



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 01:16 PM EDT

PDB ID : 7K5I  
EMDB ID : EMD-22681  
Title : SARS-COV-2 nsp1 in complex with human 40S ribosome  
Authors : Wang, L.; Shi, M.; Wu, H.  
Deposited on : 2020-09-16  
Resolution : 2.90 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](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:

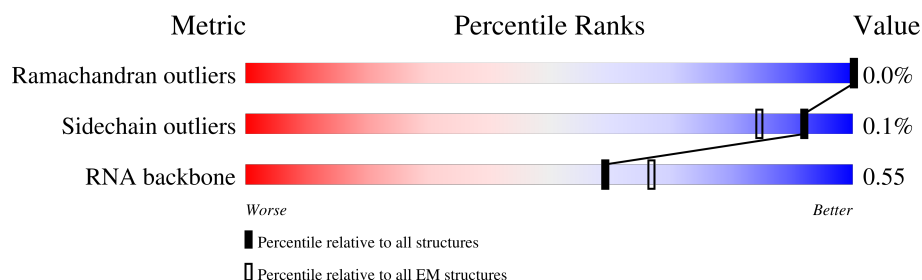
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 2.90 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.



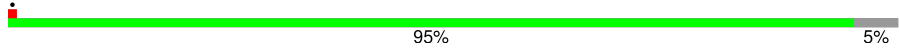
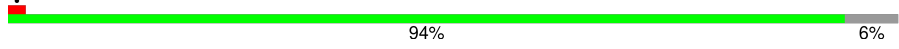
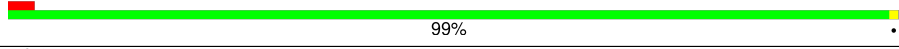




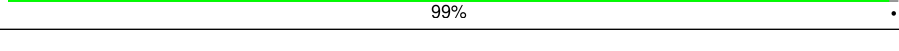
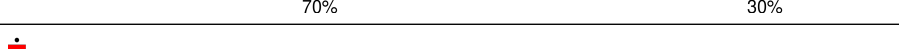
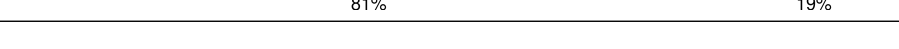
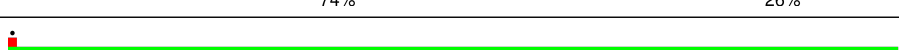
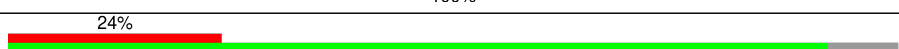
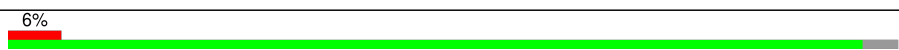
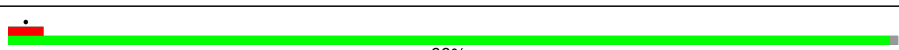
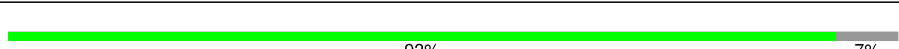

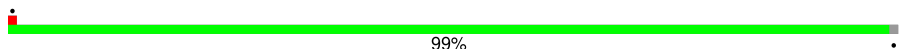

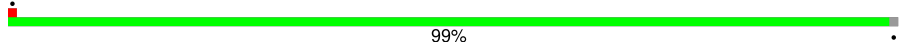
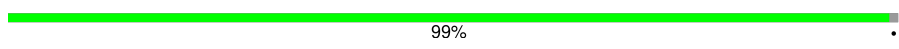
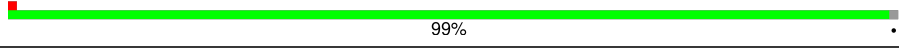
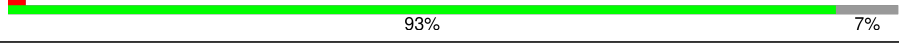
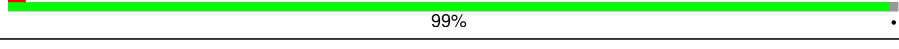
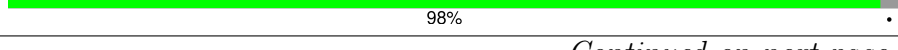

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	R	135	
2	2	1868	
3	d	56	
4	D	243	
5	F	204	
6	K	165	
7	M	132	
8	P	145	

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Mol	Chain	Length	Quality of chain
9	Q	146	
10	S	152	
11	T	145	
12	U	119	
13	Z	125	
14	c	69	
15	f	149	
16	g	317	
17	A	295	
18	B	264	
19	C	293	
20	E	263	
21	G	249	
22	H	194	
23	I	208	
24	J	194	
25	L	158	
26	N	151	
27	O	151	
28	V	83	
29	W	130	
30	X	143	
31	Y	133	
32	a	102	
33	b	84	

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Mol	Chain	Length	Quality of chain
34	e	59	<div><div></div><div>85%</div><div>15%</div></div>
35	h	25	<div><div>36%</div><div>96%</div><div>.</div></div>
36	1	180	<div><div>17%</div><div>83%</div></div>

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 74540 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 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 2 is a RNA chain called 40S ribosomal rRNA18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1665	Total	C	N	O	P	0	0
			35552	15869	6385	11633	1665		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 3 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	225	Total	C	N	O	S	0	0
			1748	1115	315	311	7		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 6 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 7 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 8 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 9 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 10 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 11 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 12 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 13 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 15 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 16 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 17 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

- Molecule 18 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 19 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	C	218	Total	C	N	O	S	0	0
			1682	1090	289	293	10		

- Molecule 20 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 21 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 22 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 23 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 24 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 27 is a protein called 40S ribosomal protein S14.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	135	Total	C	N	O	S	0	0
			1006	616	198	186	6		

- Molecule 28 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 30 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	50	Total	C	N	O	S	0	0
			397	242	89	65	1		

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 36 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	30	Total	C	N	O	S	0	0
			250	153	44	52	1		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

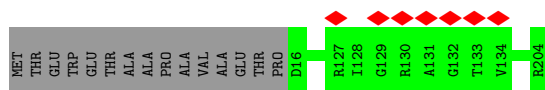
Mol	Chain	Residues	Atoms		AltConf
37	2	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

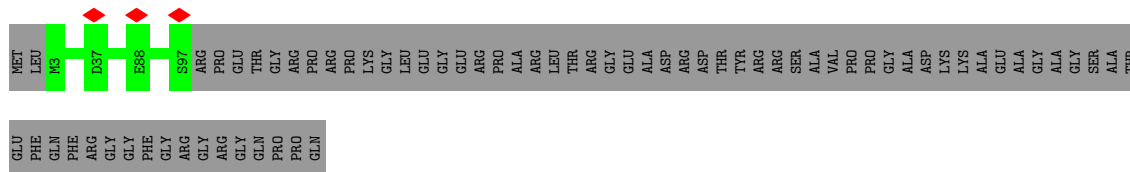
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38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	
38	a	1	Total	Zn	0
			1	1	



