



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 01:55 pm GMT

PDB ID : 5MPE
EMDB ID : EMD-3535
Title : 26S proteasome in presence of ATP (s2)
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on : 2016-12-16
Resolution : 4.50 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:

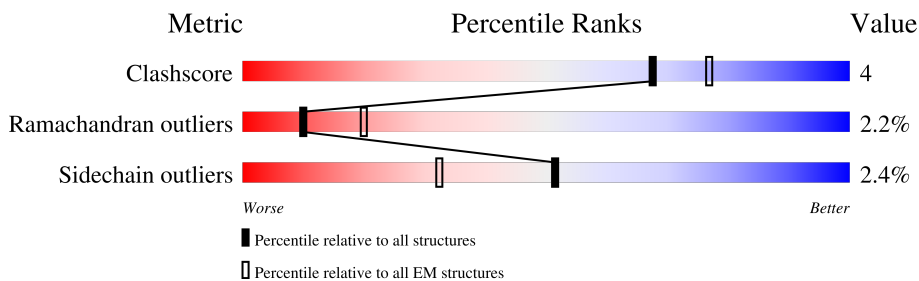
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	W	268	
2	V	306	
3	T	274	
4	X	156	
5	Y	89	
6	Z	993	
7	N	945	
8	S	523	

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Mol	Chain	Length	Quality of chain
9	P	445	<p>22% 76% 20% . .</p>
10	Q	434	<p>45% 76% 19% . .</p>
11	R	429	<p>35% 63% 20% 5% . 11%</p>
12	U	338	<p>26% 70% 17% . 12%</p>
13	O	393	<p>36% 73% 20% 5% . .</p>

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 40974 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 RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	W	197	1534	962	269	300	3	0	0

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	289	2274	1425	389	446	14	0	0

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	T	266	2192	1405	349	432	6	0	0

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	127	1032	664	169	195	4	0	0

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Y	51	435	264	69	102	0	0

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Z	906	7005	4416	1150	1409	30	0	0

- Molecule 7 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	890	6882	4373	1156	1325	28	0	0

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	S	475	3894	2488	653	738	15	0	0

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	P	440	3608	2297	604	697	10	0	0

- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	434	3499	2225	577	681	16	0	0

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	R	381	3060	1955	502	593	10	0	0

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	298	2373	1496	404	466	7	0	0

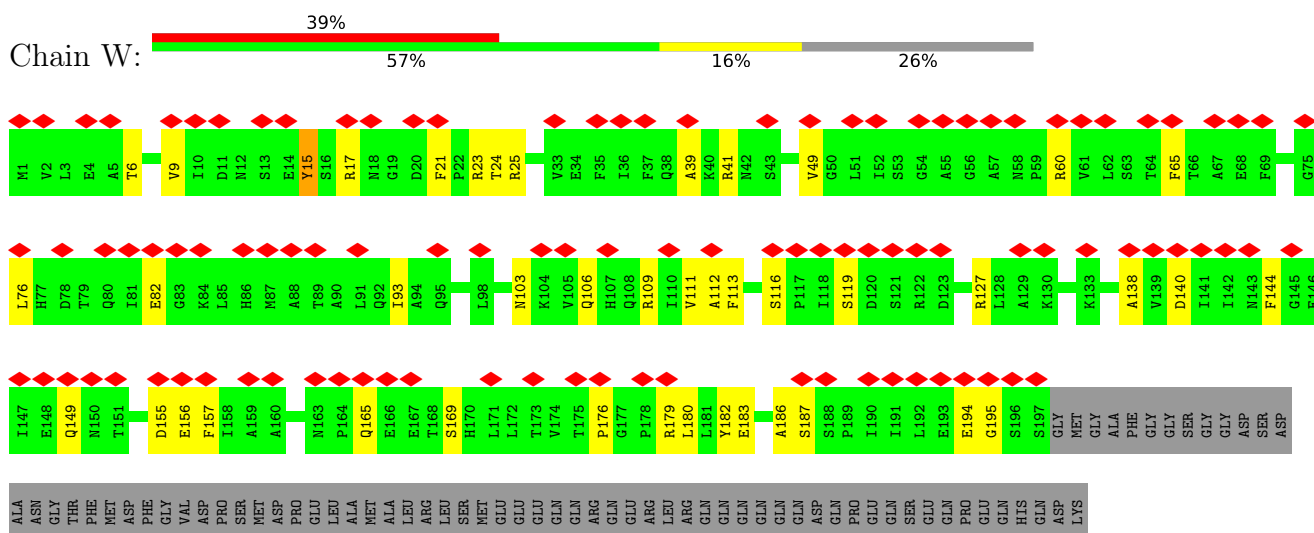
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	388	3186	2051	519	608	8	0	0

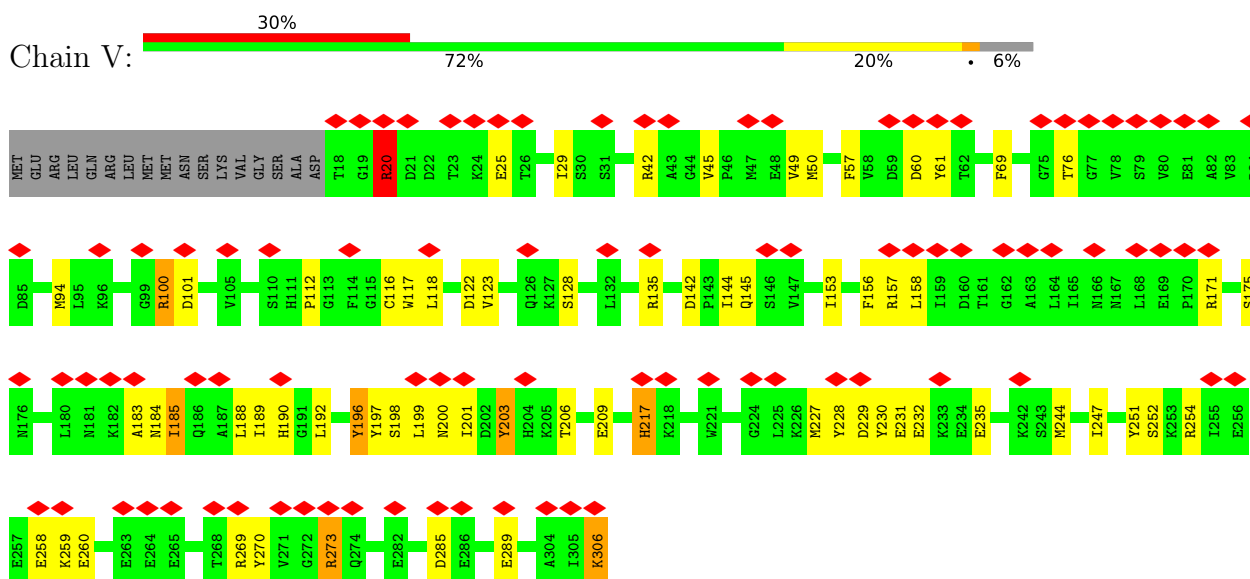
3 Residue-property plots

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.

