



## Full wwPDB EM Validation Report ⓘ

Jan 15, 2025 – 08:42 PM JST

PDB ID : 8YIZ  
EMDB ID : EMD-39334  
Title : Cryo-EM structure of human proteasome assembly intermediate preholo-2  
Authors : Han, Y.; Han, Q.; Tang, Q.; Zhang, Y.; Liu, K.  
Deposited on : 2024-02-29  
Resolution : 3.79 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](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) : 2.40

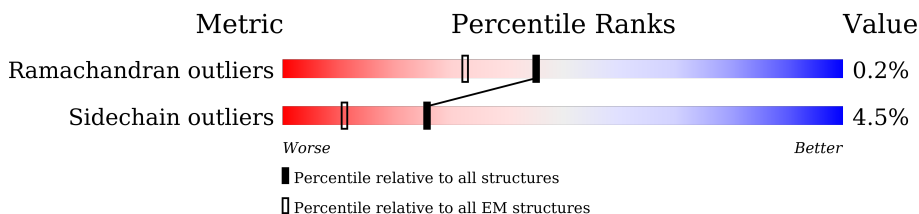
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.79 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  $\geq 3$ , 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	A	234	 5% 88% 9% ..
1	O	234	 1% 88% 9% ..
2	B	261	 7% 83% 10% • 6%
2	P	261	 11% 83% 10% • 6%
3	C	248	 1% 88% 7% ..
3	Q	248	 13% 88% 7% ..
4	D	241	 9% 89% 10% •
4	R	241	 13% 89% 10% •
5	E	263	 1% 90% 10%

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Mol	Chain	Length	Quality of chain
5	S	263	90% 10%
6	F	255	93% 6%
6	T	255	94% 6%
7	G	246	7% 91% 8%
7	U	246	6% 91% 8%
8	H	277	78% 21%
8	V	277	79% 21%
9	I	205	98%
9	W	205	98%
10	J	201	97%
10	X	201	97%
11	K	263	78% 21%
11	Y	263	78% 21%
12	L	241	88% 12%
12	Z	241	88% 12%
13	M	253	81% 19%
13	a	253	81% 19%
14	N	239	83% 16%
14	b	239	83% 16%
15	f	288	69% 95%
16	g	264	49% 98%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 52599 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	O	228	Total	C	N	O	S	0	0
			1760	1124	296	334	6		
1	A	228	Total	C	N	O	S	0	0
			1760	1124	296	334	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	245	Total	C	N	O	S	0	0
			1894	1196	321	367	10		
2	B	245	Total	C	N	O	S	0	0
			1894	1196	321	367	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	239	Total	C	N	O	S	0	0
			1849	1159	325	360	5		
3	C	239	Total	C	N	O	S	0	0
			1849	1159	325	360	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	241	Total	C	N	O	S	0	0
			1840	1159	305	364	12		
4	D	241	Total	C	N	O	S	0	0
			1840	1159	305	364	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	238	1859	1165	335	348	11	1	0
5	E	238	1859	1165	335	348	11	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	239	1858	1180	318	348	12	1	0
6	F	239	1858	1180	318	348	12	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	U	245	1893	1201	317	361	14	0	0
7	G	245	1893	1201	317	361	14	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	V	220	1655	1042	278	322	13	2	0
8	H	220	1655	1042	278	322	13	2	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	200	1576	1004	265	289	18	2	0
9	I	200	1576	1004	265	289	18	2	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	196	1581	1013	269	289	10	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	196	1581	1013	269	289	10	2	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Y	208	1631	1030	286	304	11	3	0
11	K	208	1631	1030	286	304	11	3	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Z	213	1644	1043	281	309	11	1	0
12	L	213	1644	1043	281	309	11	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	a	206	1605	1012	277	305	11	1	0
13	M	206	1605	1012	277	305	11	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	b	200	1504	943	256	292	13	1	0
14	N	200	1504	943	256	292	13	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	f	281	2239	1426	375	419	19	0	0

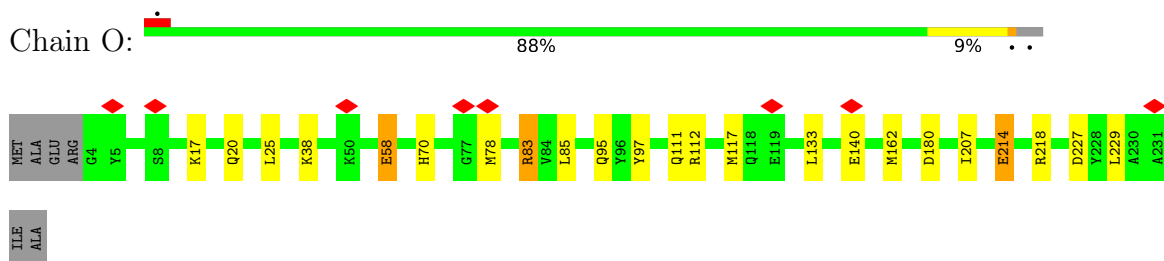
- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	g	264	2062	1323	336	388	15	0	0

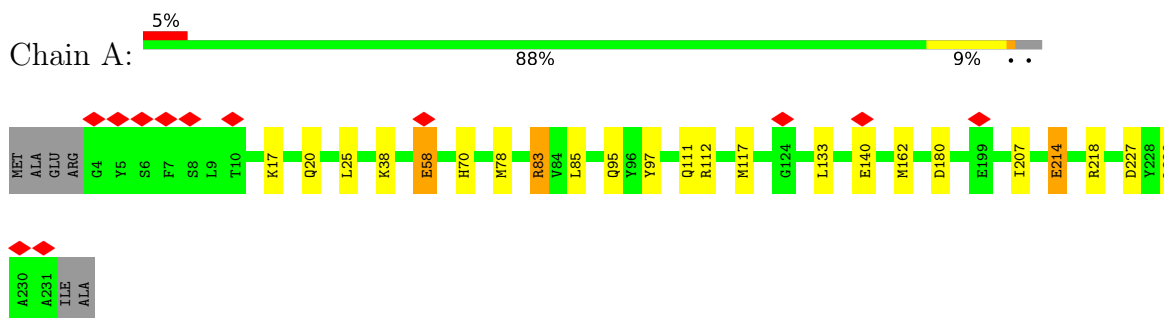
### 3 Residue-property plots [i](#)

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.

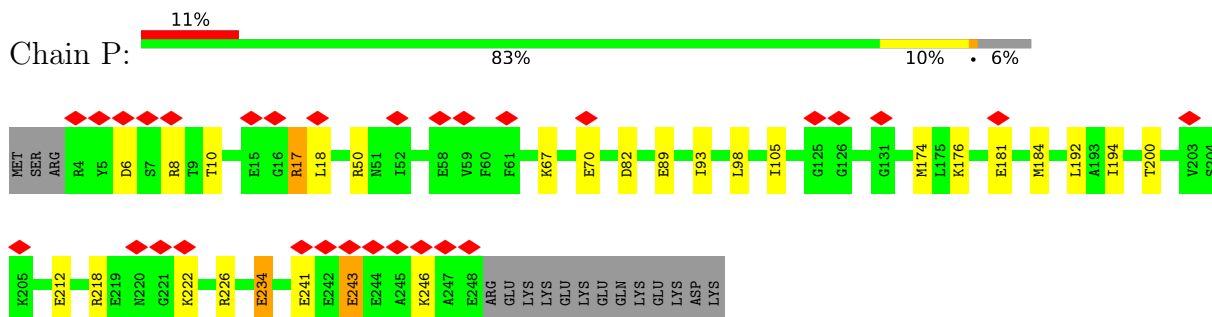
- Molecule 1: Proteasome subunit alpha type-2



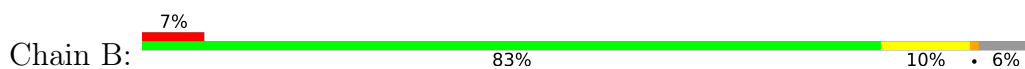
- Molecule 1: Proteasome subunit alpha type-2



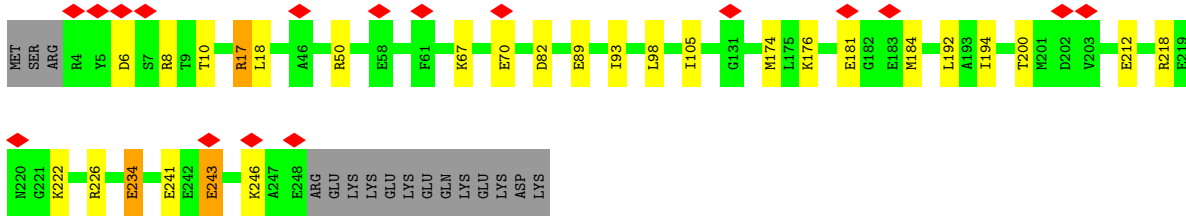
- Molecule 2: Proteasome subunit alpha type-4



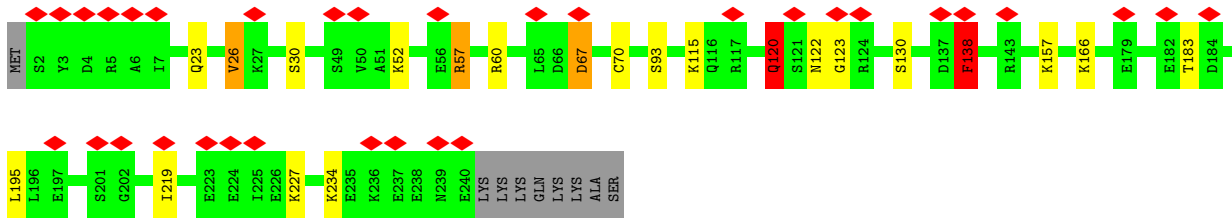
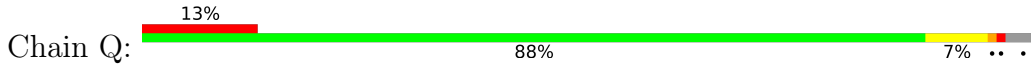
- Molecule 2: Proteasome subunit alpha type-4



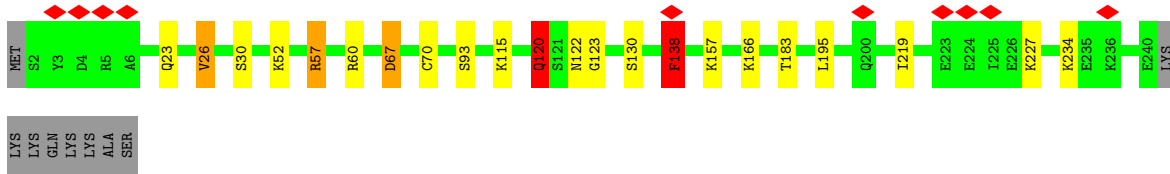
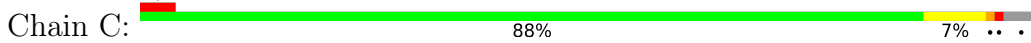




