wwPDB EM Validation Summary Report (i)

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 (i) 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 (i)) were used in the production of this report:

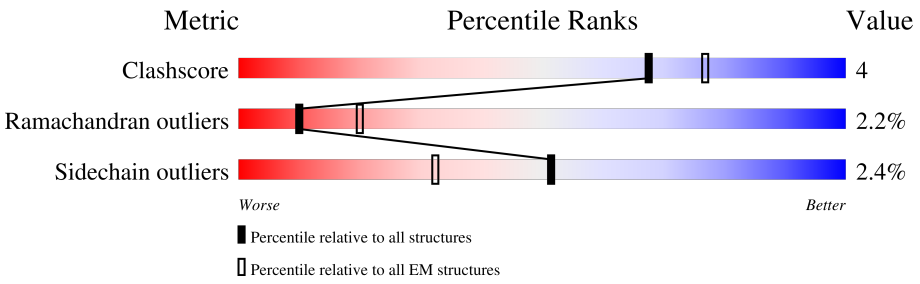
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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 <=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	39%; 57%; 16%; 26%
2	V	306	30%; 72%; 20%; • 6%
3	T	274	73%; 76%; 17%; • •
4	X	156	81%; 60%; 17%; • •; 19%
5	Y	89	39%; 36%; 18%; •; 43%
6	Z	993	85%; 72%; 16%; •; 9%
7	N	945	44%; 78%; 14%; • 6%
8	S	523	54%; 70%; 17%; •; 9%

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

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.

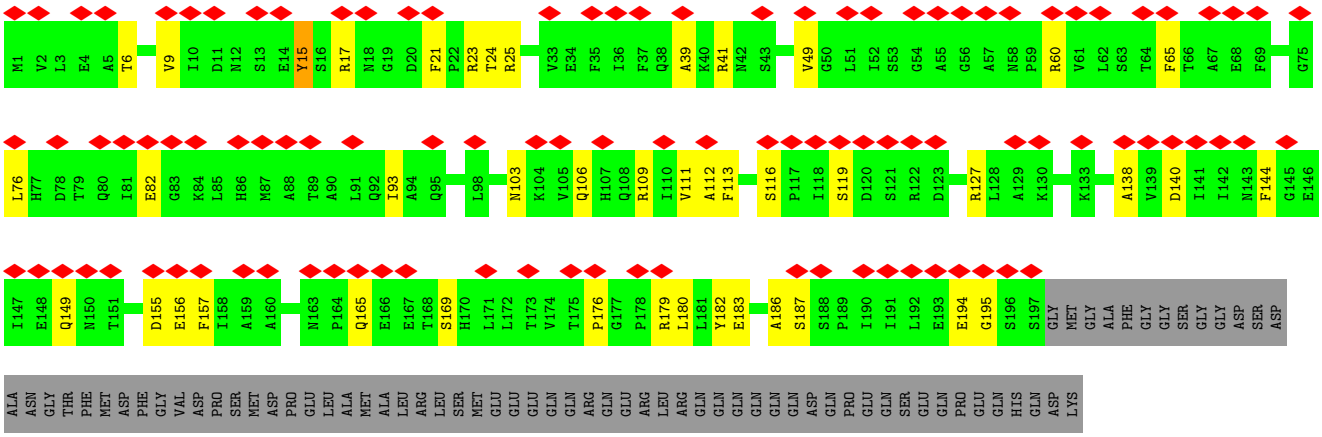
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	388	3186	2051	519	608	8	0	0

3 Residue-property plots (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.

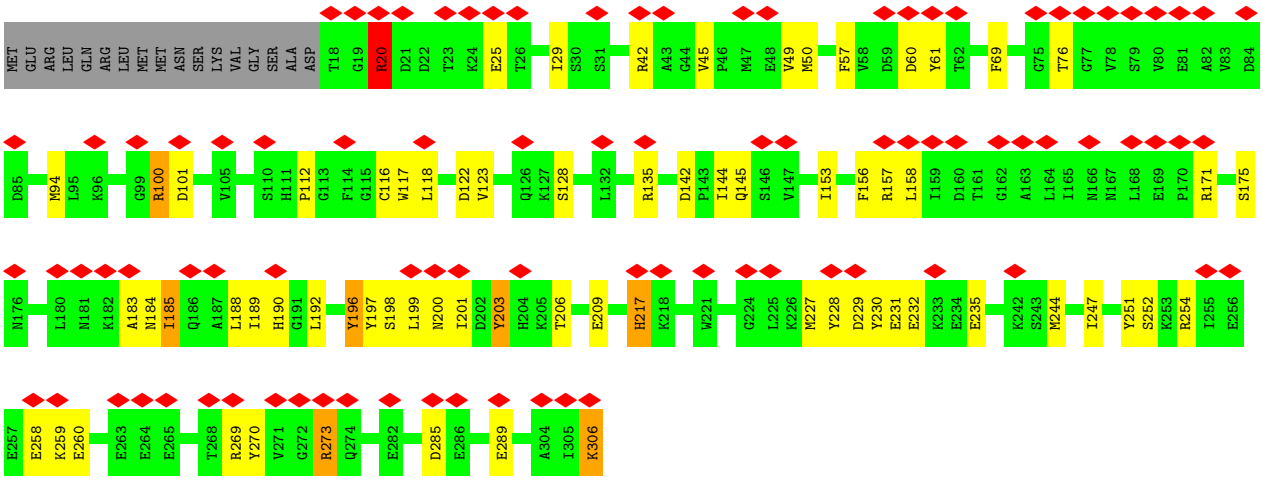
- Molecule 1: 26S proteasome regulatory subunit RPN10

