wwPDB EM Validation Summary Report

Jul 8, 2024 – 07:02 am BST

PDB ID	:	7QVE
EMDB ID	:	EMD-14175
Title	:	Spinach 20S proteasome
Authors	:	Kandolf, S.; Grishkovskaya, I.; Meinhart, A.; Haselbach, D.
Deposited on	:	2022-01-21
Resolution	:	3.30 Å(reported)
Based on initial model	:	6MSB

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

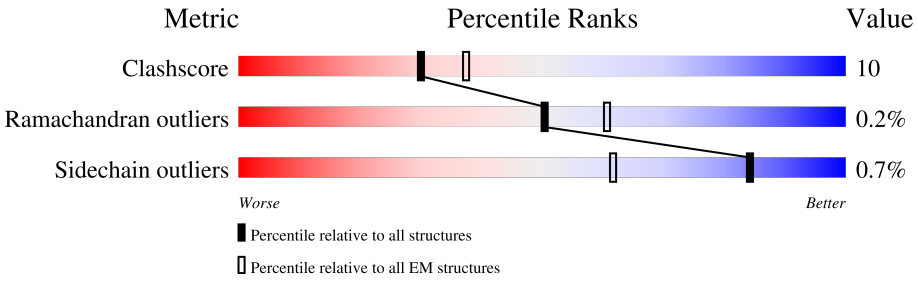
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	C	235	79% 19%
1	i	235	97%
2	D	250	72% 27%
2	j	250	99%
3	E	247	76% 20%
3	k	247	97%
4	F	237	75% 22%
4	l	237	97%

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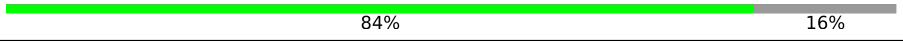
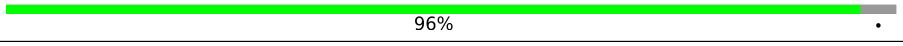
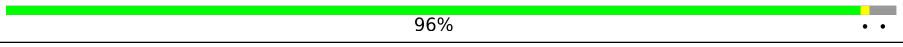
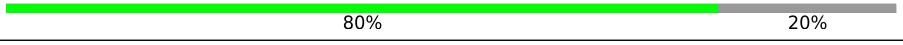
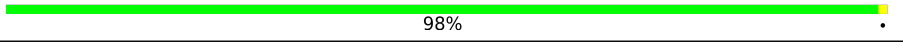
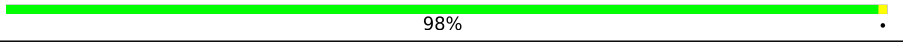
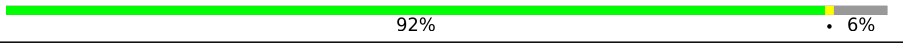
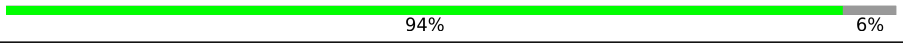
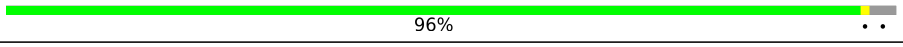
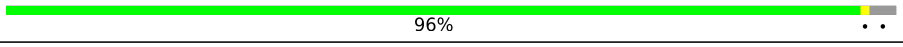
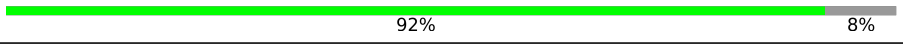
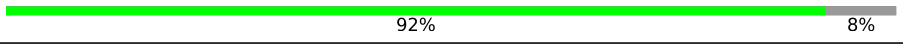
Mol	Chain	Length	Quality of chain
5	G	274	
5	m	274	
6	X	249	
6	n	249	
7	B	246	
7	h	246	
8	a	236	
8	o	236	
9	b	274	
9	p	274	
10	c	204	
10	q	204	
11	d	209	
11	r	209	
12	e	272	
12	s	272	
13	f	223	
13	t	223	
14	g	240	
14	u	240	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 48322 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	229	Total	C	N	O	S	0	0
			1754	1117	291	342	4		
1	C	229	Total	C	N	O	S	0	0
			1754	1117	291	342	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	249	Total	C	N	O	S	0	0
			1920	1209	322	380	9		
2	D	249	Total	C	N	O	S	0	0
			1920	1209	322	380	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	240	Total	C	N	O	S	0	0
			1845	1157	327	358	3		
3	E	240	Total	C	N	O	S	0	0
			1845	1157	327	358	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	l	230	Total	C	N	O	S	0	0
			1763	1104	294	357	8		
4	F	230	Total	C	N	O	S	0	0
			1763	1104	294	357	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	m	231	Total	C	N	O	S	0	0
			1794	1129	312	345	8		
5	G	231	Total	C	N	O	S	0	0
			1794	1129	312	345	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	n	239	Total	C	N	O	S	0	0
			1842	1164	320	347	11		
6	X	239	Total	C	N	O	S	0	0
			1842	1164	320	347	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	238	Total	C	N	O	S	0	0
			1861	1180	319	356	6		
7	h	238	Total	C	N	O	S	0	0
			1861	1180	319	356	6		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	212	Total	C	N	O	S	0	0
			1617	1024	273	317	3		
8	a	212	Total	C	N	O	S	0	0
			1617	1024	273	317	3		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	p	220	Total	C	N	O	S	0	0
			1648	1033	286	320	9		
9	b	220	Total	C	N	O	S	0	0
			1648	1033	286	320	9		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	203	Total	C	N	O	S	0	0
			1593	1010	269	303	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	203	Total	C	N	O	S	0	0
			1593	1010	269	303	11		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	r	196	Total	C	N	O	S	0	0
			1524	972	260	284	8		
11	d	196	Total	C	N	O	S	0	0
			1524	972	260	284	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	s	203	Total	C	N	O	S	0	0
			1553	985	270	288	10		
12	e	203	Total	C	N	O	S	0	0
			1553	985	270	288	10		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	t	217	Total	C	N	O	S	0	0
			1695	1074	286	325	10		
13	f	217	Total	C	N	O	S	0	0
			1695	1074	286	325	10		

- Molecule 14 is a protein called Proteasome subunit beta.