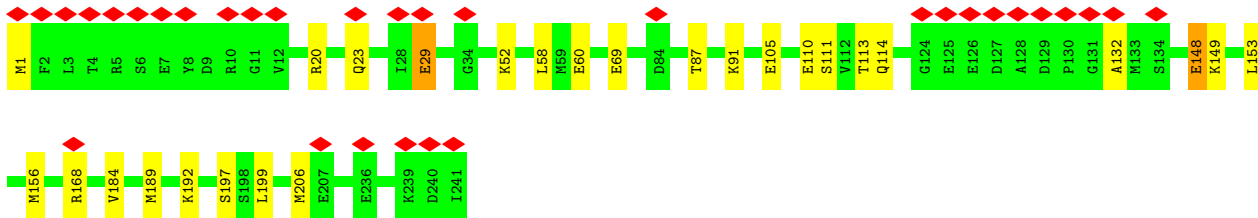
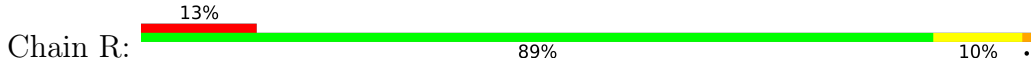
• Molecule 3: Proteasome subunit alpha type-7



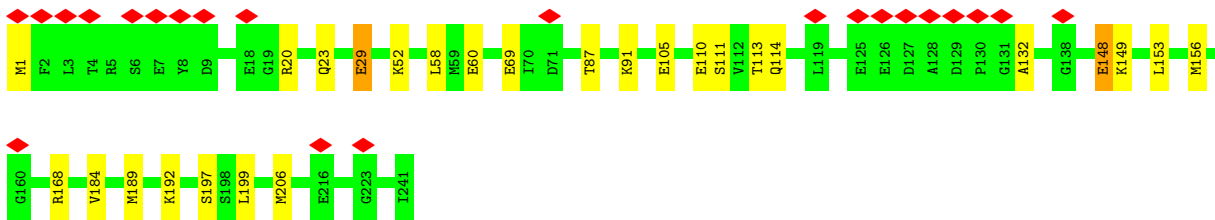
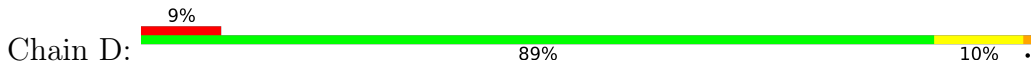
• Molecule 3: Proteasome subunit alpha type-7



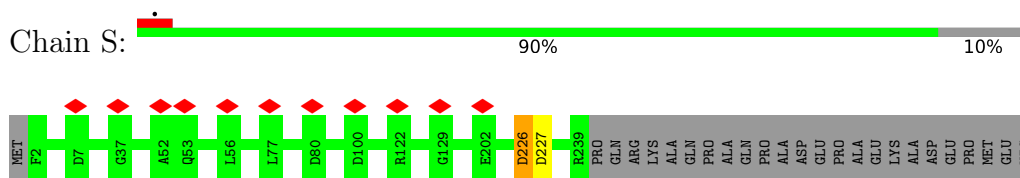
• Molecule 4: Proteasome subunit alpha type-5



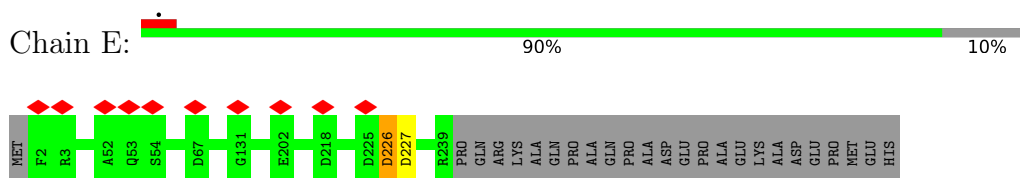
• Molecule 4: Proteasome subunit alpha type-5



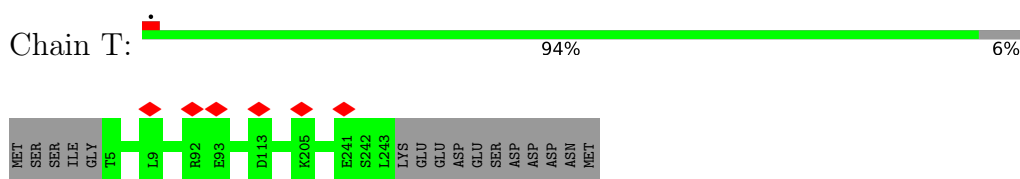
• Molecule 5: Proteasome subunit alpha type-1



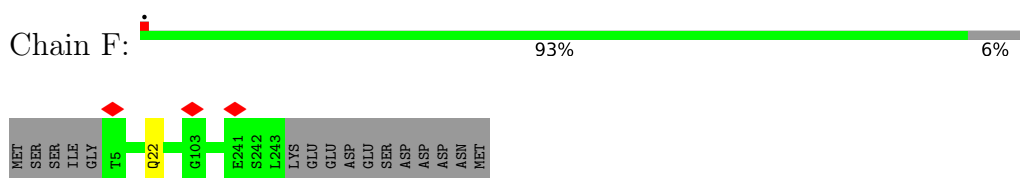
• Molecule 5: Proteasome subunit alpha type-1



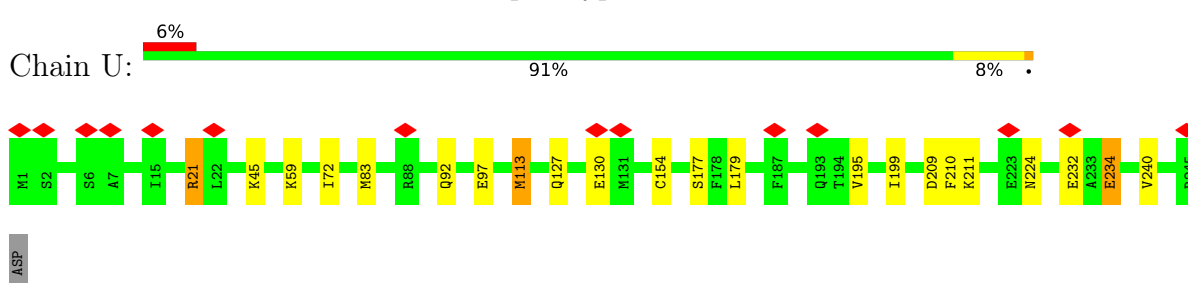
• Molecule 6: Proteasome subunit alpha type-3



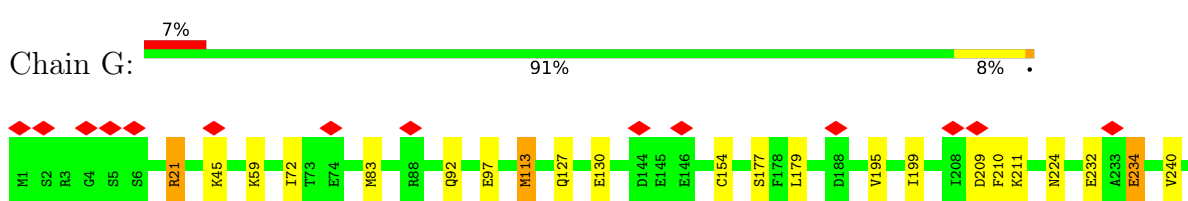
• Molecule 6: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-6

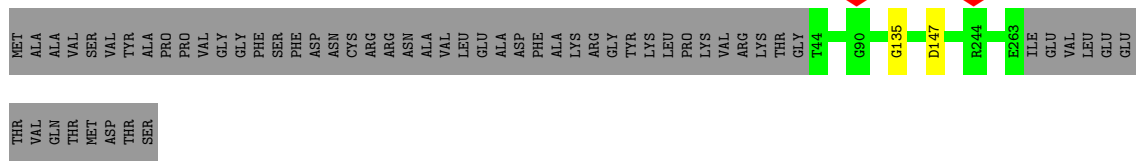
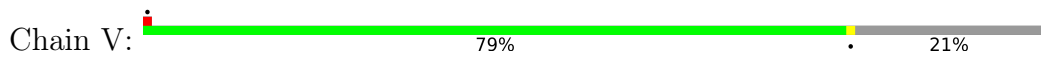


• Molecule 7: Proteasome subunit alpha type-6

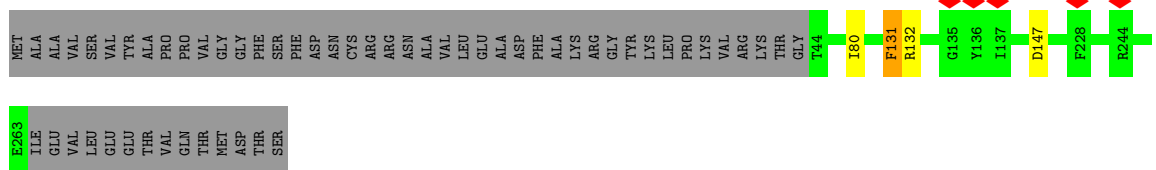
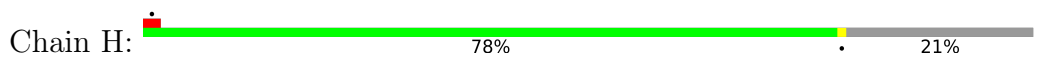




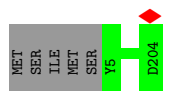
• Molecule 8: Proteasome subunit beta type-7



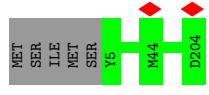
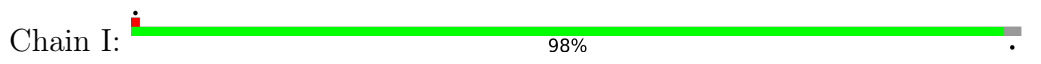
• Molecule 8: Proteasome subunit beta type-7



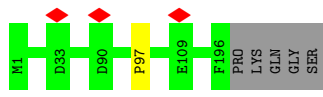
• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3

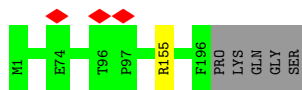


• Molecule 10: Proteasome subunit beta type-2



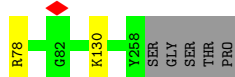
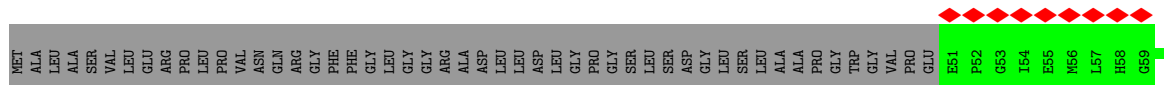
• Molecule 10: Proteasome subunit beta type-2





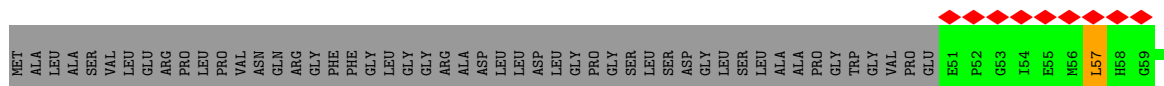
- Molecule 11: Proteasome subunit beta type-5

Chain Y: 78% 21%



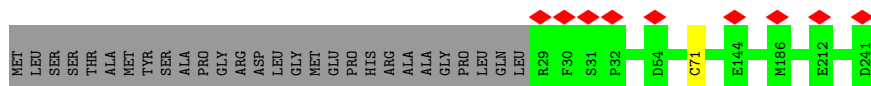
- Molecule 11: Proteasome subunit beta type-5

Chain K: 78% 21%



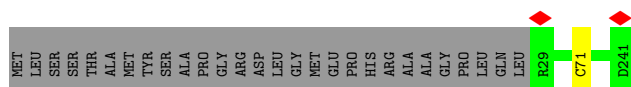
- Molecule 12: Proteasome subunit beta type-1

