



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2023 – 03:08 PM EDT

PDB ID : 5VHS
EMDB ID : EMD-8684
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2017-04-13
Resolution : 8.80 Å(reported)

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

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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:

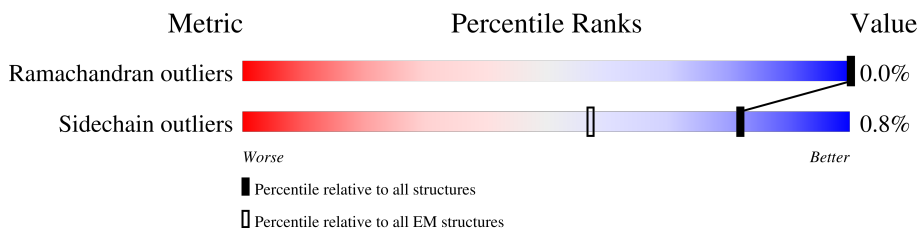
EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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 8.80 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	352	
2	B	341	
3	C	385	
4	D	368	
5	E	379	
6	F	380	
7	U	935	
8	V	488	
9	W	456	

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Mol	Chain	Length	Quality of chain
10	X	385	<p>51% 73% 27%</p>
11	Y	378	<p>55% 100%</p>
12	Z	286	<p>48% 100%</p>
13	a	374	<p>62% 100%</p>
14	b	191	<p>73% 99%</p>
15	c	287	<p>48% 100%</p>
16	d	257	<p>58% 68% 32%</p>
17	e	33	<p>42% 100%</p>
18	f	784	<p>72% 79% 19%</p>

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 47840 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	338	2665	1682	470	496	17	0	0

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	317	2476	1557	421	487	11	0	0

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	349	2752	1724	502	512	14	0	0

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	332	2649	1677	466	497	9	0	0

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	313	2493	1566	448	464	15	0	0

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	339	2647	1673	460	498	16	0	0

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	U	751	5829	3696	1001	1088	44	0	0

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	V	262	2129	1360	377	385	7	0	0

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	391	3206	2040	545	600	21	0	0

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	280	2221	1414	373	425	9	0	0

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Y	378	3115	1987	533	578	17	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Z	286	2281	1457	392	427	5	0	0

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	a	374	3003	1915	511	562	15	0	0

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	176	Total	C	N	O	S	0	0
			1452	943	232	272	5		

- Molecule 17 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	33	Total	C	N	O	S	0	0
			283	172	46	64	1		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	636	Total	C	N	O	S	0	0
			4920	3110	830	945	35		

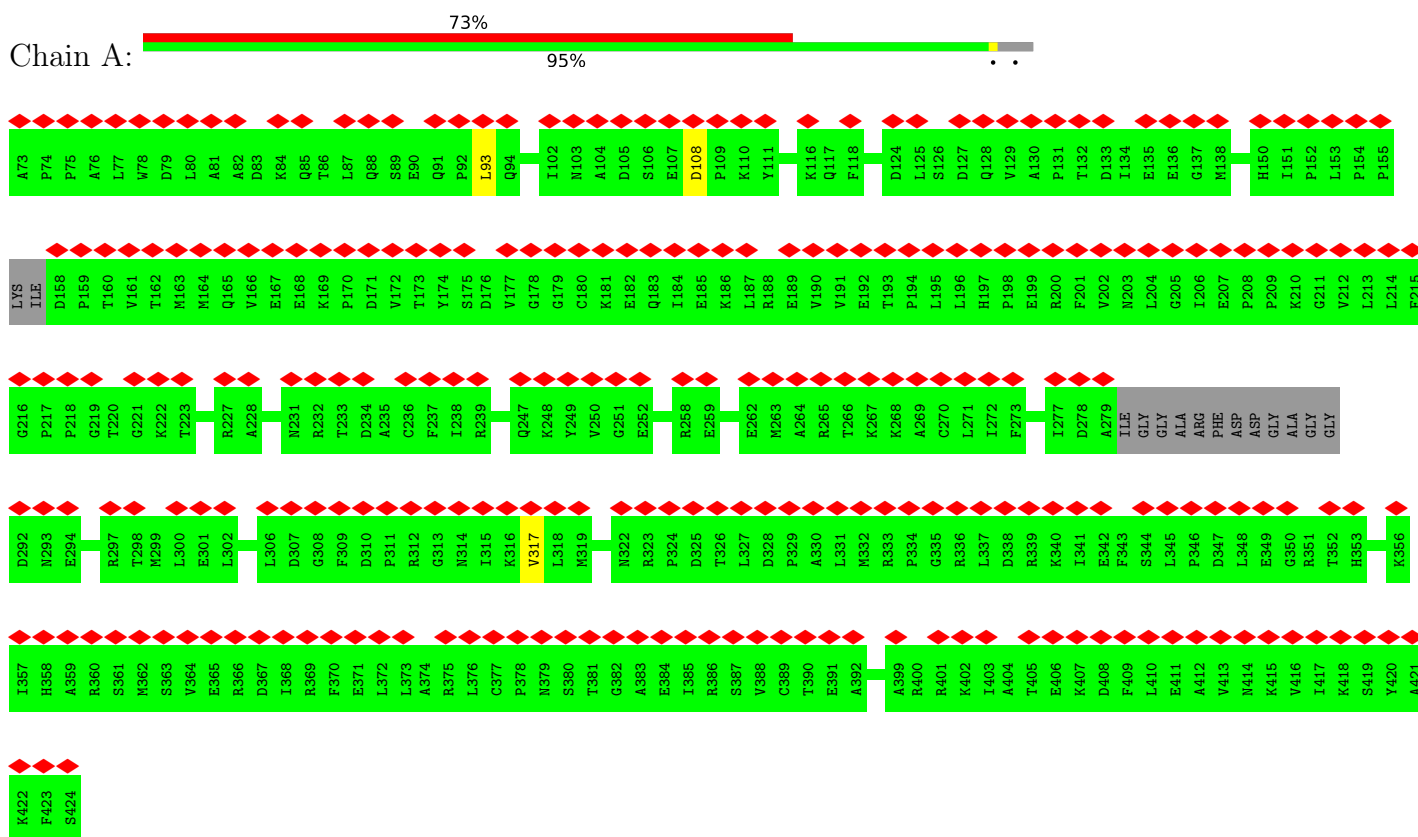
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	c	1	Total	Zn	0
			1	1	

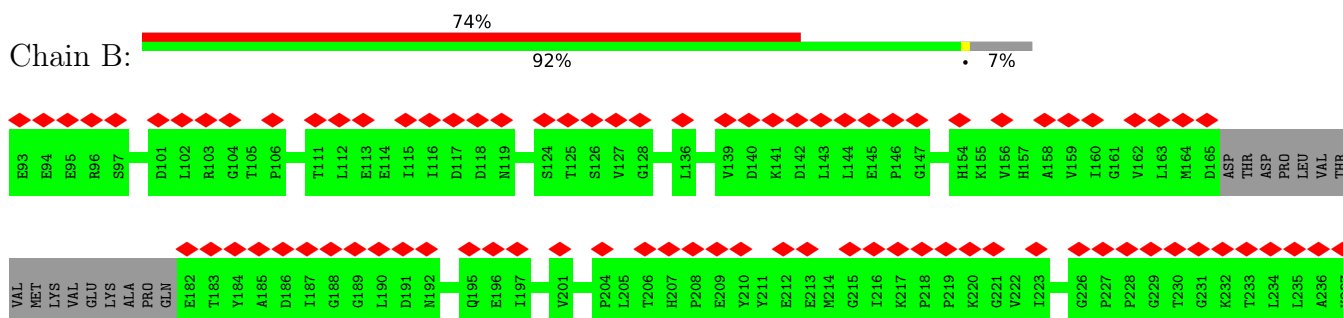
3 Residue-property plots [i](#)

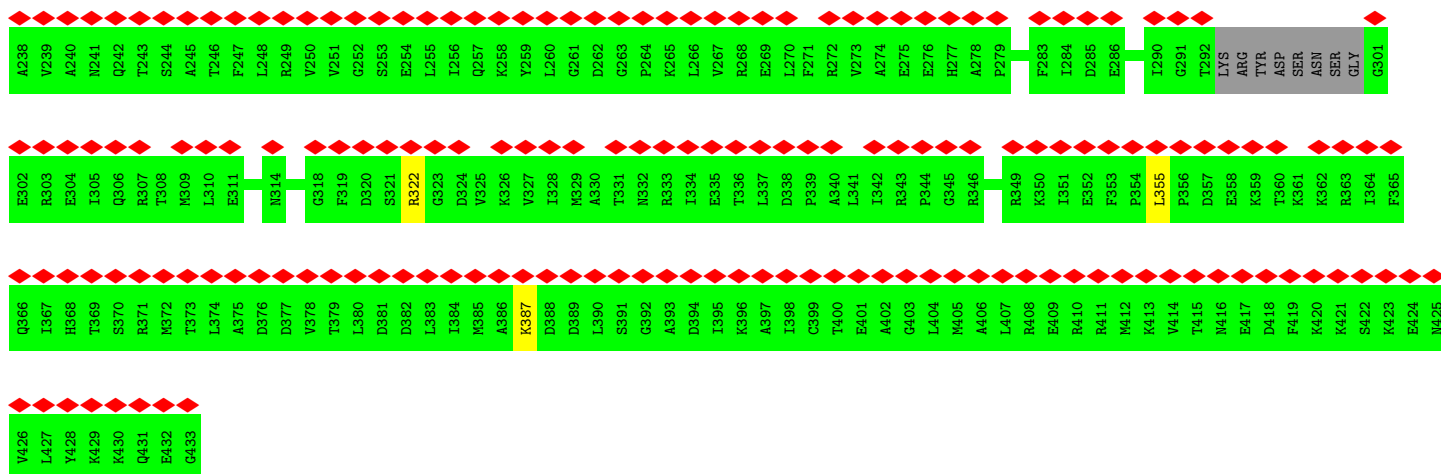
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome regulatory subunit 7

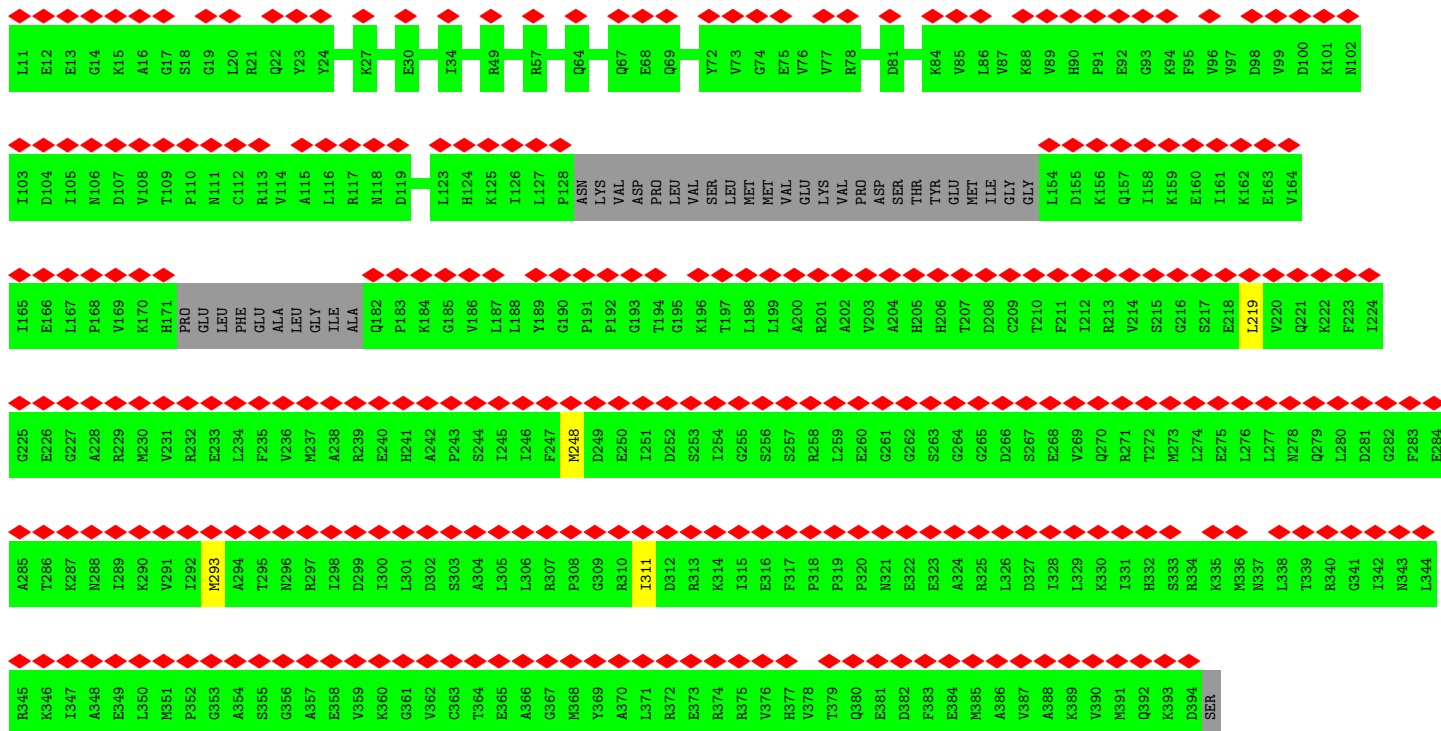
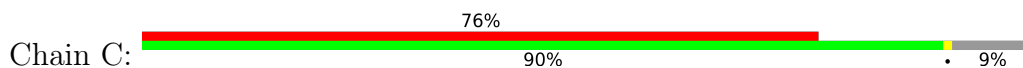


