



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 12:00 AM JST

PDB ID : 7DRW
EMDB ID : EMD-30828
Title : Bovine 20S immunoproteasome in complex with two human PA28alpha-beta activators
Authors : Cong, Y.; Xu, C.
Deposited on : 2020-12-29
Resolution : 4.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

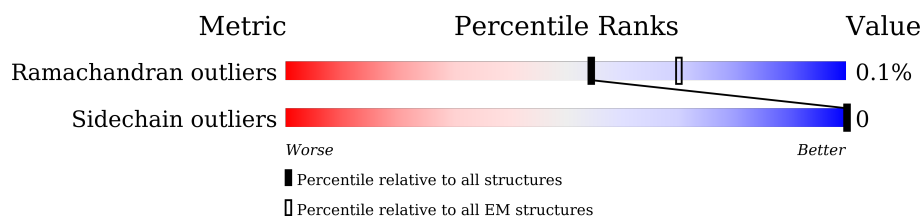
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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 $\leq 5\%$. 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	
1	f	246	
2	B	234	
2	h	234	
3	C	261	
3	j	261	
4	D	248	
4	P	248	
5	E	241	

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Mol	Chain	Length	Quality of chain
5	R	241	<div> <div>43%</div> <div>97%</div> <div>.</div> </div>
6	F	263	<div> <div>29%</div> <div>89%</div> <div>11%</div> </div>
6	b	263	<div> <div>30%</div> <div>89%</div> <div>11%</div> </div>
7	G	255	<div> <div>33%</div> <div>94%</div> <div>6%</div> </div>
7	d	255	<div> <div>35%</div> <div>94%</div> <div>6%</div> </div>
8	H	239	<div> <div>67%</div> <div>87%</div> <div>13%</div> </div>
8	K	239	<div> <div>72%</div> <div>87%</div> <div>13%</div> </div>
8	M	239	<div> <div>71%</div> <div>87%</div> <div>13%</div> </div>
8	O	239	<div> <div>85%</div> <div>87%</div> <div>13%</div> </div>
8	c	239	<div> <div>84%</div> <div>86%</div> <div>14%</div> </div>
8	g	239	<div> <div>85%</div> <div>87%</div> <div>13%</div> </div>
9	I	249	<div> <div>72%</div> <div>85%</div> <div>14%</div> </div>
9	J	249	<div> <div>57%</div> <div>83%</div> <div>17%</div> </div>
9	L	249	<div> <div>69%</div> <div>83%</div> <div>17%</div> </div>
9	N	249	<div> <div>64%</div> <div>82%</div> <div>18%</div> </div>
9	Q	249	<div> <div>83%</div> <div>86%</div> <div>14%</div> </div>
9	a	249	<div> <div>77%</div> <div>83%</div> <div>17%</div> </div>
9	e	249	<div> <div>79%</div> <div>83%</div> <div>17%</div> </div>
9	i	249	<div> <div>80%</div> <div>82%</div> <div>18%</div> </div>
10	S	205	<div> <div>32%</div> <div>99%</div> </div>
10	k	205	<div> <div>34%</div> <div>99%</div> </div>
11	T	201	<div> <div>24%</div> <div>98%</div> <div>.</div> </div>
11	l	201	<div> <div>34%</div> <div>99%</div> <div>.</div> </div>
12	U	241	<div> <div>34%</div> <div>88%</div> <div>12%</div> </div>
12	m	241	<div> <div>27%</div> <div>88%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
13	V	264	
13	n	264	
14	W	219	
14	Z	219	
15	1	273	
15	X	273	
16	2	276	
16	Y	276	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 71650 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	235	Total	C	N	O	S	0	0
			1841	1173	305	350	13		
1	f	237	Total	C	N	O	S	0	0
			1861	1184	310	354	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	226	Total	C	N	O	S	0	0
			1763	1127	298	332	6		
2	h	228	Total	C	N	O	S	0	0
			1777	1136	300	335	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	245	Total	C	N	O	S	0	0
			1927	1219	329	368	11		
3	j	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		

- 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
			1824	1149	322	348	5		
4	P	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		
5	R	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		
6	b	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		
7	d	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		

- Molecule 8 is a protein called Proteasome activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	209	Total	C	N	O	S	0	0
			1684	1084	286	310	4		
8	K	207	Total	C	N	O	S	0	0
			1678	1080	283	311	4		
8	M	209	Total	C	N	O	S	0	0
			1689	1088	286	311	4		
8	O	209	Total	C	N	O	S	0	0
			1684	1084	286	310	4		
8	c	205	Total	C	N	O	S	0	0
			1658	1066	281	308	3		
8	g	209	Total	C	N	O	S	0	0
			1689	1088	286	311	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	89	PRO	HIS	variant	UNP Q9UL46
K	89	PRO	HIS	variant	UNP Q9UL46
M	89	PRO	HIS	variant	UNP Q9UL46

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Chain	Residue	Modelled	Actual	Comment	Reference
O	89	PRO	HIS	variant	UNP Q9UL46
c	89	PRO	HIS	variant	UNP Q9UL46
g	89	PRO	HIS	variant	UNP Q9UL46

- Molecule 9 is a protein called Proteasome activator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	213	Total	C	N	O	S	0	0
			1721	1102	292	321	6		
9	J	206	Total	C	N	O	S	0	0
			1663	1063	284	310	6		
9	L	207	Total	C	N	O	S	0	0
			1672	1069	286	311	6		
9	N	205	Total	C	N	O	S	0	0
			1654	1057	283	306	8		
9	Q	213	Total	C	N	O	S	0	0
			1721	1102	292	321	6		
9	a	206	Total	C	N	O	S	0	0
			1663	1063	284	310	6		
9	e	207	Total	C	N	O	S	0	0
			1672	1069	286	311	6		
9	i	205	Total	C	N	O	S	0	0
			1654	1057	283	306	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		
10	S	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	198	Total	C	N	O	S	0	0
			1593	1023	270	292	8		
11	T	197	Total	C	N	O	S	0	0
			1584	1017	268	291	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		
12	U	213	Total	C	N	O	S	0	0
			1644	1042	282	310	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	216	Total	C	N	O	S	0	0
			1685	1065	289	319	12		
13	V	216	Total	C	N	O	S	0	0
			1682	1063	289	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		
14	Z	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		

- Molecule 15 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		
15	1	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		

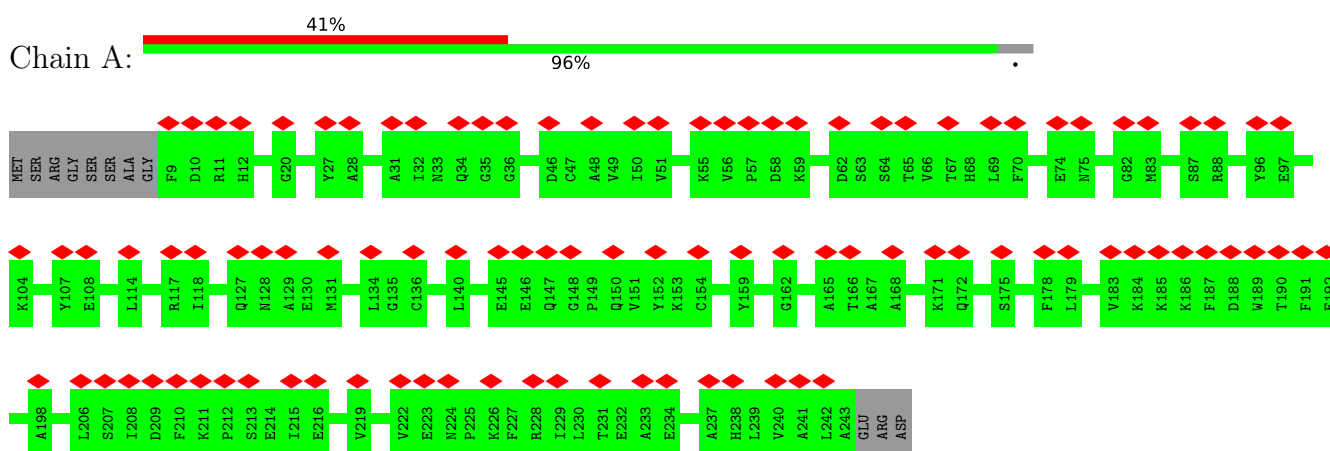
- Molecule 16 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		
16	2	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		

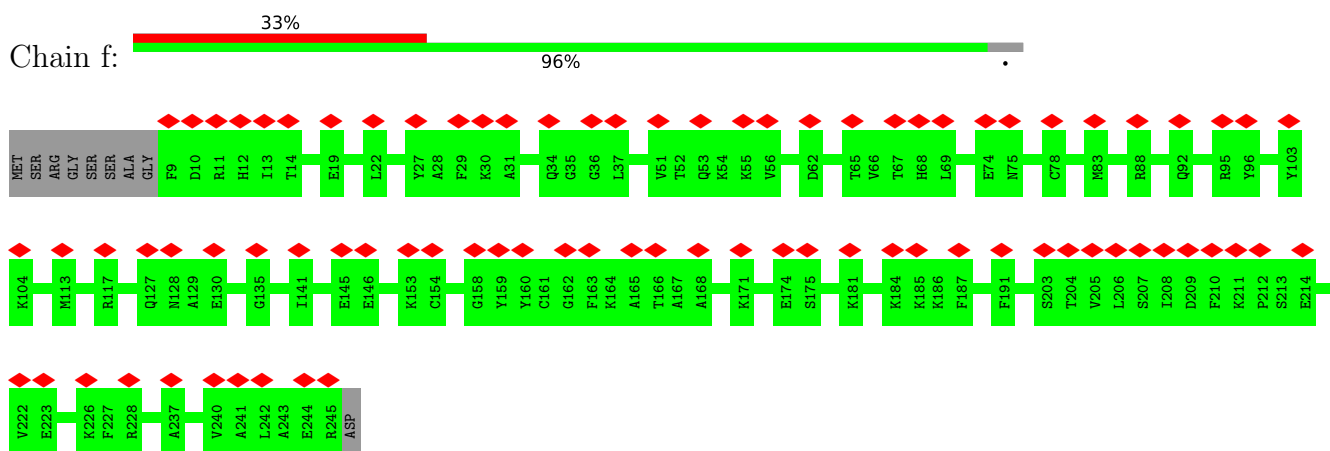
3 Residue-property plots

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.

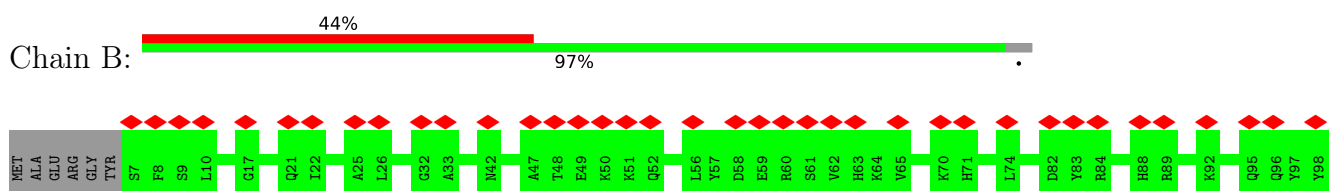
- Molecule 1: Proteasome subunit alpha type-6

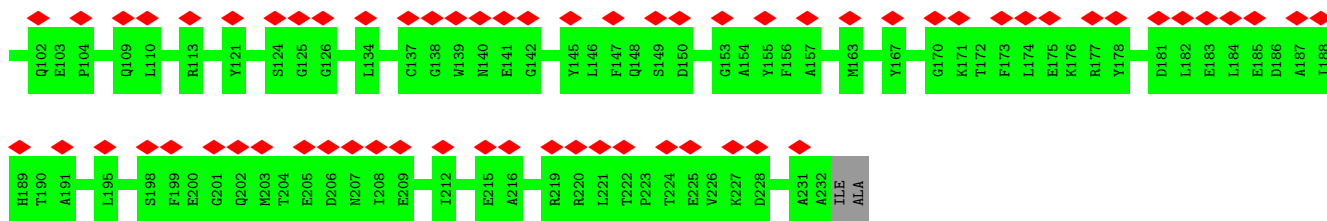


- Molecule 1: Proteasome subunit alpha type-6

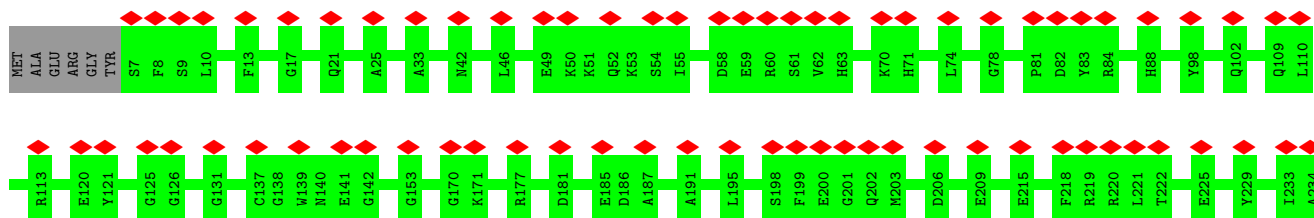


- Molecule 2: Proteasome subunit alpha type-2

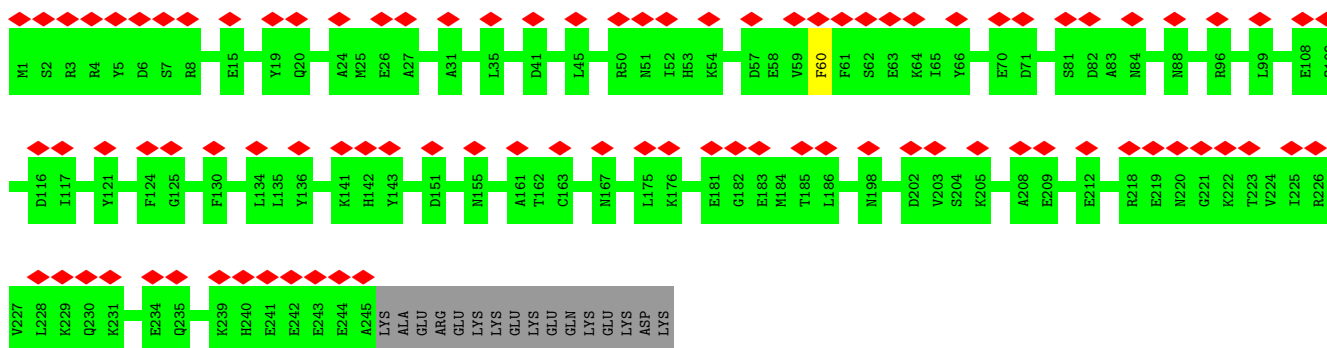
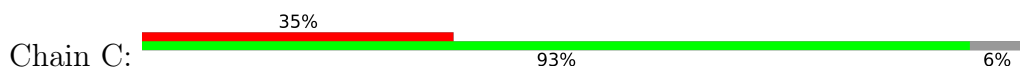




