



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:07 PM UTC

PDB ID : 7V5M / pdb_00007v5m
EMDB ID : EMD-31727
Title : 20S+monoUb-CyclinB1-NT (S2)
Authors : Xu, C.; Cong, Y.
Deposited on : 2021-08-17
Resolution : 3.88 Å(reported)

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
MolProbity : 4-5-2 with Phenix2.0
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

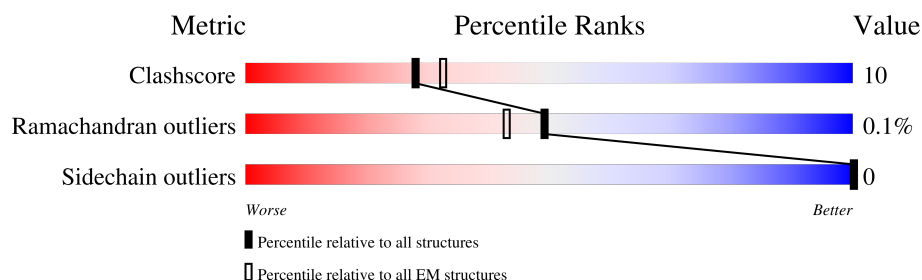
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.88 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	246	98% 80% 17% .
1	O	246	94% 82% 15% .
2	B	234	98% 79% 19% .
2	P	234	97% 78% 20% .
3	C	261	95% 78% 16% 5%
3	Q	261	91% 78% 16% 5%
4	D	248	94% 77% 16% 6%
4	R	248	79% 77% 16% 6%

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Mol	Chain	Length	Quality of chain
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	213	
13	a	213	
14	N	219	
14	b	219	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 45340 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		
5	S	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		
13	a	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		

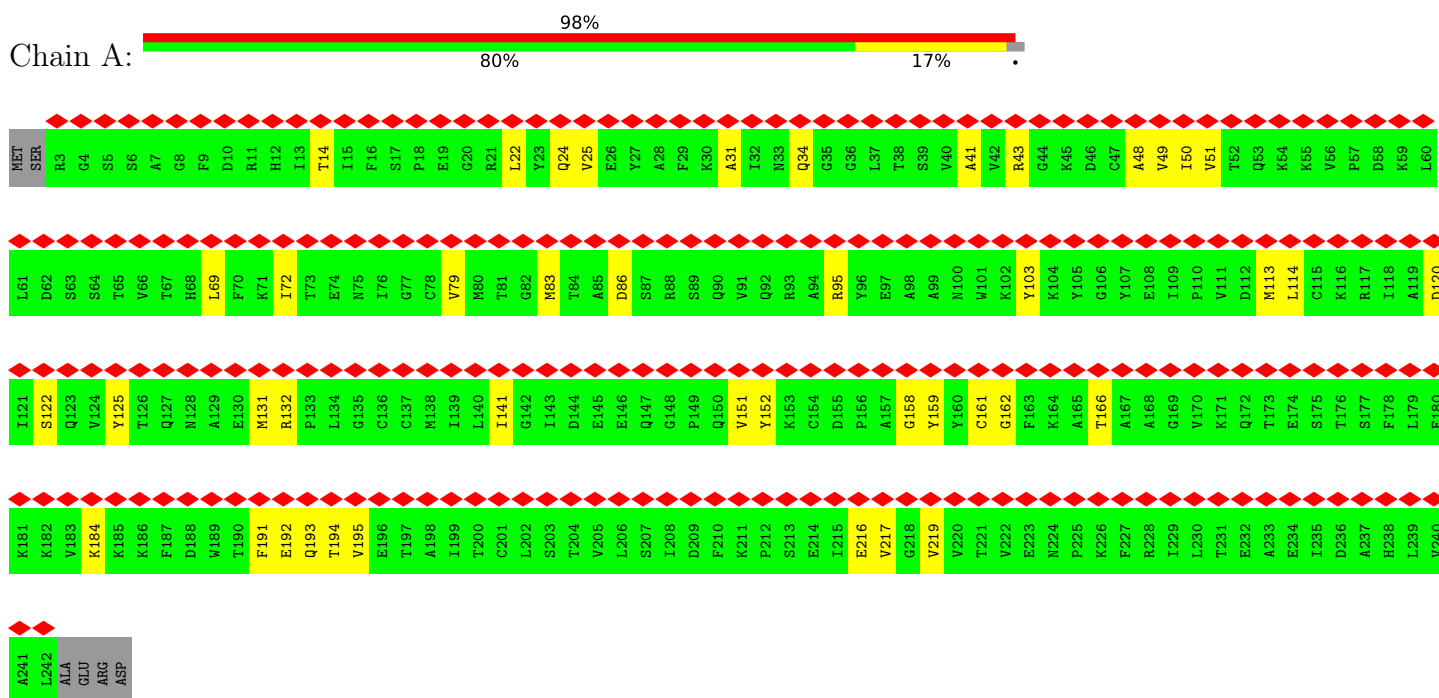
- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		

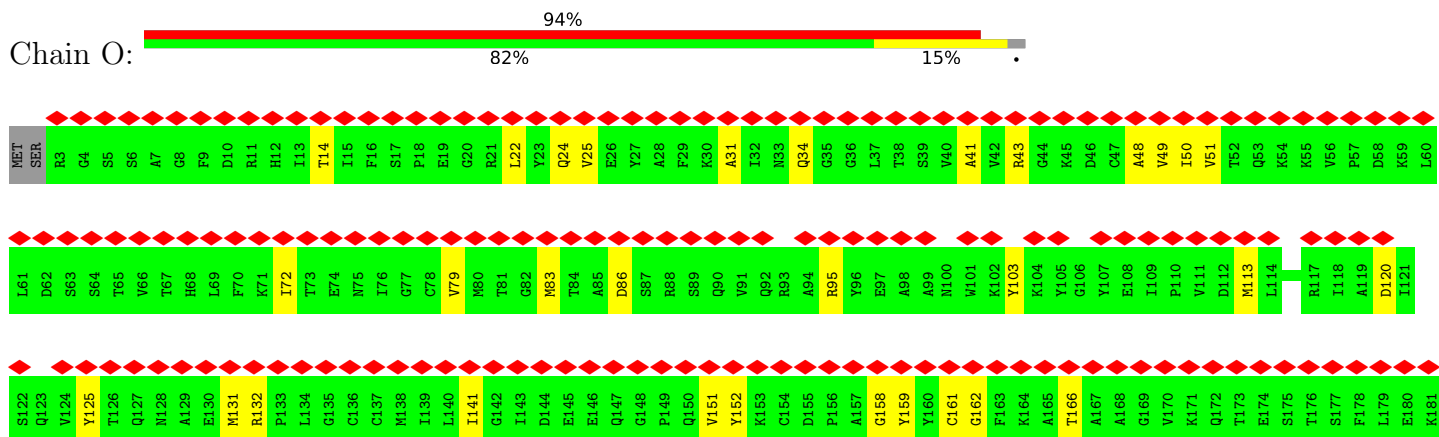
3 Residue-property plots

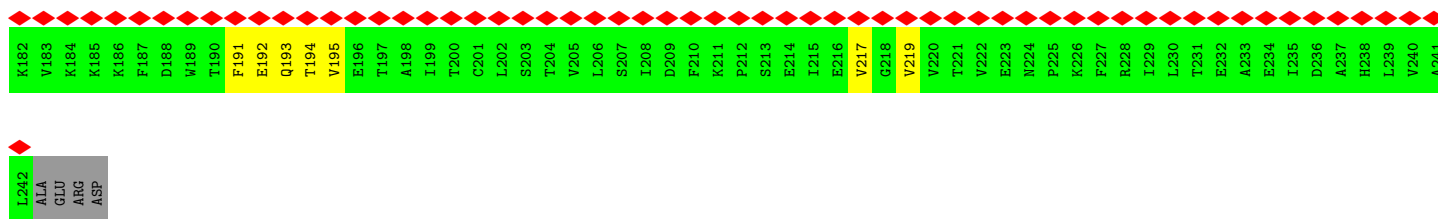
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Proteasome subunit alpha type-6

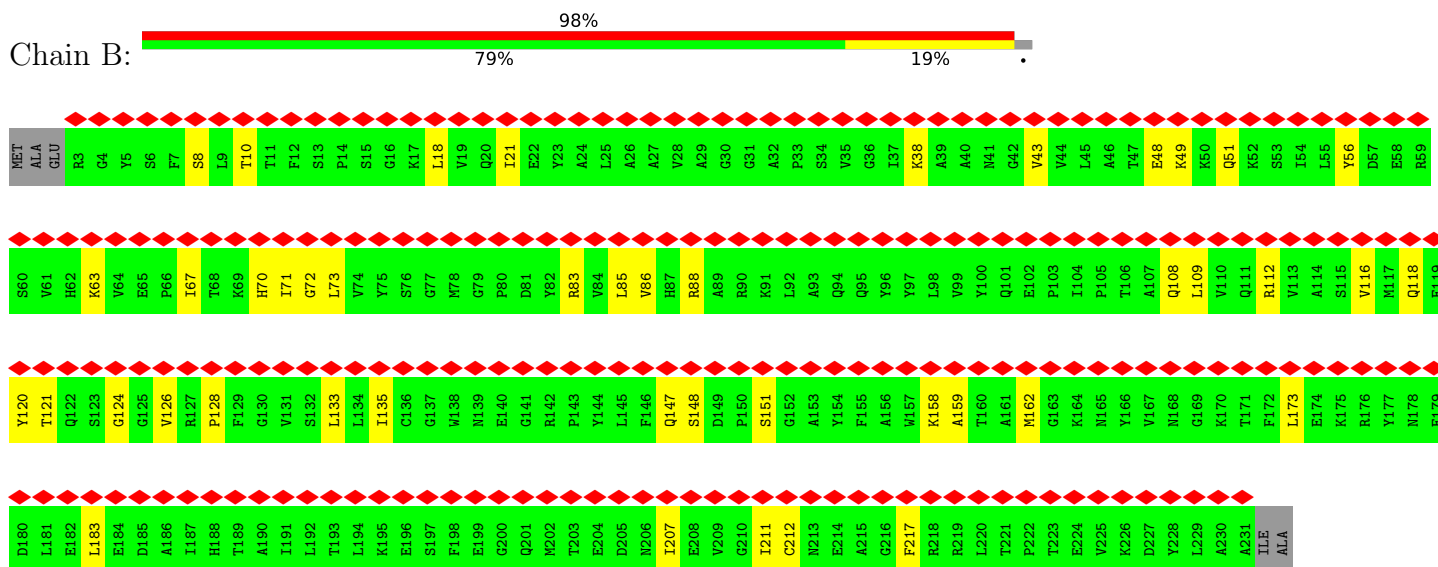


• Molecule 1: Proteasome subunit alpha type-6

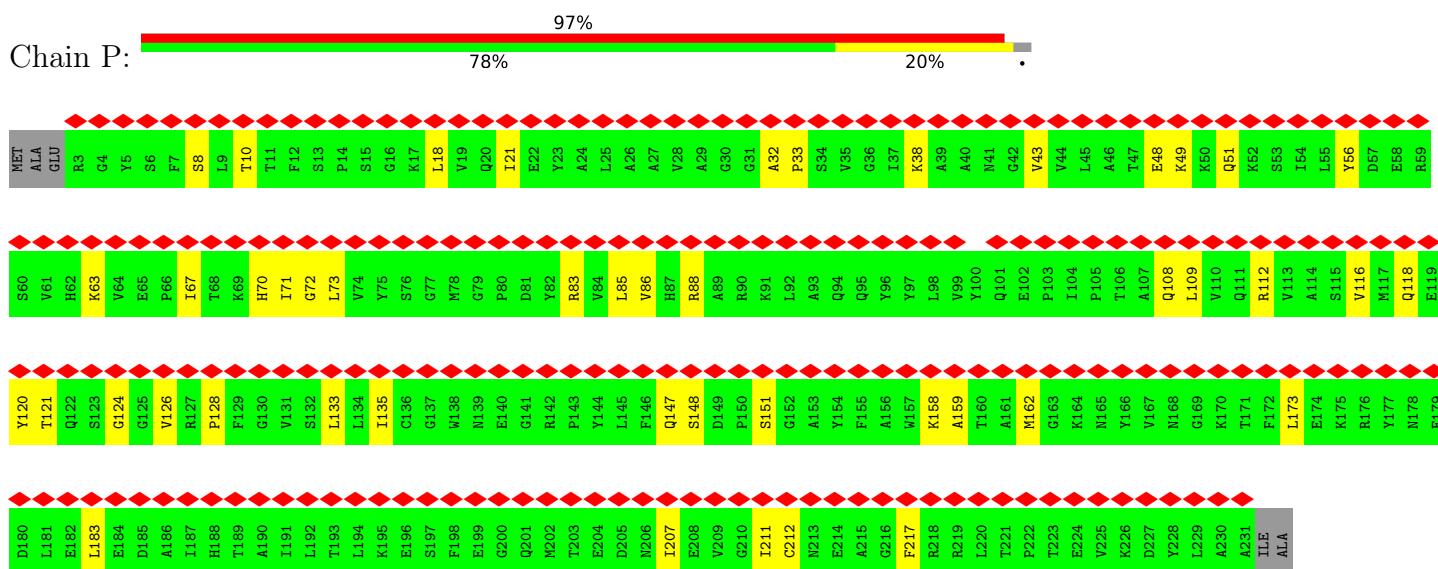




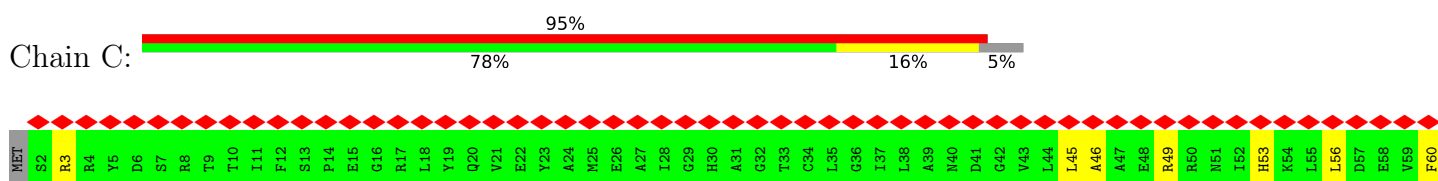
• Molecule 2: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-2