Chain Z: 88% 12%



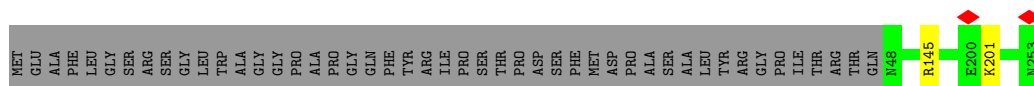
- Molecule 12: Proteasome subunit beta type-1

Chain L: 88% 12%

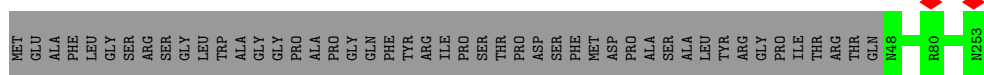
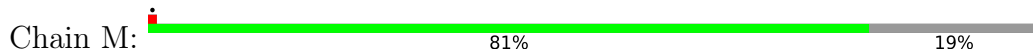


- Molecule 13: Proteasome subunit beta type-4

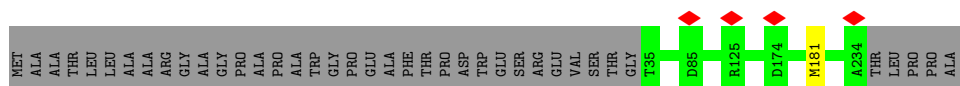
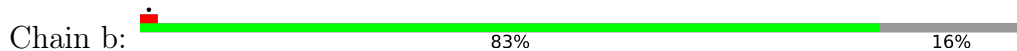
Chain a: 81% 19%



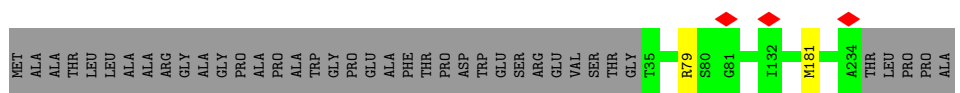
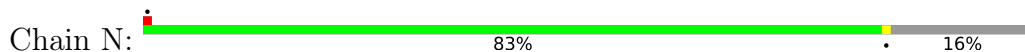
- Molecule 13: Proteasome subunit beta type-4



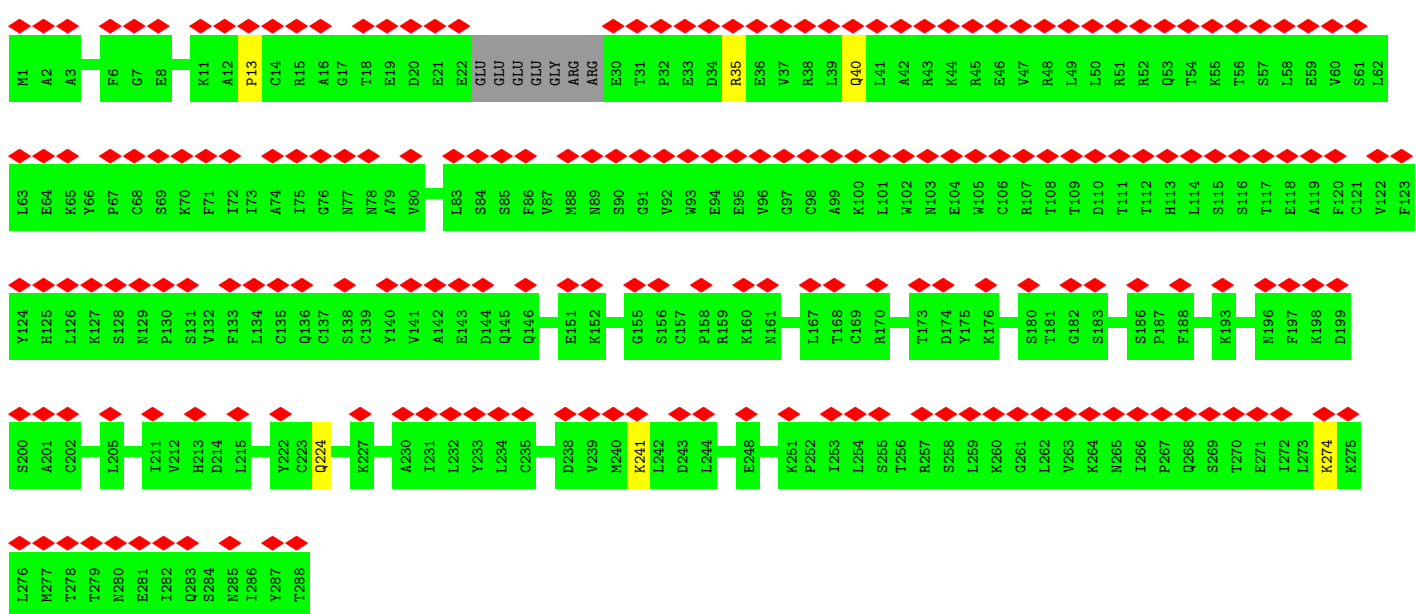
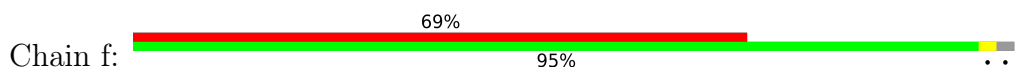
• Molecule 14: Proteasome subunit beta type-6



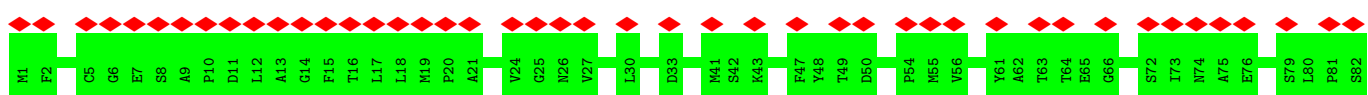
• Molecule 14: Proteasome subunit beta type-6

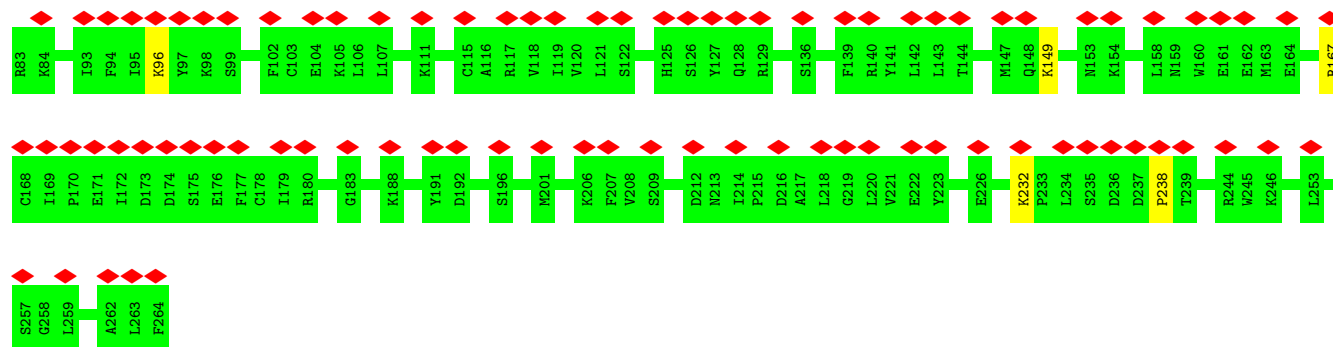


• Molecule 15: Proteasome assembly chaperone 1



• Molecule 16: Proteasome assembly chaperone 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4605	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.243	Depositor
Minimum map value	-0.612	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.328	Depositor
Map size (Å)	316.49997, 316.49997, 316.49997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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	0.40	0/1799	0.64	4/2442 (0.2%)
1	O	0.40	0/1799	0.64	4/2442 (0.2%)
2	B	0.43	0/1924	0.73	5/2602 (0.2%)
2	P	0.43	0/1924	0.73	5/2602 (0.2%)
3	C	0.39	0/1875	0.76	7/2540 (0.3%)
3	Q	0.39	0/1875	0.76	7/2540 (0.3%)
4	D	0.37	0/1869	0.65	1/2523 (0.0%)
4	R	0.37	0/1869	0.65	1/2523 (0.0%)
5	E	0.34	0/1896	0.51	0/2563
5	S	0.34	0/1896	0.53	0/2563
6	F	0.33	0/1896	0.47	0/2556
6	T	0.35	0/1896	0.50	0/2556
7	G	0.37	0/1927	0.65	4/2606 (0.2%)
7	U	0.37	0/1927	0.65	4/2606 (0.2%)
8	H	0.35	0/1688	0.58	0/2288
8	V	0.35	0/1688	0.53	0/2288
9	I	0.36	0/1608	0.54	0/2168
9	W	0.36	0/1608	0.52	0/2168
10	J	0.38	0/1620	0.50	0/2191
10	X	0.39	0/1620	0.52	0/2191
11	K	0.39	0/1673	0.52	1/2258 (0.0%)
11	Y	0.39	0/1673	0.53	0/2258
12	L	0.37	0/1677	0.51	0/2260
12	Z	0.36	0/1677	0.52	0/2260
13	M	0.36	0/1638	0.51	0/2216
13	a	0.38	0/1638	0.53	0/2216
14	N	0.38	0/1533	0.53	0/2074
14	b	0.36	0/1533	0.52	0/2074
15	f	0.29	0/2285	0.54	0/3097
16	g	0.29	0/2108	0.52	1/2858 (0.0%)
All	All	0.37	0/53639	0.59	44/72529 (0.1%)

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	A	0	1
1	O	0	1
2	B	0	1
2	P	0	1
3	C	0	3
3	Q	0	3
4	D	0	3
4	R	0	3
5	E	0	1
5	S	0	1
6	F	0	1
8	H	0	1
8	V	0	1
10	X	0	1
11	K	0	1
All	All	0	23

