



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 01:55 AM UTC

PDB ID : 9YUY / pdb_00009yuy
EMDB ID : EMD-73509
Title : Structure of the Plasmodium falciparum 20S proteasome in complex with a beta5-selective covalent syringolin analogue inhibitor.
Authors : Yan, N.L.; Gu, X.; Fajtova, P.; Tse, E.; Melo, A.; Southworth, D.R.; O'Donoghue, A.; Sello, J.K.; Gestwicki, J.E.
Deposited on : 2025-10-23
Resolution : 2.70 Å (reported)
Based on initial model : 6MUW

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:

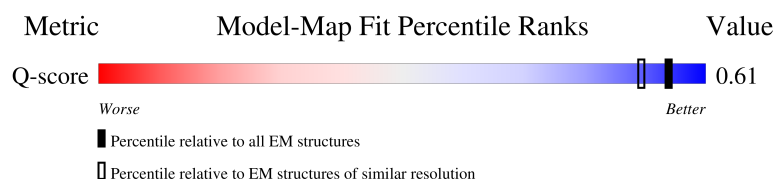
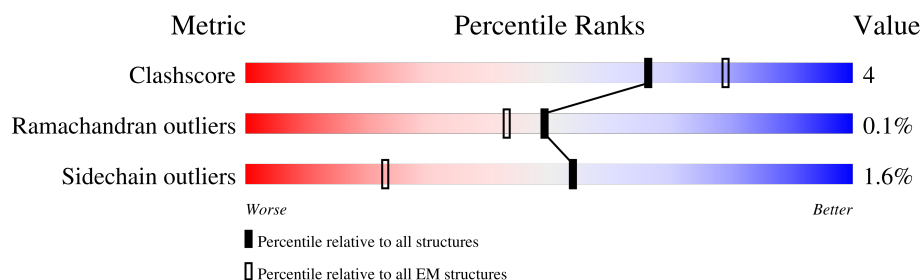
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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




The reported resolution of this entry is 2.70 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.









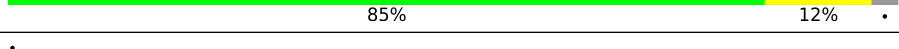
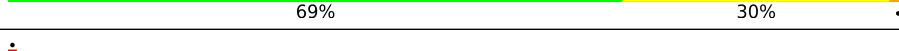
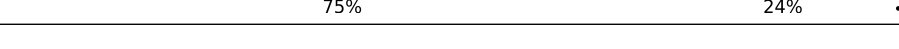
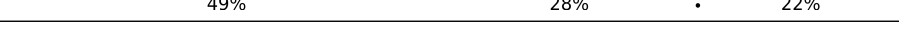
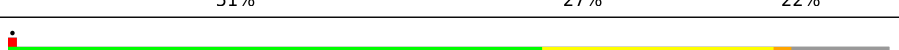

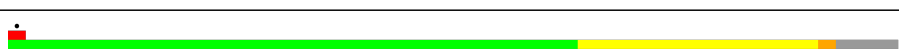

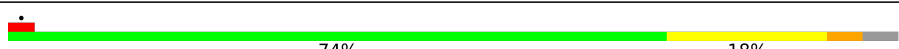





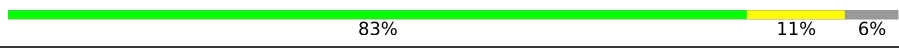
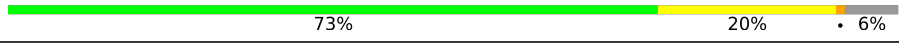



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	246	
1	Q	246	
2	D	241	

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Mol	Chain	Length	Quality of chain
2	R	241	
3	E	256	
3	S	256	
4	F	254	
4	T	254	
5	G	252	
5	U	252	
6	K	195	
6	Y	195	
7	L	271	
7	Z	271	
8	M	240	
8	a	240	
9	A	260	
9	O	260	
10	B	235	
10	P	235	
11	H	282	
11	V	282	
12	I	270	
12	W	270	
13	J	218	
13	X	218	
14	N	265	
14	b	265	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 100048 atoms, of which 49886 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	C	240	Total	C	H	N	O	S	0	0
			3828	1226	1911	312	376	3		
1	Q	240	Total	C	H	N	O	S	0	0
			3828	1226	1911	312	376	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	233	Total	C	H	N	O	S	0	0
			3724	1178	1879	312	347	8		
2	R	233	Total	C	H	N	O	S	0	0
			3724	1178	1879	312	347	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	240	Total	C	H	N	O	S	0	0
			3728	1170	1868	311	368	11		
3	S	240	Total	C	H	N	O	S	0	0
			3728	1170	1868	311	368	11		

- Molecule 4 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	237	Total	C	H	N	O	S	0	0
			3758	1194	1879	310	364	11		
4	T	237	Total	C	H	N	O	S	0	0
			3758	1194	1879	310	364	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-3, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	245	Total	C	H	N	O	S	0	0
			3958	1277	1950	335	383	13		
5	U	245	Total	C	H	N	O	S	0	0
			3958	1277	1950	335	383	13		

- Molecule 6 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	195	Total	C	H	N	O	S	0	0
			3198	1042	1584	266	298	8		
6	Y	195	Total	C	H	N	O	S	0	0
			3198	1042	1584	266	298	8		

- Molecule 7 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	211	Total	C	H	N	O	S	0	0
			3277	1060	1615	275	319	8		
7	Z	211	Total	C	H	N	O	S	0	0
			3277	1060	1615	275	319	8		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	213	Total	C	H	N	O	S	0	0
			3404	1085	1708	283	321	7		
8	a	213	Total	C	H	N	O	S	0	0
			3404	1085	1708	283	321	7		

- Molecule 9 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A	242	Total	C	H	N	O	S	0	0
			3809	1201	1899	318	377	14		
9	O	242	Total	C	H	N	O	S	0	0
			3809	1201	1899	318	377	14		

- Molecule 10 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	B	225	Total	C	H	N	O	S	0	0
			3614	1157	1816	294	341	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	P	225	Total	C	H	N	O	S	0	0
			3614	1157	1816	294	341	6		

- Molecule 11 is a protein called Proteasome subunit beta type-6, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	214	Total	C	H	N	O	S	0	0
			3461	1096	1739	297	318	11		
11	V	214	Total	C	H	N	O	S	0	0
			3461	1096	1739	297	318	11		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	218	Total	C	H	N	O	S	0	0
			3336	1055	1668	289	311	13		
12	W	218	Total	C	H	N	O	S	0	0
			3336	1055	1668	289	311	13		

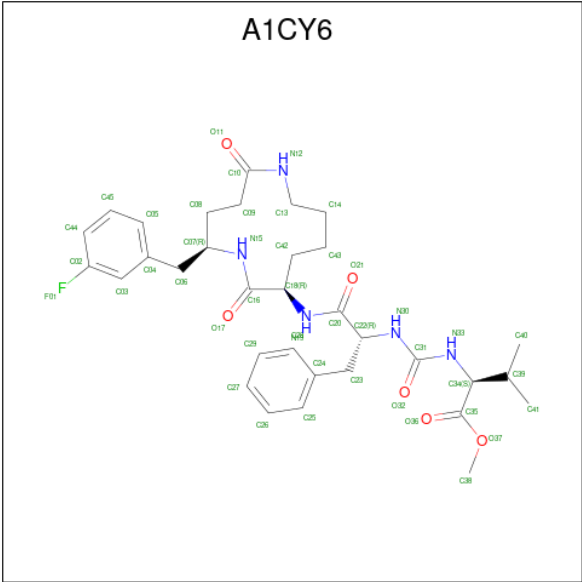
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J	205	Total	C	H	N	O	S	0	0
			3222	1029	1610	261	308	14		
13	X	205	Total	C	H	N	O	S	0	0
			3222	1029	1610	261	308	14		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	224	Total	C	H	N	O	S	0	0
			3662	1177	1817	313	348	7		
14	b	224	Total	C	H	N	O	S	0	0
			3662	1177	1817	313	348	7		

- Molecule 15 is methyl N-{[(2R)-1-({(5R,8R)-5-[(3-fluorophenyl)methyl]-2,7-dioxo-1,6-diazacyclododecan-8-yl}amino)-1-oxo-3-phenylpropan-2-yl]carbonyl}-L-valinate (CCD ID: A1CY6) (formula: C₃₃H₄₄FN₅O₆) (labeled as "Ligand of Interest" by depositor).

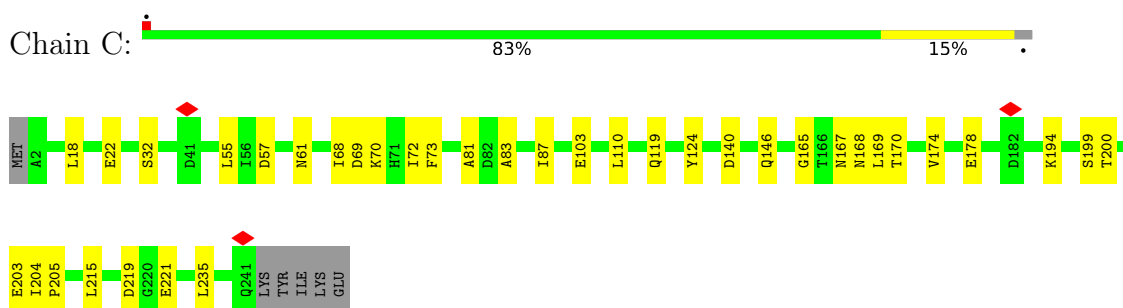


Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	F	N	O	0
			45	33	1	5	6	
15	Z	1	Total	C	F	N	O	0
			45	33	1	5	6	

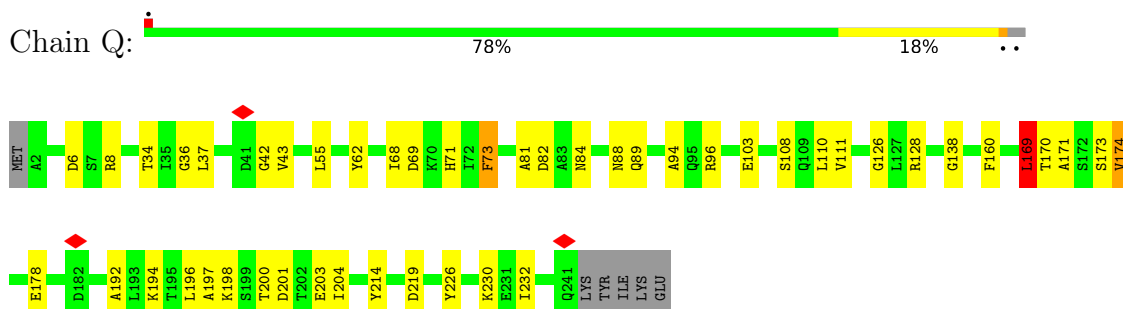
3 Residue-property plots [i](#)

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.