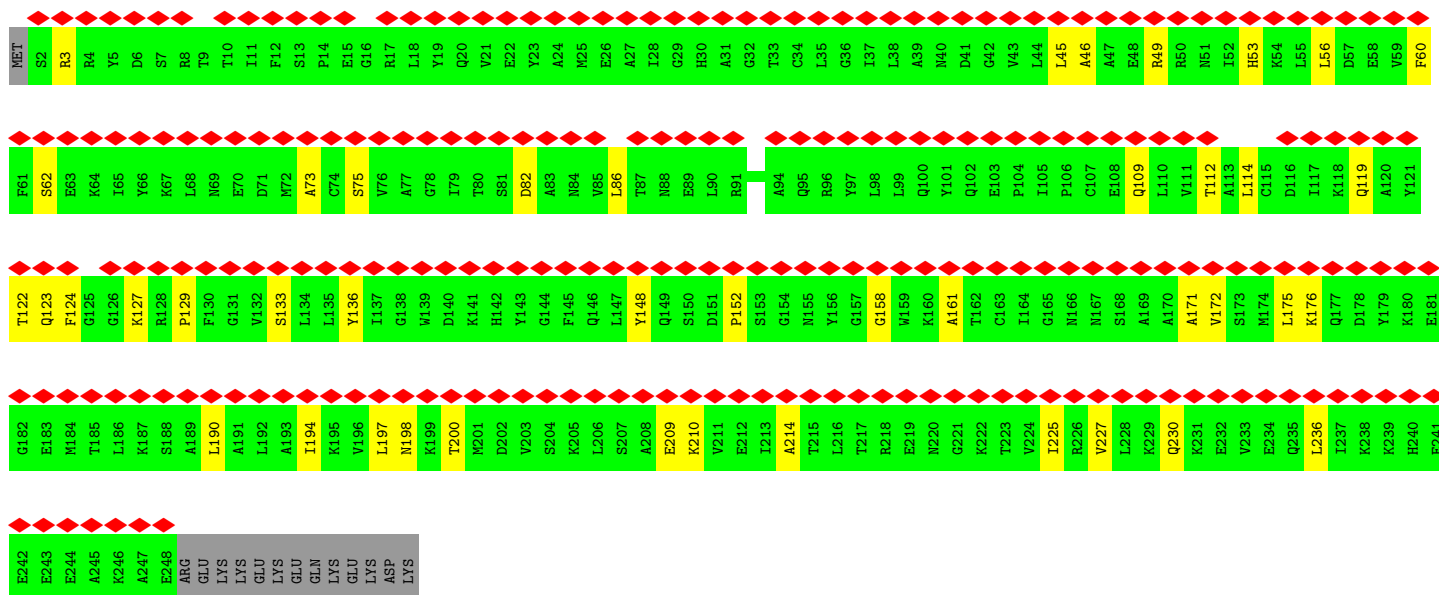
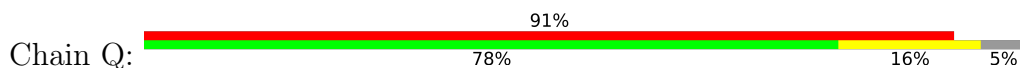


• Molecule 3: Proteasome subunit alpha type-4

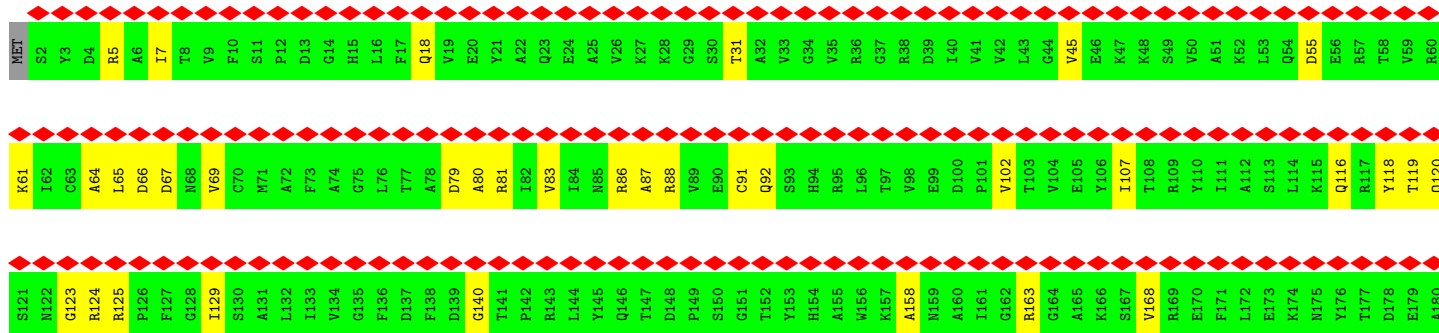
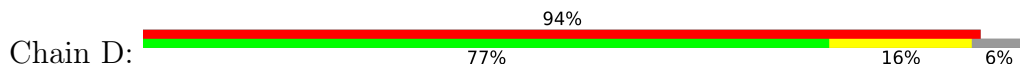


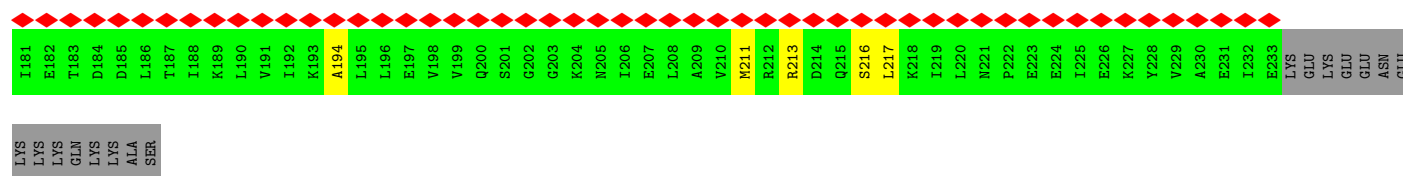


• Molecule 3: Proteasome subunit alpha type-4

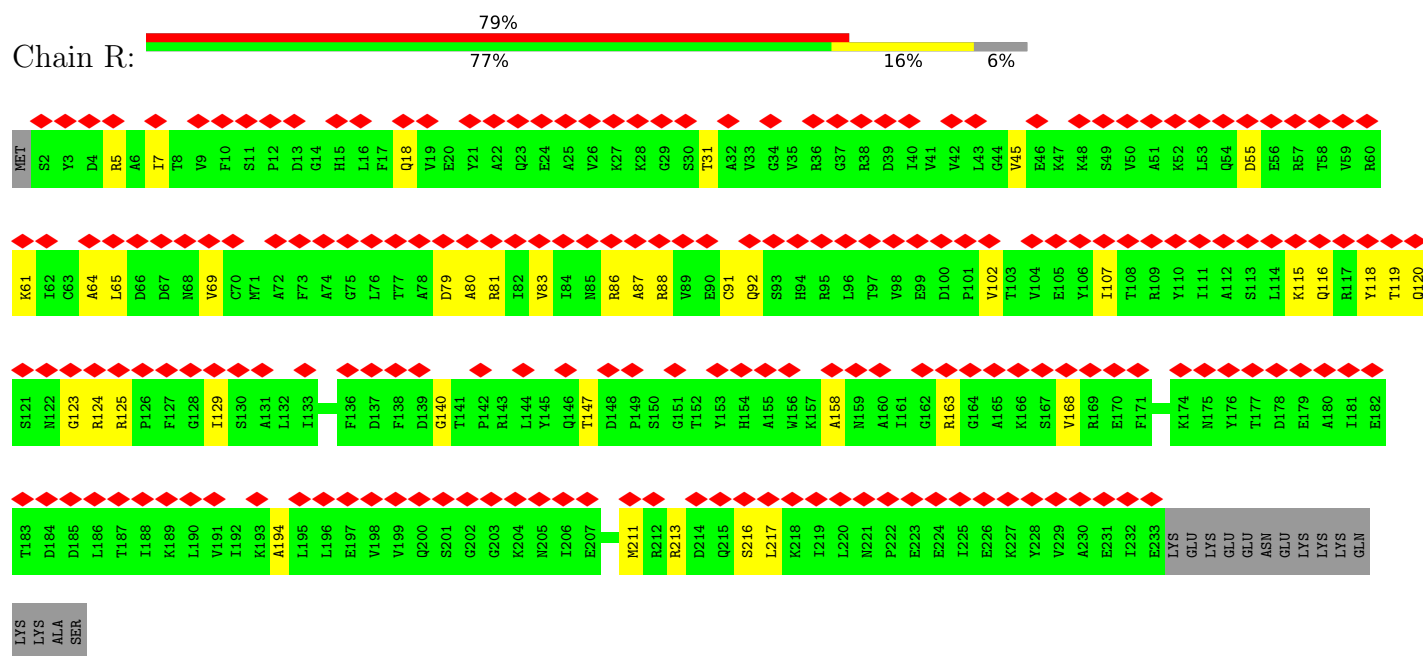


• Molecule 4: Proteasome subunit alpha type-7

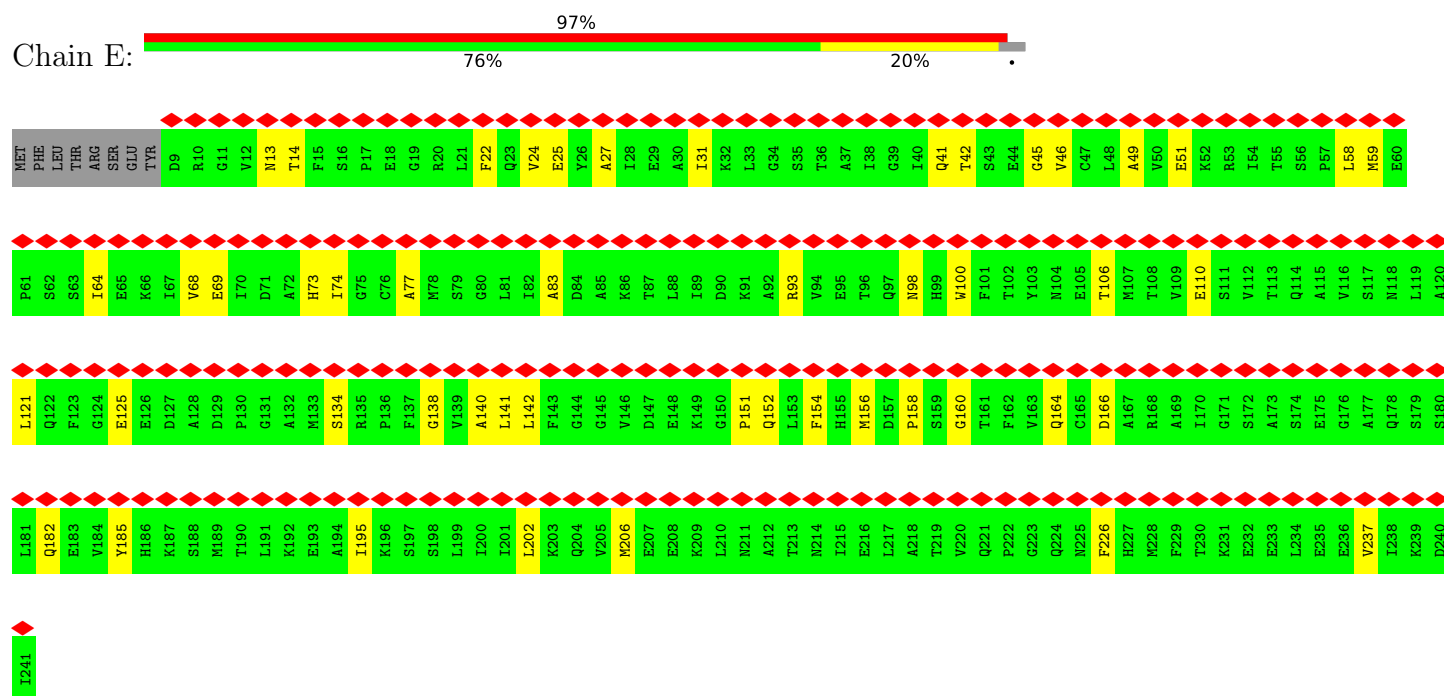




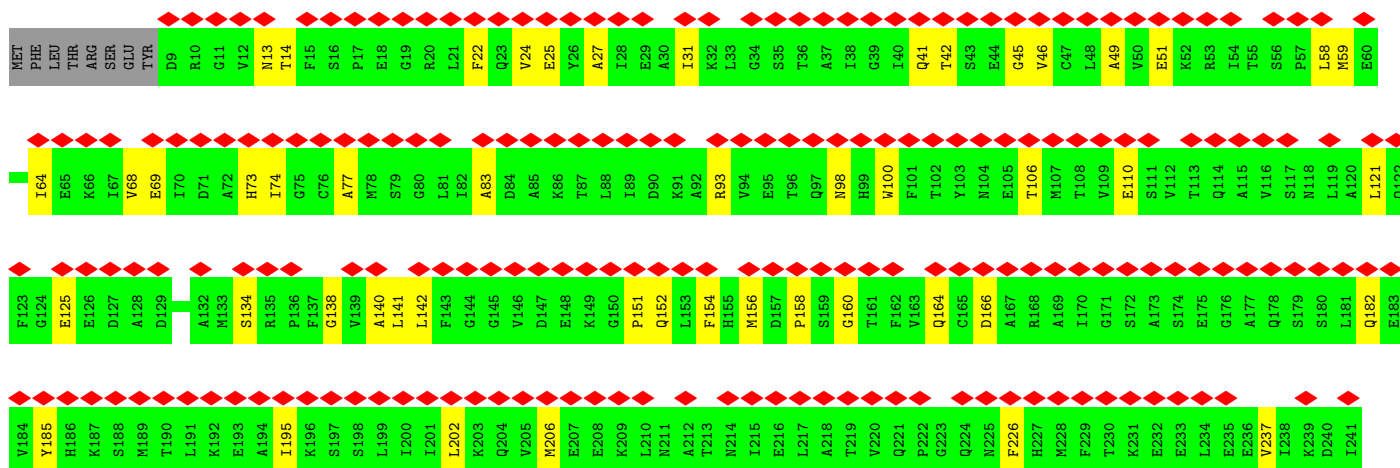
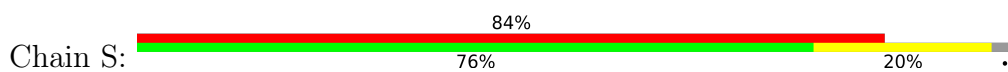
• Molecule 4: Proteasome subunit alpha type-7



