

# Full wwPDB EM Validation Report (i)

Oct 19, 2023 – 04:35 PM EDT

PDB ID : 8T0M

EMDB ID : EMD-40944

Title : Proteasome 20S core particle from Pre1-1 Pre4-1 Double mutant Authors : Walsh Jr., R.M.; Rawson, S.; Schnell, H.; Velez, B.; Hanna, J.

Deposited on : 2023-06-01

Resolution : 2.40 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

<a href="https://www.wwpdb.org/validation/2017/EMValidationReportHelp">https://www.wwpdb.org/validation/2017/EMValidationReportHelp</a>
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

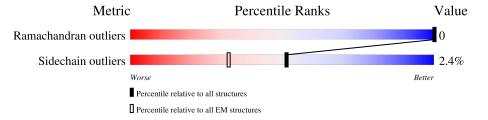
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 2.40 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	252	89%	9%
1	О	252	89%	9%
2	В	250	97%	
2	Р	250	97%	••
3	С	258	90%	• 8%
3	Q	258	90%	• 8%
4	D	254	85%	13%
4	R	254	85%	13%
5	E	260	87%	13%



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Mol	Chain	Length	Quality of chain	
5	S	260	86%	• 13%
6	F	234	96%	
6	Т	234	96%	
7	G	288	82%	• 16%
7	U	288	82%	• 16%
8	Н	215	82%	• 15%
8	V	215	82%	• 15%
9	I	261	77%	23%
9	W	261	77%	23%
10	J	205	95%	
10	X	205	95%	
11	K	198	98%	
11	Y	198	97%	
12	L	287	70%	28%
12	Z	287	69%	28%
13	M	241	90%	• 9%
13	a	241	90%	• 9%
14	N	251	82%	• 16%
14	b	251	82%	• 16%



# 2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 47538 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-1.

$\mathbf{Mol}$	Chain	Residues	$\mathbf{At}$	oms		AltConf	Trace	
1	A	229	C 1152		_	 0	0	
1	О	229	C 1152		_	 0	0	

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	248	Total 1900	C 1210	- '	O 374	$\sim$	0	0
2	Р	248	Total 1900	C 1210		_		0	0

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

Mol	Chain	Residues		Ato	AltConf	Trace			
3	С	237	Total	С	N	О	S	0	0
9	3	231	1861	1177	313	368	3	0	
2	0	237	Total	С	N	О	S	0	0
3	Q	231	1861	1177	313	368	3	0	U

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

Mol	Chain	Residues		$\mathbf{At}$	oms		AltConf	Trace	
4	D	221	Total 1727	C 1084			S 4	0	0
4	R	221	Total 1727	C 1084		_	S 4	0	0

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



Mol	Chain	Residues		Ato	oms		AltConf	Trace	
5	E	227	Total	С	N	О	S	0	0
9	E 221	221	1750	1097	294	352	7	0	
5	C	227	Total	С	N	О	S	0	0
9	b	221	1750	1097	294	352	7	0	U

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

$\mathbf{M}$	ol	Chain	Residues		Ato	oms		AltConf	Trace	
6	;	F	230	Total 1765	C 1110		O 346	,	0	0
6	;	Т	230		C 1110		_	S 4	0	0

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

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
7	G	242	1885	C 1199	328	354	4	0	0
7	U	242	Total 1885	C 1199			S 4	0	0

• Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
Q	Н	183	Total	С	N	О	S	0	0
8	11	100	1424	905	234	278	7	U	
Q	V	183	Total	С	N	О	S	0	0
0	V	100	1424	905	234	278	7	0	U

• Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
0	Т	202	Total	С	N	О	S	0	0
9	1	202	1550	985	266	293	6	0	
0	137	202	Total	С	N	О	S	0	0
9	VV	202	1550	985	266	293	6	U	U

• Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
10	J	200	Total 1551	C 991	N 254	O 298	S 8	0	0



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Mol	Chain	Residues		At	oms			AltConf	Trace
10	X	200	Total 1551	C 991	N 254	O 298	S 8	0	0

• Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms				AltConf	Trace		
11	I/	194	Total	С	N	О	S	0	0	
11	IX	194	1558	993	263	297	5	0	0	
11	V	194	Total	С	N	О	S	0	0	
11	1	194	1558	993	263	297	5	0	U	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	conflict	UNP P22141
Y	142	PHE	SER	conflict	UNP P22141

• Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
12	L	207	20001	C 1029	- '		S 7	0	0
12	Z	207	Total 1617	C 1029	- '		S 7	0	0

• Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	220		C 1101		_	S 4	0	0
13	a	220	Total 1737	C 1101	= :	_	S 4	0	0

• Molecule 14 is a protein called Proteasome subunit beta type-7.