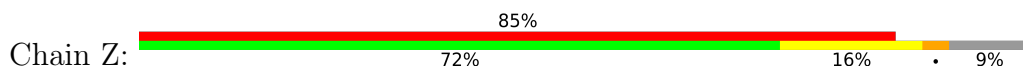
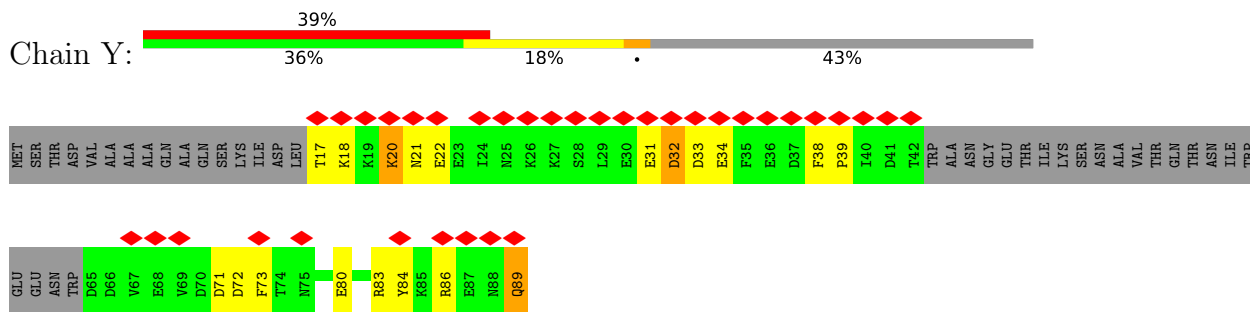
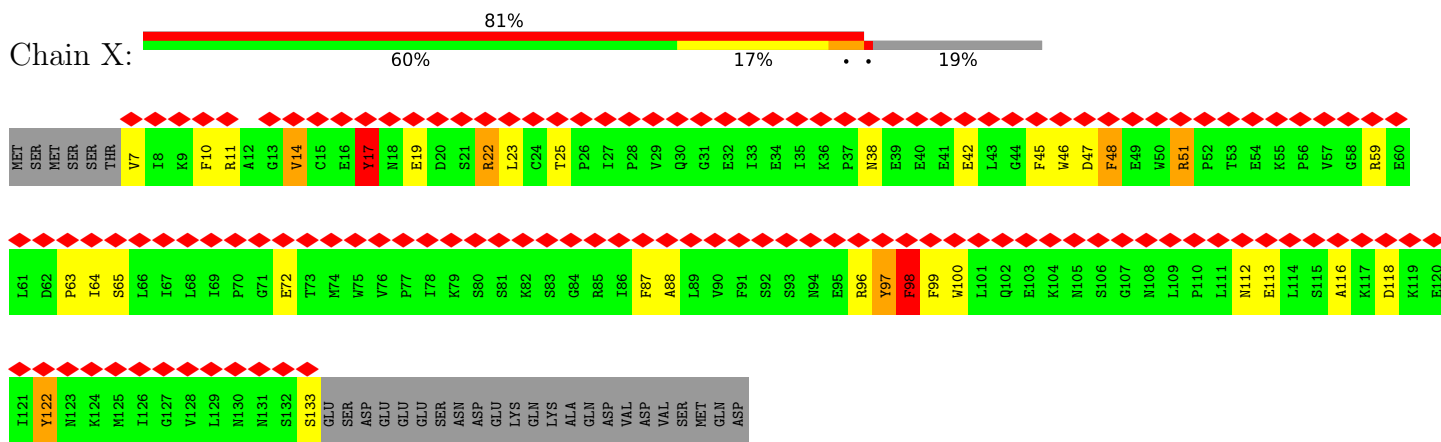
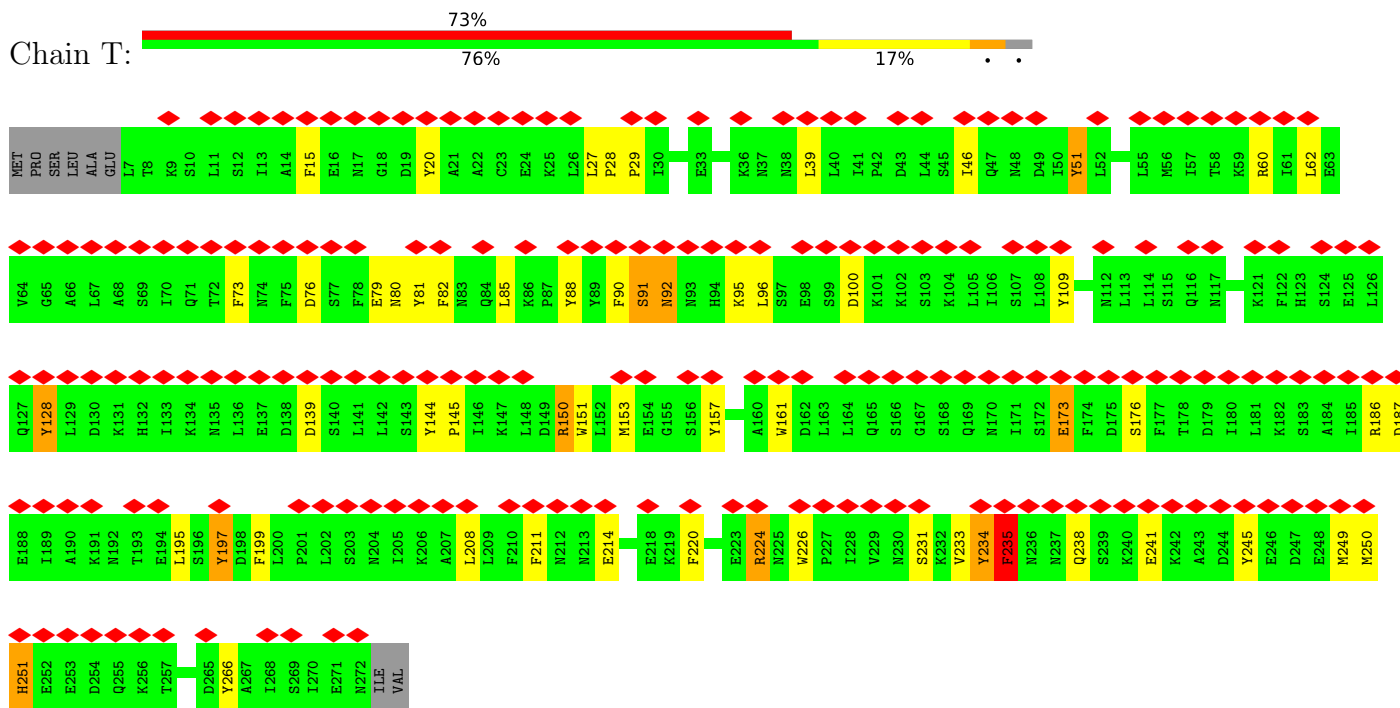
- Molecule 1: 26S proteasome regulatory subunit RPN10



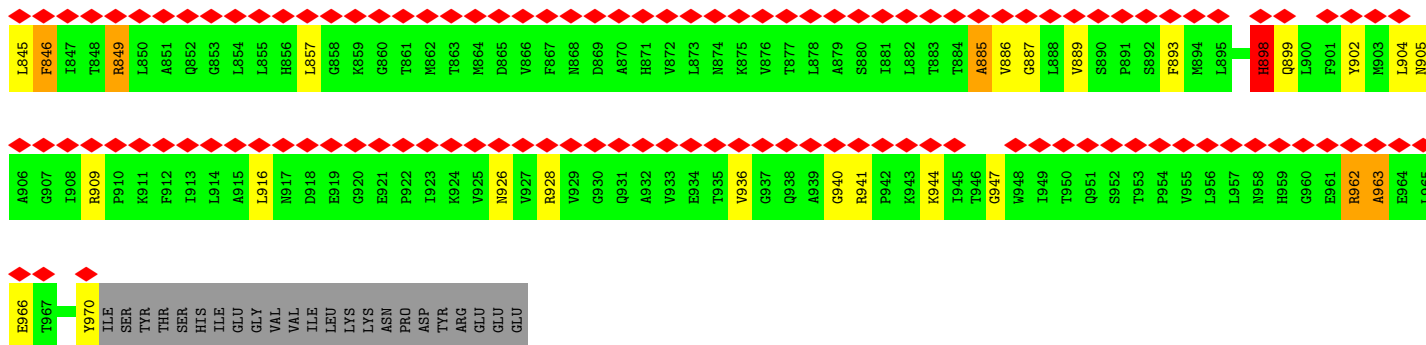
- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11



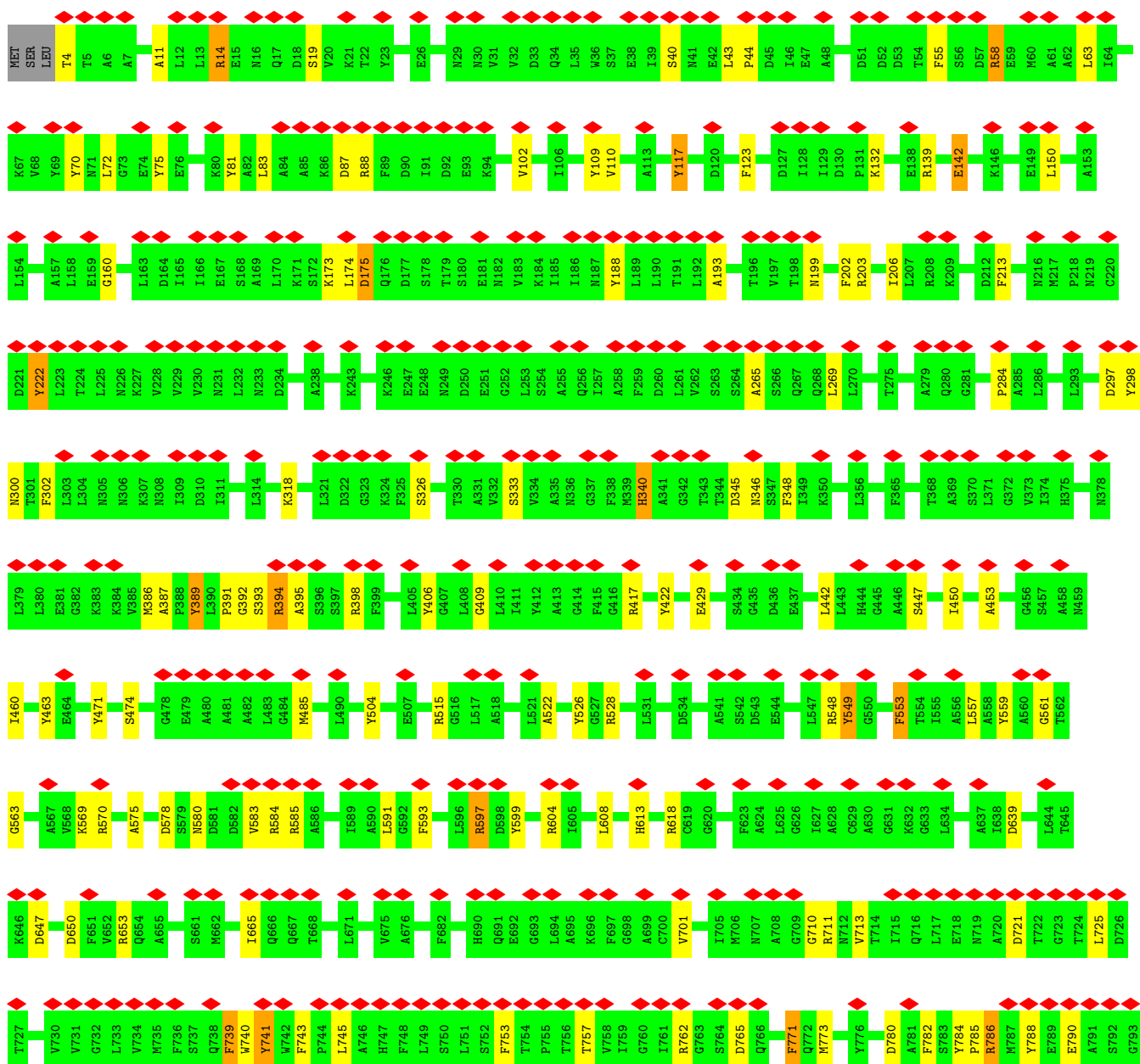
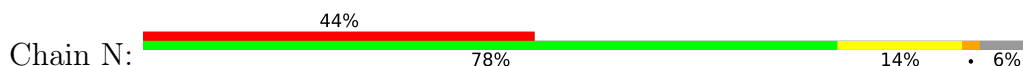
- Molecule 3: 26S proteasome regulatory subunit RPN12