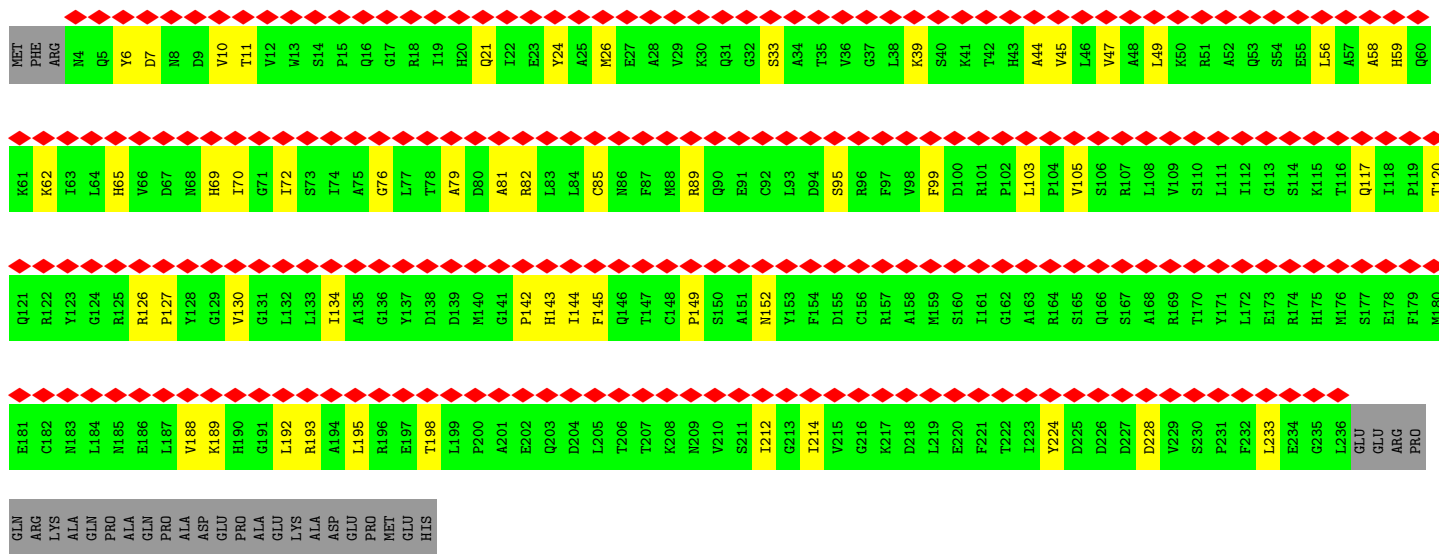
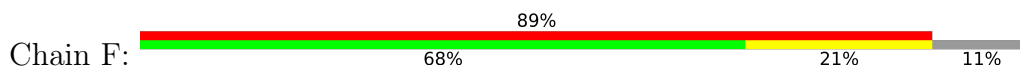
• Molecule 5: Proteasome subunit alpha type-5



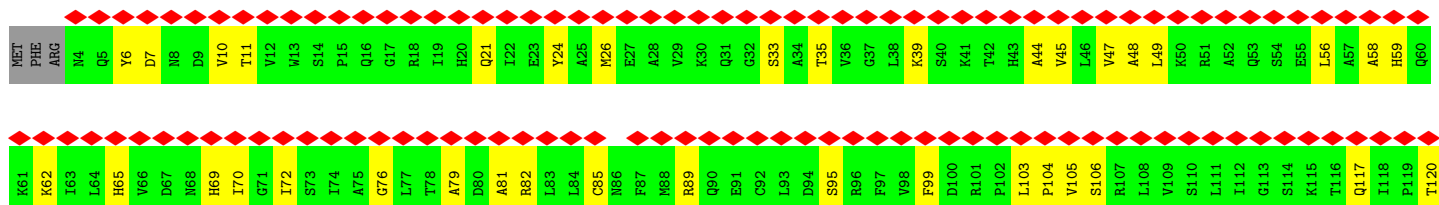
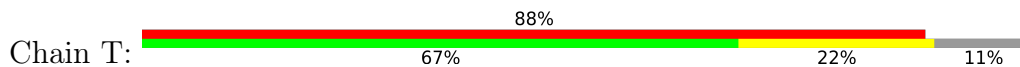
• Molecule 5: Proteasome subunit alpha type-5



• Molecule 6: Proteasome subunit alpha type-1

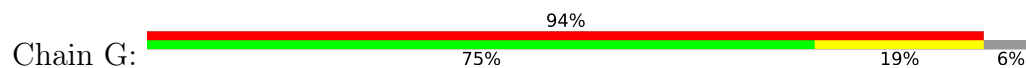


• Molecule 6: Proteasome subunit alpha type-1



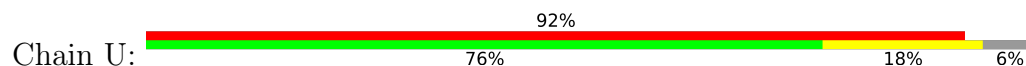
Q121	E181	GLN
R122	C182	ARG
Y123	N183	LYS
G124	L184	ALA
R125	N185	GLN
R126	E186	PRO
P127	L187	ALA
Y128	V188	GLN
G129	K189	ASP
V130	H190	GLU
G131	G191	PRO
L132	L192	ALA
L133	R193	LYS
I134	A194	ALA
A135	L195	ASP
G136	R196	GLU
Y137	E197	PRO
D138	T198	MET
D139	L199	HIS
M140	P200	
G141	A201	
P142	Q202	
H143	Q203	
I144	D204	
F145	L205	
Q146	T206	
T147	T207	
C148	K208	
P149	N209	
S150	V210	
A151	S211	
N152	I212	
Y153	G213	
F154	I214	
D155	V215	
C156	G216	
R157	K217	
A158	D218	
M159	L219	
S160	E220	
I161	F221	
G162	T222	
A163	I223	
R164	Y224	
S165	D225	
G166	D226	
S167	D227	
A168	D228	
R169	V229	
T170	S230	
Y171	P231	
L172	F232	
E173	L233	
R174	E234	
H175	G235	
M176	L236	
S177	GLU	
E178	GLU	
F179	ARG	
M180	PRO	

• Molecule 7: Proteasome subunit alpha type-3

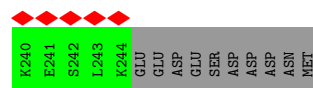


MET	G6	H120	Q180	K240
SER	Y7	A121	M181	E241
SER	D8	Y122	K182	S242
ILE	L9	T123	E183	L243
GLY	S10	L124	M184	K244
THR	A11	Y125	T185	GLU
	S12	S126	G186	GLU
	F14	A127	R187	ASP
	S15	V128	D188	GLU
	P16	R129	L189	SER
	D17	P130	V190	ASP
	G18	F131	K191	ASP
	R19	G132	E192	ASN
	T20	C133	V193	MET
	V21	S134	A194	
	Q22	F135	K195	
	V23	M136	I196	
	E24	L137	Y197	
	Y25	G138	Y198	
	A26	S139	I199	
	M27	Y140	V200	
	K28	S141	H201	
	A29	V142	D202	
	V30	N143	E203	
	E31	D144	V204	
	N32	G145	K205	
	S33	A146	D206	
	S34	Q147	K207	
	T35	L148	A208	
	A36	Y149	F209	
	I37	M150	E210	
	G38	I151	L211	
	I39	D152	L212	
	R40	P153	L213	
	C41	S154	S214	
	K42	G155	W215	
	D43	V156	V216	
	G44	S157	G217	
	V45	Y158	E218	
	W46	G159	L219	
	F47	Y160	T220	
	G48	W161	N221	
	V49	G162	G222	
	E50	C163	R223	
	K51	A164	H224	
	L52	I165	E225	
	V53	G166	L226	
	L54	K167	V227	
	S55	A168	P228	
	K56	R169	K229	
	L57	Q170	D230	
	M117	A171	I231	
	Y118	K172	R232	
		A173	E233	
		T174	E234	
		E175	A235	
		I176	E236	
		E177	K237	
		K178	Y238	
		L179	A239	

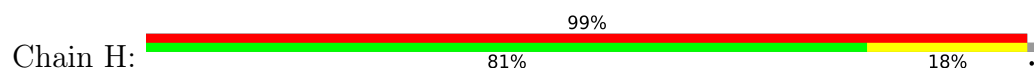
• Molecule 7: Proteasome subunit alpha type-3



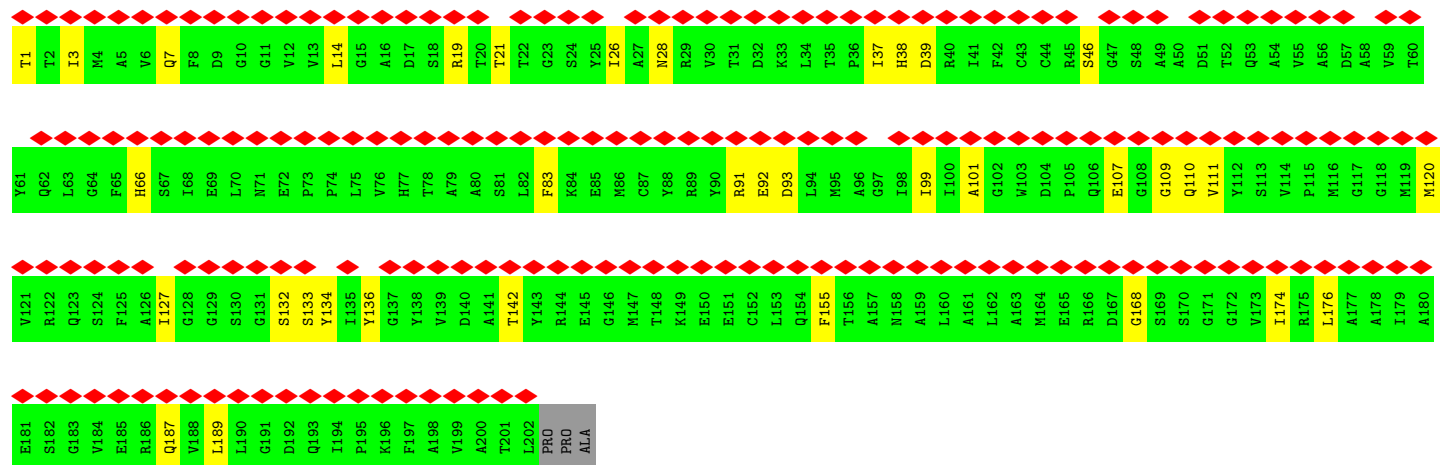
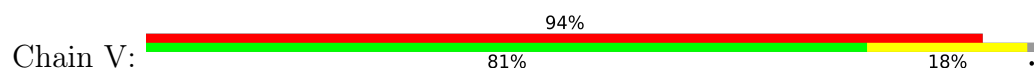
MET	G6	H120	Q180	K240
SER	Y7	A121	M181	E241
SER	D8	Y122	K182	S242
GLY	L9	T123	E183	L243
THR	S10	L124	M184	K244
	A11	Y125	T185	GLU
	S12	S126	G186	GLU
	F14	A127	R187	ASP
	S15	V128	D188	GLU
	P16	R129	L189	SER
	D17	P130	V190	ASP
	G18	F131	K191	ASP
	R19	G132	E192	ASN
	T20	C133	V193	MET
	V21	S134	A194	
	Q22	F135	K195	
	V23	M136	I196	
	E24	L137	Y197	
	Y25	G138	Y198	
	A26	S139	I199	
	M27	Y140	V200	
	K28	S141	H201	
	A29	V142	D202	
	V30	N143	E203	
	E31	D144	V204	
	N32	G145	K205	
	S33	A146	D206	
	S34	Q147	K207	
	T35	L148	A208	
	A36	Y149	F209	
	I37	M150	E210	
	G38	I151	L211	
	I39	D152	L212	
	R40	P153	L213	
	C41	S154	S214	
	K42	G155	W215	
	D43	V156	V216	
	G44	S157	G217	
	V45	Y158	E218	
	W46	G159	L219	
	F47	Y160	T220	
	G48	W161	N221	
	V49	G162	G222	
	E50	C163	R223	
	K51	A164	H224	
	L52	I165	E225	
	V53	G166	L226	
	L54	K167	V227	
	S55	A168	P228	
	K56	R169	K229	
	L57	Q170	D230	
	M117	A171	I231	
	Y118	K172	R232	
		A173	E233	
		T174	E234	
		E175	A235	
		I176	E236	
		E177	K237	
		K178	Y238	
		L179	A239	



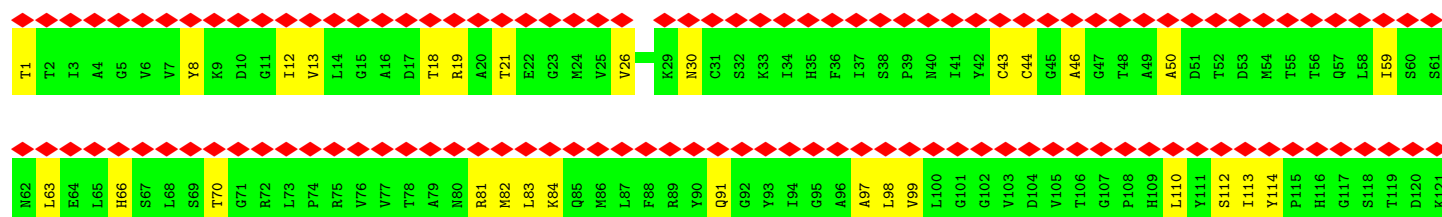
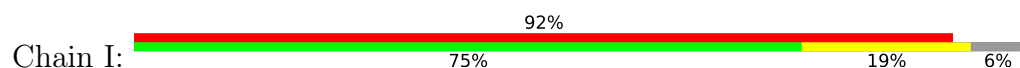
• Molecule 8: Proteasome subunit beta type-6