Chain W:



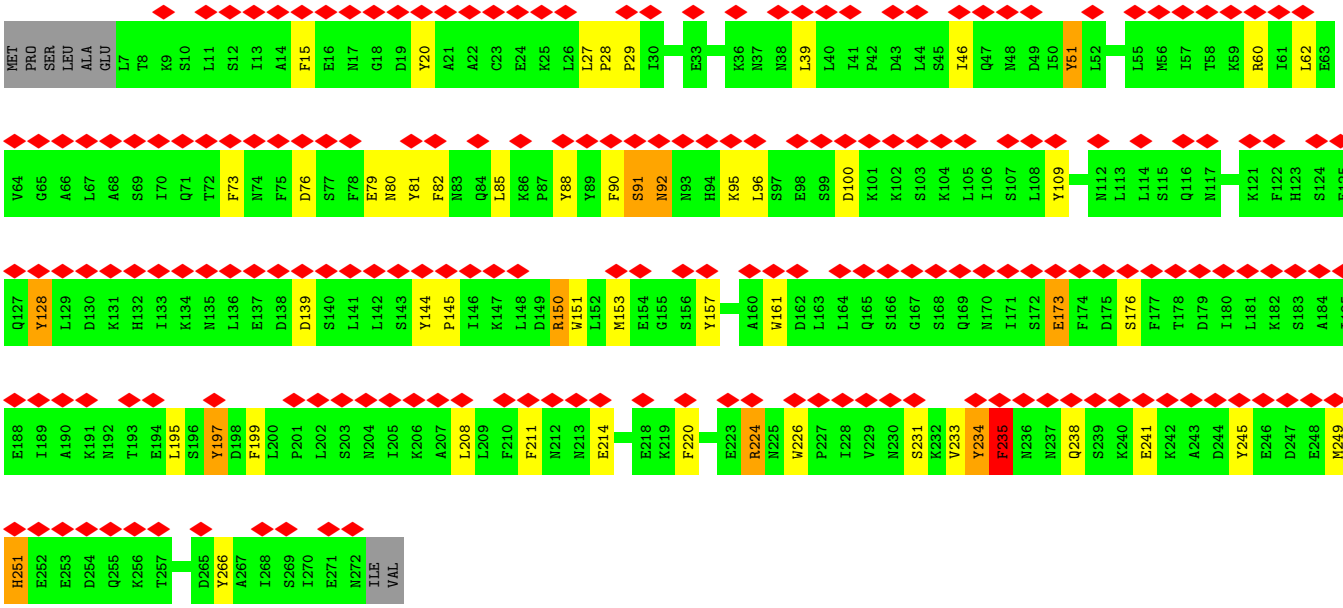
- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



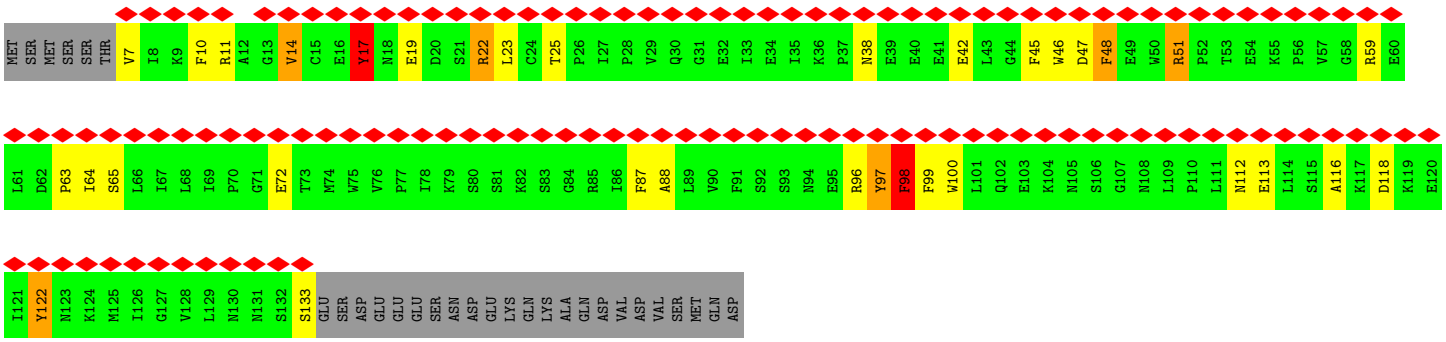
- Molecule 3: 26S proteasome regulatory subunit RPN12

Chain T:



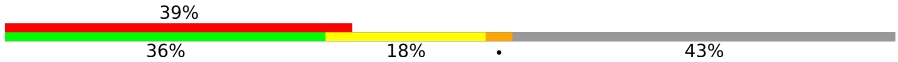
- Molecule 4: 26S proteasome regulatory subunit RPN13

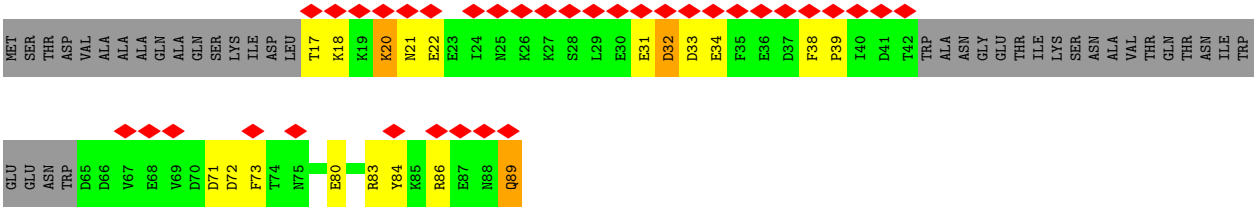
Chain X:



- Molecule 5: 26S proteasome complex subunit SEM1

Chain Y:





- Molecule 6: 26S proteasome regulatory subunit RPN1

Chain Z:

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 L38 S39 E40 E41 D42 A43 K44 L45 K46 T47 D48 L49 E50 L51 L52 V53 E54 R55 L56 K57 E58 D59 D60

S61 S62 L63 Y64 E65 A66 S67 L68 M69 A70 L71 K72 E73 S74 I75 K76 N77 S78 T79 S80 S81 M82 T83 A84 V85 P86 K87 P88 L89 K90 F91 L92 R93 P94 T95 Y96 P97 D98 L99 C100 S101 I102 Y103 D104 K105 W106 T107 D108 P109 N110 L111 K112 S113 S114 L115 A116 D117 V118 L119 S120

I121 L122 A123 M124 T125 Y126 S127 E128 N129 G130 K131 H132 D133 S134 L135 R136 Y137 R138 L139 L140 S141 D142 V143 S144 D145 F146 E147 G148 W149 G150 H151 E152 Y153 I154 R155 H156 L157 A158 L159 E160 I161 G162 E163 V164 Y165 N166 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 R202 L203 C204 L205 D206 I207 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 F264 L265 K266 T267 A268 Y269 S270 I271 Y272 L273 N276 E277 L278 T279 D280 A281 I282 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 E322 Y323 E324 G325 V326 Q327 D328 I329 I330 G331 N332 G333 K334 L335 S336 E337 H338 F339 L340 Y341 L342 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 S371 A372 G373 L374 D375 S376 A377 Q378 Q379 N380 L381 A382 S383 S384 F385 V386 N387 G388 F389 L390 N391 L392 G393 Y394 C395 N396 D397 K398 L399 I400 V401 D402 N403 D404 N405 W406 V407 Y408 K409 T410 K411 G412 D413 G414 M415 T416 S417 A418 V419 A420 S421

I422 G423 S424 I425 Y426 Q427 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 D476 Y477 V478 T479 N480 P481

D482 T483 K484 I485 S486 S487 A488 A489 I490 L491 G492 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 D503 E504 V505 L506 G507 L508 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 P519 I520 E521 T522 A523 A524 M525 A526 S527 L528 A529 L530 A531 H532 V533 F534 V535 G536 T537 C538 N539 G540 D541

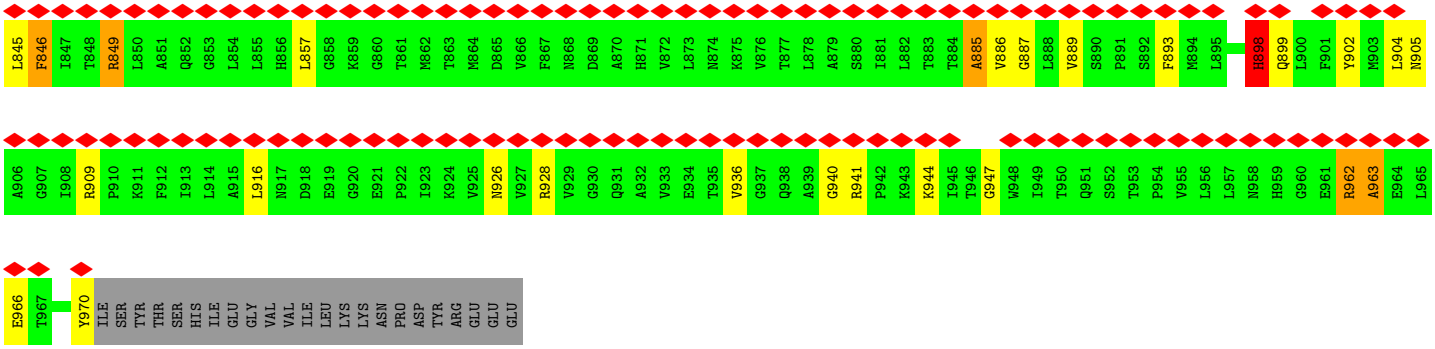
I542 T543 T544 S545 I546 M547 D548 N549 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 T560 D561 W562 V563 R564 F565 L566 A567 L568 A569 L570 G571 I572 L573 Y574 M575 G576 Q577 G578 E579 Q580 V581 D582 D583 V584 L585 E586 T587 A590 I591 E592 H593 P594 M595 T596 S597 A598 I599 E600 V601 L602

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 V629 K630 G631 E632 E633 D634 A635 ASP GLU GLU GLU THR ALA GLU GLY GLN THR ASN SER ILE SER ASP PHE LEU GLY GLU GLN VAL ASN GLU PRO THR LYS ASN

GLU GLU ALA GLU ILE GLU VAL ASP GLU MET GLU VAL ASP ALA GLU GLY GLU GLU VAL GLU VAL LYS ALA GLU ILE THR GLU LYS LYS ASN GLY GLU SER LEU GLU GLY GLU E700 I701 K702 S703 E704 E705 K706 K707 G708 K709 S710 S711 D712 K713 D714 A715 T716 T717 D718 G719 K720 N721 D722