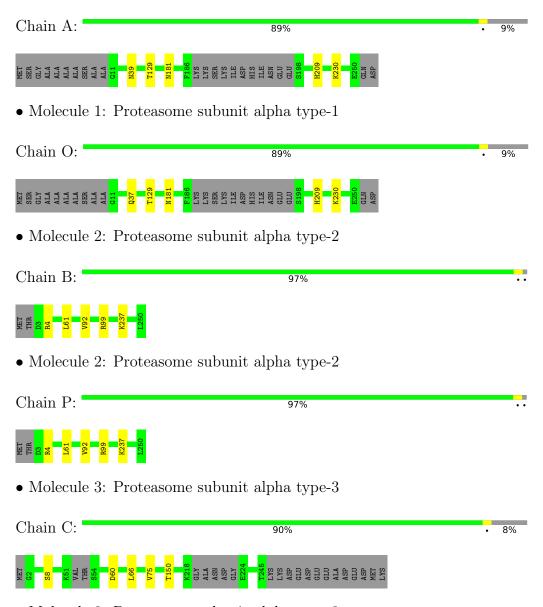
Mol	Chain	Residues	Atoms			AltConf	Trace		
1.4	N	211	Total	С	N	О	S	0	0
14	11	211	1639	1037	281	315	6	0	0
1.4	h	211	Total	С	N	О	S	0	0
14	D	211	1639	1037	281	315	6	U	U



## 3 Residue-property plots (i)

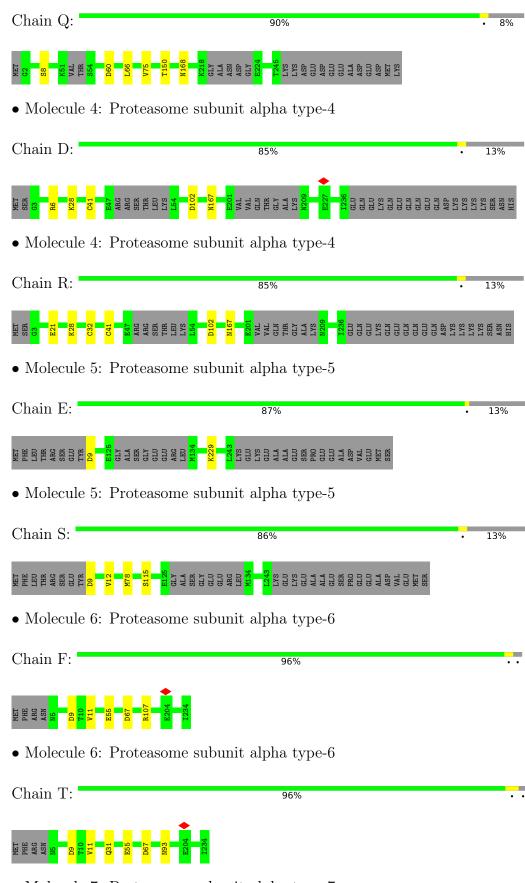
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-1



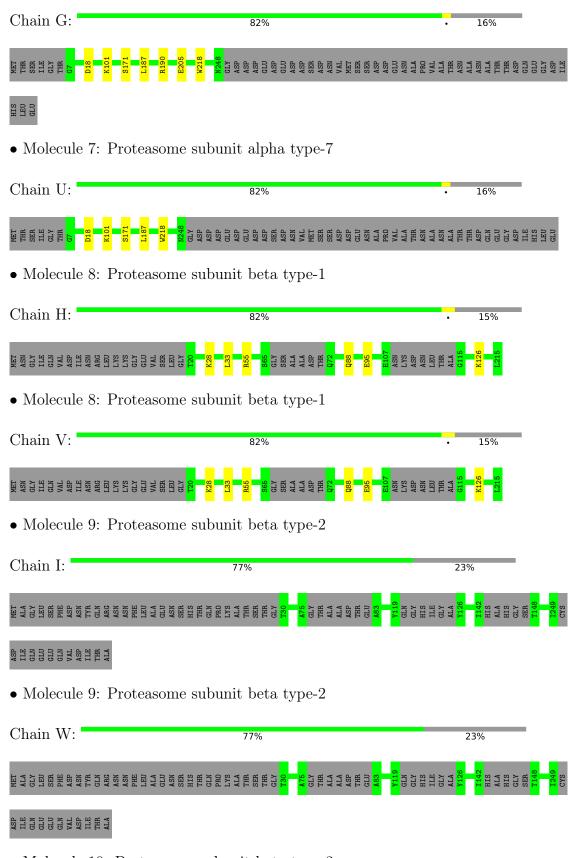
• Molecule 3: Proteasome subunit alpha type-3