• Molecule 8: Proteasome subunit beta type-6

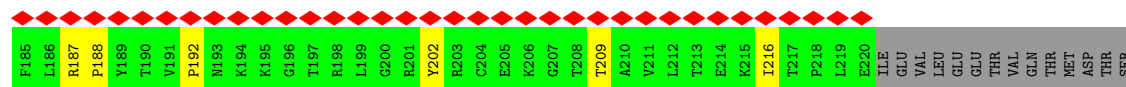
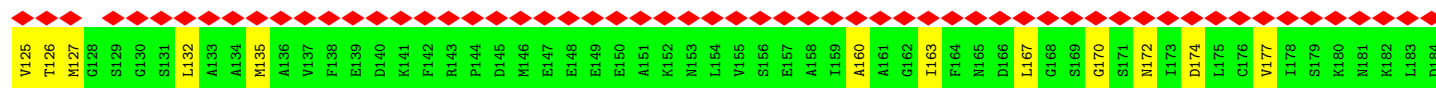
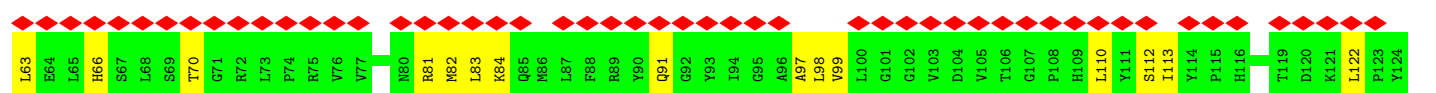
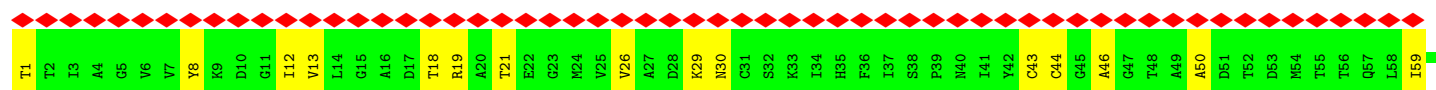
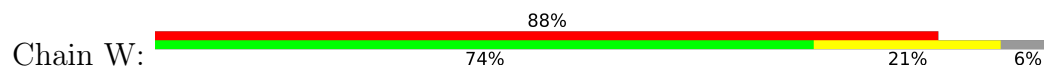


• Molecule 9: Proteasome subunit beta type-7

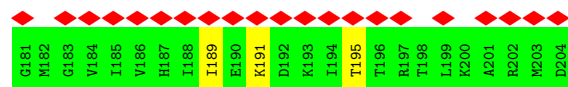
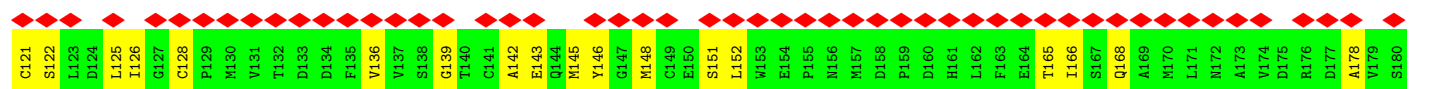
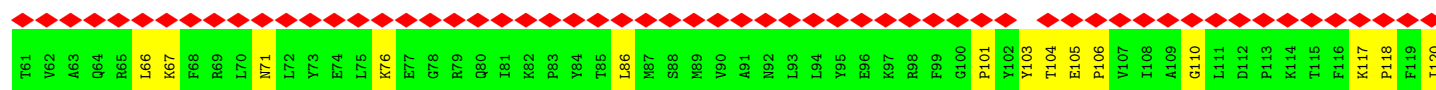
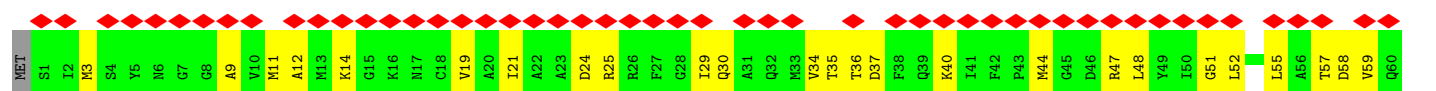




• Molecule 9: Proteasome subunit beta type-7



• Molecule 10: Proteasome subunit beta type-3

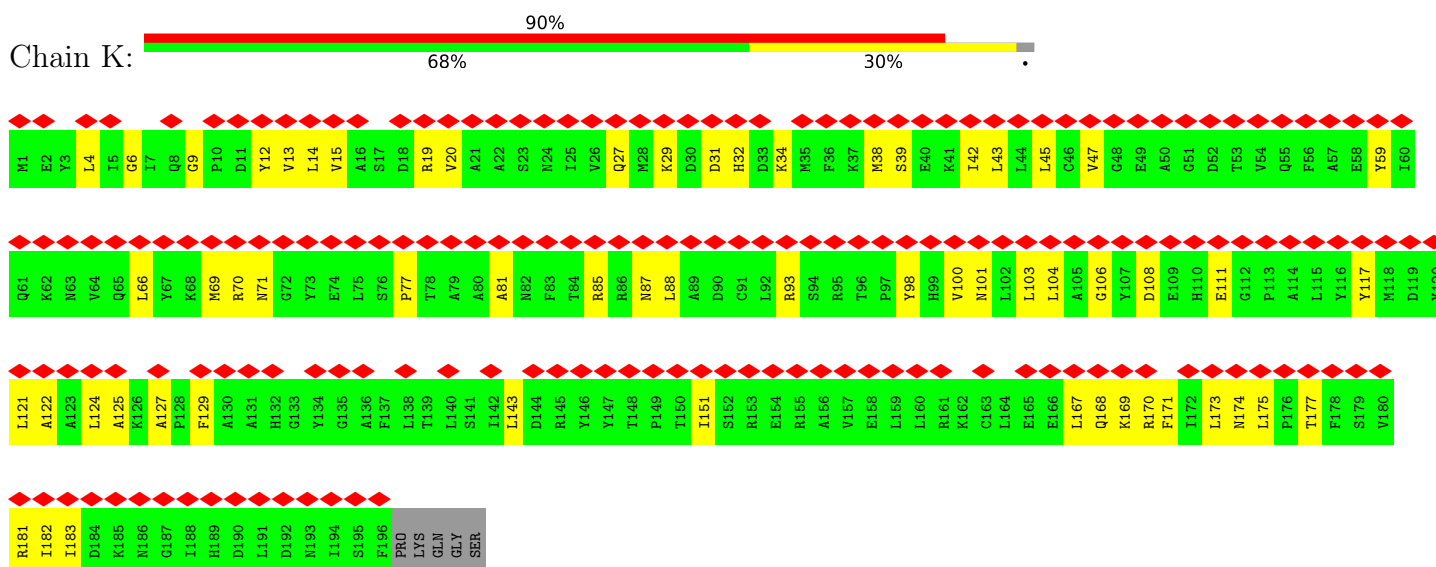


• Molecule 10: Proteasome subunit beta type-3

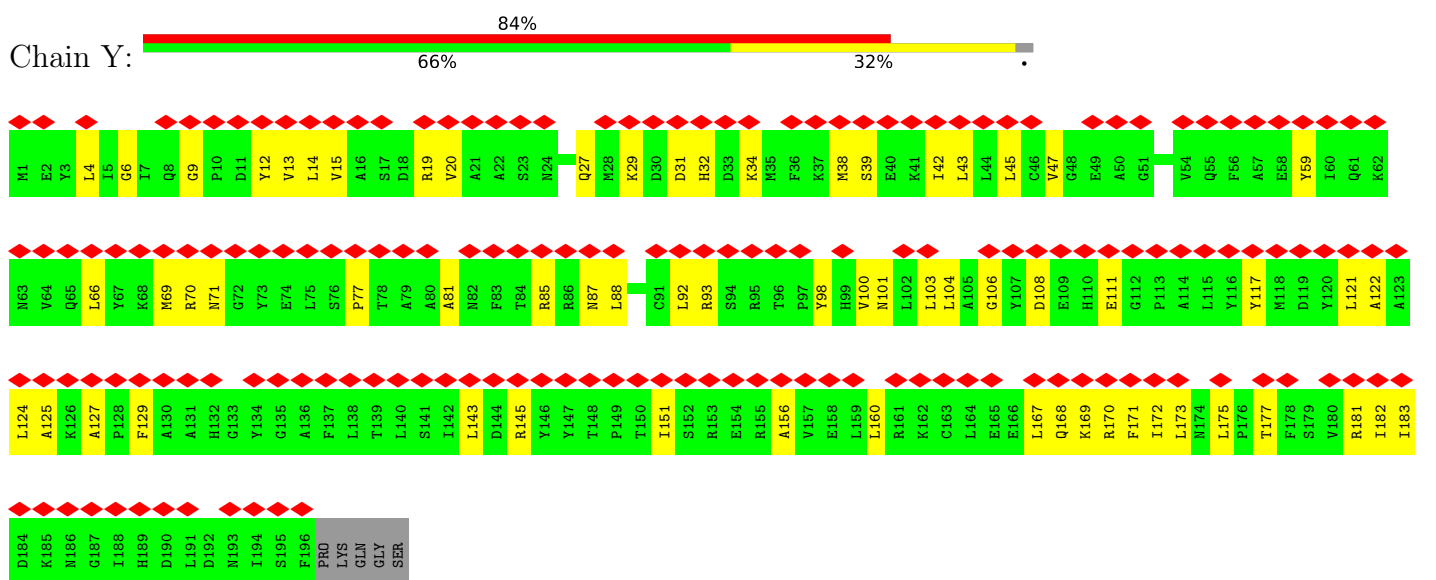




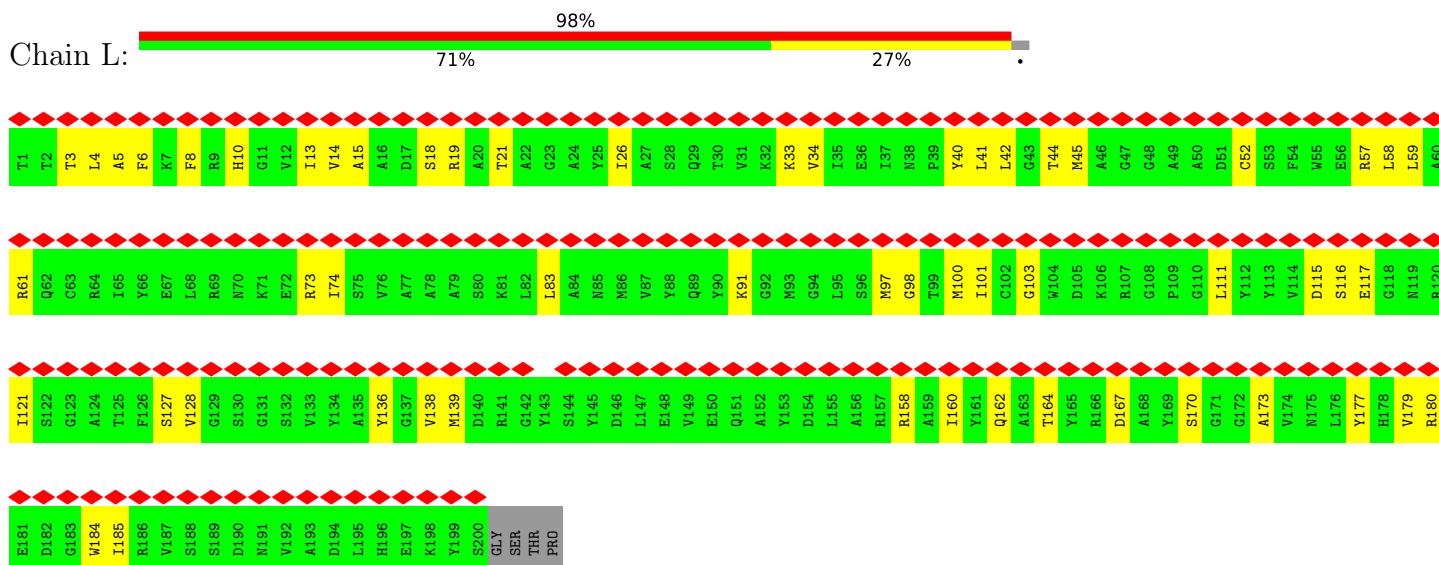
• Molecule 11: Proteasome subunit beta type-2



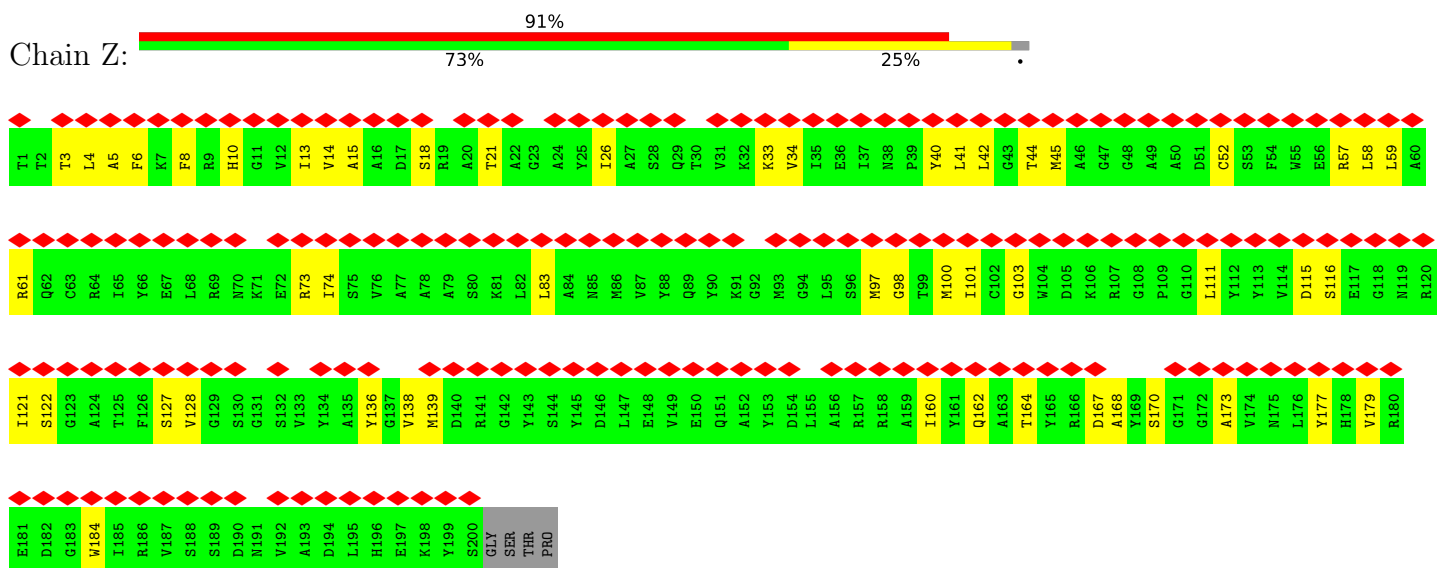
• Molecule 11: Proteasome subunit beta type-2



