



Full wwPDB EM Validation Report ⓘ

Oct 16, 2024 – 10:47 AM EDT

PDB ID : 8TM6
EMDB ID : EMD-41380
Title : Human premature 20S proteasome assembly intermediate
Authors : Zhang, H.; Zhao, J.
Deposited on : 2023-07-28
Resolution : 2.80 Å (reported)

This is a Full wwPDB EM Validation 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:

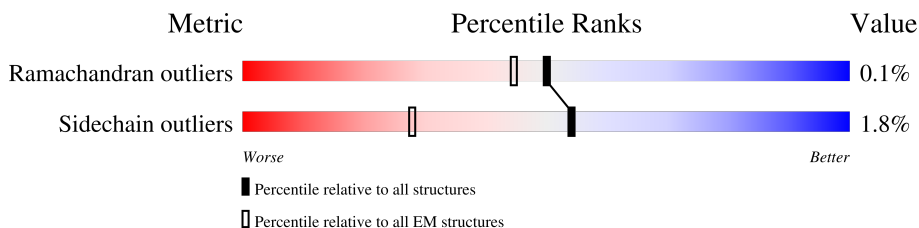
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 2.80 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

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	234	99%
1	O	234	100%
2	B	261	5% 94%
2	P	261	5% 95%
3	C	248	94%
3	Q	248	94%
4	D	241	5% 99%
4	R	241	99%
5	E	263	90% 9%

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Mol	Chain	Length	Quality of chain
5	S	263	90% 9%
6	F	255	94% 5%
6	T	255	94% 5%
7	G	246	98%
7	U	246	98%
8	H	277	12% 91% 6%
8	V	277	11% 92% 6%
9	I	205	99%
9	W	205	100%
10	J	201	97%
10	X	201	97%
11	K	263	75% 24%
11	Y	263	75% 24%
12	L	241	86% 12%
12	Z	241	88% 12%
13	M	264	81% 19%
13	a	264	81% 19%
14	N	239	7% 88% 10%
14	b	239	7% 89% 10%
15	c	288	49% 93% 5%
15	f	288	49% 92% 5%
16	d	264	16% 92% 6%
16	g	264	18% 93% 6%
17	e	141	27% 73% 27%
17	h	141	28% 72% 27%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 58074 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	234	Total	C	N	O	S	0	0
			1780	1143	305	326	6		
1	O	234	Total	C	N	O	S	0	0
			1780	1143	305	326	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	251	Total	C	N	O	S	0	0
			1929	1223	337	359	10		
2	P	251	Total	C	N	O	S	0	0
			1929	1223	337	359	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	238	Total	C	N	O	S	0	0
			1745	1101	319	320	5		
3	Q	238	Total	C	N	O	S	0	0
			1745	1101	319	320	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	241	Total	C	N	O	S	0	0
			1800	1140	303	345	12		
4	R	241	Total	C	N	O	S	0	0
			1800	1140	303	345	12		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	239	1830	1155	336	328	11	0	0
5	S	239	1830	1155	336	328	11	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	243	1847	1178	318	340	11	0	0
6	T	243	1847	1178	318	340	11	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	245	1839	1172	315	340	12	0	0
7	U	245	1839	1172	315	340	12	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	259	1910	1207	329	362	12	0	0
8	V	259	1910	1207	329	362	12	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	205	1575	1005	264	287	19	0	0
9	W	205	1575	1005	264	287	19	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	197	1564	1006	265	284	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	197	Total	C	N	O	S	0	0
			1564	1006	265	284	9		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1539	972	271	287	9		
11	Y	200	Total	C	N	O	S	0	0
			1539	972	271	287	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	0	0
			1630	1037	281	302	10		
12	Z	213	Total	C	N	O	S	0	0
			1630	1037	281	302	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	215	Total	C	N	O	S	0	0
			1642	1045	288	297	12		
13	a	215	Total	C	N	O	S	0	0
			1642	1045	288	297	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	215	Total	C	N	O	S	0	0
			1606	1006	275	313	12		
14	b	215	Total	C	N	O	S	0	0
			1606	1006	275	313	12		

- Molecule 15 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	273	Total	C	N	O	S	0	0
			2081	1336	347	381	17		
15	f	273	Total	C	N	O	S	0	0
			2081	1336	347	381	17		

- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	d	249	Total 1907	C 1231	N 312	O 352	S 12	0	0
16	g	249	Total 1907	C 1231	N 312	O 352	S 12	0	0

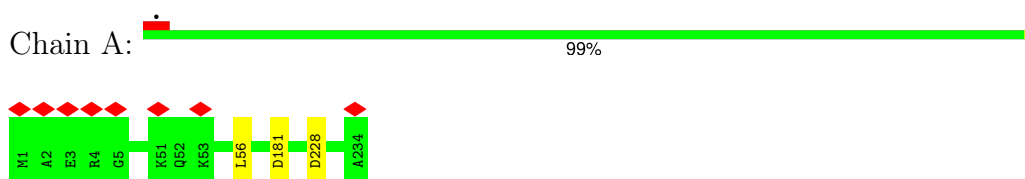
- Molecule 17 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	e	103	Total 813	C 516	N 137	O 156	S 4	0	0
17	h	103	Total 813	C 516	N 137	O 156	S 4	0	0

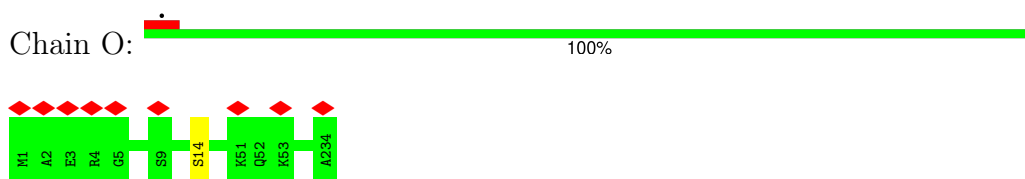
3 Residue-property plots

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.

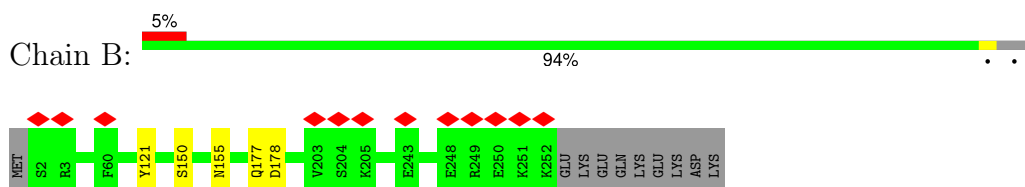
- Molecule 1: Proteasome subunit alpha type-2



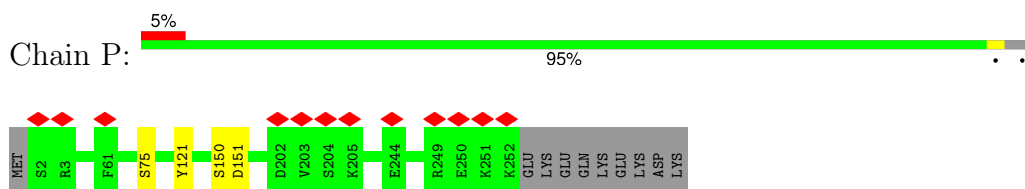
- Molecule 1: Proteasome subunit alpha type-2



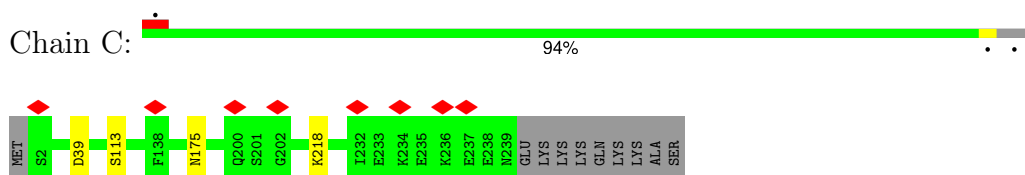
- Molecule 2: Proteasome subunit alpha type-4



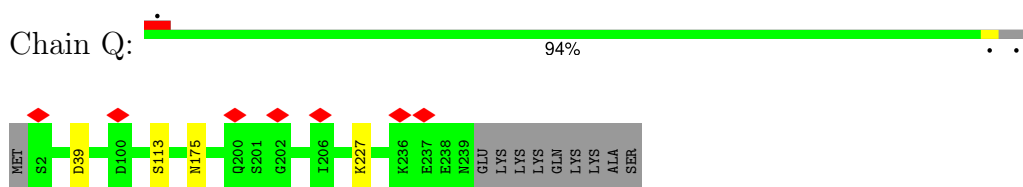
- Molecule 2: Proteasome subunit alpha type-4



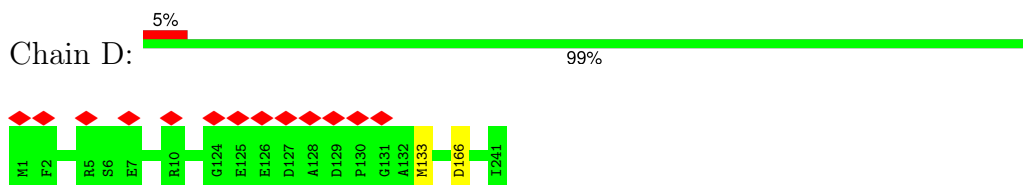
- Molecule 3: Proteasome subunit alpha type-7



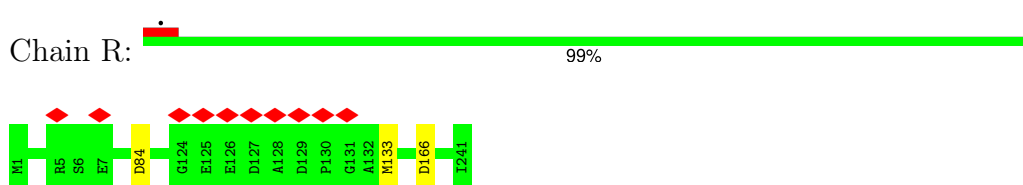
- Molecule 3: Proteasome subunit alpha type-7