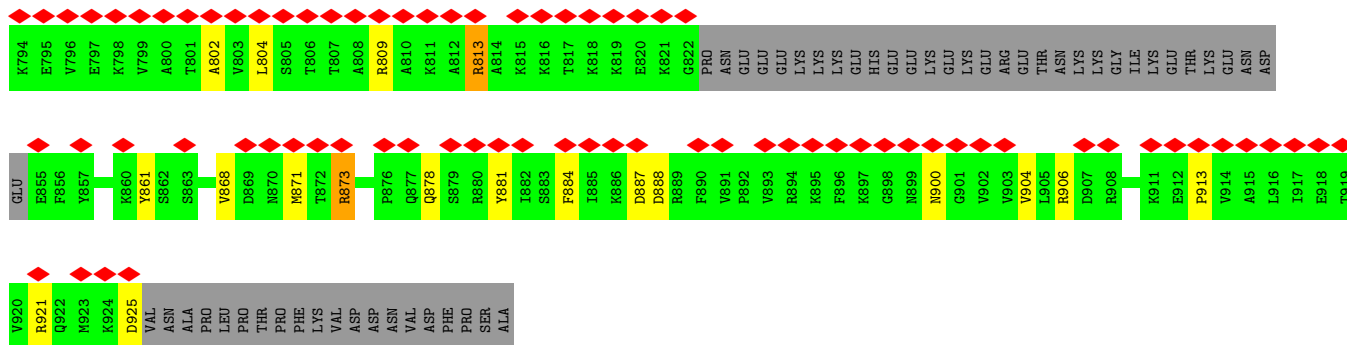


M1	V2	D3	E4	S5	D6	K7	K8	Q9	Q10	T11	I12	D13	E14	Q15	S16	Q17	I18	S19	P20	E21	K22	Q23	T24	P25	N26	K27	K28	D29	K30	K31	K32	E33	E34	E35	E36	Q37	Q38	S39	E40	E41	D42	A43	K44	L45	K46	T47	D48	M10	L49	E50	L51	L52	V53	E54	R55	L56	K57	E58	D59	D60
S61	S62	L63	Y64	E65	A66	S67	L68	N69	A70	L71	K72	S73	E74	S75	I76	K76	M77	S78	T79	S80	S81	M82	T83	A84	W85	P86	R87	P88	L89	K90	F91	L92	R93	P94	T95	Y96	P97	D98	L99	C100	E101	I102	Y103	D104	Y105	W106	T107	D108	P109	M110	L111	K112	S113	L114	L115	A116	D117	L118	S119	D120
I121	L122	A123	M124	T125	Y126	S127	E128	N129	G130	K131	H132	D133	S134	L135	L136	Y137	R138	L139	L140	S141	D142	S143	V144	D145	F146	E147	G148	W149	G150	H151	F152	Y153	I154	R155	H156	L157	A158	L159	E160	A220	I161	G162	E163	V164	Y165	M166	D167	Q168	V169	E170	K171	D172	A173	E174	D175	E176	T177	S178	S179	D180
G181	S182	K183	S184	D185	G186	S187	A188	A189	T190	S191	G192	F193	E194	F195	S196	K197	E198	D199	T200	L201	L202	L203	C204	L205	D206	L207	V208	P209	Y210	F211	L212	K213	H214	N215	G216	E217	E218	D219	A220	V221	D222	L223	L224	L225	E226	I227	E228	S229	I230	D231	K232	L233	P234	Q235	F236	V237	D238	E239	N240	
T241	F242	Q243	R244	V245	C246	Q247	Y248	M249	V250	A251	C252	V253	P254	L255	L256	P257	P258	P259	E260	D261	V262	A263	P264	L265	K266	T267	A268	S270	I271	Y272	L273	M276	E277	L278	K398	D290	A281	L282	A283	L284	A285	V286	R287	L288	G289	E290	E291	D292	M293	I294	R295	S296	V297	F298	D299	A300	T301			
S302	D303	P304	V305	M306	H307	K308	Q309	L310	A311	Y312	I313	L314	A315	A316	Q317	K318	T319	S320	F321	Y323	E324	G325	Y326	Q327	D328	I329	I330	G331	N332	G333	K334	L335	S336	E337	H338	F339	L340	Y341	A343	K344	E345	L346	N347	L348	T349	G350	P351	K352	V353	P354	E355	D356	I357	Y358	K359	S360	H361			
L362	D363	N364	S365	K366	S367	V368	F369	S370	L371	A372	G373	L374	D375	S376	A377	Q378	N380	L381	A382	E383	S384	F385	V386	N387	G388	F389	L390	N391	L392	G393	Y394	N395	N396	D397	K398	L399	I400	V401	D402	M403	D404	M405	Y406	Y407	Y408	K409	T410	K411	E291	P351	K352	V353	P354	E355	D356	I357	Y358	K359	S360	H361
I423	Q423	S424	I425	Y426	W428	N429	L430	D431	G432	L433	Q434	Q435	L436	D437	K438	Y439	L440	Y441	V442	D443	E444	P445	E446	V447	K448	A449	G450	A451	L452	L453	G454	I455	G456	I457	S458	A459	S460	G461	V462	H463	D464	G465	E466	V467	E468	P469	A470	L471	L472	L473	L474	Q475	M415	T416	Y417	V478	T479	N480	A421	
D482	T483	K484	I485	S486	S487	A488	A489	I490	L491	G492	L493	G494	I495	A496	F497	A498	S500	K501	N502	D503	E504	V505	L506	G507	L508	L509	L510	P511	L512	A513	G514	S515	T516	D517	O518	L519	I520	E521	T522	A523	A524	M525	A526	S527	L528	A529	L530	A531	H532	V533	F534	V535	G536	T537	C538	N539	G540	D541		
I542	T543	T544	S545	I546	M547	D548	N549	F550	L551	E552	R553	T554	A555	L556	E557	L558	K559	T560	D561	W562	V563	R564	F565	P566	A567	L568	A569	G571	L572	L573	Y574	M575	G576	Q577	G578	E579	Q580	V581	D582	D583	L584	L585	E586	S587	L588	A590	I591	E592	H593	P594	M595	T596	S597	A598	L599	G600	E601	L602		
V603	G604	S605	C606	A607	Y608	T609	G610	T611	G612	D613	V614	L615	L616	I617	Q618	D619	L620	L621	H622	R623	L624	T625	P626	K627	N628	G629	K630	G631	E632	E633	D634	ASP	GLU	GLU	THR	ALA	GLY	GLY	GLN	THR	ASN	ILE	SER	ASP	PHE	LEU	GLY	GLU	GLN	VAL	ASN	GLU	PRO	THR	LYS	ASN				
GLU	GLU	ALA	ILE	VAL	VAL	ASP	MET	GLU	VAL	ASP	ALA	GLY	GLU	GLU	VAL	VAL	LYS	ALA	ILE	THR	GLU	LYS	ASN	GLY	GLU	LEU	GLY	E700	I701	K702	S703	E704	E705	K706	T707	ALA	GLY	GLY	THR	ASN	ILE	SER	ASP	PHE	LEU	GLY	GLU	GLN	VAL	ASN	GLU	PRO	THR	LYS	ASN					
D723	E724	E725	E726	K727	E728	E729	A730	G731	I732	E735	Y738	A739	V740	L741	I742	G743	A744	L745	I746	A747	L748	G749	E750	N751	I752	G753	K754	E755	M756	S757	L758	R759	H760	F761	G762	H763	L764	M765	N766	H766	Y767	G768	M769	E770	H771	I772	R773	R774	M775	V776	P777	L778	A779	M780	R840	E841	Q842	D843	A844	
V785	S786	D787	P788	Q789	M790	K791	V792	F793	D794	T795	L796	T797	R798	F799	S800	H801	A802	D804	L805	E806	V807	S808	N809	N810	S811	I812	F813	A814	M815	G816	L817	C818	G819	A820	G821	T822	N823	N824	A825	R826	L827	A828	Q829	L830	L831	R832	Q833	L834	A835	S836	Y837	Y838	Y839	R840	E841	Q842	D843	A844		