- Molecule 2: 26S proteasome regulatory subunit 4

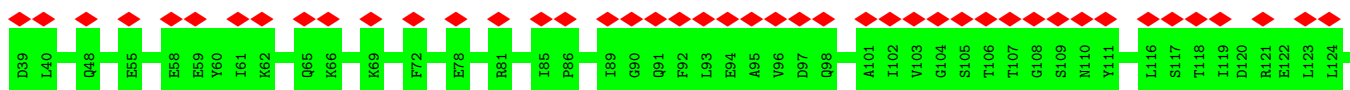
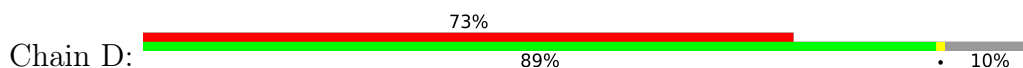


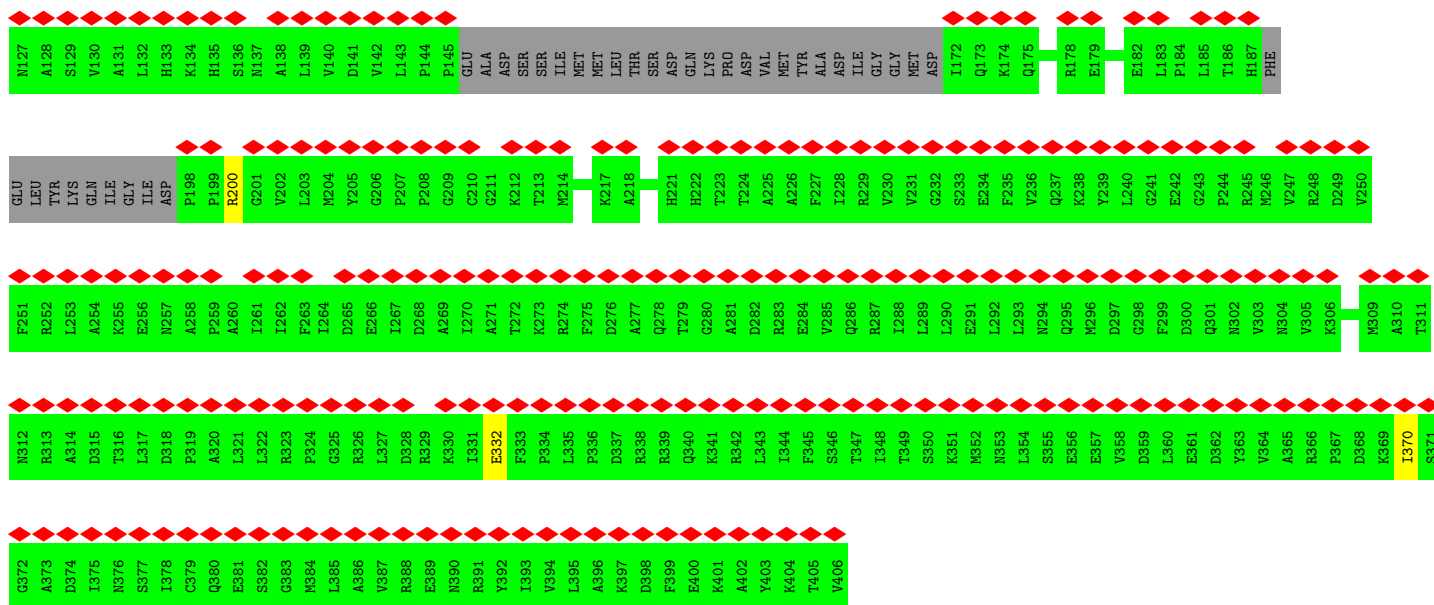


• Molecule 3: 26S proteasome regulatory subunit 8

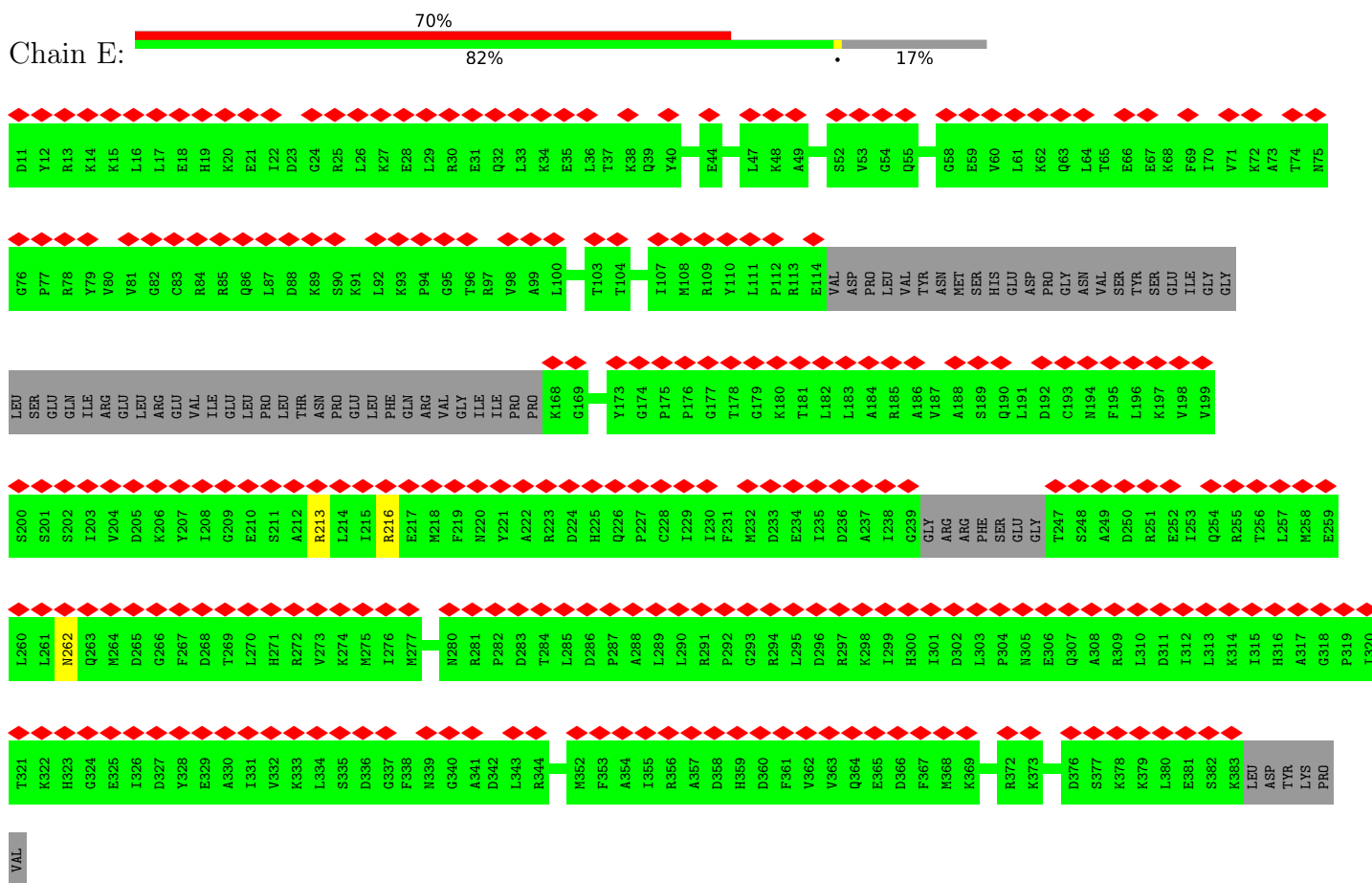


• Molecule 4: 26S proteasome regulatory subunit 6B