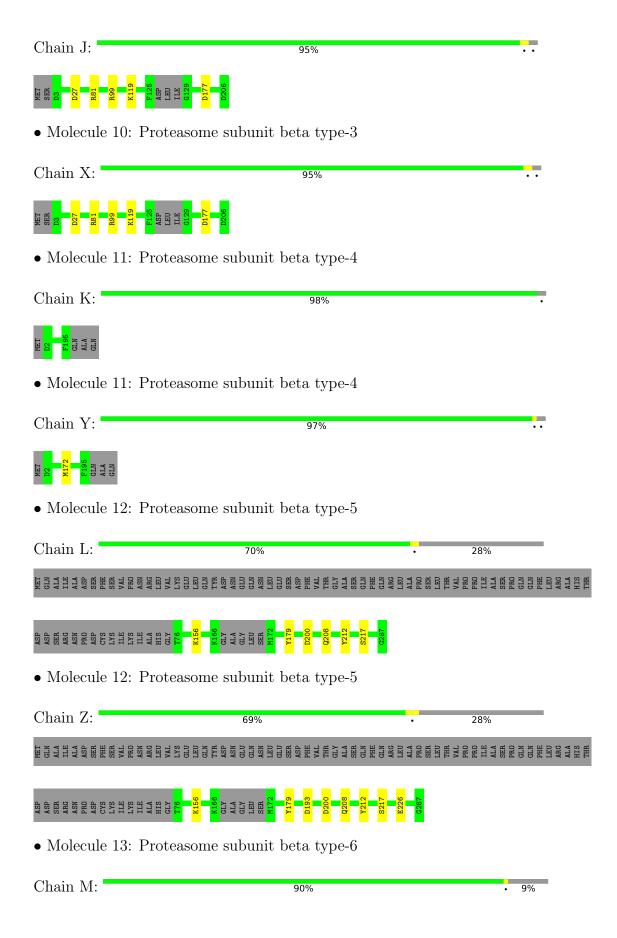
• Molecule 7: Proteasome subunit alpha type-7



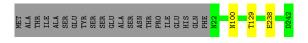


• Molecule 10: Proteasome subunit beta type-3









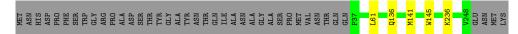
 $\bullet$  Molecule 13: Proteasome subunit beta type-6

Chain a: 90% • 9%

• Molecule 14: Proteasome subunit beta type-7

• Molecule 14: Proteasome subunit beta type-7

Chain b: 82% · 16%





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	766100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	54.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.963	Depositor
Minimum map value	-4.126	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.426	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.29	0/1841	0.50	0/2495
1	О	0.28	0/1841	0.50	0/2495
2	В	0.28	0/1937	0.48	0/2622
2	Р	0.27	0/1937	0.47	0/2622
3	С	0.27	0/1889	0.50	0/2553
3	Q	0.27	0/1889	0.49	0/2553
4	D	0.27	0/1754	0.51	0/2376
4	R	0.26	0/1754	0.50	0/2376
5	Е	0.25	0/1774	0.50	0/2392
5	S	0.25	0/1774	0.47	0/2392
6	F	0.26	0/1792	0.49	0/2422
6	Т	0.26	0/1792	0.48	0/2422
7	G	0.27	0/1925	0.46	0/2599
7	U	0.27	0/1925	0.46	0/2599
8	Н	0.26	0/1451	0.48	0/1961
8	V	0.26	0/1451	0.47	0/1961
9	I	0.26	0/1575	0.48	0/2131
9	W	0.26	0/1575	0.48	0/2131
10	J	0.28	0/1580	0.49	0/2130
10	X	0.28	0/1580	0.48	0/2130
11	K	0.27	0/1587	0.51	0/2140
11	Y	0.26	0/1587	0.52	0/2140
12	L	0.26	0/1653	0.49	0/2235
12	Z	0.26	0/1653	0.48	0/2235
13	M	0.27	0/1774	0.49	0/2392
13	a	0.27	0/1774	0.49	0/2392
14	N	0.27	0/1666	0.52	0/2262
14	b	0.27	0/1666	0.51	0/2262
All	All	0.27	0/48396	0.49	0/65420

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)