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	17	ARG	NE-CZ-NH1	-9.90	115.35	120.30
2	P	17	ARG	NE-CZ-NH1	-9.83	115.39	120.30
7	U	21	ARG	CG-CD-NE	9.43	131.61	111.80
7	G	21	ARG	CG-CD-NE	9.41	131.56	111.80
7	G	210	PHE	C-N-CA	-9.11	98.93	121.70
7	U	210	PHE	C-N-CA	-9.10	98.95	121.70
2	P	234	GLU	CA-CB-CG	8.17	131.37	113.40
2	B	234	GLU	CA-CB-CG	8.16	131.35	113.40
3	Q	57	ARG	NE-CZ-NH2	-7.81	116.40	120.30
3	C	57	ARG	NE-CZ-NH2	-7.74	116.43	120.30
3	Q	67	ASP	CB-CG-OD1	7.32	124.89	118.30
3	C	67	ASP	CB-CG-OD1	7.29	124.86	118.30
2	B	17	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	O	83	ARG	CG-CD-NE	6.85	126.18	111.80
2	P	17	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	83	ARG	CG-CD-NE	6.81	126.11	111.80
3	Q	120	GLN	CA-CB-CG	6.72	128.18	113.40
3	C	120	GLN	CA-CB-CG	6.71	128.17	113.40
3	C	138	PHE	CB-CG-CD1	6.69	125.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	138	PHE	CB-CG-CD1	6.67	125.47	120.80
2	P	243	GLU	C-N-CA	-6.40	105.69	121.70
2	B	243	GLU	C-N-CA	-6.39	105.71	121.70
1	O	83	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	214	GLU	CA-CB-CG	6.11	126.84	113.40
1	O	214	GLU	CA-CB-CG	6.10	126.81	113.40
1	A	83	ARG	NE-CZ-NH2	6.08	123.34	120.30
11	K	57	LEU	CA-CB-CG	5.85	128.75	115.30
3	Q	138	PHE	CB-CG-CD2	-5.83	116.72	120.80
3	C	138	PHE	CB-CG-CD2	-5.83	116.72	120.80
7	G	113	MET	CG-SD-CE	5.67	109.27	100.20
7	U	113	MET	CG-SD-CE	5.66	109.26	100.20
3	Q	138	PHE	N-CA-CB	-5.43	100.83	110.60
3	C	138	PHE	N-CA-CB	-5.40	100.89	110.60
1	A	83	ARG	CD-NE-CZ	5.21	130.89	123.60
7	G	234	GLU	CA-CB-CG	5.20	124.85	113.40
16	g	167	ARG	CA-CB-CG	5.20	124.84	113.40
7	U	234	GLU	CA-CB-CG	5.18	124.81	113.40
4	D	168	ARG	CB-CG-CD	5.17	125.06	111.60
4	R	168	ARG	CB-CG-CD	5.17	125.04	111.60
1	O	83	ARG	CD-NE-CZ	5.14	130.80	123.60
2	B	243	GLU	CA-CB-CG	5.09	124.60	113.40
2	P	243	GLU	CA-CB-CG	5.09	124.59	113.40
3	Q	138	PHE	CB-CA-C	5.02	120.43	110.40
3	C	138	PHE	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	GLU	Peptide
2	B	212	GLU	Peptide
3	C	120	GLN	Peptide
3	C	122	ASN	Peptide
3	C	26	VAL	Peptide
4	D	132	ALA	Peptide
4	D	148	GLU	Peptide
4	D	29	GLU	Peptide
5	E	226	ASP	Peptide
6	F	22	GLN	Peptide
8	H	131	PHE	Peptide
11	K	57	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	O	58	GLU	Peptide
2	P	212	GLU	Peptide
3	Q	120	GLN	Peptide
3	Q	122	ASN	Peptide
3	Q	26	VAL	Peptide
4	R	132	ALA	Peptide
4	R	148	GLU	Peptide
4	R	29	GLU	Peptide
5	S	226	ASP	Peptide
8	V	135	GLY	Peptide
10	X	97	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	A	226/234 (97%)	206 (91%)	20 (9%)	0	100	100
1	O	226/234 (97%)	207 (92%)	19 (8%)	0	100	100
2	B	243/261 (93%)	223 (92%)	20 (8%)	0	100	100
2	P	243/261 (93%)	223 (92%)	20 (8%)	0	100	100
3	C	237/248 (96%)	198 (84%)	37 (16%)	2 (1%)	16	49
3	Q	237/248 (96%)	198 (84%)	37 (16%)	2 (1%)	16	49
4	D	239/241 (99%)	206 (86%)	33 (14%)	0	100	100
4	R	239/241 (99%)	206 (86%)	33 (14%)	0	100	100
5	E	237/263 (90%)	215 (91%)	20 (8%)	2 (1%)	16	49
5	S	237/263 (90%)	215 (91%)	20 (8%)	2 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	238/255 (93%)	226 (95%)	12 (5%)	0	100	100
6	T	238/255 (93%)	225 (94%)	13 (6%)	0	100	100
7	G	243/246 (99%)	218 (90%)	24 (10%)	1 (0%)	30	63
7	U	243/246 (99%)	218 (90%)	24 (10%)	1 (0%)	30	63
8	H	220/277 (79%)	190 (86%)	27 (12%)	3 (1%)	9	37
8	V	220/277 (79%)	202 (92%)	18 (8%)	0	100	100
9	I	200/205 (98%)	186 (93%)	14 (7%)	0	100	100
9	W	200/205 (98%)	185 (92%)	15 (8%)	0	100	100
10	J	196/201 (98%)	185 (94%)	11 (6%)	0	100	100
10	X	196/201 (98%)	183 (93%)	13 (7%)	0	100	100
11	K	209/263 (80%)	181 (87%)	27 (13%)	1 (0%)	25	58
11	Y	209/263 (80%)	188 (90%)	21 (10%)	0	100	100
12	L	212/241 (88%)	202 (95%)	10 (5%)	0	100	100
12	Z	212/241 (88%)	198 (93%)	14 (7%)	0	100	100
13	M	205/253 (81%)	195 (95%)	10 (5%)	0	100	100
13	a	205/253 (81%)	192 (94%)	13 (6%)	0	100	100
14	N	199/239 (83%)	179 (90%)	20 (10%)	0	100	100
14	b	199/239 (83%)	181 (91%)	18 (9%)	0	100	100
15	f	277/288 (96%)	245 (88%)	31 (11%)	1 (0%)	30	63
16	g	262/264 (99%)	233 (89%)	28 (11%)	1 (0%)	30	63
All	All	6747/7406 (91%)	6109 (90%)	622 (9%)	16 (0%)	45	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	S	227	ASP
5	E	227	ASP
8	H	80	ILE
8	H	132	ARG
3	Q	138	PHE
5	S	226	ASP
3	C	138	PHE
5	E	226	ASP
8	H	131	PHE
11	K	81	ALA

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Mol	Chain	Res	Type
15	f	13	PRO
7	U	195	VAL
16	g	238	PRO
7	G	195	VAL
3	Q	123	GLY
3	C	123	GLY

### 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	182/191 (95%)	159 (87%)	23 (13%)	3	19
1	O	182/191 (95%)	159 (87%)	23 (13%)	3	19
2	B	197/221 (89%)	170 (86%)	27 (14%)	3	17
2	P	197/221 (89%)	170 (86%)	27 (14%)	3	17
3	C	193/211 (92%)	173 (90%)	20 (10%)	5	23
3	Q	193/211 (92%)	173 (90%)	20 (10%)	5	23
4	D	200/203 (98%)	175 (88%)	25 (12%)	3	19
4	R	200/203 (98%)	175 (88%)	25 (12%)	3	19
5	E	200/224 (89%)	200 (100%)	0	100	100
5	S	200/224 (89%)	200 (100%)	0	100	100
6	F	193/212 (91%)	193 (100%)	0	100	100
6	T	193/212 (91%)	193 (100%)	0	100	100
7	G	205/210 (98%)	185 (90%)	20 (10%)	6	25
7	U	205/210 (98%)	185 (90%)	20 (10%)	6	25
8	H	180/228 (79%)	178 (99%)	2 (1%)	70	79
8	V	180/228 (79%)	178 (99%)	2 (1%)	70	79
9	I	170/174 (98%)	170 (100%)	0	100	100
9	W	170/174 (98%)	170 (100%)	0	100	100
10	J	169/171 (99%)	168 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	X	169/171 (99%)	169 (100%)	0	100	100
11	K	164/202 (81%)	162 (99%)	2 (1%)	67	77
11	Y	164/202 (81%)	162 (99%)	2 (1%)	67	77
12	L	176/199 (88%)	174 (99%)	2 (1%)	70	79
12	Z	176/199 (88%)	174 (99%)	2 (1%)	70	79
13	M	170/206 (82%)	170 (100%)	0	100	100
13	a	170/206 (82%)	168 (99%)	2 (1%)	67	77
14	N	156/181 (86%)	153 (98%)	3 (2%)	52	69
14	b	156/181 (86%)	154 (99%)	2 (1%)	65	76
15	f	256/262 (98%)	251 (98%)	5 (2%)	50	68
16	g	237/237 (100%)	234 (99%)	3 (1%)	65	76
All	All	5603/6165 (91%)	5345 (95%)	258 (5%)	26	47

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	17	LYS
1	O	20	GLN
1	O	25	LEU
1	O	38	LYS
1	O	58	GLU
1	O	70	HIS
1	O	78	MET
1	O	83	ARG
1	O	85	LEU
1	O	95	GLN
1	O	97	TYR
1	O	111	GLN
1	O	112	ARG
1	O	117	MET
1	O	133	LEU
1	O	140	GLU
1	O	162	MET
1	O	180	ASP
1	O	207	ILE
1	O	214	GLU
1	O	218	ARG
1	O	227	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	229	LEU
2	P	6	ASP
2	P	8	ARG
2	P	10	THR
2	P	17	ARG
2	P	18	LEU
2	P	50	ARG
2	P	67	LYS
2	P	70	GLU
2	P	82	ASP
2	P	89	GLU
2	P	93	ILE
2	P	98	LEU
2	P	105	ILE
2	P	174	MET
2	P	176	LYS
2	P	181	GLU
2	P	184	MET
2	P	192	LEU
2	P	194	ILE
2	P	200	THR
2	P	218	ARG
2	P	222	LYS
2	P	226	ARG
2	P	234	GLU
2	P	241	GLU
2	P	243	GLU
2	P	246	LYS
3	Q	23	GLN
3	Q	26	VAL
3	Q	30	SER
3	Q	52	LYS
3	Q	57	ARG
3	Q	60	ARG
3	Q	67	ASP
3	Q	70	CYS
3	Q	93	SER
3	Q	115	LYS
3	Q	120	GLN
3	Q	130	SER
3	Q	138	PHE
3	Q	157	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	166	LYS
3	Q	183	THR
3	Q	195	LEU
3	Q	219	ILE
3	Q	227	LYS
3	Q	234	LYS
4	R	1	MET
4	R	20	ARG
4	R	23	GLN
4	R	29	GLU
4	R	52	LYS
4	R	58	LEU
4	R	60	GLU
4	R	69	GLU
4	R	87	THR
4	R	91	LYS
4	R	105	GLU
4	R	110	GLU
4	R	111	SER
4	R	113	THR
4	R	114	GLN
4	R	148	GLU
4	R	149	LYS
4	R	153	LEU
4	R	156	MET
4	R	184	VAL
4	R	189	MET
4	R	192	LYS
4	R	197	SER
4	R	199	LEU
4	R	206	MET
7	U	21	ARG
7	U	45	LYS
7	U	59	LYS
7	U	72	ILE
7	U	83	MET
7	U	92	GLN
7	U	97	GLU
7	U	113	MET
7	U	127	GLN
7	U	130	GLU
7	U	154	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	U	177	SER
7	U	179	LEU
7	U	199	ILE
7	U	209	ASP
7	U	211	LYS
7	U	224	ASN
7	U	232	GLU
7	U	234	GLU
7	U	240	VAL
8	V	147[A]	ASP
8	V	147[B]	ASP
11	Y	78	ARG
11	Y	130	LYS
12	Z	71[A]	CYS
12	Z	71[B]	CYS
13	a	145	ARG
13	a	201	LYS
14	b	181[A]	MET
14	b	181[B]	MET
15	f	35	ARG
15	f	40	GLN
15	f	224	GLN
15	f	241	LYS
15	f	274	LYS
16	g	96	LYS
16	g	149	LYS
16	g	232	LYS
1	A	17	LYS
1	A	20	GLN
1	A	25	LEU
1	A	38	LYS
1	A	58	GLU
1	A	70	HIS
1	A	78	MET
1	A	83	ARG
1	A	85	LEU
1	A	95	GLN
1	A	97	TYR
1	A	111	GLN
1	A	112	ARG
1	A	117	MET
1	A	133	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	140	GLU
1	A	162	MET
1	A	180	ASP
1	A	207	ILE
1	A	214	GLU
1	A	218	ARG
1	A	227	ASP
1	A	229	LEU
2	B	6	ASP
2	B	8	ARG
2	B	10	THR
2	B	17	ARG
2	B	18	LEU
2	B	50	ARG
2	B	67	LYS
2	B	70	GLU
2	B	82	ASP
2	B	89	GLU
2	B	93	ILE
2	B	98	LEU
2	B	105	ILE
2	B	174	MET
2	B	176	LYS
2	B	181	GLU
2	B	184	MET
2	B	192	LEU
2	B	194	ILE
2	B	200	THR
2	B	218	ARG
2	B	222	LYS
2	B	226	ARG
2	B	234	GLU
2	B	241	GLU
2	B	243	GLU
2	B	246	LYS
3	C	23	GLN
3	C	26	VAL
3	C	30	SER
3	C	52	LYS
3	C	57	ARG
3	C	60	ARG
3	C	67	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	70	CYS
3	C	93	SER
3	C	115	LYS
3	C	120	GLN
3	C	130	SER
3	C	138	PHE
3	C	157	LYS
3	C	166	LYS
3	C	183	THR
3	C	195	LEU
3	C	219	ILE
3	C	227	LYS
3	C	234	LYS
4	D	1	MET
4	D	20	ARG
4	D	23	GLN
4	D	29	GLU
4	D	52	LYS
4	D	58	LEU
4	D	60	GLU
4	D	69	GLU
4	D	87	THR
4	D	91	LYS
4	D	105	GLU
4	D	110	GLU
4	D	111	SER
4	D	113	THR
4	D	114	GLN
4	D	148	GLU
4	D	149	LYS
4	D	153	LEU
4	D	156	MET
4	D	184	VAL
4	D	189	MET
4	D	192	LYS
4	D	197	SER
4	D	199	LEU
4	D	206	MET
7	G	21	ARG
7	G	45	LYS
7	G	59	LYS
7	G	72	ILE