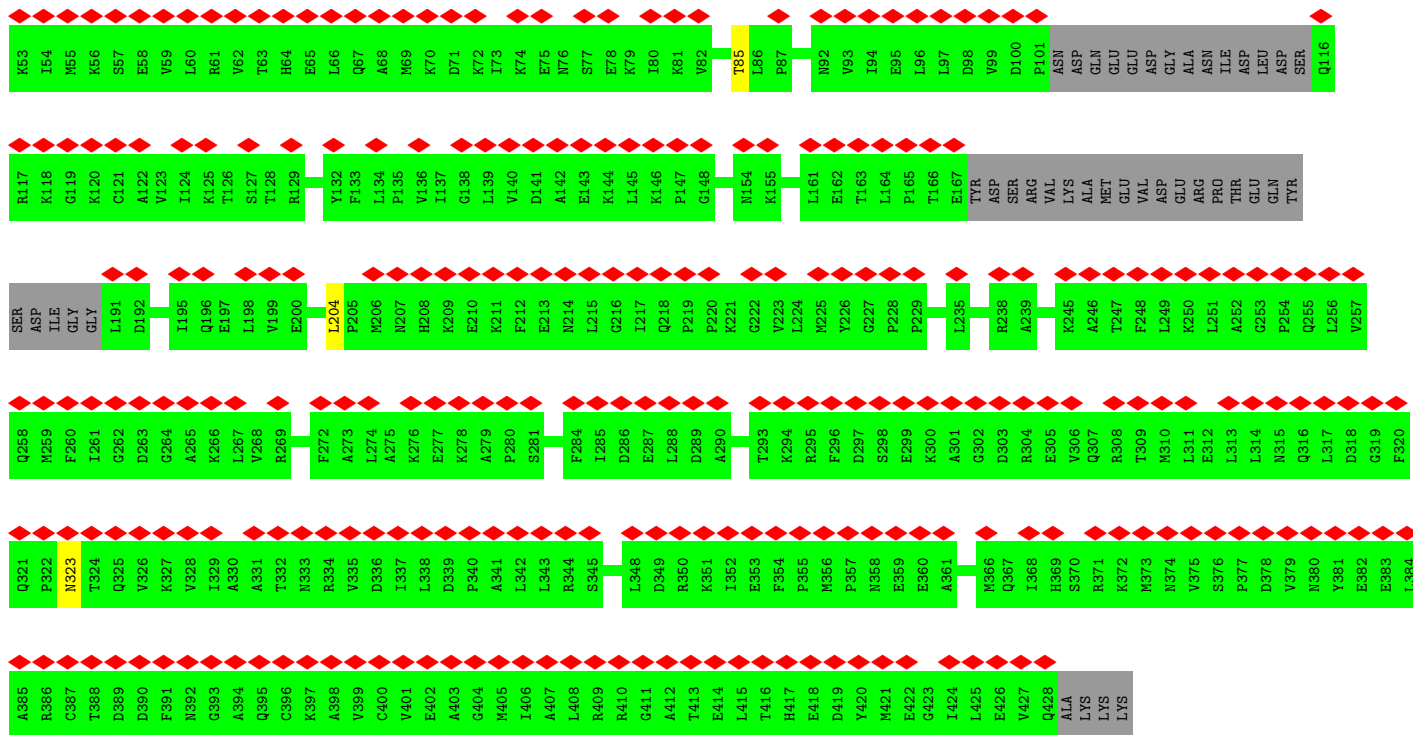


• Molecule 5: 26S proteasome regulatory subunit 10B

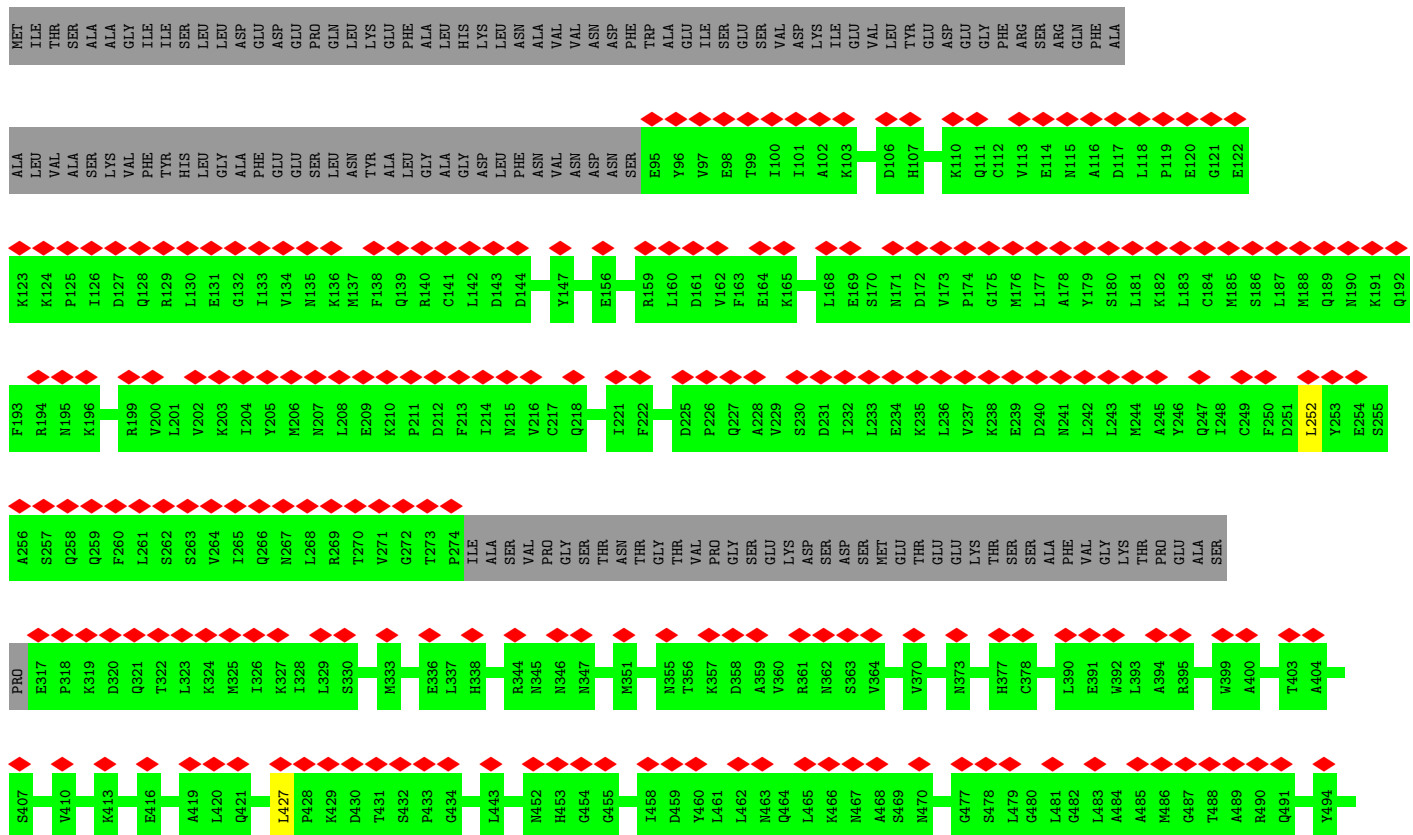
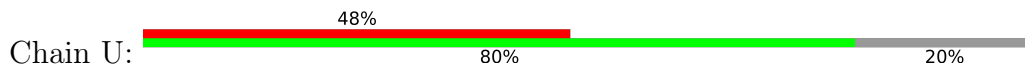


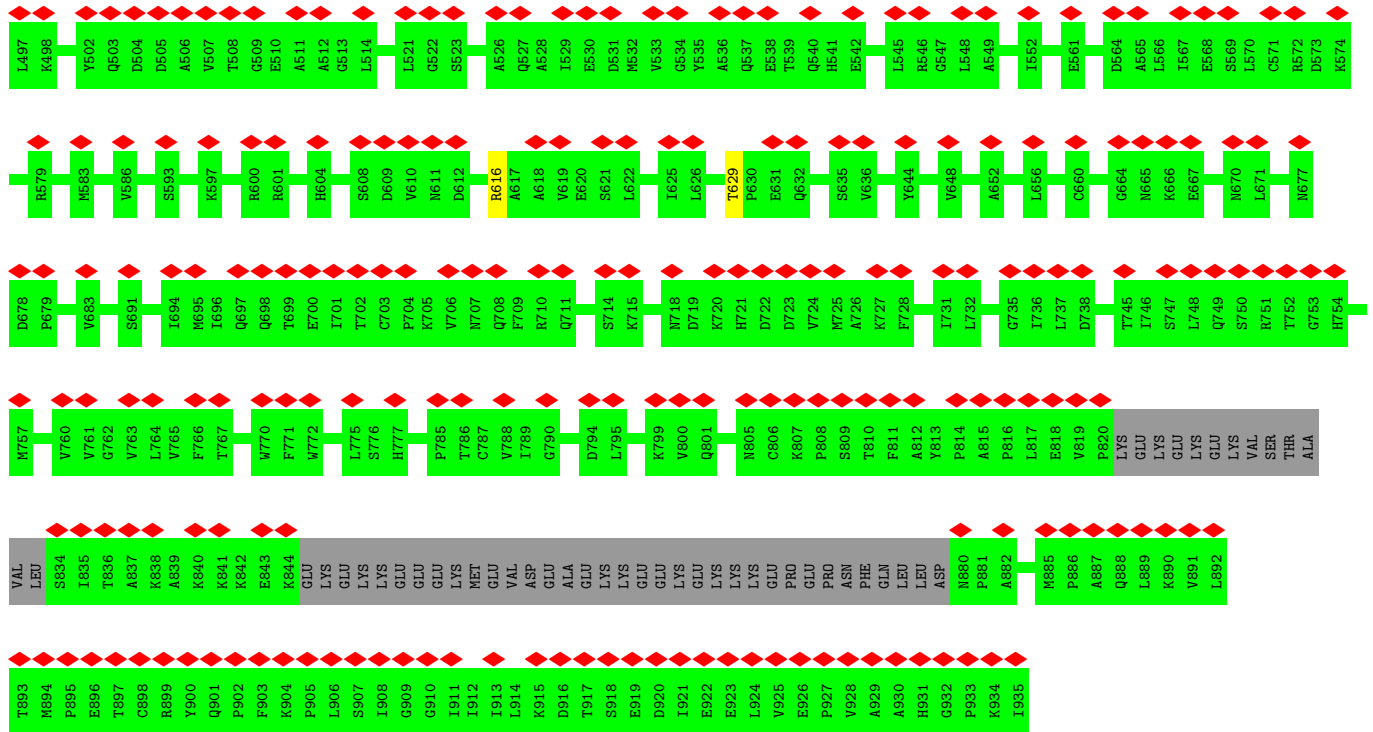
• Molecule 6: 26S proteasome regulatory subunit 6A