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	Perce	ntiles
1	A	$225/252\ (89\%)$	223 (99%)	2 (1%)	0	100	100
1	О	225/252~(89%)	224 (100%)	1 (0%)	0	100	100
2	В	246/250 (98%)	243 (99%)	3 (1%)	0	100	100
2	Р	246/250 (98%)	245 (100%)	1 (0%)	0	100	100
3	С	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
3	Q	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
4	D	215/254 (85%)	209 (97%)	6 (3%)	0	100	100
4	R	$215/254\ (85\%)$	208 (97%)	7 (3%)	0	100	100
5	Е	223/260 (86%)	221 (99%)	2 (1%)	0	100	100
5	S	223/260 (86%)	221 (99%)	2 (1%)	0	100	100
6	F	228/234~(97%)	223 (98%)	5 (2%)	0	100	100
6	Т	228/234~(97%)	225 (99%)	3 (1%)	0	100	100
7	G	240/288~(83%)	238 (99%)	2 (1%)	0	100	100
7	U	240/288 (83%)	238 (99%)	2 (1%)	0	100	100
8	Н	177/215 (82%)	176 (99%)	1 (1%)	0	100	100
8	V	177/215 (82%)	176 (99%)	1 (1%)	0	100	100
9	I	194/261 (74%)	192 (99%)	2 (1%)	0	100	100
9	W	194/261 (74%)	192 (99%)	2 (1%)	0	100	100
10	J	$196/205\ (96\%)$	190 (97%)	6 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percei	ntiles
10	X	196/205~(96%)	192 (98%)	4 (2%)	0	100	100
11	K	192/198 (97%)	190 (99%)	2 (1%)	0	100	100
11	Y	192/198~(97%)	188 (98%)	4 (2%)	0	100	100
12	L	203/287 (71%)	201 (99%)	2 (1%)	0	100	100
12	Z	$203/287 \ (71\%)$	200 (98%)	3 (2%)	0	100	100
13	M	218/241 (90%)	213 (98%)	5 (2%)	0	100	100
13	a	218/241 (90%)	214 (98%)	4 (2%)	0	100	100
14	N	209/251 (83%)	204 (98%)	5 (2%)	0	100	100
14	b	209/251 (83%)	204 (98%)	5 (2%)	0	100	100
All	All	5994/6908 (87%)	5908 (99%)	86 (1%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	$194/210\ (92\%)$	189 (97%)	5 (3%)	46 66
1	О	$194/210\ (92\%)$	189 (97%)	5 (3%)	46 66
2	В	$207/209\ (99\%)$	202 (98%)	5 (2%)	49 68
2	Р	$207/209\ (99\%)$	202 (98%)	5 (2%)	49 68
3	С	$199/216\ (92\%)$	194 (98%)	5 (2%)	47 67
3	Q	$199/216\ (92\%)$	193 (97%)	6 (3%)	41 61
4	D	$195/226\ (86\%)$	190 (97%)	5 (3%)	46 66
4	R	$195/226\ (86\%)$	189 (97%)	6 (3%)	40 60
5	E	188/215~(87%)	186 (99%)	2 (1%)	73 87
5	S	188/215~(87%)	184 (98%)	4 (2%)	53 72
6	F	$189/193\ (98\%)$	184 (97%)	5 (3%)	46 66
6	Т	$189/193\ (98\%)$	183 (97%)	6 (3%)	39 59



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
7	G	200/239~(84%)	193 (96%)	7 (4%)	36	55
7	U	200/239 (84%)	195 (98%)	5 (2%)	47	67
8	Н	153/178 (86%)	147 (96%)	6 (4%)	32	50
8	V	153/178 (86%)	147 (96%)	6 (4%)	32	50
9	Ι	169/214 (79%)	169 (100%)	0	100	100
9	W	169/214 (79%)	169 (100%)	0	100	100
10	J	168/173 (97%)	163 (97%)	5 (3%)	41	61
10	X	168/173 (97%)	163 (97%)	5 (3%)	41	61
11	K	172/175~(98%)	172 (100%)	0	100	100
11	Y	172/175 (98%)	171 (99%)	1 (1%)	86	94
12	${ m L}$	$167/235 \ (71\%)$	161 (96%)	6 (4%)	35	54
12	Z	167/235 (71%)	159 (95%)	8 (5%)	25	41
13	M	183/201 (91%)	180 (98%)	3 (2%)	62	79
13	a	183/201 (91%)	180 (98%)	3 (2%)	62	79
14	N	180/212 (85%)	176 (98%)	4 (2%)	52	71
14	b	180/212 (85%)	175 (97%)	5 (3%)	43	63
All	All	5128/5792 (88%)	5005 (98%)	123 (2%)	51	68

All (123) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	129	THR
1	A	181	ASN
1	A	209	HIS
1	A	230	LYS
2	В	4	ARG
2	В	61	LEU
2	В	92	VAL
2	В	99	ARG
2	В	237	LYS
3	С	8	SER
3	С	60	ASP
3	С	66	LEU
3	С	75	VAL
3	С	150	THR