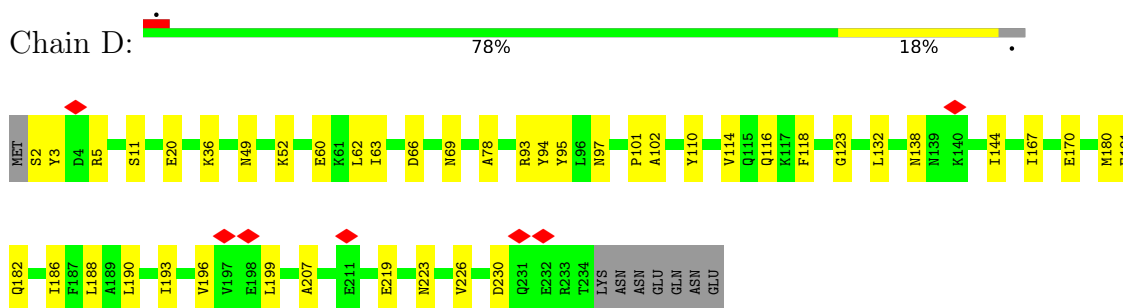
- Molecule 1: Proteasome subunit alpha type



- Molecule 1: Proteasome subunit alpha type

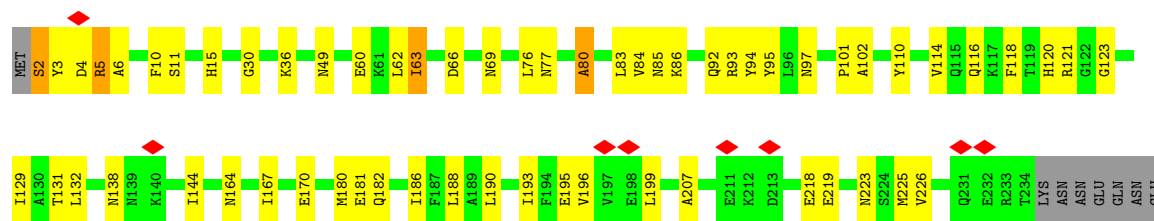


- Molecule 2: Proteasome subunit alpha type

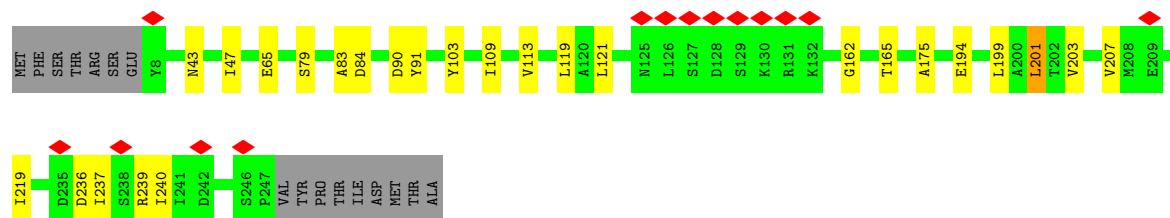
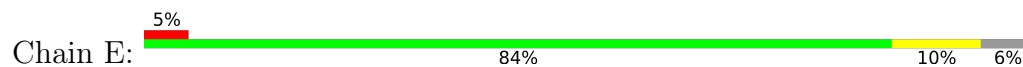


- Molecule 2: Proteasome subunit alpha type

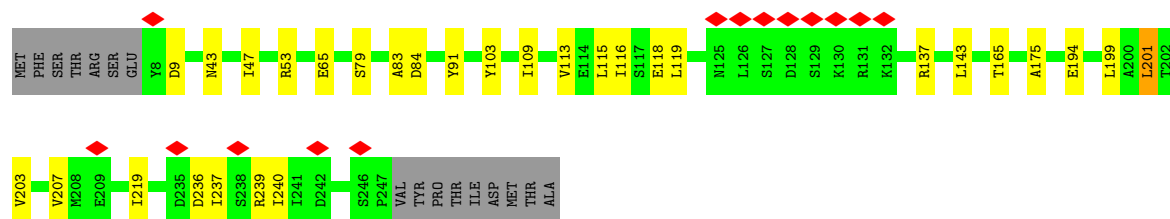
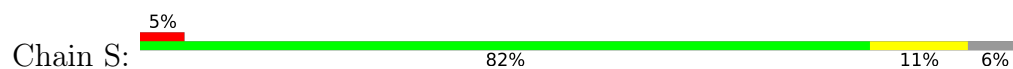




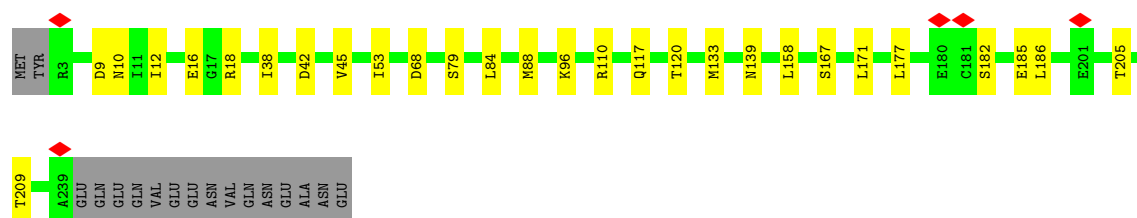
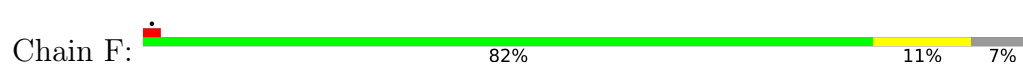
• Molecule 3: Proteasome subunit alpha type



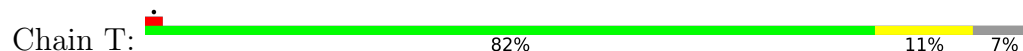
• Molecule 3: Proteasome subunit alpha type

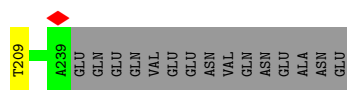


• Molecule 4: Proteasome endopeptidase complex

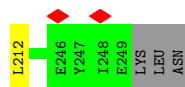
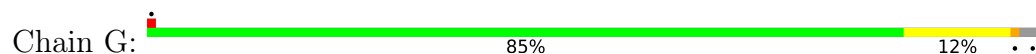


• Molecule 4: Proteasome endopeptidase complex

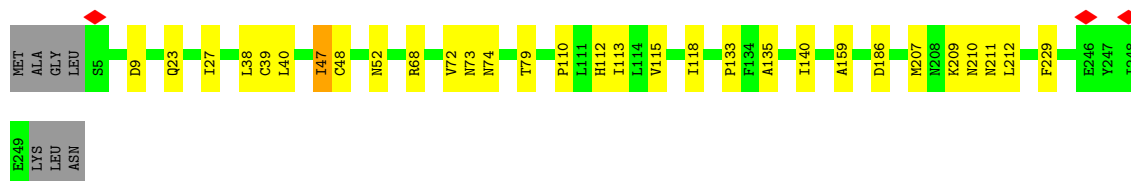
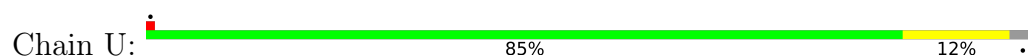




- Molecule 5: Proteasome subunit alpha type-3, putative



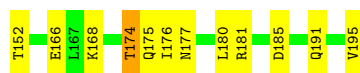
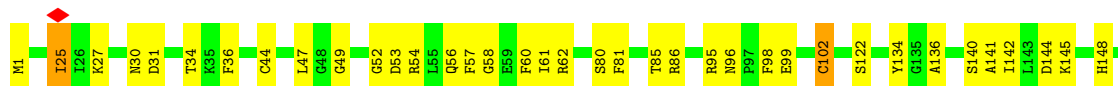
- Molecule 5: Proteasome subunit alpha type-3, putative



- Molecule 6: Proteasome subunit beta

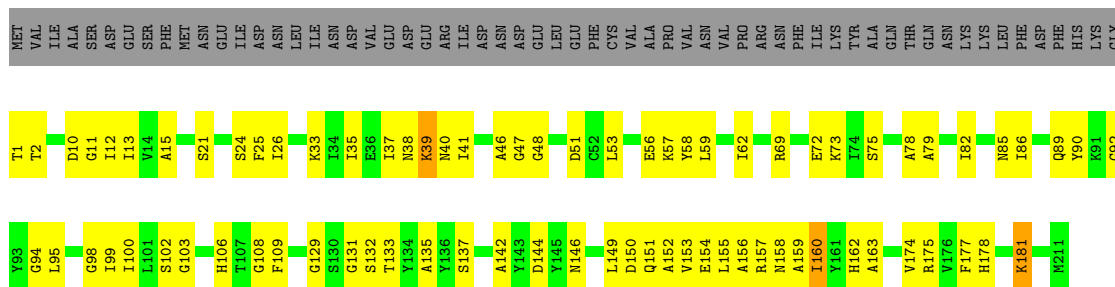


- Molecule 6: Proteasome subunit beta

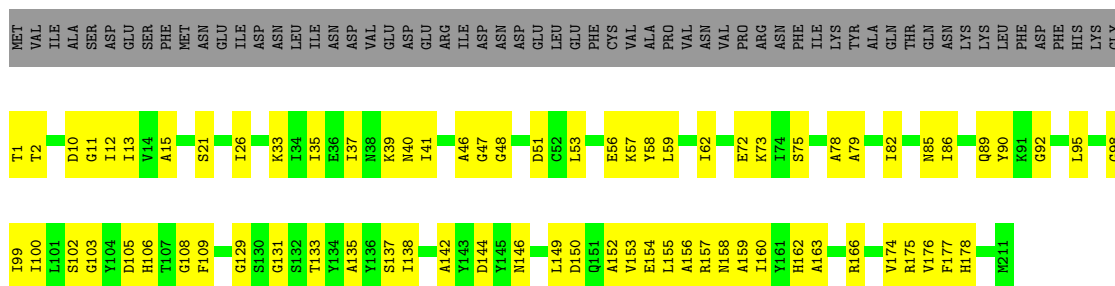


- Molecule 7: Proteasome subunit beta

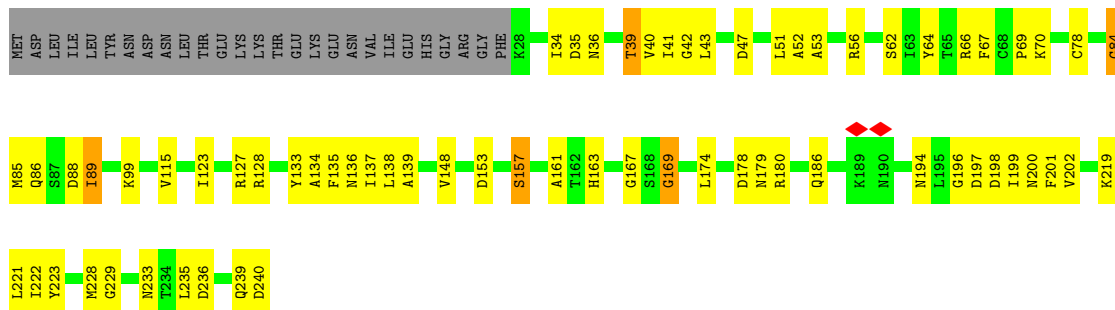




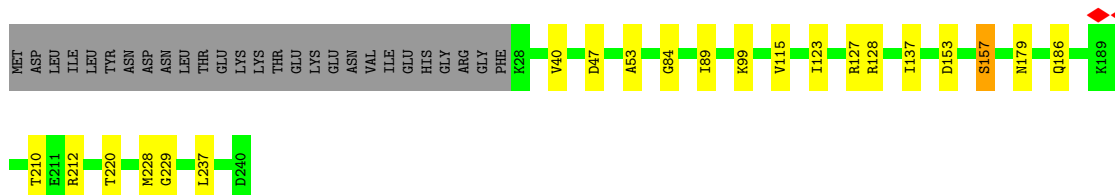
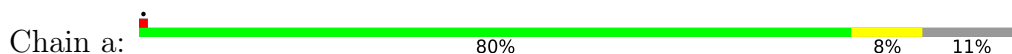
- Molecule 7: Proteasome subunit beta