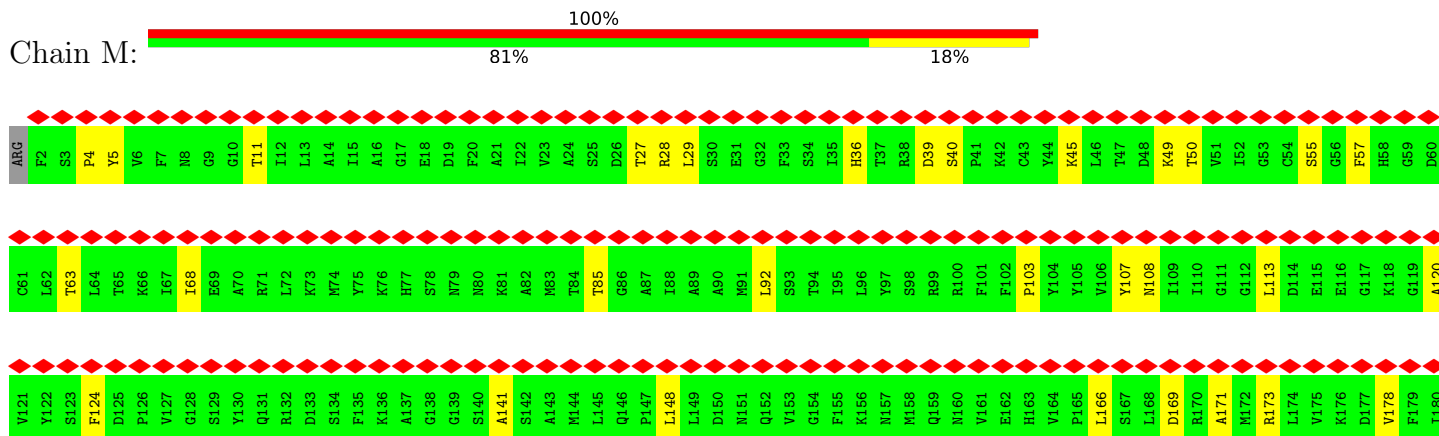
- Molecule 12: Proteasome subunit beta type-5

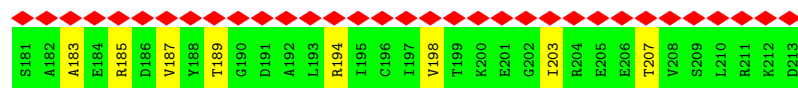


- Molecule 12: Proteasome subunit beta type-5

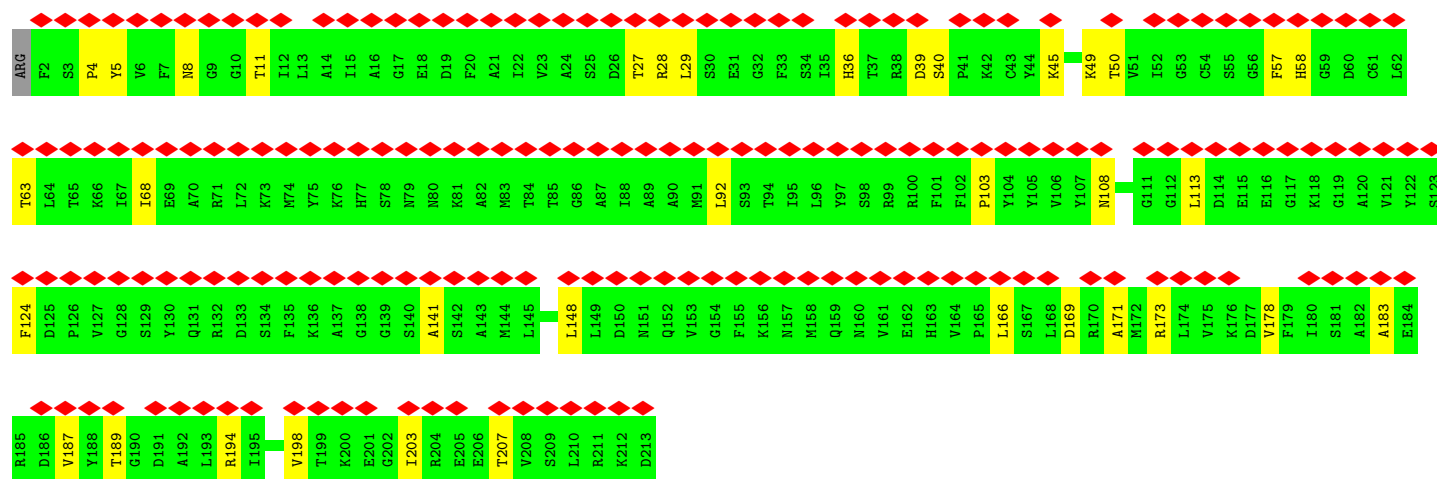
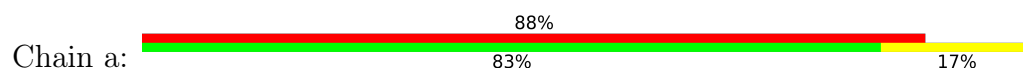


- Molecule 13: Proteasome subunit beta type-1

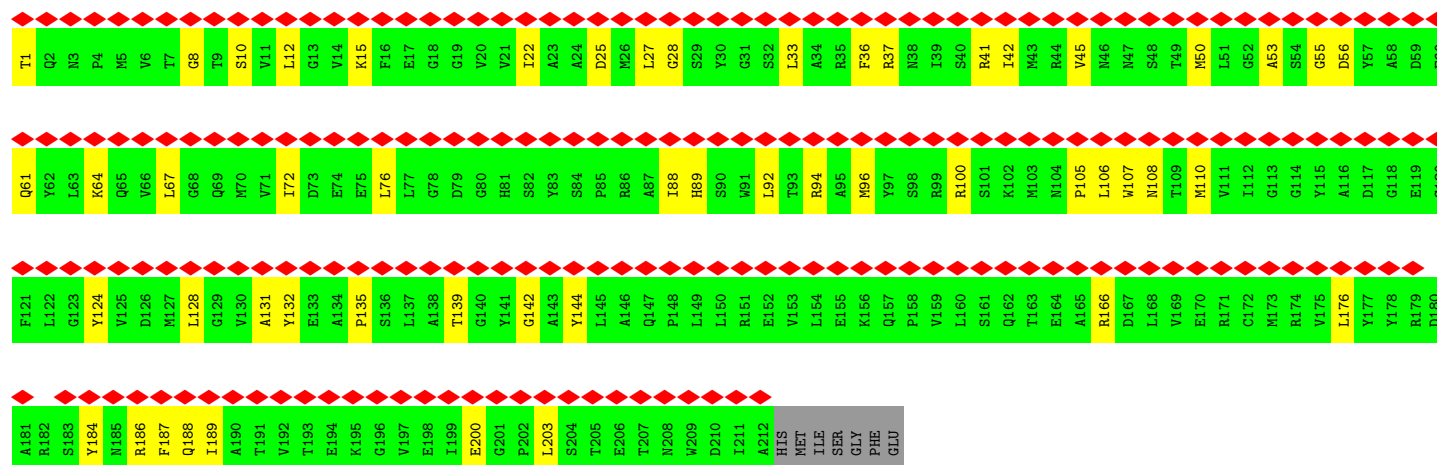
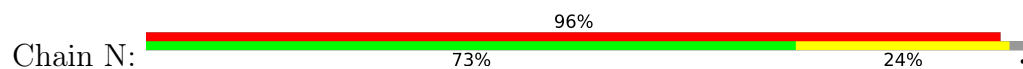




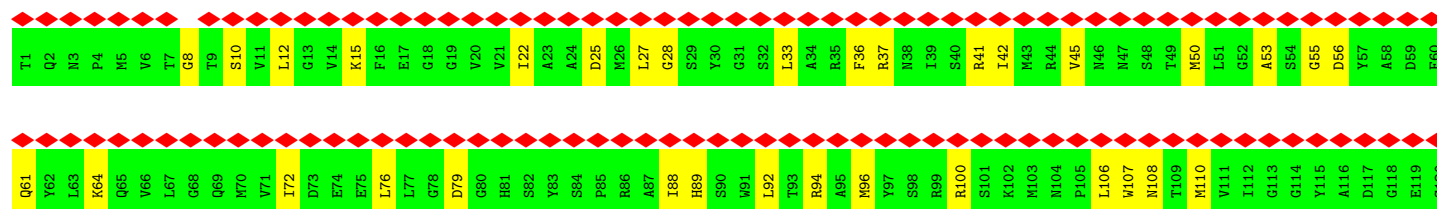
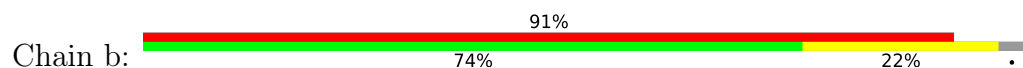
• Molecule 13: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	219.648, 219.648, 219.648	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	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	0.15	0/1763	0.42	0/2393
1	O	0.14	0/1763	0.41	0/2393
2	B	0.12	0/1701	0.37	0/2318
2	P	0.12	0/1701	0.37	0/2318
3	C	0.12	0/1815	0.38	0/2466
3	Q	0.12	0/1815	0.38	0/2466
4	D	0.14	0/1657	0.43	0/2261
4	R	0.14	0/1657	0.43	0/2261
5	E	0.12	0/1685	0.39	0/2290
5	S	0.12	0/1685	0.39	0/2290
6	F	0.13	0/1738	0.39	0/2364
6	T	0.13	0/1738	0.39	0/2364
7	G	0.11	0/1795	0.38	0/2434
7	U	0.11	0/1795	0.38	0/2434
8	H	0.12	0/1491	0.36	0/2021
8	V	0.12	0/1491	0.36	0/2021
9	I	0.13	0/1603	0.41	0/2180
9	W	0.13	0/1603	0.41	0/2180
10	J	0.14	0/1563	0.43	0/2113
10	X	0.14	0/1563	0.43	0/2113
11	K	0.14	0/1538	0.48	0/2088
11	Y	0.14	0/1538	0.47	0/2088
12	L	0.13	0/1531	0.42	0/2076
12	Z	0.13	0/1531	0.42	0/2076
13	M	0.13	0/1613	0.40	0/2178
13	a	0.13	0/1613	0.40	0/2178
14	N	0.13	0/1598	0.42	0/2170
14	b	0.13	0/1598	0.42	0/2170
All	All	0.13	0/46182	0.41	0/62704

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

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	A	1734	0	1652	27	0
1	O	1734	0	1652	24	0
2	B	1662	0	1590	30	0
2	P	1662	0	1590	31	0
3	C	1786	0	1717	26	0
3	Q	1786	0	1717	26	0
4	D	1633	0	1518	31	0
4	R	1633	0	1518	31	0
5	E	1659	0	1589	37	0
5	S	1659	0	1589	36	0
6	F	1704	0	1638	43	0
6	T	1704	0	1638	46	0
7	G	1760	0	1680	33	0
7	U	1760	0	1680	30	0
8	H	1465	0	1419	23	0
8	V	1465	0	1419	23	0
9	I	1576	0	1558	38	0
9	W	1576	0	1558	43	0
10	J	1534	0	1539	43	0
10	X	1534	0	1539	41	0
11	K	1506	0	1475	55	0
11	Y	1506	0	1475	59	0
12	L	1500	0	1441	41	0
12	Z	1500	0	1441	39	0
13	M	1583	0	1579	31	0
13	a	1583	0	1579	28	0
14	N	1568	0	1513	38	0
14	b	1568	0	1513	36	0
All	All	45340	0	43816	856	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 856 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)
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.32	1.11
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.32	1.07
5:E:121:LEU:HD12	6:F:79:ALA:HB3	1.63	0.80
5:S:121:LEU:HD12	6:T:79:ALA:HB3	1.63	0.80
4:D:211:MET:HB2	4:D:217:LEU:HD12	1.66	0.78

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	A	238/246 (97%)	229 (96%)	8 (3%)	1 (0%)	30	64
1	O	238/246 (97%)	227 (95%)	11 (5%)	0	100	100
2	B	227/234 (97%)	222 (98%)	5 (2%)	0	100	100
2	P	227/234 (97%)	222 (98%)	5 (2%)	0	100	100
3	C	245/261 (94%)	231 (94%)	14 (6%)	0	100	100
3	Q	245/261 (94%)	231 (94%)	14 (6%)	0	100	100
4	D	230/248 (93%)	223 (97%)	6 (3%)	1 (0%)	30	64
4	R	230/248 (93%)	223 (97%)	6 (3%)	1 (0%)	30	64
5	E	231/241 (96%)	225 (97%)	6 (3%)	0	100	100
5	S	231/241 (96%)	225 (97%)	6 (3%)	0	100	100
6	F	231/263 (88%)	227 (98%)	3 (1%)	1 (0%)	30	64
6	T	231/263 (88%)	227 (98%)	3 (1%)	1 (0%)	30	64
7	G	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
7	U	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
8	H	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
8	V	200/205 (98%)	197 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	218/234 (93%)	205 (94%)	13 (6%)	0	100	100
9	W	218/234 (93%)	205 (94%)	13 (6%)	0	100	100
10	J	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	X	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
11	K	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
11	Y	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
12	L	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
12	Z	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
13	M	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
13	a	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
14	N	210/219 (96%)	206 (98%)	4 (2%)	0	100	100
14	b	210/219 (96%)	206 (98%)	4 (2%)	0	100	100
All	All	6142/6458 (95%)	5954 (97%)	183 (3%)	5 (0%)	49	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	LYS
4	D	216	SER
4	R	216	SER
6	F	59	HIS
6	T	59	HIS