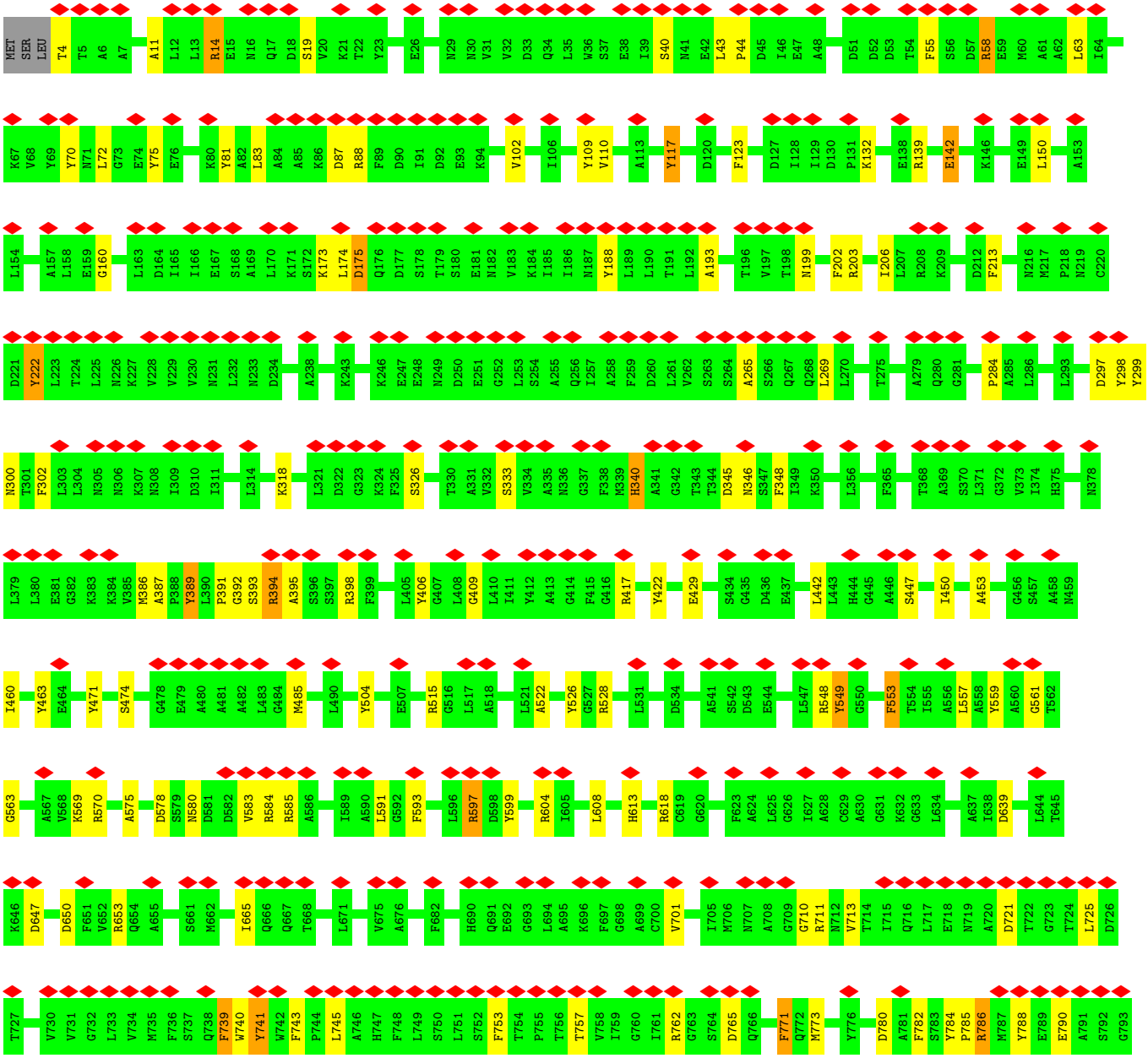
D723 E724 E725 E726 E727 K728 E729 A730 G731 I732 E735 Y738 A739 V740 L741 G742 I743 A744 L745 I746 A747 L748 G749 E750 D751 I752 G753 K754 E755 M756 S757 L758 R759 H760 F761 G762 H763 L764 M765 H766 Y767 G768 N769 E770 H771 I772 R773 R774 M775 V776 P777 L778 A779 M780 G781 I782 V783 S784

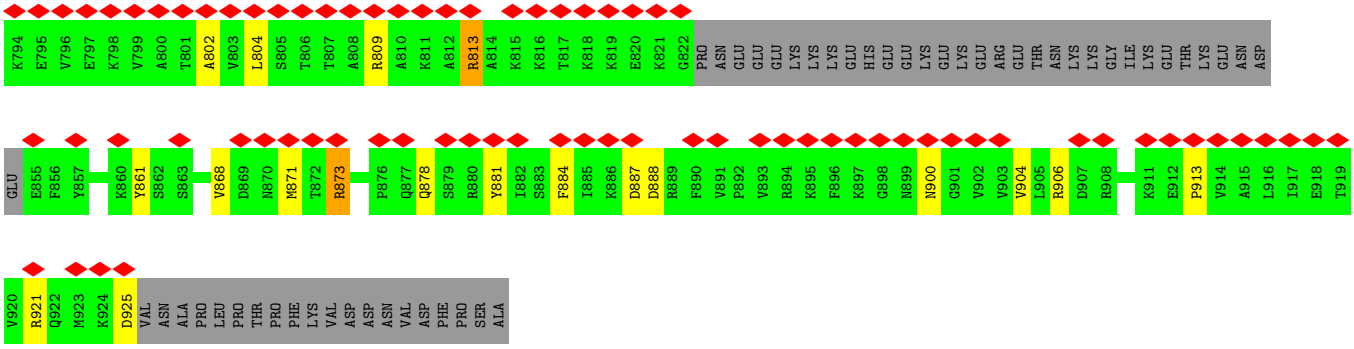
V785 S786 D787 P788 Q789 M790 K791 V792 F793 D794 T795 L796 T797 R798 F799 S800 H801 D802 A803 D804 L805 E806 V807 S808 M809 N810 S811 I812 F813 A814 M815 G816 L817 C818 G819 A820 G821 T822 N823 N824 A825 R826 L827 A828 Q829 L830 L831 R832 Q833 L834 A835 S836 Y837 Y838 S839 R840 E841 Q842 D843 A844