- Molecule 8: Proteasome subunit beta

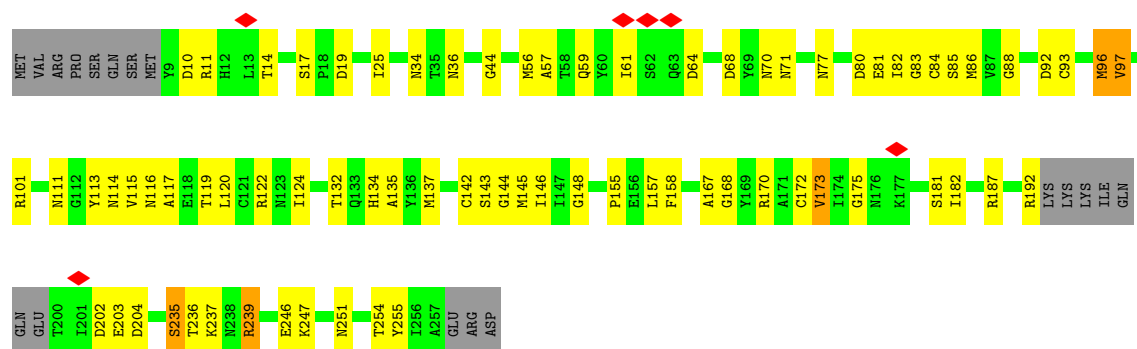


- Molecule 8: Proteasome subunit beta

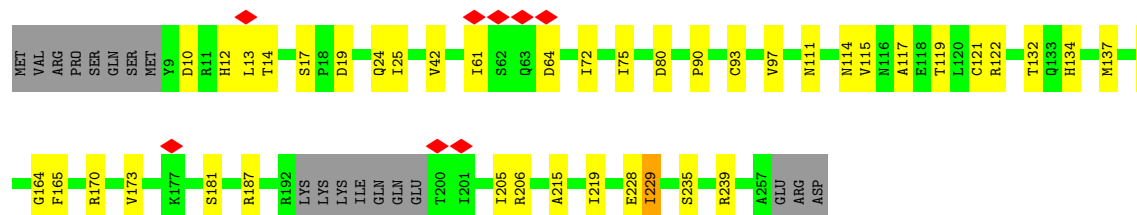
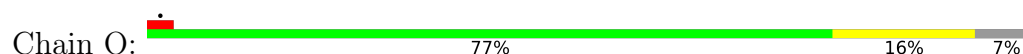


- Molecule 9: Proteasome endopeptidase complex

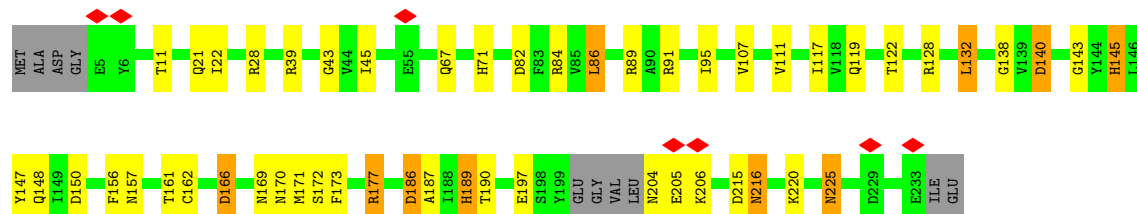
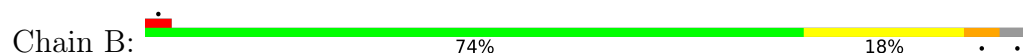




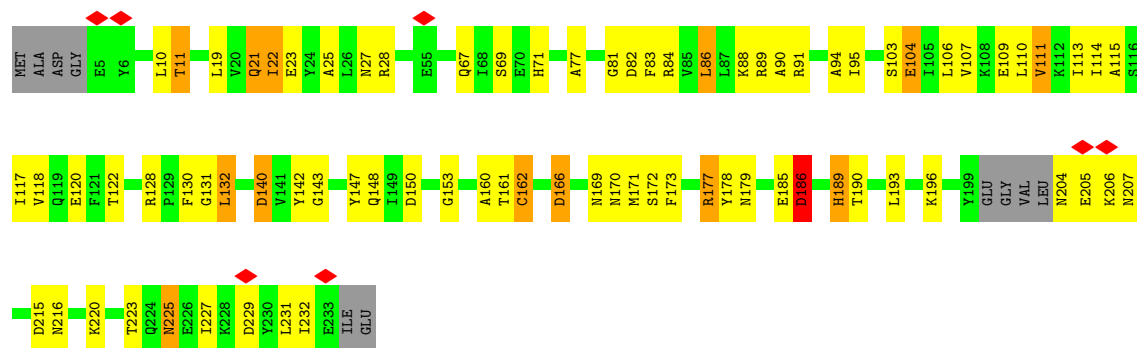
- Molecule 9: Proteasome endopeptidase complex



- Molecule 10: Proteasome endopeptidase complex

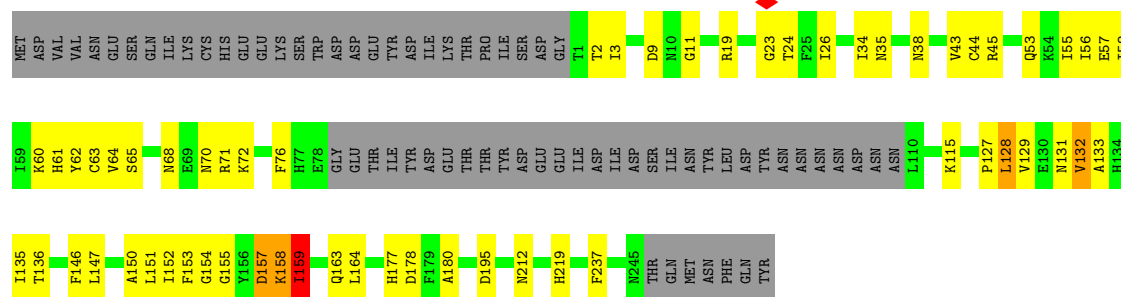


- Molecule 10: Proteasome endopeptidase complex



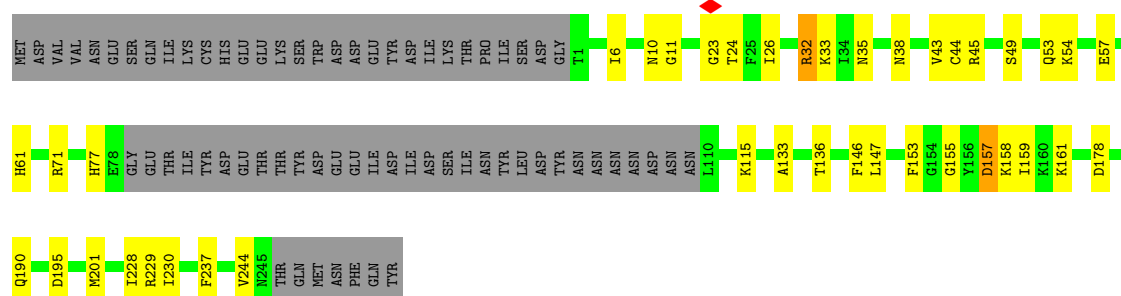
- Molecule 11: Proteasome subunit beta type-6, putative

Chain H:  55% 19% 24%



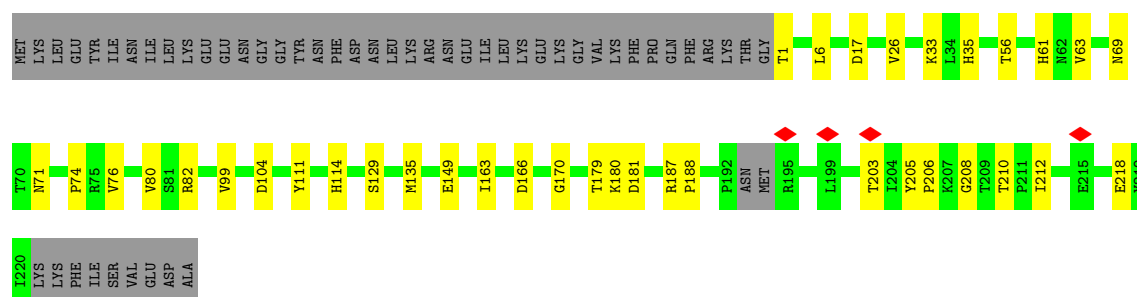
- Molecule 11: Proteasome subunit beta type-6, putative

Chain V:  62% 13% 24%



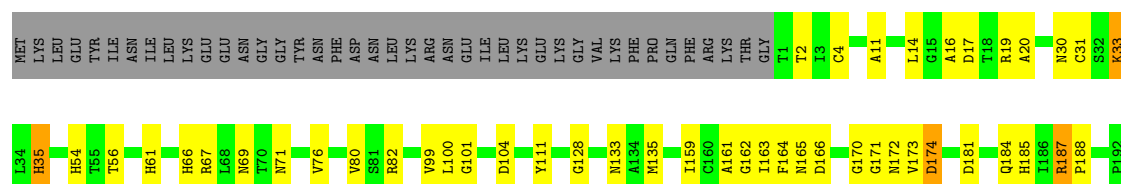
- Molecule 12: Proteasome subunit beta

Chain I:  67% 14% 19%



- Molecule 12: Proteasome subunit beta

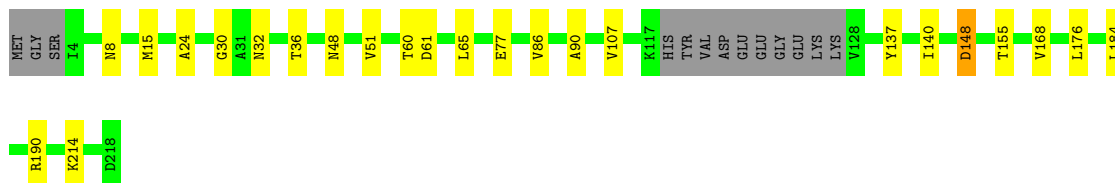
Chain W:  59% 20% 19%





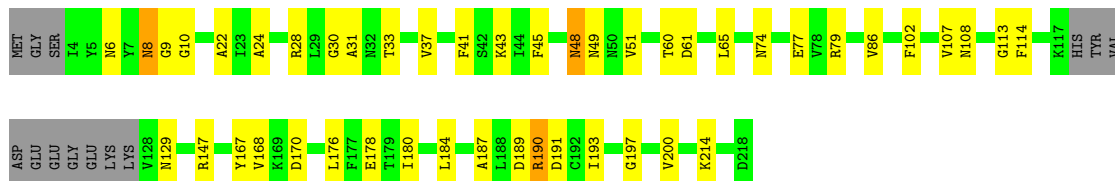
- Molecule 13: Proteasome subunit beta

Chain J: 83% 11% 6%



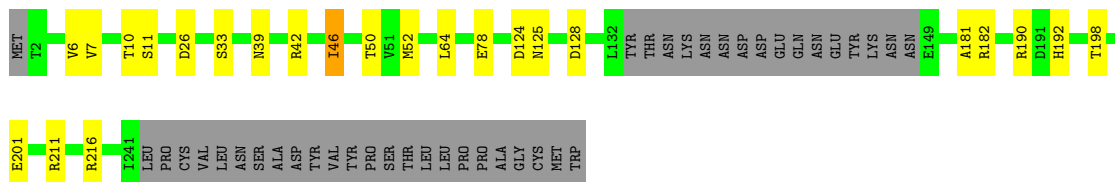
- Molecule 13: Proteasome subunit beta

Chain X: 73% 20% 6%



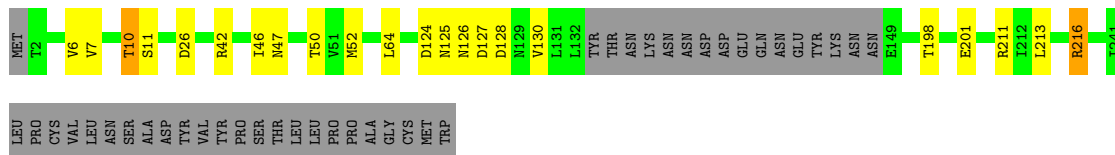
- Molecule 14: Proteasome subunit beta

Chain N: 75% 9% 15%



- Molecule 14: Proteasome subunit beta

Chain b: 76% 8% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	36364	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.727	Depositor
Minimum map value	-2.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.159	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	333.6, 333.6, 333.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.112, 1.112, 1.112	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1CY6