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Mol	Chain	Res	Type
7	G	83	MET
7	G	92	GLN
7	G	97	GLU
7	G	113	MET
7	G	127	GLN
7	G	130	GLU
7	G	154	CYS
7	G	177	SER
7	G	179	LEU
7	G	199	ILE
7	G	209	ASP
7	G	211	LYS
7	G	224	ASN
7	G	232	GLU
7	G	234	GLU
7	G	240	VAL
8	H	147[A]	ASP
8	H	147[B]	ASP
10	J	155	ARG
11	K	78	ARG
11	K	80	THR
12	L	71[A]	CYS
12	L	71[B]	CYS
14	N	79	ARG
14	N	181[A]	MET
14	N	181[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	139	ASN
1	O	165	ASN
1	O	168	ASN
2	P	240	HIS
4	R	99	HIS
5	S	146	GLN
8	V	100	GLN
9	W	92	ASN
9	W	168	GLN
11	Y	210	GLN
1	A	139	ASN
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	168	ASN
2	B	240	HIS
4	D	97	GLN
4	D	99	HIS
5	E	8	ASN
5	E	65	HIS
5	E	146	GLN
8	H	208	ASN
9	I	92	ASN
10	J	27	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.

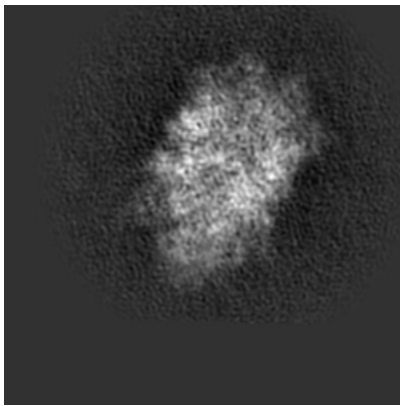
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39334. These allow visual inspection of the internal detail of the map and identification of artifacts.

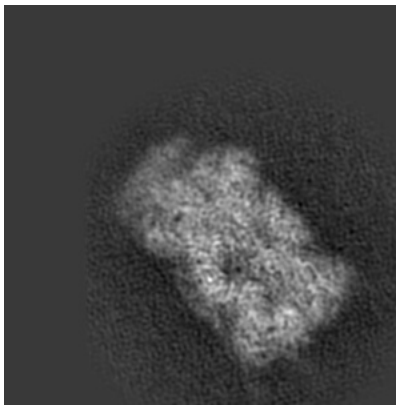
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

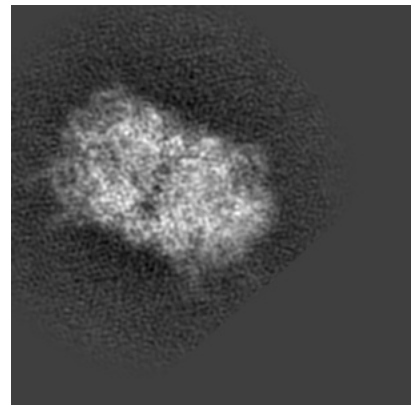
#### 6.1.1 Primary map



X

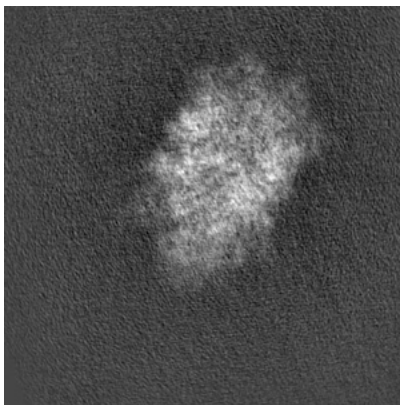


Y

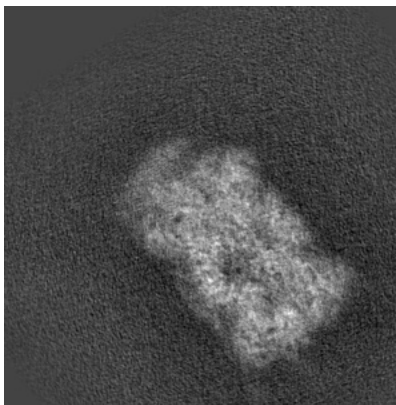


Z

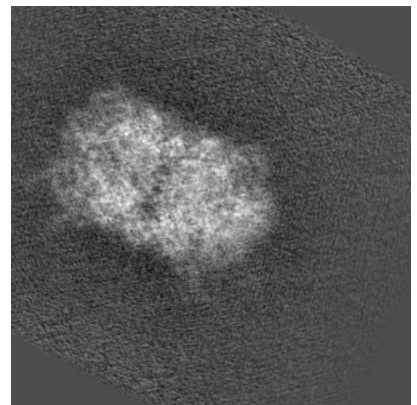
#### 6.1.2 Raw map



X



Y

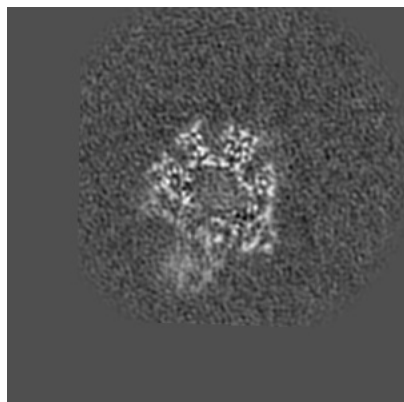


Z

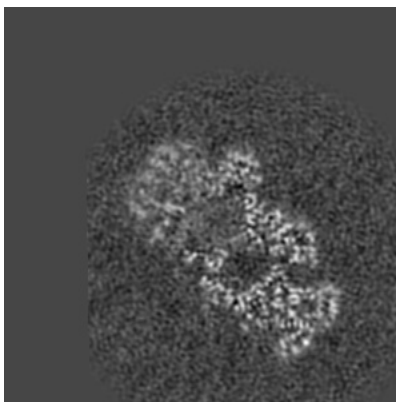
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

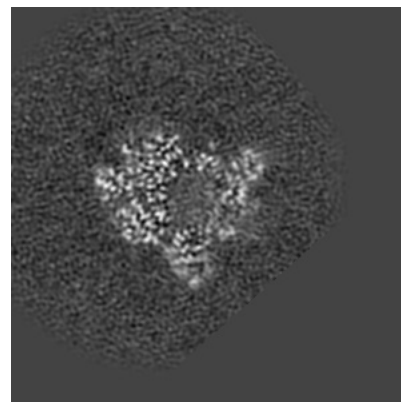
### 6.2.1 Primary map



X Index: 150

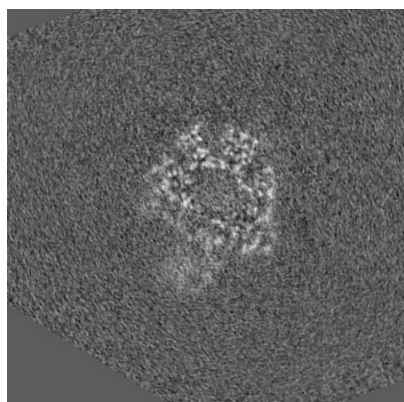


Y Index: 150

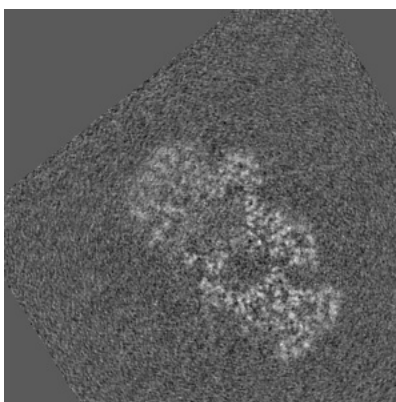


Z Index: 150

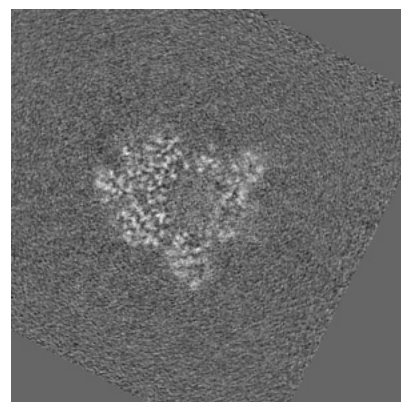
### 6.2.2 Raw map



X Index: 150



Y Index: 150

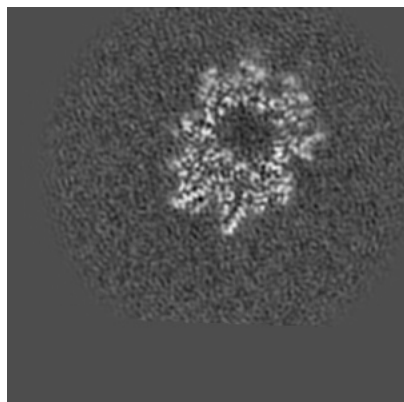


Z Index: 150

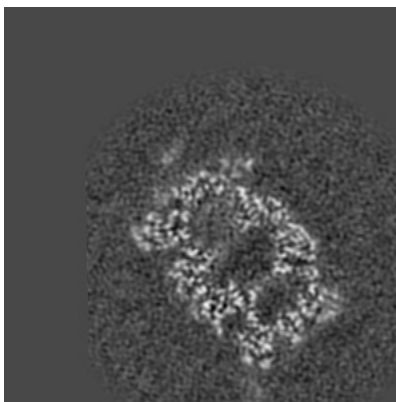
The images above show central slices of the map in three orthogonal directions.