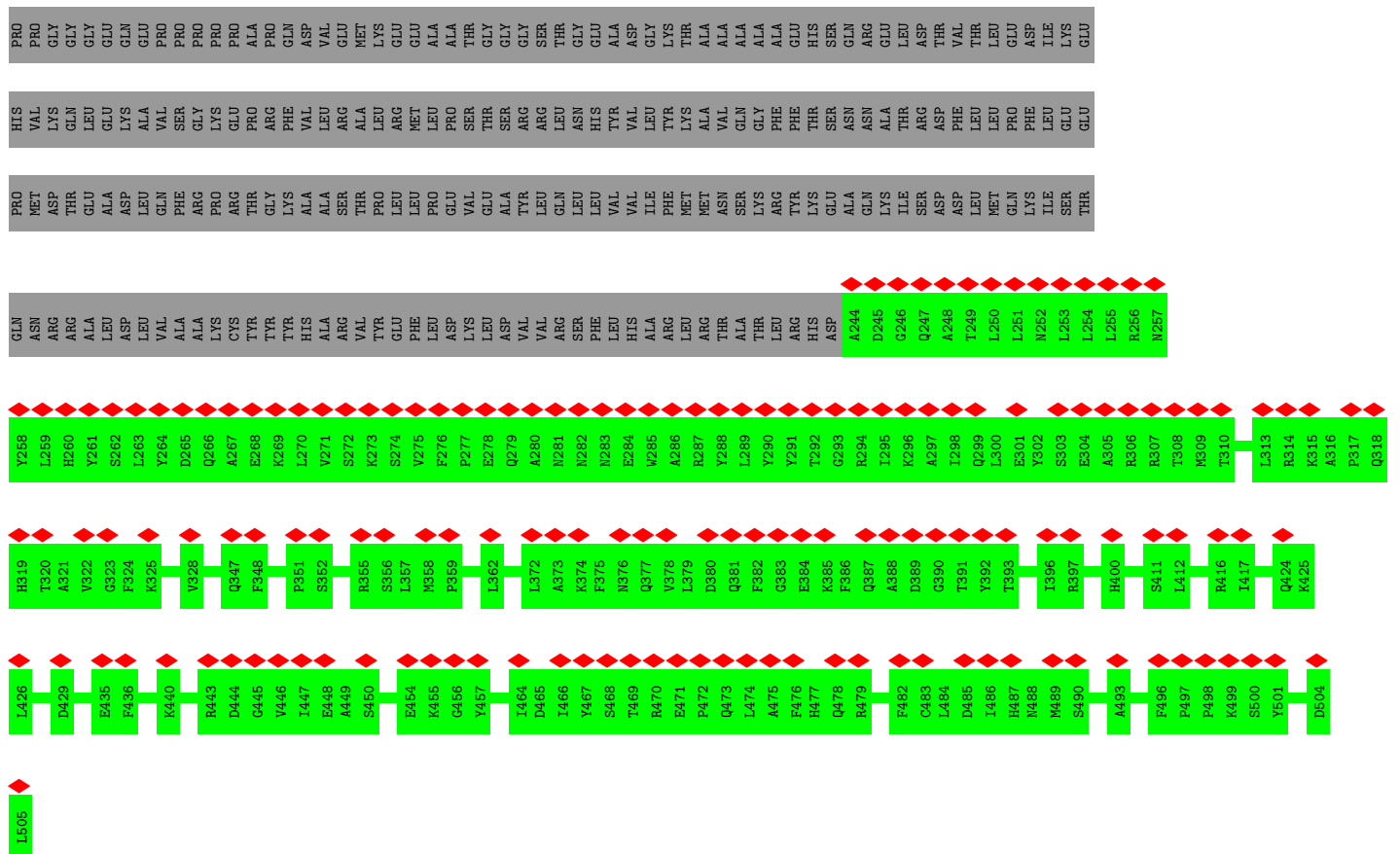


● Molecule 7: 26S proteasome non-ATPase regulatory subunit 1

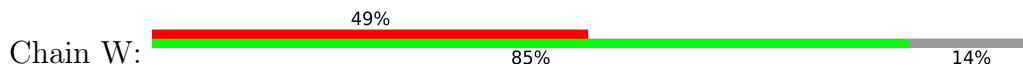




● Molecule 8: 26S proteasome non-ATPase regulatory subunit 3

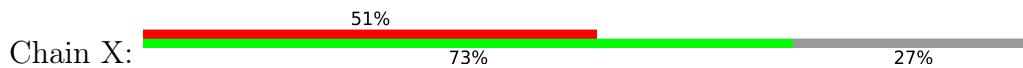


Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



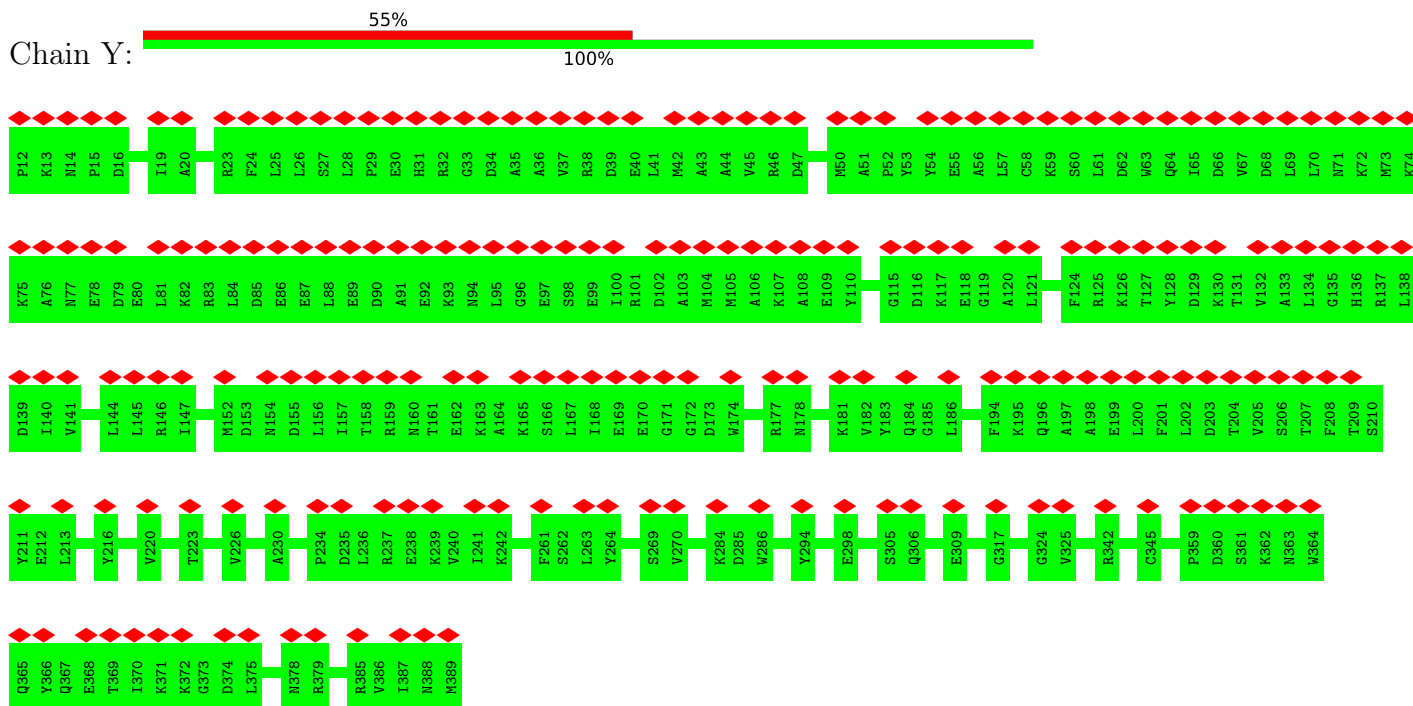
MET	ALA	ASP	GLY	GLY	SER	GLU	ARG	ALA	ASP	GLY	ARG	VAL	LEU	LEU	ASP	TYR	SER	THR	ALA	THR	VAL	ASP	GLN	ARG	LEU	PRO	LEU	GLU	GLY	CYS	ALA	LYS	LEU	LEU	ALA	LYS	GLY	ARG	LEU	GLN	VAL	ILE	LEU	THR	LEU	LEU	SER	SER	LEU	LEU	GLU	GLU	GLY	GLN	THR	THR	THR	ALA	ASP	ASP	MET
VAL	SER	THR	SER	ARG	I66	L67	V68	A69	V70	V71	K72	M73	C74	Y75	E76	A77	K78	E79	M80	D81	L82	L83	M84	E85	M86	I87	M88	L89	L90	S91	K92	R93	R94	S95	Q96	L97	K98	Q99	A100	V101	A102	A103	M104	V105	Q106	Q107	C108	C109	T110	Y111	V112	E113	E114	I115	T116	D117	P118	P119	I120		
K121	L122	R123	L124	I125	D126	T127	L128	R129	M130	V131	T132	E133	G134	K135	I136	Y137	V138	E139	I140	D141	R142	A143	R144	L145	T146	K147	L148	L149	A150	T151	I152	R93	K153	E154	Q155	M156	G157	D158	V159	K160	E161	A162	A163	S164	I165	L166	Q167	E168	L169	Q170	V171	E172	T173	Y174	G175	T176	M177	E178	K179	K180	
E181	E184	F185	D198	Y199	I200	Q203	I204	M210	T211	K212	F213	F214	Q215	E216	E217	N218	T219	E220	K221	L222	K223	L224	K225	K245	R248	A249	I250	Y251	D252	C255	I256	Q257	A258	E259	Q264	D280	N281	S284	D285	H288	R289	I290	S291	C292	D293	K294	L296														
P300	K303	D304	F309	E313	L314	M315	R316	W317	S318	E322	G325	M326	E327	L328	R329	K330	G331	S332	L333	E334	S335	P336	A337	T338	D339	V340	F341	G342	I363	R364	K368	Y369	Y370	I373	T374	Q380	L381	L382	L383	L384	S385	V386	D387	E388	S389	E390	M395														
N399	I402	F403	A404	K405	L409	A410	G411	I412	Q416	R417	P418	K419	D420	M421	N422	M423	L424	L425	W428	S429	Q430	K431	L432	L438	V439	M440	K441	H444	Q456																																

Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



ASN	ASP	GLU	GLU	ALA	VAL	GLN	VAL	LYS	GLU	GLN	SER	ILE	LEU	GLU	GLY	SER	LEU	LEU	ALA	LYS	THR	GLY	GLN	ALA	GLU	GLY	GLY	LEU	LEU	LYS	TYR	VAL	ARG	PRO	PHE	LEU	ASN	SER	ILE	SER	LYS	ALA	LYS	ALA	ALA	ARG	ARG	LEU	VAL	VAL	THR	LEU	LEU							
ASP	MET	GLU	ALA	ALA	THR	D162	K163	A164	L166	L166	V167	E168	V169	Q170	L171	L172	E173	S174	K175	T176	Y177	H178	A179	L180	S181	N182	L183	P184	K185	A186	R187	A188	A189	L190	T191	S192	A193	R194	T195	T196	A197	M198	A199	I200	C202	P203	P204	K205	L206	Q207	A208	G273	K274	L275	A276	L277	R278	Y279	A280	G281
K158	K159	M160	D161	D162	K163	A164	L166	L166	V167	E168	V169	Q170	L171	L172	E173	S174	K175	T176	Y177	H178	A179	L180	S181	N182	L183	P184	K185	A186	R187	A188	A189	L190	T191	S192	A193	R194	T195	T196	A197	M198	A199	I200	C202	P203	P204	K205	L206	Q207	A208	G273	K274	L275	A276	L277	R278	Y279	A280	G281		
A220	E221	E222	K223	D224	W225	K226	T227	A228	A228	Y229	S230	Y231	F232	Y233	E234	A235	F236	E237	G238	Y239	D240	S241	T242	D243	S244	P245	K246	A247	T248	T249	S250	L251	K252	Y253	M254	K258	L259	W260	L261	N262	T263	P264	E265	D266	V267	Q268	A269	L270	V271	S272	G273	K274	L275	A276	L277	R278	Y279	A280	G281	
R282	Q283	T284	E285	K288	C289	V290	A291	Q292	A293	S294	K295	N296	R297	A300	D301	F302	E303	K304	A305	L306	T307	D308	Y309	R310	A311	E312	L313	R314	D315	P316	L317	I318	I319	S320	T321	H322	L323	L326	Y327	E332	I336	E340	F341	L353	I354	K355	D360	D371	K372	K373										
F374	H375	V384	L385	I386	I387	F388	D389	E390	P391	F392	Y397	E398	A399	A400	L401	E402	M406	M407	F411	Y415	M416	K417	A418	K419	L421	K420	T422																																	

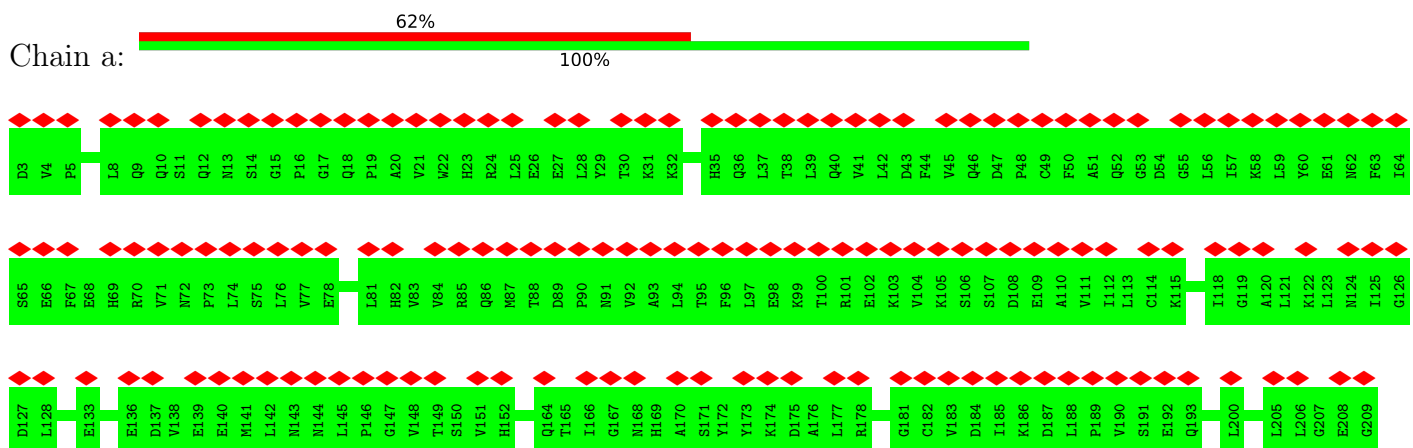
Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