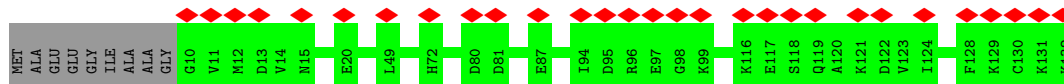




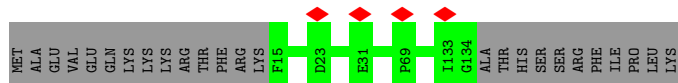
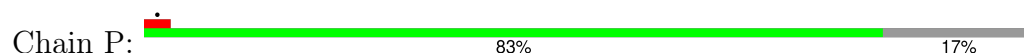
- Molecule 6: 40S ribosomal protein S10



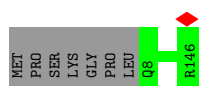
- Molecule 7: 40S ribosomal protein S12



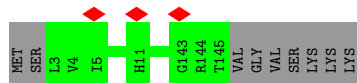
- Molecule 8: 40S ribosomal protein S15



- Molecule 9: 40S ribosomal protein S16



- Molecule 10: 40S ribosomal protein S18

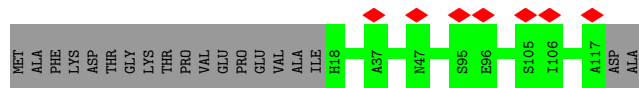
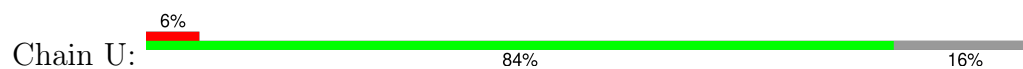


- Molecule 11: 40S ribosomal protein S19

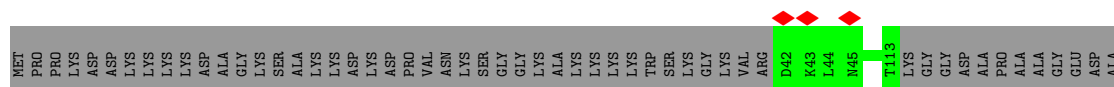




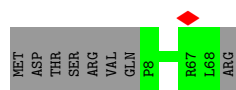
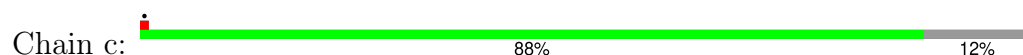
- Molecule 12: 40S ribosomal protein S20



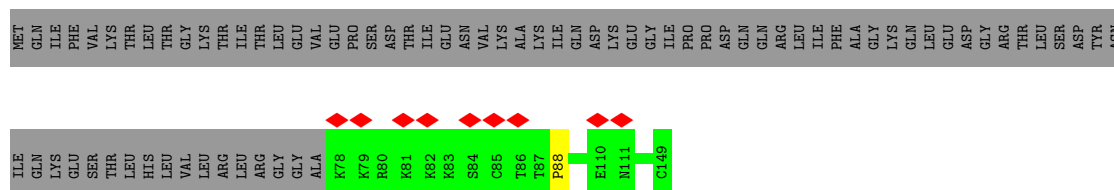
- Molecule 13: 40S ribosomal protein S25



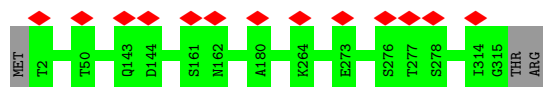
- Molecule 14: 40S ribosomal protein S28



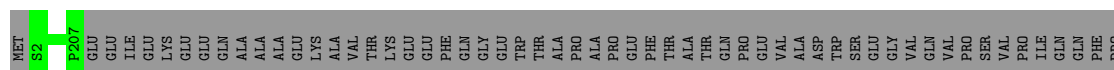
- Molecule 15: 40S ribosomal protein S27a



- Molecule 16: Receptor of activated protein C kinase 1




- Molecule 17: 40S ribosomal protein SA



THR GLU  
GLU ASP  
TRP SER  
ALA ALA  
GLN PRO  
THR GLU  
THR GLU  
ASP TRP  
SER SER  
ALA ALA  
ALA PRO  
THR THR  
GLN GLN  
ALA ALA  
THR THR  
TRP VAL  
GLY GLY  
ALA THR  
THR THR  
ASP THR  
TRP SER

- Molecule 18: 40S ribosomal protein S3a

Chain B:  81% 19%

MET ALA  
GLY VAL  
LYS LYS  
ASN ARG  
LEU THR  
GLY THR  
GLY LYS  
LYS LYS  
GLY GLY  
ALA PRO  
LYS LYS  
LYS LYS  
V21 V22  
T55 D77  
G235  
GLU GLY  
SER SER  
SER SER  
GLY GLY  
LYS LYS  
ALA THR  
THR THR  
ASP GLY  
GLU GLY  
THR THR  
GLY ALA  
LYS LYS  
VAL VAL  
GLU GLU  
ARG ARG  
ALA ALA  
ASP GLY  
TYR TYR  
GLY GLY  
PRO PRO  
PRO VAL  
GLU VAL  
SER SER  
VAL VAL

- Molecule 19: 40S ribosomal protein S2

Chain C:  74% 26%

MET ALA  
ASP ASP  
GLY VAL  
GLY VAL  
ALA ALA  
ALA ALA  
GLY THR  
GLY THR  
PRO GLN  
GLY PRO  
GLY PRO  
GLY GLY  
GLY GLY  
GLY GLY  
MET MET  
GLY MET  
ASN ASN  
ARG ARG  
GLY GLY  
PHE PHE  
ARG ARG  
GLY GLY  
PHE PHE  
GLY GLY  
GLY GLY  
SER SER  
GLY GLY  
ILE ILE  
ARG ARG  
GLY GLY  
ARG ARG  
GLY GLY  
ARG ARG  
GLY GLY  
GLY GLY  
ARG ARG  
ARG ARG  
ALA ALA  
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GLU GLU  
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LYS LYS  
E59

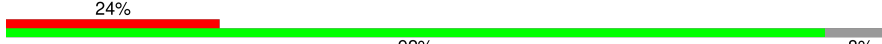
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SER SER  
VAL VAL  
GLN GLN  
ARG THR  
THR THR  
PRO PRO  
ALA ALA  
VAL VAL  
ALA THR  
THR THR

- Molecule 20: 40S ribosomal protein S4, X isoform

Chain E:  100%

MET  
A2  
S261  
S262  
Q263

- Molecule 21: 40S ribosomal protein S6

Chain G:  24% 92% 8%

M1 E17 V18 D19 D20 E21 R22 K23 L24 R25 T26 F27 Y28 E29 K30 V36 A37 A38 D39 A40 L41 G42 E43 E44 W45 K46 G47 Y48 H70 D103 A104 N105 K116 G117 E118 K119 D120 I121 P122 G123 L124 T125 D126 T127 T128 F145 K149 E150 D151 N163 K164 E165