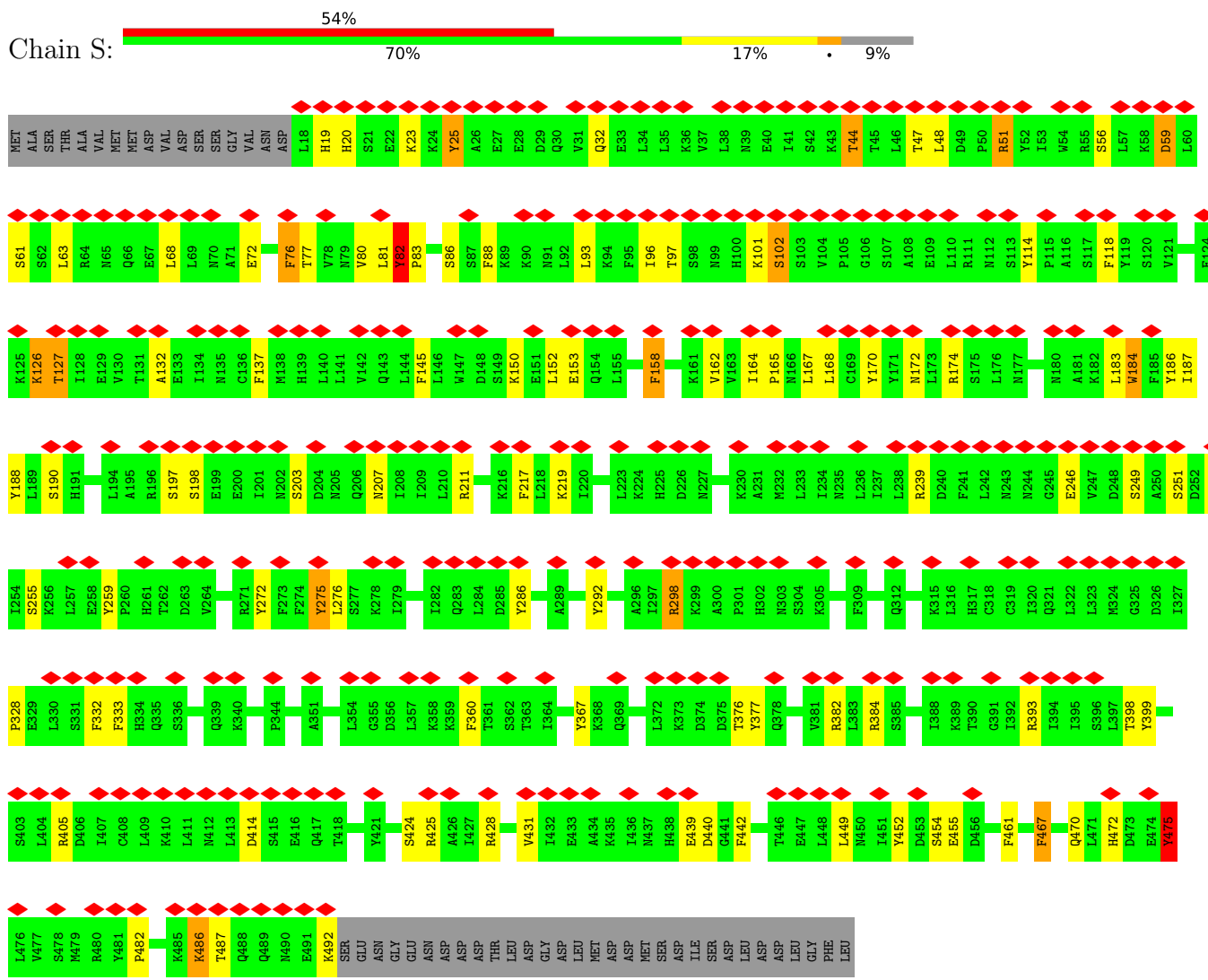


• Molecule 7: 26S proteasome regulatory subunit RPN2

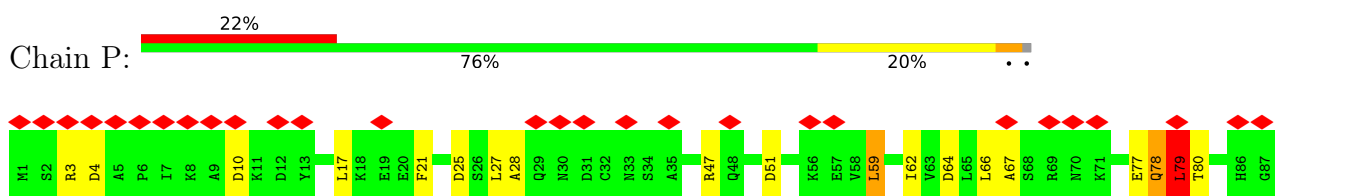


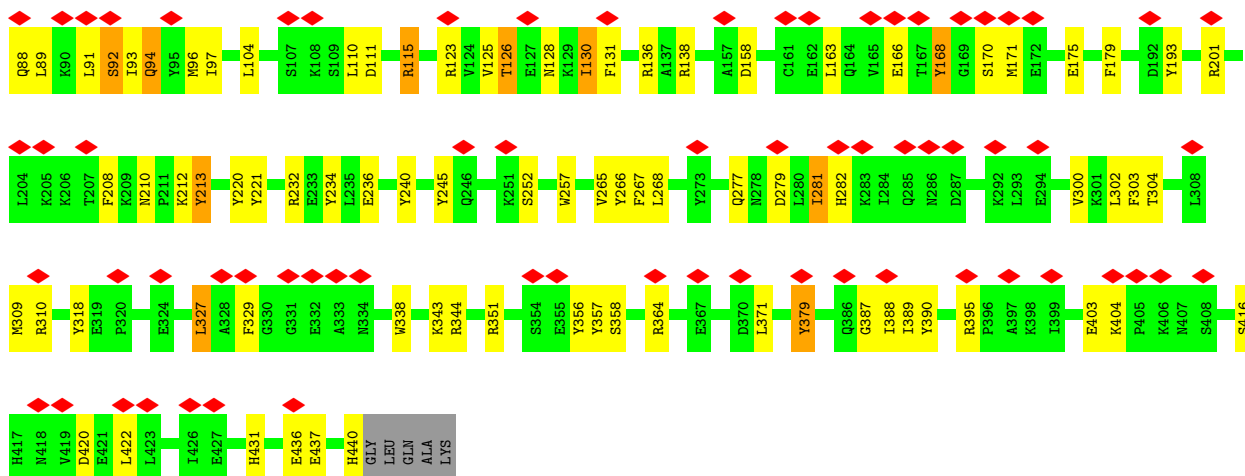


● Molecule 8: 26S proteasome regulatory subunit RPN3

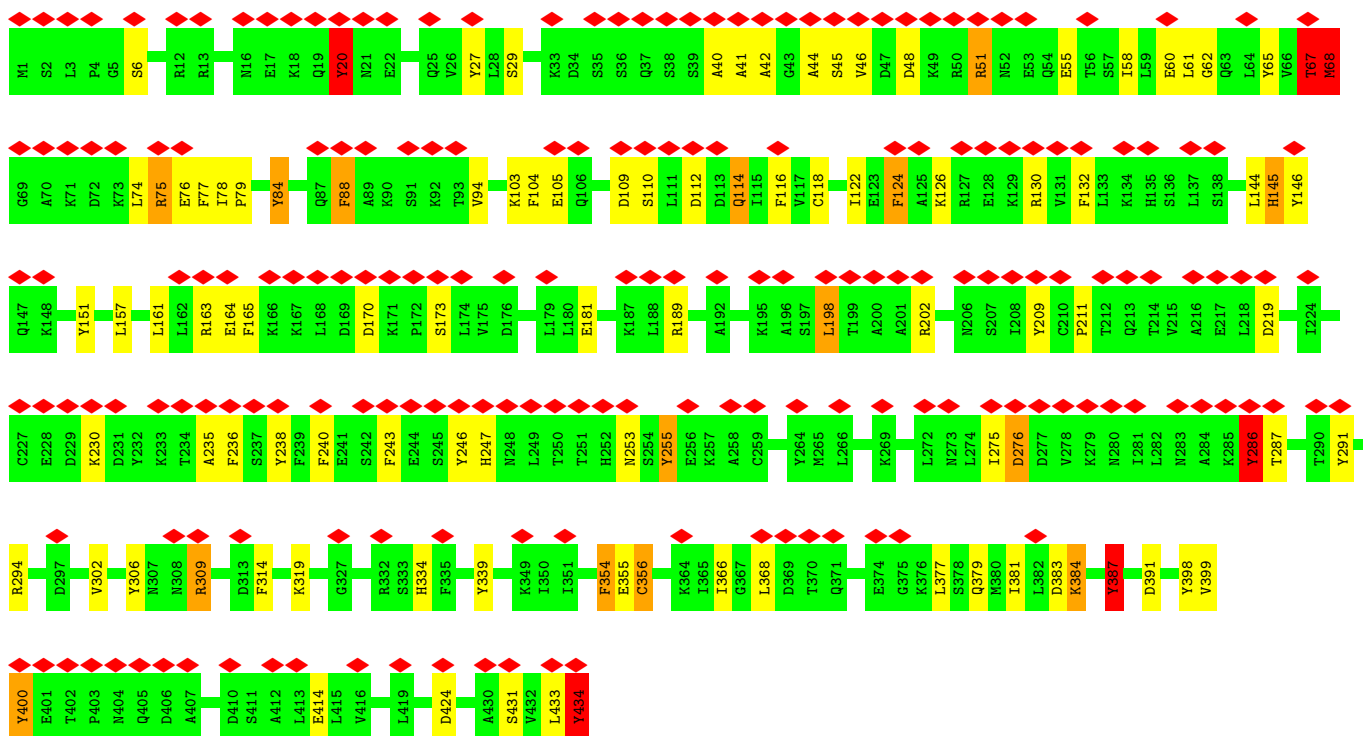
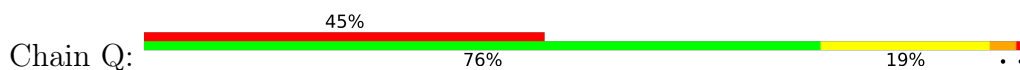