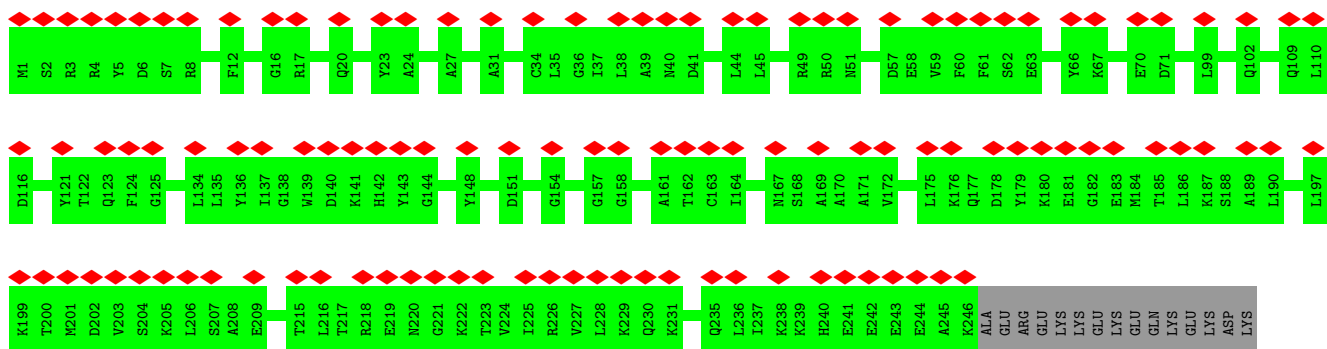
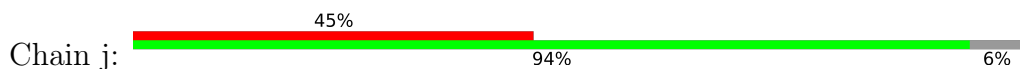
• Molecule 2: Proteasome subunit alpha type-2



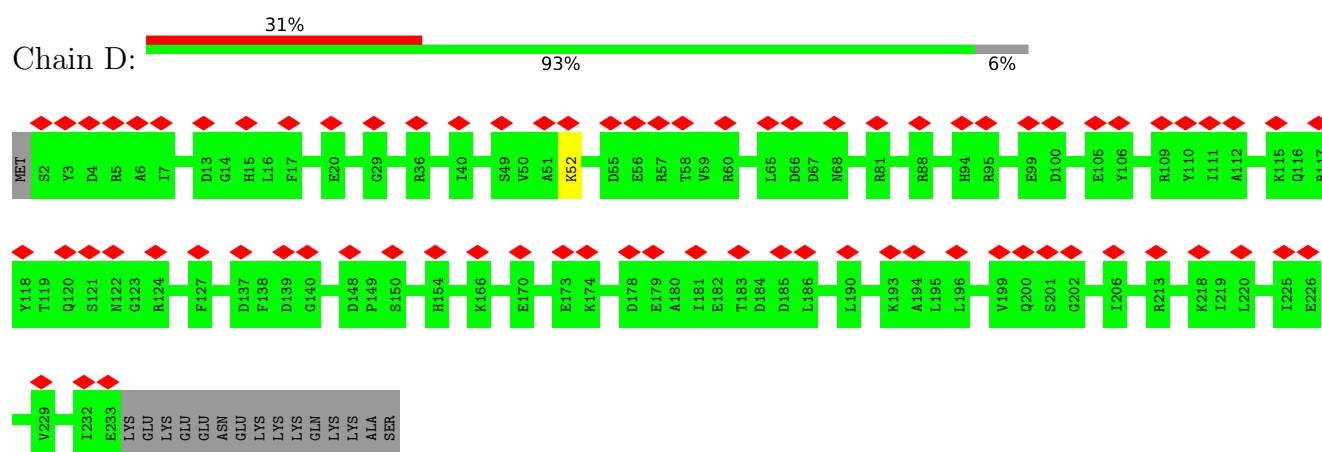
• Molecule 3: Proteasome subunit alpha type-4



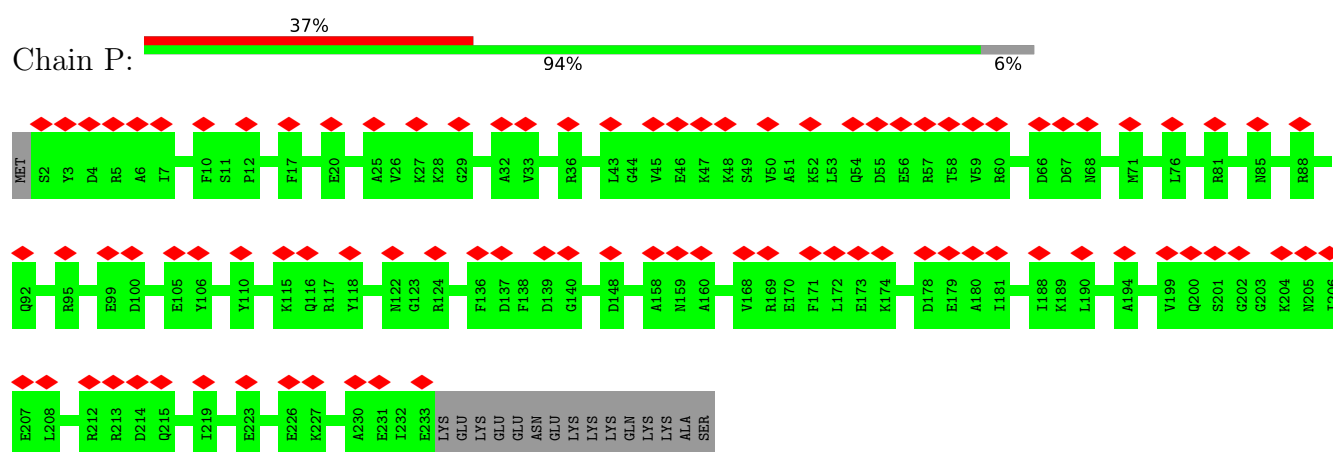
• Molecule 3: Proteasome subunit alpha type-4



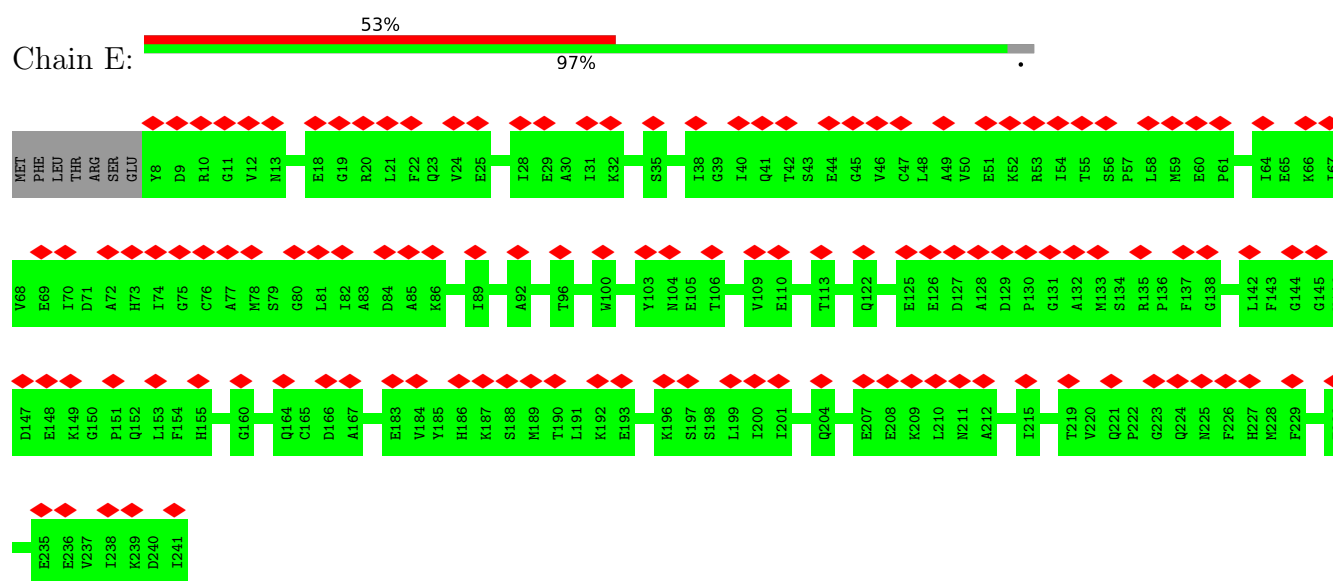
• Molecule 4: Proteasome subunit alpha type-7



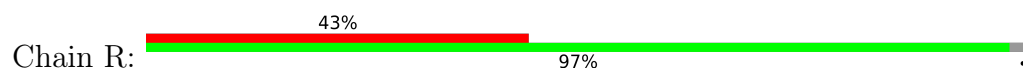
- Molecule 4: Proteasome subunit alpha type-7

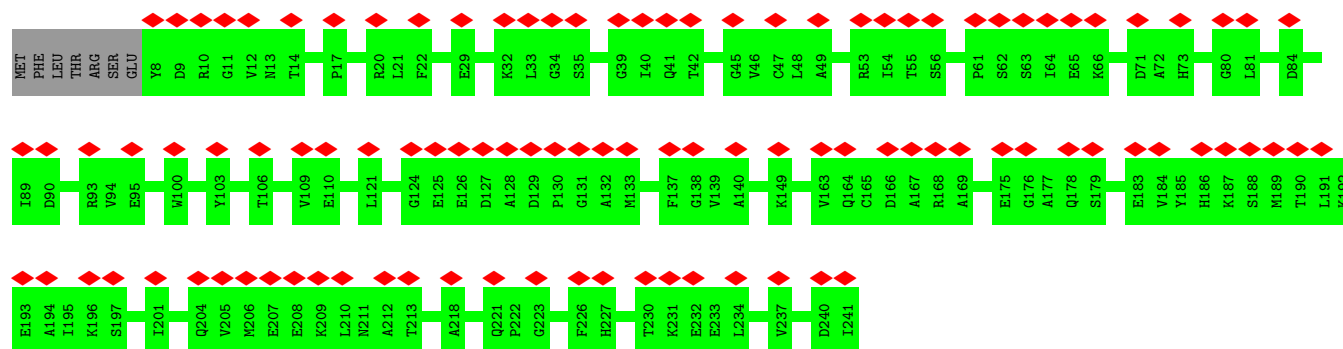


- Molecule 5: Proteasome subunit alpha type-5

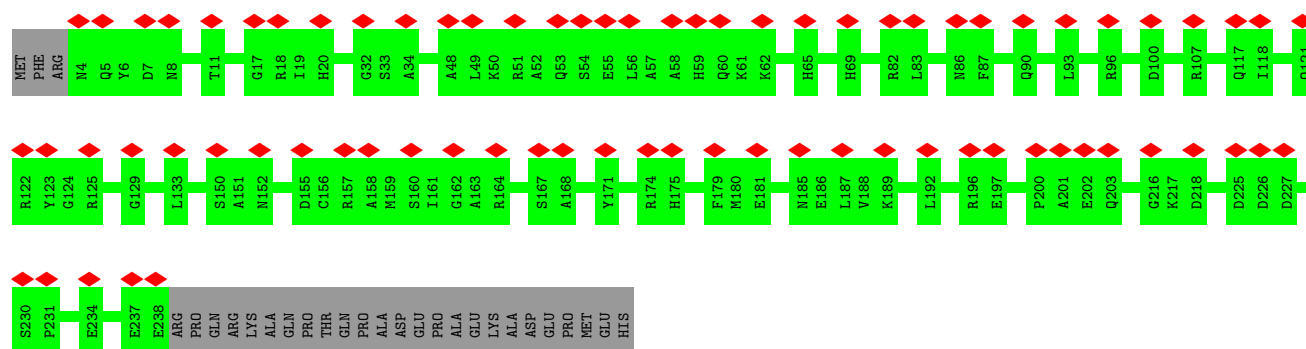
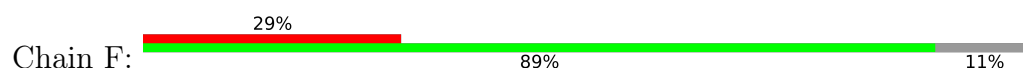


- Molecule 5: Proteasome subunit alpha type-5

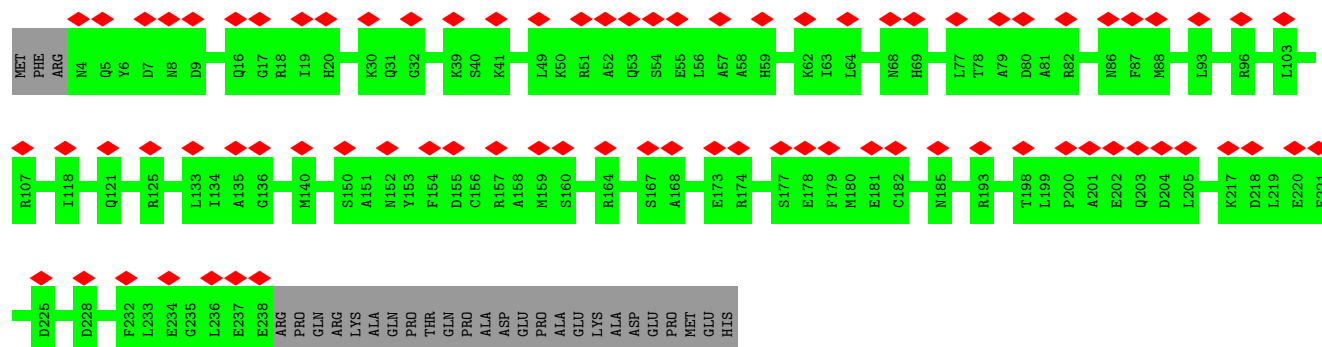
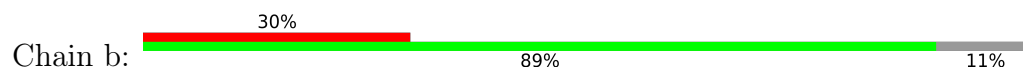




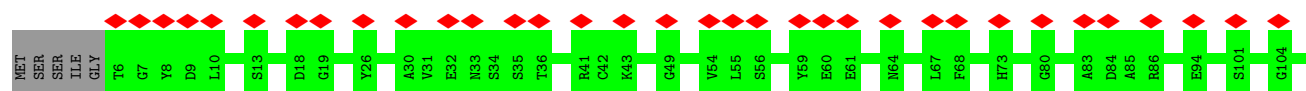
• Molecule 6: Proteasome subunit alpha type-1

