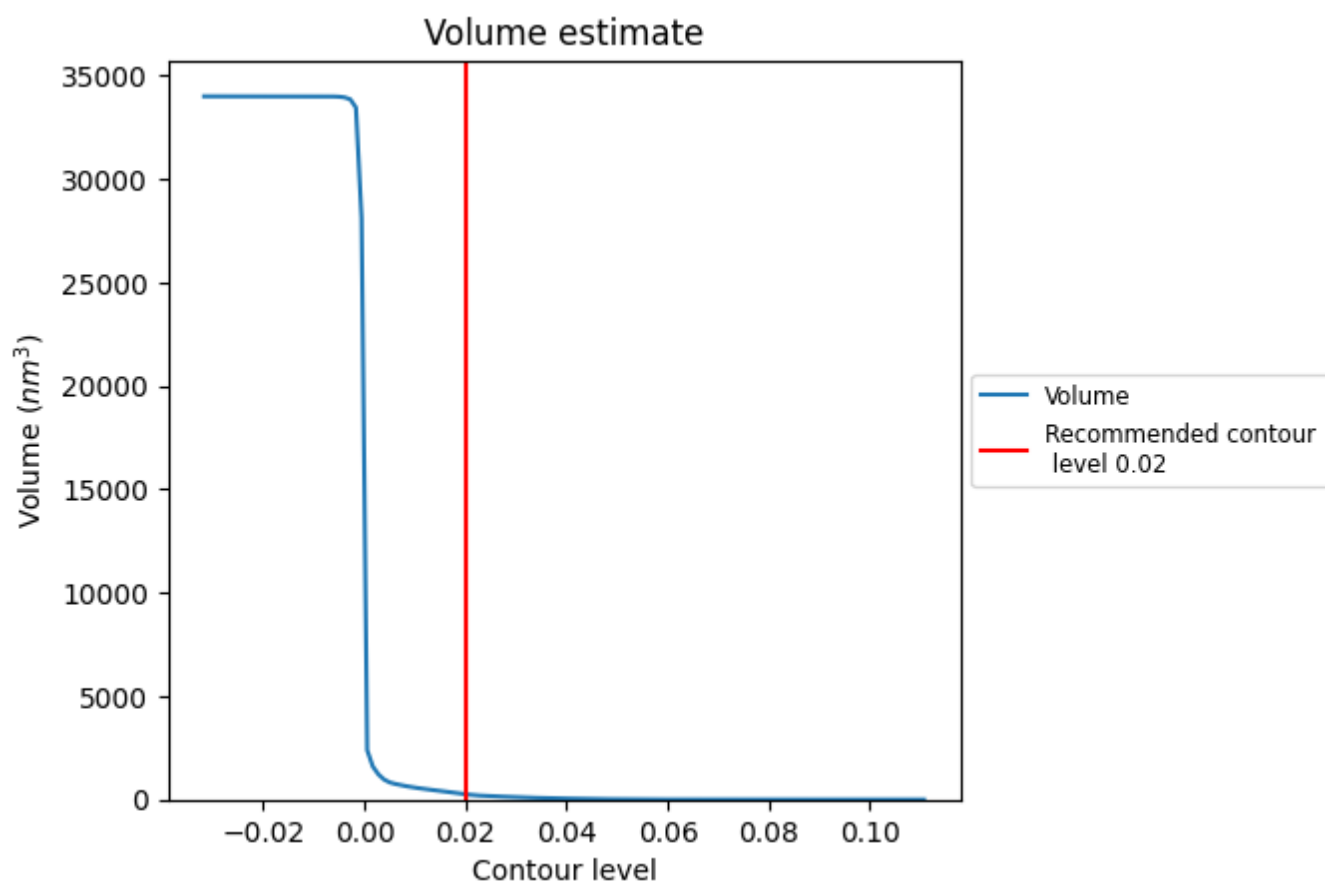
This section contains the results of statistical analysis of the map.

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.

