



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 01:41 pm GMT

PDB ID : 5MPD
EMDB ID : EMD-3534
Title : 26S proteasome in presence of ATP (s1)
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 : 4.10 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

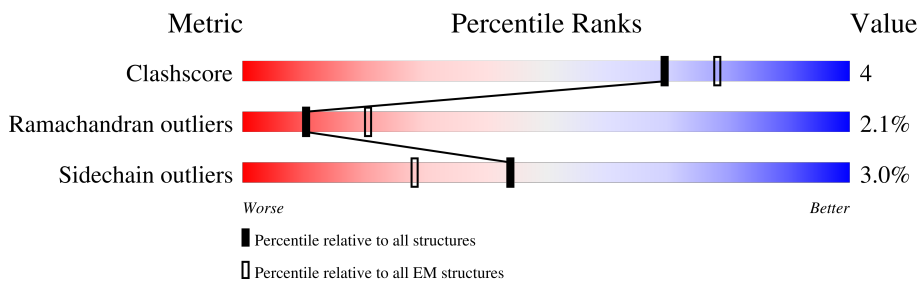
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	
10	Q	434	
11	R	429	
12	U	338	
13	O	393	

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

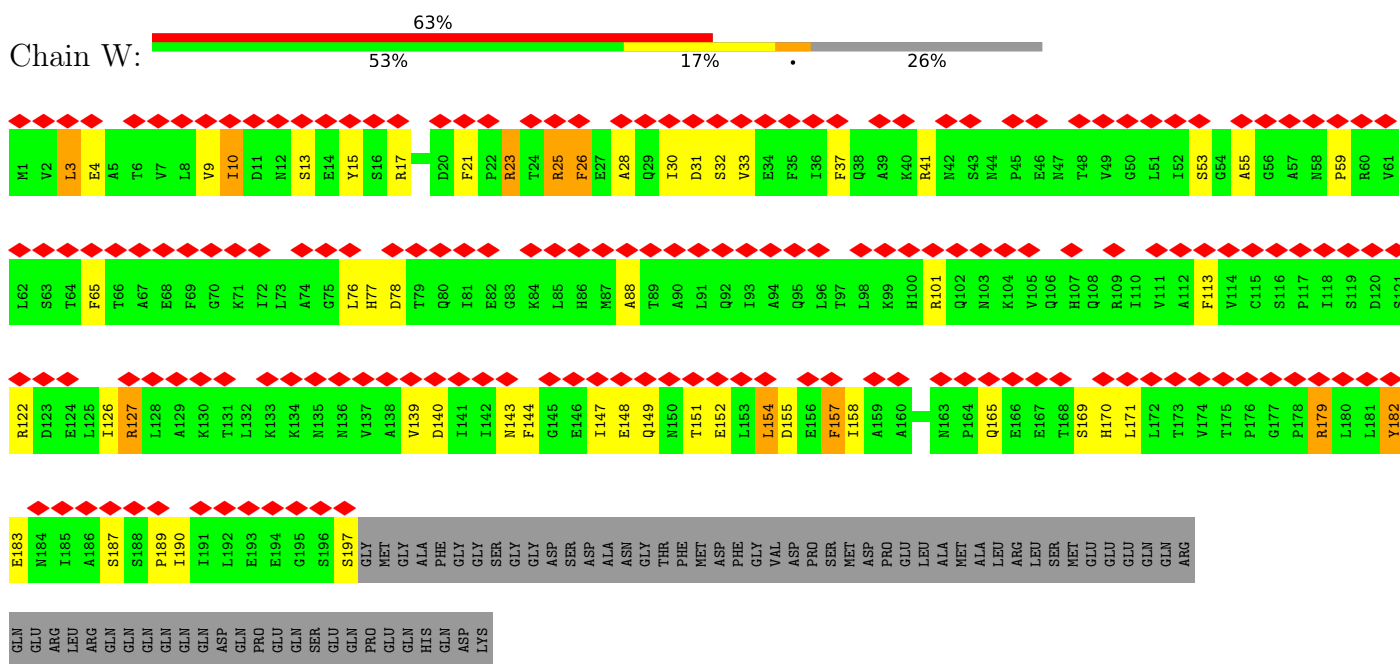
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

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

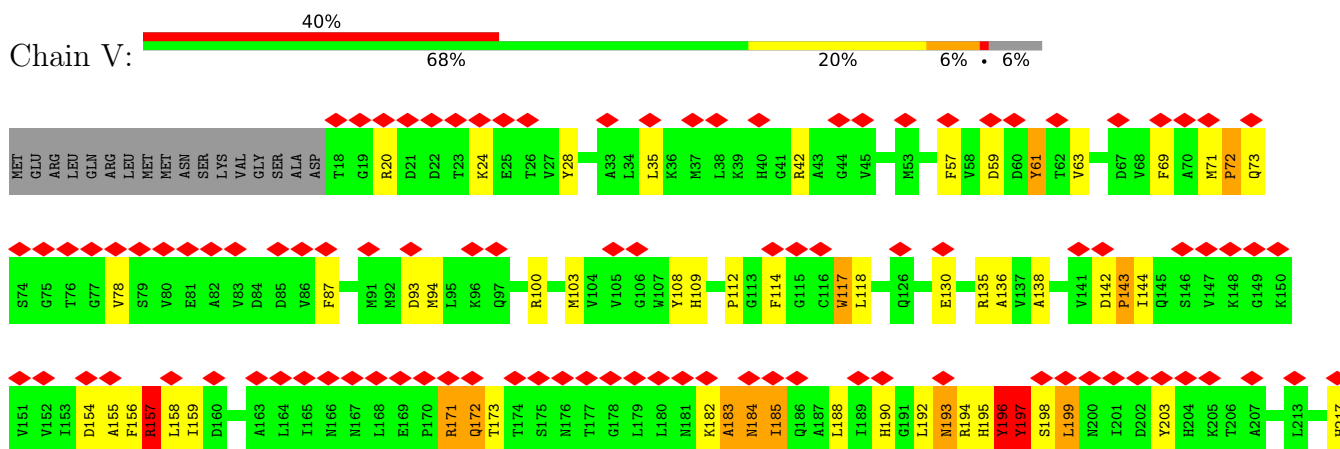
3 Residue-property plots

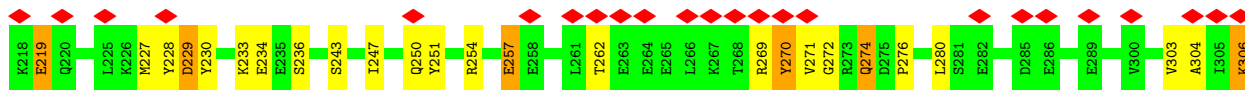
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

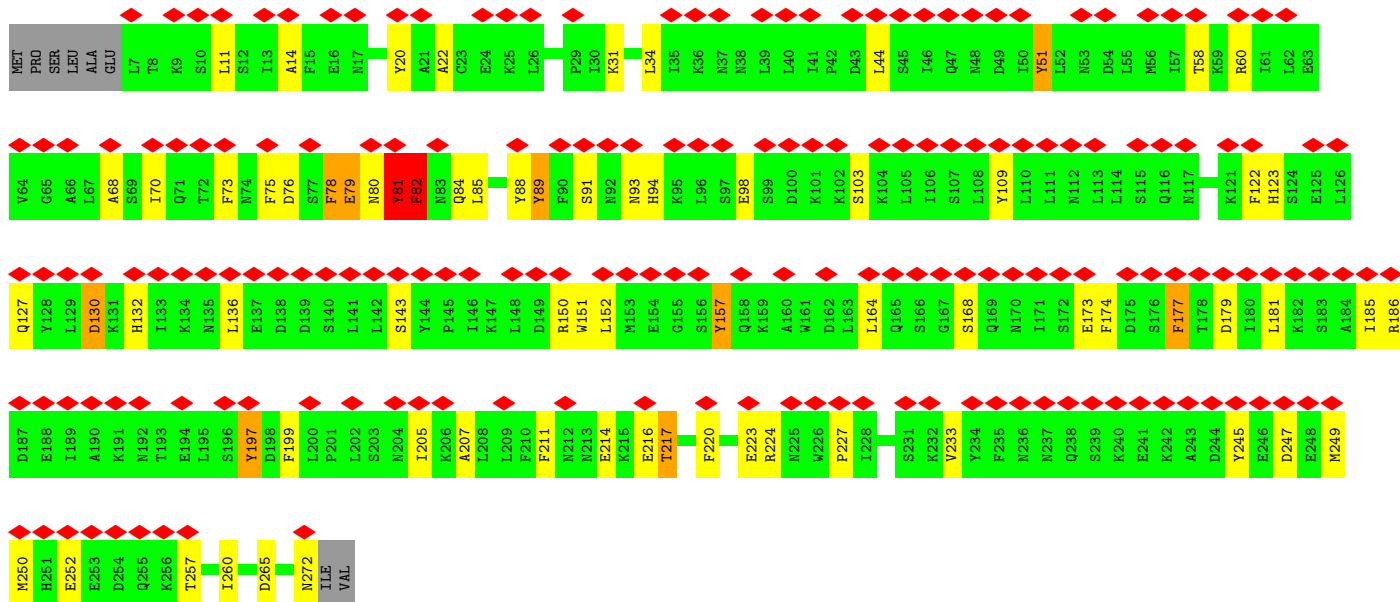


- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11

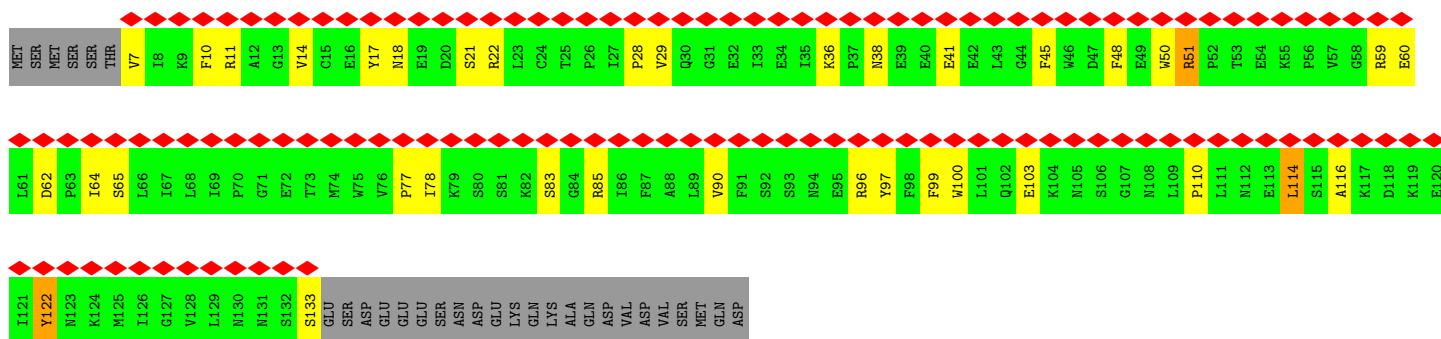
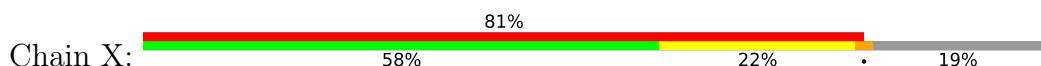