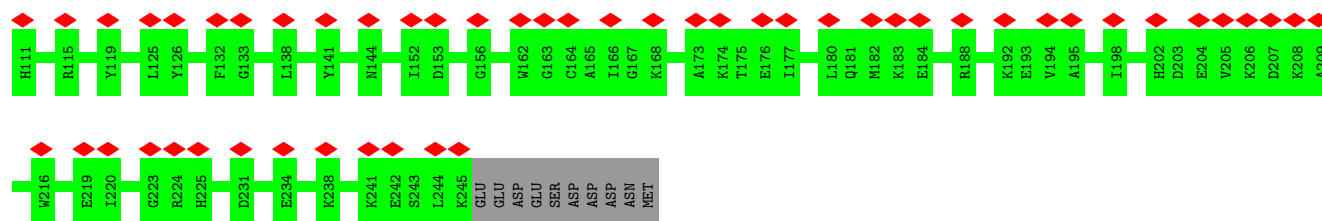


• Molecule 6: Proteasome subunit alpha type-1



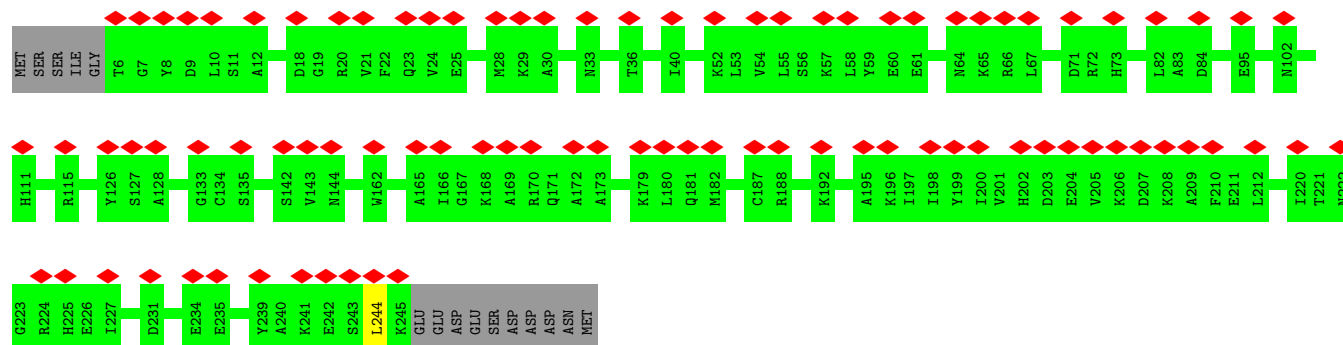
• Molecule 7: Proteasome subunit alpha type-3





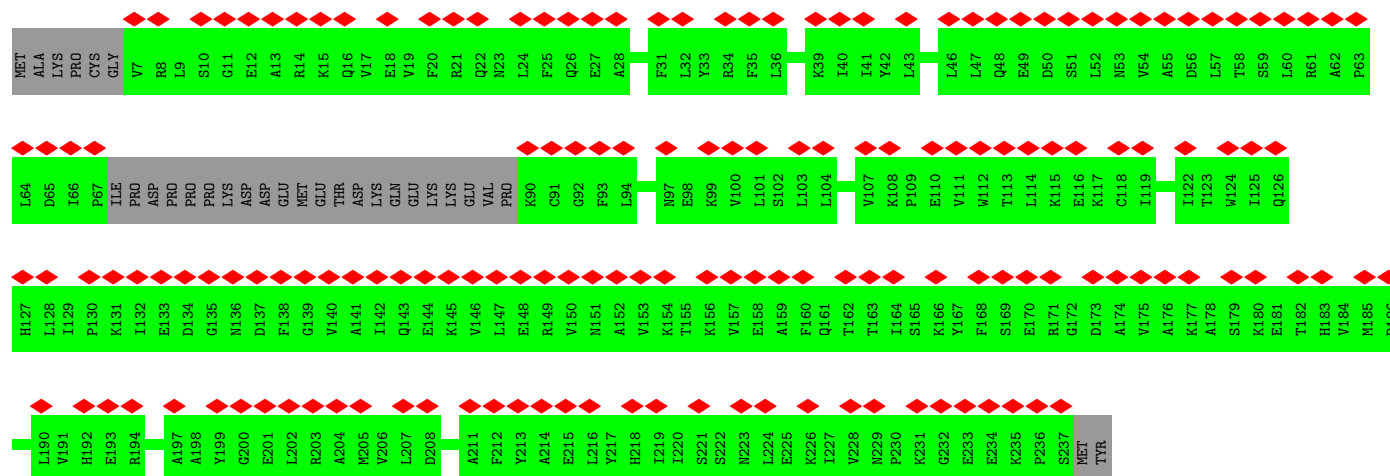
• Molecule 7: Proteasome subunit alpha type-3

Chain d:



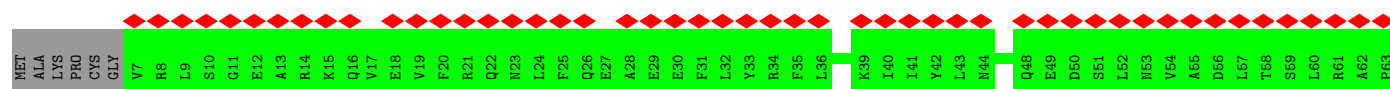
• Molecule 8: Proteasome activator complex subunit 2

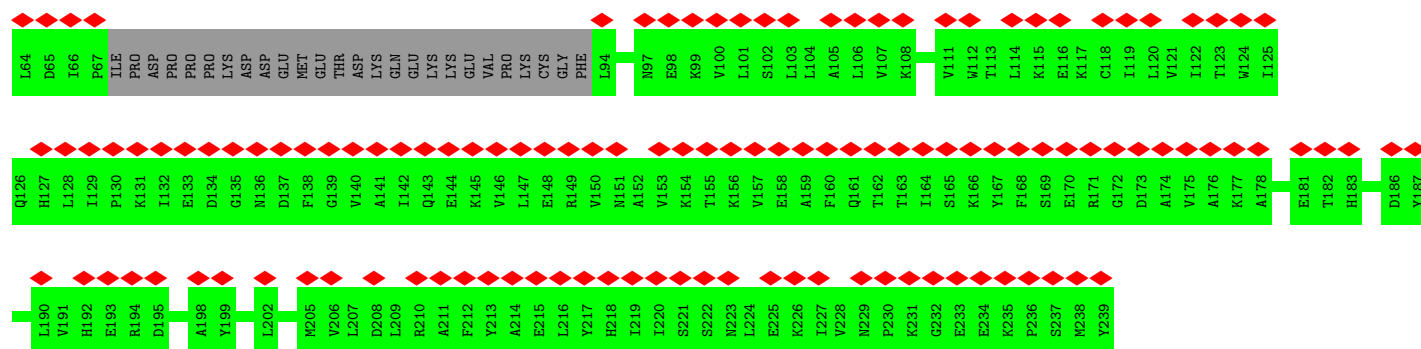
Chain H:



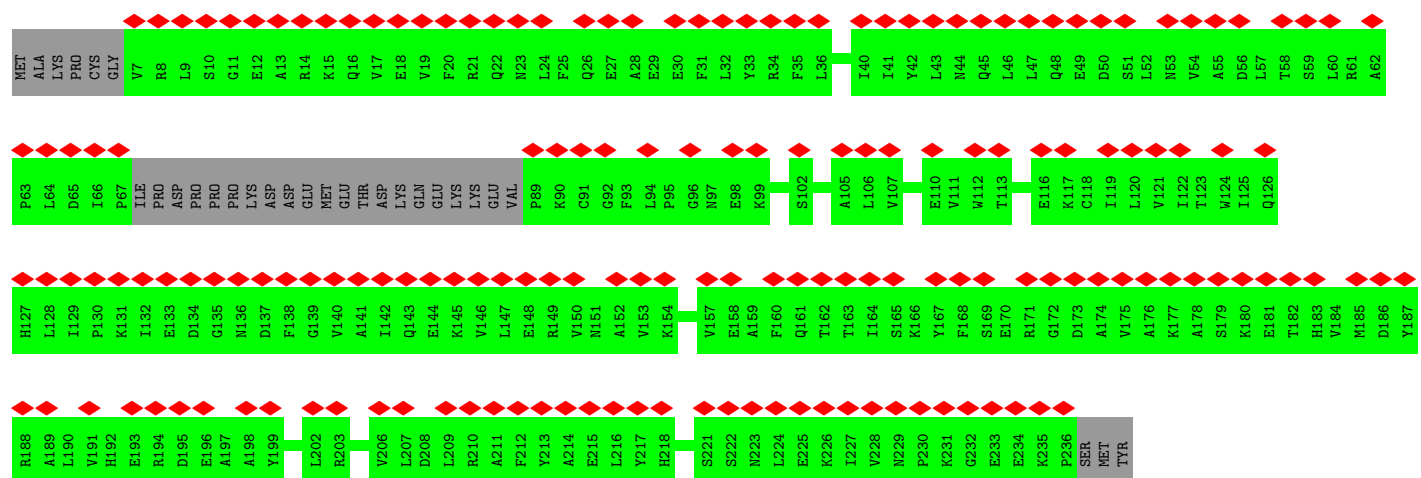
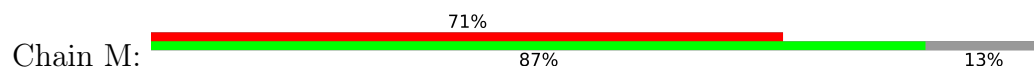
• Molecule 8: Proteasome activator complex subunit 2

Chain K:

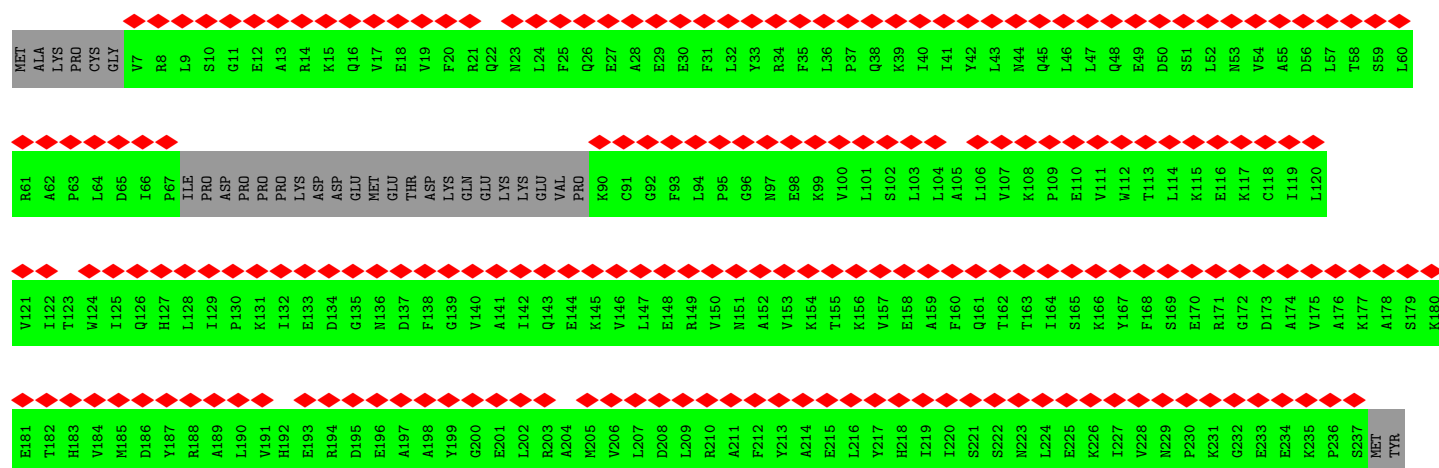
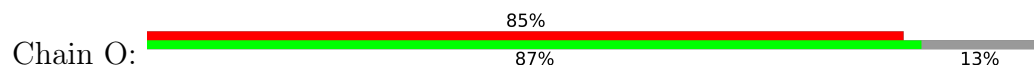




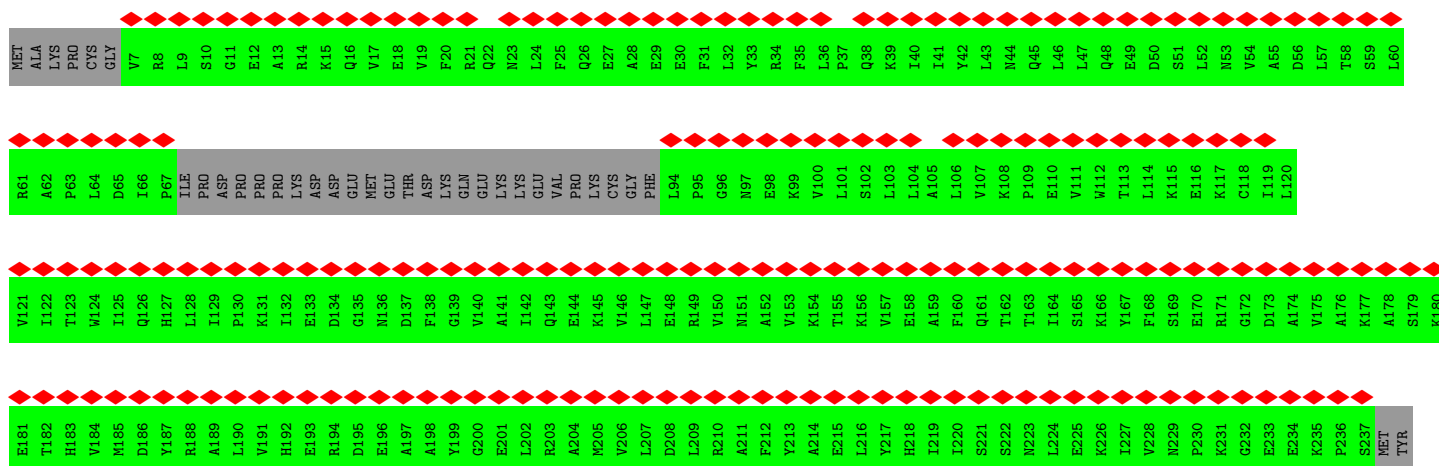
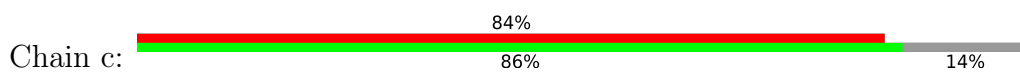
• Molecule 8: Proteasome activator complex subunit 2