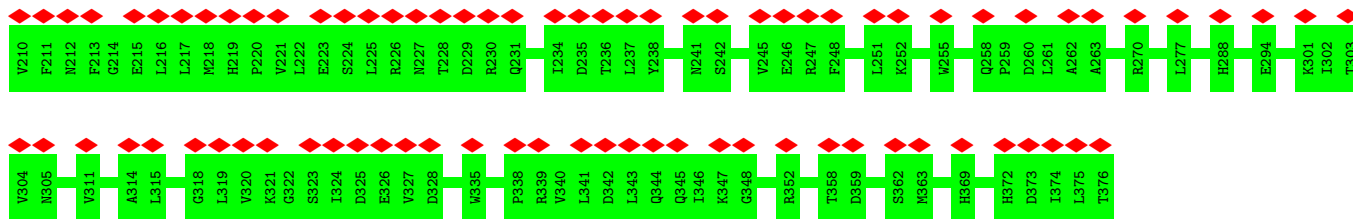


• Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

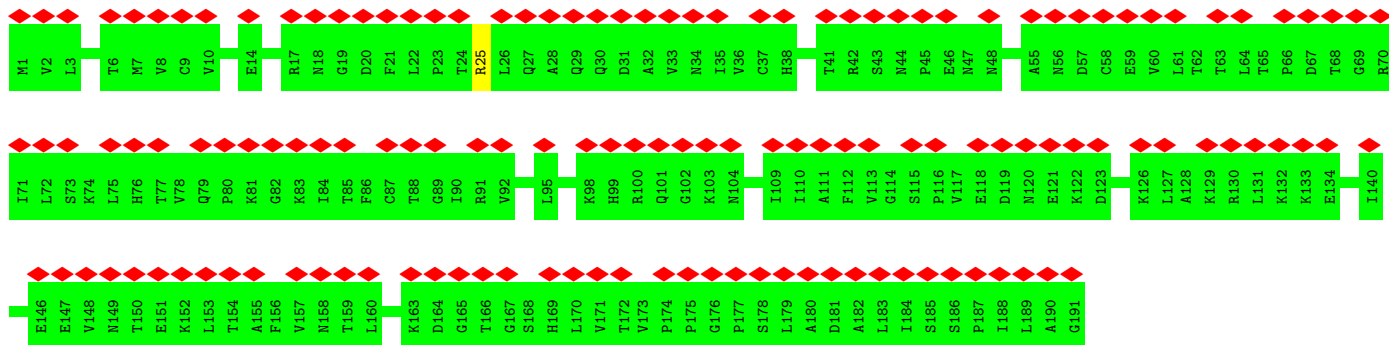


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 13

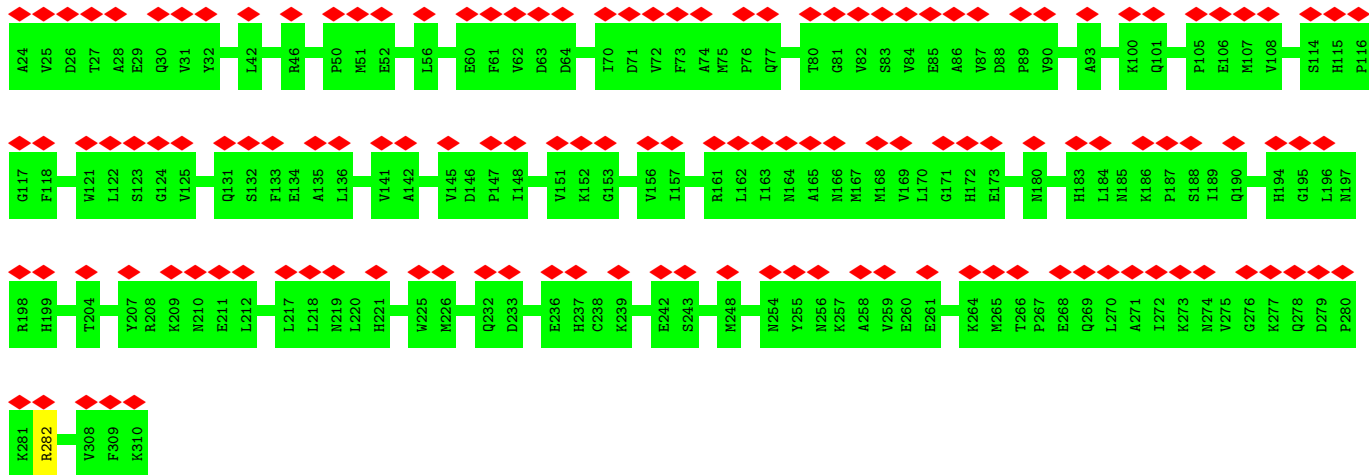




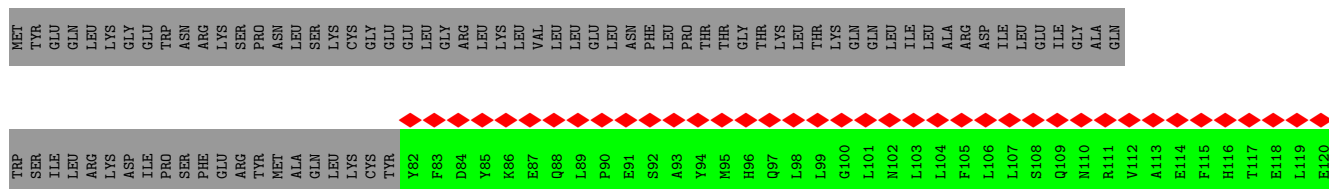
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 4

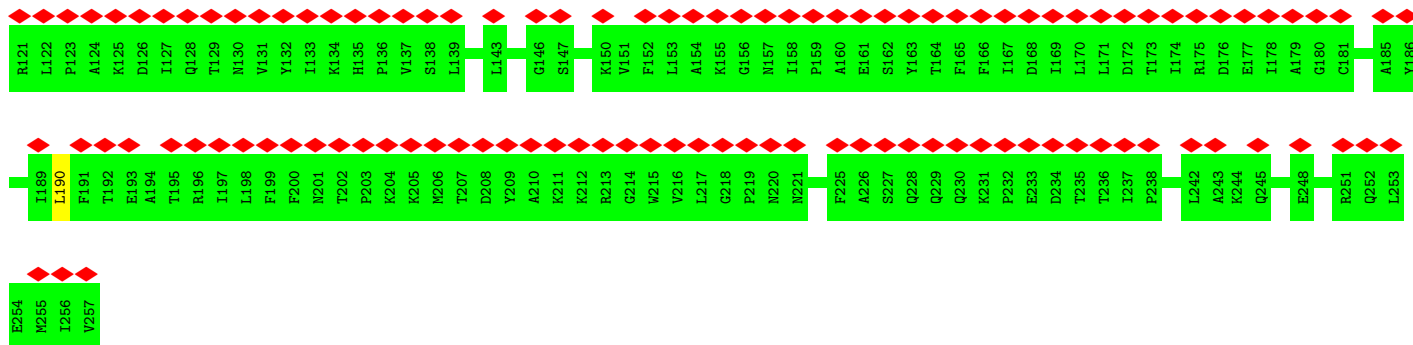


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

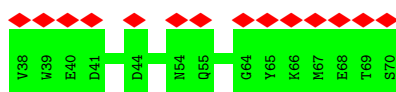
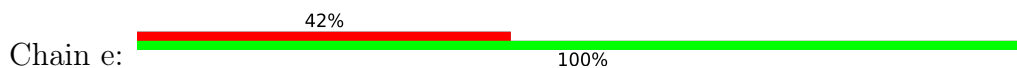


• Molecule 16: 26S proteasome non-ATPase regulatory subunit 8

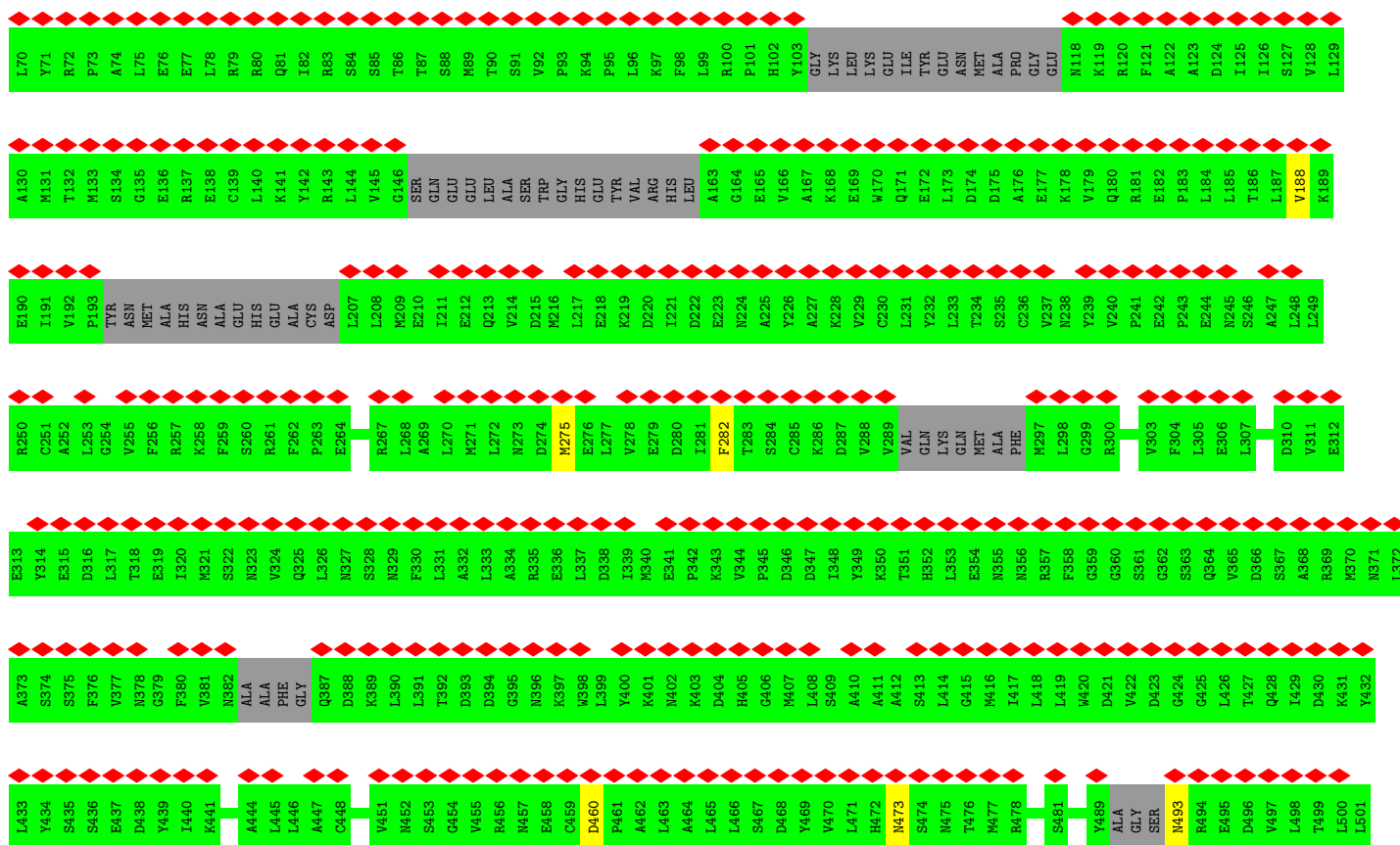
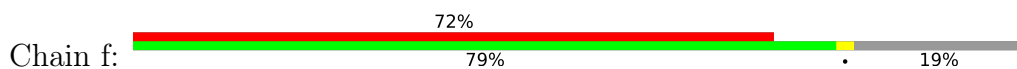