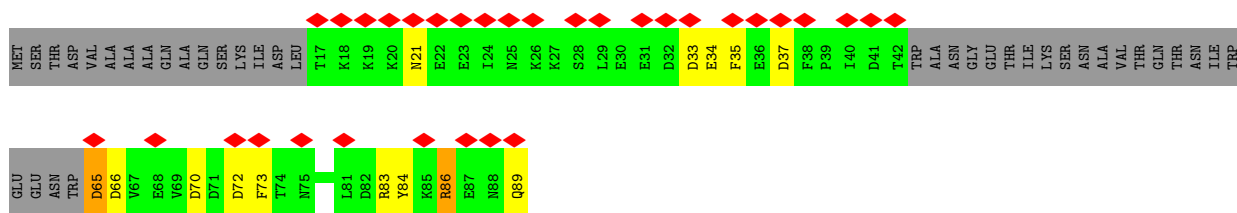
• Molecule 3: 26S proteasome regulatory subunit RPN12



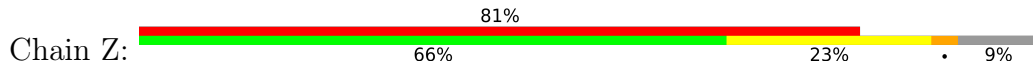
• Molecule 4: 26S proteasome regulatory subunit RPN13



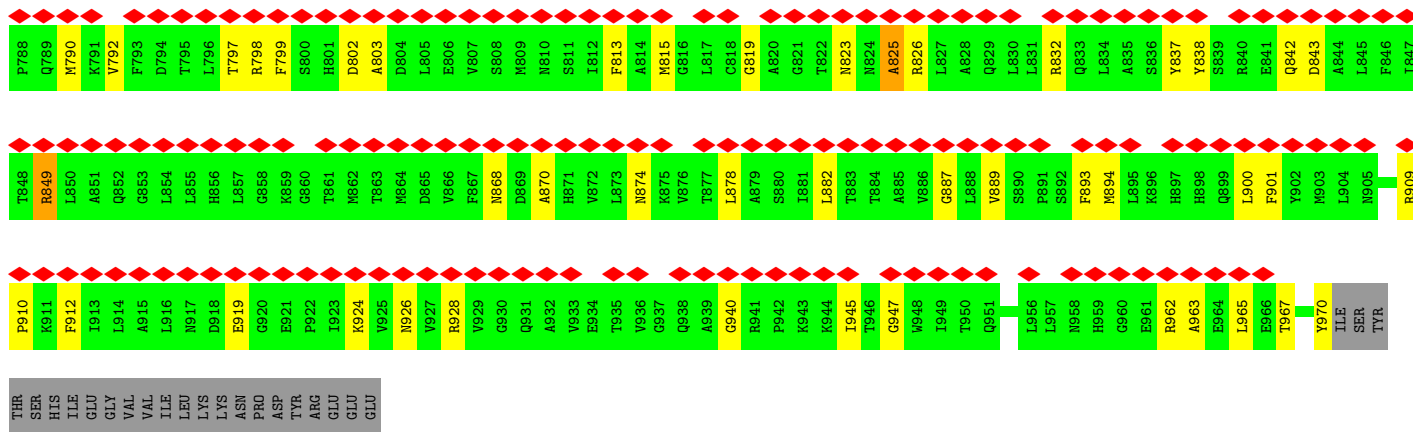
• Molecule 5: 26S proteasome complex subunit SEM1



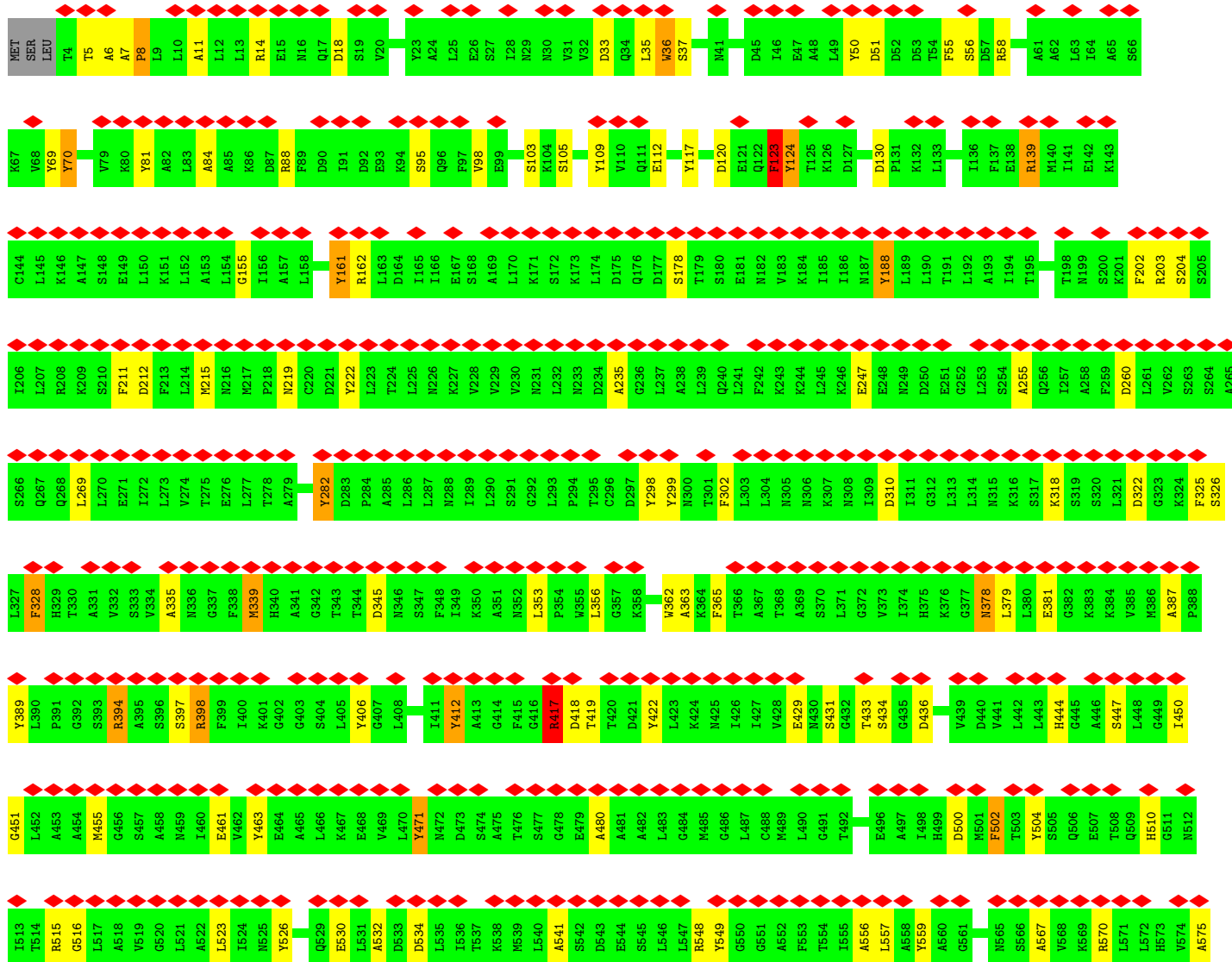
• Molecule 6: 26S proteasome regulatory subunit RPN1