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	A	163/210 (78%)	163 (100%)	0	100	100
1	O	163/210 (78%)	163 (100%)	0	100	100
2	B	150/191 (78%)	150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	150/191 (78%)	150 (100%)	0	100	100
3	C	160/221 (72%)	160 (100%)	0	100	100
3	Q	160/221 (72%)	160 (100%)	0	100	100
4	D	136/211 (64%)	136 (100%)	0	100	100
4	R	136/211 (64%)	136 (100%)	0	100	100
5	E	158/203 (78%)	158 (100%)	0	100	100
5	S	158/203 (78%)	158 (100%)	0	100	100
6	F	160/224 (71%)	160 (100%)	0	100	100
6	T	160/224 (71%)	160 (100%)	0	100	100
7	G	162/212 (76%)	162 (100%)	0	100	100
7	U	162/212 (76%)	162 (100%)	0	100	100
8	H	140/159 (88%)	140 (100%)	0	100	100
8	V	140/159 (88%)	140 (100%)	0	100	100
9	I	157/195 (80%)	157 (100%)	0	100	100
9	W	157/195 (80%)	157 (100%)	0	100	100
10	J	155/174 (89%)	155 (100%)	0	100	100
10	X	155/174 (89%)	155 (100%)	0	100	100
11	K	148/171 (86%)	148 (100%)	0	100	100
11	Y	148/171 (86%)	148 (100%)	0	100	100
12	L	138/159 (87%)	138 (100%)	0	100	100
12	Z	138/159 (87%)	138 (100%)	0	100	100
13	M	158/178 (89%)	158 (100%)	0	100	100
13	a	158/178 (89%)	158 (100%)	0	100	100
14	N	149/181 (82%)	149 (100%)	0	100	100
14	b	149/181 (82%)	149 (100%)	0	100	100
All	All	4268/5378 (79%)	4268 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
8	V	7	GLN

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Mol	Chain	Res	Type
13	a	157	ASN
8	V	123	GLN
11	Y	61	GLN
10	J	92	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](#)

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.

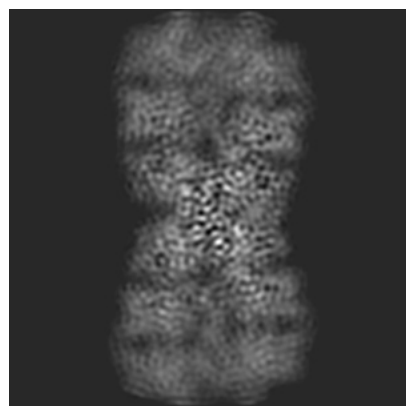
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31727. These allow visual inspection of the internal detail of the map and identification of artifacts.

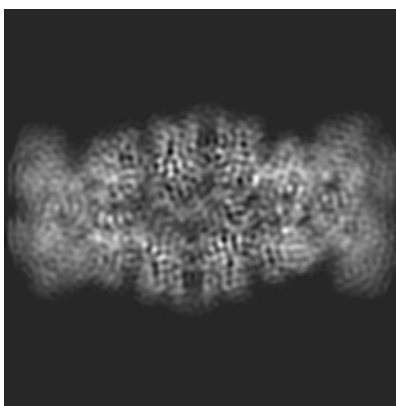
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

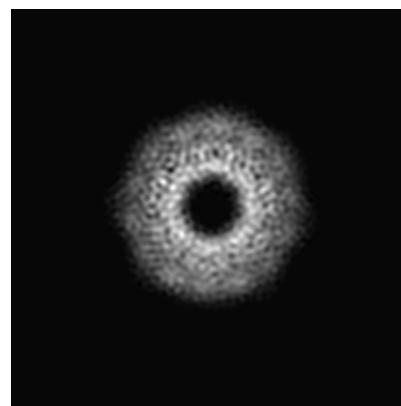
6.1.1 Primary map



X

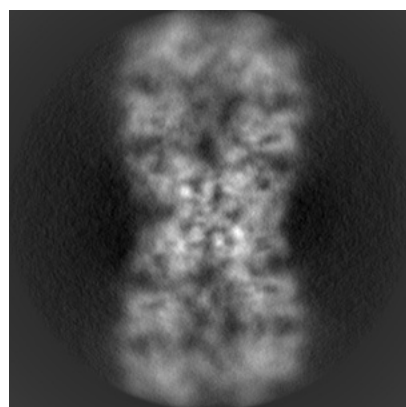


Y

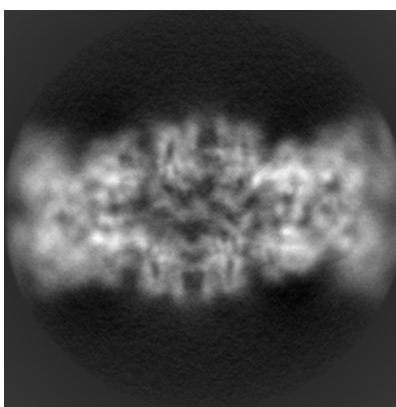


Z

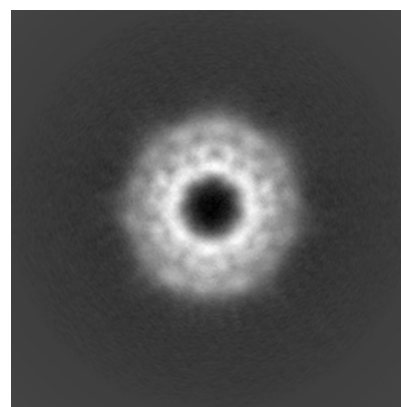
6.1.2 Raw map



X



Y

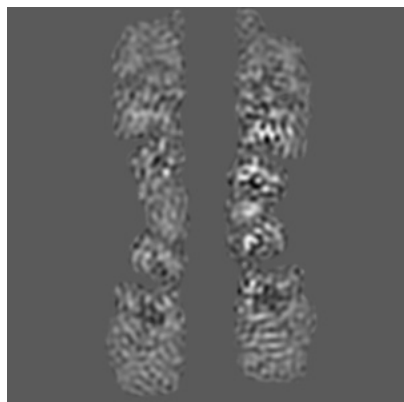


Z

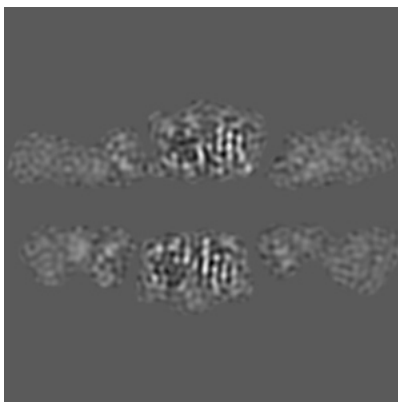
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

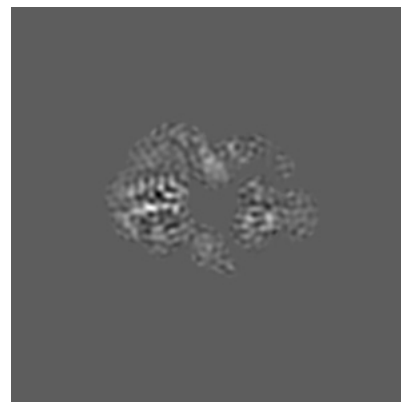
6.2.1 Primary map



X Index: 128

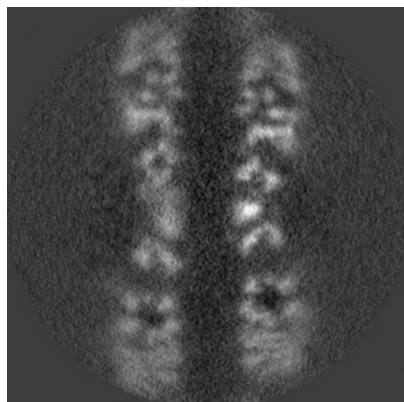


Y Index: 128

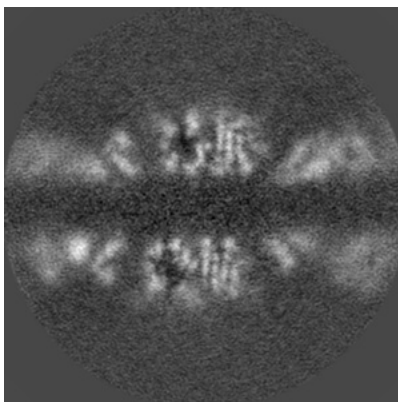


Z Index: 128

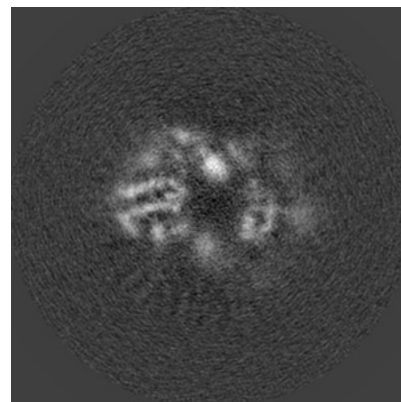
6.2.2 Raw map



X Index: 128



Y Index: 128

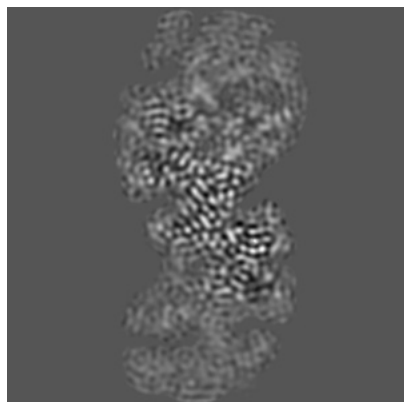


Z Index: 128

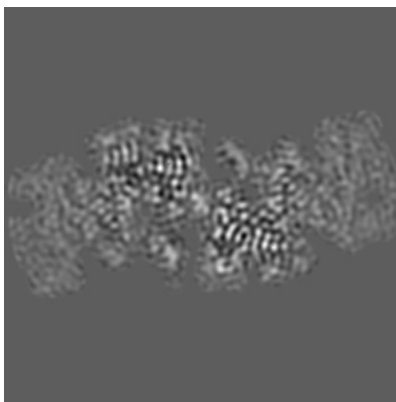
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

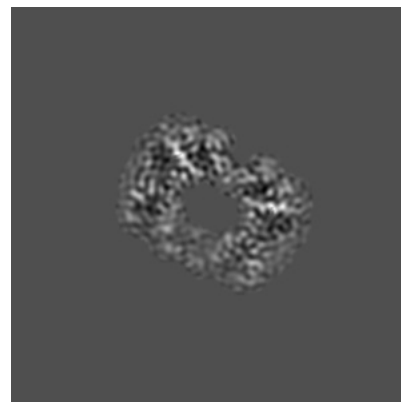
6.3.1 Primary map



X Index: 154

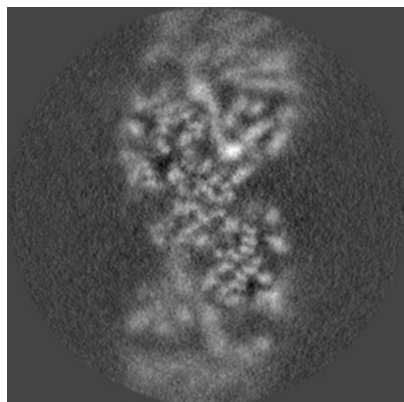


Y Index: 156

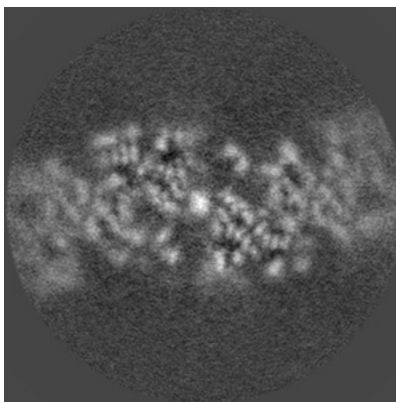


Z Index: 144

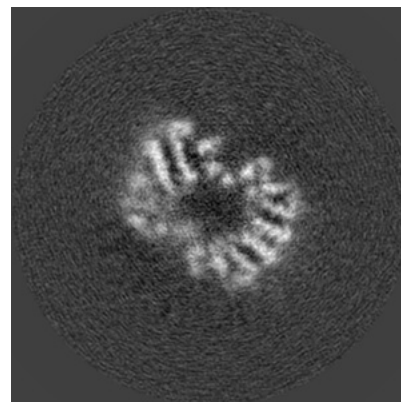
6.3.2 Raw map



X Index: 151



Y Index: 154

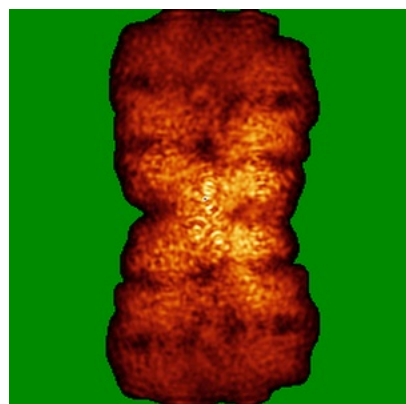


Z Index: 149

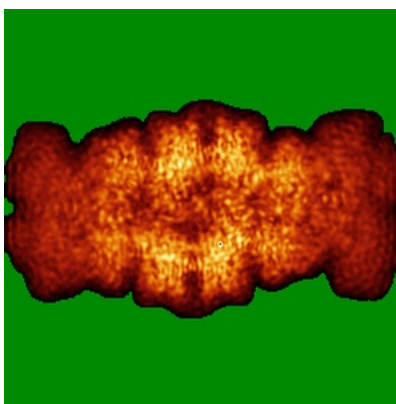
The images above show the largest variance slices of the map in three orthogonal directions.