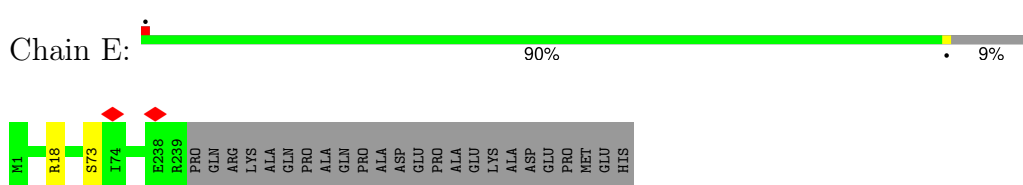
- Molecule 4: Proteasome subunit alpha type-5



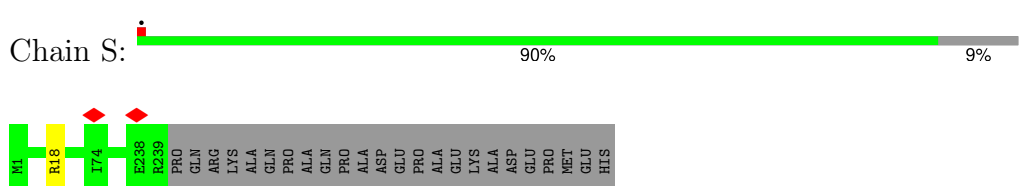
- Molecule 4: Proteasome subunit alpha type-5



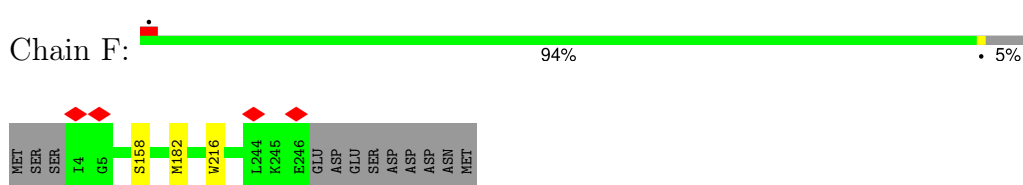
- Molecule 5: Proteasome subunit alpha type-1



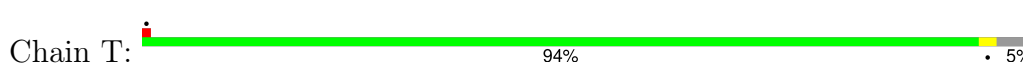
- Molecule 5: Proteasome subunit alpha type-1



- Molecule 6: Proteasome subunit alpha type-3



- Molecule 6: Proteasome subunit alpha type-3





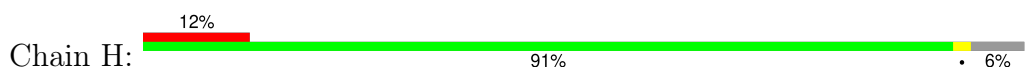
• Molecule 7: Proteasome subunit alpha type-6



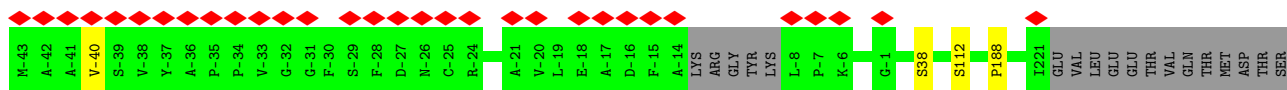
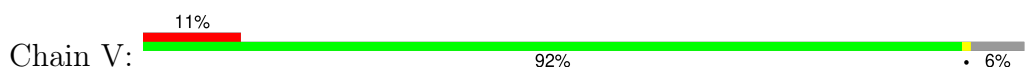
• Molecule 7: Proteasome subunit alpha type-6



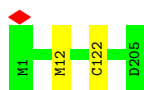
• Molecule 8: Proteasome subunit beta type-7



• Molecule 8: Proteasome subunit beta type-7

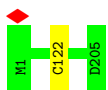


• Molecule 9: Proteasome subunit beta type-3



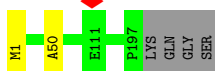
• Molecule 9: Proteasome subunit beta type-3





- Molecule 10: Proteasome subunit beta type-2

Chain J: 97%



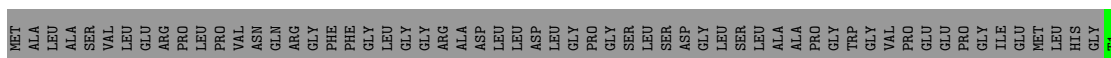
- Molecule 10: Proteasome subunit beta type-2

Chain X: 97%



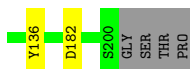
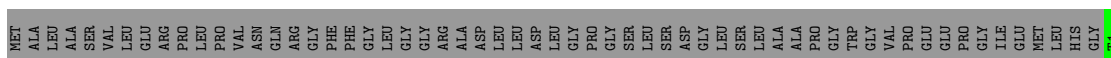
- Molecule 11: Proteasome subunit beta type-5

Chain K: 75% 24%



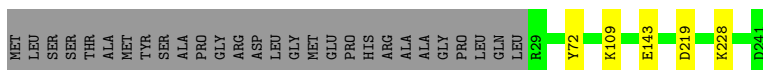
- Molecule 11: Proteasome subunit beta type-5

Chain Y: 75% 24%



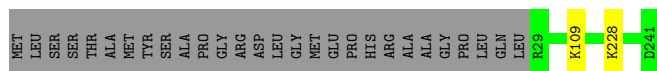
- Molecule 12: Proteasome subunit beta type-1

Chain L: 86% 12%

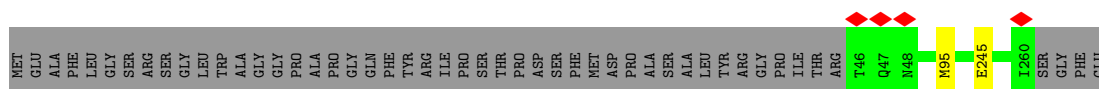
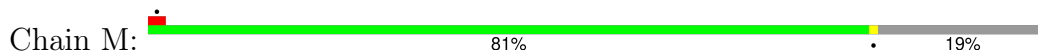


- Molecule 12: Proteasome subunit beta type-1

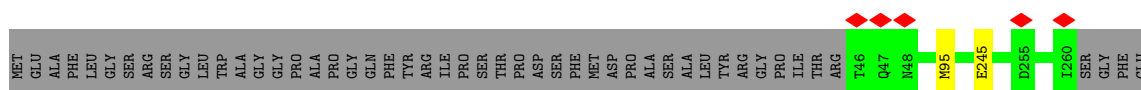
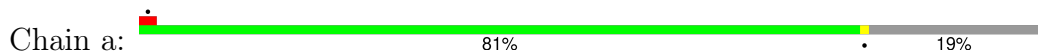
Chain Z: 88% 12%



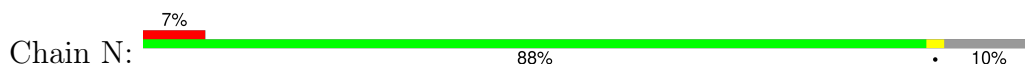
● Molecule 13: Proteasome subunit beta type-4



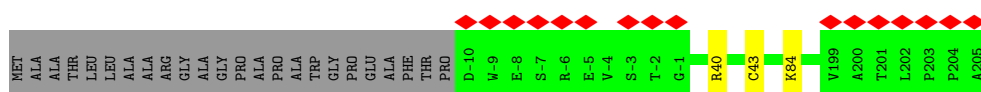
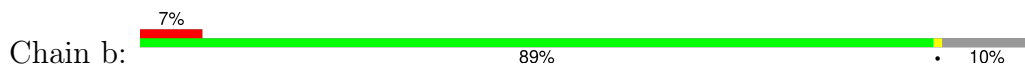
● Molecule 13: Proteasome subunit beta type-4



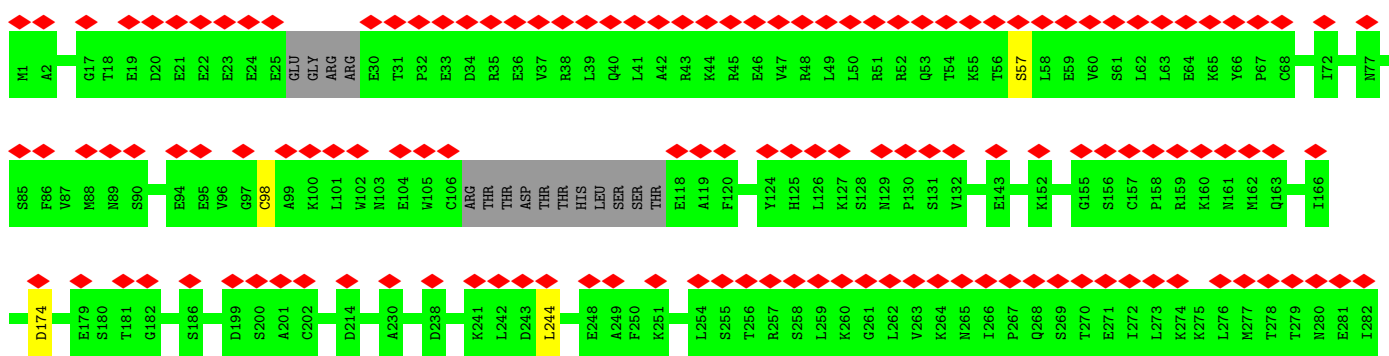
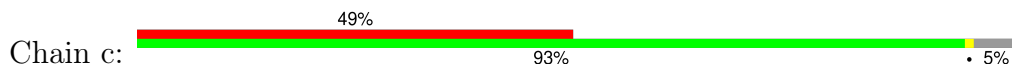
● Molecule 14: Proteasome subunit beta type-6