• Molecule 17: 26S proteasome complex subunit SEM1



• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2



L502	P503	V504	M505	G506	D507	S508	K509	S510	S511	M512	E513	V514	A515	G516	V517	T518	A519	L520	M524	V527	G528	S529	C530	M531	G532	D533	V534	T535	S536	T537	I538	L539	Q540	T541	I542	M543	E544	K545	S546	E547	T548	E549	L550	K551	D552	T553	Y554	A555	R556	W557	L558	F559	G561	L562	G563	L564										
M565	H566	L567	G568	K569	G570	E571	A572	I573	E574	A575	I576	L577	A578	A579	L580	E581	V582	V583	S584	E585	P586	F587	R588	S589	F590	A591	N592	T593	L594	V595	D596	V597	C598	A599	Y600	A601	G602	S603	G604	M605	V606	L607	K608	V609	Q610	Q611	H614	I615	C616	S617	E618	H619	F620	D621	S622	K623	E624	K625								
E626	E627	D628	K629	D630	K631	K632	E633	K634	K635	D636	K637	D638	K639	K640	E641	A642	P643	A644	D645	M646	G647	A648	H649	Q650	G651	V652	L655	G656	I657	A658	L659	I660	A661	M662	G663	E664	E665	I666	G667	A668	E669	M670	A671	L672	R673	T674	F675	G676	H677	L678	L679	R680	Y681	G682	E683	P684	T685	L686								
R687	R688	A689	V690	P691	L692	A693	L694	A695	L696	I697	S698	SER	ASN	ASN	PRO	ARG	LEU	ALA	ASN	ILE	LEU	ASP	THR	LEU	LEU	LYS	PHE	S714	H715	D716	A717	D718	P719	E720	V721	S722	V723	M724	S725	I726	F727	A728	MET	GLY	MET	VAL	GLY	SER	GLY	THR	ASN	ASN	A739	R740	L741	A742	A743	M744	L745	R746						
Q747	L748	A749	Q750	Y751	A753	K754	ASP	PRO	ASN	ASN	ASN	PHE	ALA	ALA	MET	VAL	GLN	ARG	PRO	ARG	LEU	ALA	GLN	MET	LEU	GLY	LEU	THR	PHE	ASP	GLU	LEU	GLY	K773	G774	I775	L776	I777	L778	C779	P780	Y781	H782	S783	D784	R785	Q786	L787	M788	S789	Q790	V791	A792	V793	L796	L797	T798	V799	L800	V801	S802	F803	L804	ASP	VAL	ARG
ASN	ILE	ILE	LEU	GLY	LYS	SER	HIS	TYR	VAL	LEU	TYR	GLY	LEU	VAL	ALA	ALA	MET	GLN	PRO	ARG	ARG	LEU	MET	LEU	VAL	THR	PHE	ASP	GLU	LEU	GLY	ARG	PRO	LEU	PRO	VAL	SER	VAL	ARG	VAL	GLY	GLN	ALA	VAL	ASP	VAL	VAL	S789	Q790	V791	A792	V793	L796	L797	T798	V799	L800	V801	S802	F803	L804	ASP	VAL	ARG		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.009	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (\AA)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/2710	0.42	0/3659
2	B	0.23	0/2509	0.42	0/3383
3	C	0.23	0/2784	0.41	0/3737
4	D	0.24	0/2690	0.41	1/3630 (0.0%)
5	E	0.23	0/2525	0.40	0/3387
6	F	0.23	0/2681	0.41	0/3611
7	U	0.23	0/5930	0.40	0/8021
8	V	0.23	0/2170	0.39	0/2929
9	W	0.24	0/3251	0.41	1/4370 (0.0%)
10	X	0.23	0/2255	0.36	0/3041
11	Y	0.23	0/3173	0.37	0/4273
12	Z	0.23	0/2324	0.39	0/3150
13	a	0.23	0/3061	0.37	0/4144
14	b	0.23	0/1478	0.40	0/2001
15	c	0.23	0/2302	0.39	0/3110
16	d	0.24	0/1486	0.37	0/2010
17	e	0.21	0/289	0.41	0/389
18	f	0.24	0/4989	0.42	0/6729
All	All	0.23	0/48607	0.40	2/65574 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	221	LYS	C-N-CA	5.92	136.51	121.70
4	D	332	GLU	C-N-CA	5.16	134.59	121.70

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	332/352 (94%)	299 (90%)	33 (10%)	0	100	100
2	B	311/341 (91%)	271 (87%)	40 (13%)	0	100	100
3	C	343/385 (89%)	323 (94%)	20 (6%)	0	100	100
4	D	326/368 (89%)	315 (97%)	11 (3%)	0	100	100
5	E	307/379 (81%)	290 (94%)	17 (6%)	0	100	100
6	F	333/380 (88%)	311 (93%)	22 (7%)	0	100	100
7	U	743/935 (80%)	716 (96%)	27 (4%)	0	100	100
8	V	260/488 (53%)	237 (91%)	23 (9%)	0	100	100
9	W	387/456 (85%)	359 (93%)	26 (7%)	2 (0%)	29	69
10	X	276/385 (72%)	269 (98%)	7 (2%)	0	100	100
11	Y	376/378 (100%)	359 (96%)	17 (4%)	0	100	100
12	Z	284/286 (99%)	272 (96%)	12 (4%)	0	100	100
13	a	372/374 (100%)	351 (94%)	21 (6%)	0	100	100
14	b	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
15	c	285/287 (99%)	277 (97%)	8 (3%)	0	100	100
16	d	174/257 (68%)	160 (92%)	14 (8%)	0	100	100
17	e	31/33 (94%)	28 (90%)	3 (10%)	0	100	100
18	f	616/784 (79%)	556 (90%)	60 (10%)	0	100	100
All	All	5945/7059 (84%)	5568 (94%)	375 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	W	221	LYS
9	W	222	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/300 (98%)	290 (99%)	3 (1%)	76	86
2	B	276/298 (93%)	273 (99%)	3 (1%)	73	84
3	C	302/333 (91%)	298 (99%)	4 (1%)	69	81
4	D	290/321 (90%)	288 (99%)	2 (1%)	84	90
5	E	273/333 (82%)	270 (99%)	3 (1%)	73	84
6	F	291/326 (89%)	288 (99%)	3 (1%)	76	86
7	U	639/798 (80%)	635 (99%)	4 (1%)	86	92
8	V	231/422 (55%)	231 (100%)	0	100	100
9	W	361/416 (87%)	360 (100%)	1 (0%)	92	95
10	X	243/331 (73%)	243 (100%)	0	100	100
11	Y	334/334 (100%)	334 (100%)	0	100	100
12	Z	257/257 (100%)	256 (100%)	1 (0%)	91	94
13	a	334/334 (100%)	334 (100%)	0	100	100
14	b	167/167 (100%)	166 (99%)	1 (1%)	86	92
15	c	252/252 (100%)	251 (100%)	1 (0%)	91	94
16	d	158/231 (68%)	157 (99%)	1 (1%)	86	92
17	e	31/31 (100%)	31 (100%)	0	100	100
18	f	538/660 (82%)	525 (98%)	13 (2%)	49	69
All	All	5270/6144 (86%)	5230 (99%)	40 (1%)	82	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	f	275	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	f	583	VAL
18	f	282	PHE
18	f	493	ASN
18	f	662	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
8	V	329	HIS
18	f	301	HIS
10	X	406	ASN
18	f	273	ASN
18	f	493	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	1
10	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	205:ILE	C	206:SER	N	3.21
1	X	311:ALA	C	312:GLU	N	3.20

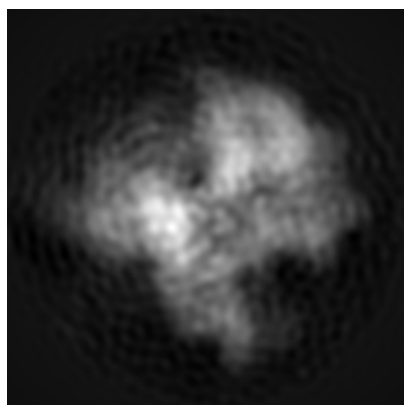
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8684. These allow visual inspection of the internal detail of the map and identification of artifacts.

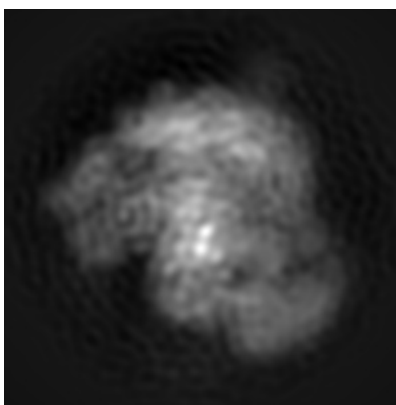
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

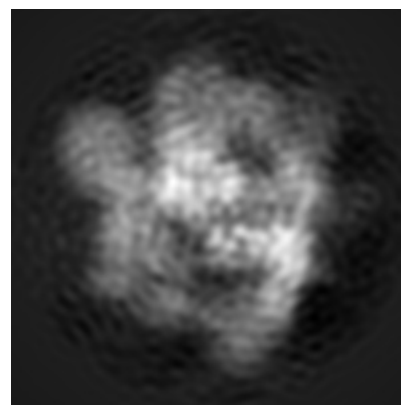
6.1.1 Primary map



X



Y

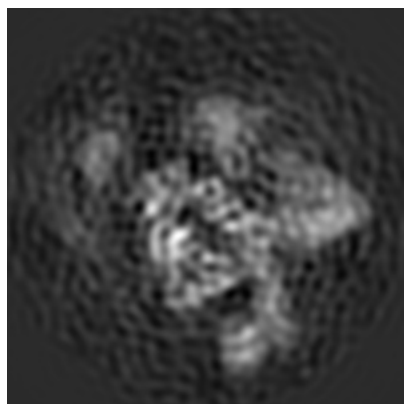


Z

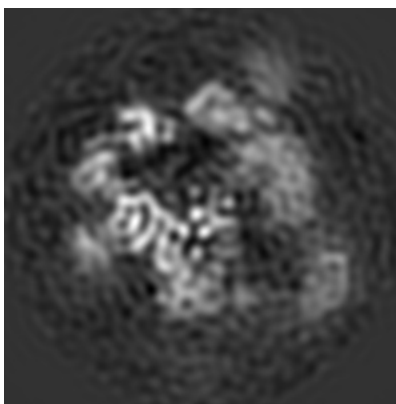
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

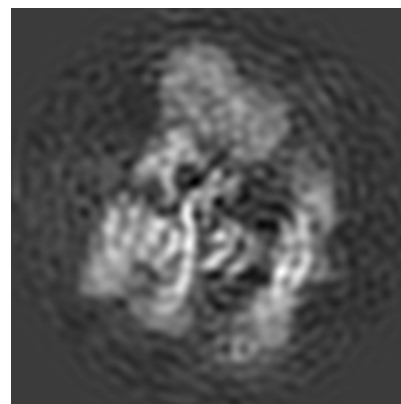
6.2.1 Primary map



X Index: 150



Y Index: 150

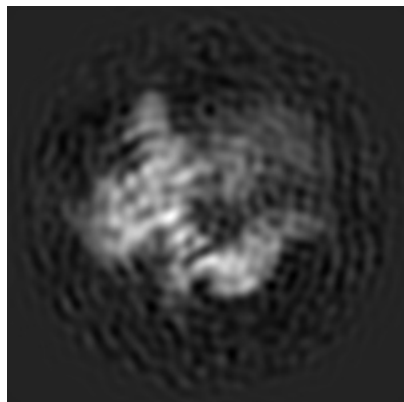


Z Index: 150

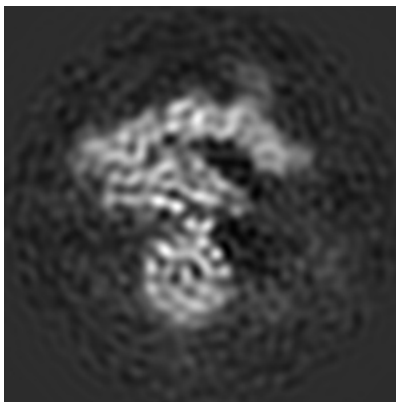
The images above show central slices of the map in three orthogonal directions.

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

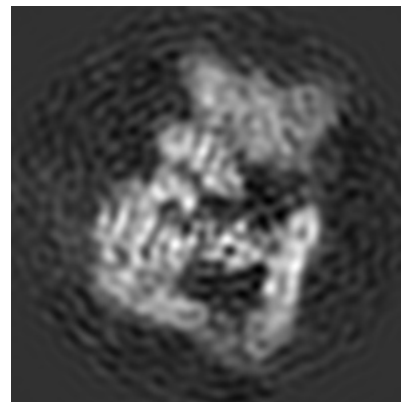
6.3.1 Primary map



X Index: 209



Y Index: 128

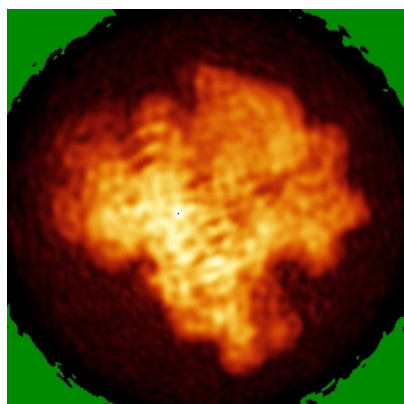


Z Index: 135

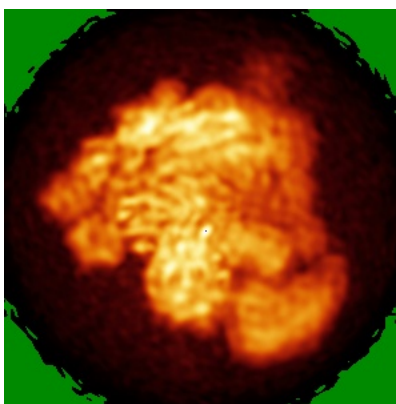
The images above show the largest variance slices of the map in three orthogonal directions.