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

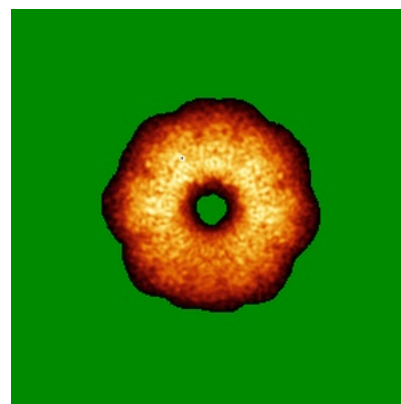
6.4.1 Primary map



X

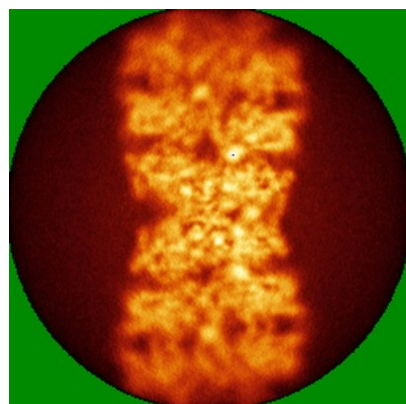


Y

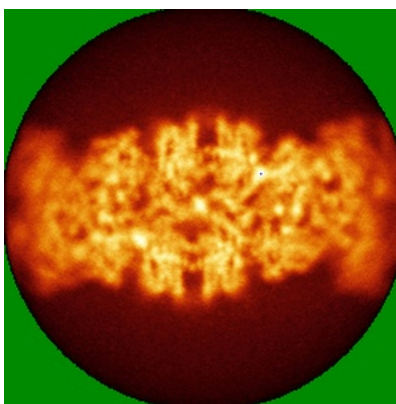


Z

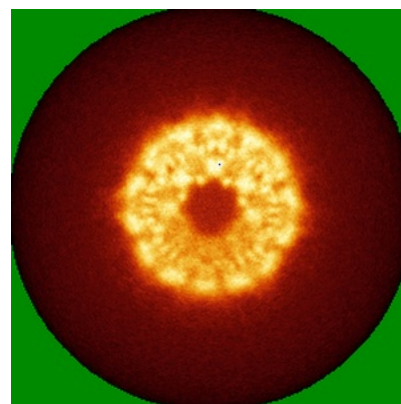
6.4.2 Raw map



X



Y



Z

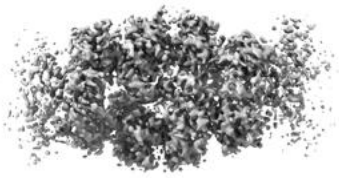
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



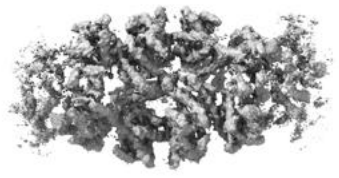
Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

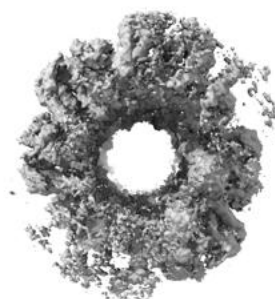
6.5.2 Raw map



X



Y



Z

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.

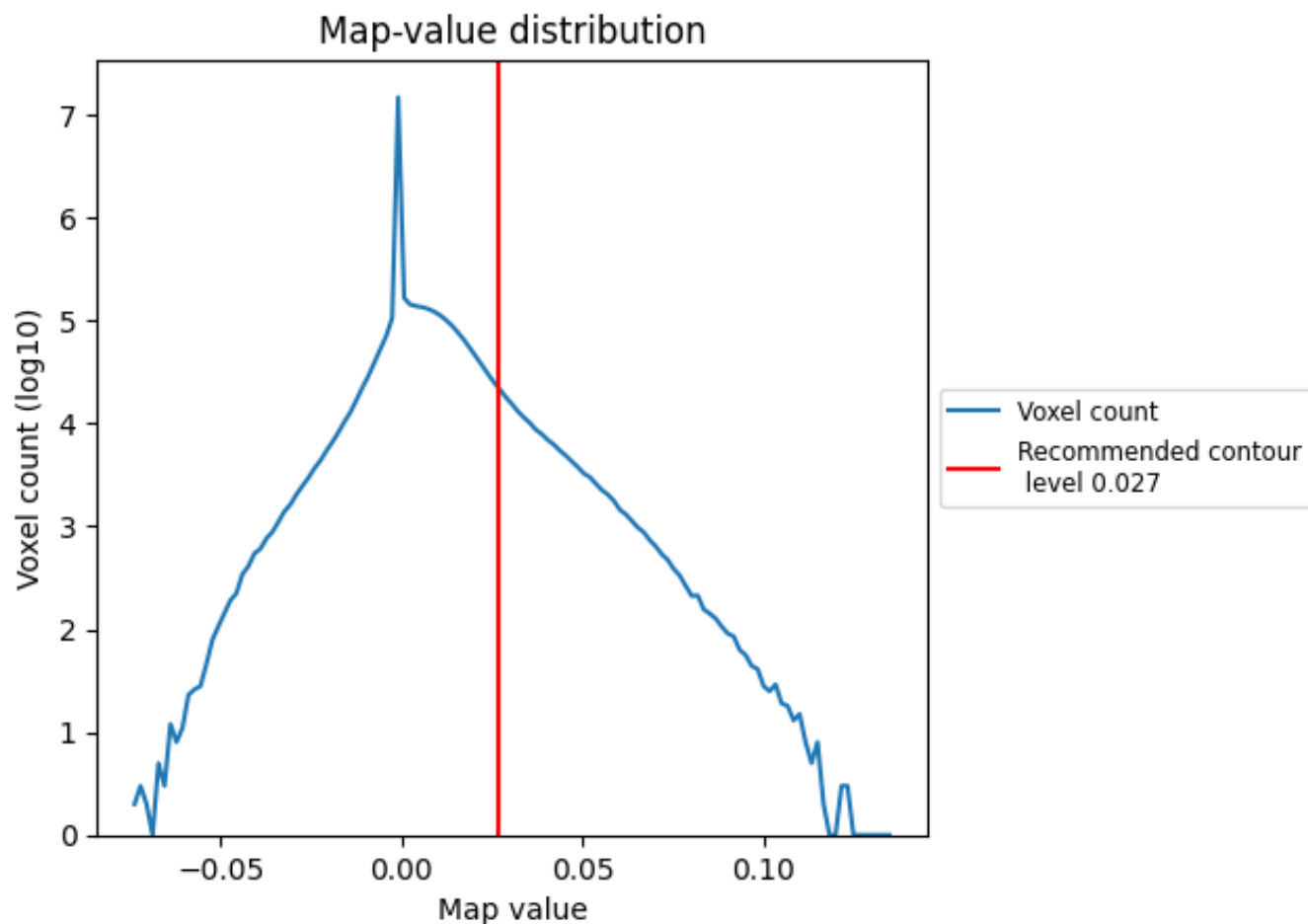
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

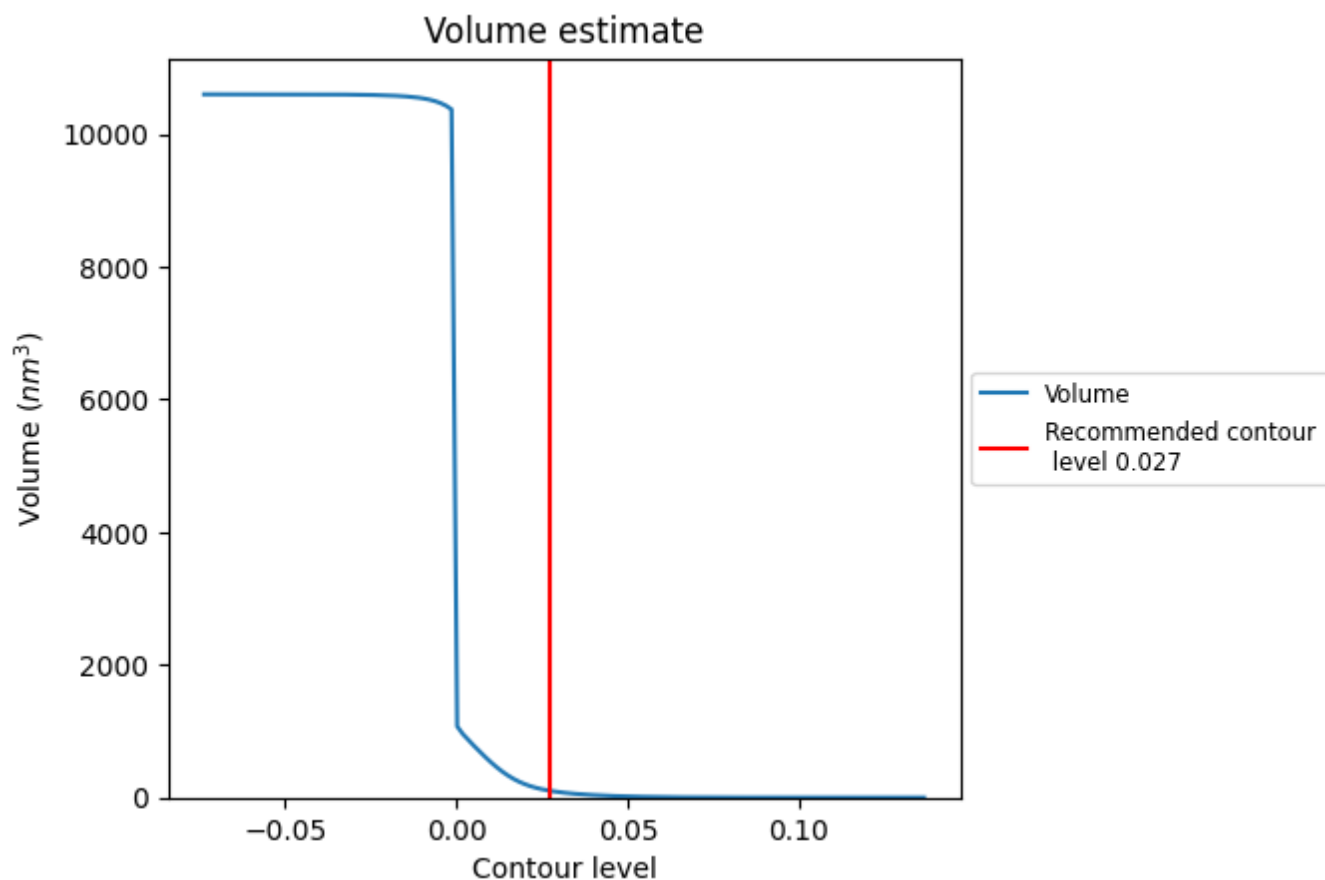
This section contains the results of statistical analysis of the map.

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.

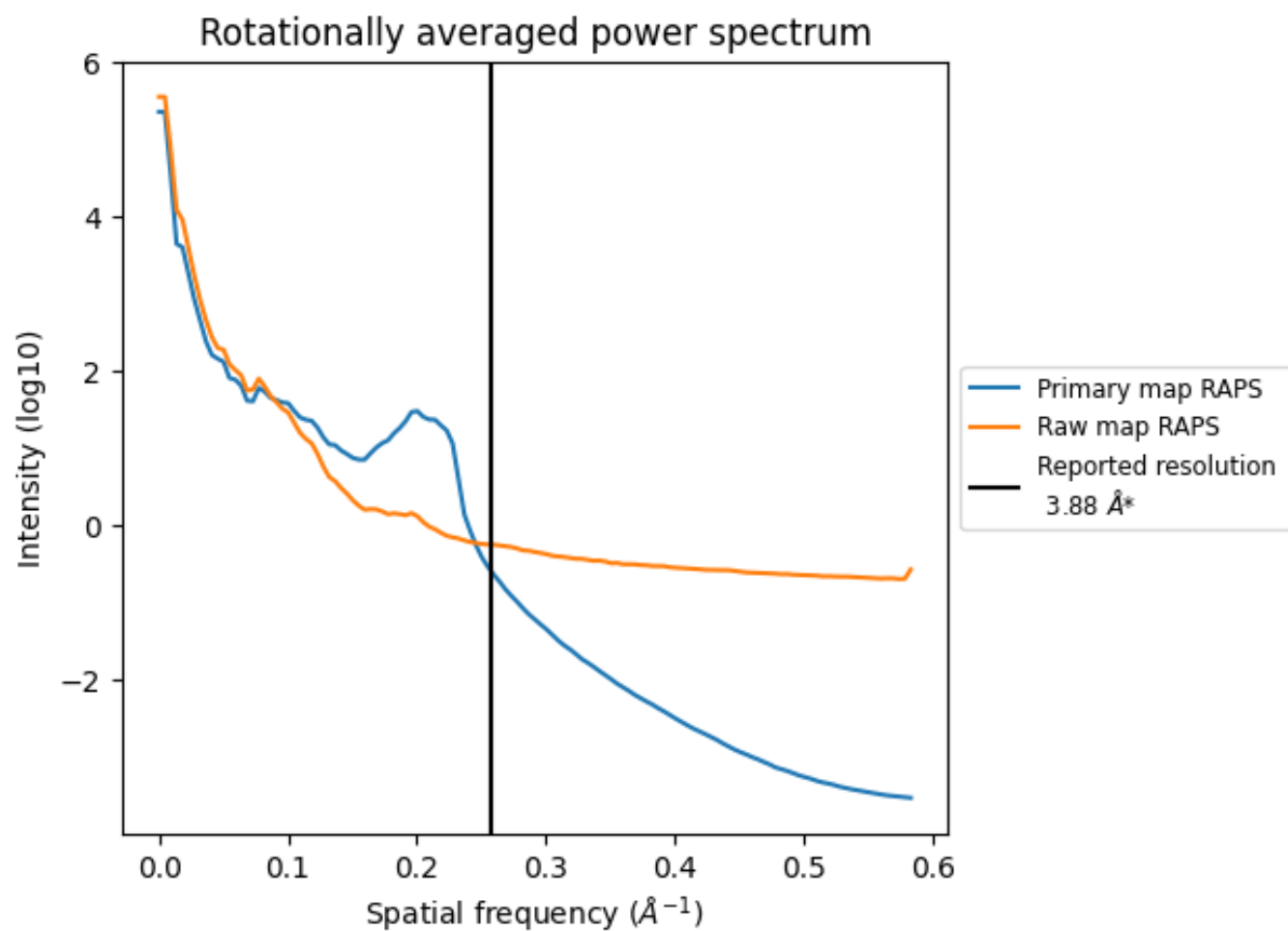
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 ⓘ