- Molecule 7: 26S proteasome regulatory subunit RPN2

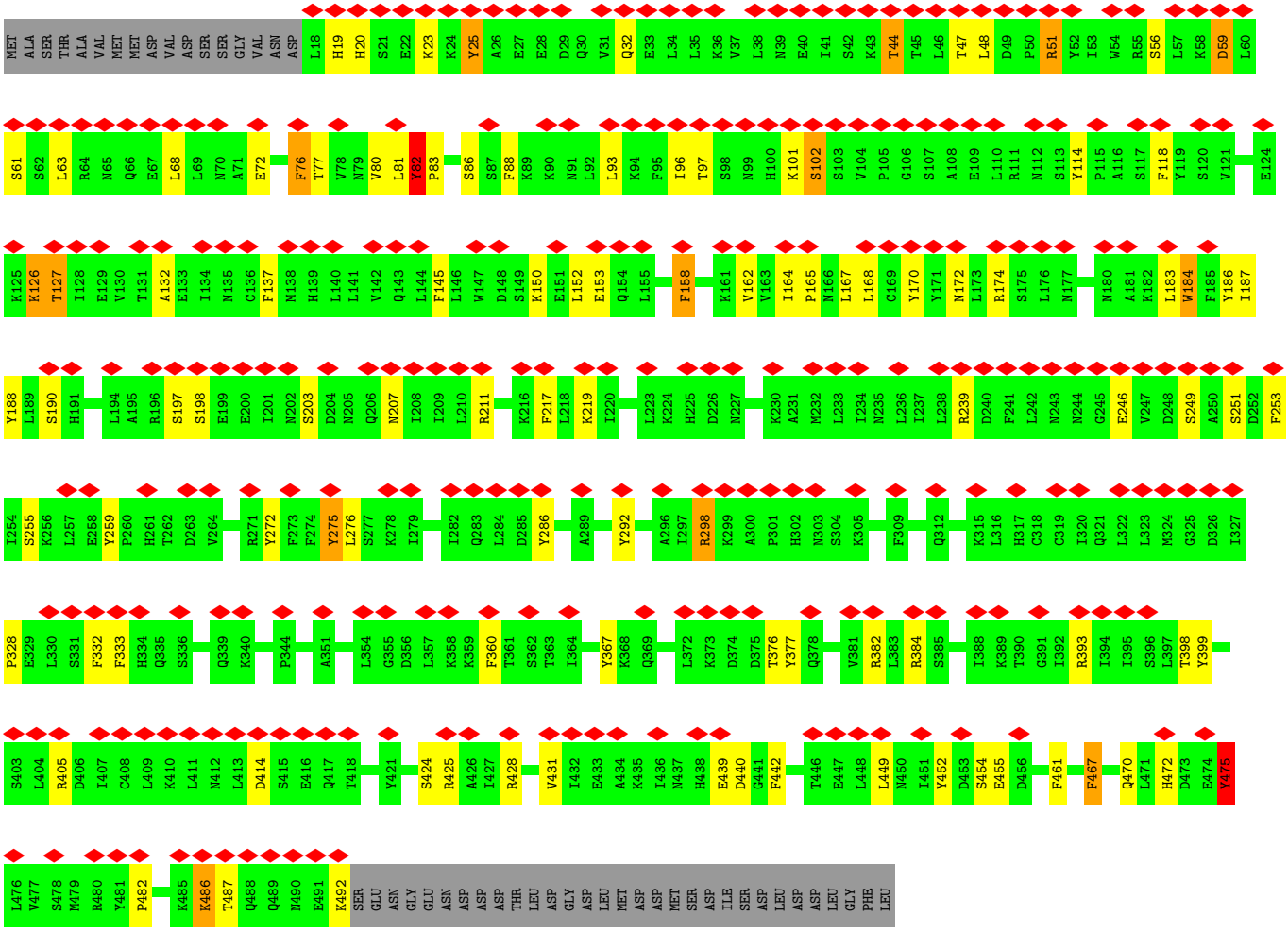
Chain N:





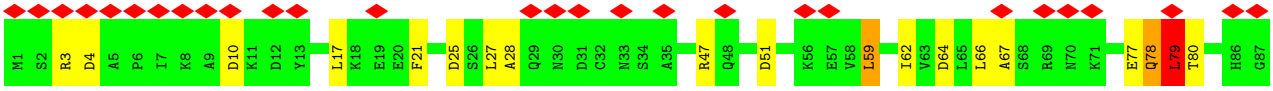
- Molecule 8: 26S proteasome regulatory subunit RPN3