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

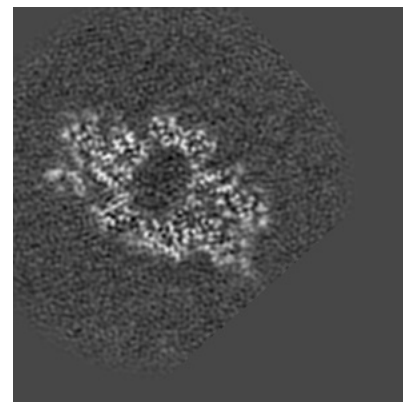
### 6.3.1 Primary map



X Index: 87

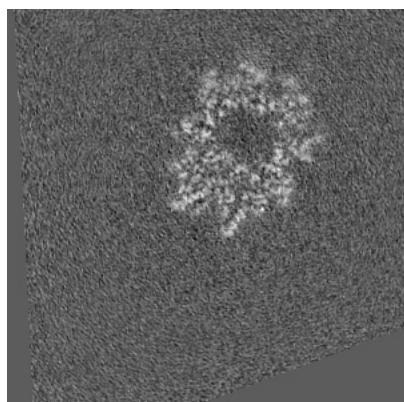


Y Index: 164

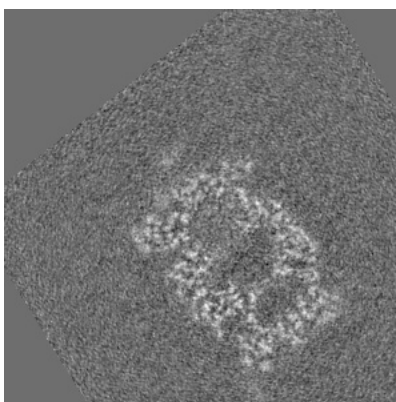


Z Index: 179

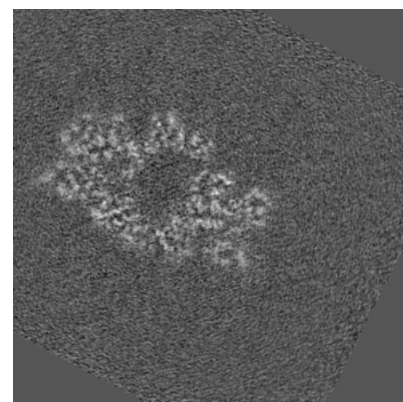
### 6.3.2 Raw map



X Index: 87



Y Index: 164



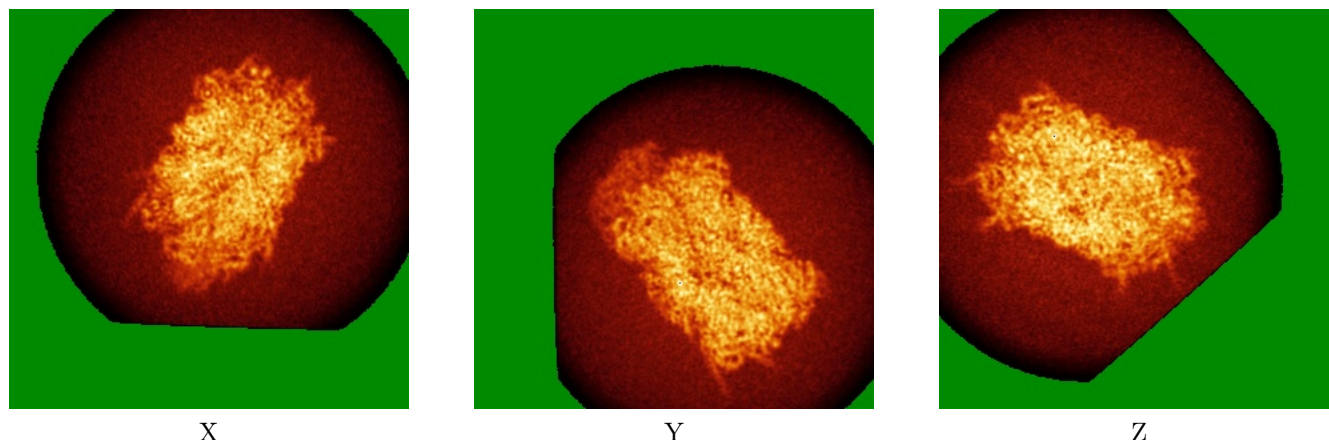
Z Index: 182

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

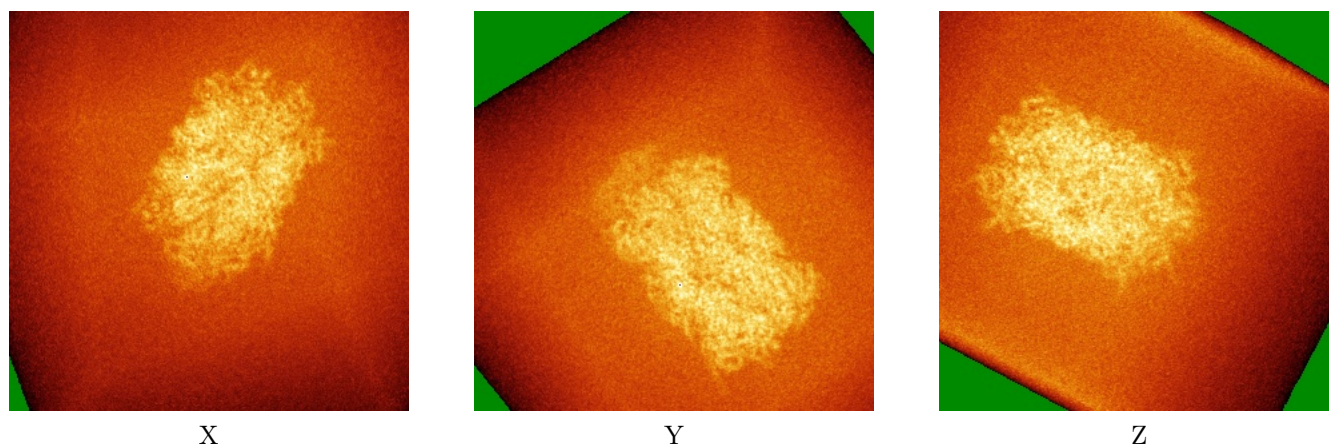


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 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.

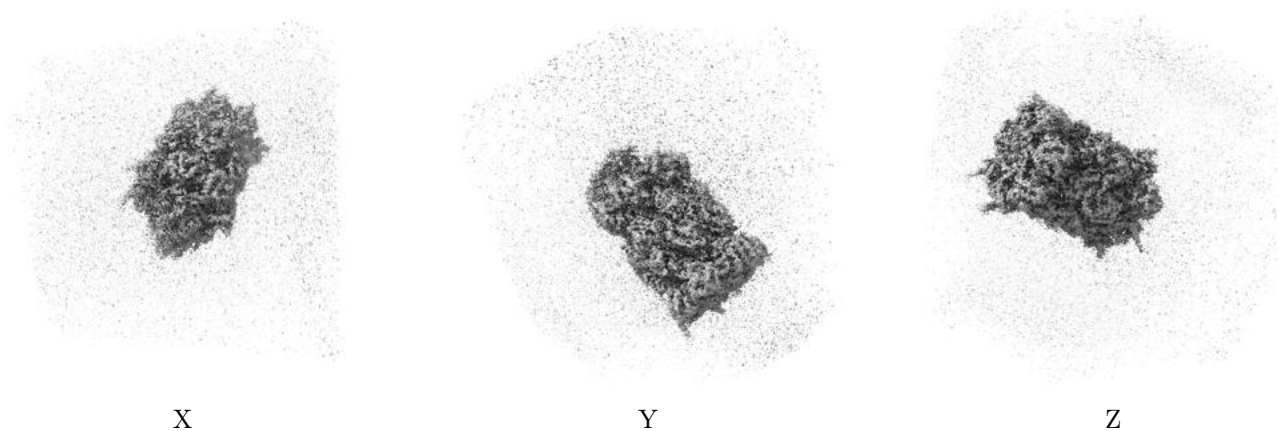
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.328. 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.

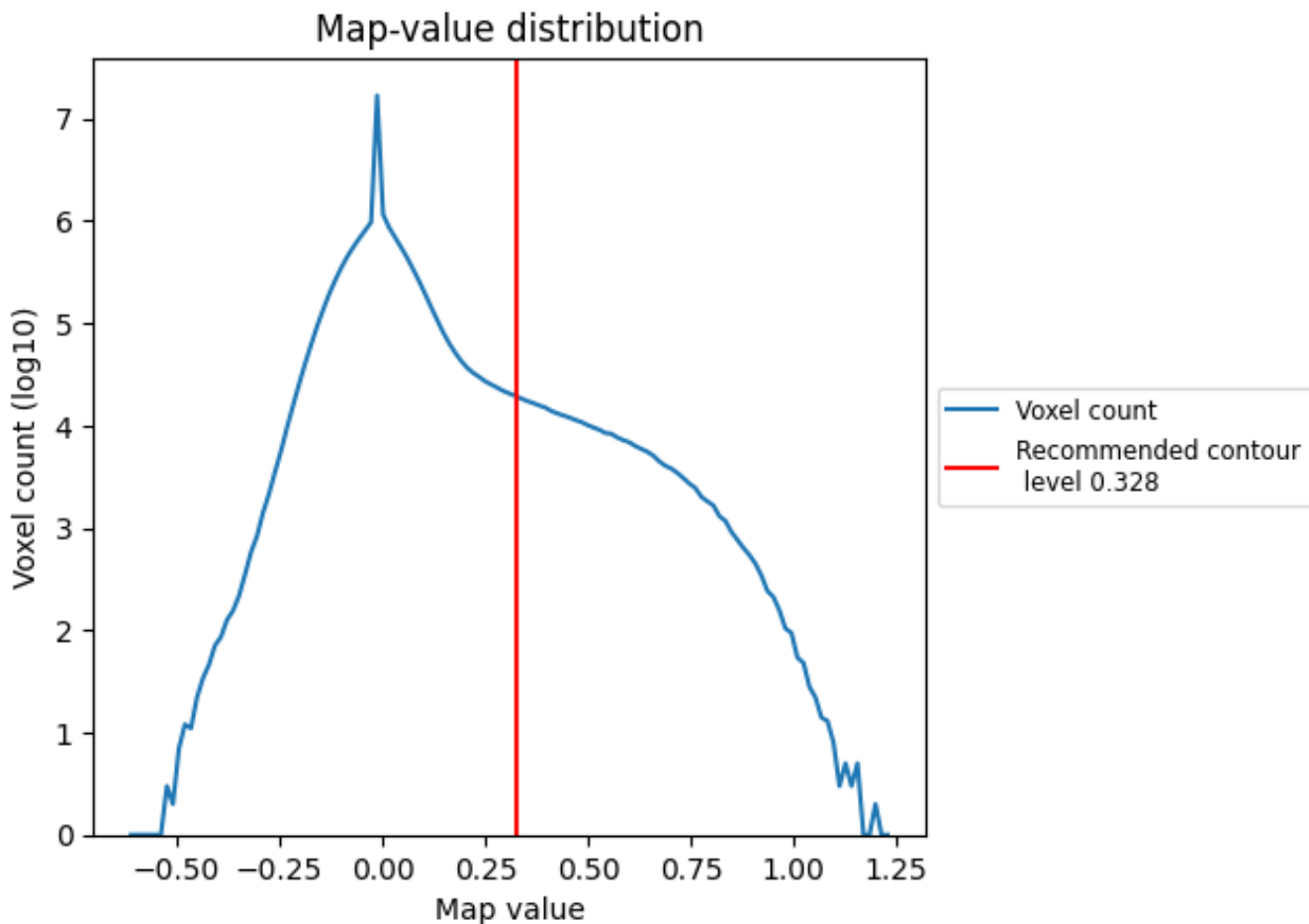
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