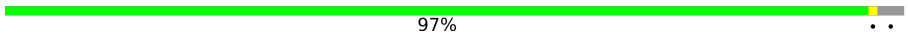
Mol	Chain	Residues	Atoms					AltConf	Trace
14	u	221	Total	C	N	O	S	0	0
			1752	1120	300	326	6		
14	g	221	Total	C	N	O	S	0	0
			1752	1120	300	326	6		

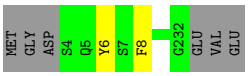
3 Residue-property plots (i)

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

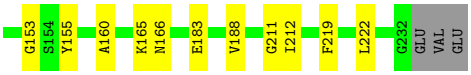
Chain i:





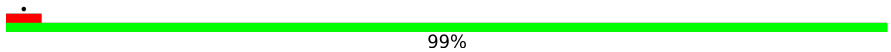
• Molecule 1: Proteasome subunit alpha type

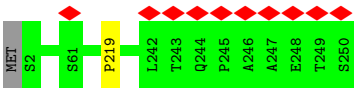
Chain C:



• Molecule 2: Proteasome subunit alpha type

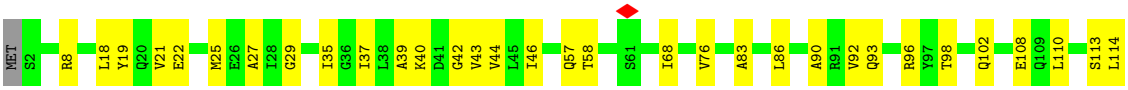
Chain j:

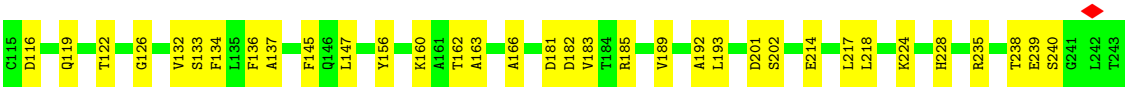


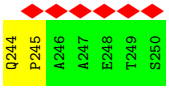


• Molecule 2: Proteasome subunit alpha type

Chain D:

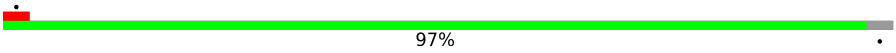


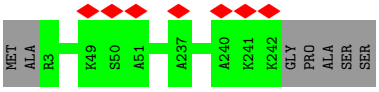




• Molecule 3: Proteasome subunit alpha type

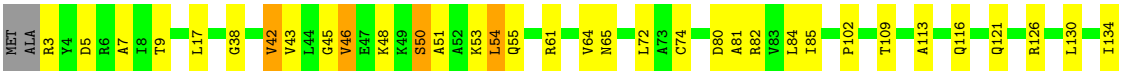
Chain k:





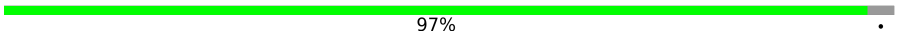
• Molecule 3: Proteasome subunit alpha type

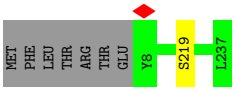
Chain E:



• Molecule 4: Proteasome subunit alpha type

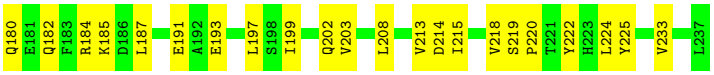
Chain l:





• Molecule 4: Proteasome subunit alpha type

Chain F:

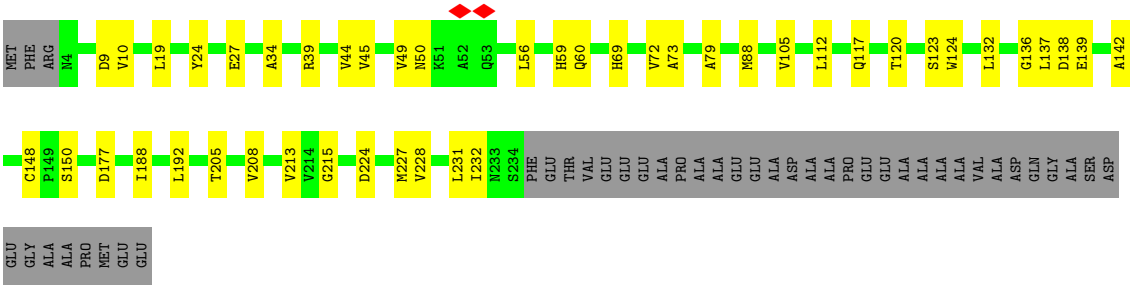


• Molecule 5: Proteasome subunit alpha type

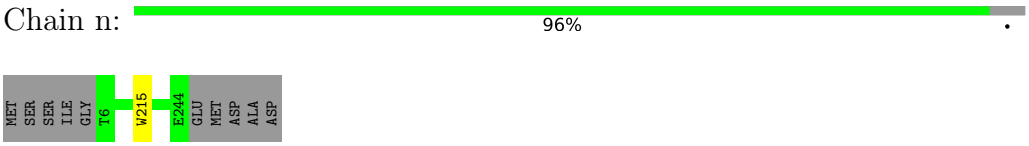
Chain m:

• Molecule 5: Proteasome subunit alpha type

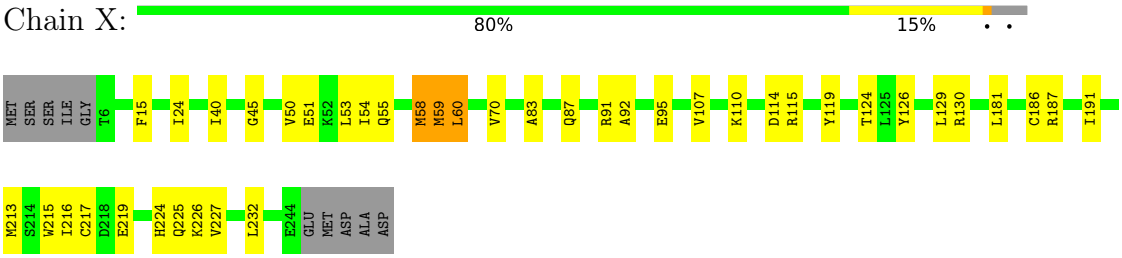
Chain G:



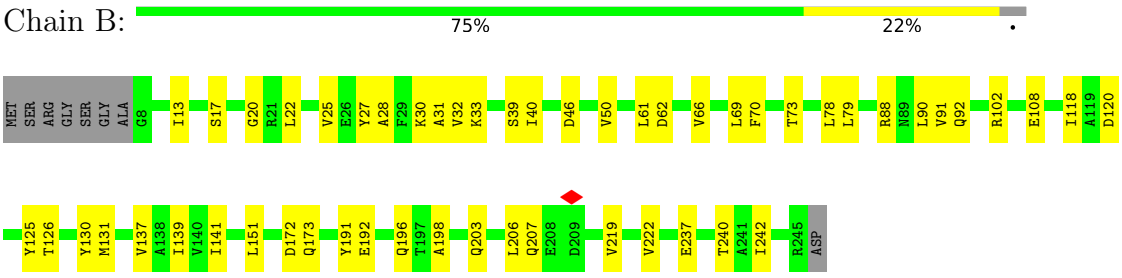
• Molecule 6: Proteasome subunit alpha type-3