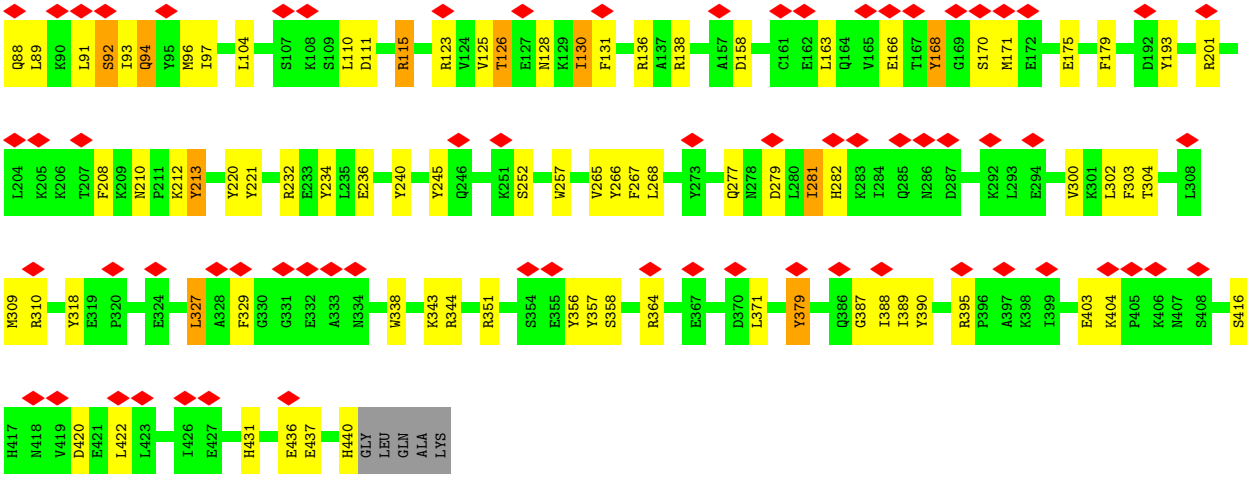
Chain S:



- Molecule 9: 26S proteasome regulatory subunit RPN5

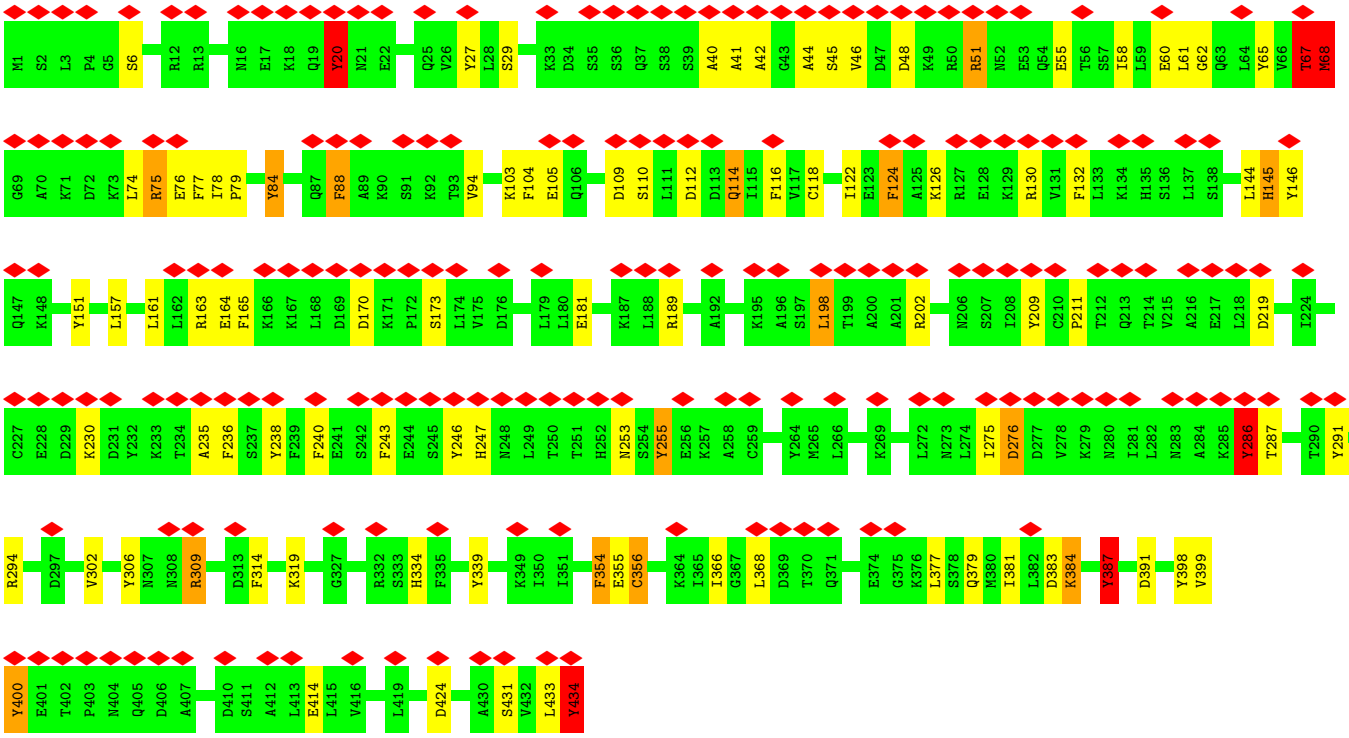
Chain P:





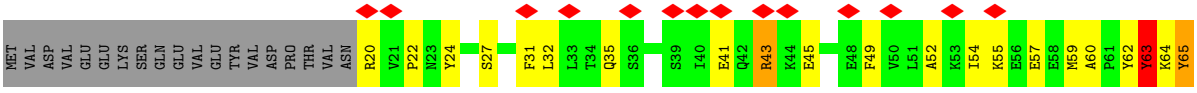
- Molecule 10: 26S proteasome regulatory subunit RPN6