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Mol	Chain	Res	Type	
4	D	6	ARG	
4	D	28	LYS	
4	D	41	CYS	
4	D	102	CYS ASP ASN	
4	D	167	ASN	
5	Е	9	ASP LYS	
5	Е	229	LYS	
6	F F	9	ASP VAL	
6	F	11	VAL	
6	F F G	55	GLU	
6	F	67	ASP	
6	F	107	ARG	
7	G	18	ASP	
7	G	101	LYS	
7	G	171	SER	
7 7 7 7	G	187	LEU	
7	G G	190	ARG	
7	G	205	GLU	
7	G	218	TRP	
8	Н	28	LYS	
8	Н	33	LEU	
8	Н	55	ARG	
8	Н	88	GLN	
8	Н	95	GLU	
8	Н	126	LYS ASP	
10	J	27	ASP	
10	J	81	ARG	
10	J	99	ARG	
10	J	119	LYS	
10	J	177	ASP	
12	L	156	LYS	
12	L	179	TYR	
12	L	200	ASP	
12	L	208	GLN	
12	L	212	TYR	
12	L	217	SER	
13	M	100	ASN	
13	M	129	THR	
13	M	238	GLU	
14	N	61	LEU	
14	N	136	GLN	
14	N	140	LYS	

14 | N | 140 | LYS | Continued on next page...



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Mol	Chain	$\operatorname{Res}$	Type TRP GLN THR	
14	N	145	TRP	
1	О	37	GLN	
1	О	129	THR	
1 1	О	129 181 209	ASN HIS	
	О	209	HIS	
1	O O O O O P P P P P Q Q Q Q Q R R R R	230	LYS ARG LEU VAL	
2 2 2 2 2 2 3	Р	4	ARG	
2	Р	61 92	LEU	
2	Р	92	VAL	
2	Р	99	ARG LYS SER ASP LEU VAL	
2	Р	237	LYS	
3	Q	8	SER	
3	Q	60	ASP	
3	Q	66	LEU	
3	Q	75	VAL	
3	Q	150	THR ASN GLU LYS CYS CYS ASP ASN ASP VAL MET	
3	Q	168	ASN	
4 4	R	21	GLU	
4	R	28	LYS	
4	R	32	CYS	
4	R R	32 41 102	CYS	
4	R	102	ASP	
4	R R	167	ASN	
5	S S S S	9	ASP	
5	S	12	VAL	
5	S	78	MET	
5 6	S	115	SER	
6	Т	9	SER ASP	
6	Т	11	VAL	
6	Т	31	GLN	
6	Т	55	GLU	
6	Т	67	ASP	
6	T T T U	93	ASN	
7	U	18	ASP	
7	U	101	LYS	
7	U	171	SER	
7	U U	187	LEU	
7	U	218	TRP	
8	V	28	LYS	
8	V	33	LEU	
8	V	55	ARG	
8	V	88	GLN	

8 V 88 GLN

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Mol	Chain	Res	Type
8	V	95	GLU
8	V	126	LYS
10	X	27	ASP
10	X	81	ARG
10	X	99	ARG
10	X	119	LYS
10	X	177	ASP
11	Y	172	MET
12	Z	156	LYS
12	Z	179	TYR
12	Z	193	ASP
12	Z	200	ASP
12	Z	208	GLN
12	Z	212	TYR
12	Z	217	SER
12	Z	226	GLU
13	a	100	ASN
13	a	129	THR
13	a	238	GLU
14	b	61	LEU
14	b	136	GLN
14	b	141	MET
14	b	145	TRP
14	b	236	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
11	K	166	GLN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

# 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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



### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



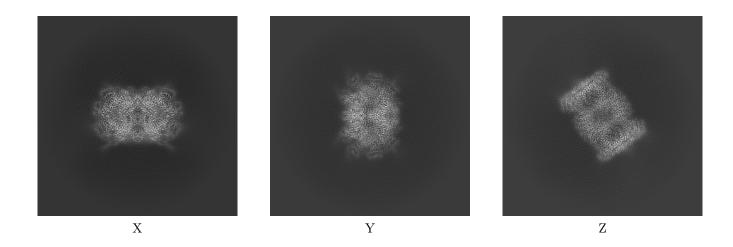
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40944. These allow visual inspection of the internal detail of the map and identification of artifacts.

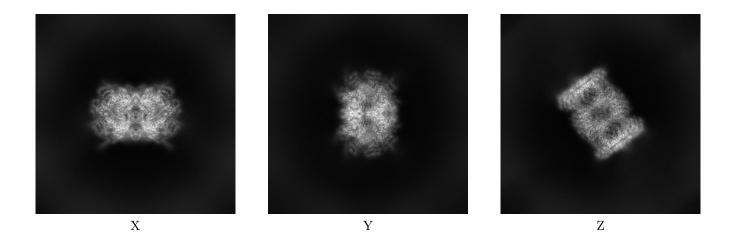
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



#### 6.1.2 Raw map



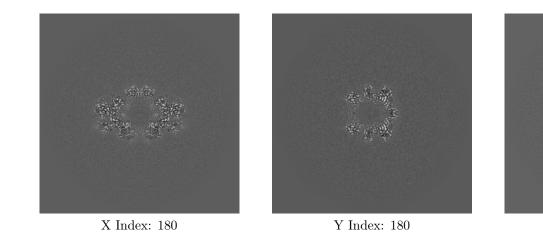
The images above show the map projected in three orthogonal directions.