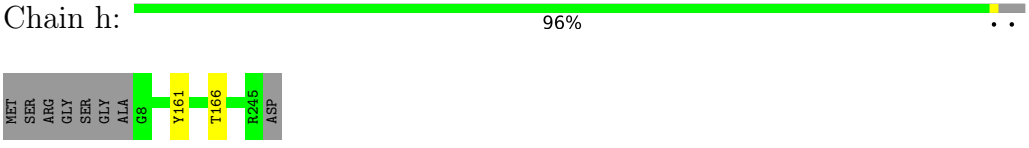
• Molecule 6: Proteasome subunit alpha type-3



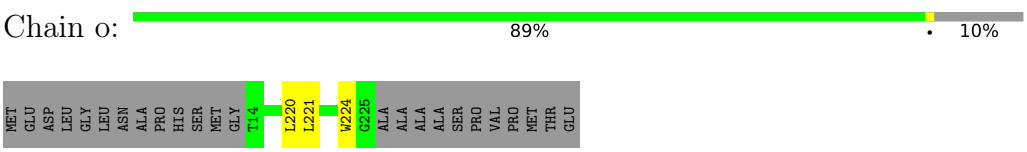
• Molecule 7: Proteasome subunit alpha type



• Molecule 7: Proteasome subunit alpha type



• Molecule 8: Proteasome subunit beta

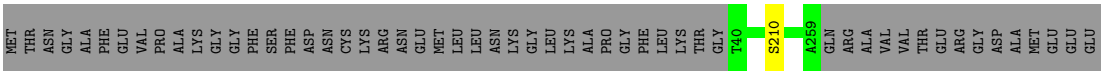


• Molecule 8: Proteasome subunit beta

Chain a:

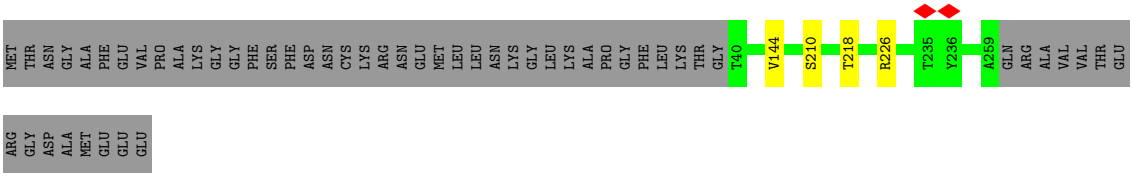
• Molecule 9: Proteasome subunit beta

Chain p:



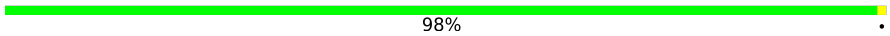
• Molecule 9: Proteasome subunit beta

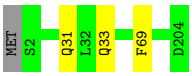
Chain b:



• Molecule 10: Proteasome subunit beta

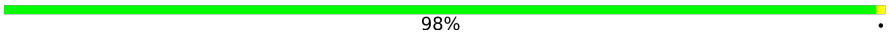
Chain q:

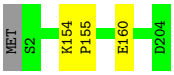




• Molecule 10: Proteasome subunit beta

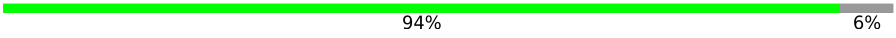
Chain c:





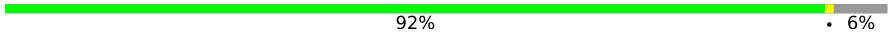
• Molecule 11: Proteasome subunit beta

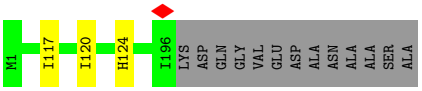
Chain r:



• Molecule 11: Proteasome subunit beta

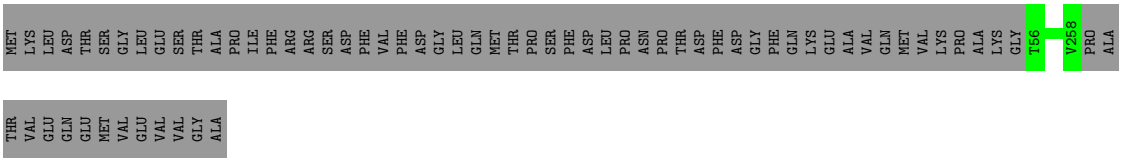
Chain d:





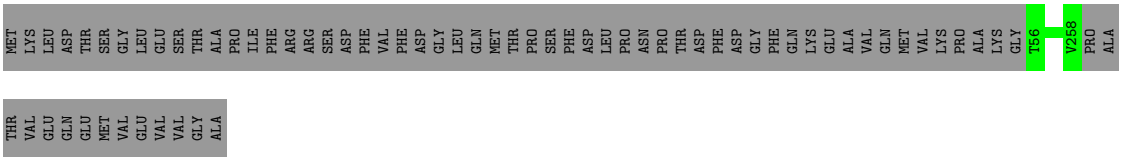
• Molecule 12: Proteasome subunit beta type-5

Chain s:



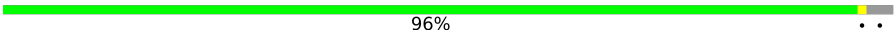
• Molecule 12: Proteasome subunit beta type-5

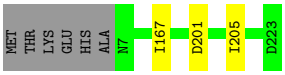
Chain e:



• Molecule 13: Proteasome subunit beta

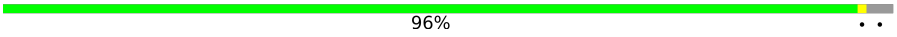
Chain t:

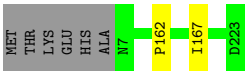




• Molecule 13: Proteasome subunit beta

Chain f:





• Molecule 14: Proteasome subunit beta

Chain u:

• Molecule 14: Proteasome subunit beta

Chain g:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	951422	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 ($e^-/Å^2$)	80, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.932	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0168	Depositor
Map size (Å)	541.696, 541.696, 541.696	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2311273, 1.2311273, 1.2311273	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.41	0/1785	0.48	0/2414
1	i	0.42	0/1785	0.51	0/2414
2	D	0.42	0/1953	0.48	0/2640
2	j	0.41	0/1953	0.50	0/2640
3	E	0.44	0/1870	0.52	0/2526
3	k	0.41	0/1870	0.49	0/2526
4	F	0.47	0/1794	0.56	0/2428
4	l	0.49	0/1794	0.52	0/2428
5	G	0.46	0/1827	0.49	0/2470
5	m	0.50	0/1827	0.53	0/2470
6	X	0.46	0/1876	0.52	0/2529
6	n	0.45	0/1876	0.53	0/2529
7	B	0.46	0/1897	0.55	0/2565
7	h	0.45	0/1897	0.51	0/2565
8	a	0.56	0/1648	0.55	0/2238
8	o	0.55	0/1648	0.59	0/2238
9	b	0.53	0/1679	0.60	0/2282
9	p	0.48	0/1679	0.57	0/2282
10	c	0.53	0/1624	0.59	0/2189
10	q	0.50	0/1624	0.60	0/2189
11	d	0.49	0/1553	0.59	0/2099
11	r	0.49	0/1553	0.53	0/2099
12	e	0.54	0/1589	0.54	0/2146
12	s	0.52	0/1589	0.54	0/2146
13	f	0.54	0/1730	0.59	0/2340
13	t	0.55	0/1730	0.57	0/2340
14	g	0.54	0/1792	0.60	0/2422
14	u	0.54	0/1792	0.54	0/2422
All	All	0.49	0/49234	0.54	0/66576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1754	0	1775	29	0
1	i	1754	0	1775	0	0
2	D	1920	0	1910	48	0
2	j	1920	0	1910	0	0
3	E	1845	0	1872	49	0
3	k	1845	0	1872	0	0
4	F	1763	0	1728	53	0
4	l	1763	0	1728	0	0
5	G	1794	0	1769	34	0
5	m	1794	0	1769	0	0
6	X	1842	0	1847	39	0
6	n	1842	0	1847	0	0
7	B	1861	0	1848	45	0
7	h	1861	0	1848	0	0
8	a	1617	0	1594	0	0
8	o	1617	0	1594	0	0
9	b	1648	0	1640	0	0
9	p	1648	0	1640	0	0
10	c	1593	0	1570	0	0
10	q	1593	0	1570	0	0
11	d	1524	0	1520	0	0
11	r	1524	0	1520	0	0
12	e	1553	0	1518	0	0
12	s	1553	0	1518	0	0
13	f	1695	0	1665	0	0
13	t	1695	0	1665	0	0
14	g	1752	0	1732	0	0
14	u	1752	0	1732	0	0
All	All	48322	0	47976	271	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 271 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:SER:CB	3:E:53:LYS:HD3	1.79	1.11
4:F:78:MET:HB3	4:F:139:LEU:CD2	1.87	1.03
3:E:50:SER:HB3	3:E:53:LYS:HD3	1.38	1.03
4:F:85:ALA:HB2	4:F:137:VAL:HG11	1.50	0.93
3:E:46:VAL:HG12	3:E:206:GLU:HB3	1.48	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	227/235 (97%)	219 (96%)	8 (4%)	0	100	100
1	i	227/235 (97%)	214 (94%)	13 (6%)	0	100	100
2	D	247/250 (99%)	238 (96%)	9 (4%)	0	100	100
2	j	247/250 (99%)	234 (95%)	13 (5%)	0	100	100
3	E	238/247 (96%)	228 (96%)	9 (4%)	1 (0%)	34	66
3	k	238/247 (96%)	230 (97%)	8 (3%)	0	100	100
4	F	228/237 (96%)	213 (93%)	15 (7%)	0	100	100
4	l	228/237 (96%)	216 (95%)	11 (5%)	1 (0%)	34	66
5	G	229/274 (84%)	220 (96%)	9 (4%)	0	100	100
5	m	229/274 (84%)	218 (95%)	11 (5%)	0	100	100
6	X	237/249 (95%)	219 (92%)	17 (7%)	1 (0%)	34	66
6	n	237/249 (95%)	220 (93%)	17 (7%)	0	100	100
7	B	236/246 (96%)	225 (95%)	11 (5%)	0	100	100
7	h	236/246 (96%)	224 (95%)	12 (5%)	0	100	100
8	a	210/236 (89%)	191 (91%)	17 (8%)	2 (1%)	15	46
8	o	210/236 (89%)	196 (93%)	13 (6%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	b	218/274 (80%)	199 (91%)	18 (8%)	1 (0%)	29 61
9	p	218/274 (80%)	205 (94%)	12 (6%)	1 (0%)	29 61
10	c	201/204 (98%)	184 (92%)	16 (8%)	1 (0%)	29 61
10	q	201/204 (98%)	178 (89%)	22 (11%)	1 (0%)	29 61
11	d	194/209 (93%)	179 (92%)	15 (8%)	0	100 100
11	r	194/209 (93%)	181 (93%)	13 (7%)	0	100 100
12	e	201/272 (74%)	193 (96%)	8 (4%)	0	100 100
12	s	201/272 (74%)	192 (96%)	9 (4%)	0	100 100
13	f	215/223 (96%)	198 (92%)	17 (8%)	0	100 100
13	t	215/223 (96%)	201 (94%)	13 (6%)	1 (0%)	29 61
14	g	219/240 (91%)	202 (92%)	17 (8%)	0	100 100
14	u	219/240 (91%)	198 (90%)	21 (10%)	0	100 100
All	All	6200/6792 (91%)	5815 (94%)	374 (6%)	11 (0%)	50 77

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	t	201	ASP
10	c	160	GLU
4	l	219	SER
8	a	224	TRP
9	p	210	SER

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	C	192/197 (98%)	192 (100%)	0	100 100
1	i	192/197 (98%)	190 (99%)	2 (1%)	76 86
2	D	208/209 (100%)	208 (100%)	0	100 100
2	j	208/209 (100%)	207 (100%)	1 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	194/198 (98%)	190 (98%)	4 (2%)	53 75
3	k	194/198 (98%)	194 (100%)	0	100 100
4	F	194/201 (96%)	191 (98%)	3 (2%)	65 81
4	l	194/201 (96%)	194 (100%)	0	100 100
5	G	193/220 (88%)	193 (100%)	0	100 100
5	m	193/220 (88%)	193 (100%)	0	100 100
6	X	191/199 (96%)	189 (99%)	2 (1%)	76 86
6	n	191/199 (96%)	190 (100%)	1 (0%)	88 93
7	B	199/204 (98%)	199 (100%)	0	100 100
7	h	199/204 (98%)	197 (99%)	2 (1%)	76 86
8	a	171/188 (91%)	168 (98%)	3 (2%)	59 78
8	o	171/188 (91%)	169 (99%)	2 (1%)	71 83
9	b	180/222 (81%)	177 (98%)	3 (2%)	60 78
9	p	180/222 (81%)	180 (100%)	0	100 100
10	c	171/172 (99%)	169 (99%)	2 (1%)	71 83
10	q	171/172 (99%)	169 (99%)	2 (1%)	71 83
11	d	160/168 (95%)	157 (98%)	3 (2%)	57 77
11	r	160/168 (95%)	160 (100%)	0	100 100
12	e	158/217 (73%)	158 (100%)	0	100 100
12	s	158/217 (73%)	158 (100%)	0	100 100
13	f	181/186 (97%)	179 (99%)	2 (1%)	73 85
13	t	181/186 (97%)	179 (99%)	2 (1%)	73 85
14	g	186/205 (91%)	185 (100%)	1 (0%)	88 93
14	u	186/205 (91%)	186 (100%)	0	100 100
All	All	5156/5572 (92%)	5121 (99%)	35 (1%)	84 90

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	d	120	ILE
11	d	124	HIS
14	g	28	ILE
6	X	60	LEU
6	X	58	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
9	b	148	HIS
10	q	75	GLN
9	p	211	ASN
8	o	217	GLN
10	q	33	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.