● Molecule 9: 26S proteasome regulatory subunit RPN5

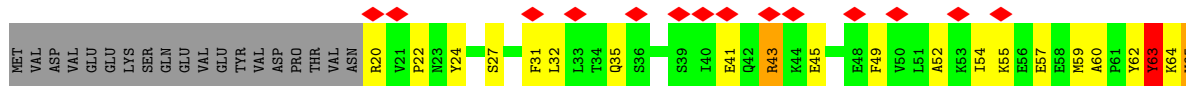


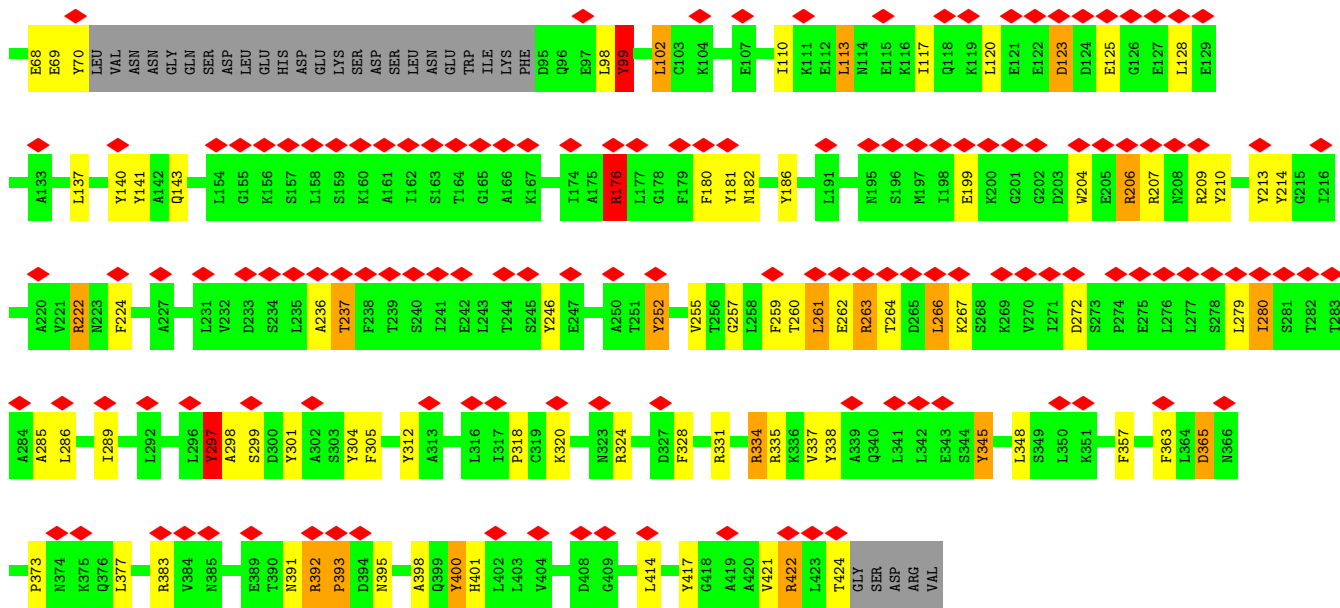


• Molecule 10: 26S proteasome regulatory subunit RPN6

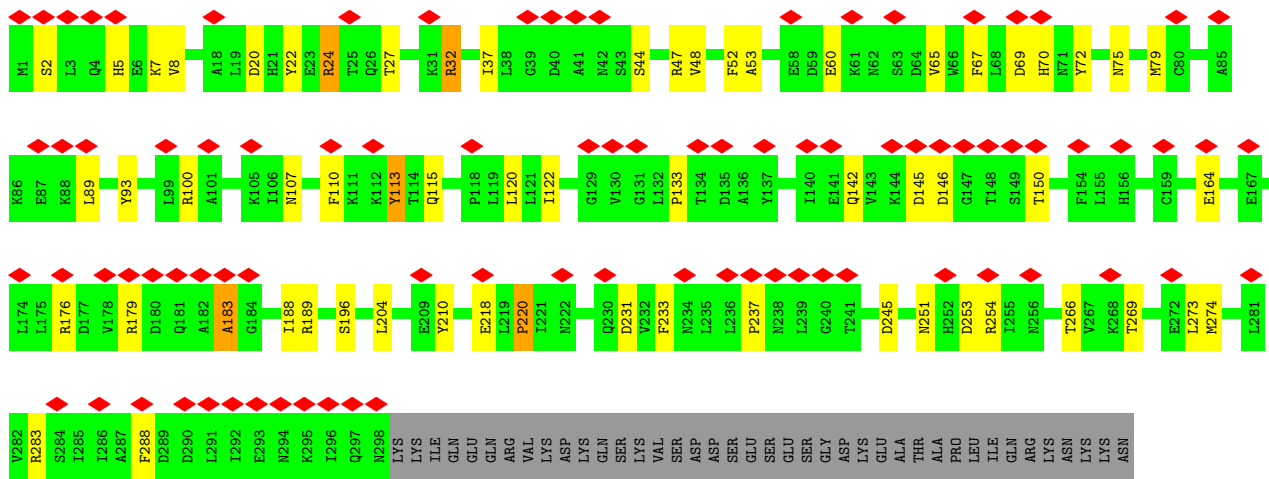


• Molecule 11: 26S proteasome regulatory subunit RPN7

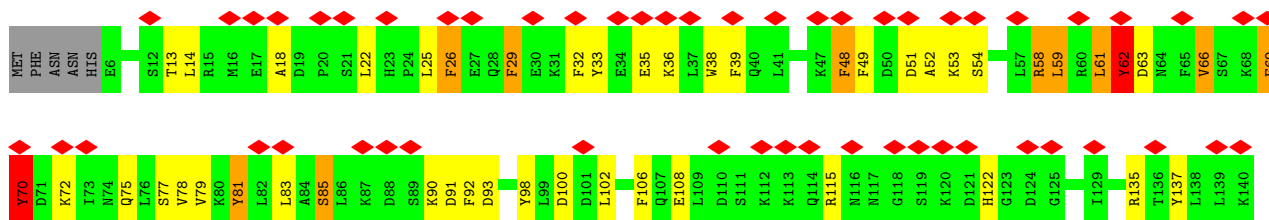
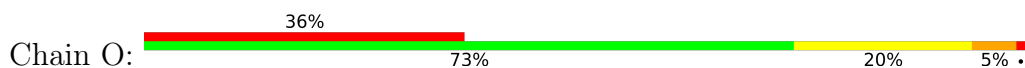


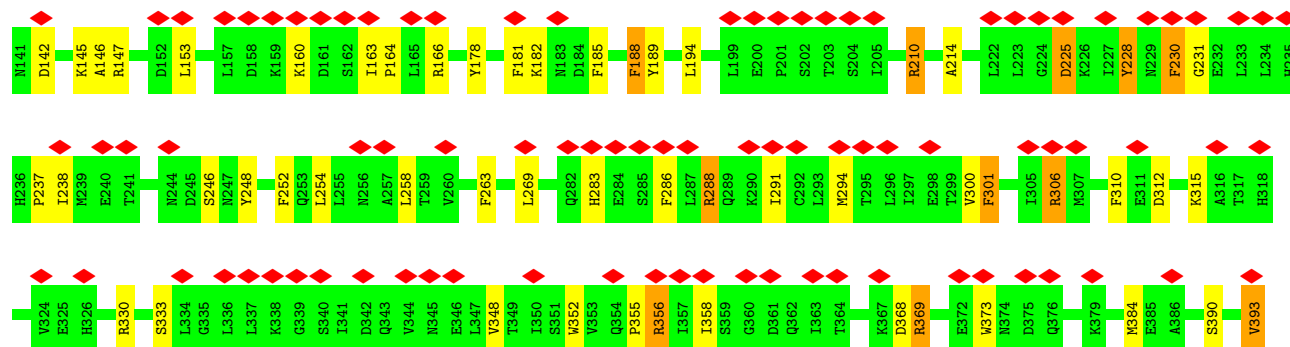


• Molecule 12: 26S proteasome regulatory subunit RPN8



• Molecule 13: 26S proteasome regulatory subunit RPN9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	193337	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (\AA)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.38, 1.38, 1.38	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	W	1.69	17/1557 (1.1%)	1.87	34/2111 (1.6%)
2	V	1.62	16/2309 (0.7%)	1.77	38/3115 (1.2%)
3	T	1.62	12/2235 (0.5%)	1.78	43/3017 (1.4%)
4	X	1.83	12/1058 (1.1%)	1.96	29/1432 (2.0%)
5	Y	1.83	7/438 (1.6%)	1.83	9/583 (1.5%)
6	Z	1.61	45/7122 (0.6%)	1.78	124/9645 (1.3%)
7	N	1.62	63/6994 (0.9%)	1.71	108/9455 (1.1%)
8	S	1.69	30/3966 (0.8%)	1.81	91/5355 (1.7%)
9	P	1.66	31/3663 (0.8%)	1.79	84/4940 (1.7%)
10	Q	1.66	28/3556 (0.8%)	1.80	68/4787 (1.4%)
11	R	2.09	27/3110 (0.9%)	1.95	82/4193 (2.0%)
12	U	1.57	18/2407 (0.7%)	1.74	32/3258 (1.0%)
13	O	1.63	26/3247 (0.8%)	1.79	77/4380 (1.8%)
All	All	1.68	332/41662 (0.8%)	1.79	819/56271 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	2
2	V	0	7
3	T	0	9
4	X	0	7
5	Y	0	1
6	Z	0	19
7	N	0	13
8	S	0	10
9	P	0	5
10	Q	0	11
11	R	0	18
12	U	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	13
All	All	0	118

The worst 5 of 332 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	99	TYR	CE1-CZ	54.44	2.09	1.38
11	R	99	TYR	CZ-OH	39.26	2.04	1.37
8	S	59	ASP	CA-CB	-19.85	1.10	1.53
9	P	78	GLN	C-N	18.16	1.75	1.34
8	S	127	THR	CA-CB	17.50	1.98	1.53

The worst 5 of 819 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	99	TYR	CE1-CZ-OH	-25.48	51.30	120.10
2	V	61	TYR	CB-CG-CD2	-19.36	109.39	121.00
6	Z	188	ALA	CB-CA-C	-18.32	82.62	110.10
13	O	62	TYR	CB-CA-C	-15.89	78.61	110.40
9	P	266	TYR	CB-CG-CD2	-15.64	111.62	121.00

There are no chirality outliers.