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	0.28	0/1952	0.45	1/2644 (0.0%)
1	Q	1.73	17/1952 (0.9%)	1.92	48/2644 (1.8%)
2	D	0.68	4/1875 (0.2%)	0.74	8/2530 (0.3%)
2	R	1.47	13/1875 (0.7%)	1.52	24/2530 (0.9%)
3	E	0.12	0/1886	0.39	0/2546
3	S	0.36	1/1886 (0.1%)	0.48	1/2546 (0.0%)
4	F	0.10	0/1913	0.32	0/2576
4	T	0.10	0/1913	0.33	0/2576
5	G	0.69	2/2052 (0.1%)	0.80	12/2774 (0.4%)
5	U	0.31	1/2052 (0.0%)	0.45	0/2774
6	K	1.79	11/1649 (0.7%)	2.01	70/2223 (3.1%)
6	Y	1.73	11/1649 (0.7%)	1.94	57/2223 (2.6%)
7	L	1.98	24/1696 (1.4%)	2.05	106/2286 (4.6%)
7	Z	1.94	26/1696 (1.5%)	2.01	101/2286 (4.4%)
8	M	1.74	21/1728 (1.2%)	1.83	85/2339 (3.6%)
8	a	0.36	3/1728 (0.2%)	0.43	2/2339 (0.1%)
9	A	1.82	24/1936 (1.2%)	1.98	90/2614 (3.4%)
9	O	1.03	5/1936 (0.3%)	1.12	14/2614 (0.5%)
10	B	1.78	13/1831 (0.7%)	1.97	47/2471 (1.9%)
10	P	2.16	26/1831 (1.4%)	2.34	120/2471 (4.9%)
11	H	1.76	15/1751 (0.9%)	1.98	70/2349 (3.0%)
11	V	1.49	7/1751 (0.4%)	1.68	23/2349 (1.0%)
12	I	0.59	1/1703 (0.1%)	0.68	2/2315 (0.1%)
12	W	1.87	27/1703 (1.6%)	1.89	53/2315 (2.3%)
13	J	0.42	0/1638	0.58	3/2211 (0.1%)
13	X	1.77	10/1638 (0.6%)	1.98	35/2211 (1.6%)
14	N	0.75	9/1882 (0.5%)	0.78	6/2538 (0.2%)
14	b	0.71	2/1882 (0.1%)	0.83	2/2538 (0.1%)
All	All	1.31	273/50984 (0.5%)	1.43	980/68832 (1.4%)

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	Q	0	2
6	K	0	2
6	Y	0	1
All	All	0	5

The worst 5 of 273 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	112	HIS	CE1-NE2	-8.86	1.23	1.32
7	Z	106	HIS	CE1-NE2	-8.86	1.23	1.32
7	L	162	HIS	CE1-NE2	-8.81	1.23	1.32
7	L	106	HIS	CE1-NE2	-8.79	1.23	1.32
10	P	71	HIS	ND1-CE1	-8.75	1.23	1.32

The worst 5 of 980 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	143	SER	CA-C-N	8.58	128.96	121.58
9	A	143	SER	C-N-CA	8.58	128.96	121.58
9	A	82	ILE	CA-C-N	8.25	129.30	121.46
9	A	82	ILE	C-N-CA	8.25	129.30	121.46
6	Y	98	PHE	CA-CB-CG	7.89	121.69	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	K	170	ARG	Sidechain
6	K	54	ARG	Sidechain
1	Q	226	TYR	Sidechain
1	Q	62	TYR	Sidechain
6	Y	54	ARG	Sidechain

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	1917	1911	1910	22	0
1	Q	1917	1911	1910	7	0
2	D	1845	1879	1878	26	0
2	R	1845	1879	1878	24	0
3	E	1860	1868	1867	23	0
3	S	1860	1868	1867	22	0
4	F	1879	1879	1878	19	0
4	T	1879	1879	1878	17	0
5	G	2008	1950	1949	15	0
5	U	2008	1950	1949	18	0
6	K	1614	1584	1584	10	0
6	Y	1614	1584	1584	8	0
7	L	1662	1615	1617	8	0
7	Z	1662	1615	1617	6	0
8	M	1696	1708	1707	13	0
8	a	1696	1708	1707	16	0
9	A	1910	1899	1897	14	0
9	O	1910	1899	1897	18	0
10	B	1798	1816	1814	15	0
10	P	1798	1816	1814	10	0
11	H	1722	1739	1740	10	0
11	V	1722	1739	1740	14	0
12	I	1668	1668	1669	26	0
12	W	1668	1668	1669	17	0
13	J	1612	1610	1608	15	0
13	X	1612	1610	1608	12	0
14	N	1845	1817	1814	11	0
14	b	1845	1817	1814	12	0
15	L	45	0	0	2	0
15	Z	45	0	0	2	0
All	All	50162	49886	49864	387	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 4.

The worst 5 of 387 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:65:GLU:OE1	3:E:65:GLU:N	2.08	0.87
4:T:68:ASP:OD2	4:T:96:LYS:NZ	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:68:ASP:OD2	4:F:96:LYS:NZ	2.08	0.86
13:J:8:ASN:ND2	13:J:30:GLY:O	2.10	0.85
3:S:65:GLU:N	3:S:65:GLU:OE1	2.11	0.83

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	238/246 (97%)	235 (99%)	3 (1%)	0	100	100
1	Q	238/246 (97%)	234 (98%)	4 (2%)	0	100	100
2	D	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
2	R	231/241 (96%)	220 (95%)	11 (5%)	0	100	100
3	E	238/256 (93%)	231 (97%)	7 (3%)	0	100	100
3	S	238/256 (93%)	232 (98%)	6 (2%)	0	100	100
4	F	235/254 (92%)	230 (98%)	5 (2%)	0	100	100
4	T	235/254 (92%)	231 (98%)	4 (2%)	0	100	100
5	G	243/252 (96%)	232 (96%)	11 (4%)	0	100	100
5	U	243/252 (96%)	233 (96%)	10 (4%)	0	100	100
6	K	193/195 (99%)	184 (95%)	7 (4%)	2 (1%)	12	32
6	Y	193/195 (99%)	183 (95%)	8 (4%)	2 (1%)	12	32
7	L	209/271 (77%)	206 (99%)	3 (1%)	0	100	100
7	Z	209/271 (77%)	206 (99%)	3 (1%)	0	100	100
8	M	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
8	a	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
9	A	238/260 (92%)	233 (98%)	4 (2%)	1 (0%)	30	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	O	238/260 (92%)	230 (97%)	7 (3%)	1 (0%)	30	54
10	B	221/235 (94%)	216 (98%)	4 (2%)	1 (0%)	24	48
10	P	221/235 (94%)	217 (98%)	3 (1%)	1 (0%)	24	48
11	H	210/282 (74%)	203 (97%)	7 (3%)	0	100	100
11	V	210/282 (74%)	204 (97%)	6 (3%)	0	100	100
12	I	214/270 (79%)	202 (94%)	12 (6%)	0	100	100
12	W	214/270 (79%)	200 (94%)	14 (6%)	0	100	100
13	J	201/218 (92%)	195 (97%)	6 (3%)	0	100	100
13	X	201/218 (92%)	194 (96%)	7 (4%)	0	100	100
14	N	220/265 (83%)	214 (97%)	6 (3%)	0	100	100
14	b	220/265 (83%)	214 (97%)	6 (3%)	0	100	100
All	All	6204/6970 (89%)	6009 (97%)	187 (3%)	8 (0%)	49	73

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	P	206	LYS
10	B	206	LYS
6	K	99	GLU
6	Y	99	GLU
9	A	61	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	207/213 (97%)	204 (99%)	3 (1%)	59	82
1	Q	207/213 (97%)	201 (97%)	6 (3%)	37	67
2	D	199/207 (96%)	197 (99%)	2 (1%)	68	86
2	R	199/207 (96%)	193 (97%)	6 (3%)	36	66
3	E	208/223 (93%)	206 (99%)	2 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	208/223 (93%)	205 (99%)	3 (1%)	59	82
4	F	211/227 (93%)	210 (100%)	1 (0%)	81	92
4	T	211/227 (93%)	208 (99%)	3 (1%)	59	82
5	G	224/229 (98%)	223 (100%)	1 (0%)	84	93
5	U	224/229 (98%)	223 (100%)	1 (0%)	84	93
6	K	174/174 (100%)	169 (97%)	5 (3%)	37	67
6	Y	174/174 (100%)	169 (97%)	5 (3%)	37	67
7	L	176/232 (76%)	174 (99%)	2 (1%)	65	85
7	Z	176/232 (76%)	175 (99%)	1 (1%)	78	91
8	M	191/216 (88%)	188 (98%)	3 (2%)	55	80
8	a	191/216 (88%)	190 (100%)	1 (0%)	81	92
9	A	213/231 (92%)	210 (99%)	3 (1%)	59	82
9	O	213/231 (92%)	207 (97%)	6 (3%)	38	68
10	B	198/205 (97%)	191 (96%)	7 (4%)	32	61
10	P	198/205 (97%)	190 (96%)	8 (4%)	28	56
11	H	194/260 (75%)	191 (98%)	3 (2%)	57	81
11	V	194/260 (75%)	190 (98%)	4 (2%)	47	75
12	I	184/231 (80%)	182 (99%)	2 (1%)	65	85
12	W	184/231 (80%)	178 (97%)	6 (3%)	33	63
13	J	180/191 (94%)	178 (99%)	2 (1%)	65	85
13	X	180/191 (94%)	179 (99%)	1 (1%)	78	91
14	N	201/239 (84%)	200 (100%)	1 (0%)	81	92
14	b	201/239 (84%)	199 (99%)	2 (1%)	68	86
All	All	5520/6156 (90%)	5430 (98%)	90 (2%)	54	80

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	159	ILE
10	P	162	CYS
12	I	210	THR
9	O	72	ILE
10	P	189	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
4	T	227	GLN
10	P	157	ASN
7	Z	30	ASN
10	P	148	GLN
12	W	30	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	A1CY6	Z	301	7	47,47,47	0.21	0	62,62,62	0.63	1 (1%)
15	A1CY6	L	301	7	47,47,47	0.22	0	62,62,62	0.62	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1CY6	Z	301	7	-	13/55/55/55	0/2/3/3
15	A1CY6	L	301	7	-	13/55/55/55	0/2/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	A1CY6	C13-N12-C10	2.42	127.33	122.82
15	Z	301	A1CY6	C13-N12-C10	2.40	127.29	122.82