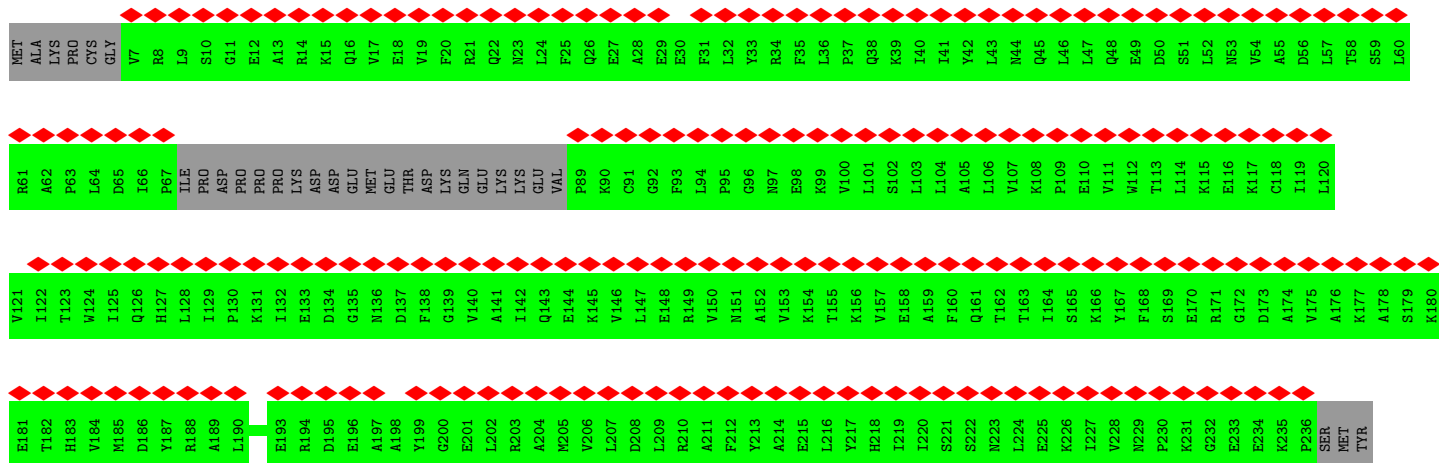
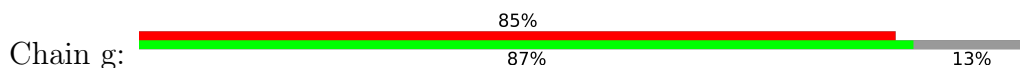
• Molecule 8: Proteasome activator complex subunit 2



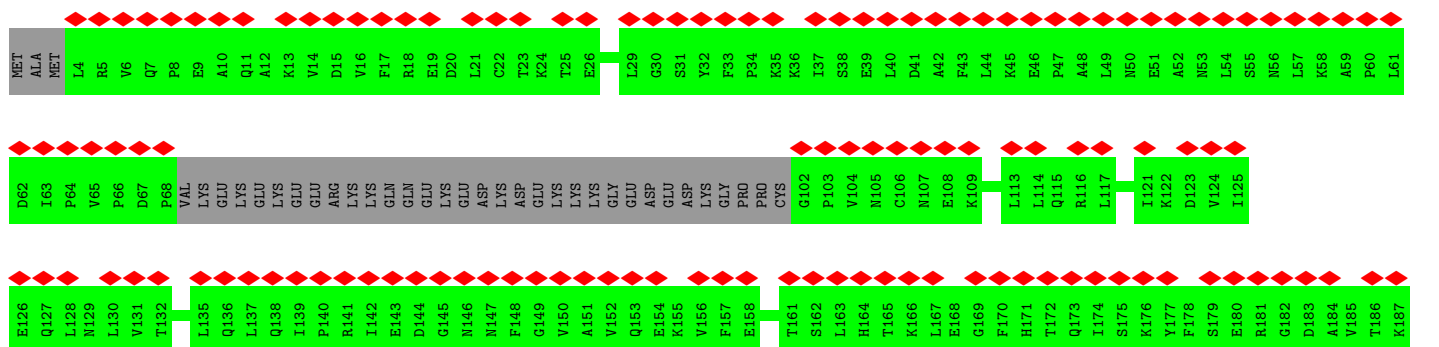
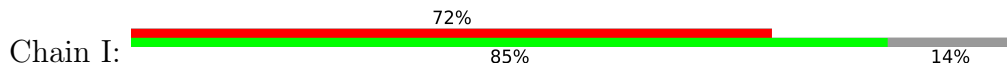
• Molecule 8: Proteasome activator complex subunit 2

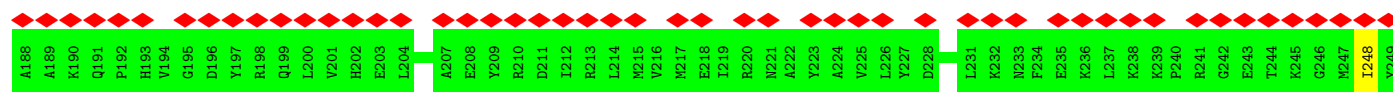


• Molecule 8: Proteasome activator complex subunit 2

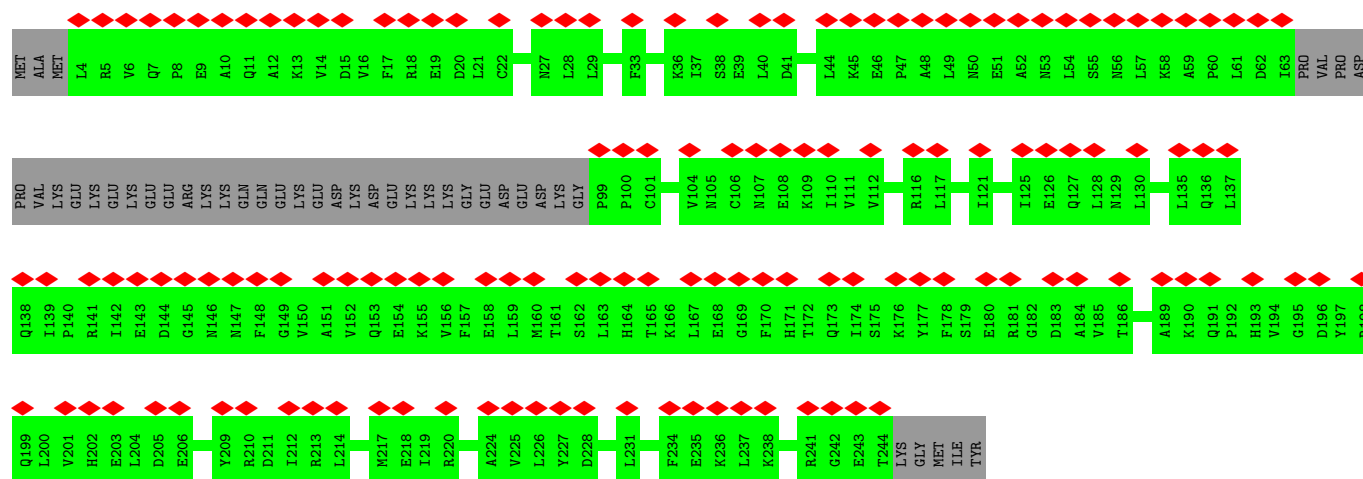
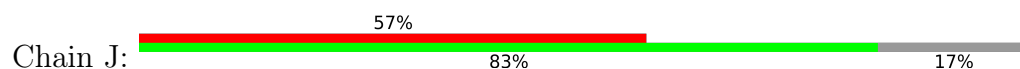


• Molecule 9: Proteasome activator complex subunit 1

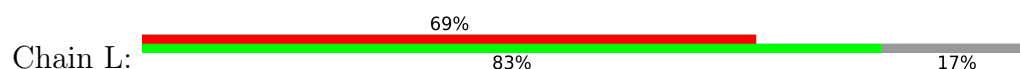




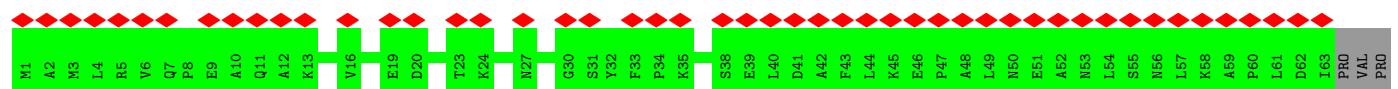
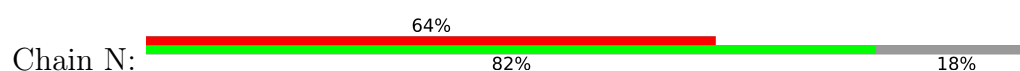
• Molecule 9: Proteasome activator complex subunit 1

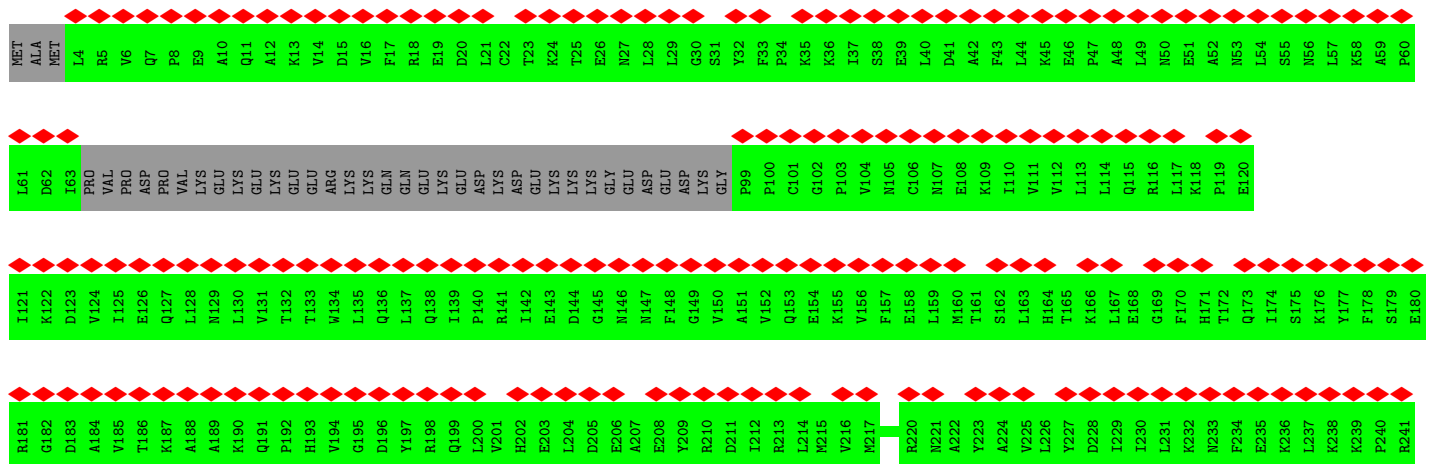


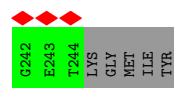
• Molecule 9: Proteasome activator complex subunit 1



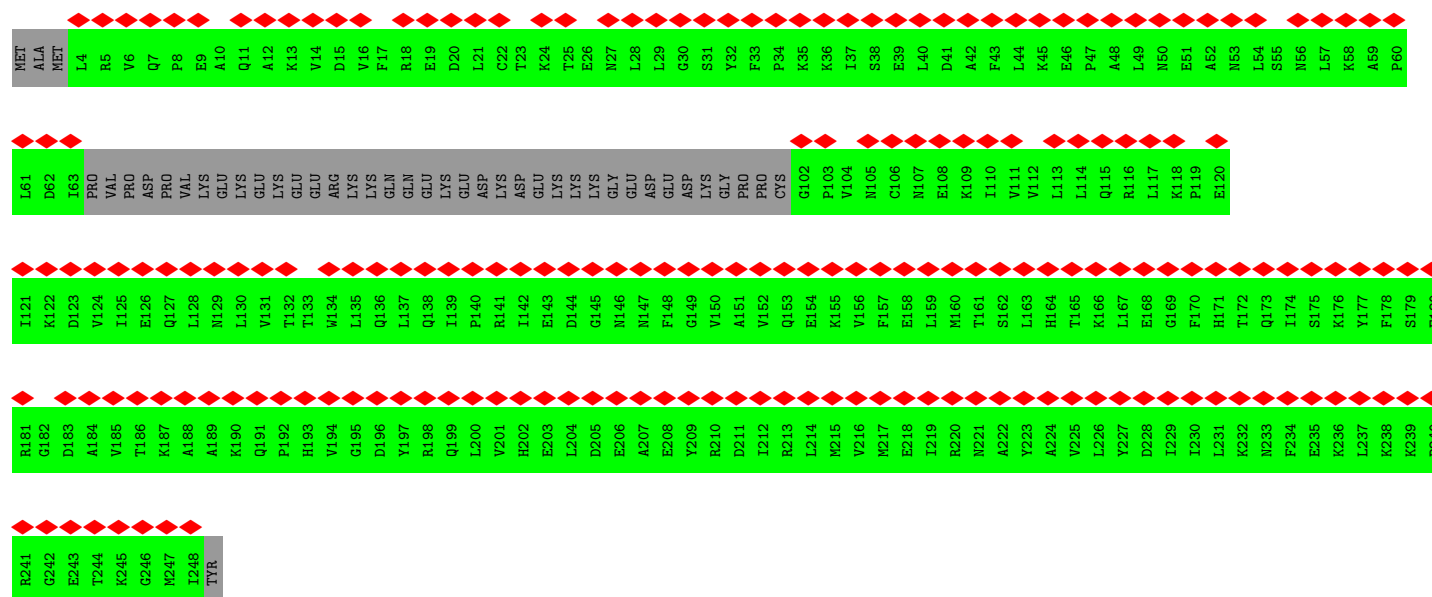
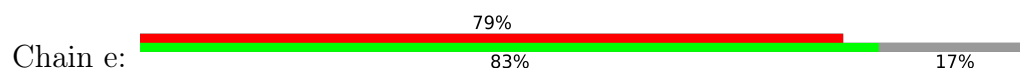
• Molecule 9: Proteasome activator complex subunit 1