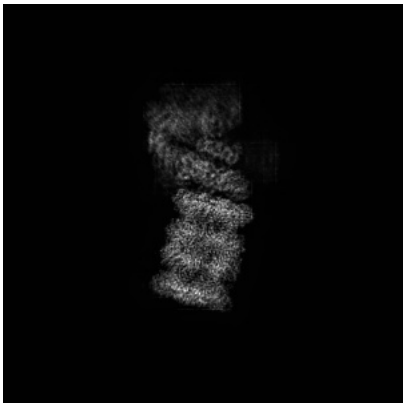
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14175. These allow visual inspection of the internal detail of the map and identification of artifacts.

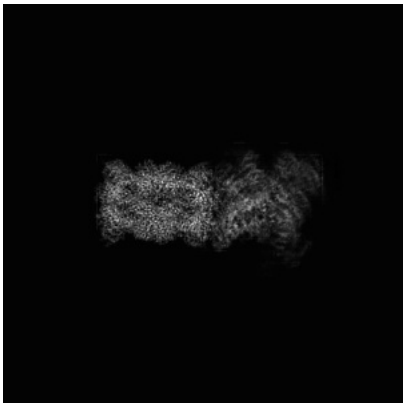
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

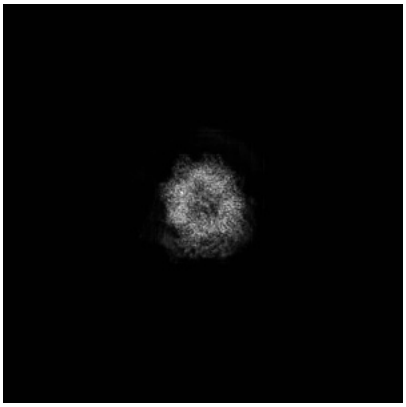
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 220

Y Index: 220

Z Index: 220

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: 199

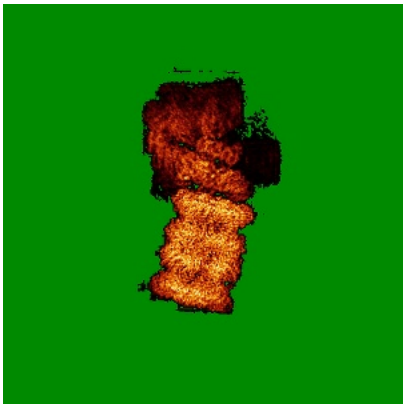
Y Index: 200

Z Index: 210

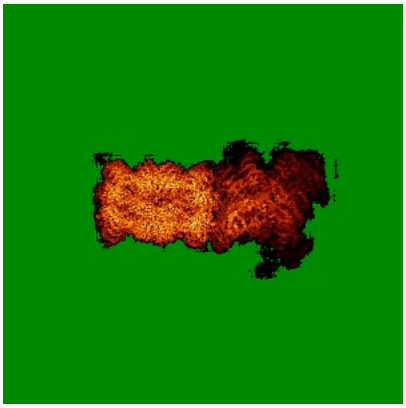
The images above show the largest variance slices of the map in three orthogonal directions.

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

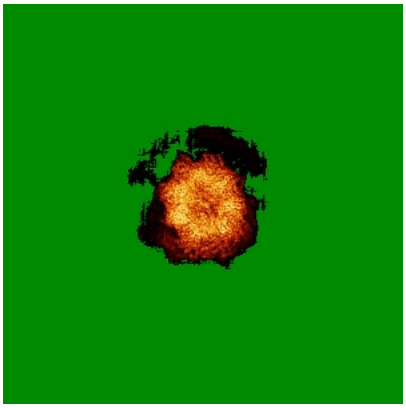
6.4.1 Primary map



X



Y

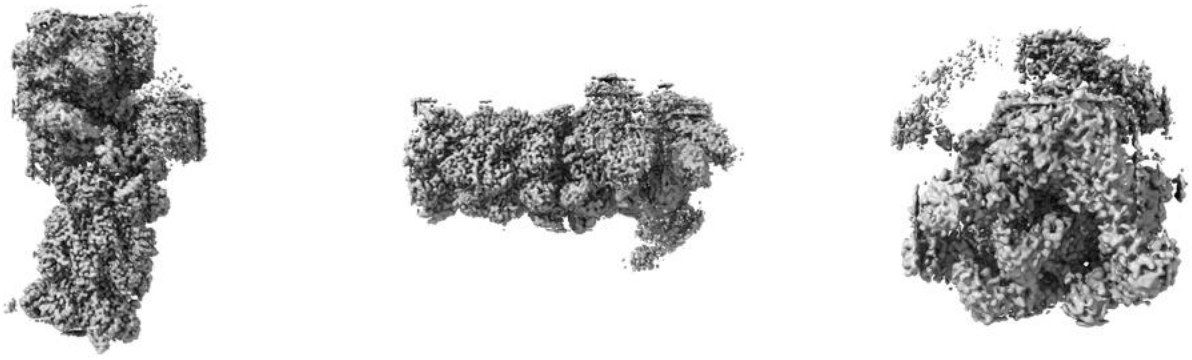


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0168. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