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

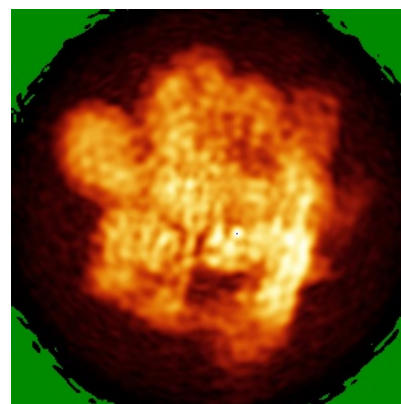
6.4.1 Primary map



X



Y

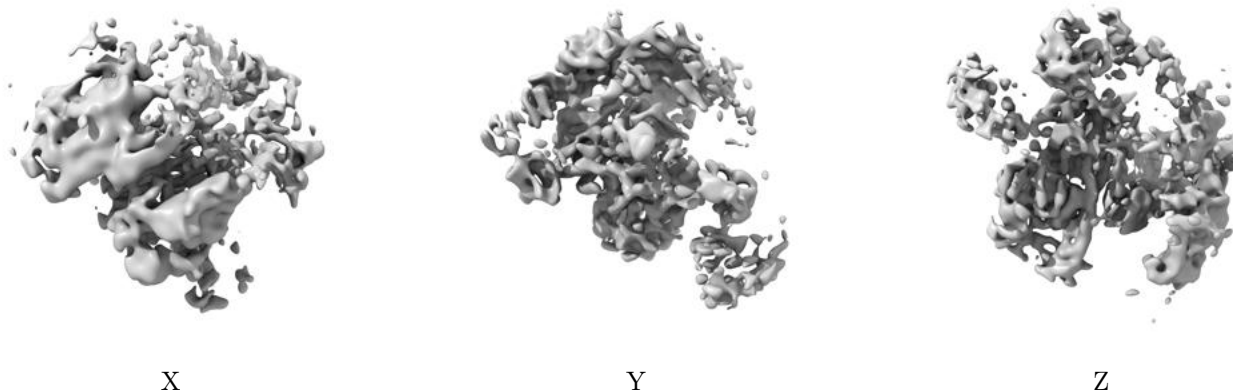


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

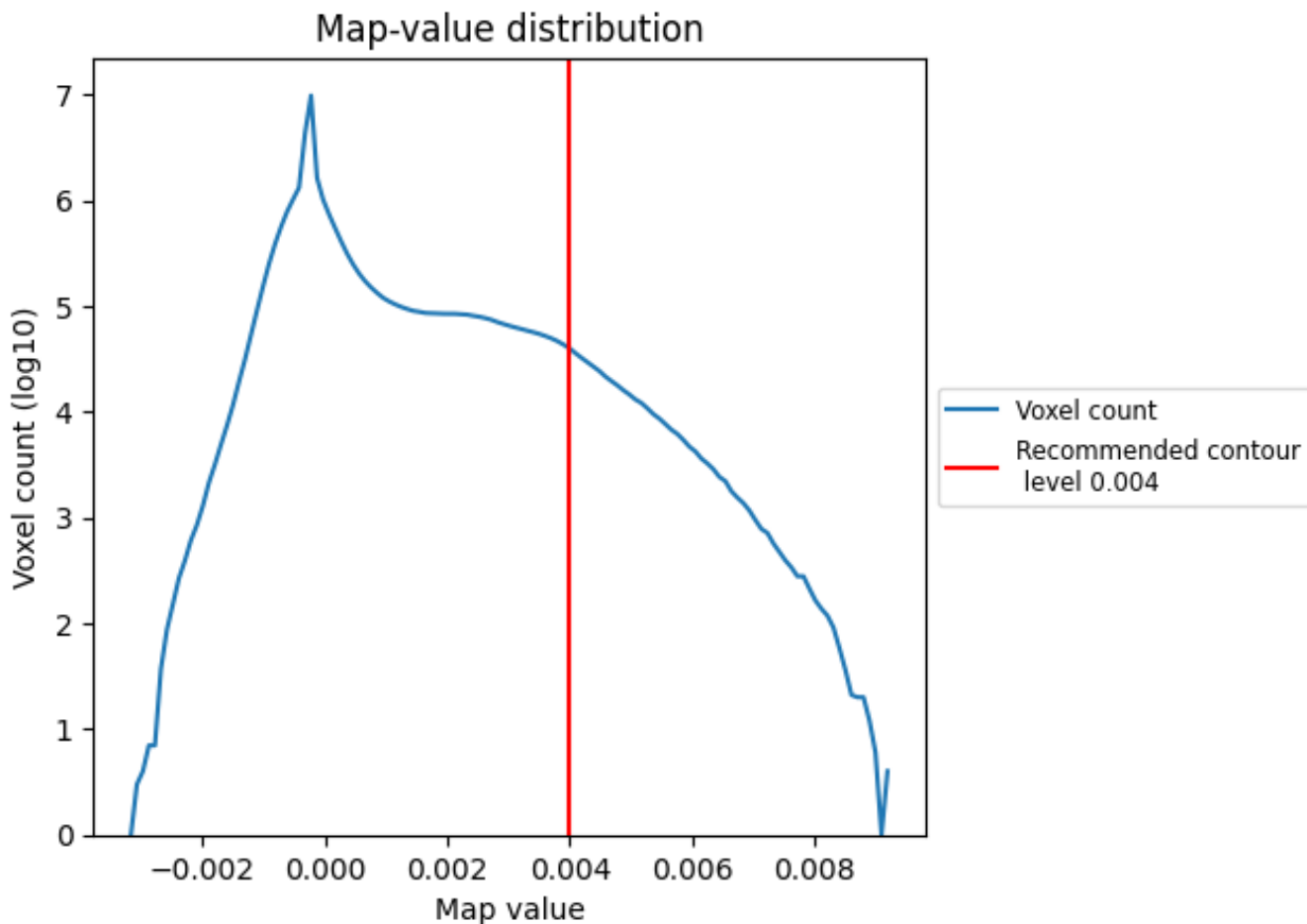
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

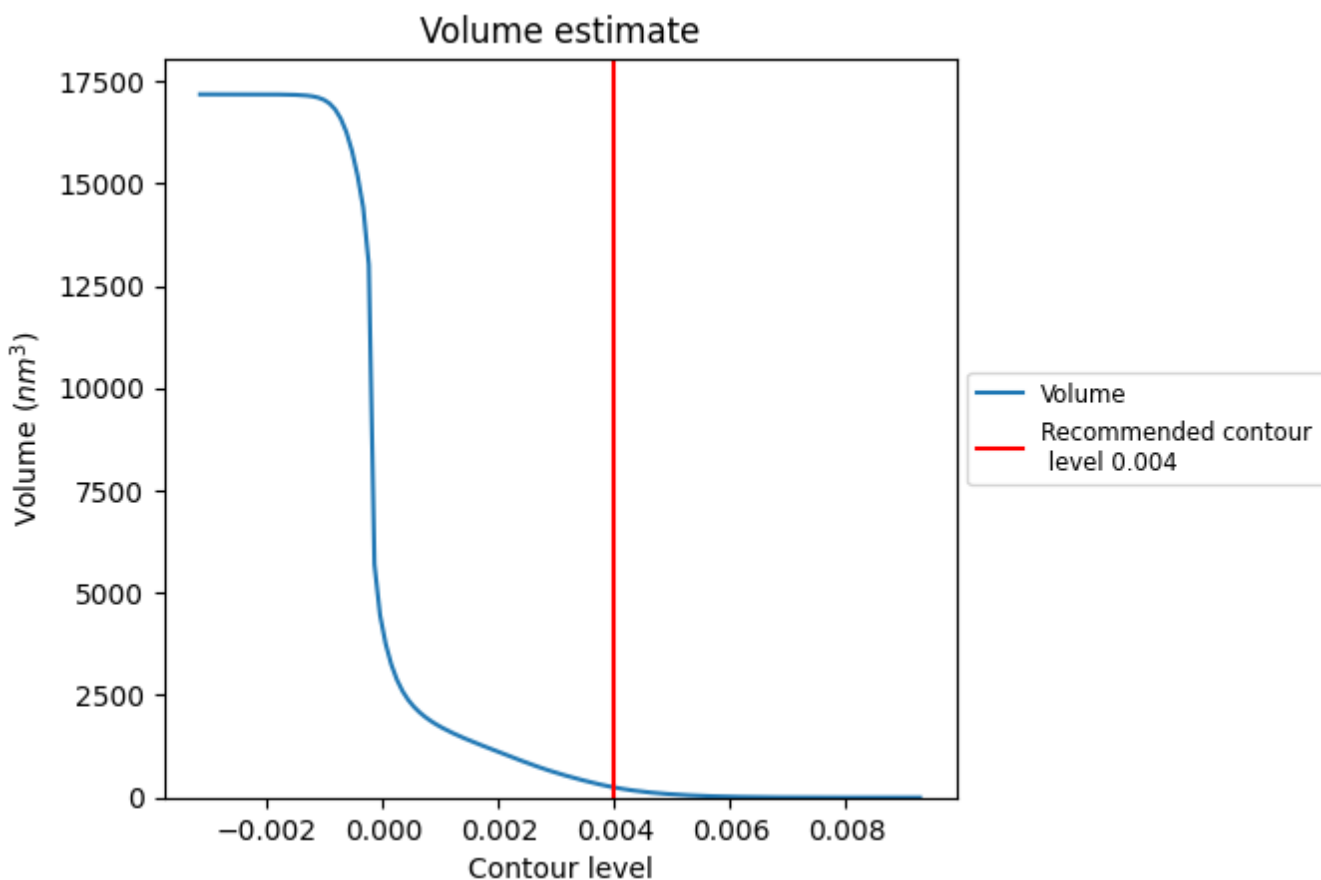
This section contains the results of statistical analysis of the map.

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.