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

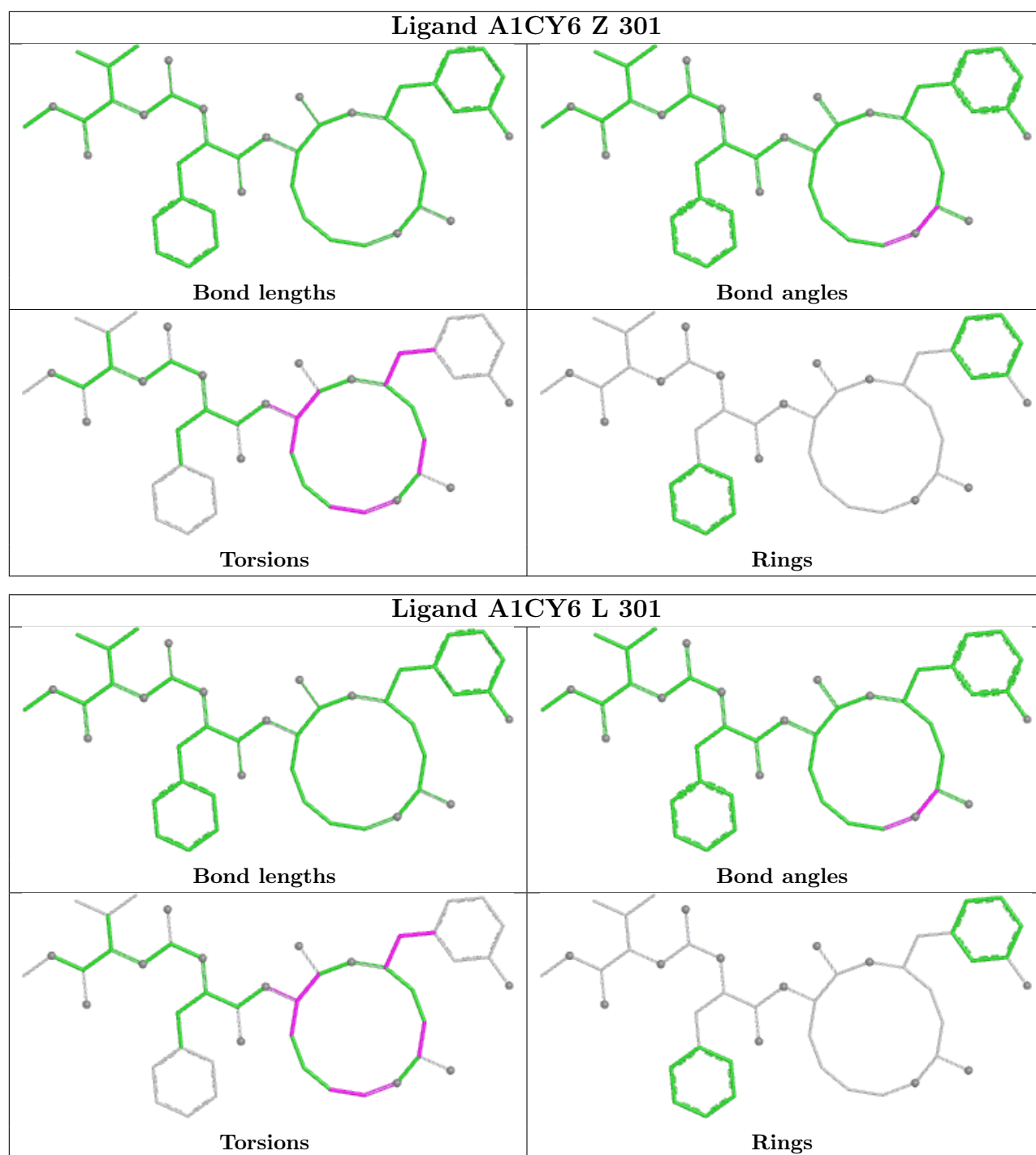
Mol	Chain	Res	Type	Atoms
15	L	301	A1CY6	C16-C18-C42-C43
15	Z	301	A1CY6	C16-C18-C42-C43
15	L	301	A1CY6	C14-C13-N12-C10
15	Z	301	A1CY6	C14-C13-N12-C10
15	L	301	A1CY6	N19-C18-C42-C43

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Z	301	A1CY6	2	0
15	L	301	A1CY6	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

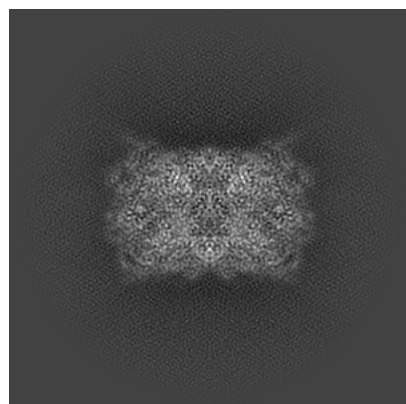
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73509. These allow visual inspection of the internal detail of the map and identification of artifacts.

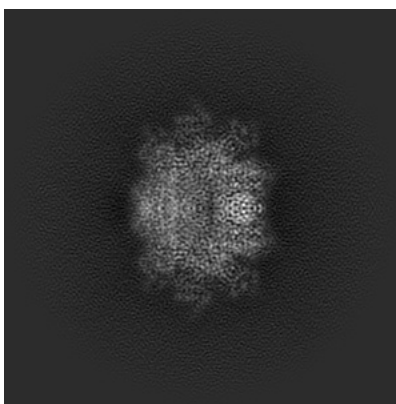
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

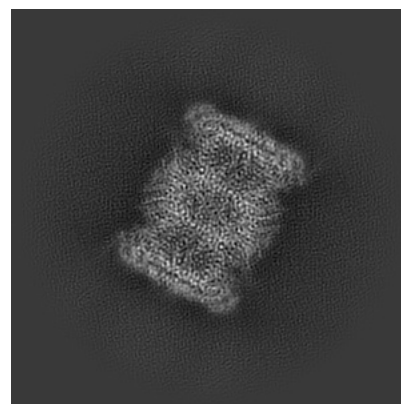
6.1.1 Primary map



X

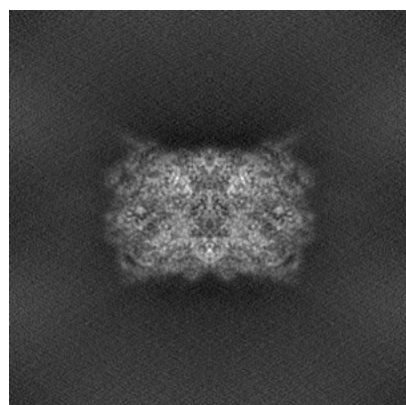


Y

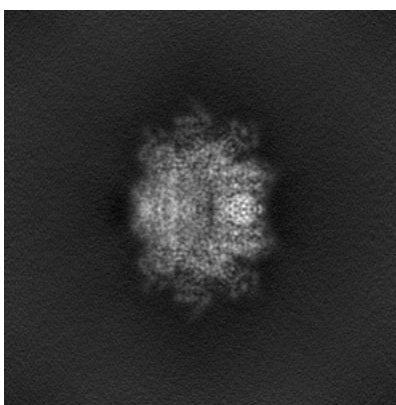


Z

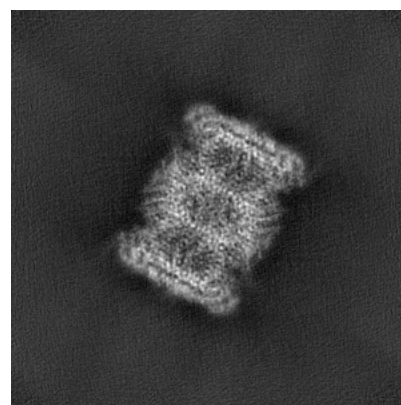
6.1.2 Raw map



X



Y

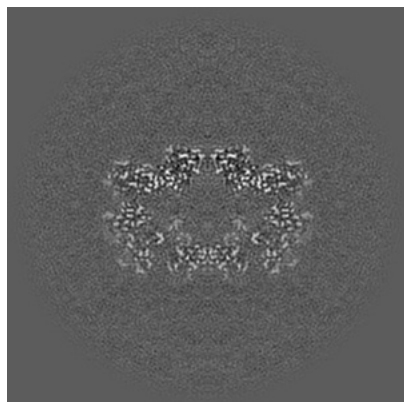


Z

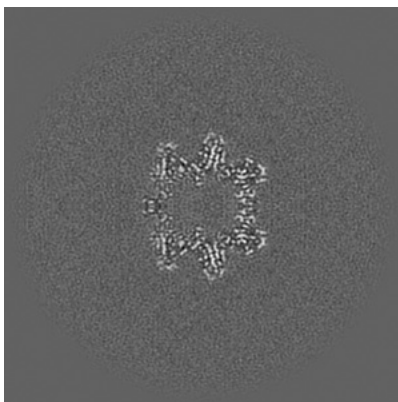
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

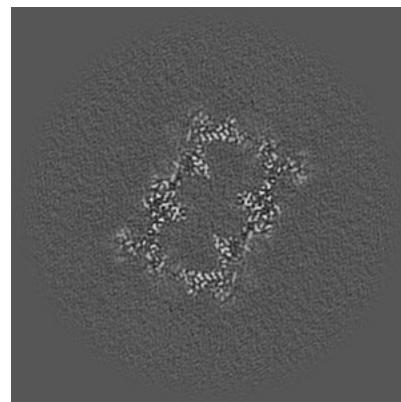
6.2.1 Primary map



X Index: 150

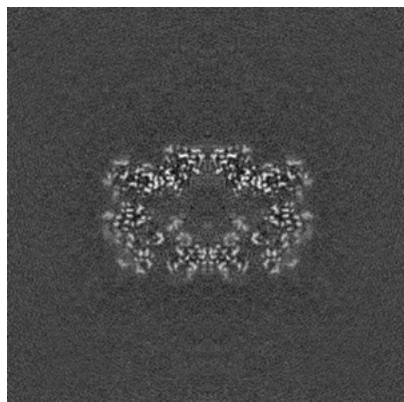


Y Index: 150

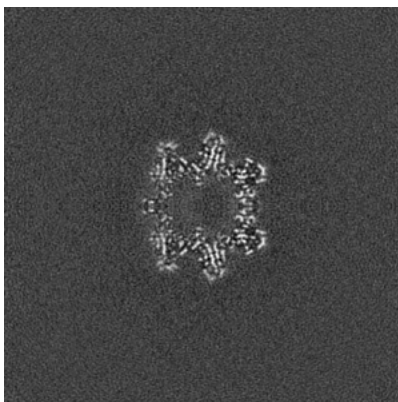


Z Index: 150

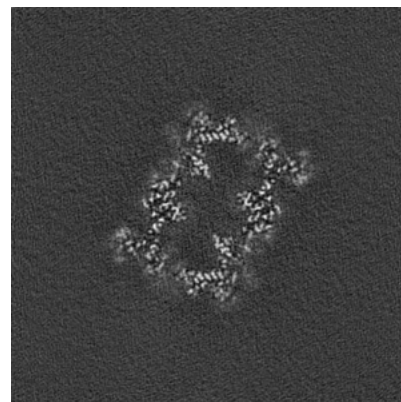
6.2.2 Raw map



X Index: 150



Y Index: 150

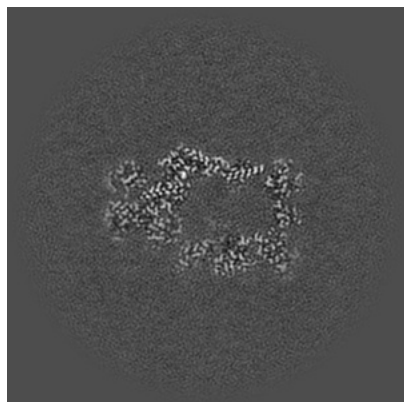


Z Index: 150

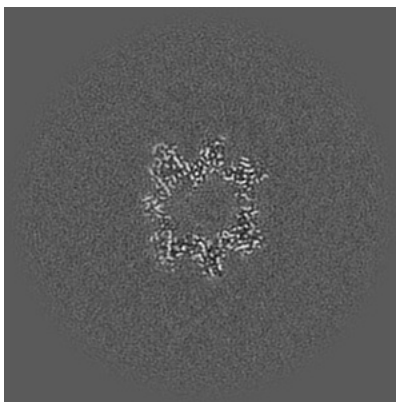
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