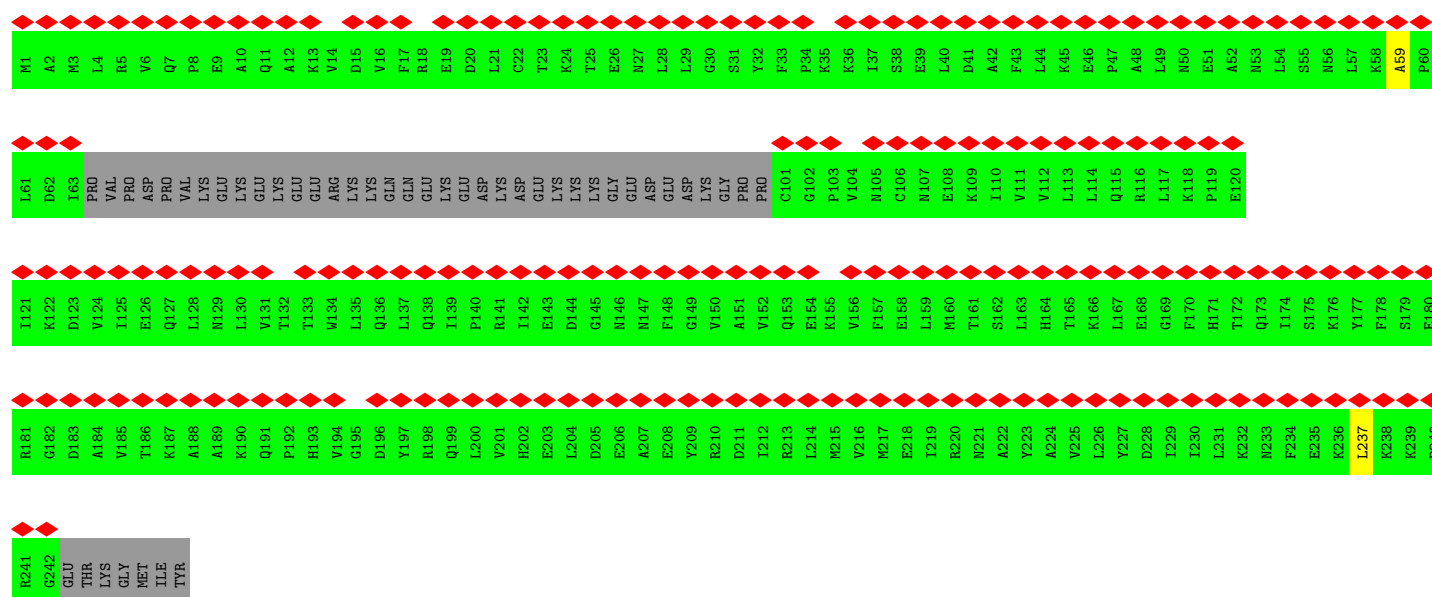
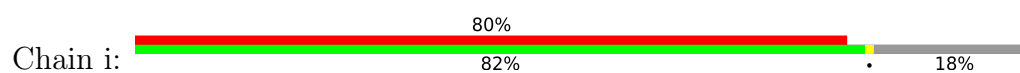




• Molecule 9: Proteasome activator complex subunit 1

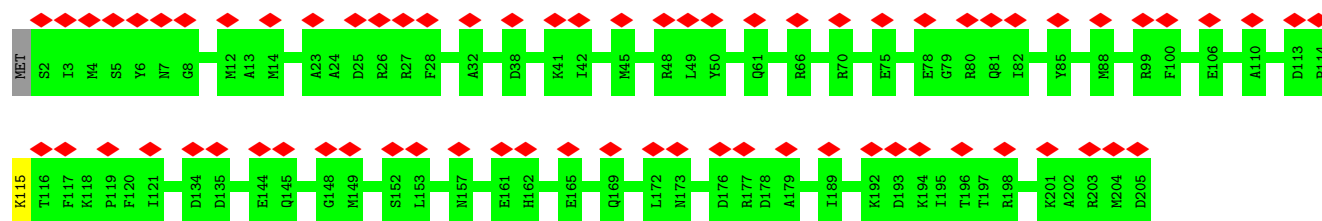


• Molecule 9: Proteasome activator complex subunit 1

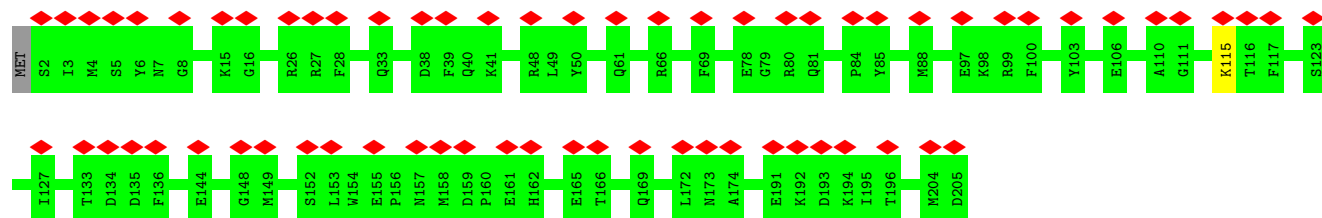


• Molecule 10: Proteasome subunit beta type-3

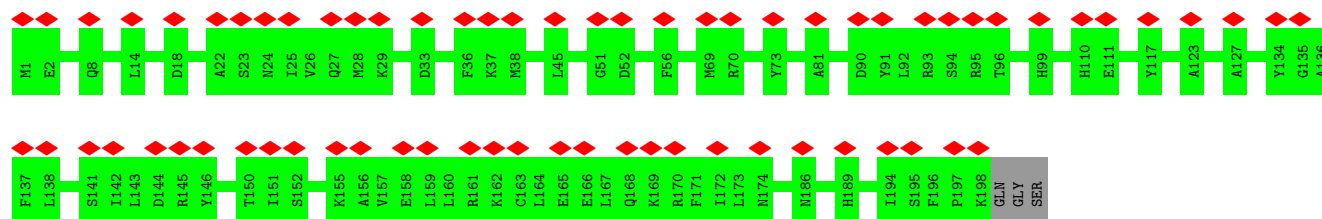




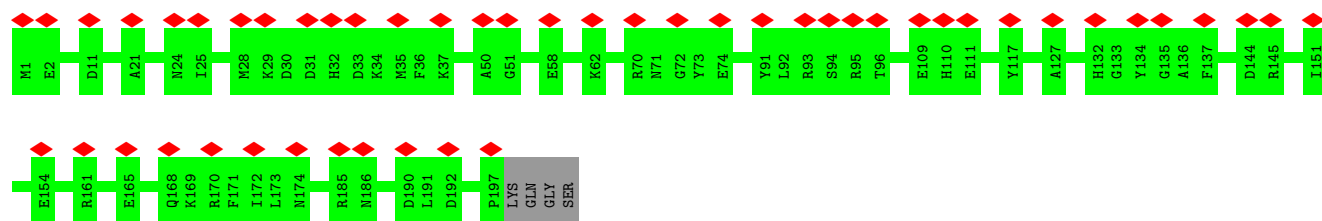
• Molecule 10: Proteasome subunit beta type-3



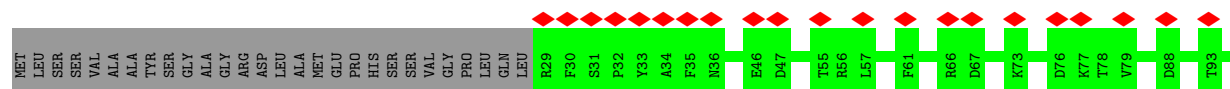
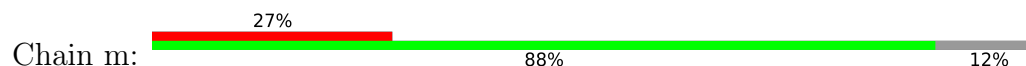
• Molecule 11: Proteasome subunit beta type-2

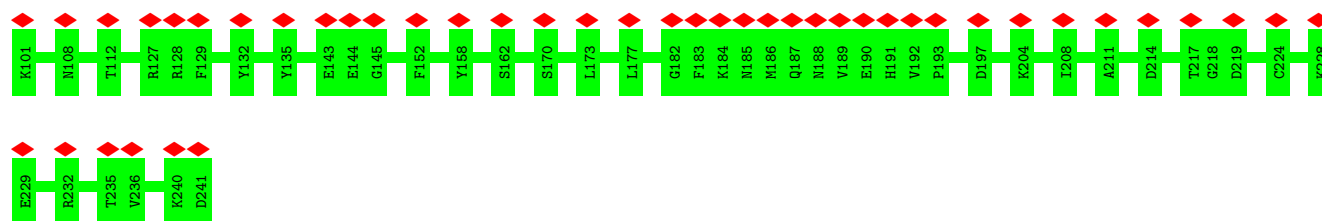


• Molecule 11: Proteasome subunit beta type-2

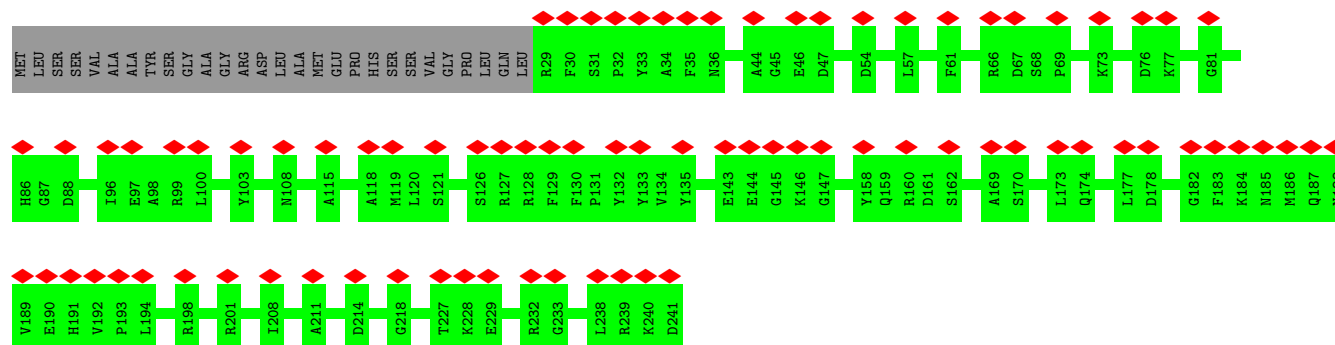
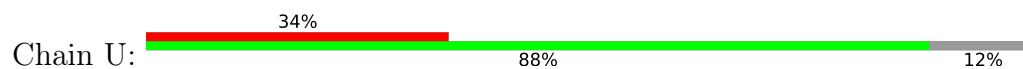


• Molecule 12: Proteasome subunit beta type-1

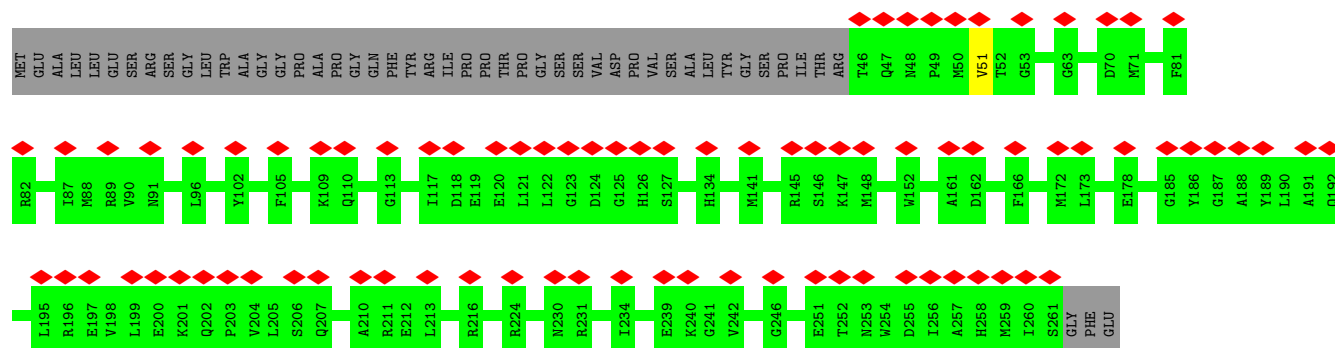
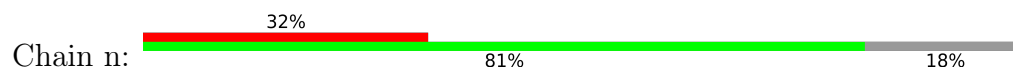




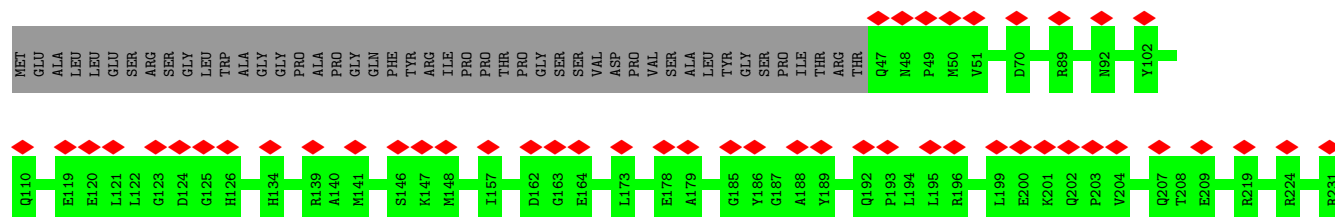
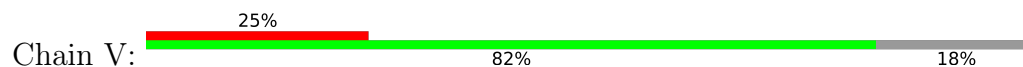
• Molecule 12: Proteasome subunit beta type-1

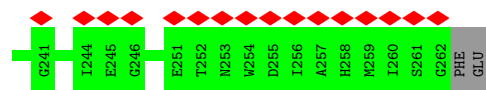


• Molecule 13: Proteasome subunit beta type-4

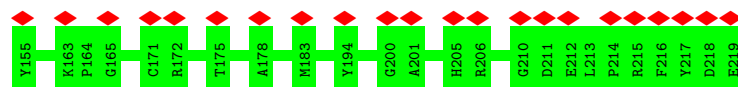
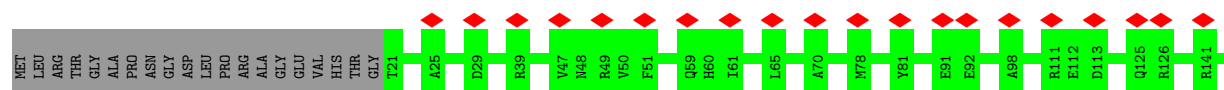


• Molecule 13: Proteasome subunit beta type-4

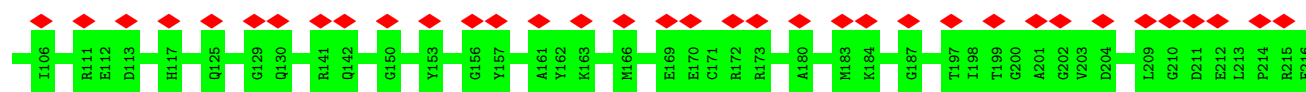
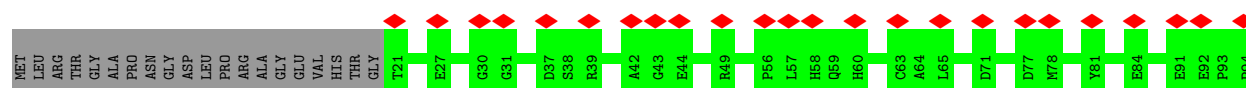