G166 R224 Q225 E226 Q227 T228 A229 K230 ARG ARG ARG LEU LEU SER SER LEU ARG ALA ALA THR THR SER SER LYS LYS SER SER GLU GLU SER SER GLN LYS

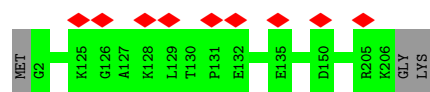
- Molecule 22: 40S ribosomal protein S7

Chain H:  6% 96%

MET PHE  
SER SER  
SER SER  
ALA ALA  
LYS LYS  
T8 N12 G13 E14 K15 P16 D17 D35 G55 R109 T110 K111 N112 F192 Q193 LEU

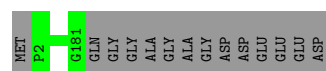
- Molecule 23: 40S ribosomal protein S8

Chain I:  99%



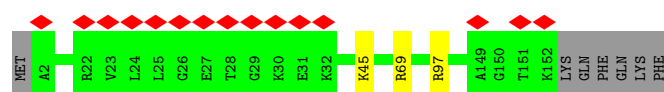
- Molecule 24: 40S ribosomal protein S9

Chain J: 93% 7%



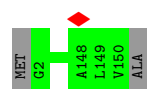
- Molecule 25: 40S ribosomal protein S11

Chain L: 9% 94% . .



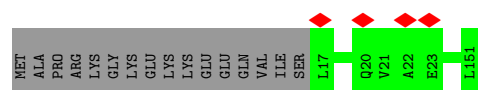
- Molecule 26: 40S ribosomal protein S13

Chain N: 99% .



- Molecule 27: 40S ribosomal protein S14

Chain O: 89% 11% .



- Molecule 28: 40S ribosomal protein S21

Chain V: 99% .



- Molecule 29: 40S ribosomal protein S15a

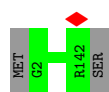
Chain W: 99% .



- Molecule 30: 40S ribosomal protein S23

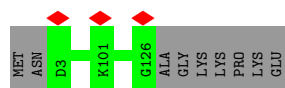


Chain X:  99%



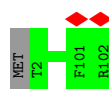
- Molecule 31: 40S ribosomal protein S24

Chain Y:  93%  7%



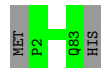
- Molecule 32: 40S ribosomal protein S26

Chain a:  99%





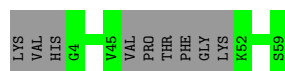
- Molecule 33: 40S ribosomal protein S27

Chain b:  98%



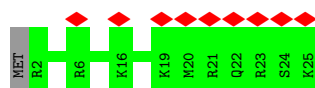
- Molecule 34: 40S ribosomal protein S30

Chain e:  85%  15%



- Molecule 35: 60S ribosomal protein L41

Chain h:  36%  96%



- Molecule 36: Host translation inhibitor nsp1

Chain 1:  17%  83%



LEU PRO GLN LEU LEU GLN GLN GLN PRO TYR VAL VAL ILE ILE LYS ARG SER SER ASP ALA ALA THR THR ALA ASP PRO HIS GLY HIS VAL MET VAL GLU LEU VAL VAL ALA ALA GLU LEU LEU GLY ILE ILE GLN TYR GLY ARG SER GLY THR LEU GLY VAL VAL VAL PRO HIS VAL GLY GLU ILE ILE PRO VAL ALA TYR ARG LYS

VAL LEU LEU ARG LYS ASN GLY ASN LYS GLY ALA GLY GLY HIS SER TYR GLY ALA ASP LEU LYS SER PHE ASP LEU GLY GLU L149 N178 GLY GLY

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	794651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.459	Depositor
Minimum map value	-5.531	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.199	Depositor
Recommended contour level	0.54	Depositor
Map size ( $\text{\AA}$ )	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	R	0.27	0/1080	0.55	0/1449
2	2	0.38	0/39755	0.84	32/61954 (0.1%)
3	d	0.32	0/466	0.63	1/618 (0.2%)
4	D	0.27	0/1776	0.53	0/2392
5	F	0.25	0/1516	0.54	0/2037
6	K	0.27	0/824	0.55	0/1112
7	M	0.25	0/963	0.49	0/1291
8	P	0.27	0/1003	0.54	0/1341
9	Q	0.28	0/1126	0.55	0/1506
10	S	0.26	0/1202	0.59	0/1610
11	T	0.26	0/1142	0.52	0/1530
12	U	0.26	0/805	0.58	0/1081
13	Z	0.26	0/580	0.50	0/780
14	c	0.29	0/481	0.61	0/643
15	f	0.26	0/595	0.55	0/785
16	g	0.26	0/2497	0.54	0/3399
17	A	0.27	0/1661	0.52	0/2259
18	B	0.27	0/1756	0.52	0/2350
19	C	0.28	0/1718	0.52	0/2322
20	E	0.27	0/2118	0.54	0/2849
21	G	0.25	0/1885	0.55	0/2510
22	H	0.26	0/1524	0.52	0/2042
23	I	0.27	0/1711	0.57	0/2282
24	J	0.27	0/1524	0.56	0/2035
25	L	0.29	0/1250	0.56	0/1673
26	N	0.26	0/1226	0.51	0/1649
27	O	0.26	0/1019	0.57	0/1367
28	V	0.27	0/631	0.53	0/844
29	W	0.27	0/1051	0.56	0/1406
30	X	0.28	0/1116	0.55	0/1490
31	Y	0.27	0/1031	0.53	0/1370
32	a	0.30	0/828	0.57	0/1109

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	b	0.26	0/653	0.54	0/876
34	e	0.28	0/399	0.57	0/520
35	h	0.22	0/232	0.71	0/295
36	1	0.29	0/255	0.45	0/344
All	All	0.33	0/79399	0.72	33/115120 (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
1	R	0	1

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	501	C	C2-N1-C1'	9.48	129.23	118.80
2	2	501	C	N1-C2-O2	8.39	123.93	118.90
2	2	356	C	C2-N1-C1'	7.85	127.43	118.80
2	2	293	C	C2-N1-C1'	7.35	126.89	118.80
2	2	293	C	N1-C2-O2	7.19	123.21	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	42	PRO	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	R	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
3	d	52/56 (93%)	49 (94%)	3 (6%)	0	100	100
4	D	223/243 (92%)	216 (97%)	7 (3%)	0	100	100
5	F	187/204 (92%)	176 (94%)	11 (6%)	0	100	100
6	K	93/165 (56%)	92 (99%)	1 (1%)	0	100	100
7	M	121/132 (92%)	113 (93%)	8 (7%)	0	100	100
8	P	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
9	Q	137/146 (94%)	124 (90%)	13 (10%)	0	100	100
10	S	141/152 (93%)	134 (95%)	7 (5%)	0	100	100
11	T	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
12	U	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
13	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
14	c	59/69 (86%)	58 (98%)	1 (2%)	0	100	100
15	f	70/149 (47%)	64 (91%)	5 (7%)	1 (1%)	9	31
16	g	312/317 (98%)	294 (94%)	18 (6%)	0	100	100
17	A	204/295 (69%)	198 (97%)	6 (3%)	0	100	100
18	B	211/264 (80%)	204 (97%)	7 (3%)	0	100	100
19	C	216/293 (74%)	209 (97%)	7 (3%)	0	100	100
20	E	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
21	G	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
22	H	184/194 (95%)	181 (98%)	3 (2%)	0	100	100
23	I	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
24	J	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
25	L	149/158 (94%)	136 (91%)	13 (9%)	0	100	100
26	N	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
27	O	133/151 (88%)	126 (95%)	7 (5%)	0	100	100
28	V	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
29	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
30	X	139/143 (97%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
32	a	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
33	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
34	e	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
35	h	22/25 (88%)	22 (100%)	0	0	100	100
36	1	28/180 (16%)	27 (96%)	1 (4%)	0	100	100
All	All	4809/5661 (85%)	4631 (96%)	177 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	f	88	PRO