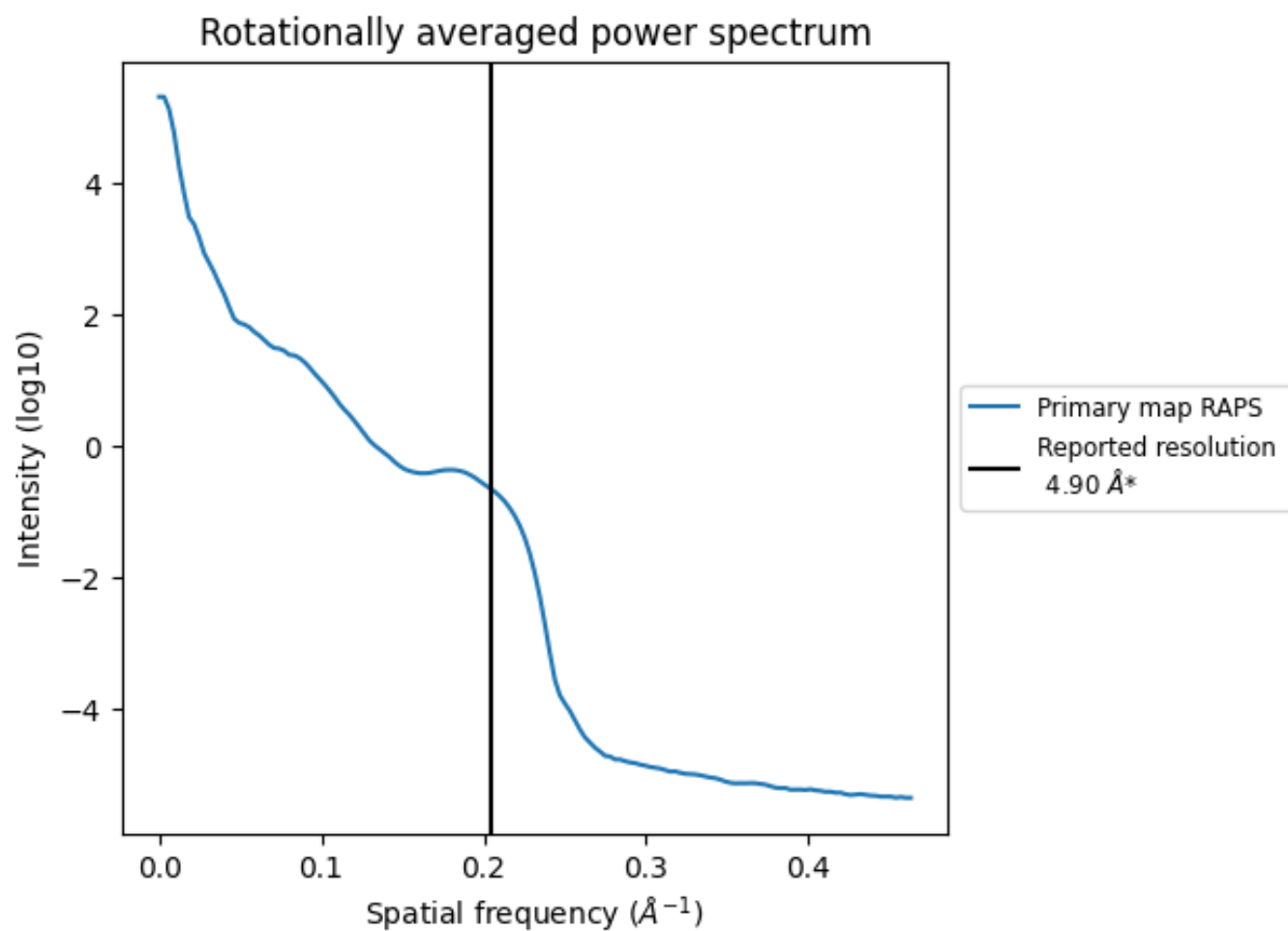
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm³; this corresponds to an approximate mass of 231 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 0.204 Å⁻¹

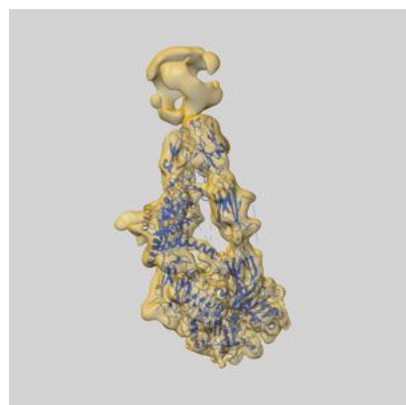
8 Fourier-Shell correlation

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

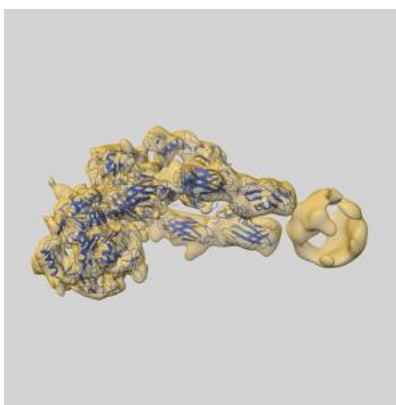
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25429 and PDB model 7STI. Per-residue inclusion information can be found in section [3](#) on page [4](#).