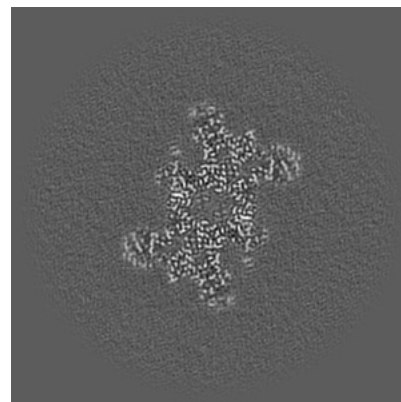
6.3.1 Primary map



X Index: 158

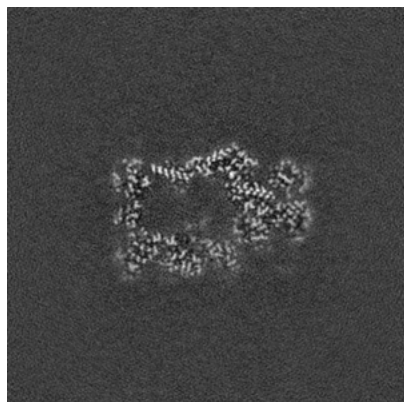


Y Index: 152

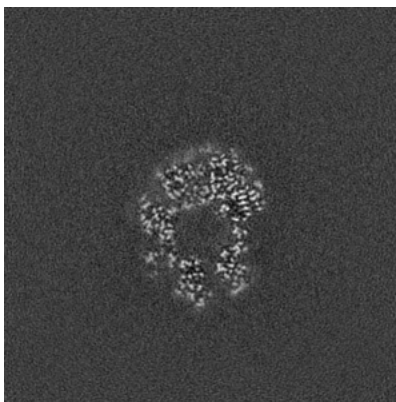


Z Index: 172

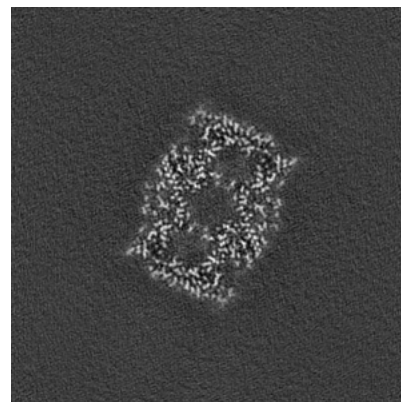
6.3.2 Raw map



X Index: 142



Y Index: 126

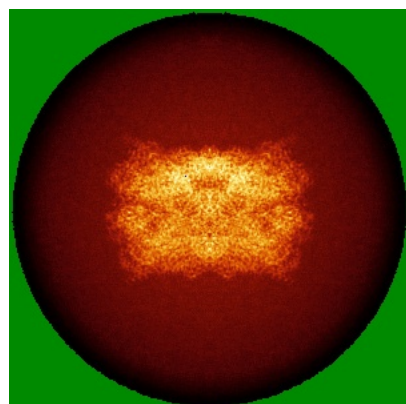


Z Index: 164

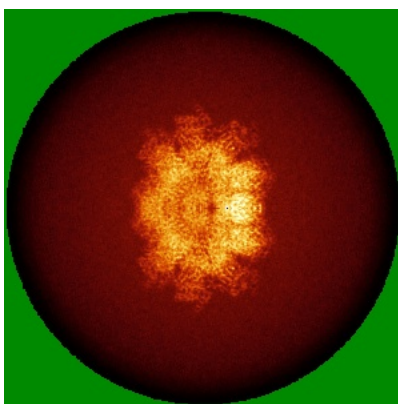
The images above show the largest variance slices of the map in three orthogonal directions.

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

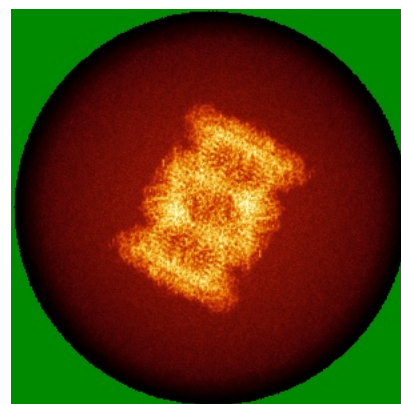
6.4.1 Primary map



X

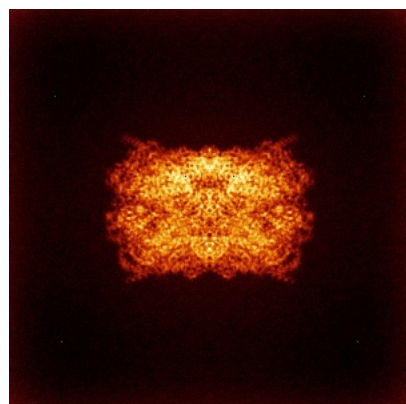


Y

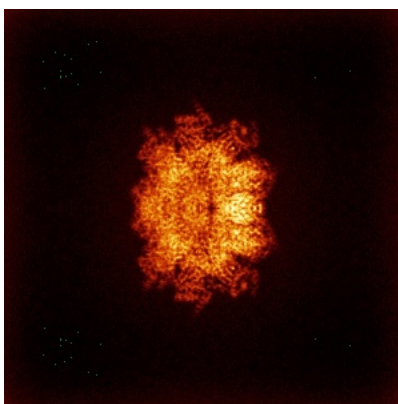


Z

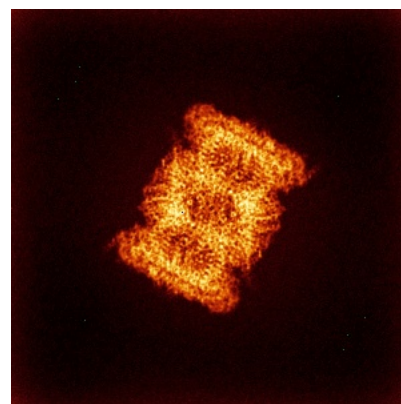
6.4.2 Raw map



X



Y

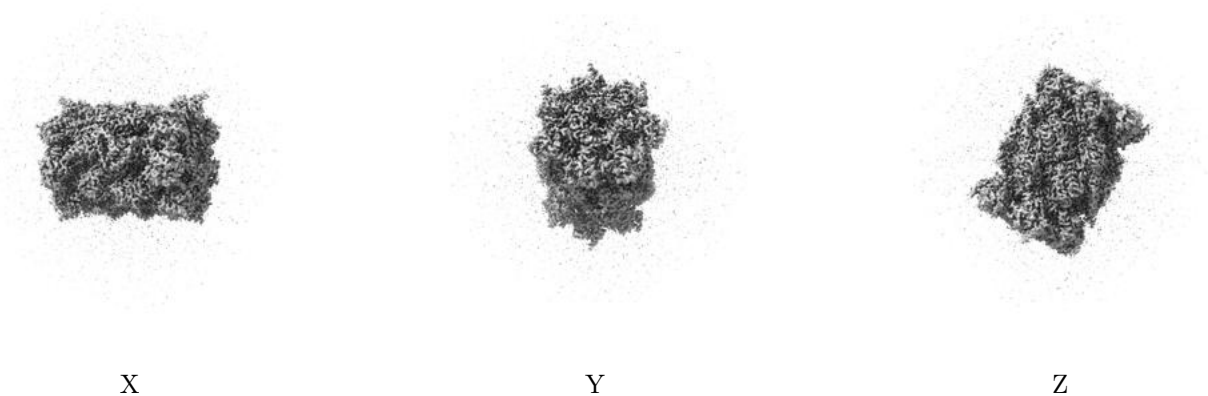


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

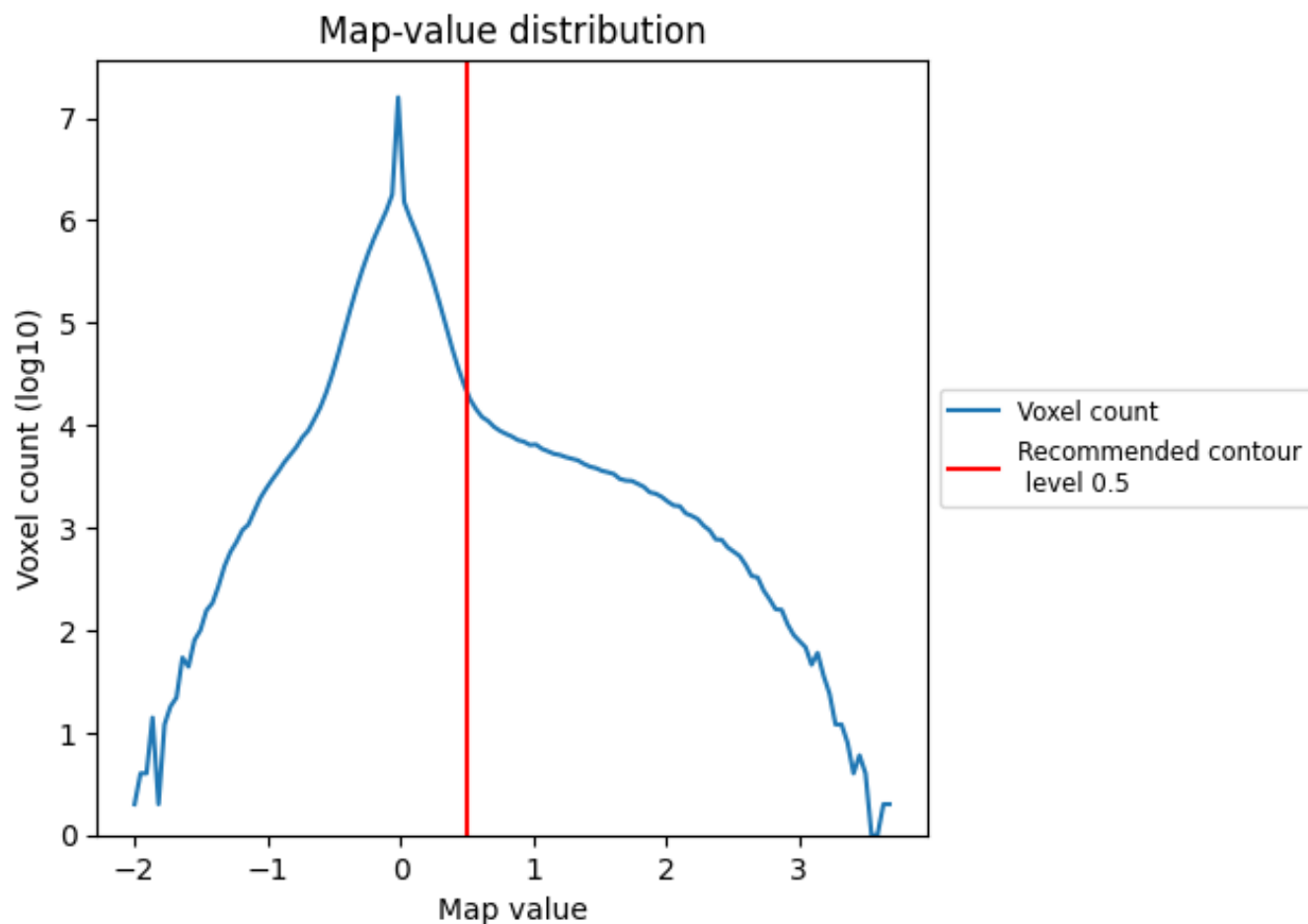
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