### 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	R	118/122 (97%)	118 (100%)	0	100	100
3	d	48/49 (98%)	48 (100%)	0	100	100
4	D	188/202 (93%)	187 (100%)	1 (0%)	86	96
5	F	159/170 (94%)	159 (100%)	0	100	100
6	K	86/136 (63%)	86 (100%)	0	100	100
7	M	104/108 (96%)	104 (100%)	0	100	100
8	P	107/130 (82%)	107 (100%)	0	100	100
9	Q	115/121 (95%)	115 (100%)	0	100	100
10	S	124/132 (94%)	124 (100%)	0	100	100
11	T	114/115 (99%)	113 (99%)	1 (1%)	75	92
12	U	92/107 (86%)	92 (100%)	0	100	100
13	Z	64/103 (62%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	c	54/62 (87%)	54 (100%)	0	100	100
15	f	65/133 (49%)	65 (100%)	0	100	100
16	g	272/275 (99%)	272 (100%)	0	100	100
17	A	172/243 (71%)	172 (100%)	0	100	100
18	B	194/231 (84%)	194 (100%)	0	100	100
19	C	182/225 (81%)	182 (100%)	0	100	100
20	E	224/225 (100%)	224 (100%)	0	100	100
21	G	200/218 (92%)	200 (100%)	0	100	100
22	H	167/174 (96%)	167 (100%)	0	100	100
23	I	178/180 (99%)	178 (100%)	0	100	100
24	J	160/168 (95%)	160 (100%)	0	100	100
25	L	135/142 (95%)	132 (98%)	3 (2%)	47	78
26	N	130/131 (99%)	130 (100%)	0	100	100
27	O	104/119 (87%)	104 (100%)	0	100	100
28	V	66/67 (98%)	66 (100%)	0	100	100
29	W	112/113 (99%)	112 (100%)	0	100	100
30	X	113/115 (98%)	113 (100%)	0	100	100
31	Y	108/115 (94%)	108 (100%)	0	100	100
32	a	88/89 (99%)	88 (100%)	0	100	100
33	b	74/76 (97%)	74 (100%)	0	100	100
34	e	40/48 (83%)	40 (100%)	0	100	100
35	h	23/24 (96%)	23 (100%)	0	100	100
36	l	28/151 (18%)	28 (100%)	0	100	100
All	All	4208/4819 (87%)	4203 (100%)	5 (0%)	92	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	54	ARG
11	T	24	LYS
25	L	45	LYS
25	L	69	ARG
25	L	97	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
16	g	191	HIS
34	e	44	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1655/1868 (88%)	365 (22%)	35 (2%)

5 of 365 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	A
2	2	3	C
2	2	17	C
2	2	23	G
2	2	33	G

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1431	G
2	2	1438	A
2	2	1494	U
2	2	590	A
2	2	554	A

## 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](#)

Of 4 ligands modelled in this entry, 4 are 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.

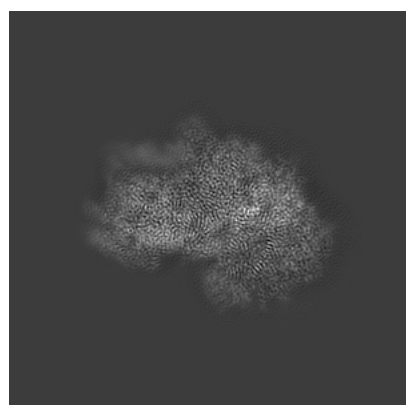
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22681. These allow visual inspection of the internal detail of the map and identification of artifacts.

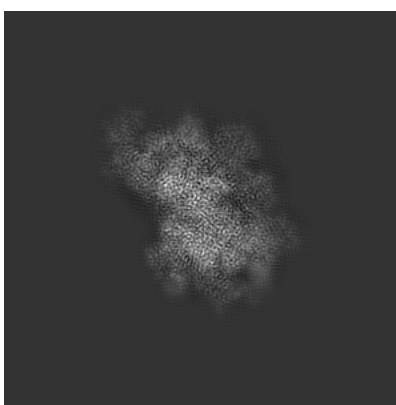
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

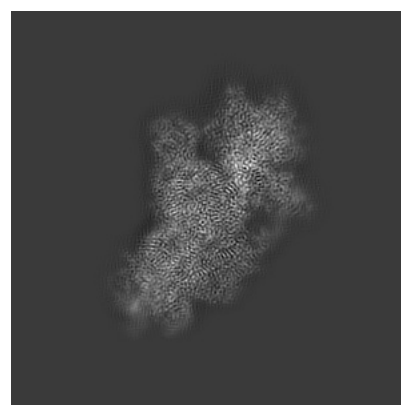
#### 6.1.1 Primary map



X



Y

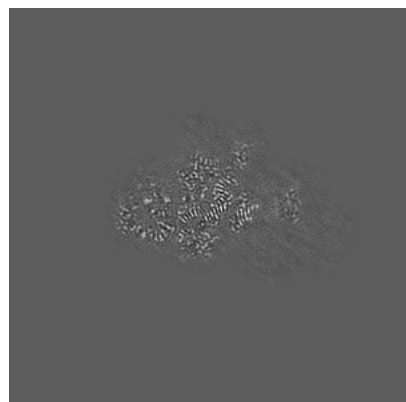


Z

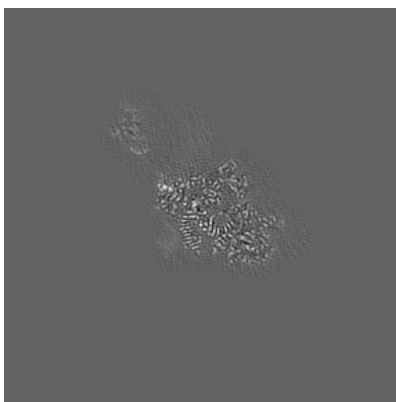
The images above show the map projected in three orthogonal directions.