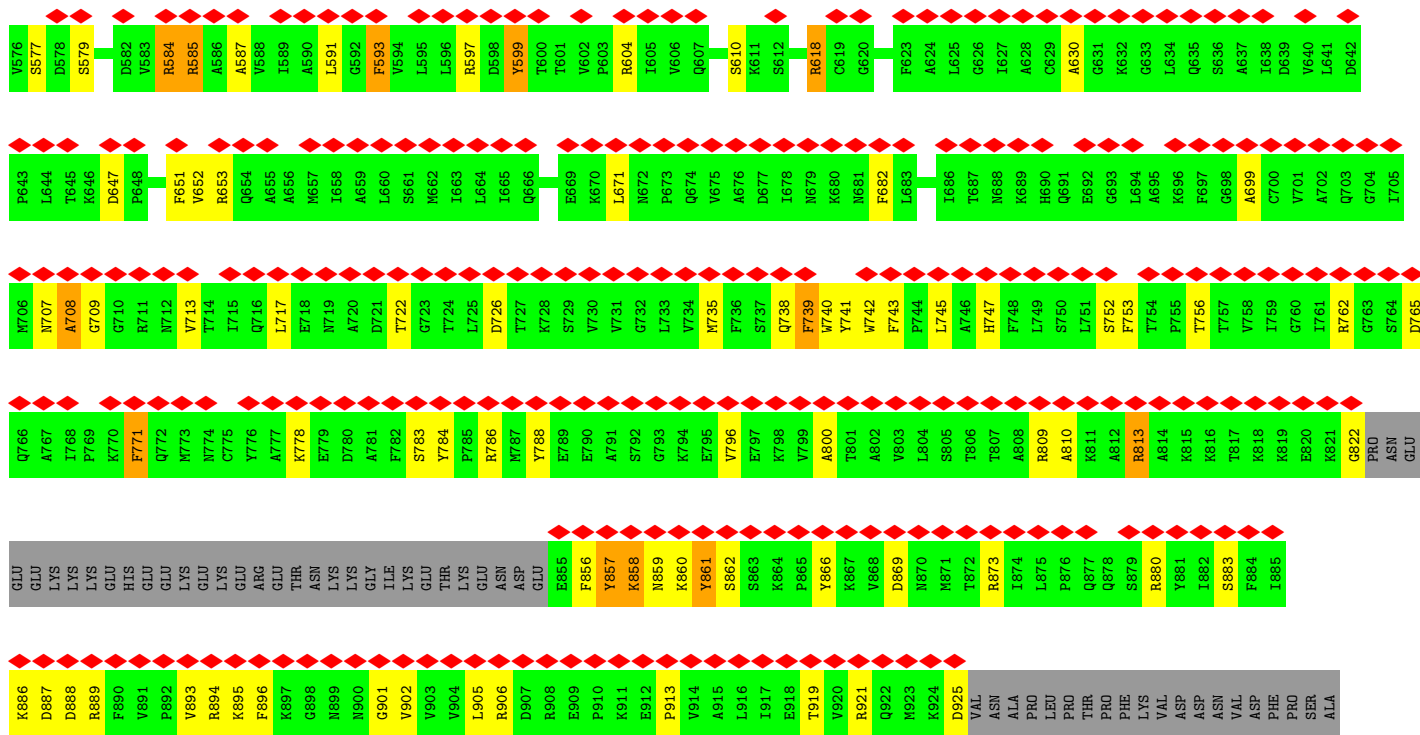


M1	S61	I121	G181	T241	P304	R364	I425	I485	S545	A607	I1E	E727
V2	S62	L122	S182	F242	V305	S365	Y426	S485	I546	Y608	GLU	K728
D3	L63	A123	K183	Q243	M306	K366	Q427	S487	H547	T609	ASP	E729
E4	Y64	M124	S184	R244	H307	S367	V428	A488	D548	G610	GLU	A730
S5	E65	T125	D185	V245	Q308	V368	M429	A489	H549	T611	NET	G731
D6	A66	Y126	G186	Y248	Q309	F369	L430	A490	F550	G612	GLU	I732
K8	S67	S127	L68	M249	L310	S370	D431	A491	L551	D613	ASP	V733
Q9	L69	E128	A188	V250	A311	S371	Q432	Q492	E552	D614	ALA	D734
Q10	N69	M129	A189	A251	Y312	A372	L433	Q493	H553	V615	GLU	L736
T11	A70	G130	T190	C252	L313	G373	Q434	Q494	T554	I617	GLY	L737
I12	L71	K131	S191	V253	L314	L374	Q435	L495	A555	G618	GLU	A738
D13	L72	H132	G192	P254	A315	D375	L436	L496	I556	D619	VAL	E739
E14	K73	D133	F193	L255	Q317	S376	K438	F497	E557	G620	GLU	L741
Q15	S74	S134	E194	L256	K318	A377	K439	A498	L558	L620	VAL	G742
S16	I76	L135	F195	P257	T319	Q378	Y439	G499	K559	L621	LYS	I743
Q17	K76	R136	S196	P258	S320	Q379	L440	S500	T560	H622	ALA	A744
I18	N77	Y137	K197	P259	F321	L381	Y441	X501	D561	R623	GLU	A745
S19	S78	R138	E198	E260	E322	A382	Y442	N502	V562	L624	THR	L745
P20	T79	L139	D199	D261	E323	S383	E443	D503	H563	T625	GLU	I746
E21	S80	L140	T200	V262	Y323	S384	P444	E504	H564	P626	LYS	A747
K22	S81	S141	L201	V263	G324	S385	E445	V505	F565	R627	ASN	L748
Q23	M82	D142	R202	F264	G325	V386	V447	L506	L566	H628	GLY	G749
T24	T83	V143	L203	L265	Q327	Q328	K448	G507	A567	V629	SER	E750
P25	A84	A144	C204	K266	D328	F389	A449	G508	L568	H630	LEU	D751
N26	V85	D145	L205	T267	L329	L390	A450	L509	A569	G631	GLU	I752
K27	K87	F146	D206	A268	G330	N391	G451	L510	L570	E532	GLY	G753
K28	P88	E147	I207	Y269	G331	L392	A451	P511	G571	E533	GLU	K754
D29	L89	G148	V208	Y272	N332	L393	L452	L512	I572	D634	GLU	E755
K30	K90	W149	P209	L273	G333	G394	L453	A513	L573	A635	ASP	M756
K31	L91	G150	Y210	S274	K334	Y394	G454	A514	Y574	GLU	GLU	S757
K32	F91	H151	F211	Q275	L335	C395	G455	S515	H575	GLU	GLU	L758
E33	L92	H152	L212	N276	S336	N396	G456	T516	G576	THR	THR	E759
E34	R93	Y153	K213	E277	E337	D397	L457	D517	Q577	ALA	ALA	K760
E35	P94	I154	H214	N278	H338	L398	S458	L518	G578	L459	GLU	K707
E36	T95	R155	N215	L279	F339	L400	S460	P519	E579	G460	GLY	G708
E37	Y96	H156	G216	T279	L340	V401	G461	L520	O580	G461	GLN	K709
Q37	P97	L157	E217	A281	Y341	D402	V462	T522	V581	D402	THR	S710
L38	D98	A158	E218	L282	L342	M403	H463	A523	D582	D403	ASN	S711
S39	L99	L159	D219	A283	A343	D404	D464	A524	E583	D404	SER	D712
E40	C100	E160	A220	L284	K344	M405	G465	N525	E586	D405	ILE	D713
E41	S101	I161	V221	L284	E345	V406	E466	A526	T587	D406	ASP	K713
D42	I102	G162	D222	R287	L346	Y407	V467	S527	T588	D407	PHE	D714
A43	Y103	E163	L223	L288	L347	Y408	E468	L528	S589	D408	LEU	A715
K44	D104	V164	L224	G289	N348	K409	P469	T410	A529	D409	GLY	A716
L45	K105	Y165	L225	E290	T349	L410	L470	L410	A530	D410	GLU	T717
K46	W106	M166	E226	E291	G350	P351	A470	G411	A531	D411	GLN	D718
T47	T107	D167	I227	E292	P352	G412	L471	G412	A532	D412	VAL	H718
D48	Q168	Q168	E228	M293	K352	D413	L472	D413	H532	D413	ASN	G719
L49	P109	V169	S229	I294	V353	G414	L473	G414	A533	D414	GLU	K720
E50	N110	E170	I230	R296	E354	M415	L474	M415	V534	D415	PRO	G721
L51	L111	K171	D231	S297	E355	T416	Q475	T416	F534	D416	THR	L722
L52	K112	D172	K232	V297	D356	S417	D476	S417	G536	D417	LYS	D723
V63	S113	A173	L233	F298	L357	A418	Y477	A418	T537	D418	ASN	D724
E54	S114	E174	P234	D299	Y358	V419	V478	V419	C538	D419	GLU	E725
R55	L115	D175	Q235	A300	K359	A420	T479	A420	N539	D420	ALA	E726
L56	A116	D176	F236	T301	S360	S421	N480	N480	G540	D421	GLU	L778
K57	D117	T177	V237	S302	H361	I422	P481	P481	D541	D422	GLU	A779
E58	V118	S178	D238	D303	L363	G423	T483	T483	I542	D423	ALA	M780
D60	L119	S179	N240	D303	D363	S424	K484	K484	T544	D424	GLU	I782
												G781
												I782
												V783
												S784
												V785
												S786
												D787