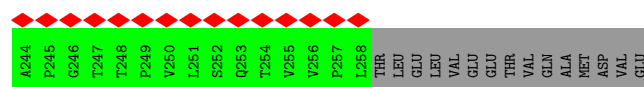
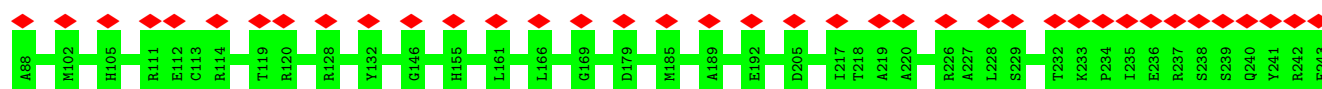
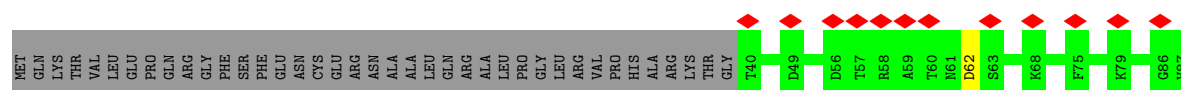
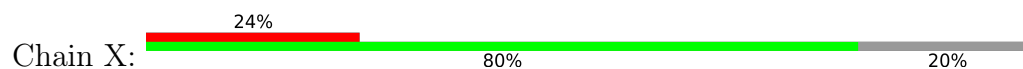
• Molecule 14: Proteasome subunit beta type-9



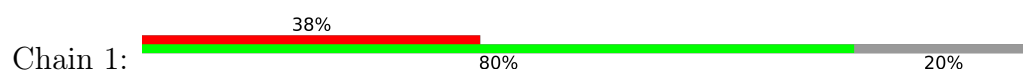
• Molecule 14: Proteasome subunit beta type-9

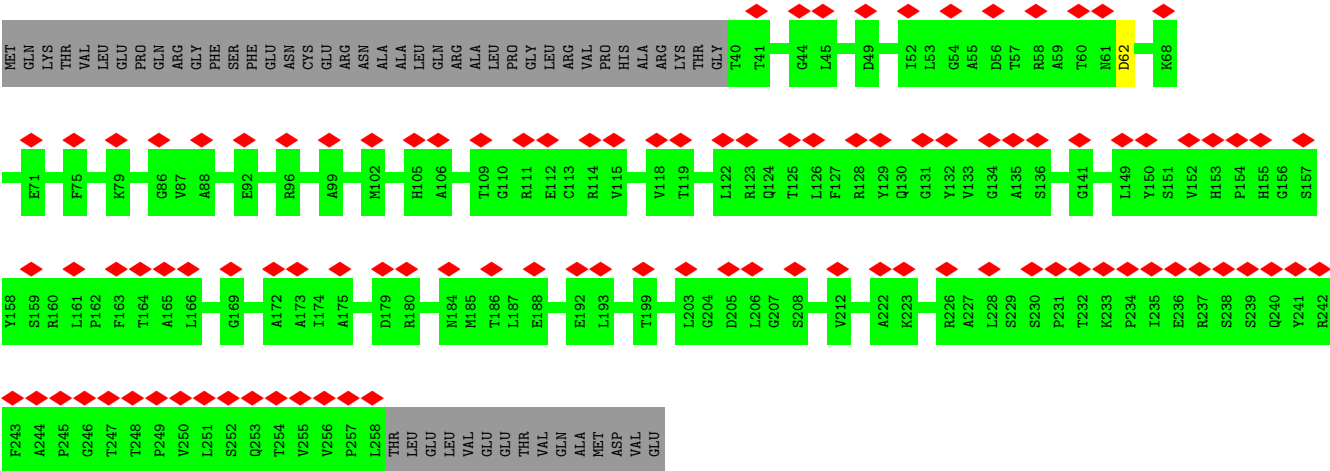


• Molecule 15: Proteasome subunit beta type-10

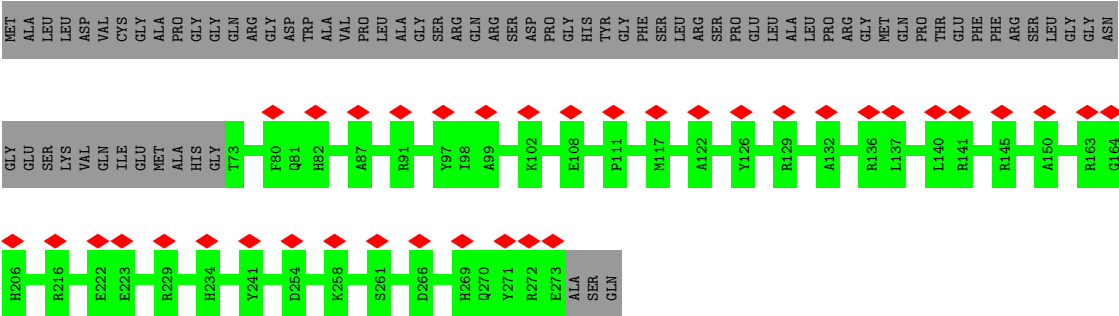


• Molecule 15: Proteasome subunit beta type-10

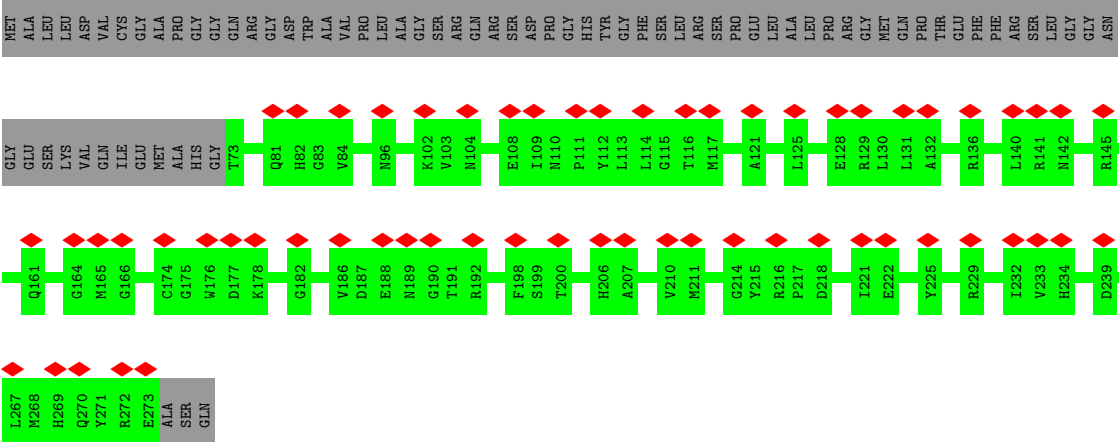




• Molecule 16: Proteasome subunit beta type-8



• Molecule 16: Proteasome subunit beta type-8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24657	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	2.421	Depositor
Minimum map value	-1.431	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.666	Depositor
Map size (Å)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	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	A	0.24	0/1875	0.40	0/2536
1	f	0.24	0/1895	0.40	0/2562
2	B	0.25	0/1801	0.41	0/2440
2	h	0.25	0/1815	0.41	0/2458
3	C	0.24	0/1957	0.41	0/2637
3	j	0.23	0/1966	0.40	0/2648
4	D	0.23	0/1851	0.43	0/2501
4	P	0.24	0/1851	0.44	0/2501
5	E	0.24	0/1818	0.42	0/2455
5	R	0.24	0/1818	0.42	0/2455
6	F	0.23	0/1880	0.42	0/2541
6	b	0.23	0/1880	0.42	0/2541
7	G	0.24	0/1914	0.40	0/2578
7	d	0.24	0/1914	0.40	0/2578
8	H	0.23	0/1714	0.36	0/2315
8	K	0.23	0/1708	0.36	0/2308
8	M	0.23	0/1720	0.35	0/2323
8	O	0.24	0/1714	0.37	0/2315
8	c	0.23	0/1687	0.36	0/2280
8	g	0.23	0/1720	0.36	0/2323
9	I	0.24	0/1752	0.36	0/2366
9	J	0.24	0/1692	0.36	0/2285
9	L	0.28	1/1699 (0.1%)	0.37	0/2291
9	N	0.23	0/1681	0.37	0/2267
9	Q	0.25	0/1752	0.38	0/2366
9	a	0.24	0/1692	0.36	0/2285
9	e	0.27	0/1699	0.36	0/2291
9	i	0.28	1/1681 (0.1%)	0.38	0/2267
10	S	0.24	0/1623	0.42	0/2188
10	k	0.24	0/1623	0.42	0/2188
11	T	0.24	0/1618	0.40	0/2190
11	l	0.24	0/1627	0.40	0/2201
12	U	0.24	0/1675	0.44	0/2257
12	m	0.24	0/1676	0.43	0/2258

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	V	0.24	0/1715	0.42	0/2319
13	n	0.24	0/1718	0.44	0/2324
14	W	0.24	0/1529	0.41	0/2071
14	Z	0.24	0/1529	0.41	0/2071
15	1	0.24	0/1637	0.43	0/2225
15	X	0.24	0/1637	0.43	0/2225
16	2	0.23	0/1592	0.41	0/2145
16	Y	0.23	0/1592	0.41	0/2145
All	All	0.24	2/72937 (0.0%)	0.40	0/98520

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	59	ALA	C-N	5.85	1.45	1.34
9	L	191	GLN	C-N	5.09	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/246 (95%)	222 (95%)	11 (5%)	0	100	100
1	f	235/246 (96%)	224 (95%)	11 (5%)	0	100	100
2	B	224/234 (96%)	221 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	226/234 (97%)	224 (99%)	2 (1%)	0	100	100
3	C	243/261 (93%)	231 (95%)	11 (4%)	1 (0%)	34	72
3	j	244/261 (94%)	232 (95%)	12 (5%)	0	100	100
4	D	230/248 (93%)	224 (97%)	5 (2%)	1 (0%)	34	72
4	P	230/248 (93%)	221 (96%)	9 (4%)	0	100	100
5	E	232/241 (96%)	226 (97%)	6 (3%)	0	100	100
5	R	232/241 (96%)	226 (97%)	6 (3%)	0	100	100
6	F	233/263 (89%)	223 (96%)	10 (4%)	0	100	100
6	b	233/263 (89%)	223 (96%)	10 (4%)	0	100	100
7	G	238/255 (93%)	230 (97%)	8 (3%)	0	100	100
7	d	238/255 (93%)	228 (96%)	9 (4%)	1 (0%)	34	72
8	H	205/239 (86%)	202 (98%)	3 (2%)	0	100	100
8	K	203/239 (85%)	196 (97%)	7 (3%)	0	100	100
8	M	205/239 (86%)	202 (98%)	3 (2%)	0	100	100
8	O	205/239 (86%)	201 (98%)	4 (2%)	0	100	100
8	c	201/239 (84%)	196 (98%)	5 (2%)	0	100	100
8	g	205/239 (86%)	202 (98%)	3 (2%)	0	100	100
9	I	209/249 (84%)	204 (98%)	4 (2%)	1 (0%)	29	68
9	J	202/249 (81%)	197 (98%)	5 (2%)	0	100	100
9	L	203/249 (82%)	195 (96%)	8 (4%)	0	100	100
9	N	201/249 (81%)	193 (96%)	8 (4%)	0	100	100
9	Q	209/249 (84%)	204 (98%)	5 (2%)	0	100	100
9	a	202/249 (81%)	197 (98%)	5 (2%)	0	100	100
9	e	203/249 (82%)	195 (96%)	8 (4%)	0	100	100
9	i	201/249 (81%)	195 (97%)	5 (2%)	1 (0%)	29	68
10	S	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	29	68
10	k	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	29	68
11	T	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
11	l	196/201 (98%)	190 (97%)	6 (3%)	0	100	100
12	U	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
12	m	211/241 (88%)	205 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	V	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
13	n	214/264 (81%)	207 (97%)	6 (3%)	1 (0%)	29	68
14	W	197/219 (90%)	194 (98%)	3 (2%)	0	100	100
14	Z	197/219 (90%)	194 (98%)	3 (2%)	0	100	100
15	1	217/273 (80%)	207 (95%)	9 (4%)	1 (0%)	29	68
15	X	217/273 (80%)	207 (95%)	9 (4%)	1 (0%)	29	68
16	2	199/276 (72%)	194 (98%)	5 (2%)	0	100	100
16	Y	199/276 (72%)	194 (98%)	5 (2%)	0	100	100
All	All	8996/10280 (88%)	8718 (97%)	268 (3%)	10 (0%)	54	85