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

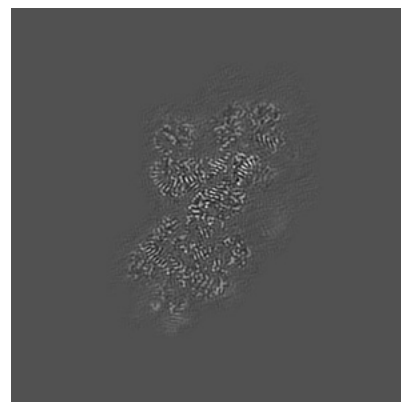
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

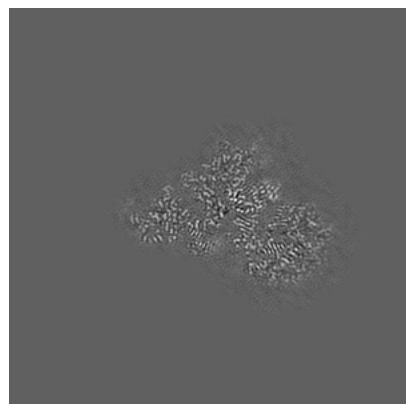


Z Index: 180

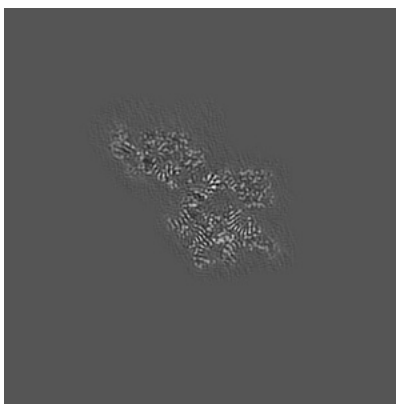
The images above show central slices of the map in three orthogonal directions.

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

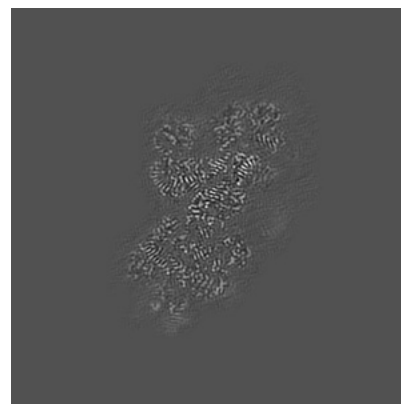
### 6.3.1 Primary map



X Index: 203



Y Index: 203

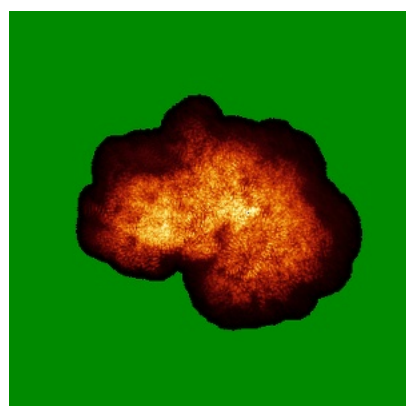


Z Index: 180

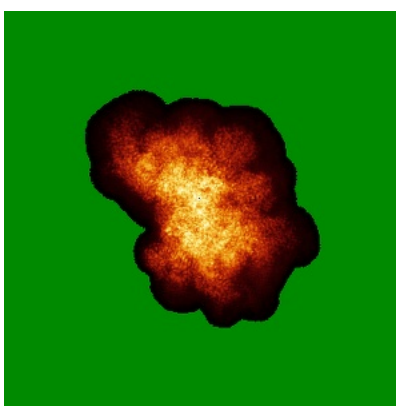
The images above show the largest variance slices of the map in three orthogonal directions.