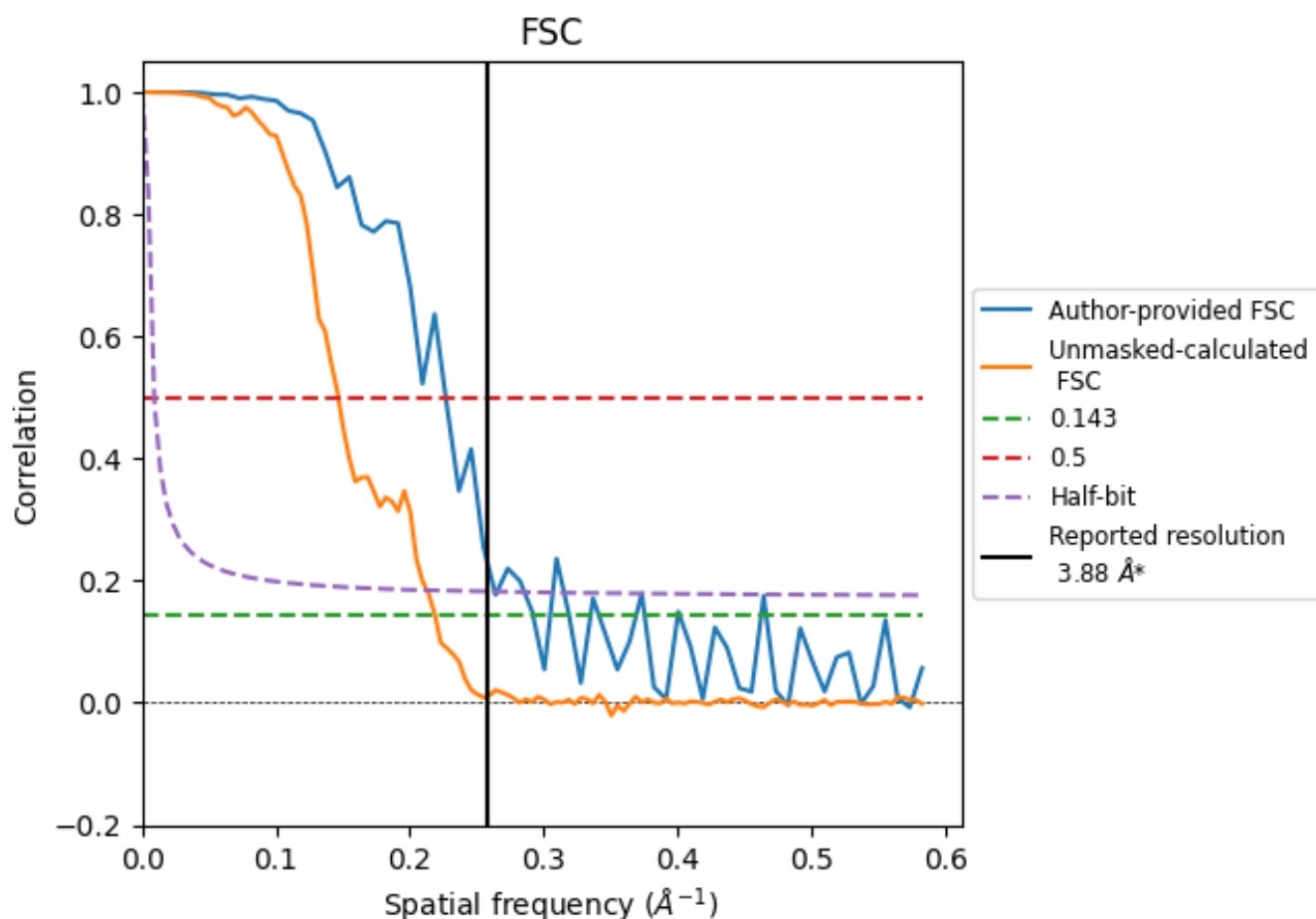


*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

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 0.258 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.88	-	-
Author-provided FSC curve	3.42	4.41	3.81
Unmasked-calculated*	4.57	6.83	4.70

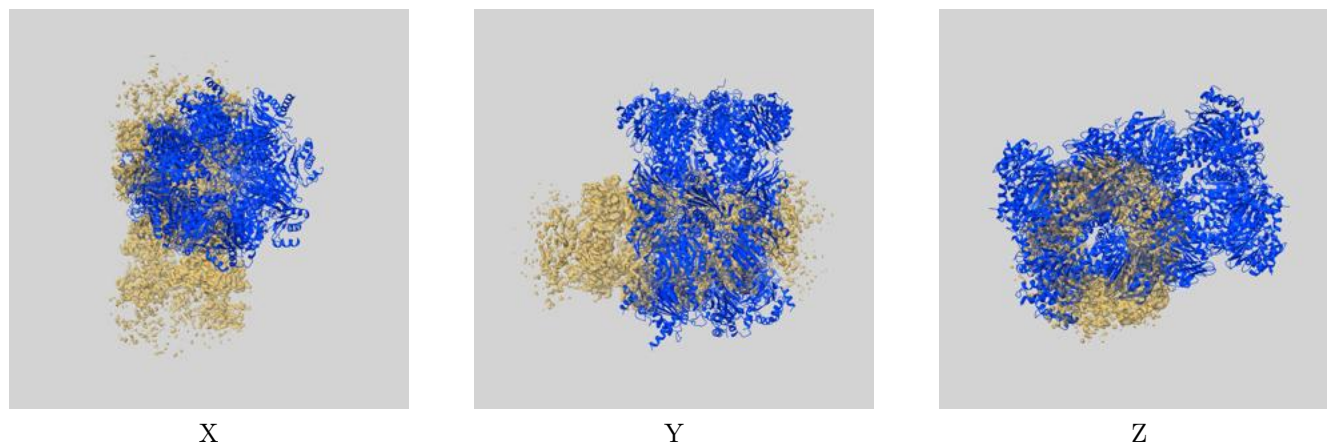
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.88 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.88 by more than 10 %

9 Map-model fit [i](#)

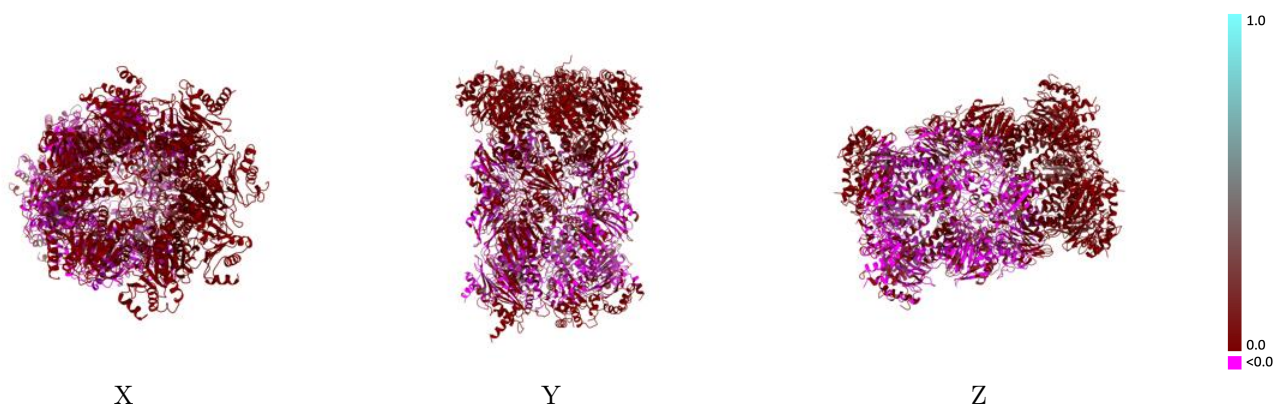
This section contains information regarding the fit between EMDB map EMD-31727 and PDB model 7V5M. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



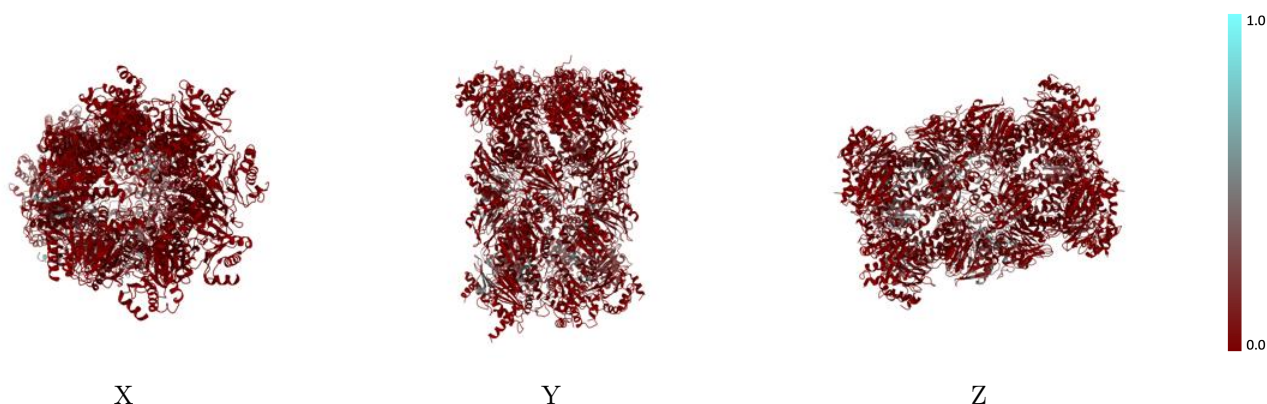
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



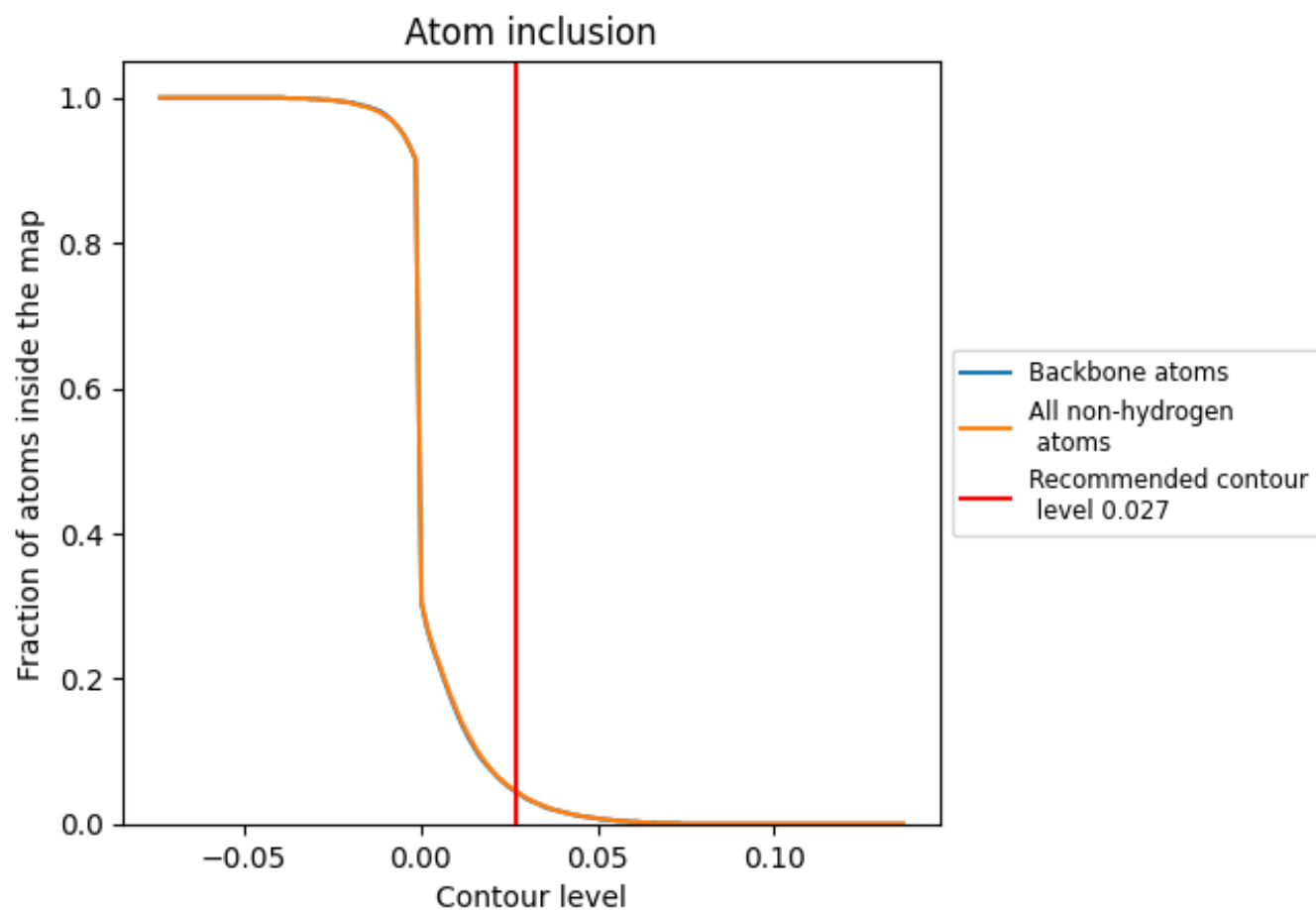
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 4% of all backbone atoms, 4% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0450	-0.0060
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	-0.0010
D	0.0000	0.0000
E	0.0000	0.0000
F	0.0000	0.0000
G	0.0000	0.0000
H	0.0080	-0.0180
I	0.0260	0.0010
J	0.0980	-0.0040
K	0.0920	-0.0070
L	0.0180	-0.0030
M	0.0010	0.0010
N	0.0120	-0.0020
O	0.0360	-0.0030
P	0.0120	-0.0070
Q	0.0470	-0.0030
R	0.1570	-0.0510
S	0.1170	-0.0110
T	0.0110	-0.0200
U	0.0310	-0.0250
V	0.0900	-0.0020
W	0.0720	-0.0030
X	0.0440	-0.0010
Y	0.1430	0.0110
Z	0.0770	-0.0170
a	0.1120	-0.0100
b	0.0840	0.0090