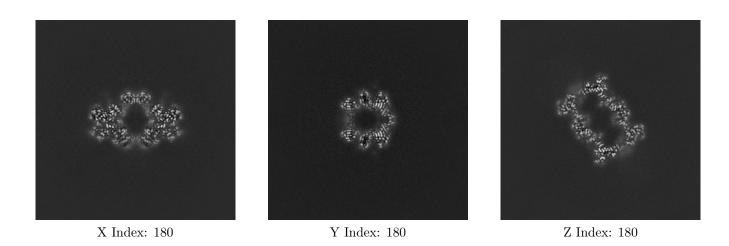
Z Index: 180

### 6.2 Central slices (i)

#### 6.2.1 Primary map



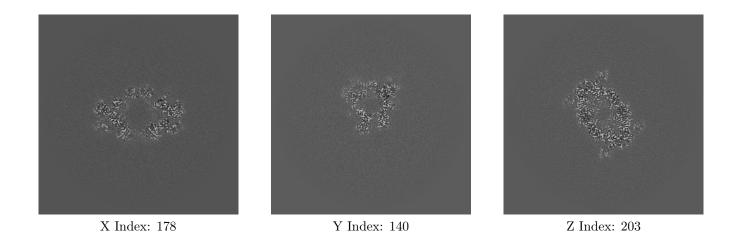
#### 6.2.2 Raw map



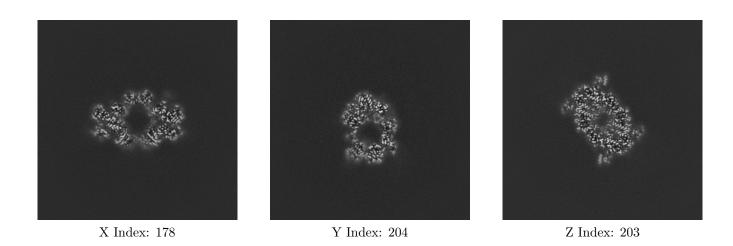
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



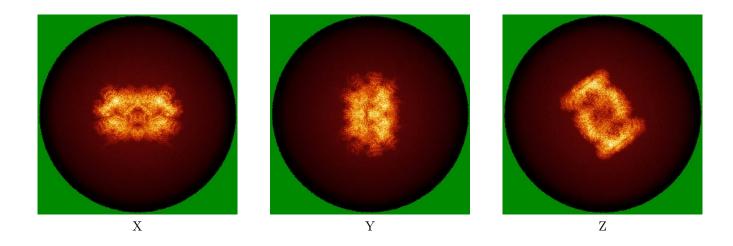
#### 6.3.2 Raw map



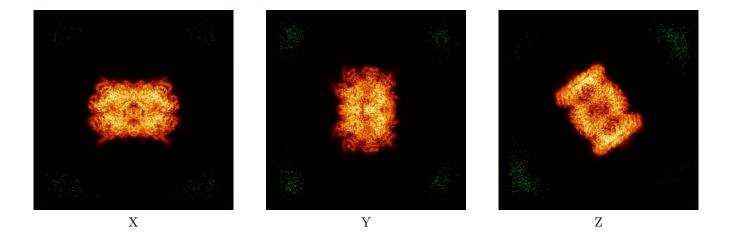
The images above show the largest variance slices of the map in three orthogonal directions.

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

#### 6.4.1 Primary map



#### 6.4.2 Raw map

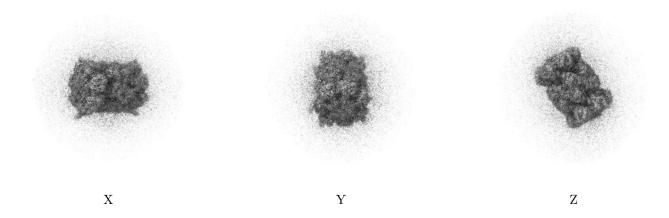


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



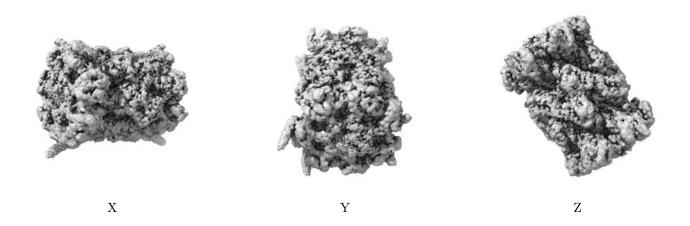
### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.426. 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)