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	52	LYS
3	C	60	PHE
9	i	237	LEU
7	d	244	LEU
13	n	51	VAL
15	X	62	ASP
15	1	62	ASP
10	k	115	LYS
10	S	115	LYS
9	I	248	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	A	202/210 (96%)	202 (100%)	0	100	100
1	f	204/210 (97%)	204 (100%)	0	100	100
2	B	186/191 (97%)	186 (100%)	0	100	100
2	h	187/191 (98%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	206/221 (93%)	206 (100%)	0	100	100
3	j	207/221 (94%)	207 (100%)	0	100	100
4	D	196/211 (93%)	196 (100%)	0	100	100
4	P	196/211 (93%)	196 (100%)	0	100	100
5	E	196/203 (97%)	196 (100%)	0	100	100
5	R	196/203 (97%)	196 (100%)	0	100	100
6	F	201/225 (89%)	201 (100%)	0	100	100
6	b	201/225 (89%)	201 (100%)	0	100	100
7	G	198/212 (93%)	198 (100%)	0	100	100
7	d	198/212 (93%)	198 (100%)	0	100	100
8	H	183/212 (86%)	183 (100%)	0	100	100
8	K	183/212 (86%)	183 (100%)	0	100	100
8	M	184/212 (87%)	184 (100%)	0	100	100
8	O	183/212 (86%)	183 (100%)	0	100	100
8	c	181/212 (85%)	181 (100%)	0	100	100
8	g	184/212 (87%)	184 (100%)	0	100	100
9	I	191/224 (85%)	191 (100%)	0	100	100
9	J	185/224 (83%)	185 (100%)	0	100	100
9	L	185/224 (83%)	185 (100%)	0	100	100
9	N	183/224 (82%)	183 (100%)	0	100	100
9	Q	191/224 (85%)	191 (100%)	0	100	100
9	a	185/224 (83%)	185 (100%)	0	100	100
9	e	185/224 (83%)	185 (100%)	0	100	100
9	i	183/224 (82%)	183 (100%)	0	100	100
10	S	174/175 (99%)	174 (100%)	0	100	100
10	k	174/175 (99%)	174 (100%)	0	100	100
11	T	168/171 (98%)	168 (100%)	0	100	100
11	l	169/171 (99%)	169 (100%)	0	100	100
12	U	176/198 (89%)	176 (100%)	0	100	100
12	m	177/198 (89%)	177 (100%)	0	100	100
13	V	177/215 (82%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	n	178/215 (83%)	178 (100%)	0	100	100
14	W	153/167 (92%)	153 (100%)	0	100	100
14	Z	153/167 (92%)	153 (100%)	0	100	100
15	1	170/216 (79%)	170 (100%)	0	100	100
15	X	170/216 (79%)	170 (100%)	0	100	100
16	2	166/222 (75%)	166 (100%)	0	100	100
16	Y	166/222 (75%)	166 (100%)	0	100	100
All	All	7731/8738 (88%)	7731 (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. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	123	GLN
1	A	150	GLN
2	B	52	GLN
2	B	102	GLN
3	C	102	GLN
3	C	146	GLN
3	C	167	ASN
4	D	15	HIS
5	E	114	GLN
5	E	182	GLN
6	F	65	HIS
6	F	117	GLN
6	F	166	GLN
7	G	225	HIS
8	K	126	GLN
9	L	193	HIS
9	N	7	GLN
9	N	153	GLN
9	Q	199	GLN
8	c	192	HIS
8	g	38	GLN
9	i	7	GLN
4	P	15	HIS
4	P	94	HIS

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Mol	Chain	Res	Type
5	R	122	GLN
6	b	65	HIS
6	b	117	GLN
6	b	166	GLN
6	b	175	HIS
7	d	225	HIS
1	f	150	GLN
2	h	52	GLN
2	h	102	GLN
2	h	109	GLN
3	j	102	GLN
3	j	146	GLN
3	j	167	ASN
10	k	169	GLN
12	m	108	ASN
13	n	91	ASN
13	n	192	GLN
12	U	108	ASN
13	V	91	ASN
13	V	114	GLN
13	V	192	GLN
16	Y	110	ASN
16	Y	234	HIS
16	Y	247	ASN
14	Z	105	ASN
16	2	96	ASN
16	2	110	ASN
16	2	234	HIS
16	2	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

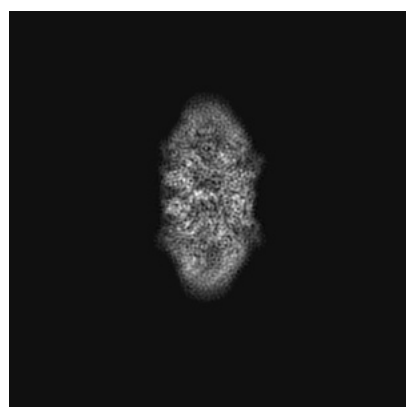
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30828. These allow visual inspection of the internal detail of the map and identification of artifacts.

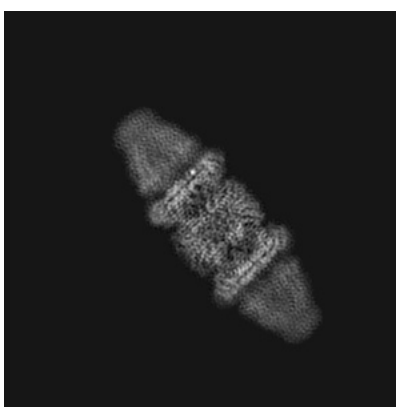
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

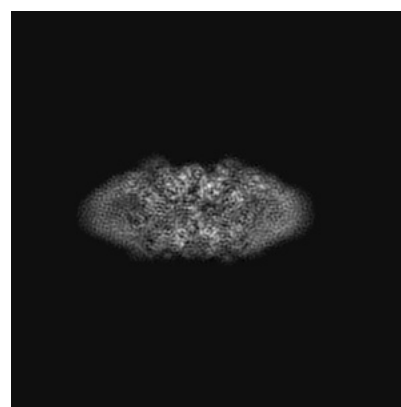
6.1.1 Primary map



X



Y



Z

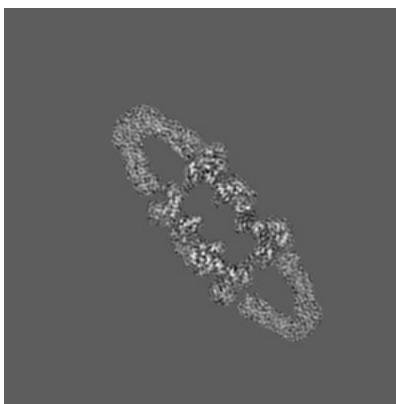
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

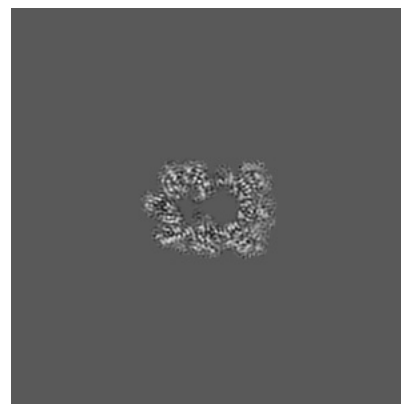
6.2.1 Primary map



X Index: 180



Y Index: 180

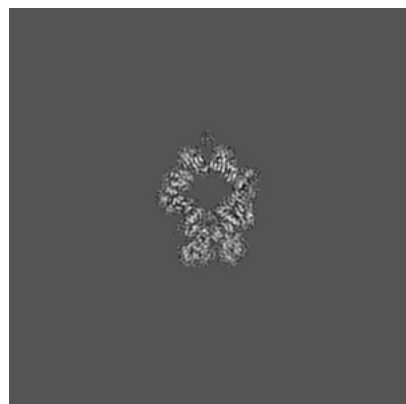


Z Index: 180

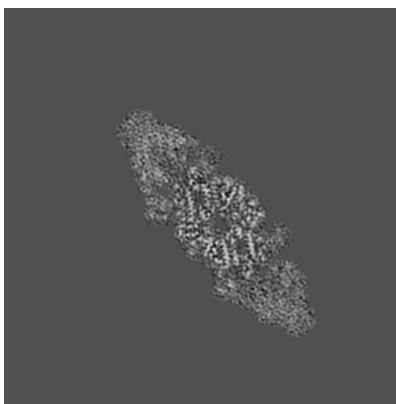
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 171



Y Index: 161



Z Index: 194

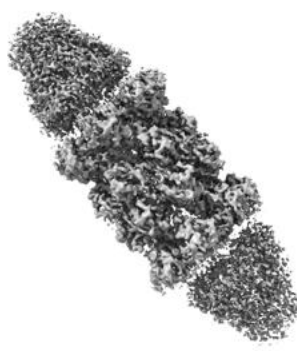
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.666. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

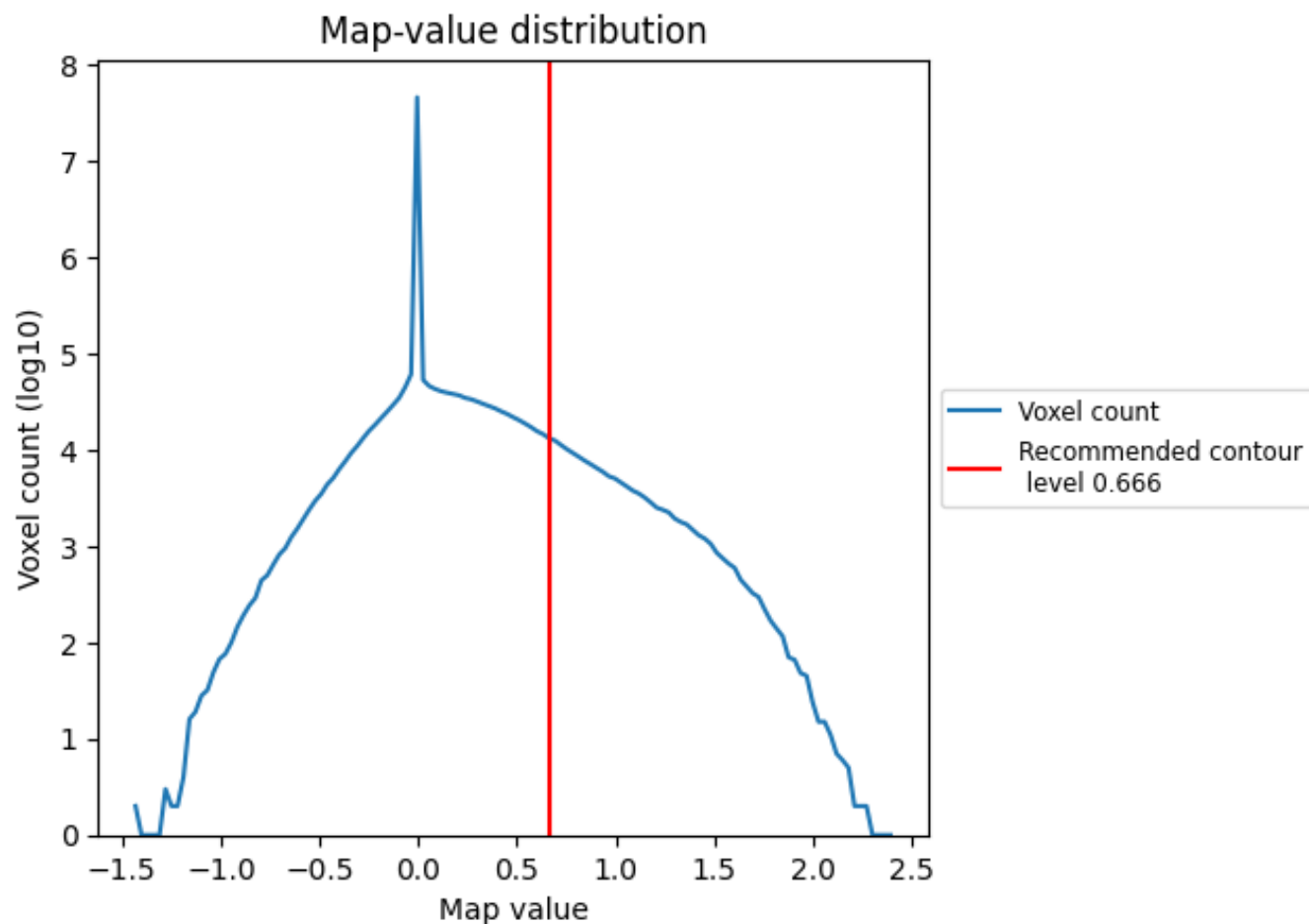
6.5 Mask visualisation

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

7 Map analysis [i](#)

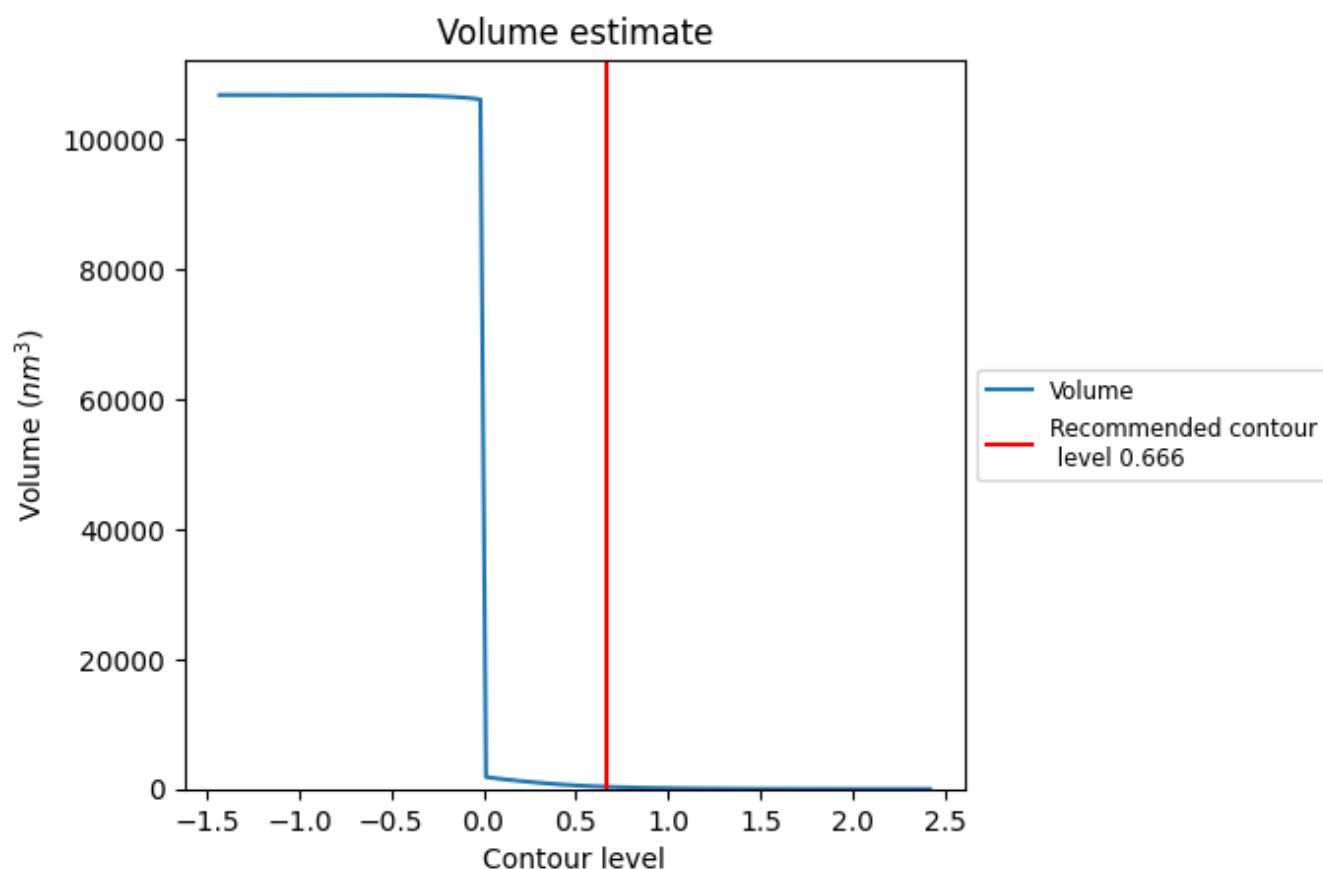
This section contains the results of statistical analysis of the map.