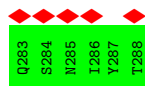


● Molecule 14: Proteasome subunit beta type-6

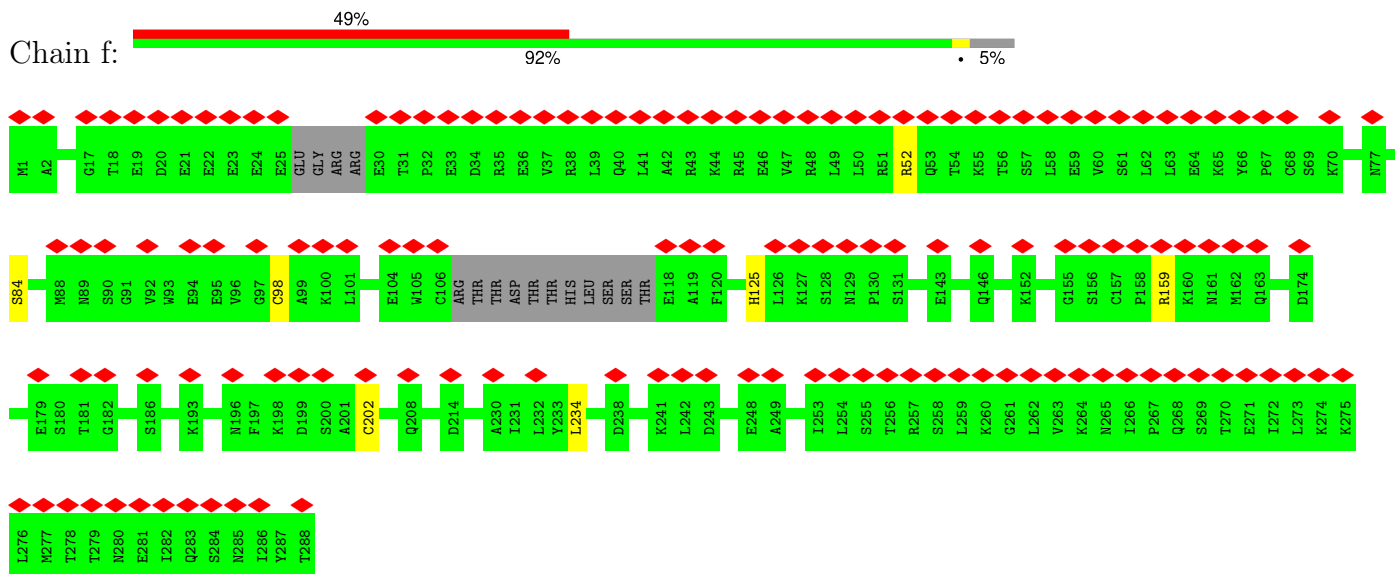


● Molecule 15: Proteasome assembly chaperone 1

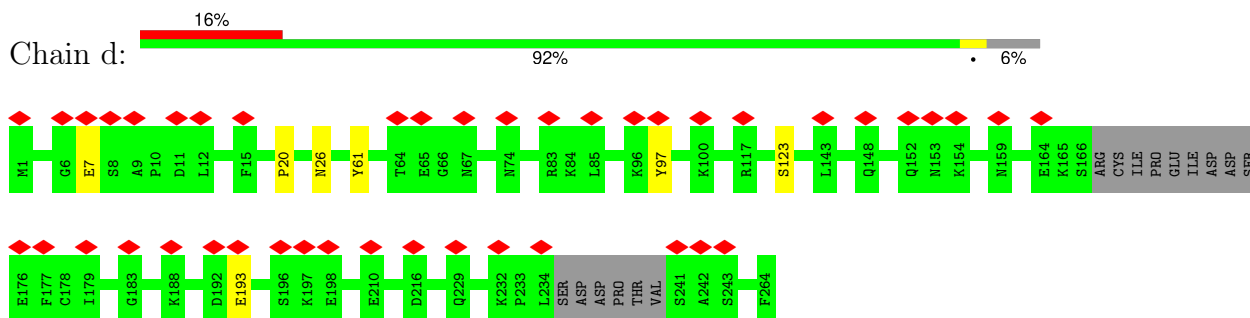




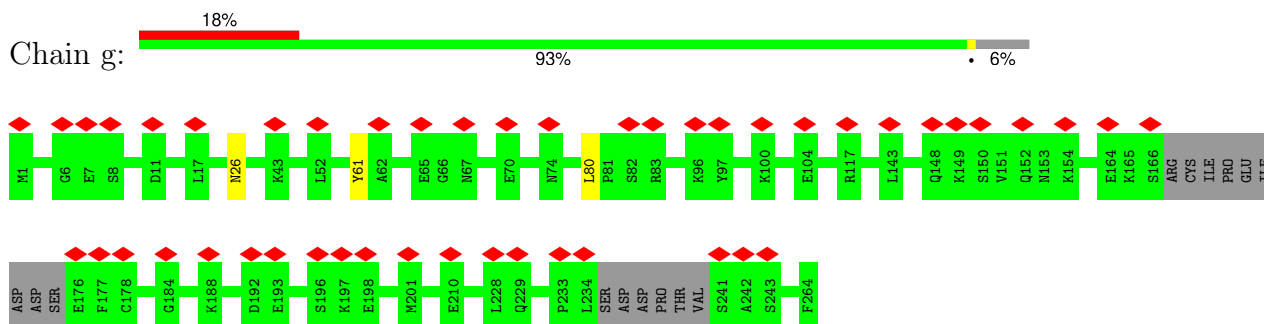
- Molecule 15: Proteasome assembly chaperone 1



- Molecule 16: Proteasome assembly chaperone 2

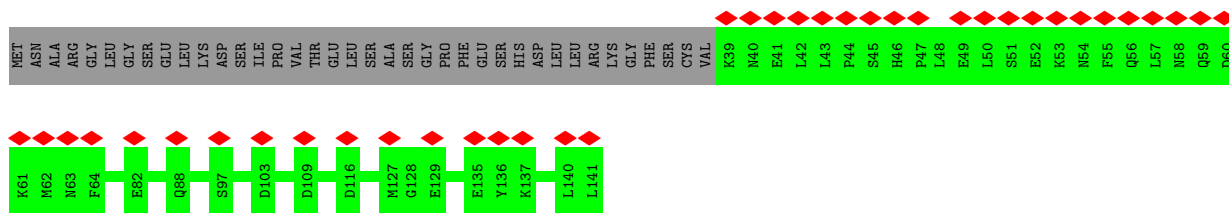


- Molecule 16: Proteasome assembly chaperone 2

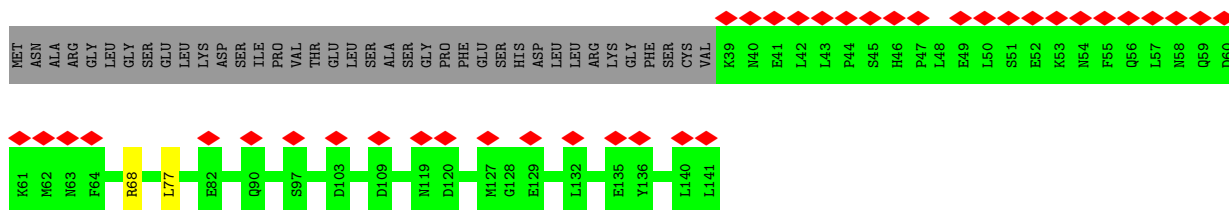


- Molecule 17: Proteasome maturation protein





● Molecule 17: Proteasome maturation protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115008	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.717	Depositor
Minimum map value	-14.922	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	Depositor
Map size (\AA)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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	0.26	0/1819	0.47	0/2470
1	O	0.26	0/1819	0.47	0/2470
2	B	0.25	0/1959	0.47	0/2646
2	P	0.25	0/1959	0.47	0/2646
3	C	0.25	0/1770	0.49	0/2407
3	Q	0.25	0/1770	0.50	0/2407
4	D	0.25	0/1828	0.46	0/2472
4	R	0.25	0/1828	0.46	0/2472
5	E	0.25	0/1865	0.50	0/2525
5	S	0.25	0/1865	0.50	0/2525
6	F	0.26	0/1882	0.47	0/2543
6	T	0.25	0/1882	0.48	0/2543
7	G	0.27	0/1871	0.48	0/2535
7	U	0.27	0/1871	0.49	0/2535
8	H	0.25	0/1942	0.50	0/2635
8	V	0.25	0/1942	0.51	0/2635
9	I	0.25	0/1604	0.48	0/2166
9	W	0.26	0/1604	0.49	0/2166
10	J	0.26	0/1597	0.49	0/2163
10	X	0.26	0/1597	0.50	0/2163
11	K	0.25	0/1570	0.52	0/2125
11	Y	0.25	0/1570	0.51	0/2125
12	L	0.26	0/1660	0.49	0/2240
12	Z	0.25	0/1660	0.49	0/2240
13	M	0.25	0/1675	0.51	0/2270
13	a	0.25	0/1675	0.52	0/2270
14	N	0.25	0/1636	0.49	0/2218
14	b	0.25	0/1636	0.49	0/2218
15	c	0.25	0/2125	0.48	0/2893
15	f	0.25	0/2125	0.47	0/2893
16	d	0.27	0/1948	0.52	2/2645 (0.1%)
16	g	0.25	0/1948	0.47	0/2645
17	e	0.26	0/827	0.46	0/1117
17	h	0.25	0/827	0.42	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.25	0/59156	0.49	2/80140 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	U	0	1
17	h	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	d	20	PRO	CA-N-CD	-9.54	98.14	111.50
16	d	20	PRO	N-CD-CG	-5.33	95.21	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	U	153	LYS	Peptide
17	h	68	ARG	Sidechain

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	A	232/234 (99%)	229 (99%)	3 (1%)	0	100	100
1	O	232/234 (99%)	225 (97%)	7 (3%)	0	100	100
2	B	249/261 (95%)	243 (98%)	6 (2%)	0	100	100
2	P	249/261 (95%)	244 (98%)	5 (2%)	0	100	100
3	C	236/248 (95%)	233 (99%)	3 (1%)	0	100	100
3	Q	236/248 (95%)	233 (99%)	3 (1%)	0	100	100
4	D	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
4	R	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	237/263 (90%)	233 (98%)	4 (2%)	0	100	100
5	S	237/263 (90%)	232 (98%)	5 (2%)	0	100	100
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100	100
6	T	241/255 (94%)	238 (99%)	3 (1%)	0	100	100
7	G	243/246 (99%)	241 (99%)	2 (1%)	0	100	100
7	U	243/246 (99%)	241 (99%)	2 (1%)	0	100	100
8	H	255/277 (92%)	244 (96%)	10 (4%)	1 (0%)	30	61
8	V	255/277 (92%)	243 (95%)	11 (4%)	1 (0%)	30	61
9	I	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
9	W	203/205 (99%)	194 (96%)	9 (4%)	0	100	100
10	J	195/201 (97%)	190 (97%)	4 (2%)	1 (0%)	25	56
10	X	195/201 (97%)	190 (97%)	4 (2%)	1 (0%)	25	56
11	K	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
11	Y	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
12	L	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
12	Z	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
13	M	213/264 (81%)	207 (97%)	6 (3%)	0	100	100
13	a	213/264 (81%)	207 (97%)	6 (3%)	0	100	100
14	N	213/239 (89%)	210 (99%)	3 (1%)	0	100	100
14	b	213/239 (89%)	210 (99%)	3 (1%)	0	100	100
15	c	267/288 (93%)	256 (96%)	11 (4%)	0	100	100
15	f	267/288 (93%)	256 (96%)	11 (4%)	0	100	100
16	d	243/264 (92%)	233 (96%)	10 (4%)	0	100	100
16	g	243/264 (92%)	235 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	e	101/141 (72%)	99 (98%)	2 (2%)	0	100	100
17	h	101/141 (72%)	98 (97%)	3 (3%)	0	100	100
All	All	7552/8262 (91%)	7377 (98%)	171 (2%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	-40	VAL
8	V	-40	VAL
10	X	50	ALA
10	J	50	ALA