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

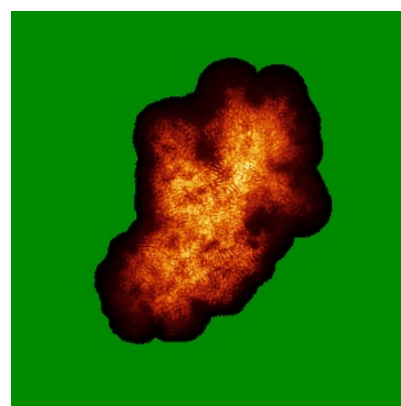
### 6.4.1 Primary map



X



Y

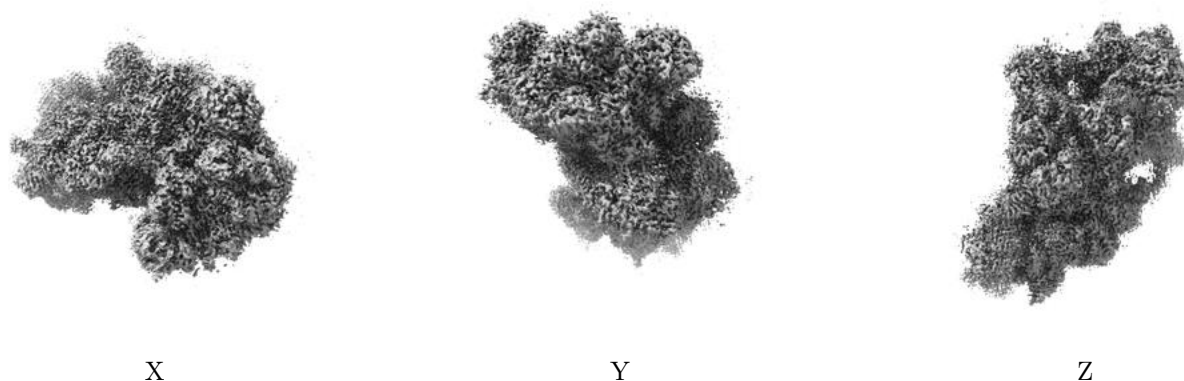


Z

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

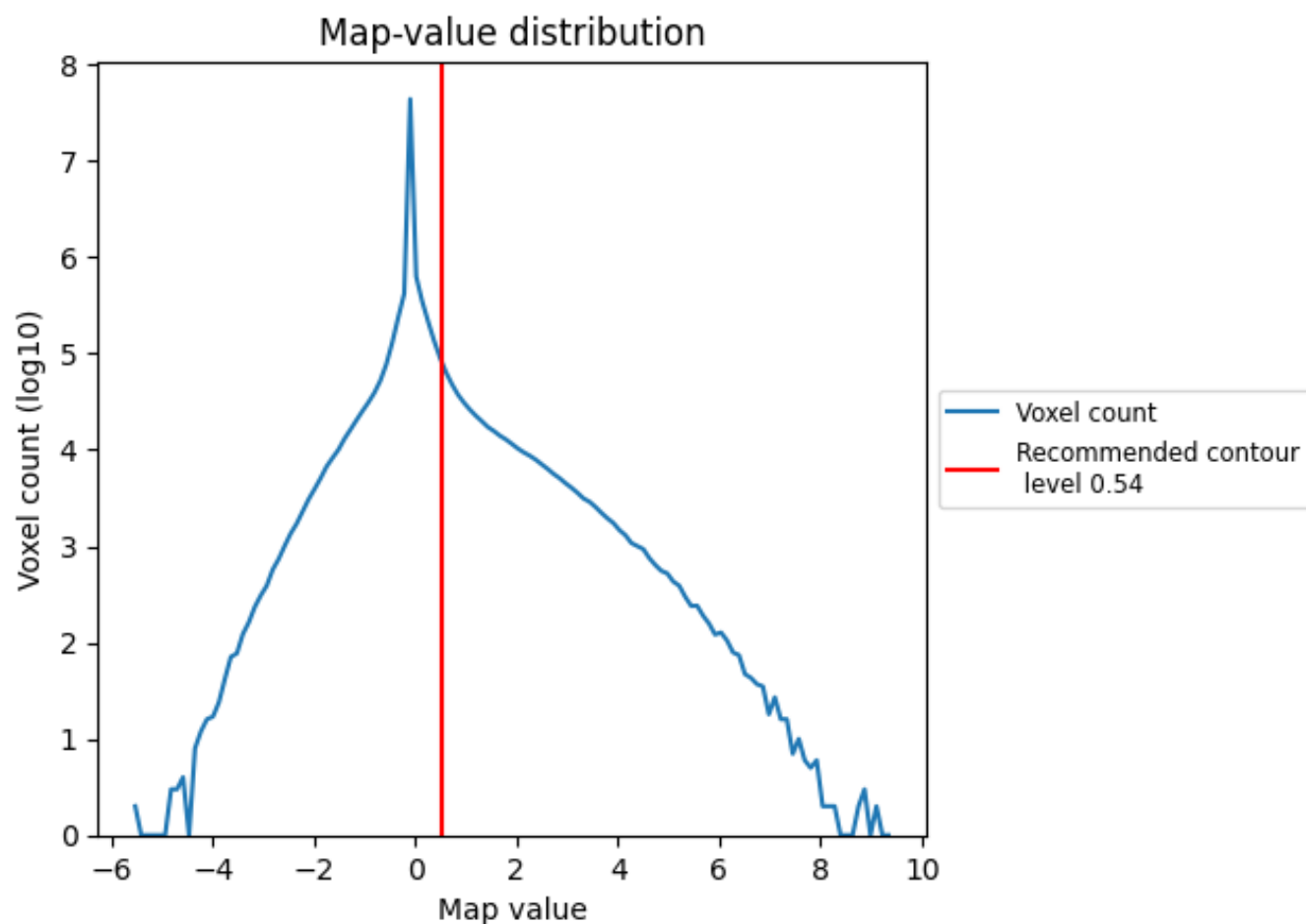
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

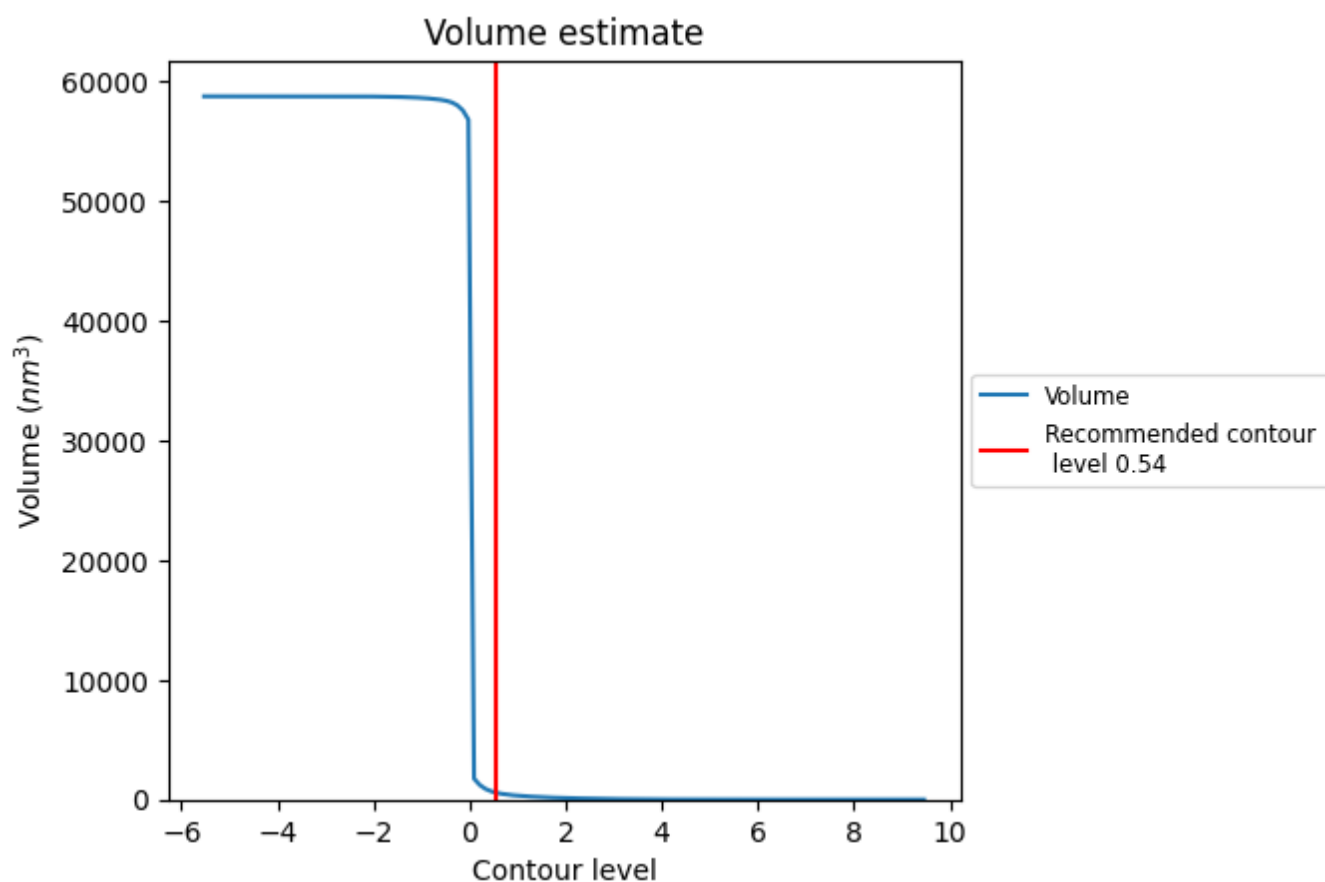
This section contains the results of statistical analysis of the map.