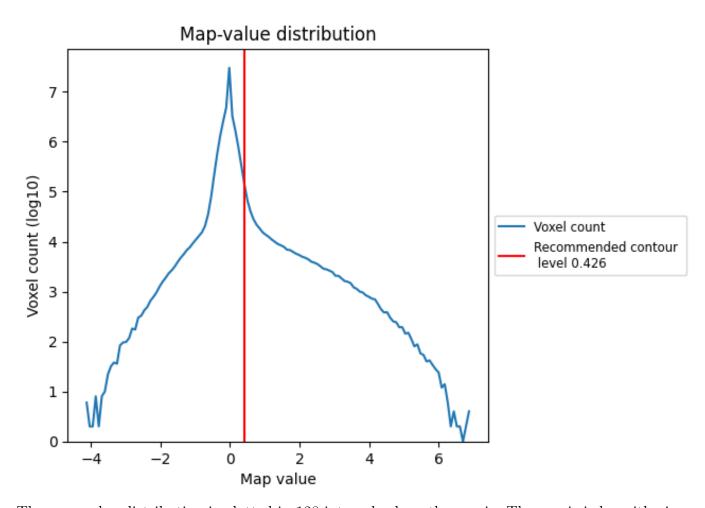
This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

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

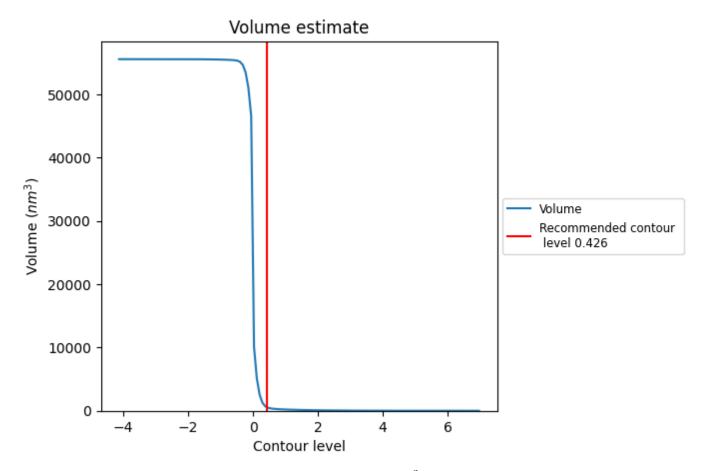
### 7.1 Map-value distribution (i)



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)

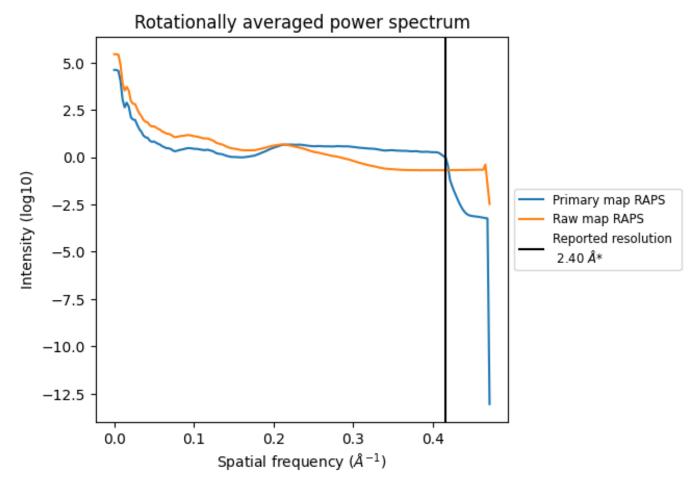


The volume at the recommended contour level is  $579~\mathrm{nm}^3$ ; this corresponds to an approximate mass of  $523~\mathrm{kDa}$ .

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)



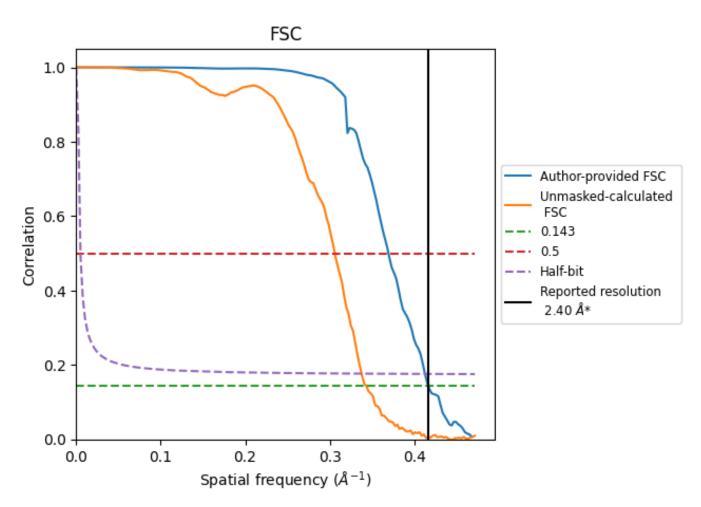
\*Reported resolution corresponds to spatial frequency of 0.417  $\rm \mathring{A}^{-1}$ 