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	176/191 (92%)	173 (98%)	3 (2%)	56	84
1	O	176/191 (92%)	175 (99%)	1 (1%)	84	95
2	B	192/221 (87%)	187 (97%)	5 (3%)	41	75
2	P	192/221 (87%)	188 (98%)	4 (2%)	48	80
3	C	161/211 (76%)	157 (98%)	4 (2%)	42	75
3	Q	161/211 (76%)	157 (98%)	4 (2%)	42	75
4	D	184/203 (91%)	182 (99%)	2 (1%)	70	90
4	R	184/203 (91%)	181 (98%)	3 (2%)	58	85
5	E	186/224 (83%)	184 (99%)	2 (1%)	70	90
5	S	186/224 (83%)	185 (100%)	1 (0%)	86	95
6	F	182/212 (86%)	179 (98%)	3 (2%)	58	85
6	T	182/212 (86%)	178 (98%)	4 (2%)	47	79
7	G	184/210 (88%)	180 (98%)	4 (2%)	47	79
7	U	184/210 (88%)	180 (98%)	4 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	200/228 (88%)	195 (98%)	5 (2%)	42	75
8	V	200/228 (88%)	197 (98%)	3 (2%)	60	86
9	I	167/174 (96%)	165 (99%)	2 (1%)	67	89
9	W	167/174 (96%)	166 (99%)	1 (1%)	84	95
10	J	163/171 (95%)	162 (99%)	1 (1%)	84	95
10	X	163/171 (95%)	161 (99%)	2 (1%)	67	89
11	K	149/202 (74%)	145 (97%)	4 (3%)	40	74
11	Y	149/202 (74%)	147 (99%)	2 (1%)	65	88
12	L	171/199 (86%)	166 (97%)	5 (3%)	37	71
12	Z	171/199 (86%)	169 (99%)	2 (1%)	67	89
13	M	165/215 (77%)	163 (99%)	2 (1%)	67	89
13	a	165/215 (77%)	163 (99%)	2 (1%)	67	89
14	N	164/181 (91%)	159 (97%)	5 (3%)	36	70
14	b	164/181 (91%)	161 (98%)	3 (2%)	54	83
15	c	220/262 (84%)	216 (98%)	4 (2%)	54	83
15	f	220/262 (84%)	213 (97%)	7 (3%)	34	68
16	d	209/237 (88%)	203 (97%)	6 (3%)	37	71
16	g	209/237 (88%)	206 (99%)	3 (1%)	62	87
17	e	92/128 (72%)	92 (100%)	0	100	100
17	h	92/128 (72%)	91 (99%)	1 (1%)	70	90
All	All	5930/6938 (86%)	5826 (98%)	104 (2%)	54	83

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	181	ASP
1	A	228	ASP
2	B	121	TYR
2	B	150	SER
2	B	155	ASN
2	B	177	GLN
2	B	178	ASP
3	C	39	ASP
3	C	113	SER

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Mol	Chain	Res	Type
3	C	175	ASN
3	C	218	LYS
4	D	133	MET
4	D	166	ASP
5	E	18	ARG
5	E	73	SER
6	F	158	SER
6	F	182	MET
6	F	216	TRP
7	G	75	ASN
7	G	89	SER
7	G	112	ASP
7	G	155	ASP
8	H	-23	ARG
8	H	38	SER
8	H	112	SER
8	H	127	MET
8	H	188	PRO
9	I	12	MET
9	I	122	CYS
10	J	1	MET
11	K	136	TYR
11	K	154	ASP
11	K	182	ASP
11	K	197	GLU
12	L	72	TYR
12	L	109	LYS
12	L	143	GLU
12	L	219	ASP
12	L	228	LYS
13	M	95	MET
13	M	245	GLU
14	N	-10	ASP
14	N	43	CYS
14	N	67	SER
14	N	84	LYS
14	N	190	LEU
1	O	14	SER
2	P	75	SER
2	P	121	TYR
2	P	150	SER
2	P	151	ASP

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Mol	Chain	Res	Type
3	Q	39	ASP
3	Q	113	SER
3	Q	175	ASN
3	Q	227	LYS
4	R	84	ASP
4	R	133	MET
4	R	166	ASP
5	S	18	ARG
6	T	102	ASN
6	T	164	CYS
6	T	182	MET
6	T	216	TRP
7	U	63	SER
7	U	75	ASN
7	U	112	ASP
7	U	155	ASP
8	V	38	SER
8	V	112	SER
8	V	188	PRO
9	W	122	CYS
10	X	1	MET
10	X	179	SER
11	Y	136	TYR
11	Y	182	ASP
12	Z	109	LYS
12	Z	228	LYS
13	a	95	MET
13	a	245	GLU
14	b	40	ARG
14	b	43	CYS
14	b	84	LYS
15	c	57	SER
15	c	98	CYS
15	c	174	ASP
15	c	244	LEU
16	d	7	GLU
16	d	26	ASN
16	d	61	TYR
16	d	97	TYR
16	d	123	SER
16	d	193	GLU
15	f	52	ARG

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Mol	Chain	Res	Type
15	f	84	SER
15	f	98	CYS
15	f	125	HIS
15	f	159	ARG
15	f	202	CYS
15	f	234	LEU
16	g	26	ASN
16	g	61	TYR
16	g	80	LEU
17	h	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	109	GLN
3	C	116	GLN
7	G	12	HIS
10	J	174	ASN
2	P	51	ASN
2	P	109	GLN
3	Q	116	GLN
7	U	12	HIS
10	X	27	GLN
10	X	174	ASN
15	c	89	ASN
15	f	103	ASN
15	f	145	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

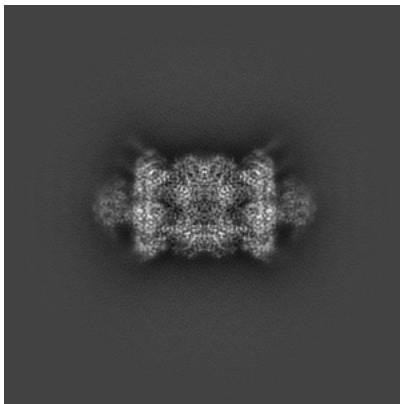
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41380. These allow visual inspection of the internal detail of the map and identification of artifacts.

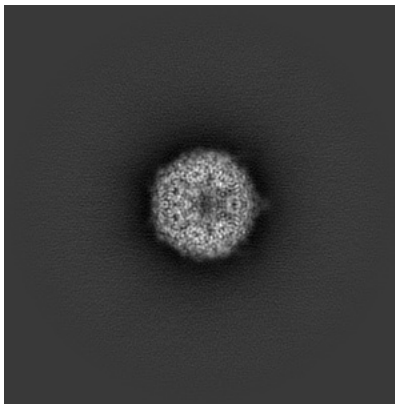
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

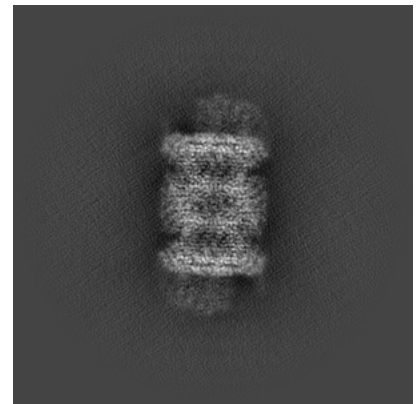
6.1.1 Primary map



X

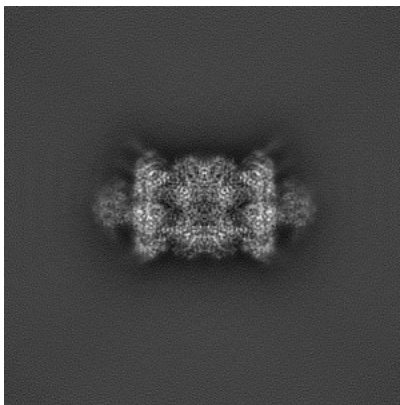


Y

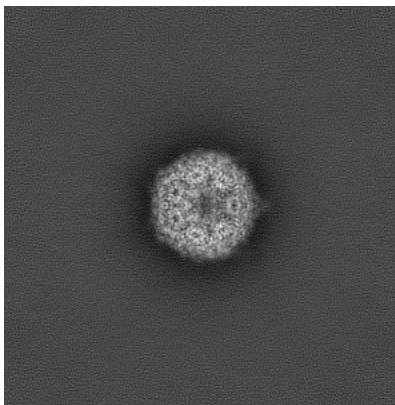


Z

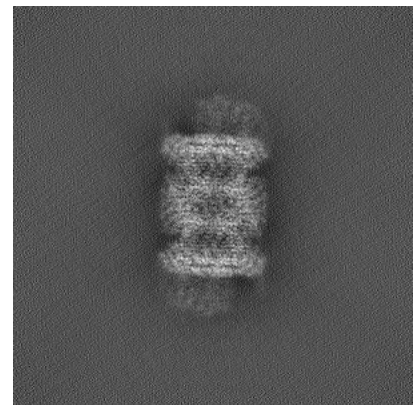
6.1.2 Raw map



X



Y

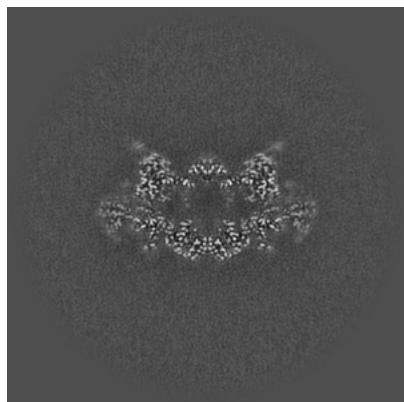


Z

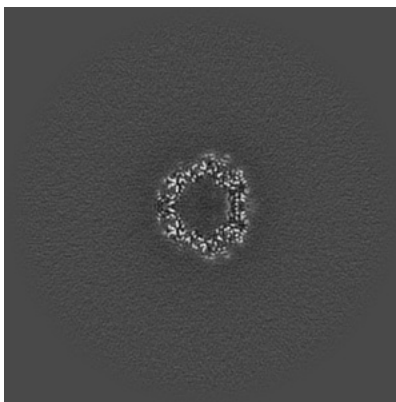
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