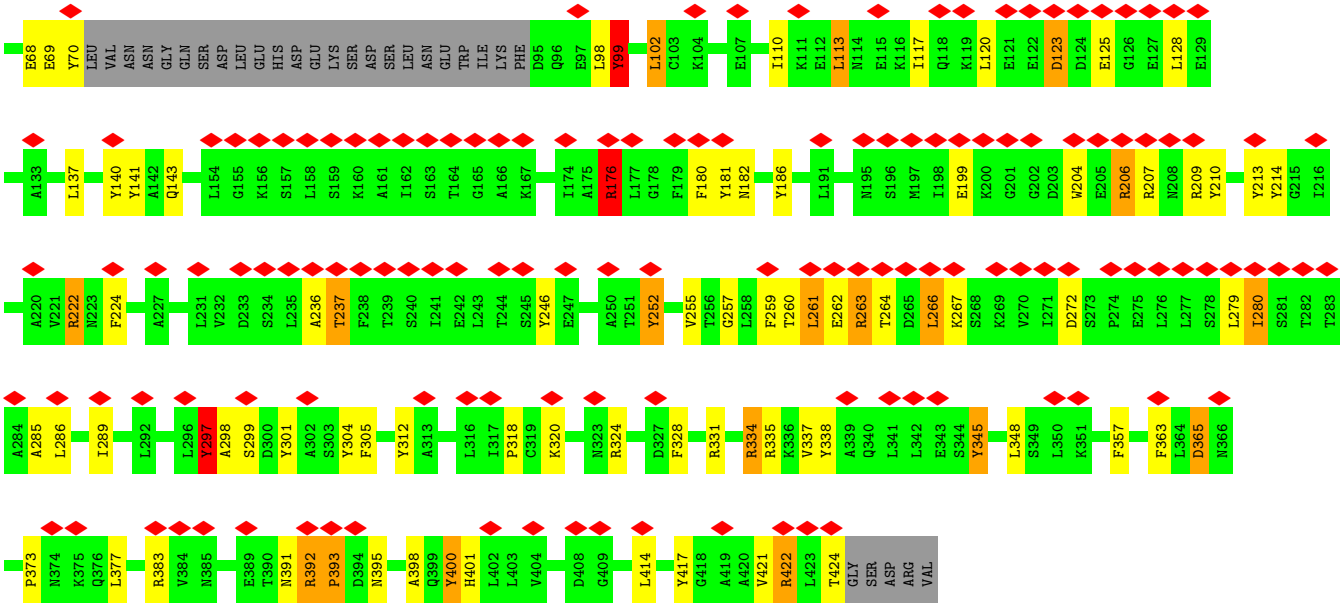
Chain Q:



- Molecule 11: 26S proteasome regulatory subunit RPN7

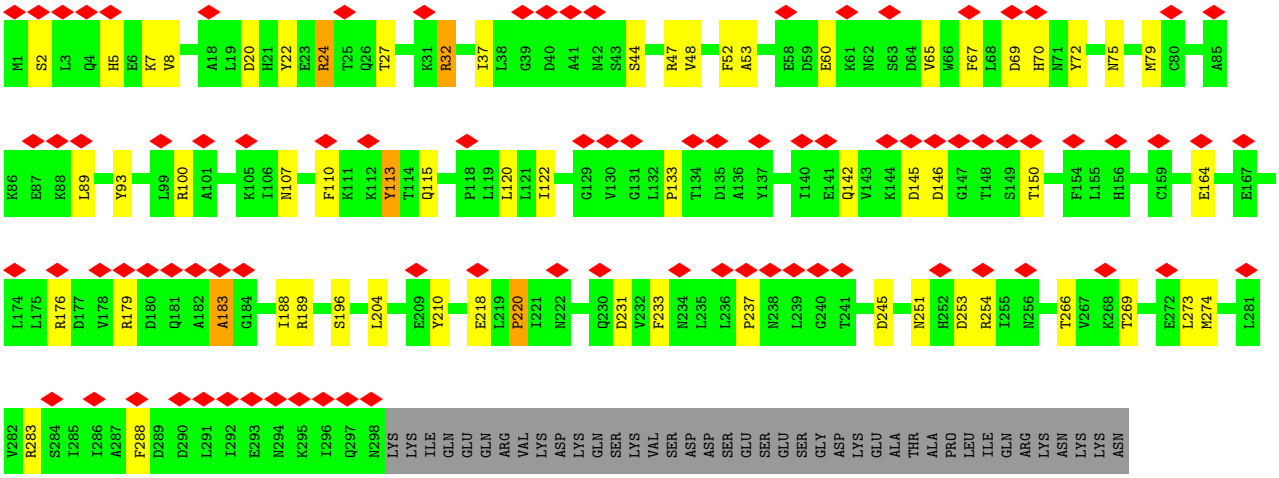
Chain R:





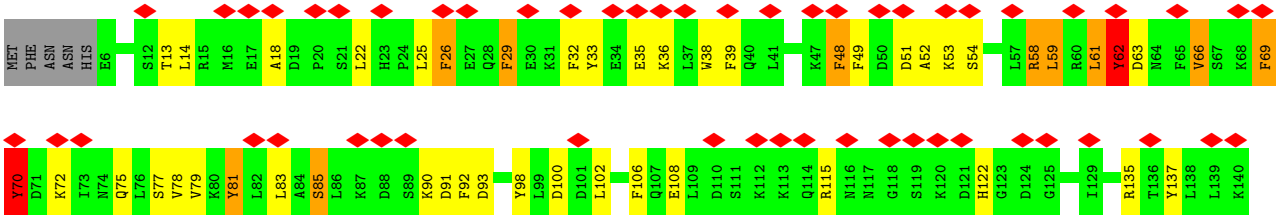
- Molecule 12: 26S proteasome regulatory subunit RPN8