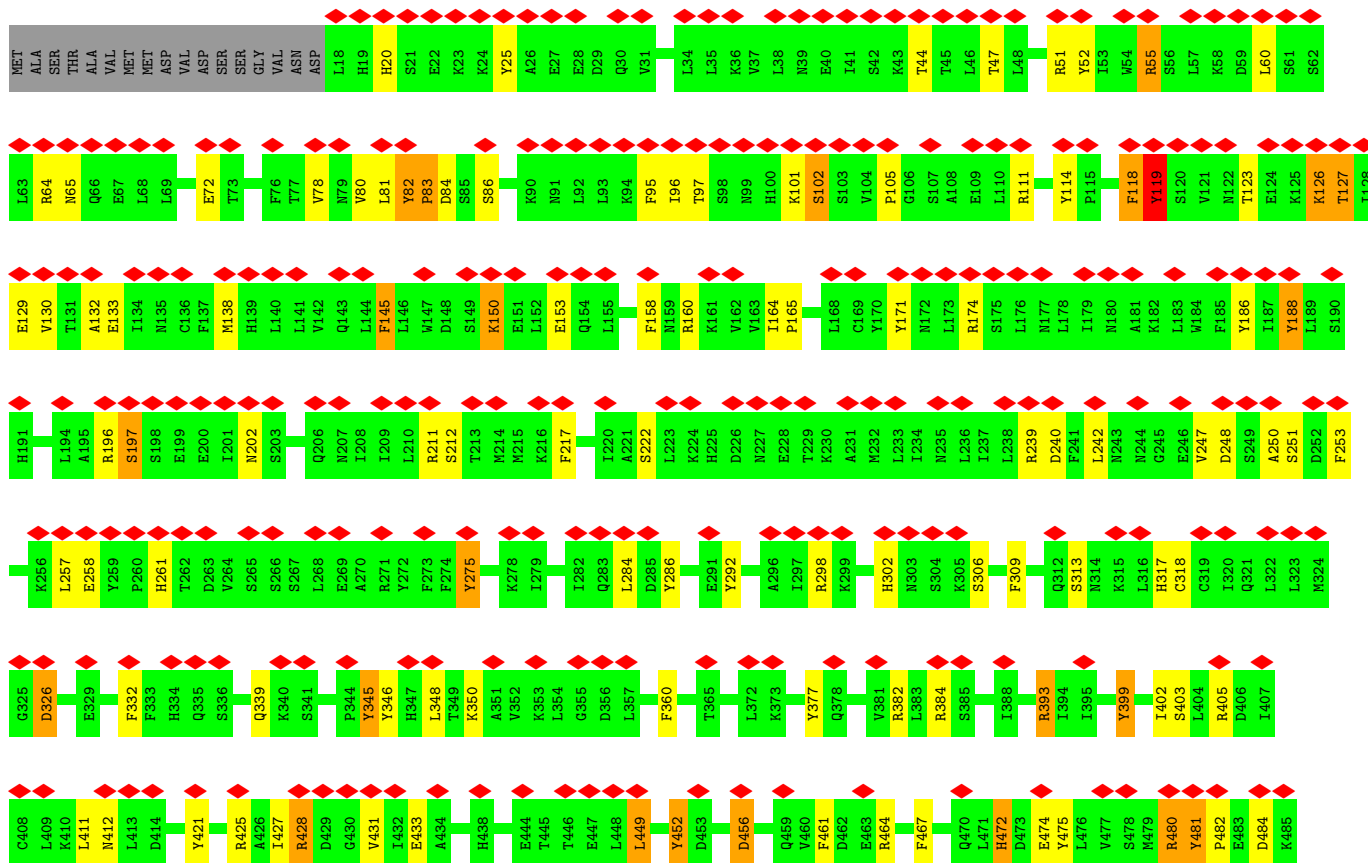


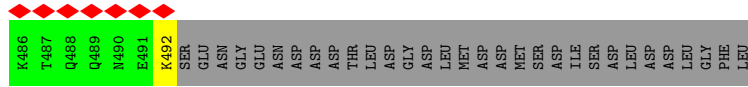
● Molecule 7: 26S proteasome regulatory subunit RPN2



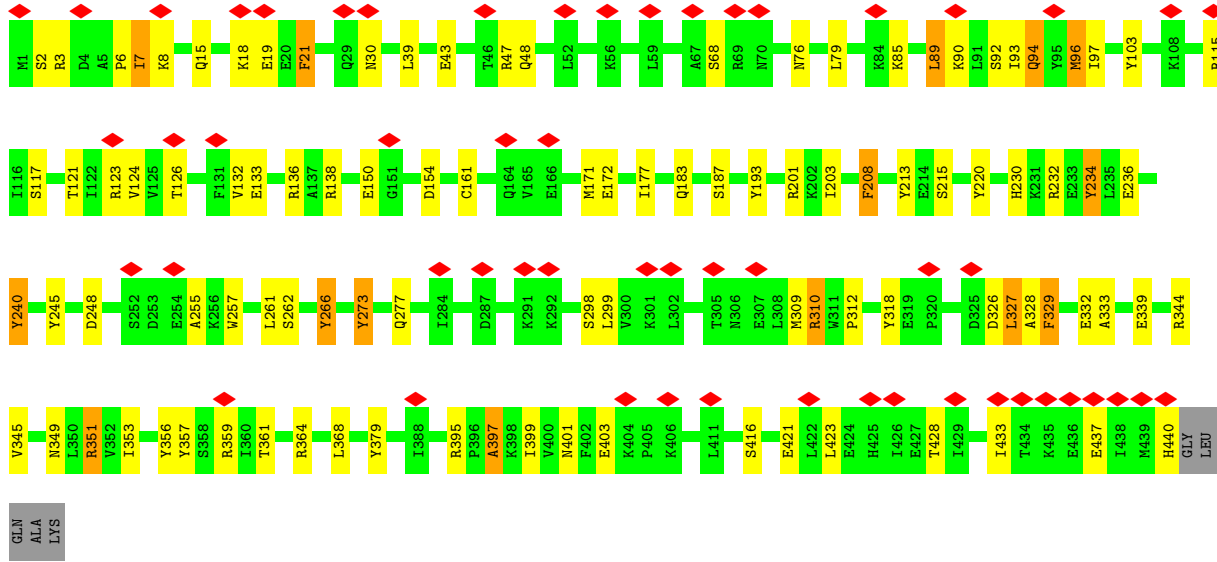
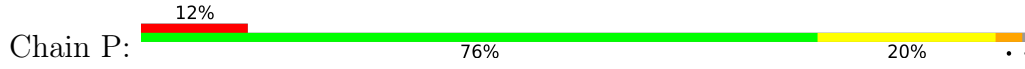


• Molecule 8: 26S proteasome regulatory subunit RPN3

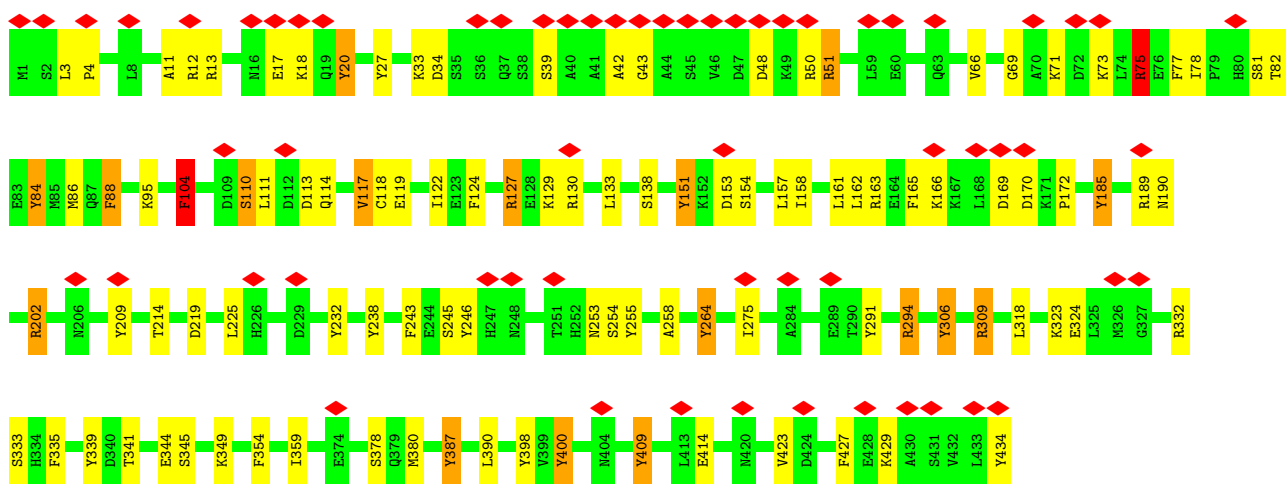
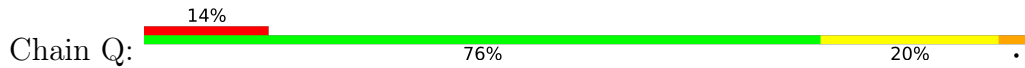




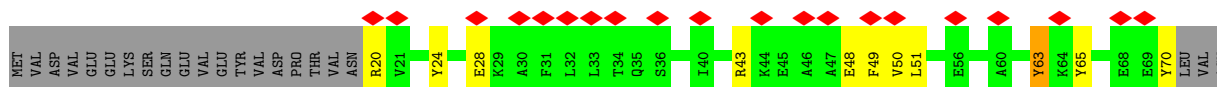
• Molecule 9: 26S proteasome regulatory subunit RPN5