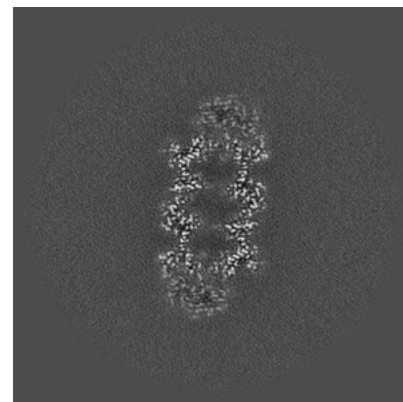
6.2.1 Primary map



X Index: 200

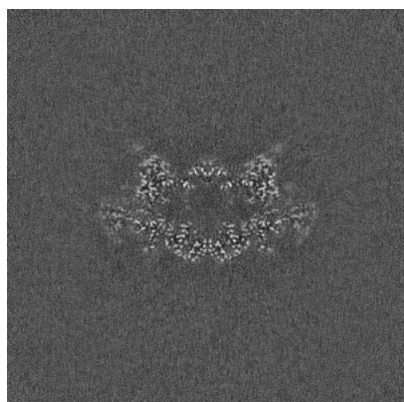


Y Index: 200

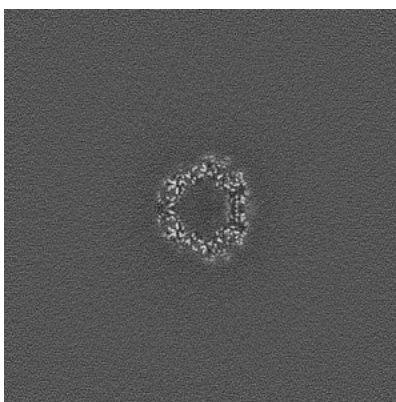


Z Index: 200

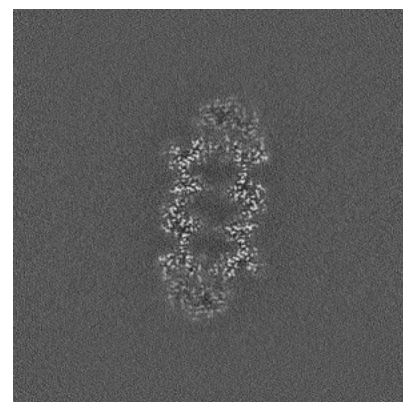
6.2.2 Raw map



X Index: 200



Y Index: 200

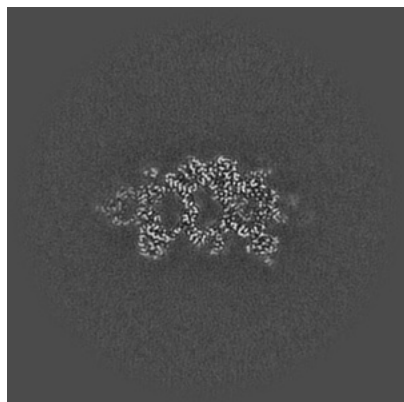


Z Index: 200

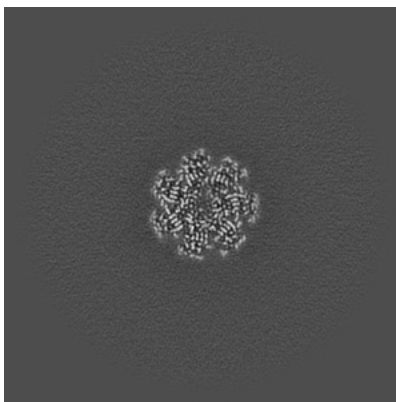
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

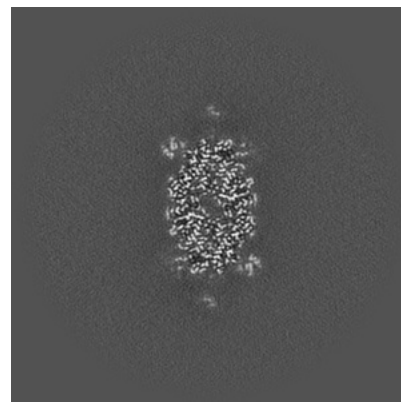
6.3.1 Primary map



X Index: 182

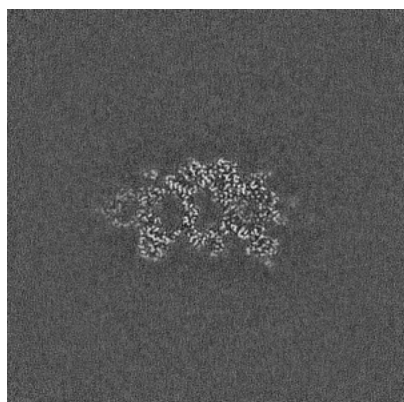


Y Index: 254

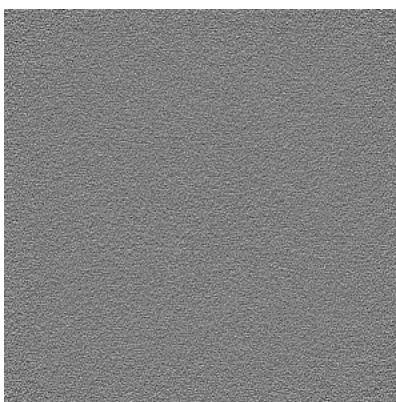


Z Index: 175

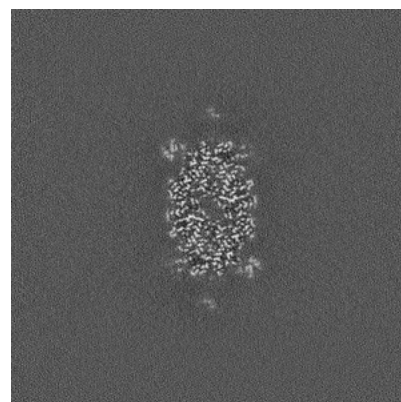
6.3.2 Raw map



X Index: 182



Y Index: 0

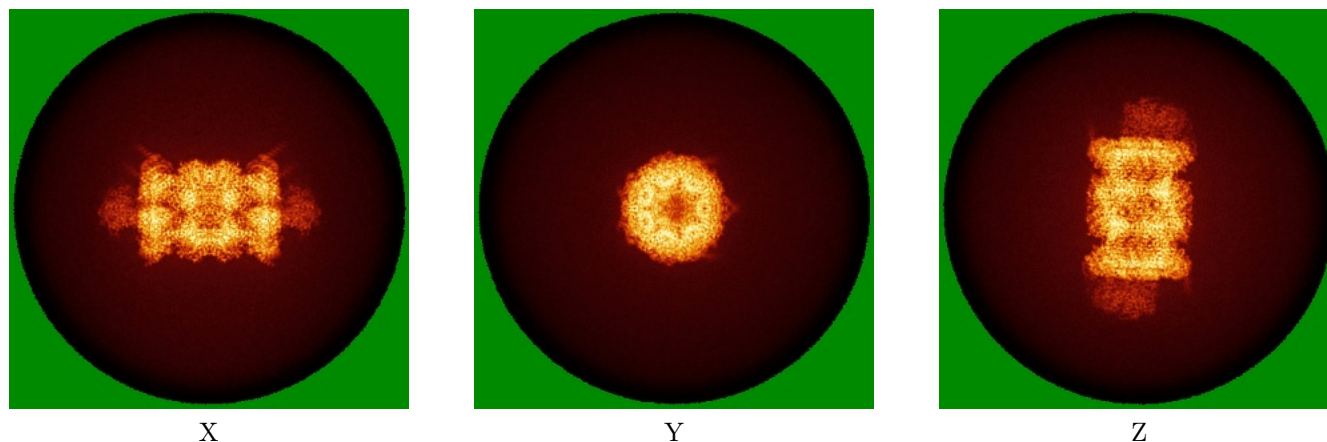


Z Index: 175

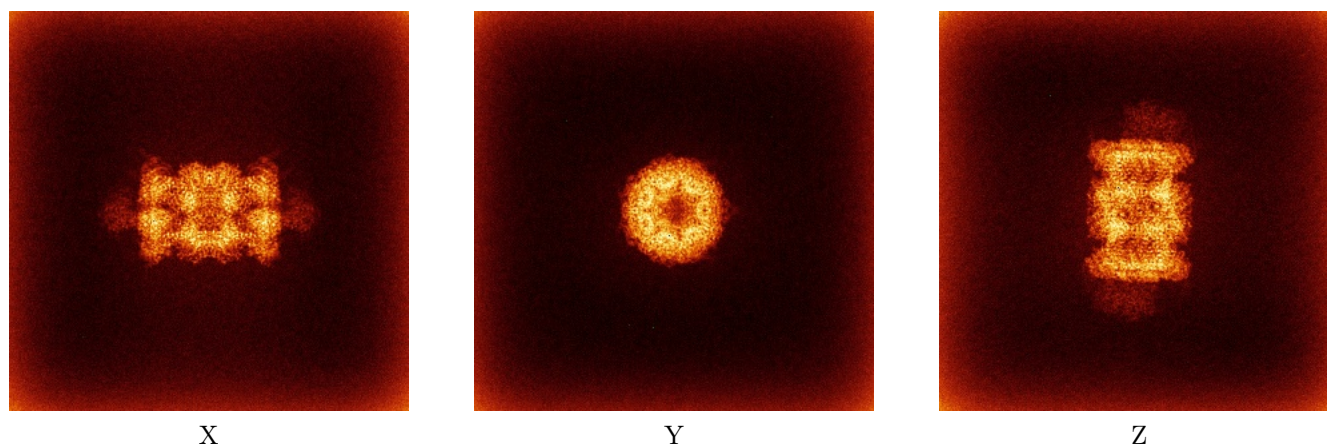
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



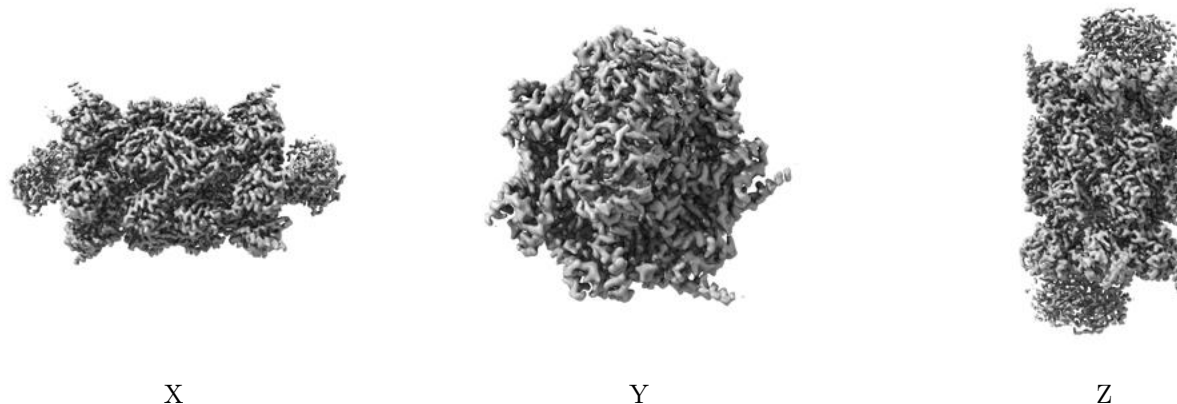
6.4.2 Raw map



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.