5 of 118 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	100	ARG	Sidechain
2	V	156	PHE	Sidechain
2	V	20	ARG	Sidechain
1	W	15	TYR	Sidechain
1	W	21	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1534	0	1542	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	2274	0	2273	25	0
3	T	2192	0	2161	7	0
4	X	1032	0	1017	4	0
5	Y	435	0	393	9	0
6	Z	7005	0	6932	71	0
7	N	6882	0	6959	24	0
8	S	3894	0	3938	23	0
9	P	3608	0	3693	20	0
10	Q	3499	0	3524	24	0
11	R	3060	0	3083	50	0
12	U	2373	0	2403	16	0
13	O	3186	0	3213	58	0
All	All	40974	0	41131	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 318 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:P:78:GLN:C	9:P:79:LEU:N	1.75	1.39
11:R:99:TYR:CE1	11:R:99:TYR:CZ	2.09	1.39
8:S:127:THR:CB	8:S:127:THR:CA	1.98	1.37
11:R:99:TYR:CE1	11:R:99:TYR:OH	1.79	1.32
9:P:212:LYS:O	9:P:213:TYR:CD1	1.92	1.22

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	W	195/268 (73%)	179 (92%)	12 (6%)	4 (2%)	7	39
2	V	287/306 (94%)	263 (92%)	18 (6%)	6 (2%)	7	39
3	T	264/274 (96%)	236 (89%)	21 (8%)	7 (3%)	5	34
4	X	125/156 (80%)	107 (86%)	12 (10%)	6 (5%)	2	23
5	Y	47/89 (53%)	43 (92%)	3 (6%)	1 (2%)	7	39
6	Z	902/993 (91%)	820 (91%)	55 (6%)	27 (3%)	4	31
7	N	886/945 (94%)	849 (96%)	30 (3%)	7 (1%)	19	60
8	S	473/523 (90%)	436 (92%)	24 (5%)	13 (3%)	5	34
9	P	438/445 (98%)	408 (93%)	22 (5%)	8 (2%)	8	42
10	Q	432/434 (100%)	388 (90%)	26 (6%)	18 (4%)	3	25
11	R	377/429 (88%)	352 (93%)	17 (4%)	8 (2%)	7	39
12	U	296/338 (88%)	280 (95%)	11 (4%)	5 (2%)	9	43
13	O	386/393 (98%)	368 (95%)	16 (4%)	2 (0%)	29	68
All	All	5108/5593 (91%)	4729 (93%)	267 (5%)	112 (2%)	10	38

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	200	ASN
3	T	92	ASN
3	T	96	LEU
3	T	173	GLU
4	X	116	ALA

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	W	171/230 (74%)	168 (98%)	3 (2%)	59	77
2	V	253/268 (94%)	250 (99%)	3 (1%)	71	84
3	T	249/256 (97%)	241 (97%)	8 (3%)	39	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	116/144 (81%)	115 (99%)	1 (1%)	78	87
5	Y	50/81 (62%)	48 (96%)	2 (4%)	31	56
6	Z	773/850 (91%)	753 (97%)	20 (3%)	46	67
7	N	745/797 (94%)	731 (98%)	14 (2%)	57	75
8	S	447/489 (91%)	436 (98%)	11 (2%)	47	68
9	P	412/415 (99%)	404 (98%)	8 (2%)	57	75
10	Q	391/391 (100%)	380 (97%)	11 (3%)	43	65
11	R	333/379 (88%)	321 (96%)	12 (4%)	35	60
12	U	271/308 (88%)	266 (98%)	5 (2%)	59	77
13	O	363/368 (99%)	353 (97%)	10 (3%)	43	65
All	All	4574/4976 (92%)	4466 (98%)	108 (2%)	51	69

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	414	ASP
10	Q	88	PHE
13	O	61	LEU
8	S	470	GLN
9	P	302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
9	P	323	ASN
10	Q	247	HIS
9	P	342	GLN
9	P	431	HIS
11	R	35	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	78:GLN	C	79:LEU	N	1.75

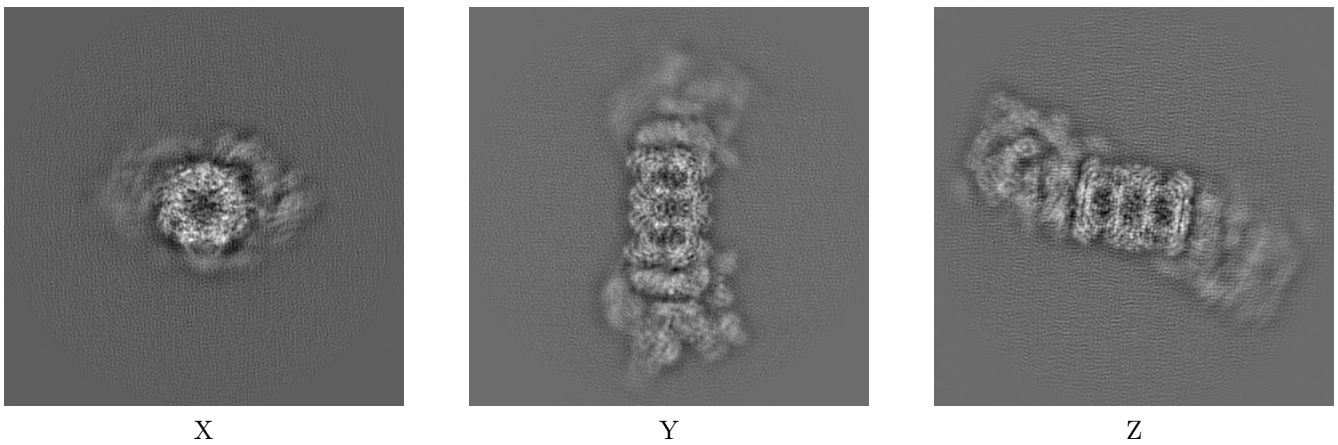
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3535. 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](#)

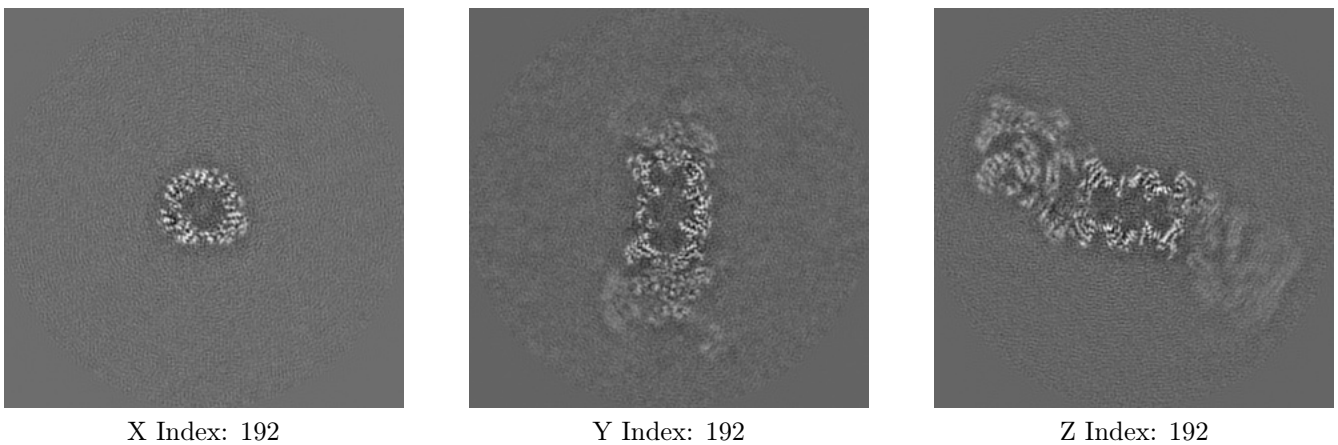
6.1.1 Primary map



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

6.2 Central slices [i](#)

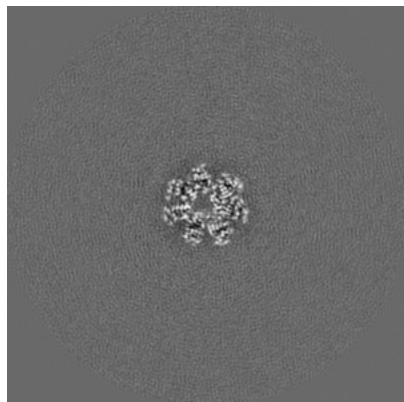
6.2.1 Primary map



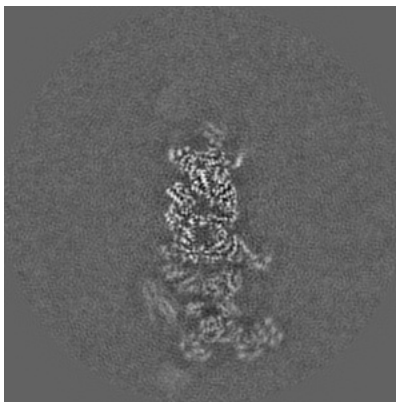
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

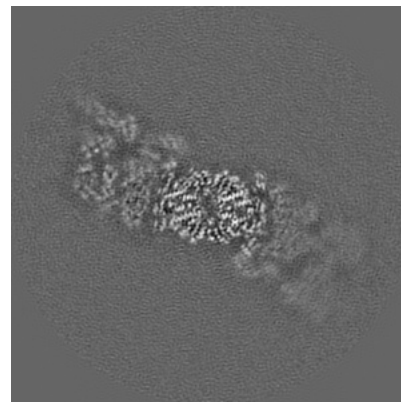
6.3.1 Primary map



X Index: 206



Y Index: 210



Z Index: 210

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 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