### 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.

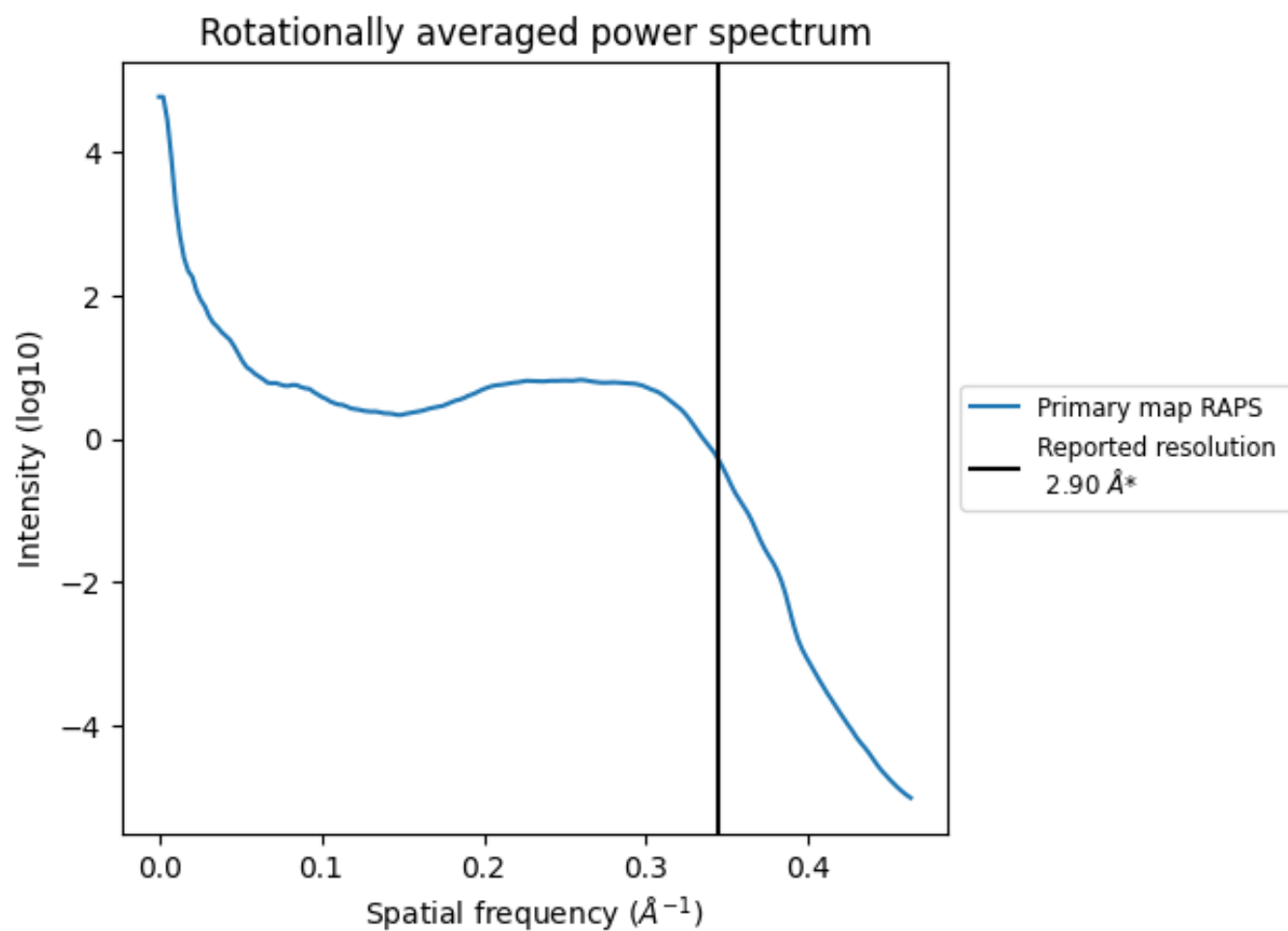
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 587 nm<sup>3</sup>; this corresponds to an approximate mass of 530 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 0.345 Å⁻¹



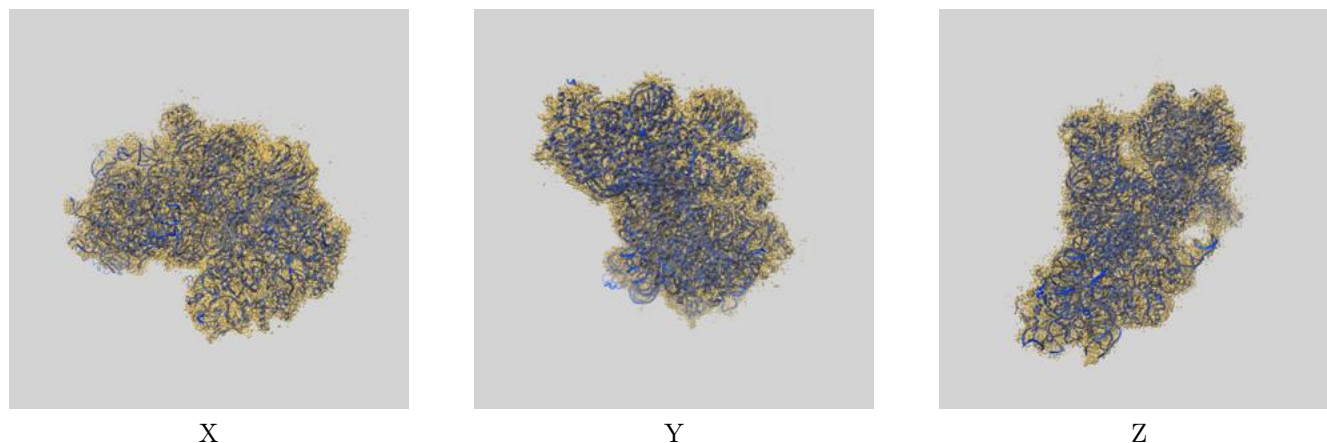
## 8 Fourier-Shell correlation

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

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

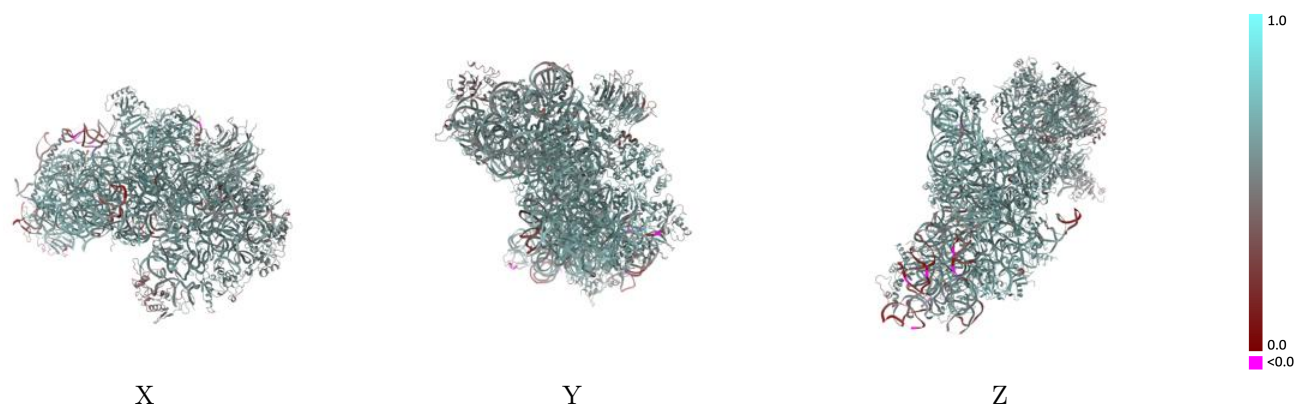
This section contains information regarding the fit between EMDB map EMD-22681 and PDB model 7K5I. Per-residue inclusion information can be found in section 3 on page 11.