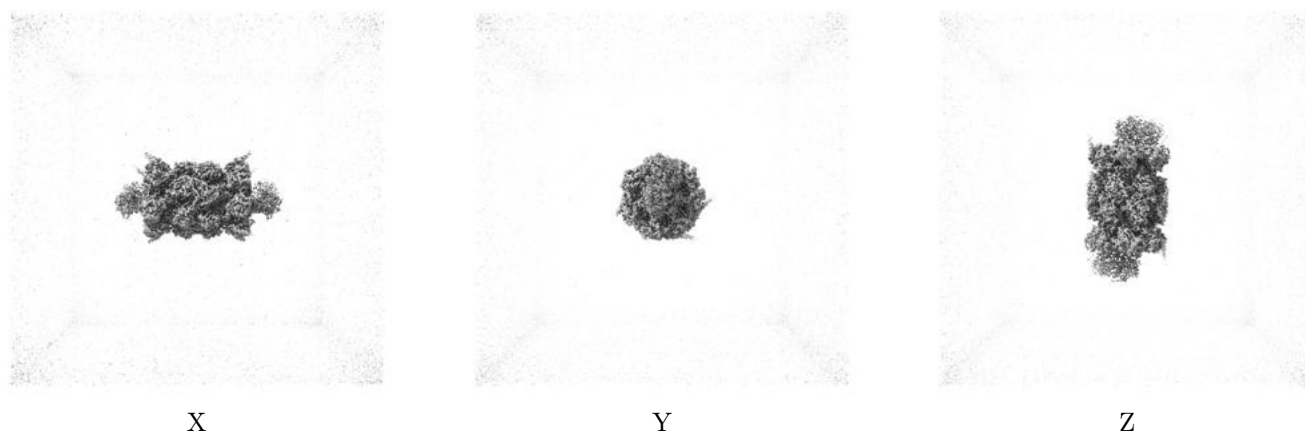
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

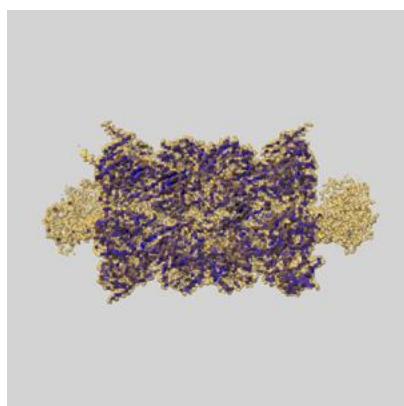
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

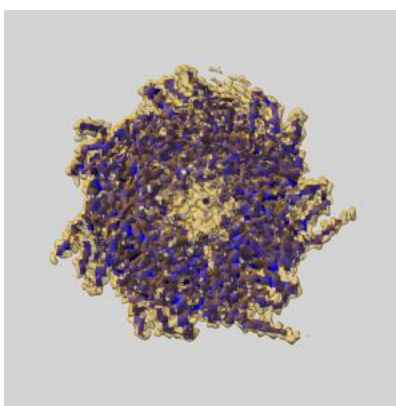
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

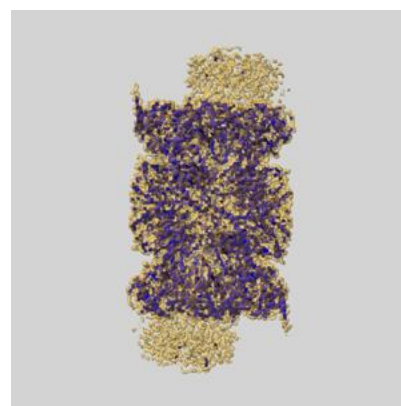
6.6.1 emd_41380_msk_1.map [i](#)