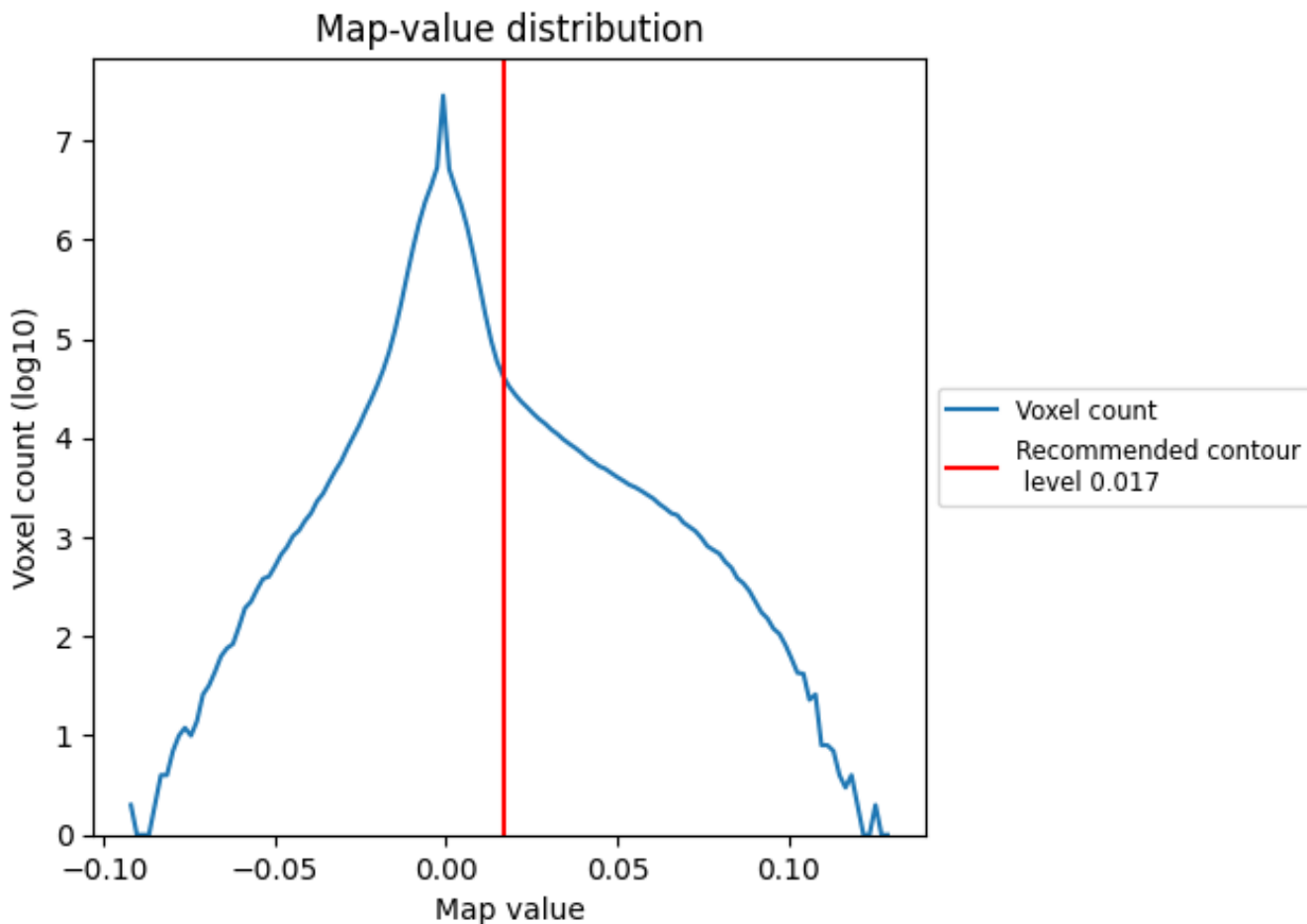
6.5 Mask visualisation

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

7 Map analysis [i](#)

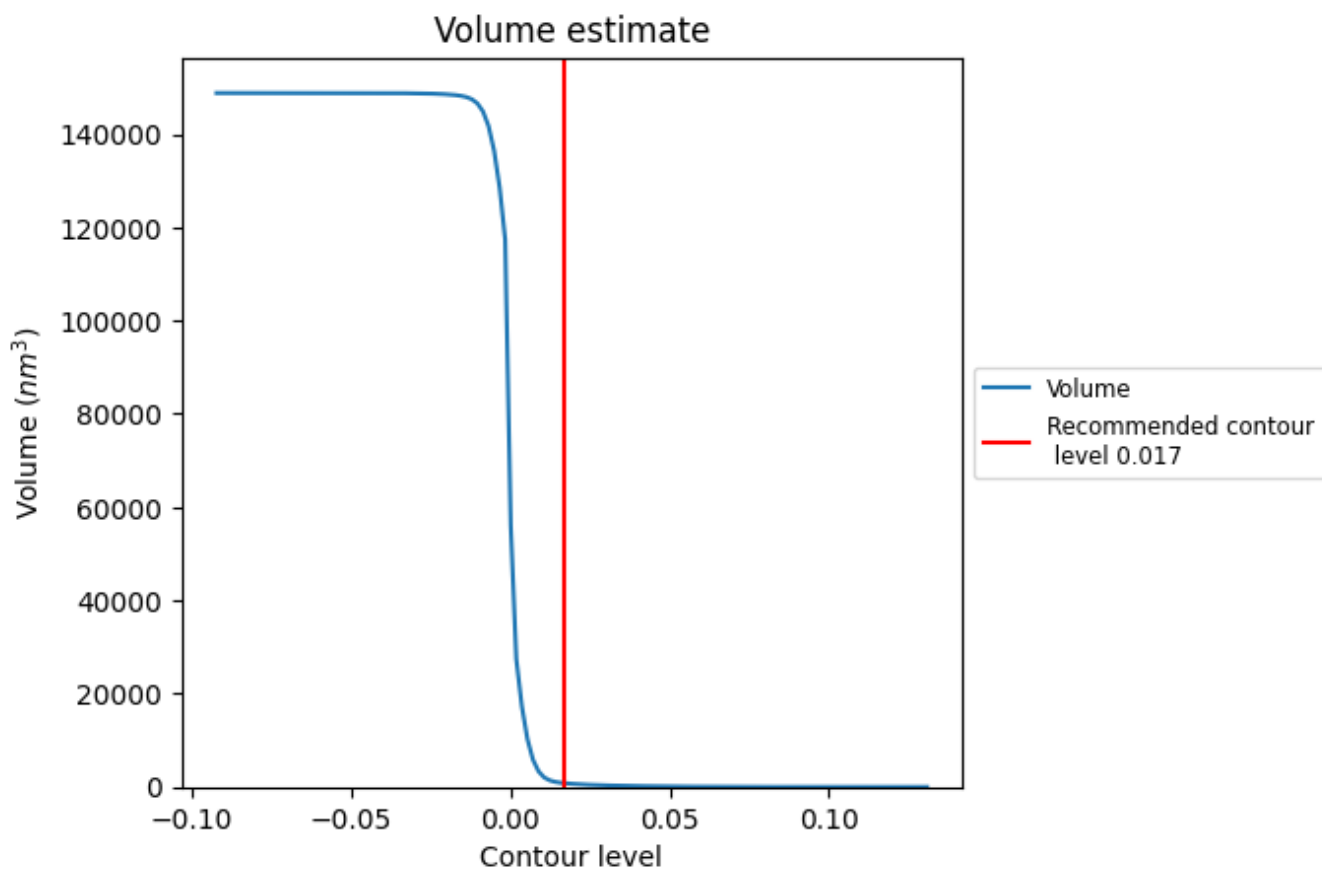
This section contains the results of statistical analysis of the map.

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.

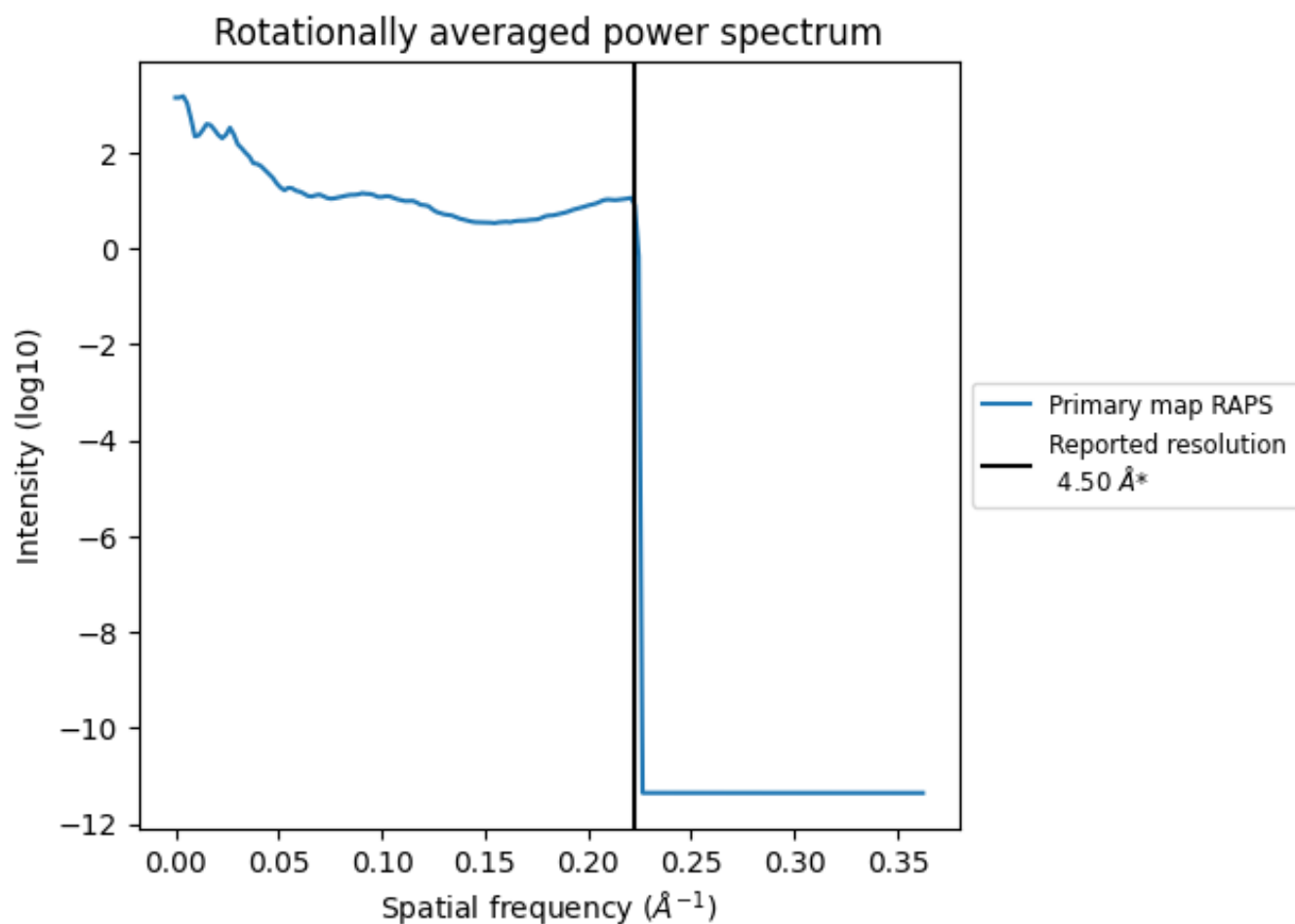
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 813 nm³; this corresponds to an approximate mass of 734 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 0.222 Å⁻¹