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



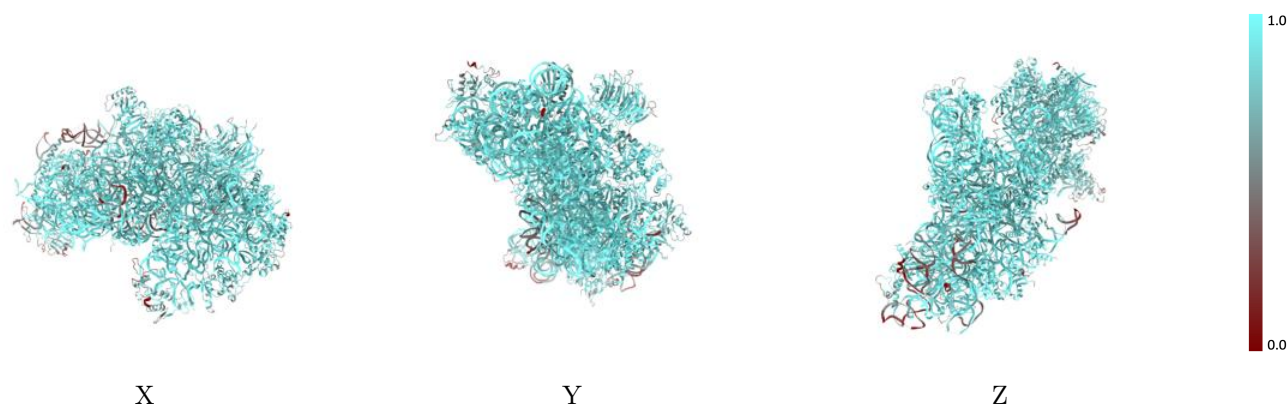
The images above show the 3D surface view of the map at the recommended contour level 0.54 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



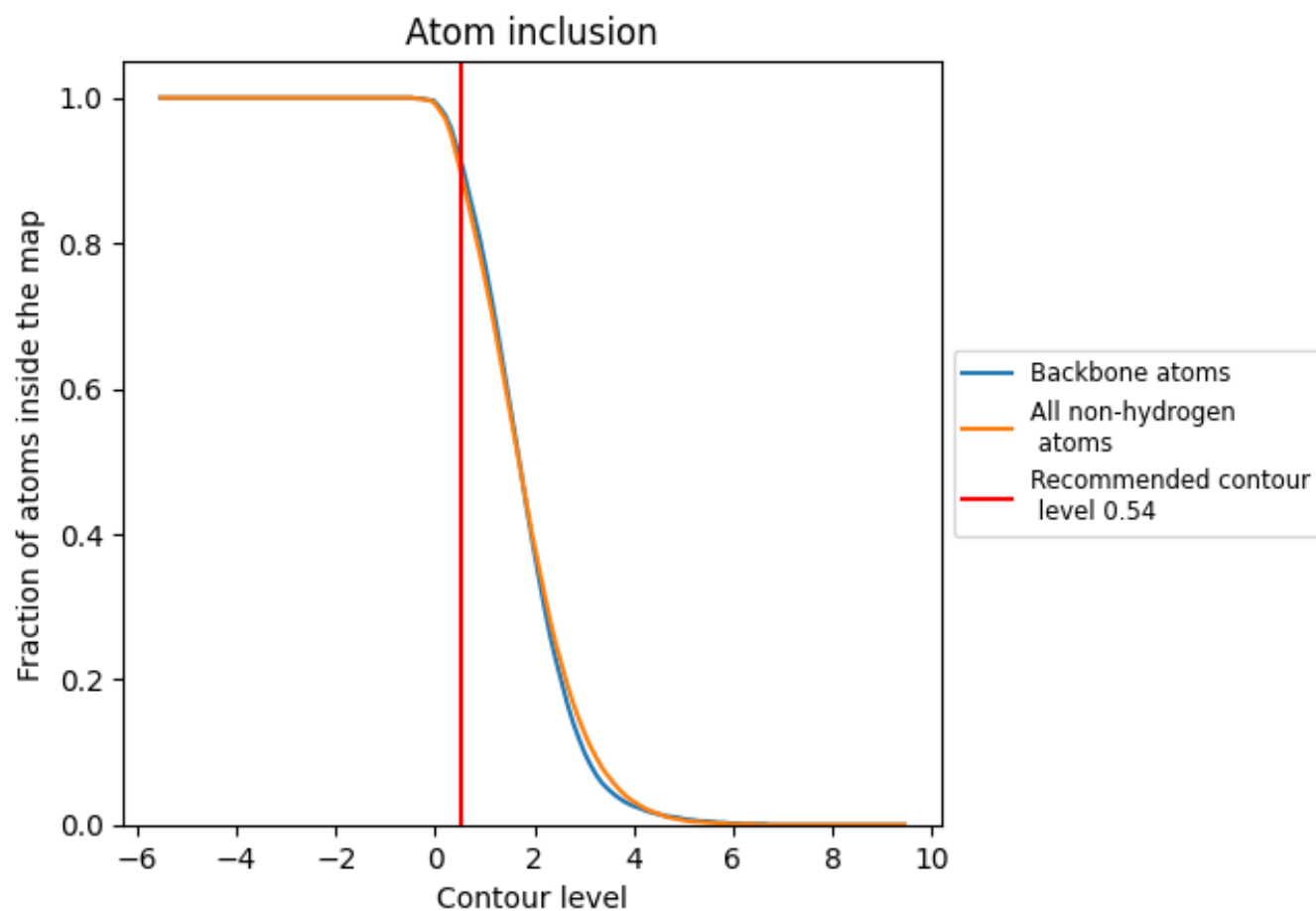
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.54).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.5700
1	 0.9340	 0.5990
2	 0.9140	 0.5710
A	 0.9600	 0.6220
B	 0.8880	 0.5970
C	 0.9610	 0.6260
D	 0.8720	 0.5590
E	 0.9530	 0.6260
F	 0.8820	 0.5610
G	 0.6590	 0.4830
H	 0.8020	 0.5400
I	 0.8660	 0.5600
J	 0.9530	 0.6290
K	 0.8950	 0.5590
L	 0.8660	 0.5820
M	 0.5900	 0.4100
N	 0.9290	 0.5990
O	 0.9240	 0.5950
P	 0.8510	 0.5380
Q	 0.9250	 0.5750
R	 0.8550	 0.5300
S	 0.8240	 0.5150
T	 0.8600	 0.5440
U	 0.7980	 0.5160
V	 0.9200	 0.6170
W	 0.9760	 0.6410
X	 0.9570	 0.6320
Y	 0.9490	 0.6240
Z	 0.8070	 0.4980
a	 0.9410	 0.6090
b	 0.9040	 0.5960
c	 0.8610	 0.5590
d	 0.9340	 0.6100
e	 0.9320	 0.6050
f	 0.7050	 0.4690



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Chain	Atom inclusion	Q-score
g	 0.8360	 0.5260
h	 0.4710	 0.5010