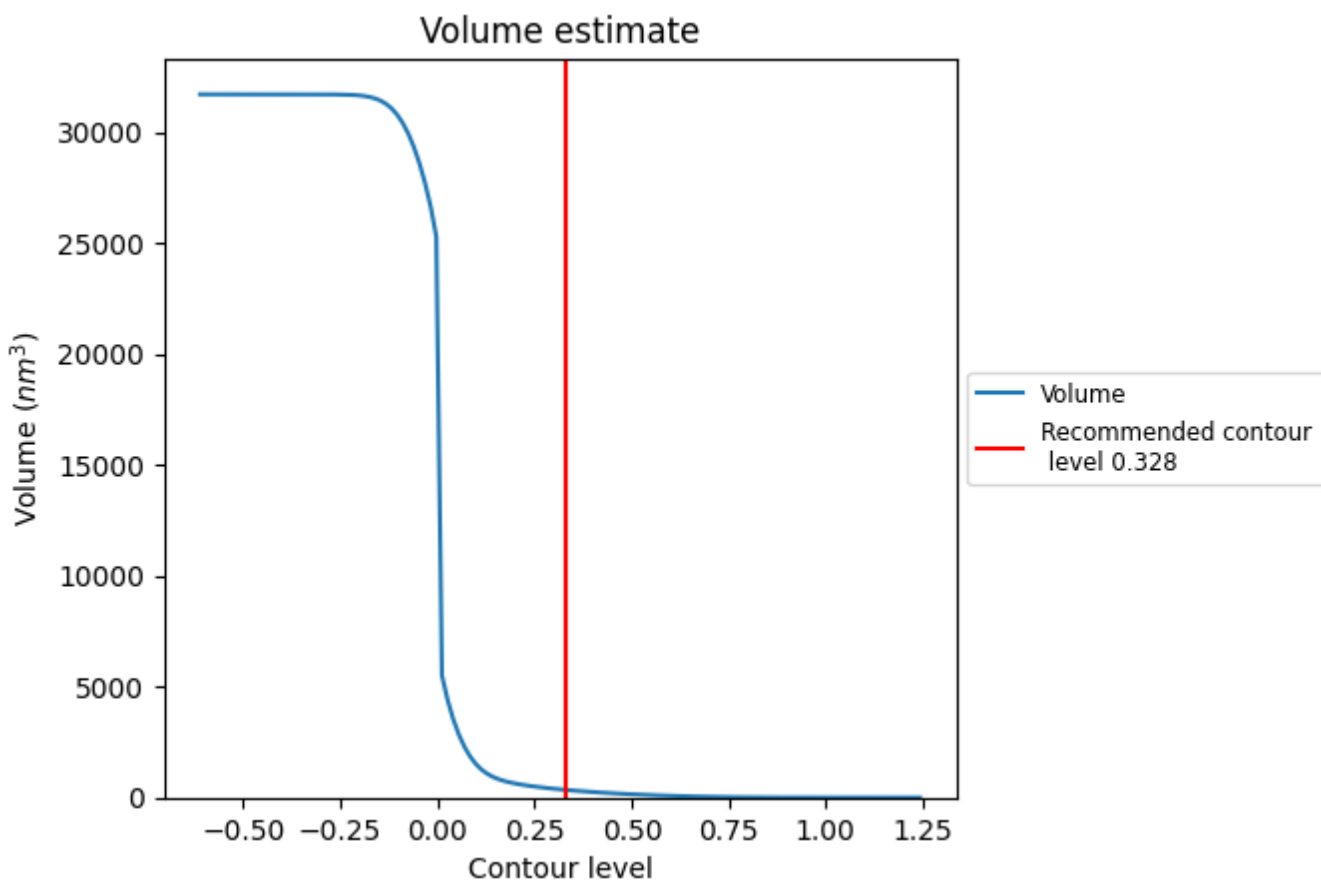
This section contains the results of statistical analysis of the map.

### 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.

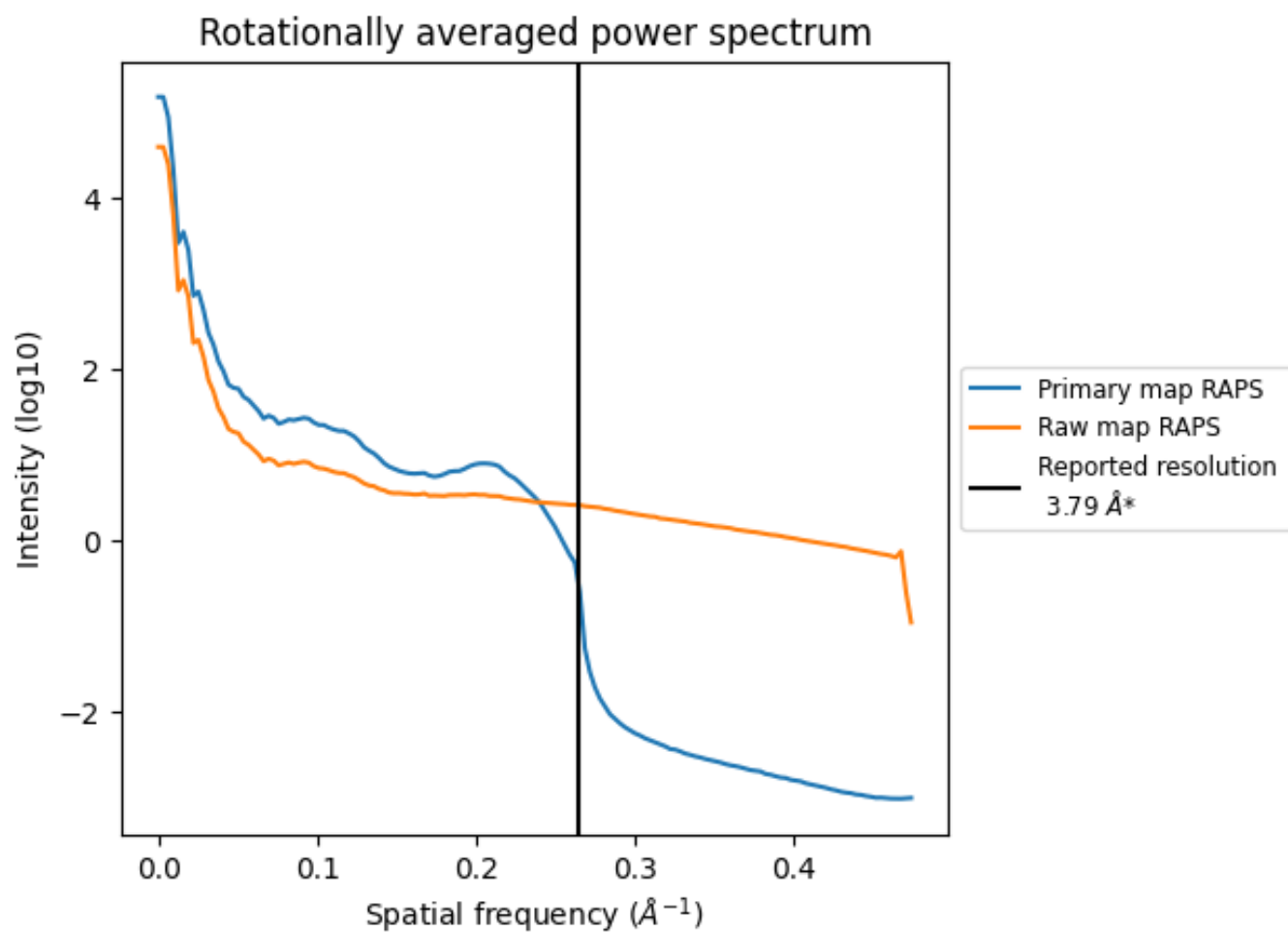
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm<sup>3</sup>; this corresponds to an approximate mass of 315 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