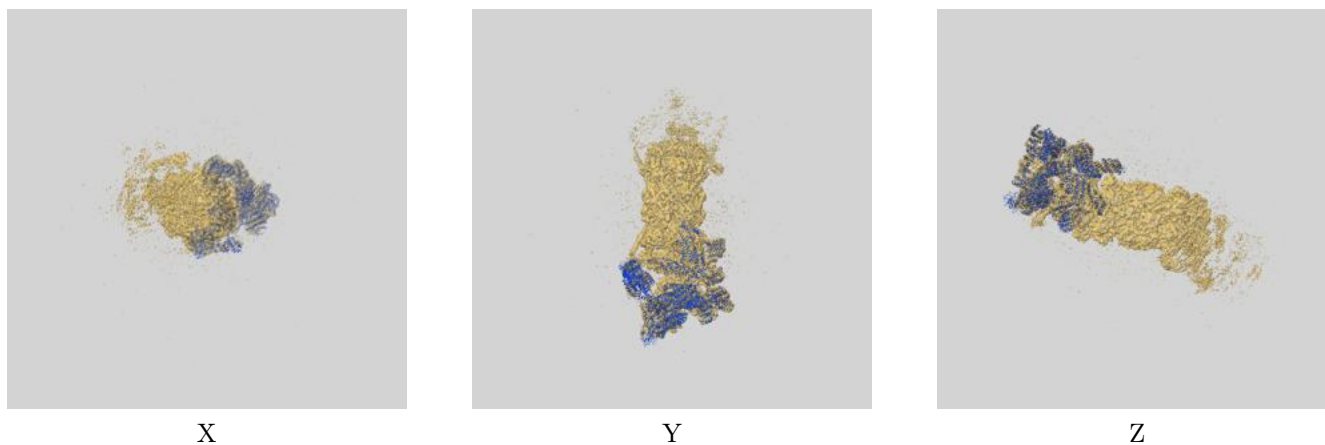
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

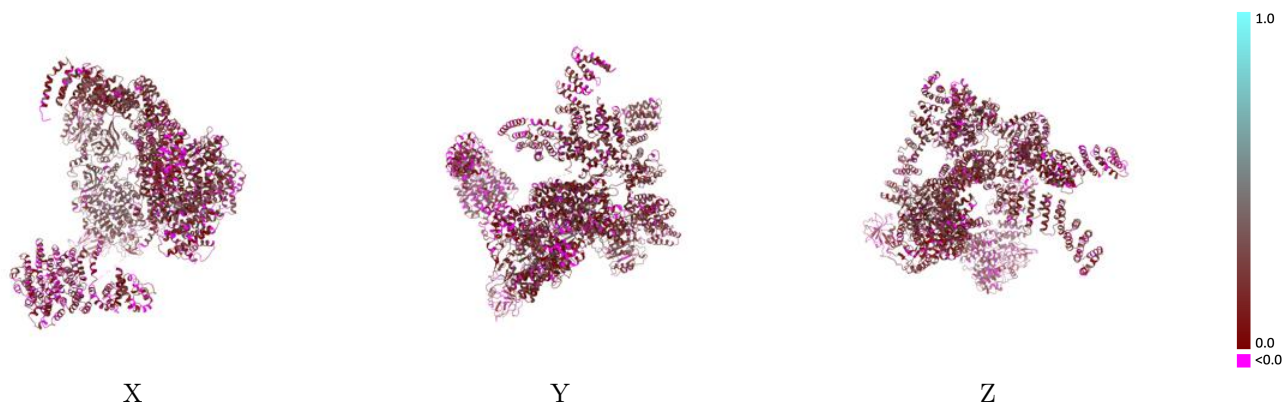
This section contains information regarding the fit between EMDB map EMD-3535 and PDB model 5MPE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



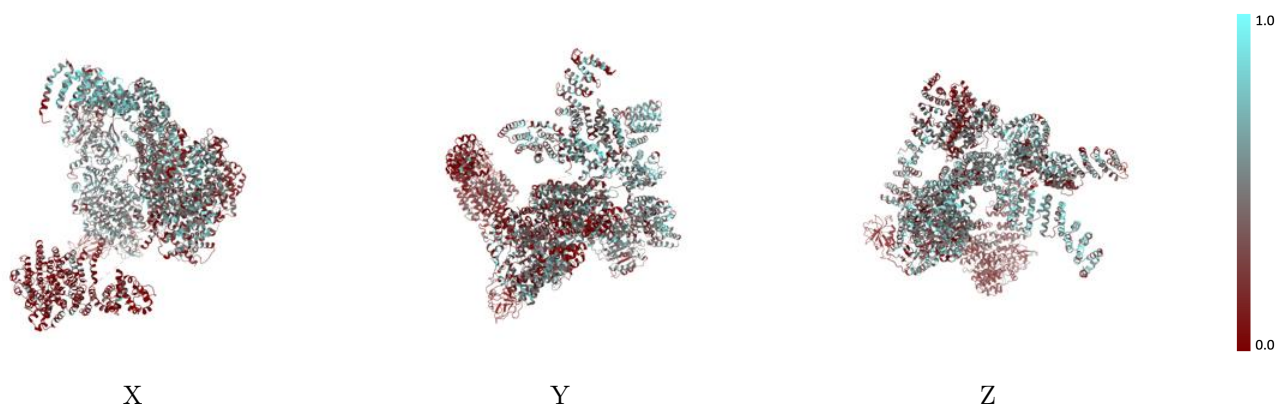
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



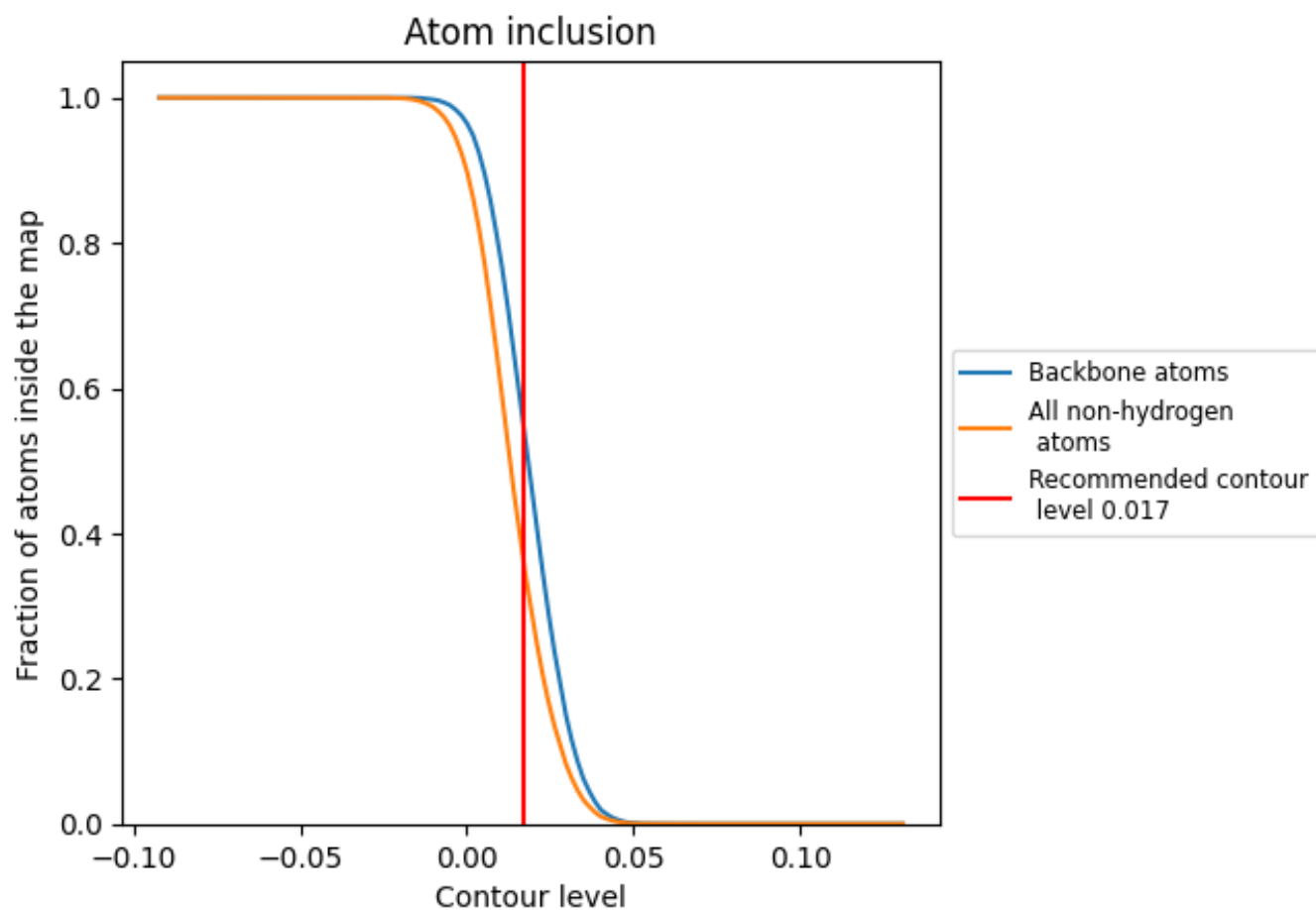
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).





























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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3627	 0.1550
N	 0.4284	 0.1860
O	 0.4686	 0.1680
P	 0.5634	 0.1960
Q	 0.4326	 0.1430
R	 0.4582	 0.1670
S	 0.3407	 0.1390
T	 0.2140	 0.1130
U	 0.4783	 0.2160
V	 0.4873	 0.2080
W	 0.3988	 0.1820
X	 0.0168	 0.0660
Y	 0.2814	 0.1360
Z	 0.0978	 0.0930