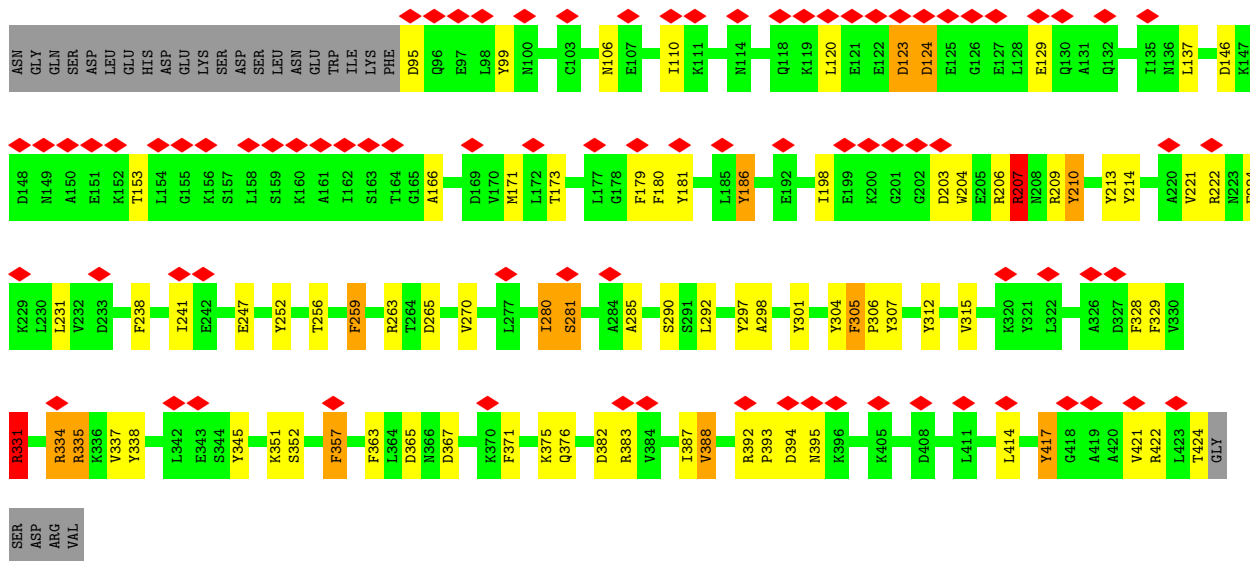


• Molecule 10: 26S proteasome regulatory subunit RPN6

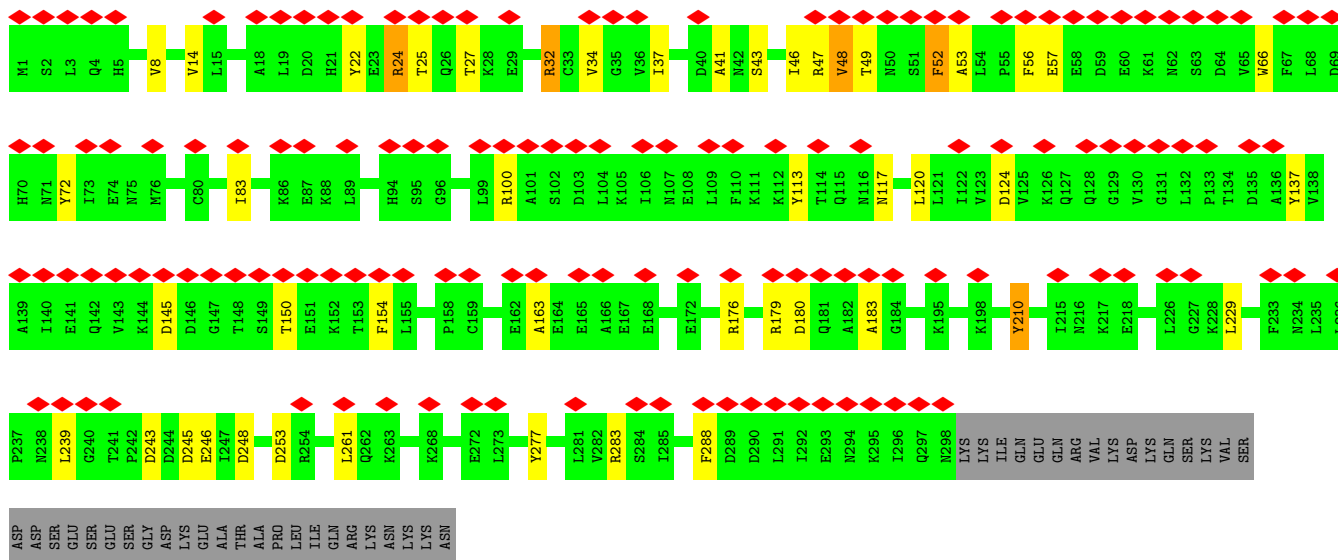
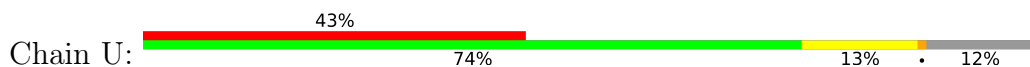


• Molecule 11: 26S proteasome regulatory subunit RPN7

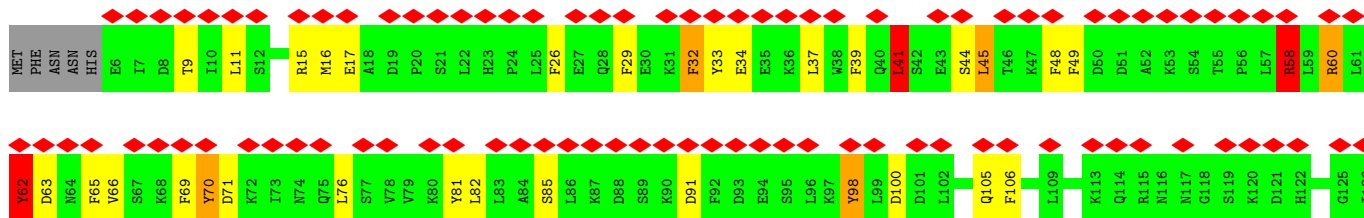
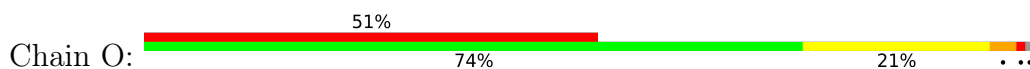


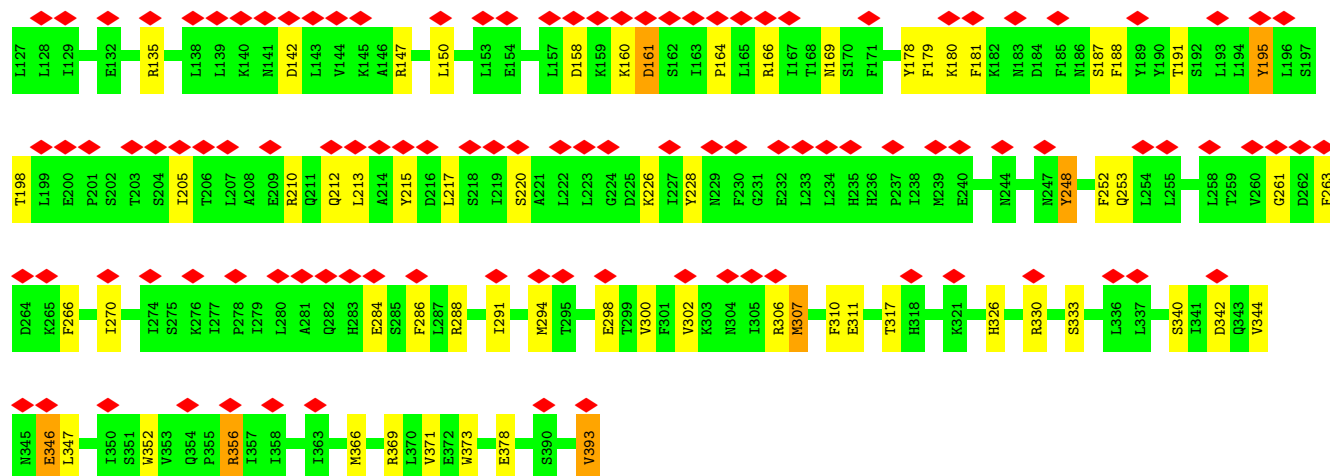


• Molecule 12: 26S proteasome regulatory subunit RPN8



• 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	286500	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 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.133	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	1.70	14/1557 (0.9%)	1.79	29/2111 (1.4%)
2	V	1.74	22/2309 (1.0%)	2.02	64/3115 (2.1%)
3	T	1.71	27/2235 (1.2%)	1.82	45/3017 (1.5%)
4	X	1.75	12/1058 (1.1%)	1.90	24/1432 (1.7%)
5	Y	1.90	7/438 (1.6%)	1.92	10/583 (1.7%)
6	Z	1.66	59/7122 (0.8%)	1.88	169/9645 (1.8%)
7	N	1.74	61/6994 (0.9%)	1.84	142/9455 (1.5%)
8	S	1.68	33/3966 (0.8%)	1.84	98/5355 (1.8%)
9	P	1.67	29/3663 (0.8%)	1.77	60/4940 (1.2%)
10	Q	1.68	28/3556 (0.8%)	1.89	77/4787 (1.6%)
11	R	1.73	31/3110 (1.0%)	1.95	83/4193 (2.0%)
12	U	1.58	11/2407 (0.5%)	1.76	41/3258 (1.3%)
13	O	1.68	36/3247 (1.1%)	1.93	86/4380 (2.0%)
All	All	1.69	370/41662 (0.9%)	1.86	928/56271 (1.6%)

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	6
2	V	0	5
3	T	0	6
4	X	0	2
5	Y	0	1
6	Z	0	12
7	N	0	23
8	S	0	14
9	P	0	8
10	Q	0	19
11	R	0	12
12	U	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	11
All	All	0	123

The worst 5 of 370 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	8	PRO	CA-CB	32.16	2.17	1.53
5	Y	89	GLN	C-OXT	-12.08	1.00	1.23
9	P	440	HIS	C-O	-12.08	1.00	1.23
3	T	272	ASN	C-O	-12.07	1.00	1.23
13	O	393	VAL	C-O	-12.07	1.00	1.23

The worst 5 of 928 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	8	PRO	N-CA-CB	-29.24	68.21	103.30
2	V	196	TYR	CB-CA-C	-25.02	60.37	110.40
2	V	157	ARG	NE-CZ-NH1	16.47	128.53	120.30
13	O	330	ARG	NE-CZ-NH1	16.47	128.53	120.30
10	Q	409	TYR	CB-CG-CD2	-16.00	111.40	121.00

There are no chirality outliers.

5 of 123 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	W	122	ARG	Sidechain
1	W	127	ARG	Sidechain
1	W	23	ARG	Sidechain
1	W	25	ARG	Sidechain
1	W	77	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1534	0	1542	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	2274	0	2272	51	0
3	T	2192	0	2157	12	0
4	X	1032	0	1017	5	0
5	Y	435	0	394	17	0
6	Z	7005	0	6932	85	0
7	N	6882	0	6959	42	0
8	S	3894	0	3937	32	0
9	P	3608	0	3694	15	0
10	Q	3499	0	3524	18	0
11	R	3060	0	3083	12	0
12	U	2373	0	2403	6	0
13	O	3186	0	3213	11	0
All	All	40974	0	41127	301	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 301 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)
8:S:127:THR:CB	8:S:127:THR:CA	1.80	1.58
6:Z:30:LYS:CG	6:Z:37:GLN:HB3	1.22	1.55
6:Z:24:THR:HB	6:Z:25:PRO:CD	1.36	1.51
2:V:118:LEU:HB2	2:V:195:HIS:CD2	1.47	1.49
2:V:118:LEU:CB	2:V:195:HIS:NE2	1.80	1.44