## 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 0.417  $\rm \mathring{A}^{-1}$ 



### 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.71	2.42
Unmasked-calculated*	2.91	3.27	2.96

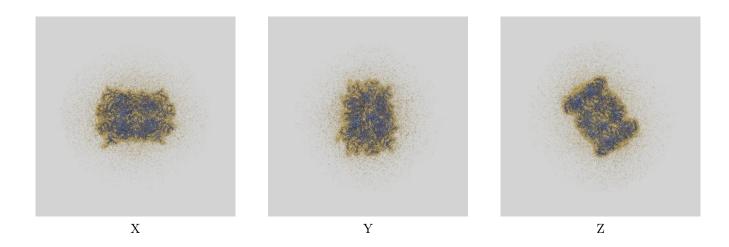
<sup>\*</sup>Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.91 differs from the reported value 2.4 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40944 and PDB model 8T0M. Per-residue inclusion information can be found in section 3 on page 7.

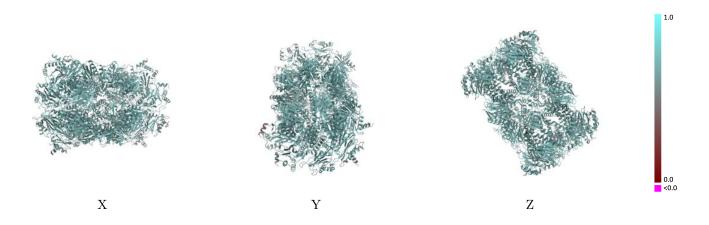
### 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.426 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.

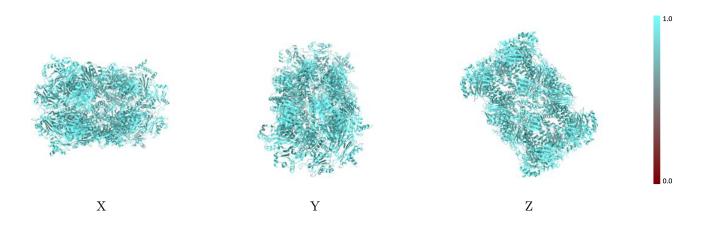


### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

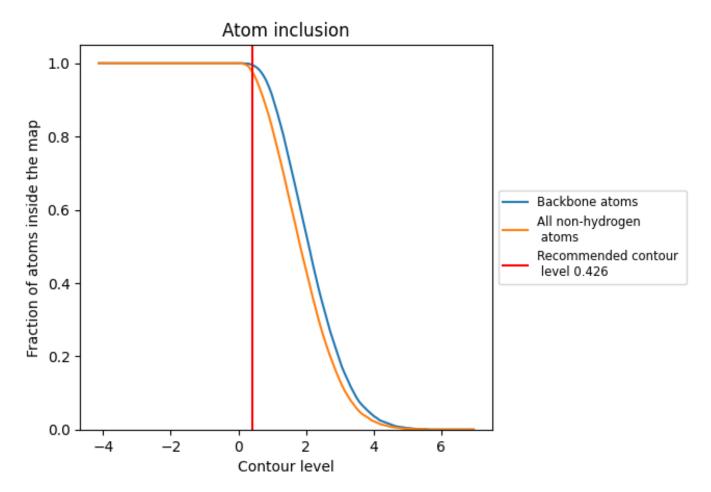
### 9.3 Atom inclusion mapped to coordinate model (i)



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 (0.426).



### 9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.



### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.426) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.6600
A	0.9890	0.6690
В	0.9780	0.6680
С	0.9700	0.6520
D	0.9590	0.6190
Е	0.9590	0.6270
F	0.9720	0.6520
G	0.9700	0.6610
Н	0.9800	0.6610
I	0.9820	0.6730
J	0.9840	0.6840
K	0.9690	0.6520
L	0.9810	0.6690
M	0.9770	0.6680
N	0.9830	0.6780
О	0.9880	0.6710
P	0.9800	0.6710
Q	0.9730	0.6550
R	0.9600	0.6200
S	0.9600	0.6300
Т	0.9710	0.6520
U	0.9710	0.6600
V	0.9790	0.6600
W	0.9810	0.6730
X	0.9840	0.6840
Y	0.9690	0.6540
Z	0.9800	0.6710
a	0.9740	0.6700
b	0.9830	0.6790