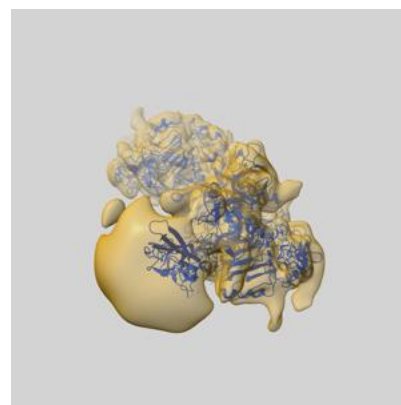
9.1 Map-model overlay [i](#)



X



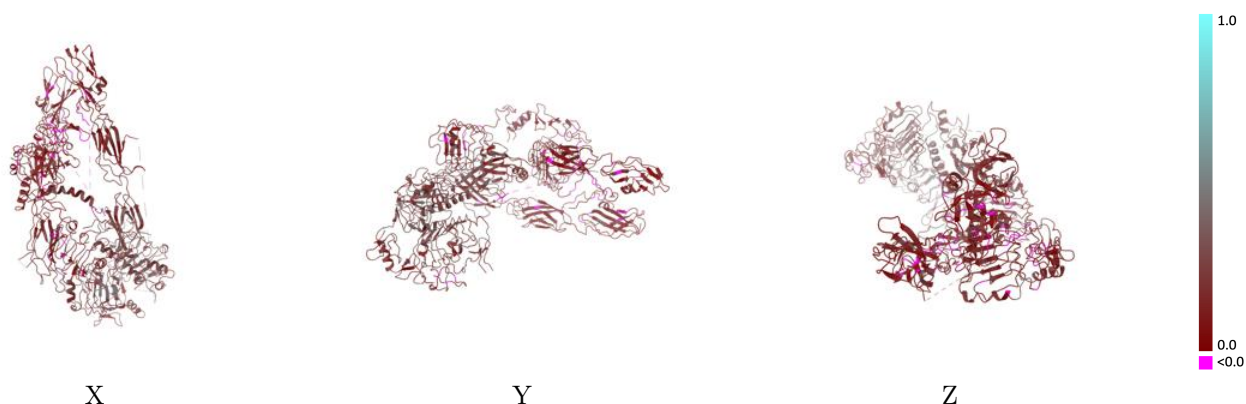
Y



Z

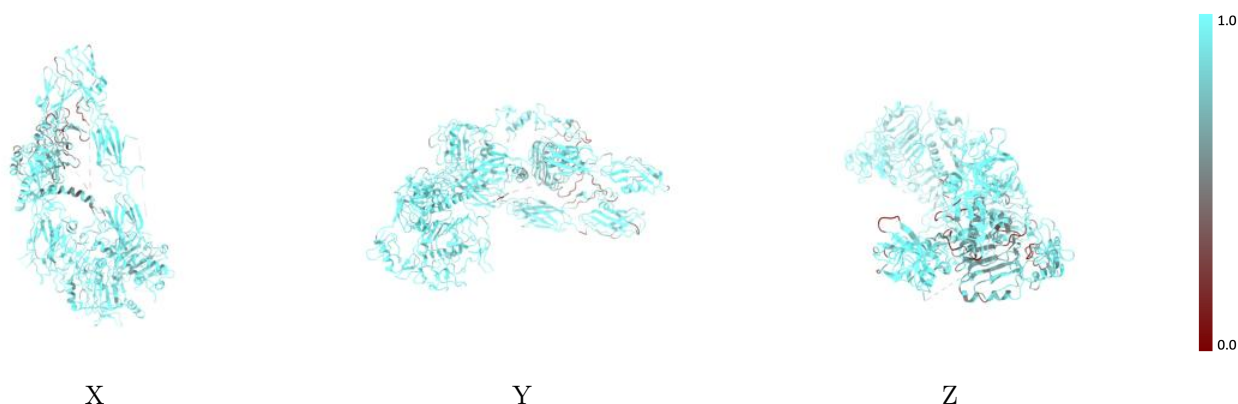
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