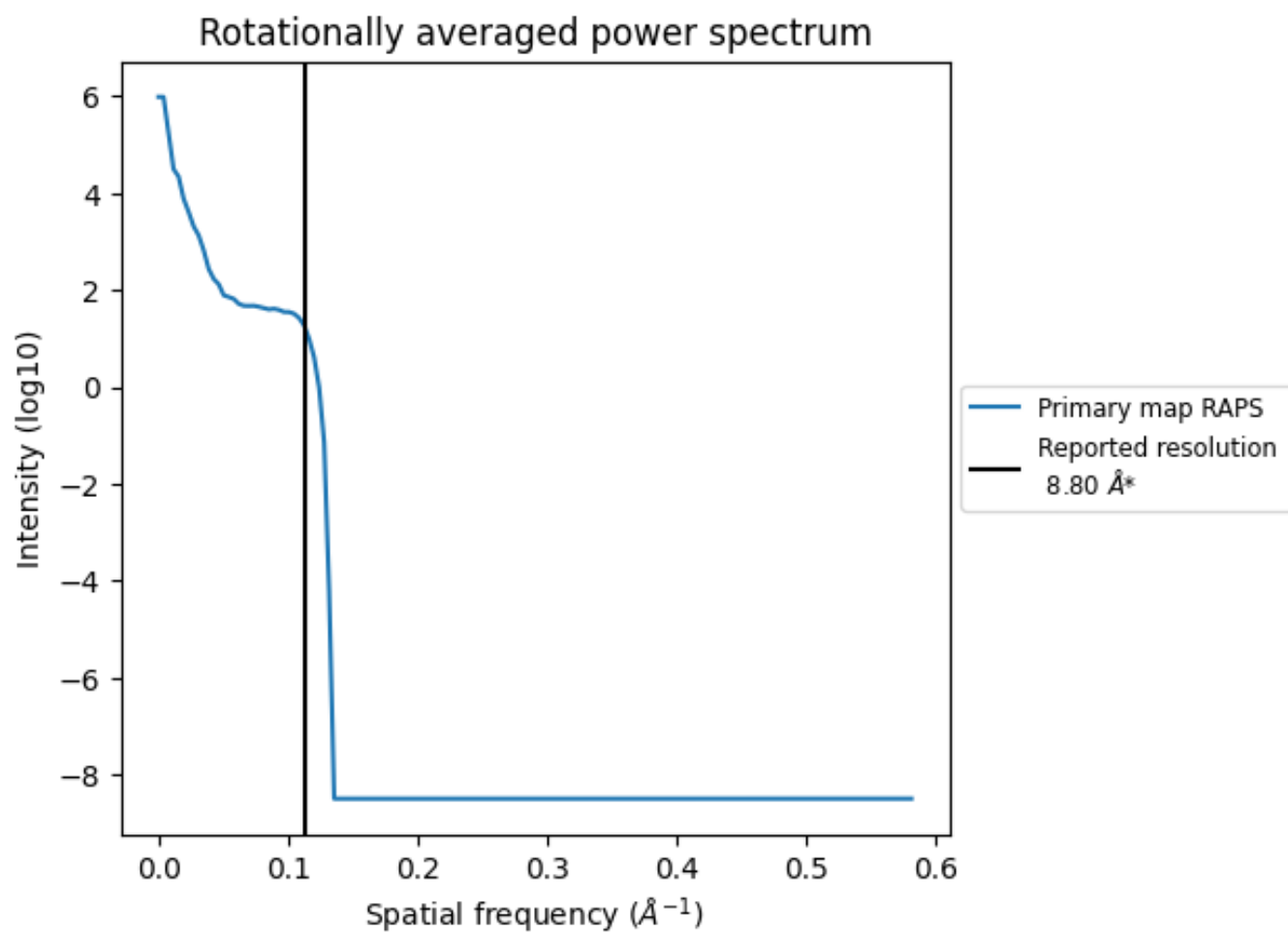
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 248 nm³; this corresponds to an approximate mass of 224 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

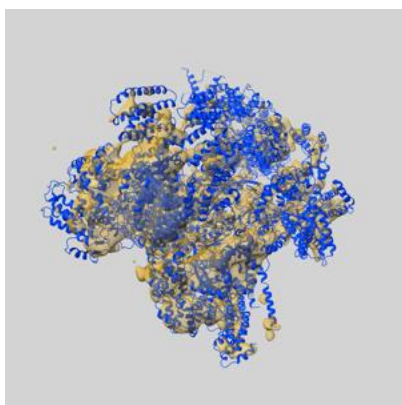
8 Fourier-Shell correlation

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

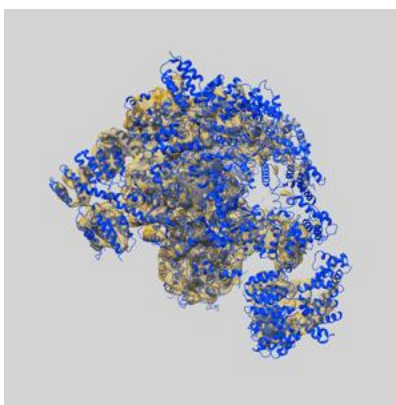
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8684 and PDB model 5VHS. Per-residue inclusion information can be found in section 3 on page 7.

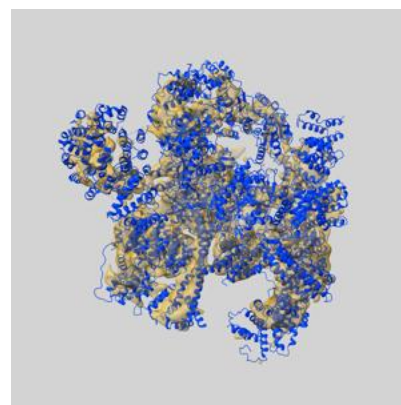
9.1 Map-model overlay [i](#)



X



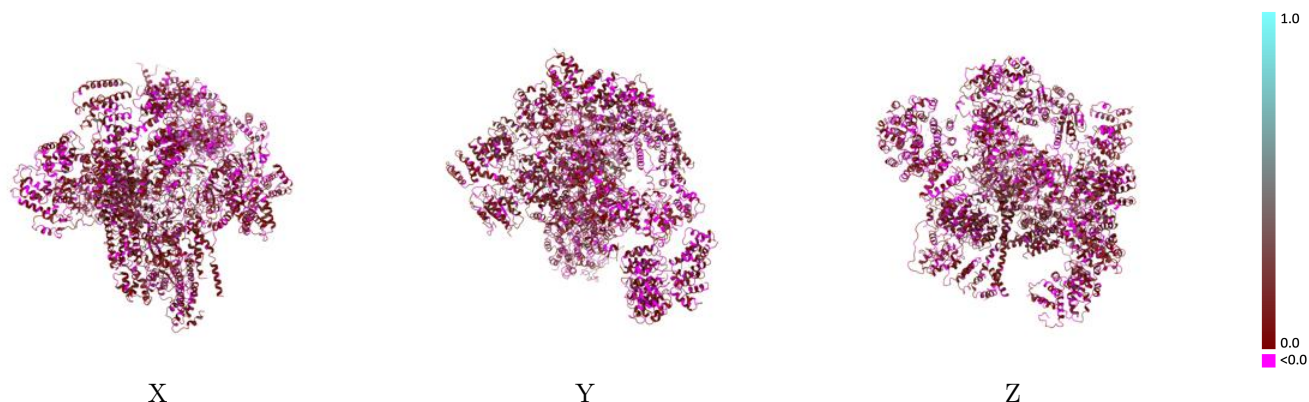
Y



Z

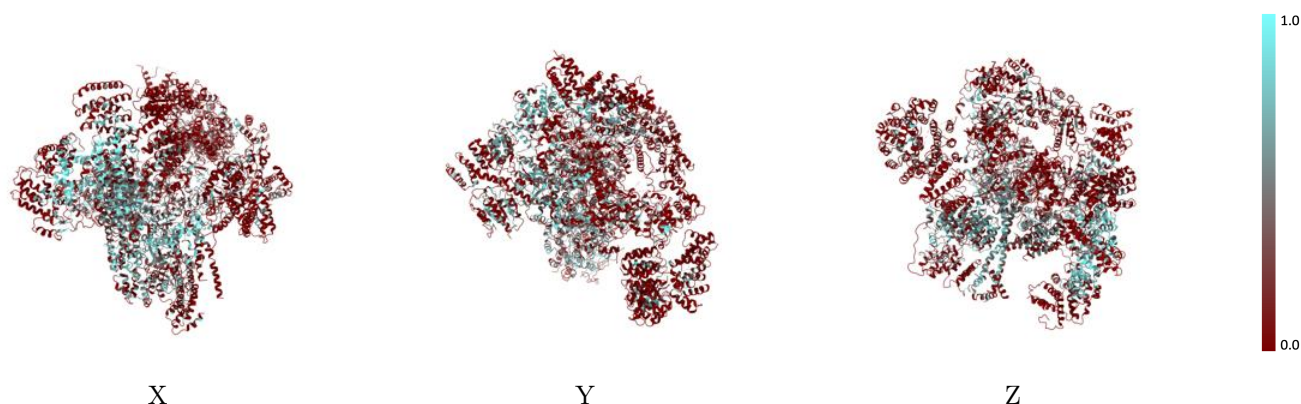
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



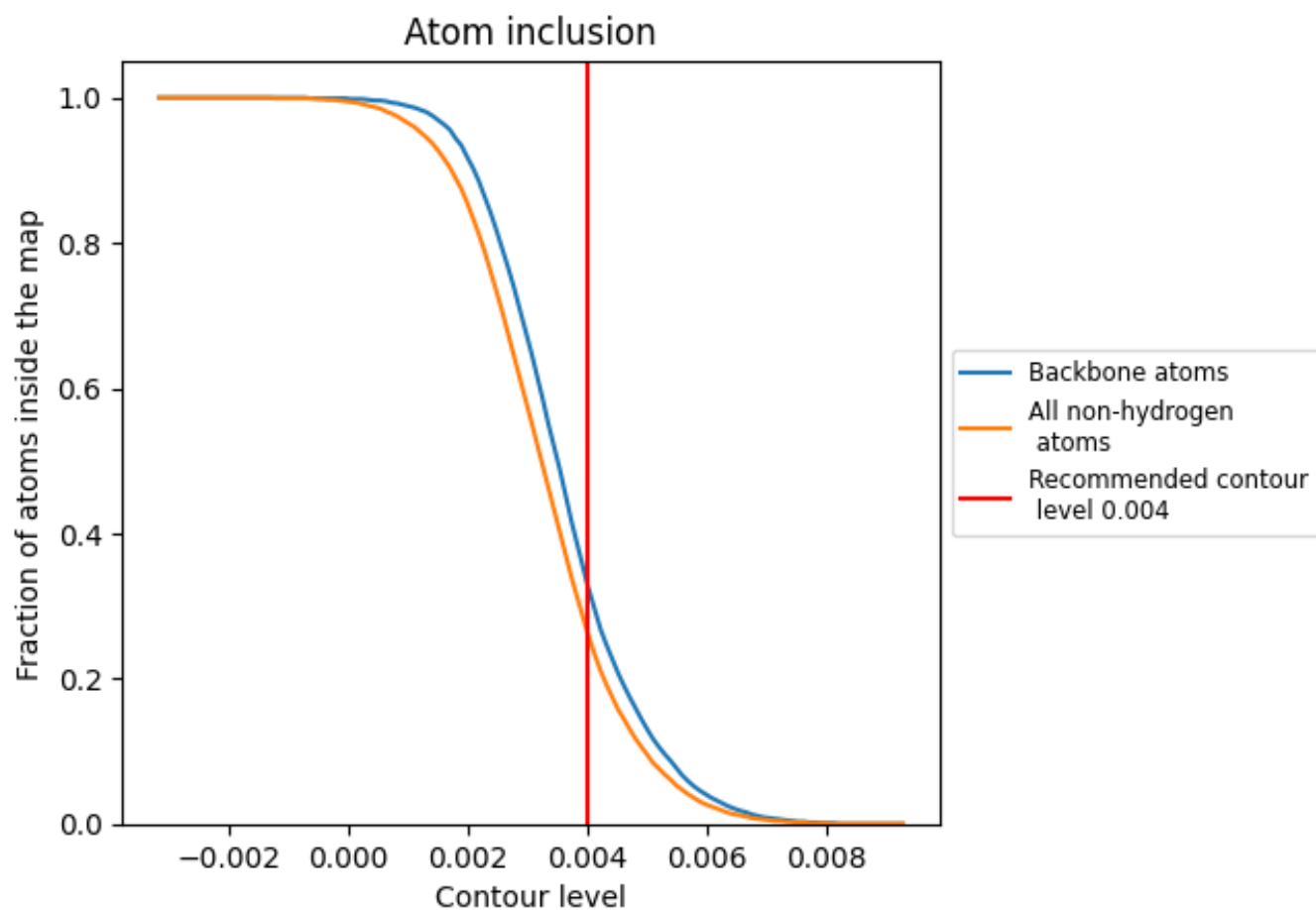
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 26% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2640	 0.0810
A	 0.2060	 0.0660
B	 0.1870	 0.0520
C	 0.1350	 0.0890
D	 0.1710	 0.0710
E	 0.1210	 0.0800
F	 0.1970	 0.0870
U	 0.3520	 0.0840
V	 0.3630	 0.0530
W	 0.3720	 0.1050
X	 0.2600	 0.0780
Y	 0.4020	 0.0940
Z	 0.4240	 0.1220
a	 0.3310	 0.1080
b	 0.2460	 0.0840
c	 0.4200	 0.1130
d	 0.1420	 0.0550
e	 0.5290	 0.1110
f	 0.1040	 0.0460