X



Y

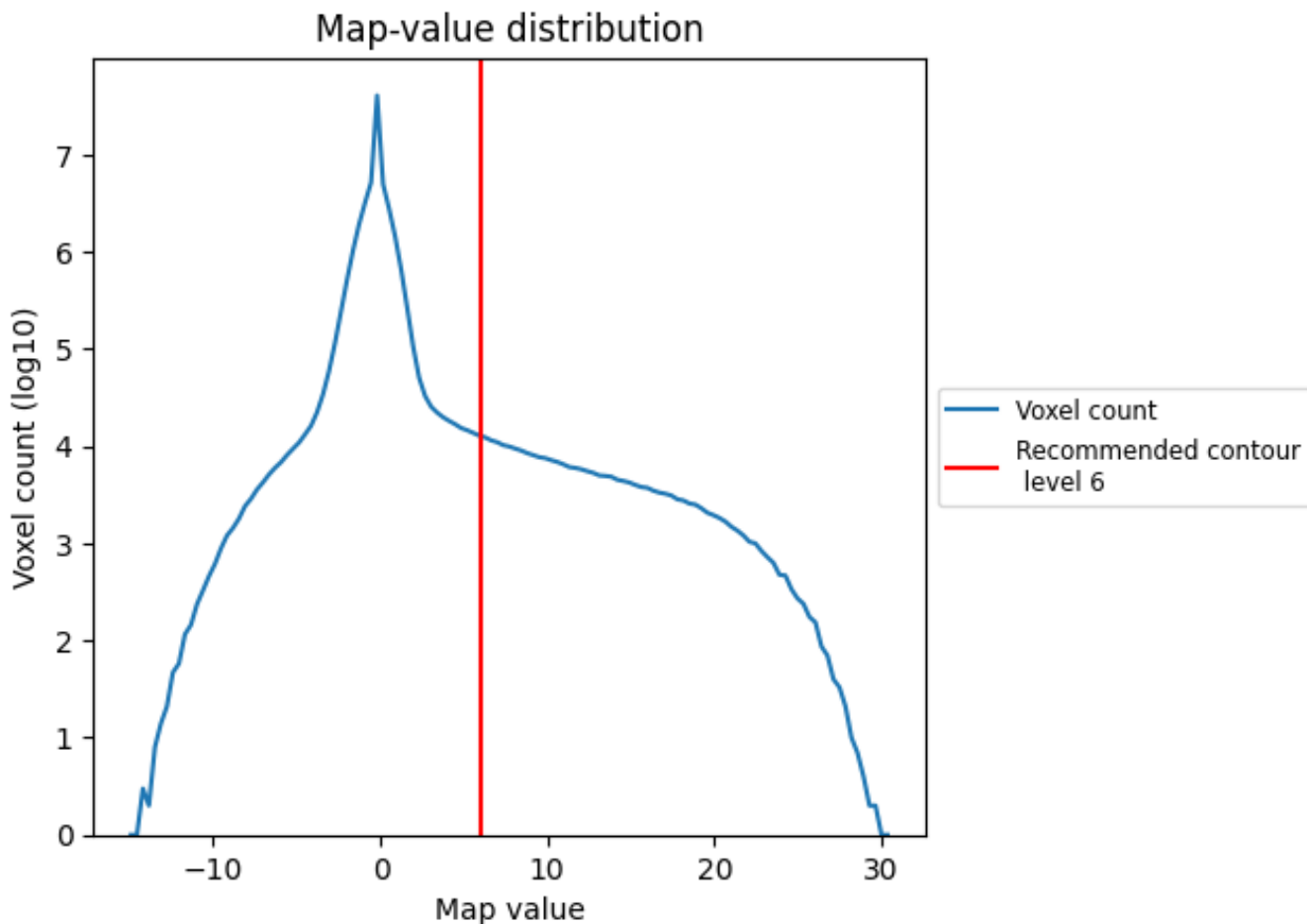


Z

7 Map analysis [i](#)

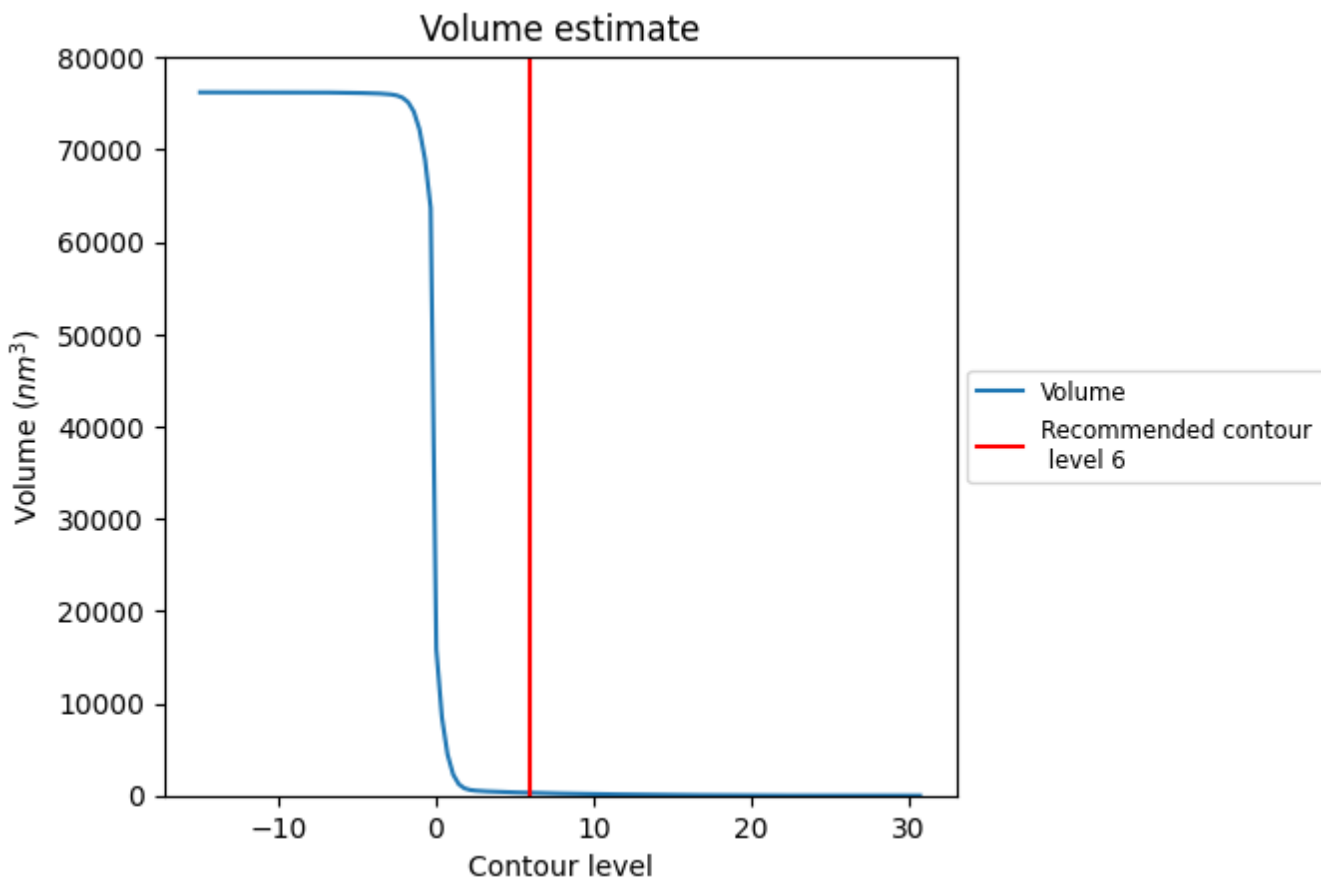
This section contains the results of statistical analysis of the map.

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.

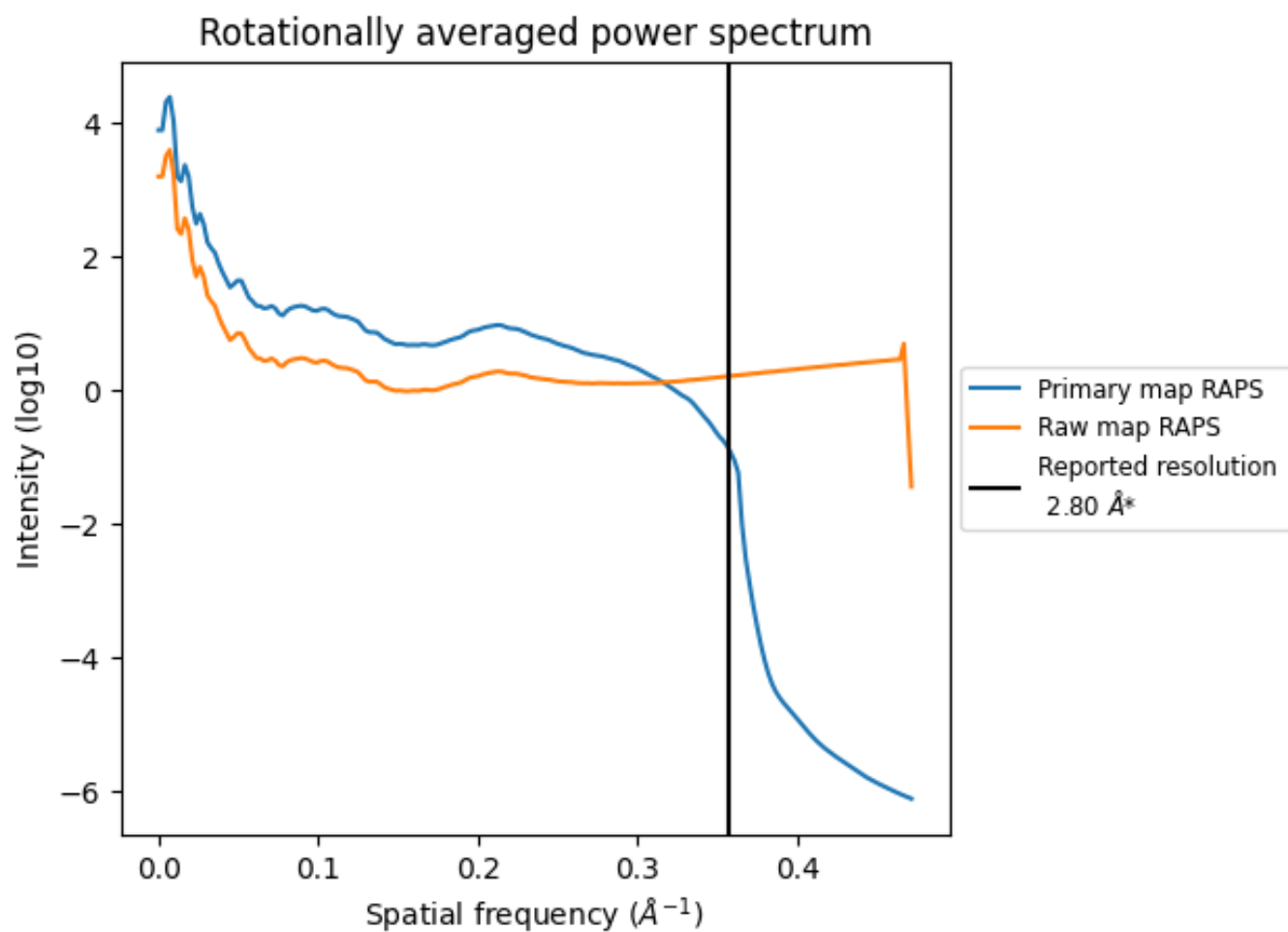
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm³; this corresponds to an approximate mass of 268 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