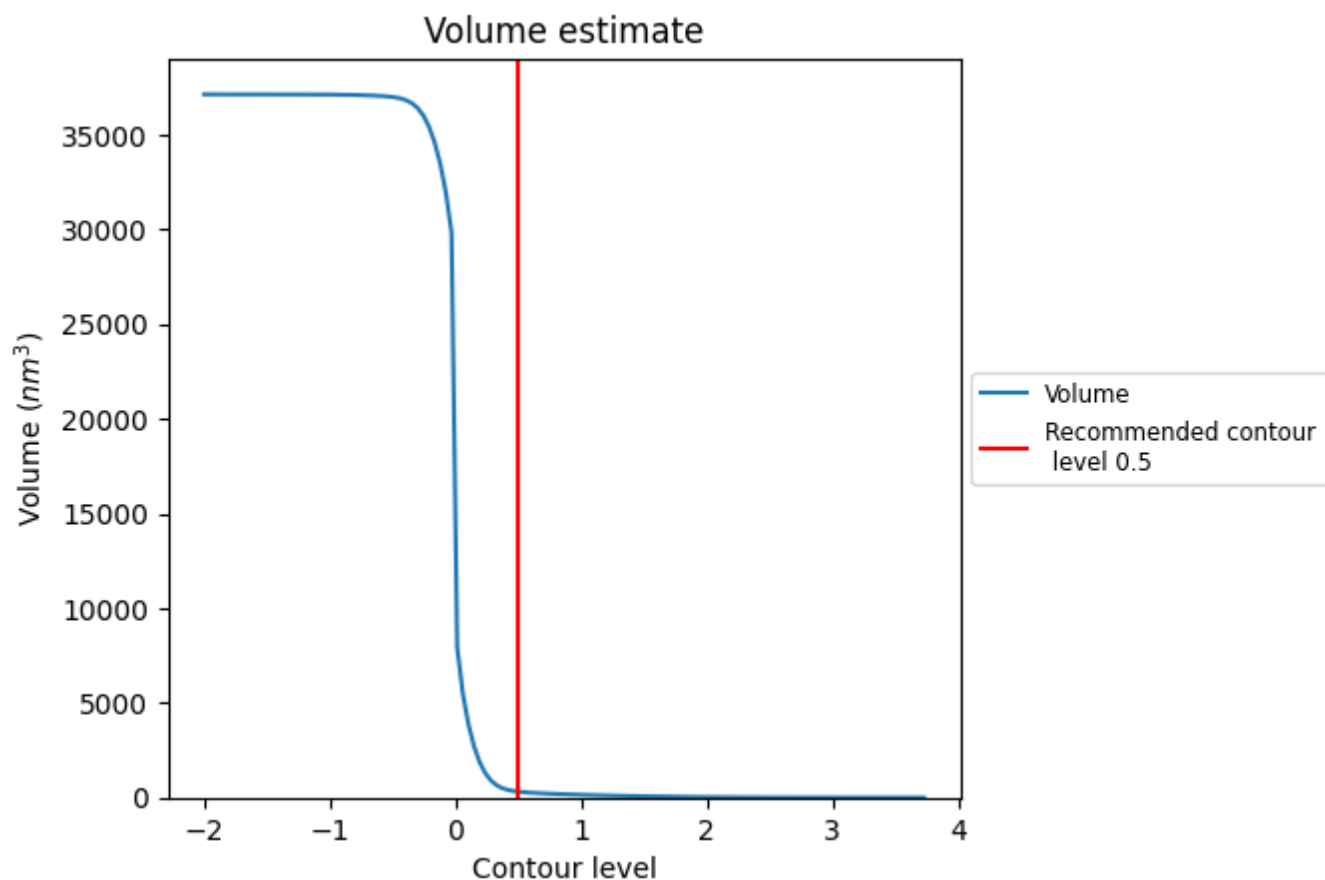
This section contains the results of statistical analysis of the map.

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.

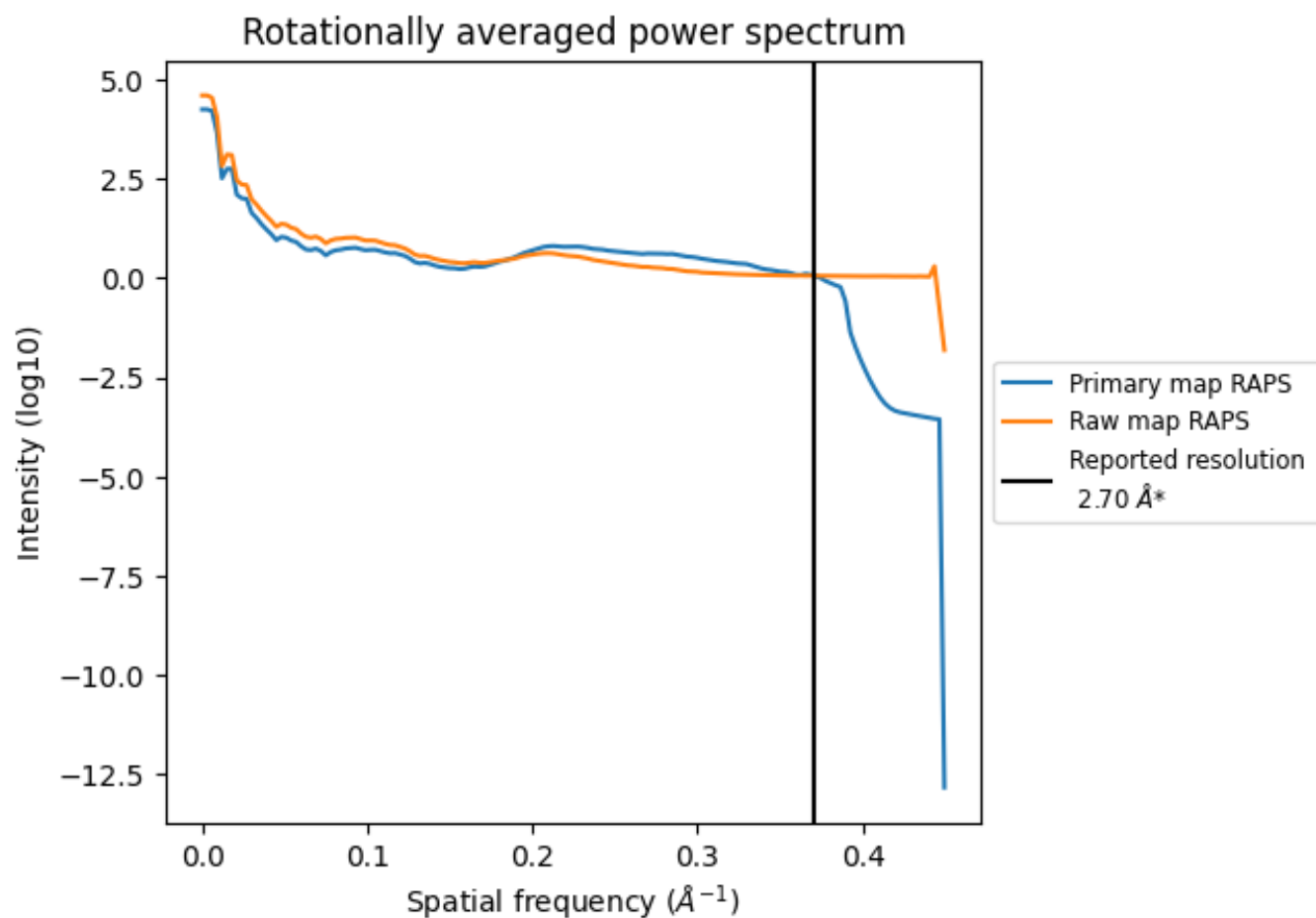
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm³; this corresponds to an approximate mass of 281 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