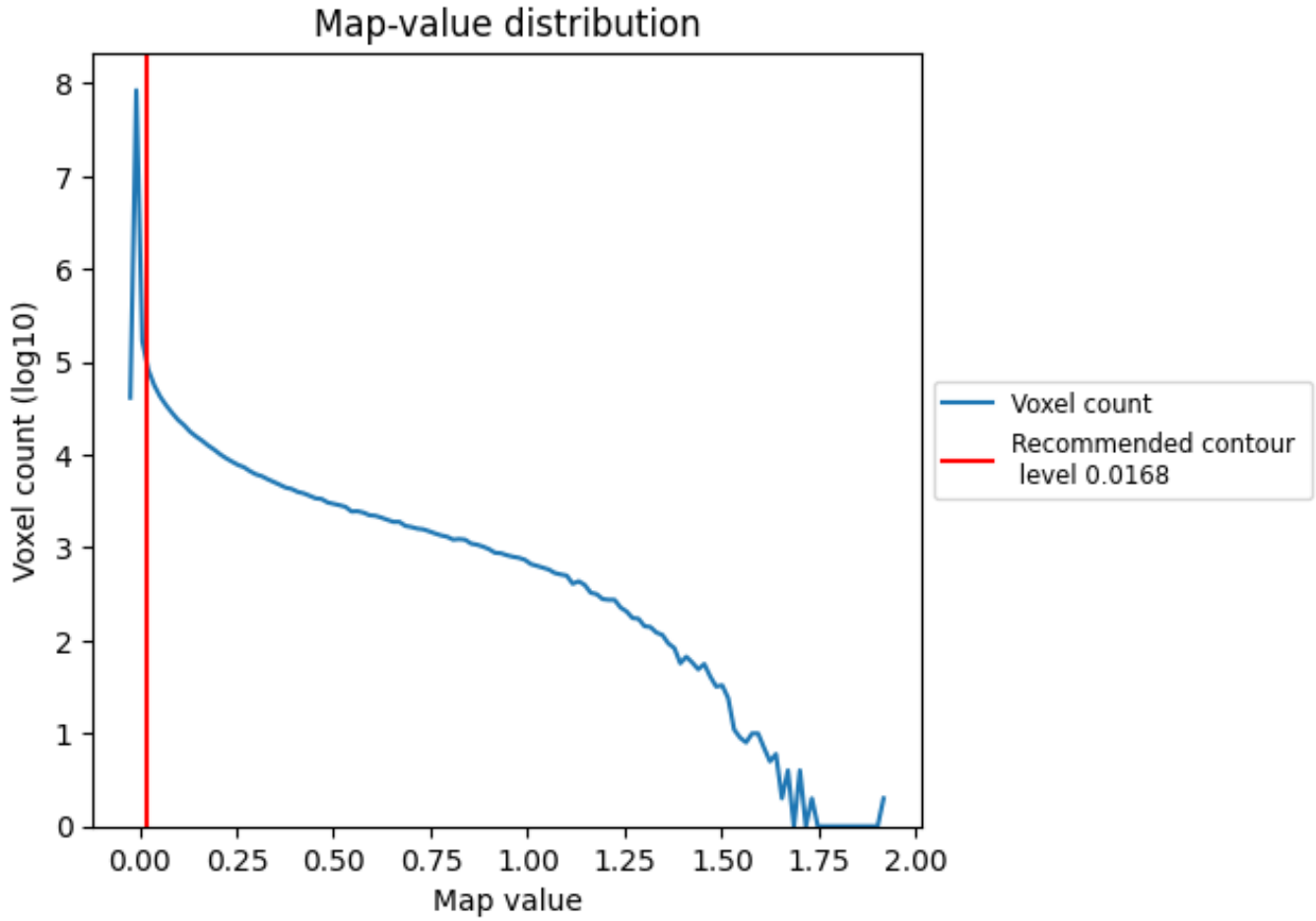
6.6 Mask visualisation (i)

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

7 Map analysis

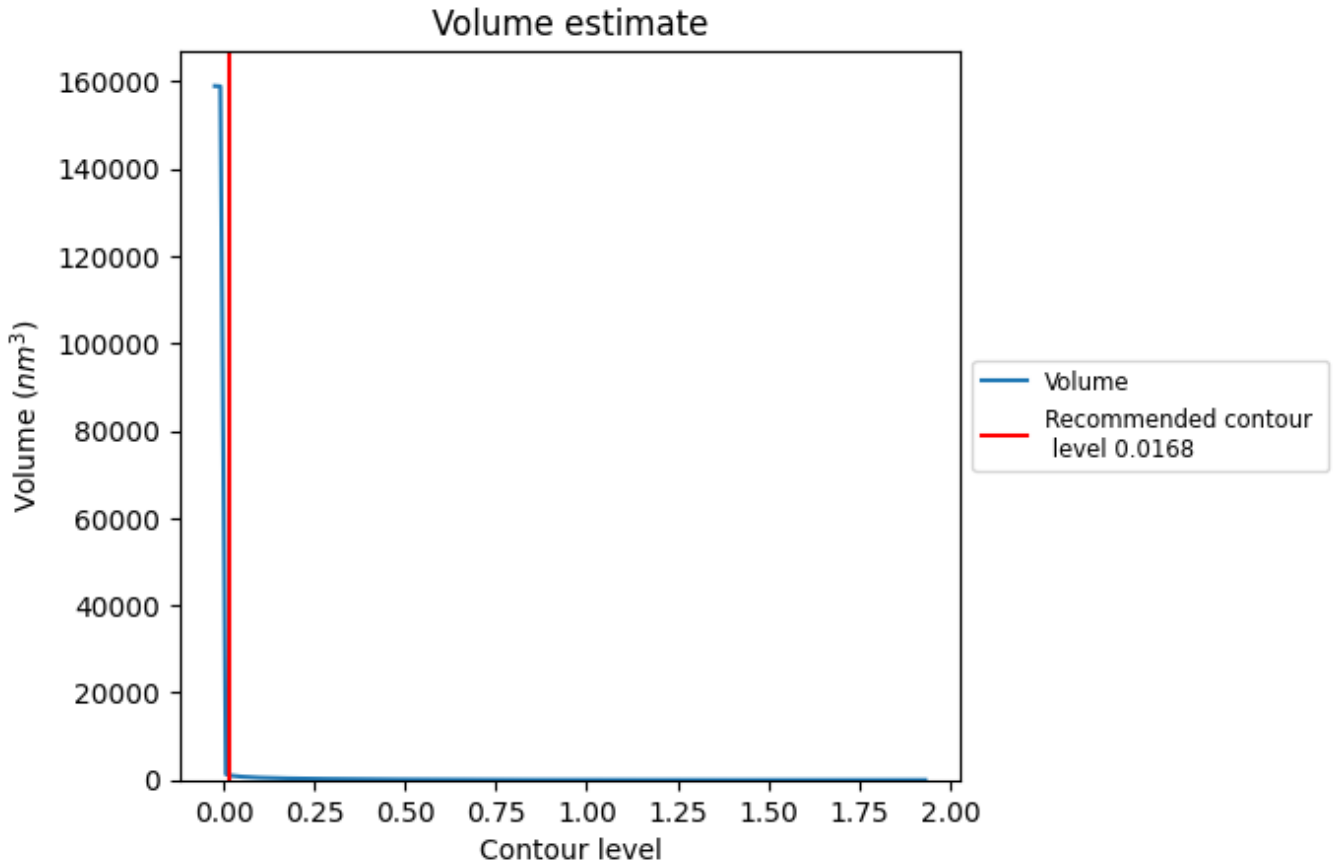
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