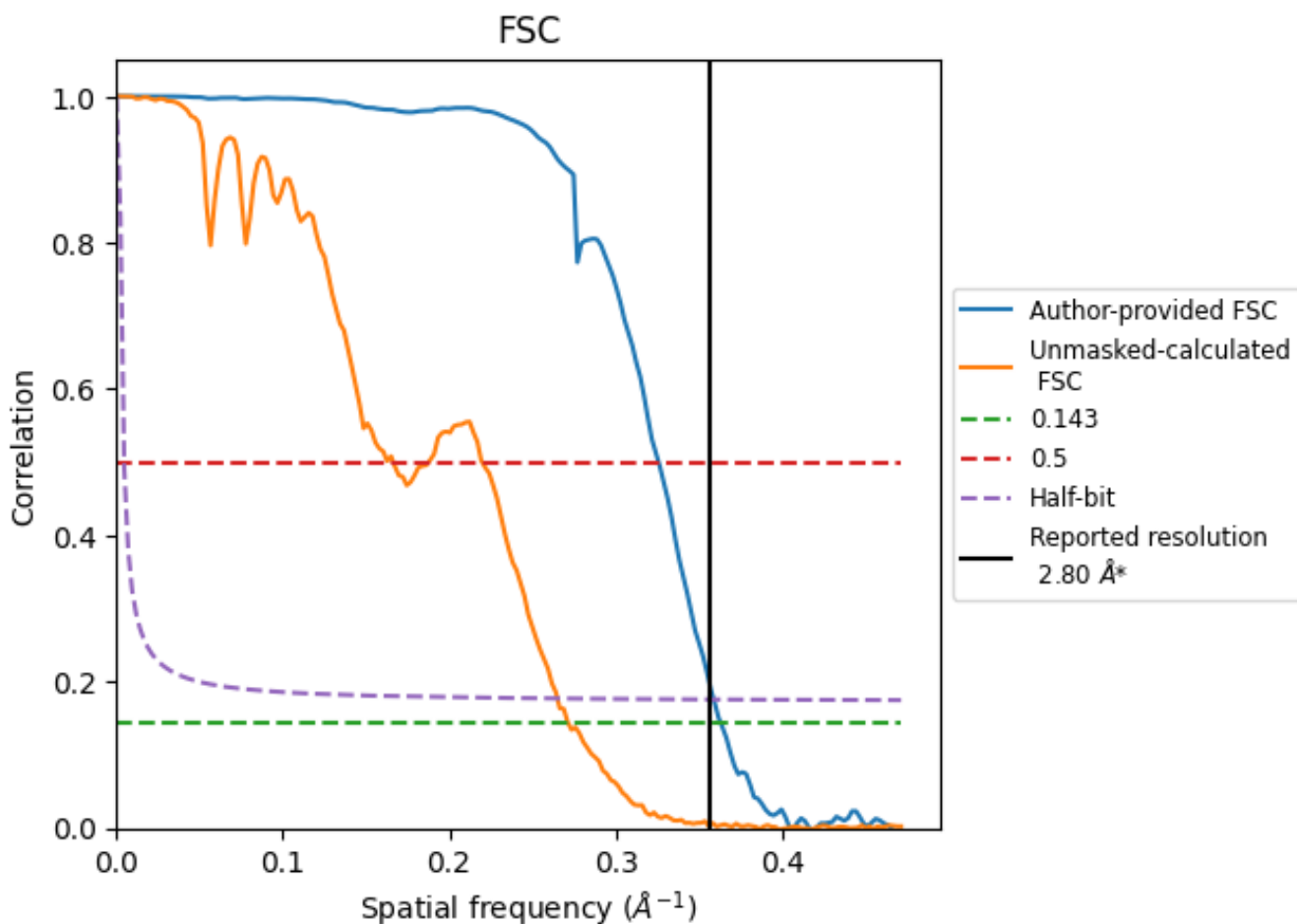


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357\AA^{-1}

8.2 Resolution estimates [i](#)

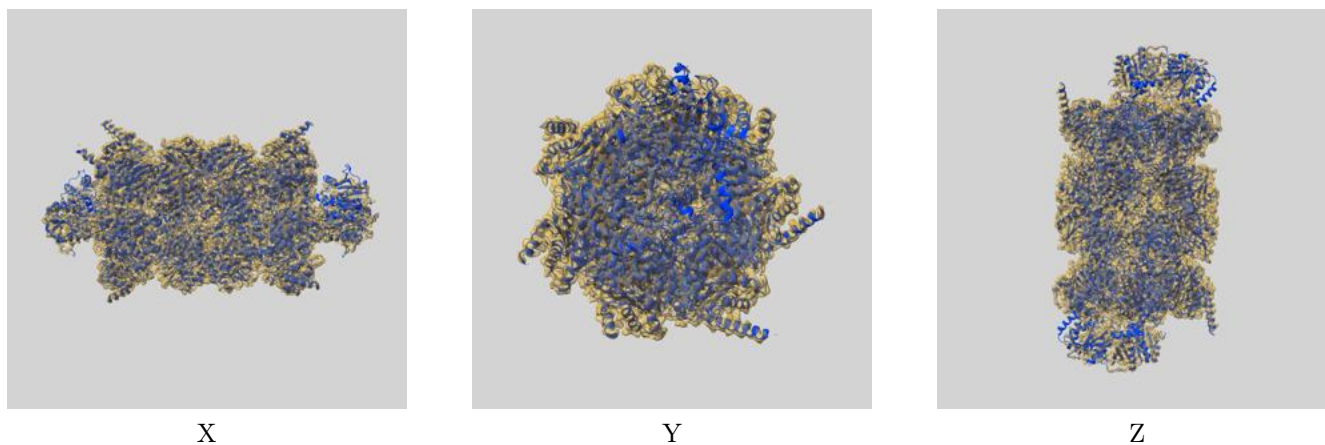
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.75	3.07	2.79
Unmasked-calculated*	3.68	6.01	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

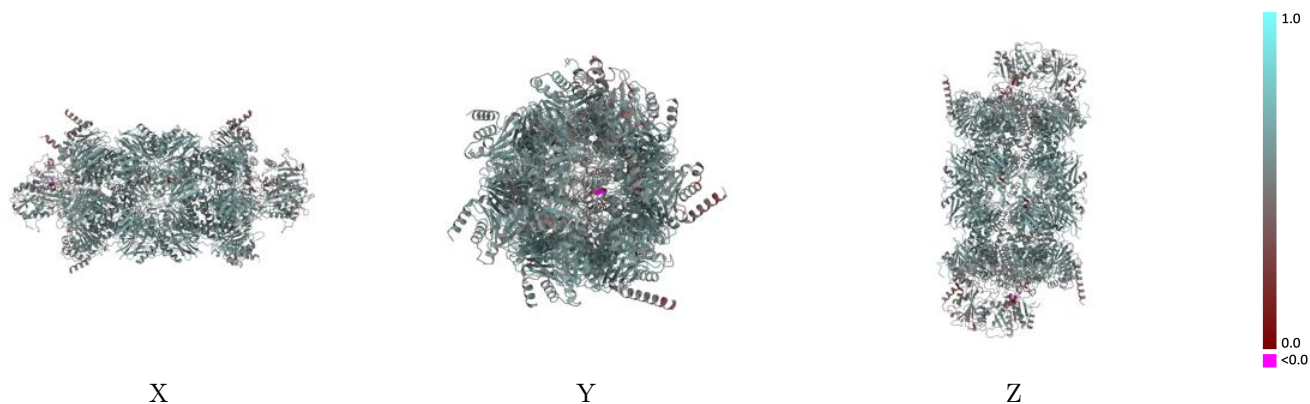
This section contains information regarding the fit between EMDB map EMD-41380 and PDB model 8TM6. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



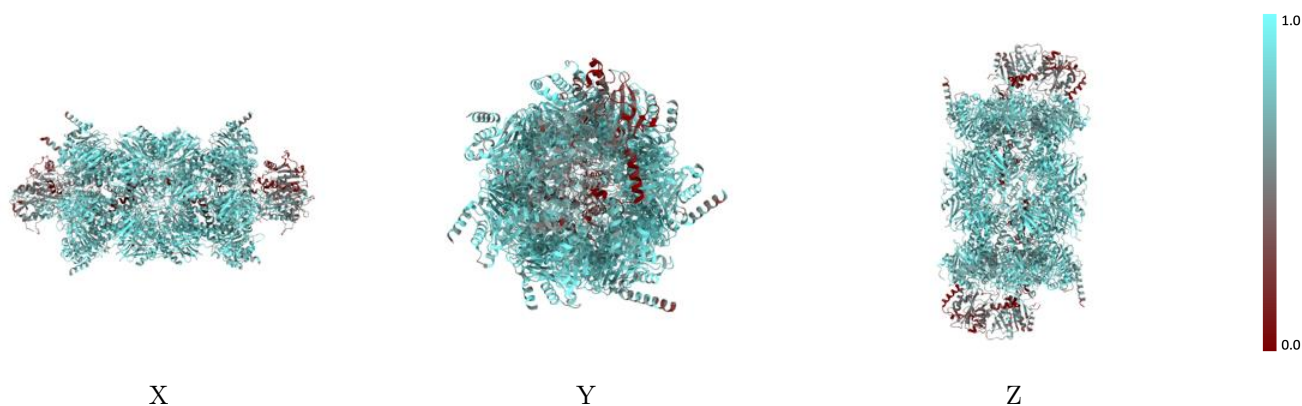
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



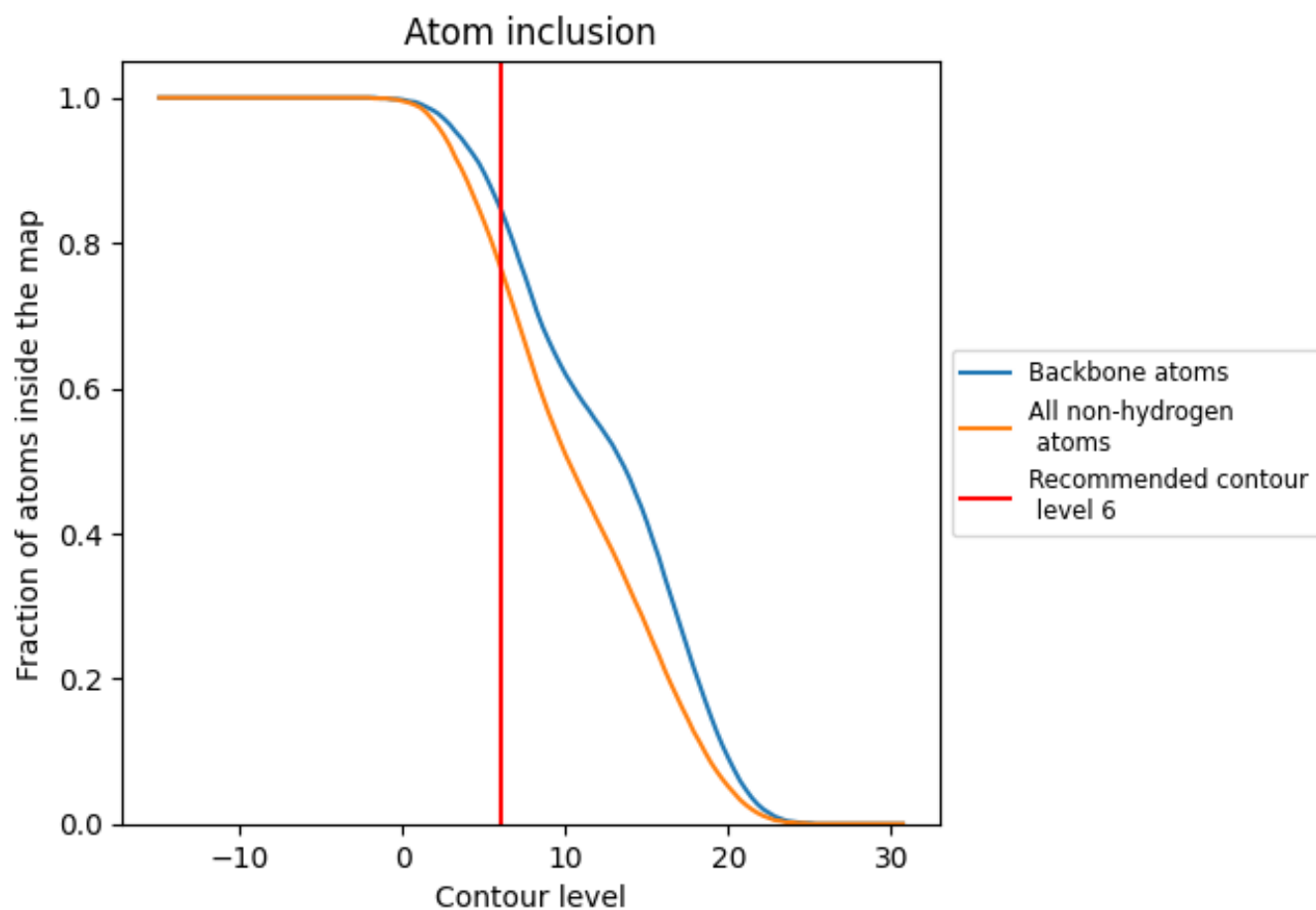
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.5520
A	 0.8410	 0.5580
B	 0.7920	 0.5500
C	 0.7900	 0.5300
D	 0.7660	 0.5440
E	 0.8440	 0.5670
F	 0.8200	 0.5590
G	 0.8240	 0.5580
H	 0.7700	 0.5600
I	 0.8840	 0.5870
J	 0.8850	 0.5910
K	 0.8920	 0.5860
L	 0.8650	 0.5830
M	 0.8790	 0.5840
N	 0.8190	 0.5710
O	 0.8270	 0.5520
P	 0.7840	 0.5440
Q	 0.7940	 0.5290
R	 0.7710	 0.5420
S	 0.8380	 0.5610
T	 0.8230	 0.5570
U	 0.8180	 0.5530
V	 0.7680	 0.5520
W	 0.8760	 0.5860
X	 0.8750	 0.5850
Y	 0.8920	 0.5870
Z	 0.8720	 0.5860
a	 0.8870	 0.5820
b	 0.8120	 0.5690
c	 0.3640	 0.4750
d	 0.5550	 0.5160
e	 0.4520	 0.5370
f	 0.3660	 0.4500
g	 0.5560	 0.5080
h	 0.4490	 0.5330