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.

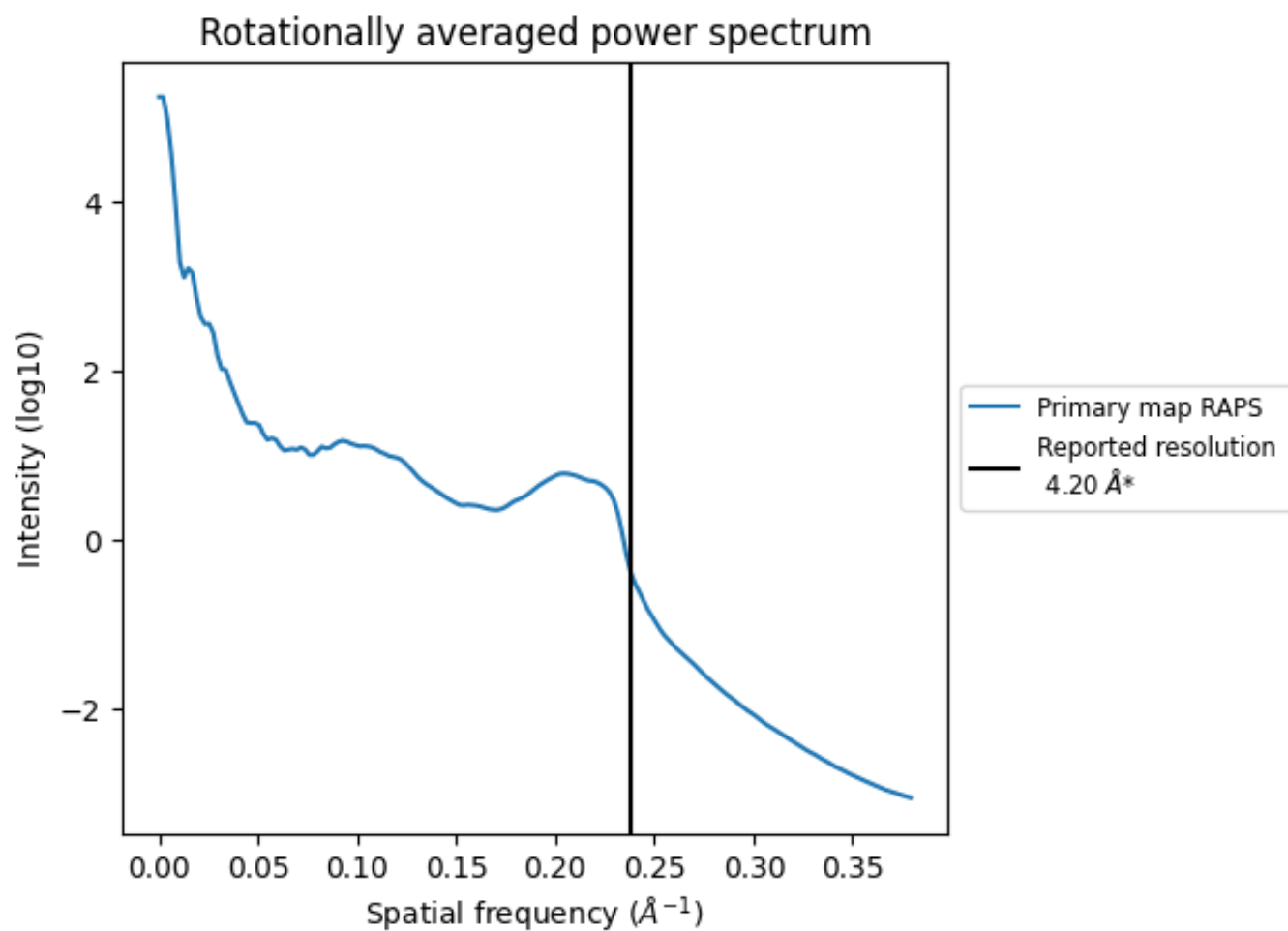
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm³; this corresponds to an approximate mass of 300 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 0.238 Å⁻¹

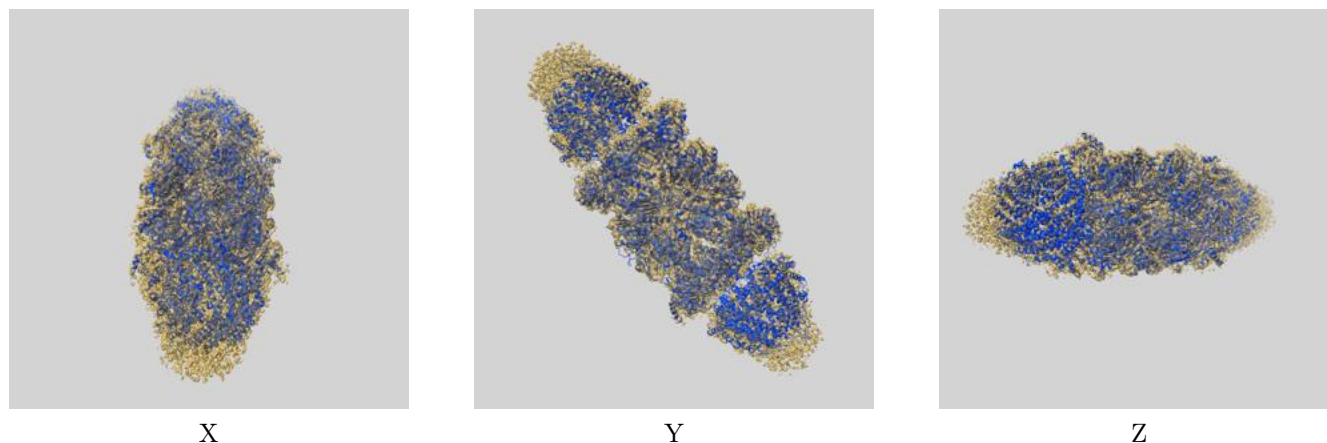
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

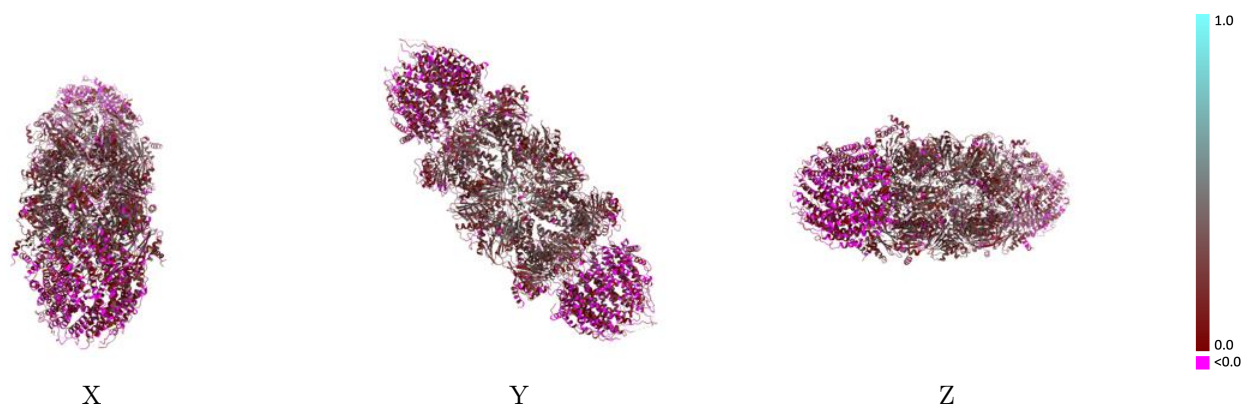
This section contains information regarding the fit between EMDB map EMD-30828 and PDB model 7DRW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



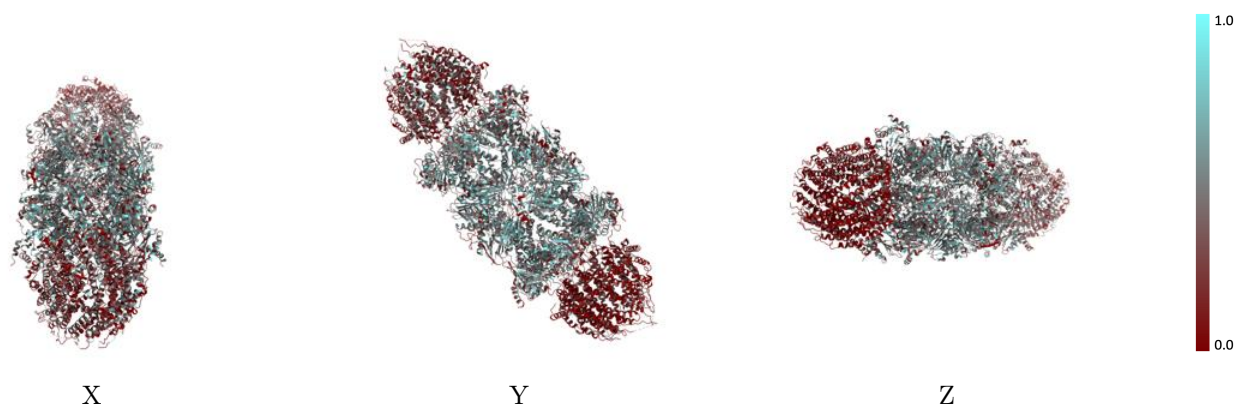
The images above show the 3D surface view of the map at the recommended contour level 0.666 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



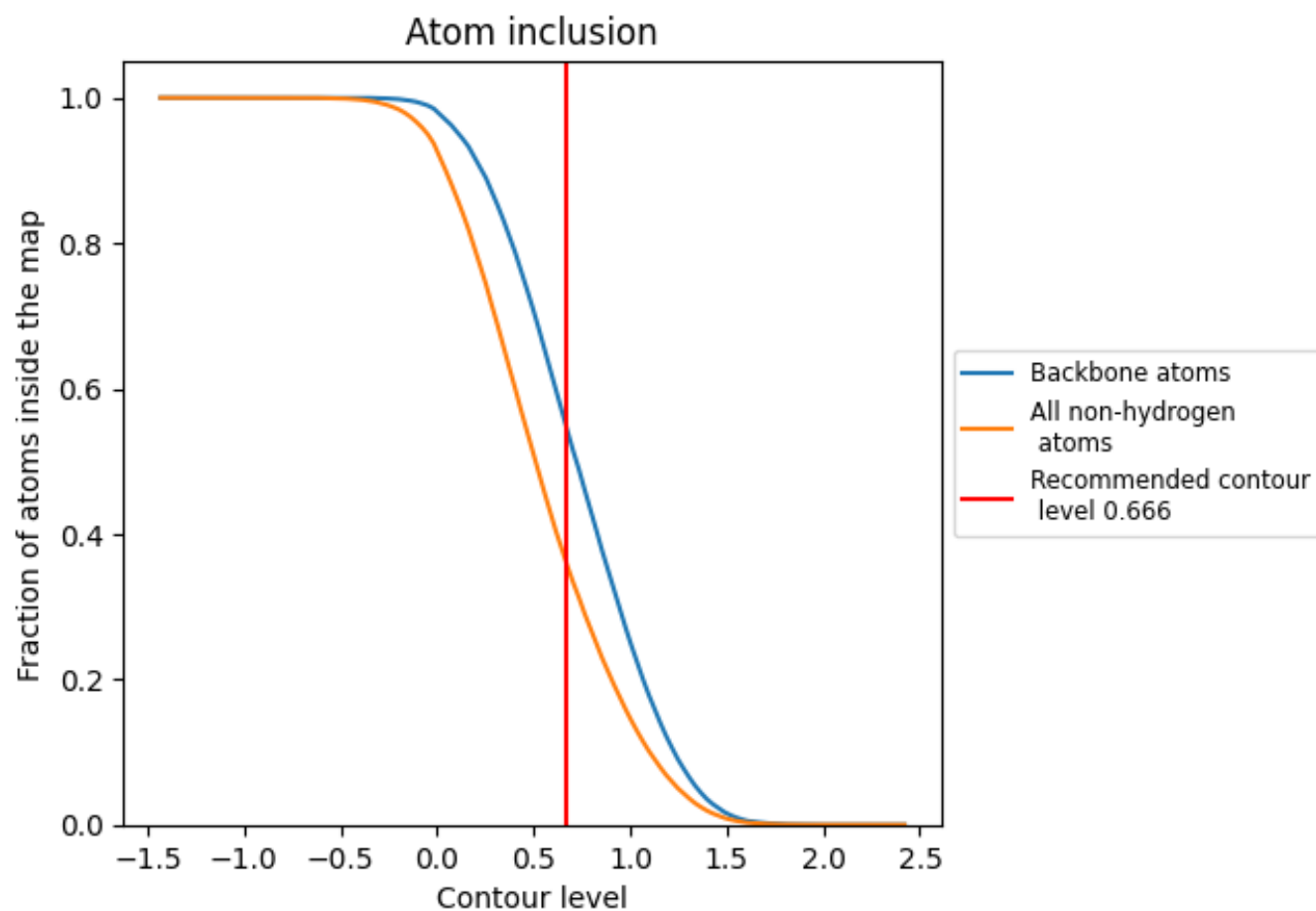
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.666).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 36% 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 (0.666) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3626	 0.1790
1	 0.4269	 0.2090
2	 0.4763	 0.2200
A	 0.4224	 0.1910
B	 0.4334	 0.2110
C	 0.4564	 0.2310
D	 0.4697	 0.2440
E	 0.3666	 0.1370
F	 0.4936	 0.2540
G	 0.4603	 0.2430
H	 0.2263	 0.1050
I	 0.2079	 0.0870
J	 0.2903	 0.1150
K	 0.2005	 0.0790
L	 0.2103	 0.0550
M	 0.2165	 0.0740
N	 0.2391	 0.0860
O	 0.1047	 0.0680
P	 0.4584	 0.2280
Q	 0.0774	 0.0610
R	 0.4191	 0.1980
S	 0.4812	 0.2600
T	 0.5162	 0.2870
U	 0.4547	 0.2350
V	 0.4835	 0.2620
W	 0.5368	 0.2840
X	 0.4813	 0.2500
Y	 0.5270	 0.2870
Z	 0.4952	 0.2440
a	 0.1094	 0.0170
b	 0.4632	 0.2360
c	 0.0836	 0.0390
d	 0.4554	 0.2380
e	 0.0900	 0.0420
f	 0.4615	 0.2370



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Chain	Atom inclusion	Q-score
g	 0.0850	 0.0390
h	 0.4759	 0.2320
i	 0.0830	 0.0350
j	 0.3984	 0.1940
k	 0.4875	 0.2480
l	 0.4849	 0.2480
m	 0.4680	 0.2560
n	 0.4430	 0.2390