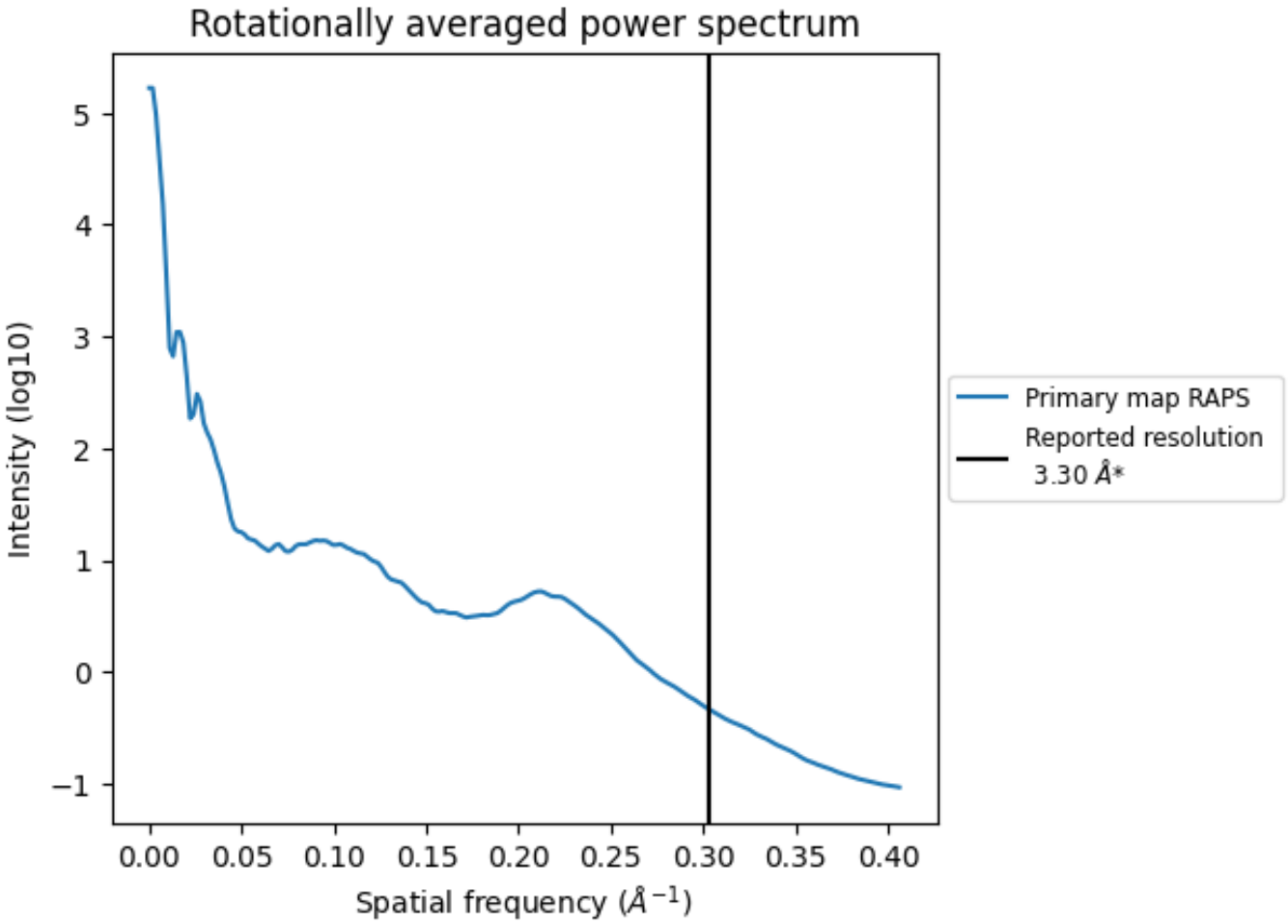
7.2 Volume estimate



The volume at the recommended contour level is 1112 nm^3; this corresponds to an approximate mass of 1004 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 0.303 Å^{-1}

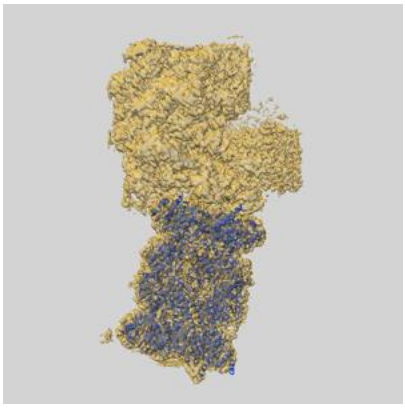
8 Fourier-Shell correlation (i)

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

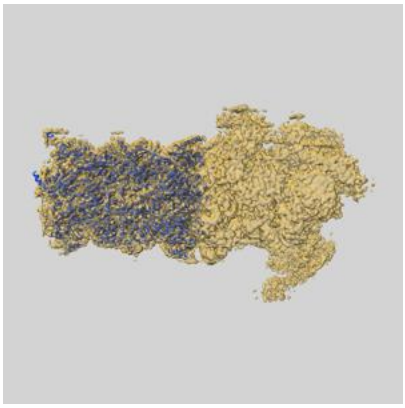
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14175 and PDB model 7QVE. Per-residue inclusion information can be found in section 3 on page 7.

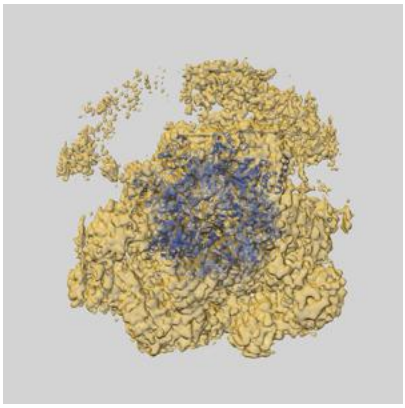
9.1 Map-model overlay



X



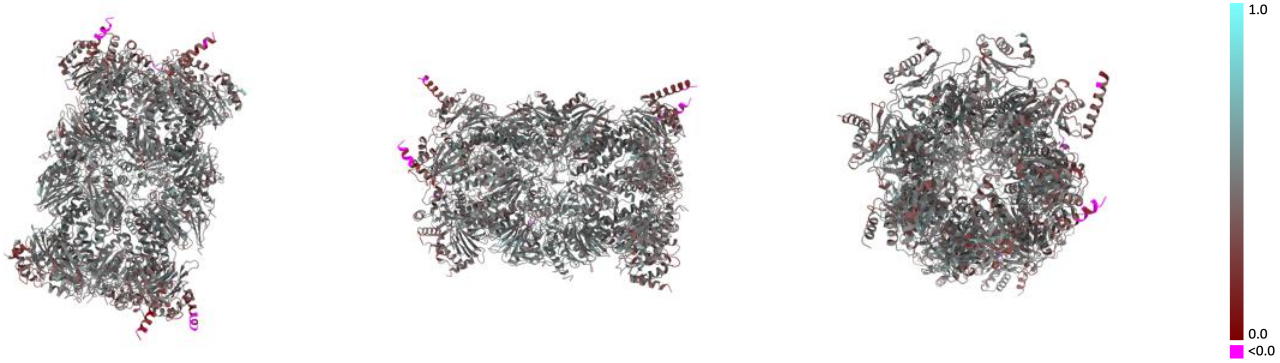
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0168 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.