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%)	175 (90%)	13 (7%)	7 (4%)	3	28
2	V	287/306 (94%)	262 (91%)	15 (5%)	10 (4%)	3	28
3	T	264/274 (96%)	240 (91%)	20 (8%)	4 (2%)	10	44
4	X	125/156 (80%)	105 (84%)	19 (15%)	1 (1%)	19	58
5	Y	47/89 (53%)	39 (83%)	6 (13%)	2 (4%)	2	24
6	Z	902/993 (91%)	813 (90%)	66 (7%)	23 (2%)	5	34
7	N	886/945 (94%)	842 (95%)	31 (4%)	13 (2%)	10	44
8	S	473/523 (90%)	441 (93%)	17 (4%)	15 (3%)	4	30
9	P	438/445 (98%)	405 (92%)	22 (5%)	11 (2%)	5	34
10	Q	432/434 (100%)	392 (91%)	32 (7%)	8 (2%)	8	39
11	R	377/429 (88%)	353 (94%)	16 (4%)	8 (2%)	7	38
12	U	296/338 (88%)	282 (95%)	12 (4%)	2 (1%)	22	60
13	O	386/393 (98%)	366 (95%)	17 (4%)	3 (1%)	19	58
All	All	5108/5593 (91%)	4715 (92%)	286 (6%)	107 (2%)	10	38

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	184	ASN
2	V	197	TYR
2	V	274	GLN
4	X	116	ALA
6	Z	24	THR

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%)	165 (96%)	6 (4%)	36	61
2	V	253/268 (94%)	242 (96%)	11 (4%)	29	56
3	T	249/256 (97%)	239 (96%)	10 (4%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	116/144 (81%)	112 (97%)	4 (3%)	37	61
5	Y	50/81 (62%)	48 (96%)	2 (4%)	31	57
6	Z	773/850 (91%)	745 (96%)	28 (4%)	35	60
7	N	745/797 (94%)	724 (97%)	21 (3%)	43	65
8	S	447/489 (91%)	436 (98%)	11 (2%)	47	68
9	P	412/415 (99%)	402 (98%)	10 (2%)	49	69
10	Q	391/391 (100%)	382 (98%)	9 (2%)	50	70
11	R	333/379 (88%)	325 (98%)	8 (2%)	49	69
12	U	271/308 (88%)	269 (99%)	2 (1%)	84	90
13	O	363/368 (99%)	349 (96%)	14 (4%)	32	58
All	All	4574/4976 (92%)	4438 (97%)	136 (3%)	44	64

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	R	146	ASP
11	R	352	SER
13	O	105	GLN
6	Z	548	ASP
6	Z	445	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
8	S	317	HIS
9	P	431	HIS
8	S	334	HIS
9	P	296	GLN
10	Q	247	HIS

5.3.3 RNA

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](#)

There are no chain breaks in this entry.

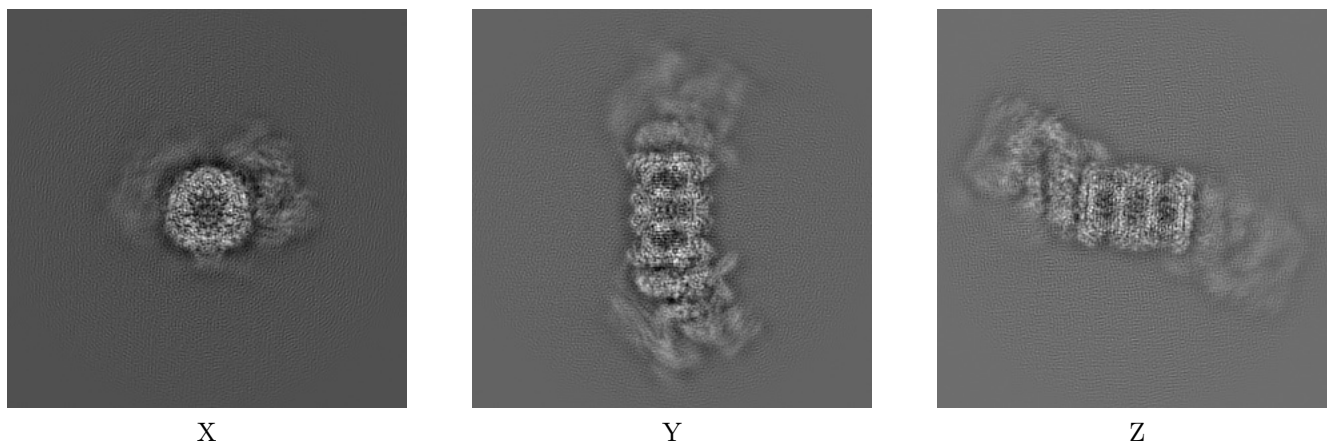
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3534. 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](#)

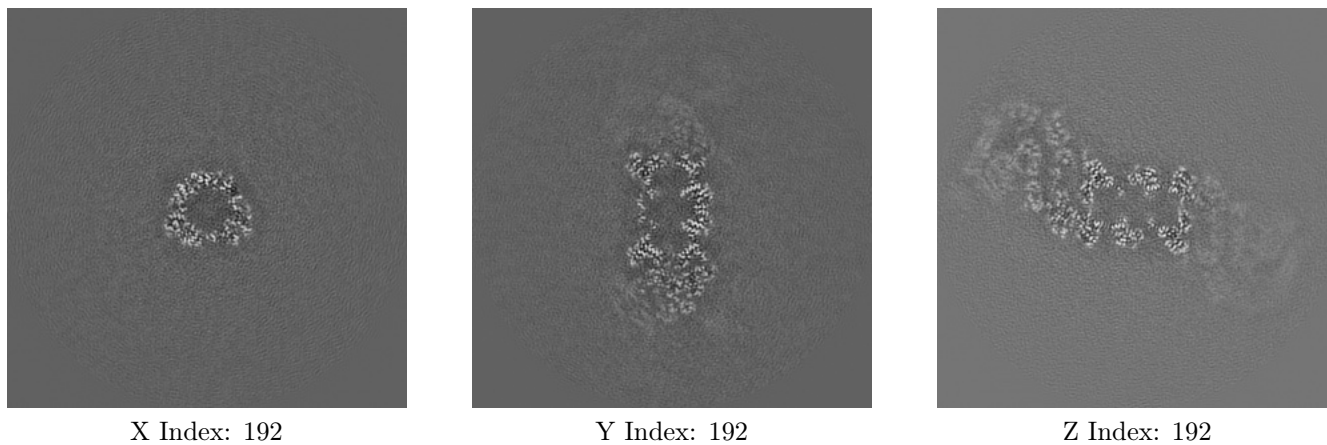
6.1.1 Primary map



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

6.2 Central slices [i](#)

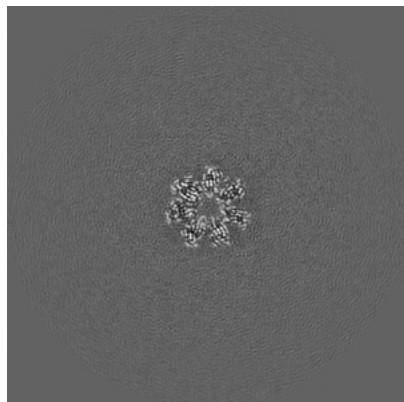
6.2.1 Primary map



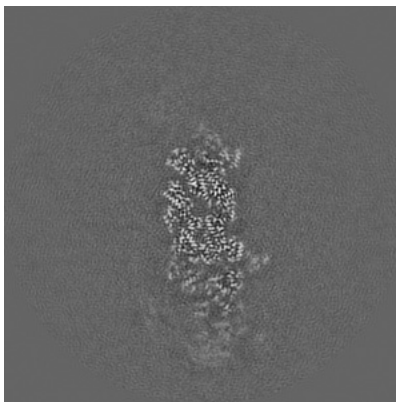
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

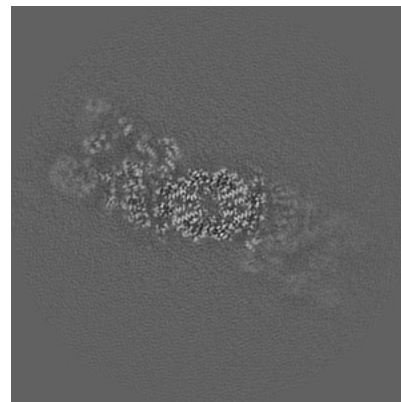
6.3.1 Primary map



X Index: 177



Y Index: 212



Z Index: 208

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

6.4 Orthogonal surface views [i](#)

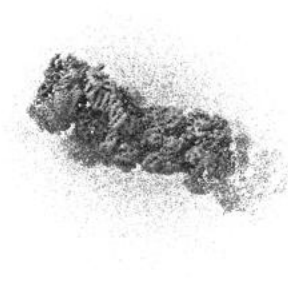
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