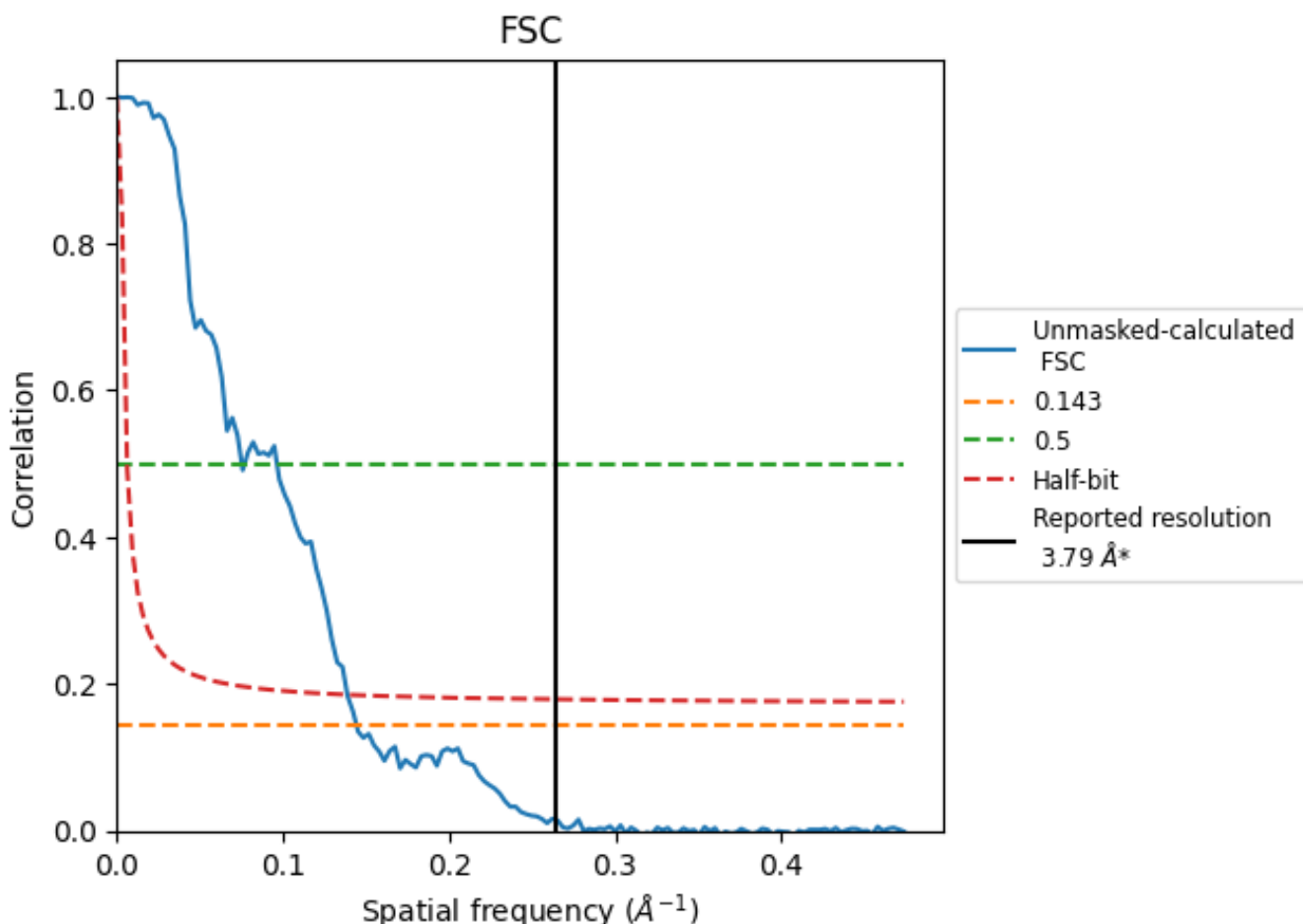


\*Reported resolution corresponds to spatial frequency of 0.264 Å<sup>-1</sup>

## 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 0.264 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

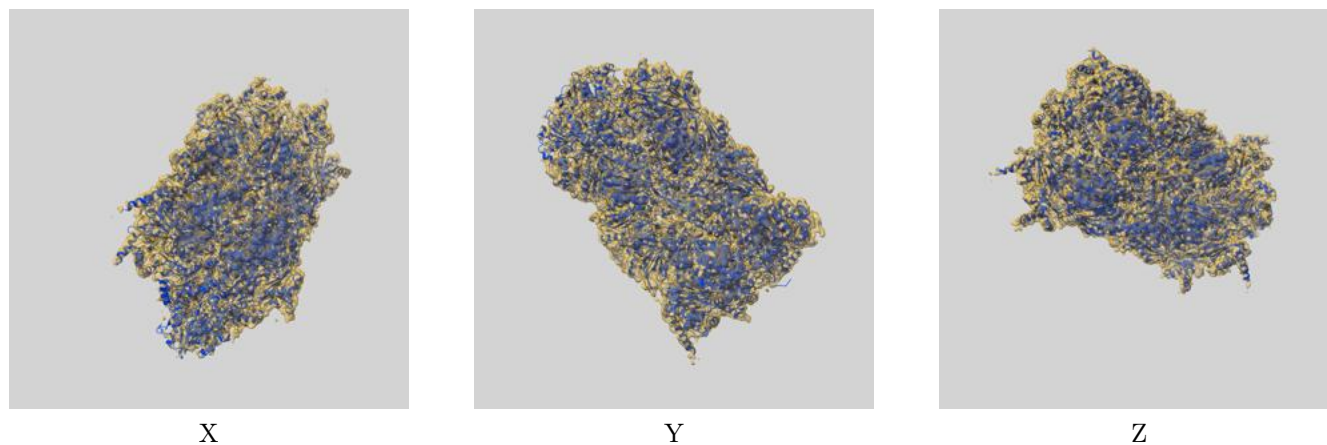
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.93	13.30	7.20

\*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 6.93 differs from the reported value 3.79 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-39334 and PDB model 8YIZ. Per-residue inclusion information can be found in section 3 on page 8.

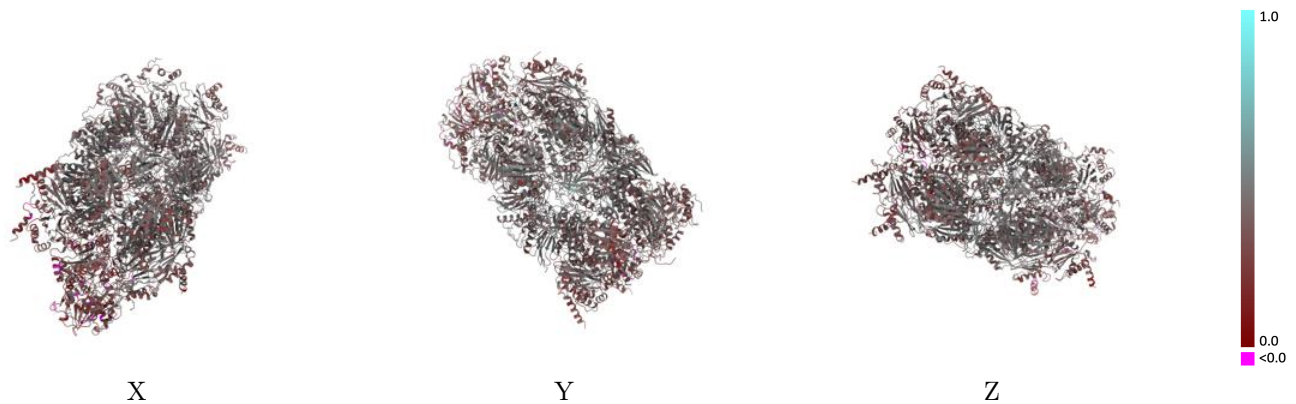
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.328 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.

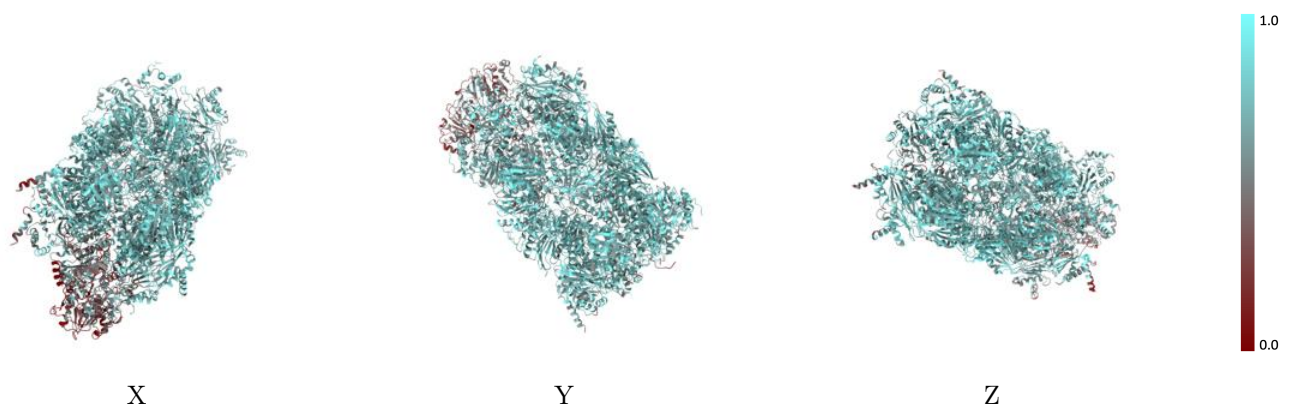


## 9.2 Q-score mapped to coordinate model [i](#)



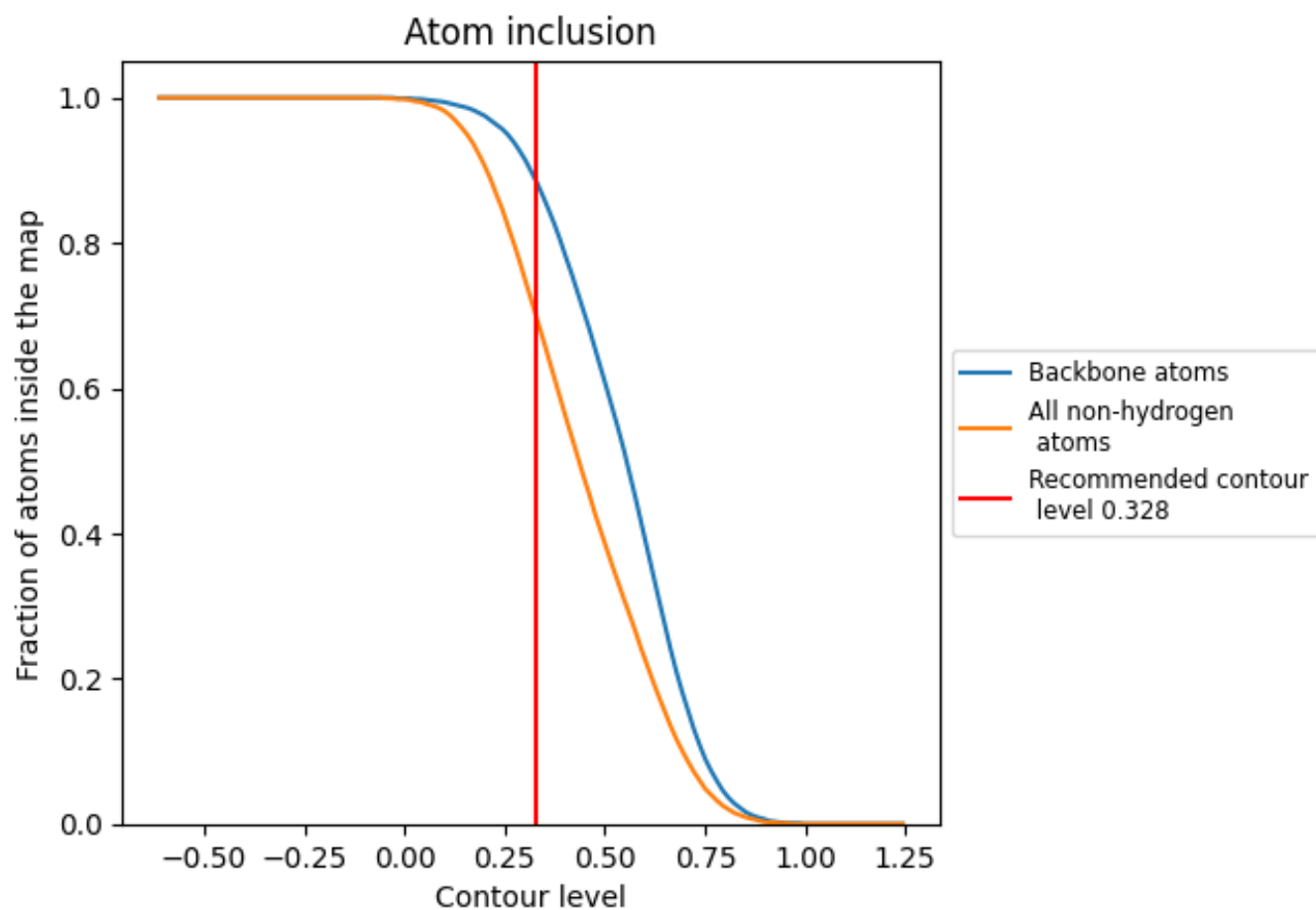
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.328).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 70% 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 (0.328) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.3930
A	 0.7280	 0.3640
B	 0.7100	 0.3790
C	 0.7220	 0.3740
D	 0.6860	 0.3760
E	 0.7540	 0.3960
F	 0.7480	 0.4080
G	 0.7240	 0.3440
H	 0.7740	 0.4240
I	 0.7590	 0.4400
J	 0.7740	 0.4330
K	 0.7750	 0.4300
L	 0.7590	 0.4350
M	 0.7830	 0.4370
N	 0.7720	 0.4350
O	 0.7300	 0.3860
P	 0.6590	 0.3500
Q	 0.6270	 0.3200
R	 0.6190	 0.3380
S	 0.7140	 0.4020
T	 0.7470	 0.3940
U	 0.7160	 0.3810
V	 0.7580	 0.4260
W	 0.7630	 0.4480
X	 0.7650	 0.4430
Y	 0.7540	 0.4260
Z	 0.7560	 0.4310
a	 0.7760	 0.4310
b	 0.7680	 0.4350
f	 0.2570	 0.2910
g	 0.3890	 0.3150