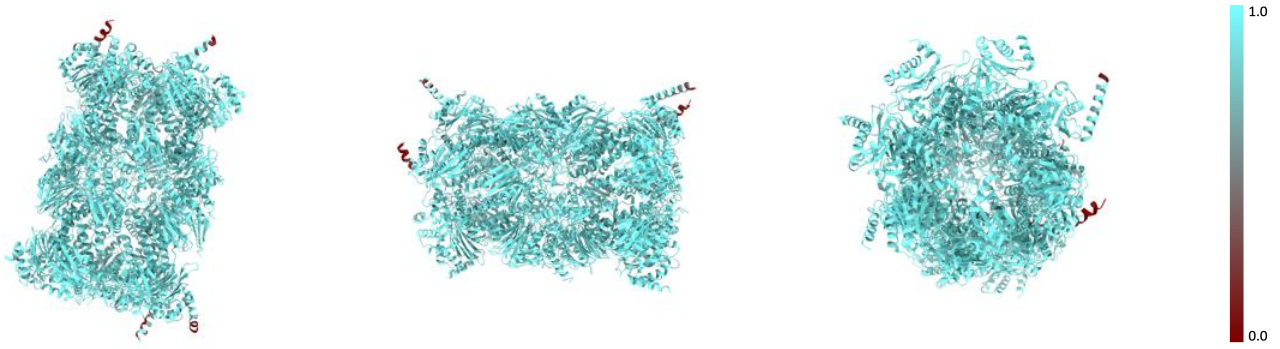
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

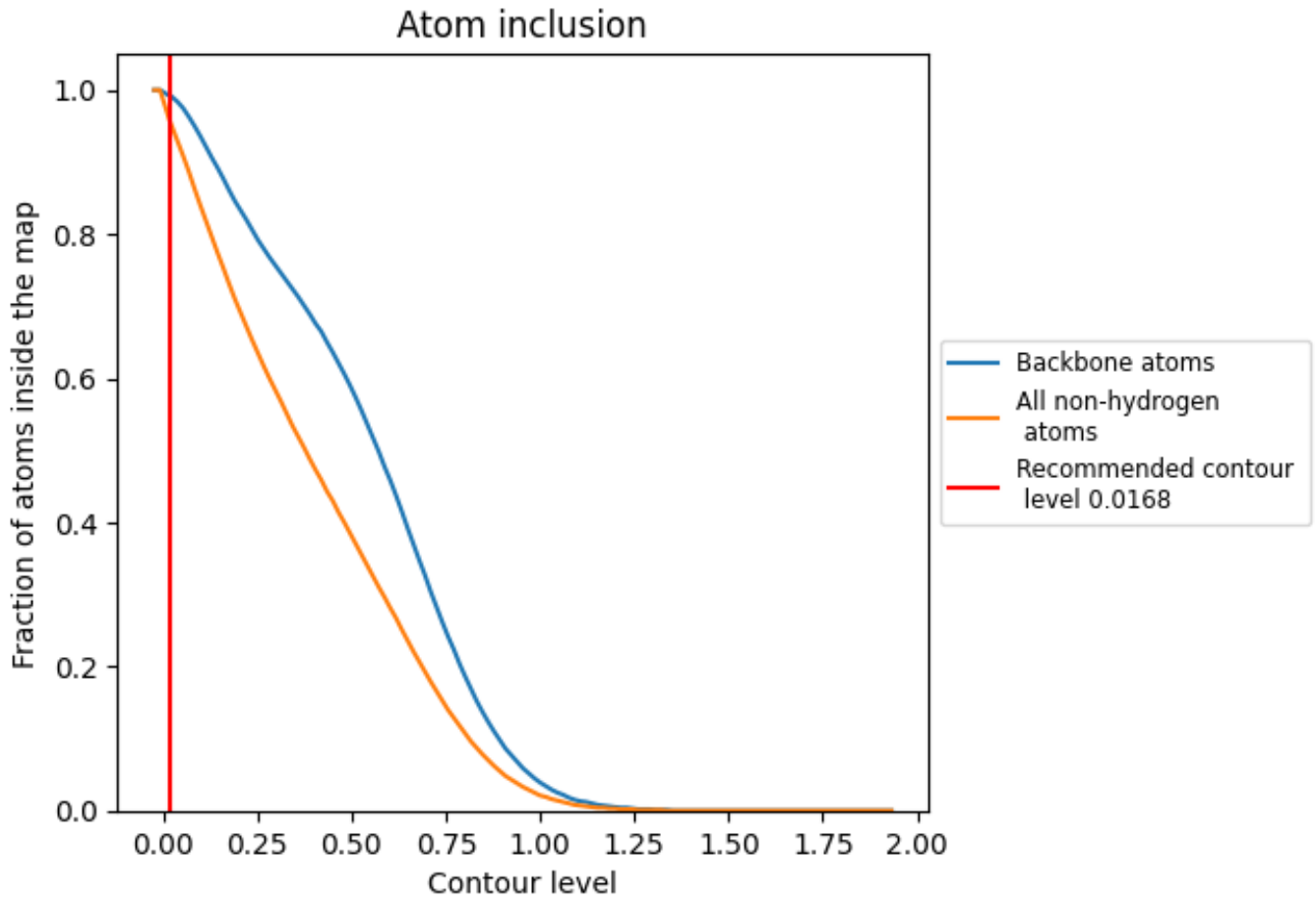
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0168).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.0168) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9590	0.4500
B	0.9570	0.4350
C	0.9580	0.4350
D	0.9230	0.4040
E	0.9170	0.4070
F	0.9570	0.4510
G	0.9490	0.4270
X	0.9440	0.4180
a	0.9810	0.4990
b	0.9620	0.4690
c	0.9800	0.4730
d	0.9670	0.4660
e	0.9820	0.4710
f	0.9770	0.4830
g	0.9780	0.4930
h	0.9570	0.4390
i	0.9430	0.4100
j	0.8980	0.3880
k	0.9250	0.4070
l	0.9620	0.4410
m	0.9700	0.4550
n	0.9560	0.4460
o	0.9860	0.4890
p	0.9640	0.4580
q	0.9710	0.4670
r	0.9740	0.4640
s	0.9800	0.4690
t	0.9840	0.4840
u	0.9790	0.4860