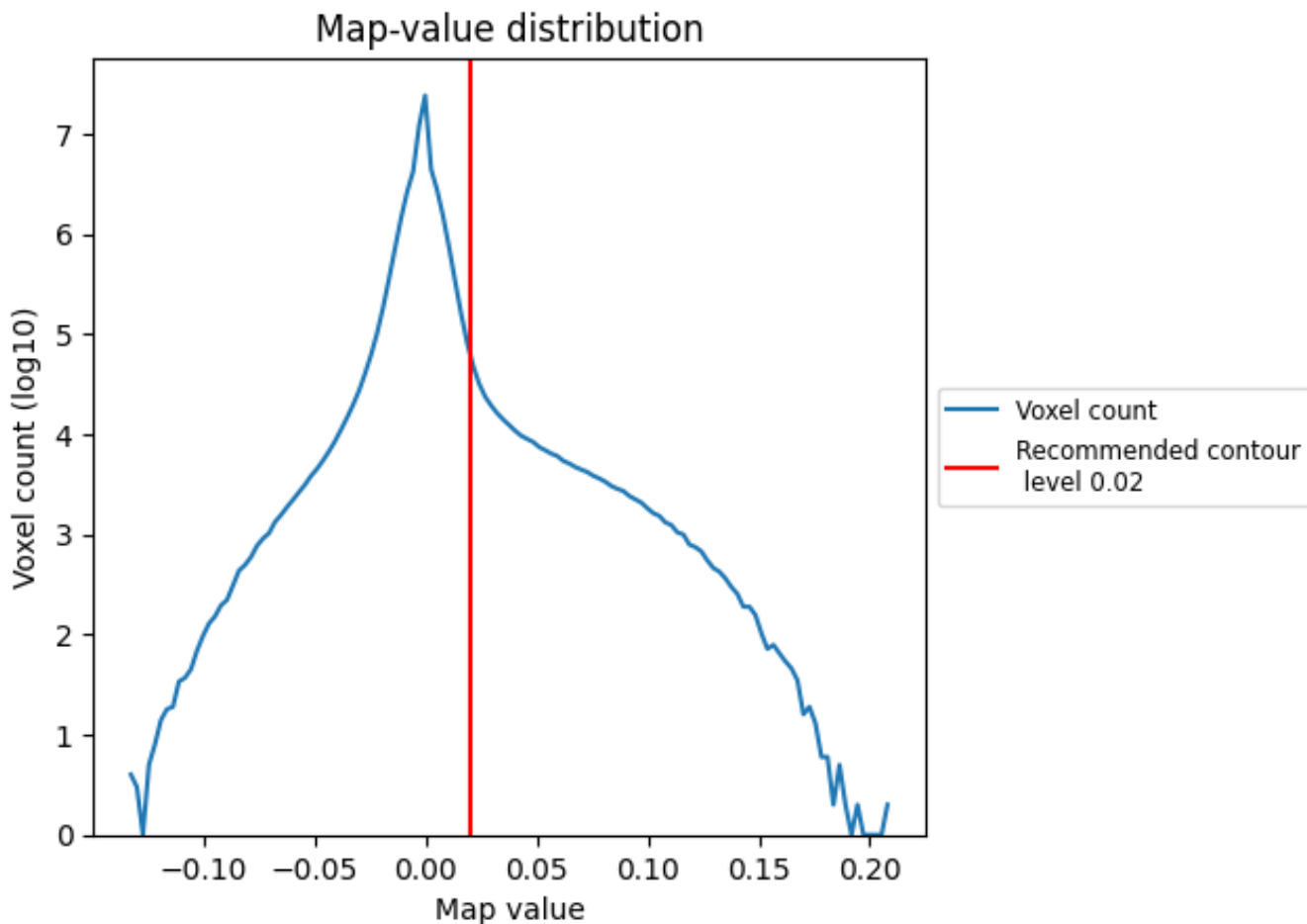
6.5 Mask visualisation

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

7 Map analysis [i](#)

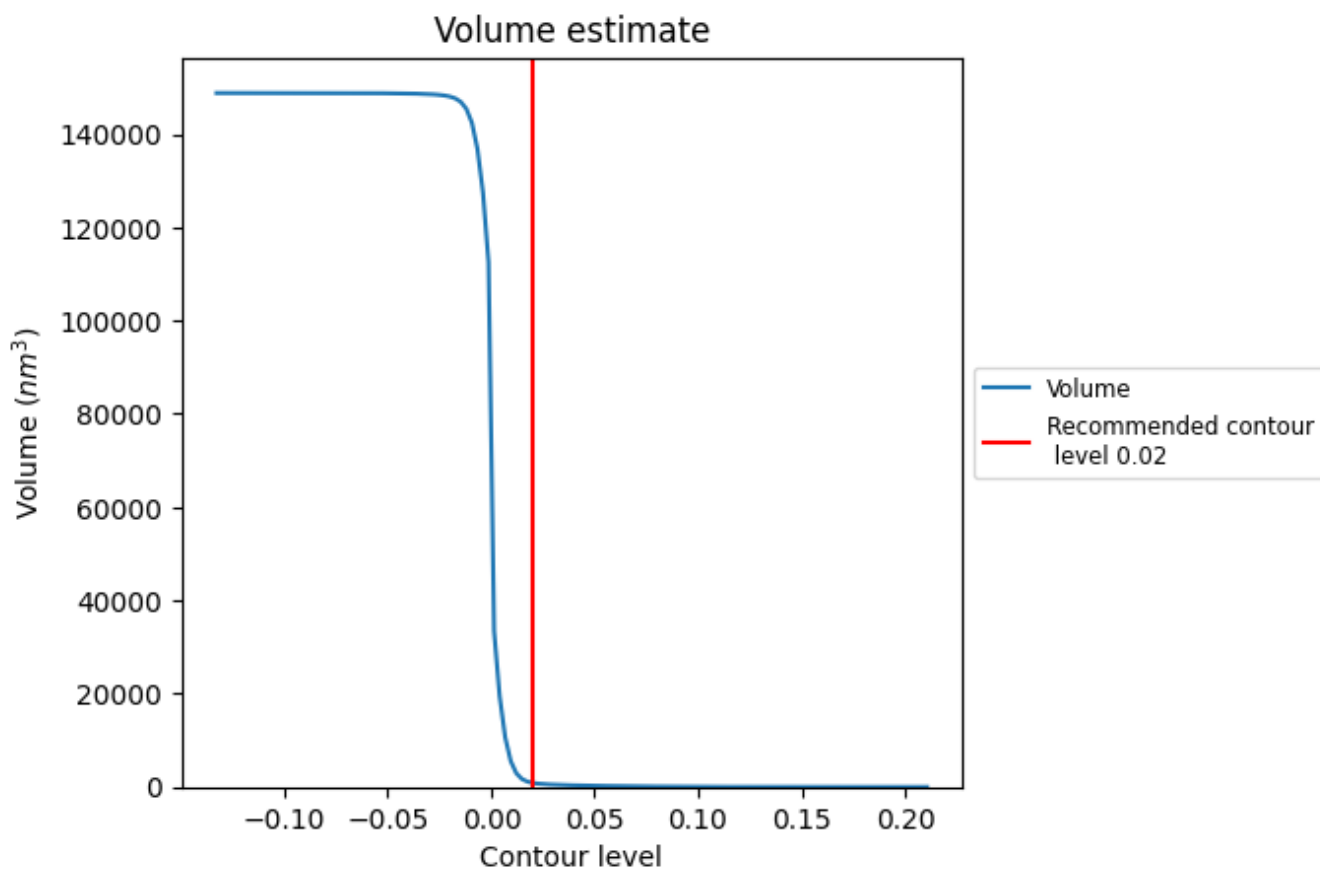
This section contains the results of statistical analysis of the map.

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.

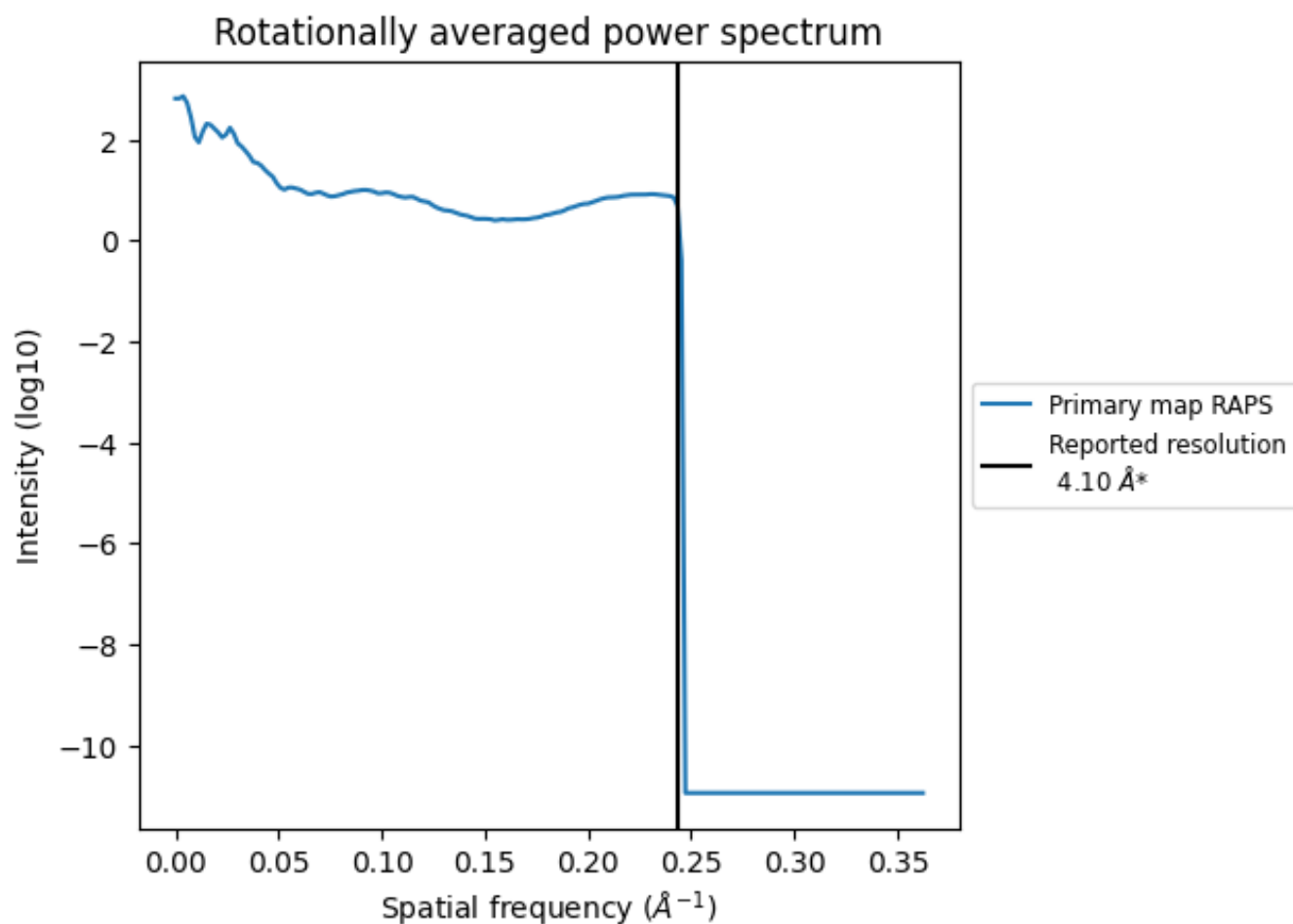
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 881 nm³; this corresponds to an approximate mass of 796 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 0.244 Å⁻¹