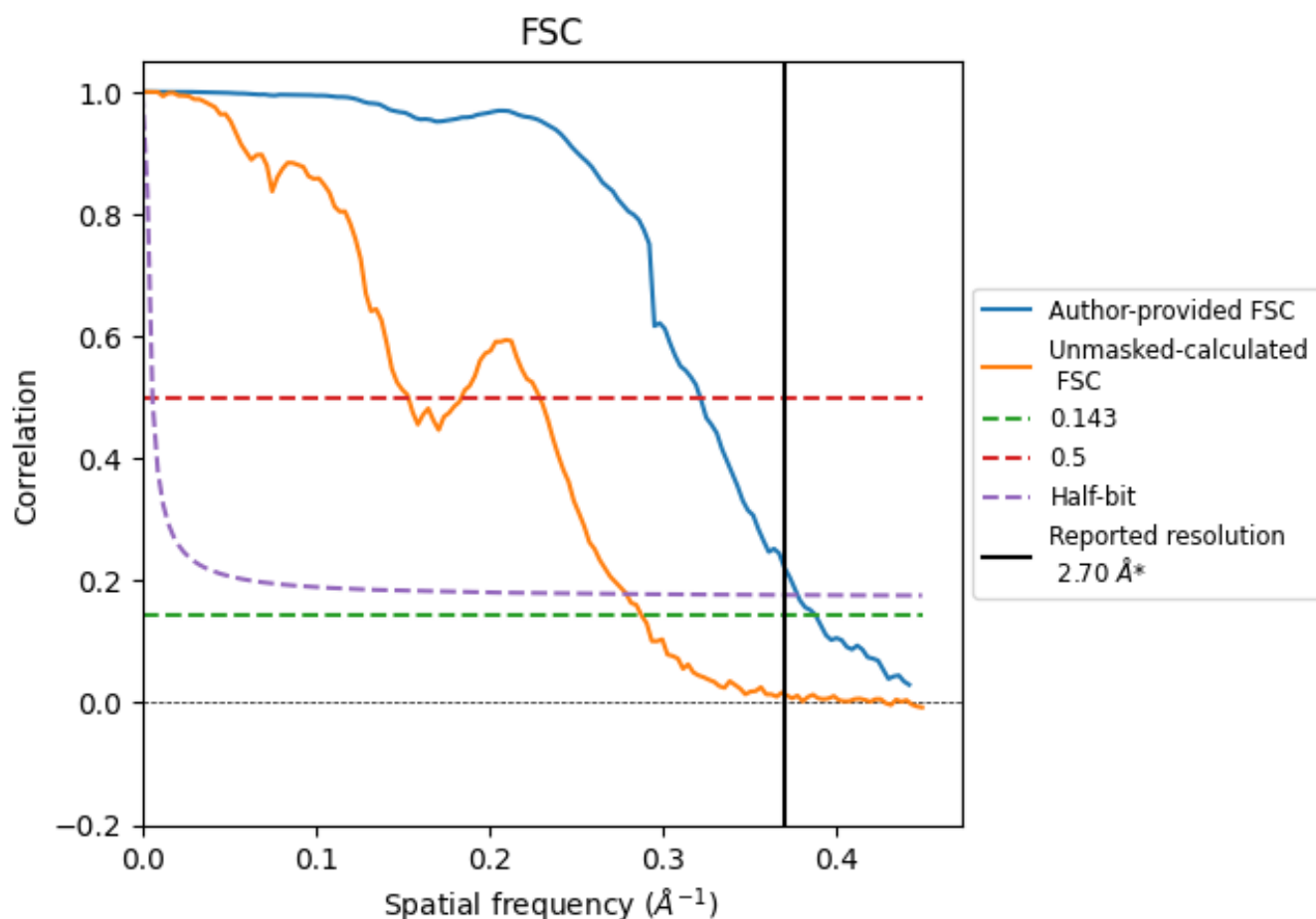


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

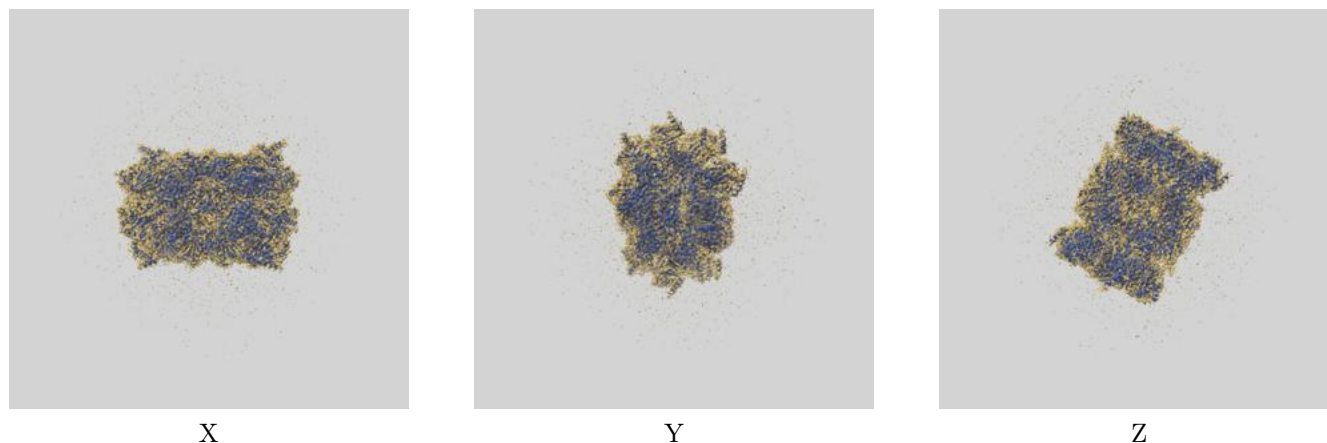
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.58	3.11	2.65
Unmasked-calculated*	3.47	6.52	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

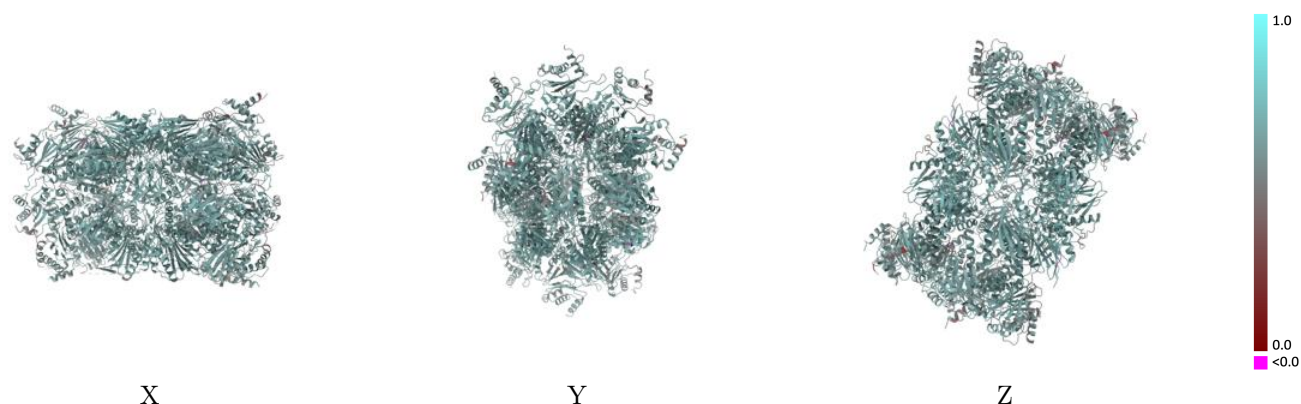
This section contains information regarding the fit between EMDB map EMD-73509 and PDB model 9YUY. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



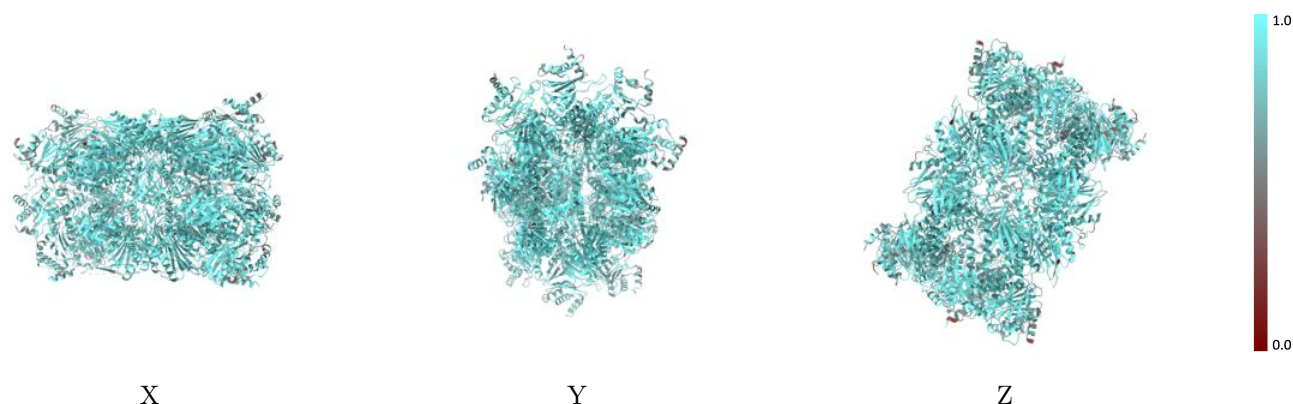
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



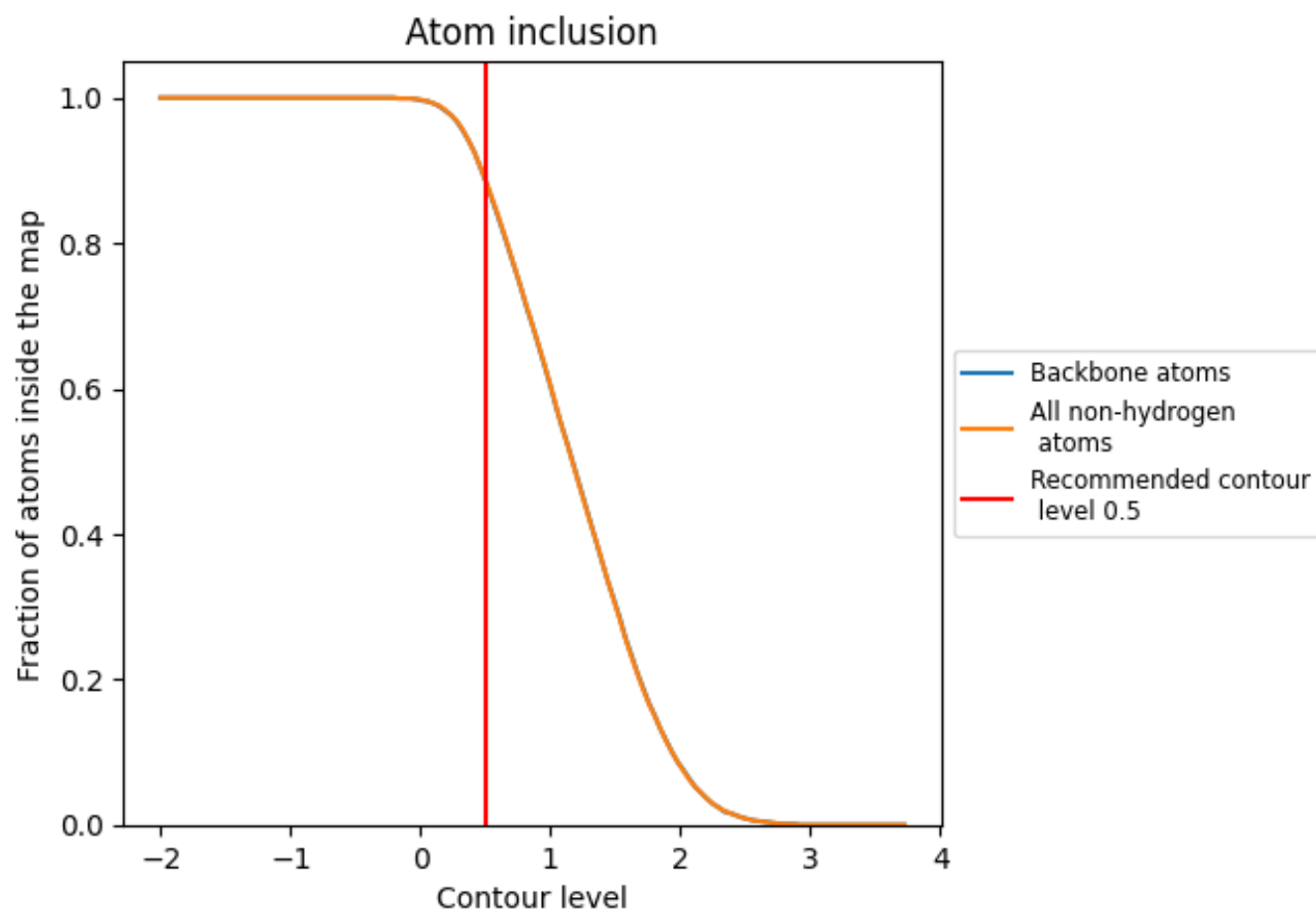
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.6100
A	 0.8420	 0.5930
B	 0.8400	 0.5890
C	 0.8580	 0.5990
D	 0.8450	 0.5920
E	 0.8070	 0.5650
F	 0.8770	 0.6060
G	 0.8860	 0.6080
H	 0.8910	 0.6180
I	 0.8860	 0.5930
J	 0.9430	 0.6310
K	 0.9510	 0.6360
L	 0.9590	 0.6490
M	 0.9400	 0.6390
N	 0.9370	 0.6310
O	 0.8410	 0.5910
P	 0.8400	 0.5880
Q	 0.8630	 0.6010
R	 0.8480	 0.5970
S	 0.8050	 0.5650
T	 0.8770	 0.6080
U	 0.8860	 0.6060
V	 0.8910	 0.6170
W	 0.8870	 0.5930
X	 0.9420	 0.6340
Y	 0.9510	 0.6350
Z	 0.9610	 0.6500
a	 0.9360	 0.6340
b	 0.9380	 0.6330