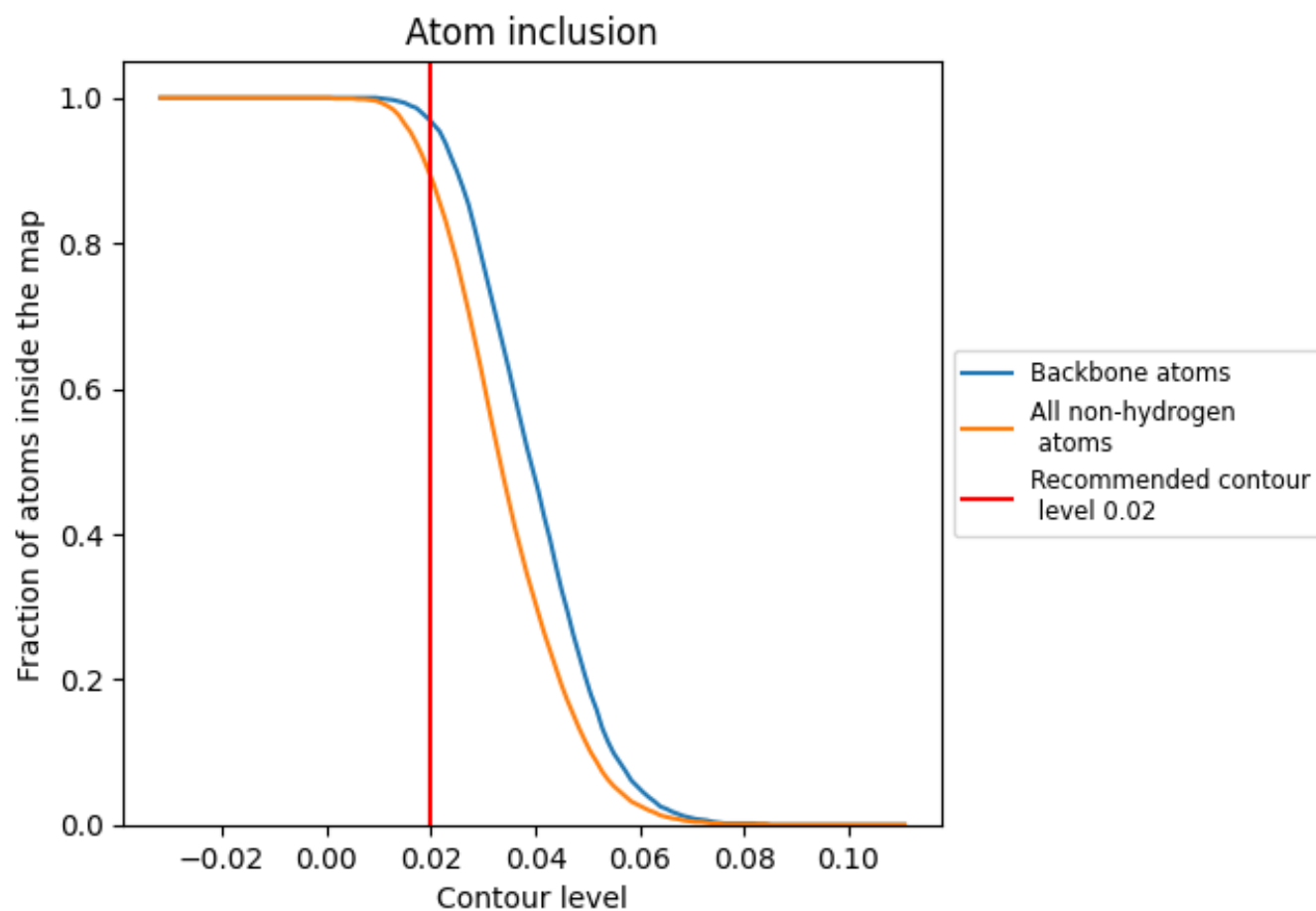
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 97% of all backbone atoms, 89% 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	<div></div> 0.8910	<div></div> 0.2090
A	<div></div> 0.8550	<div></div> 0.1870
B	<div></div> 0.9230	<div></div> 0.2280
C	<div></div> 0.9680	<div></div> 0.2680