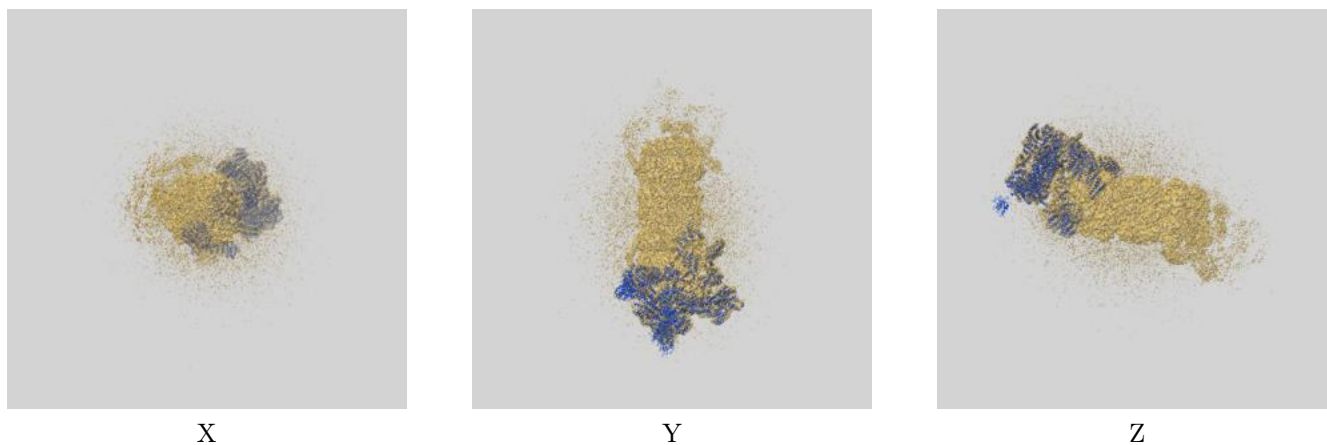
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

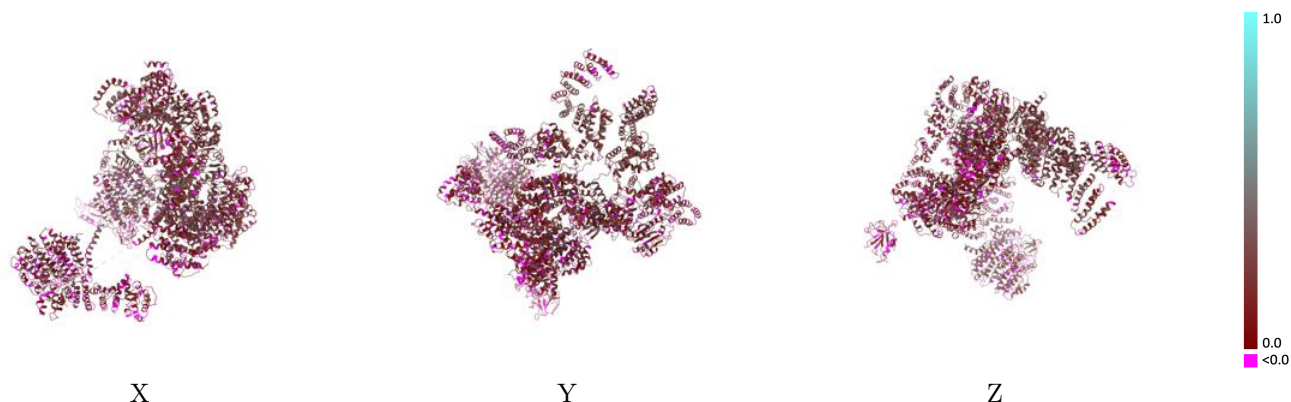
This section contains information regarding the fit between EMDB map EMD-3534 and PDB model 5MPD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



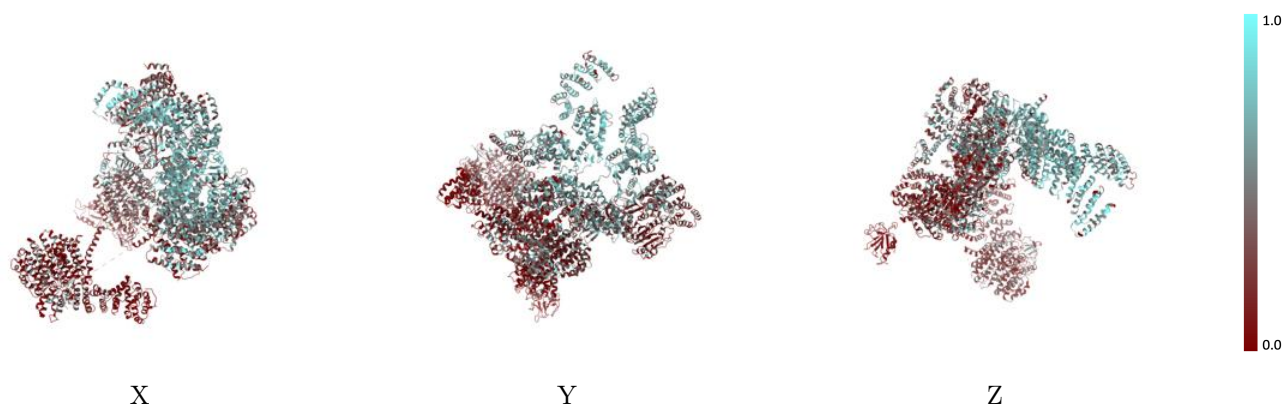
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



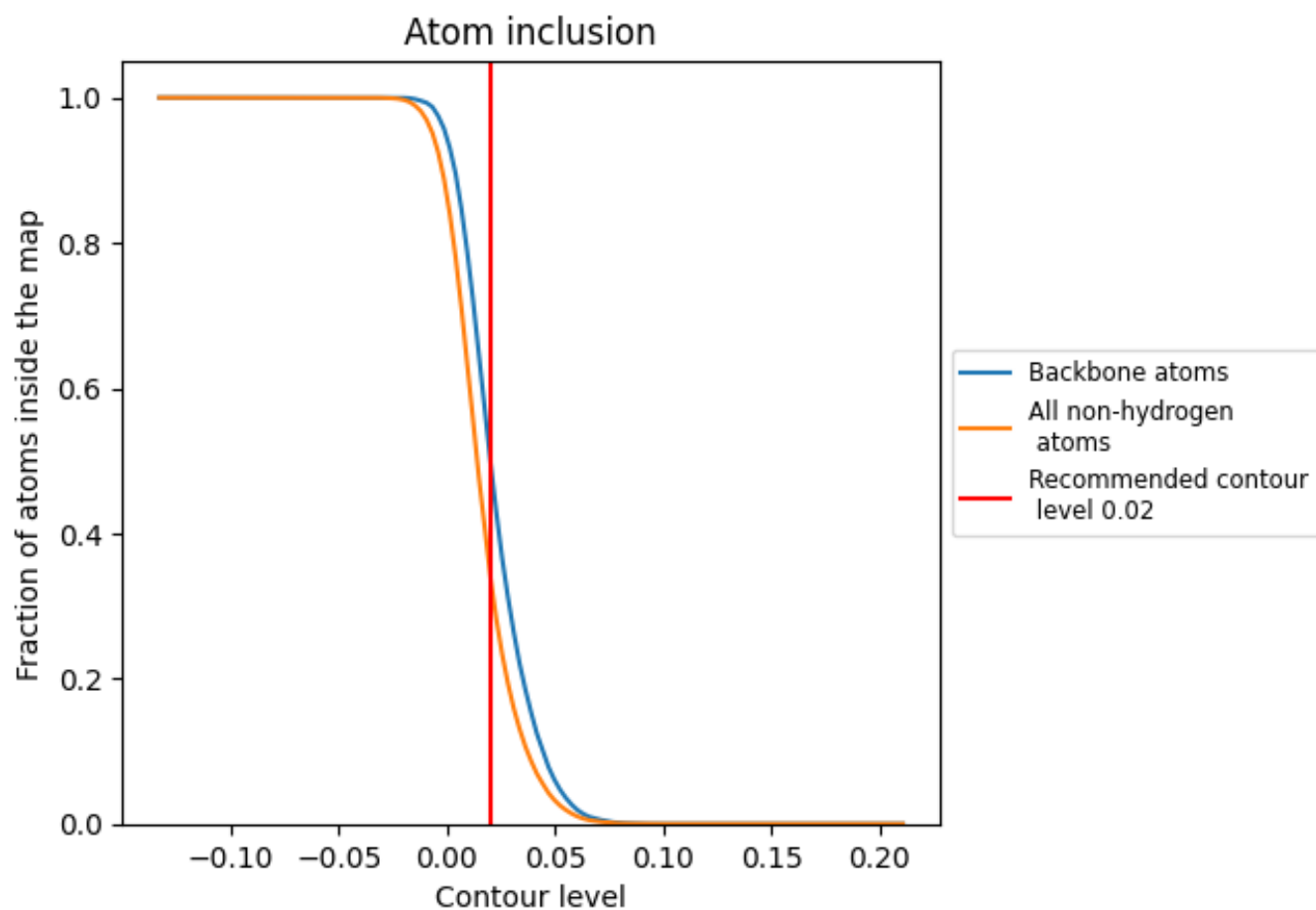
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 34% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3444	 0.1690
N	 0.2124	 0.1430
O	 0.3944	 0.1720
P	 0.6352	 0.2450
Q	 0.6213	 0.2300
R	 0.5315	 0.2040
S	 0.3548	 0.1570
T	 0.2901	 0.1490
U	 0.4071	 0.1900
V	 0.4418	 0.2060
W	 0.1739	 0.1320
X	 0.0049	 0.0660
Y	 0.3163	 0.1370
Z	 0.1294	 0.1250