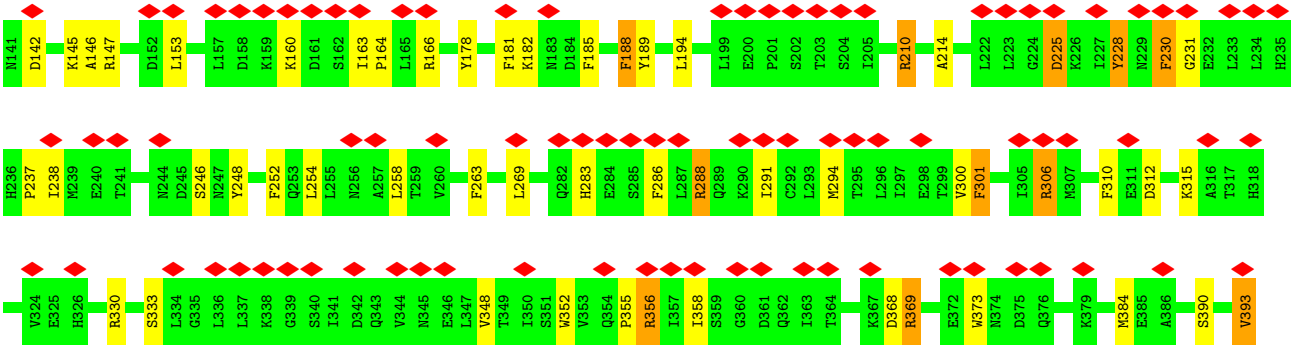
Chain U:



- Molecule 13: 26S proteasome regulatory subunit RPN9

Chain O:

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H236 P237 I238 M239 E240 T241 N244 D245 S246 N247 Y248 F252 Q253 L254 L255 N256 A257 L258 T259 V260 F263 L269 Q282 H283 E284 S285 F286 L287 R288 Q289 K290 I291 C292 L293 M294 T295 L296 I297 E298 T299 V300 F301 I305 R306 M307 F310 E311 D312 K315 A316 T317 H318
V324 E325 H326 R330 S333 L334 G335 L336 L337 K338 G339 S340 I341 D342 Q343 V344 N345 E346 L347 V348 T349 I350 S351 W352 V353 Q354 P355 R356 I357 I358 S359 G360 D361 Q362 I363 T364 K367 D368 R369 E372 W373 N374 D375 Q376 K379 M384 E385 A386 S390 V393

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (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	1.69	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(^{o})	Ideal(^{o})
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

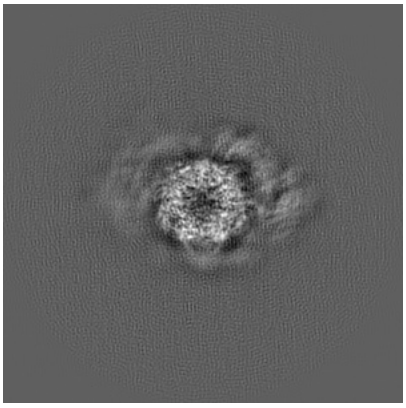
6 Map visualisation (i)

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.

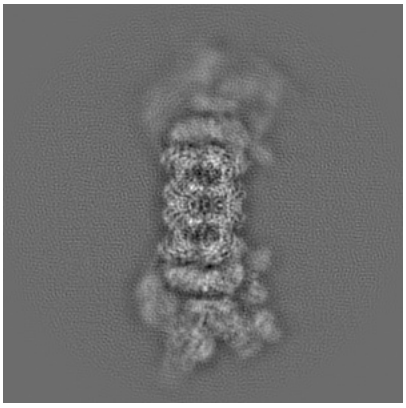
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

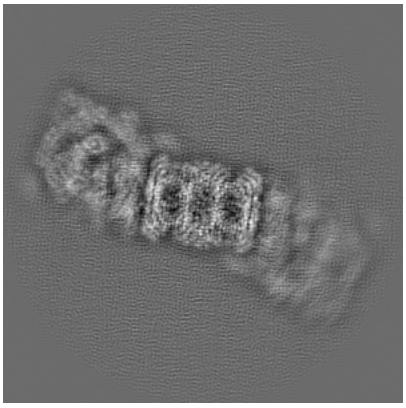
6.1.1 Primary map



X



Y

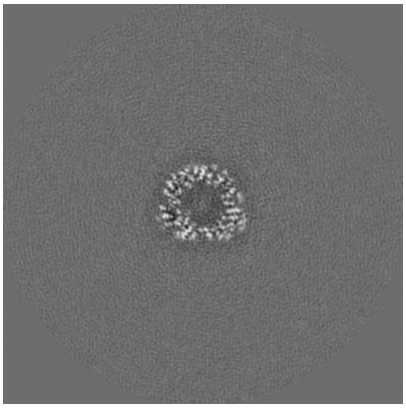


Z

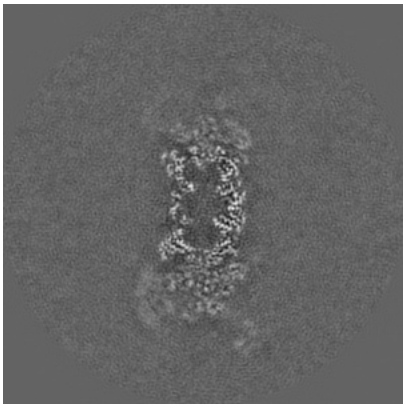
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

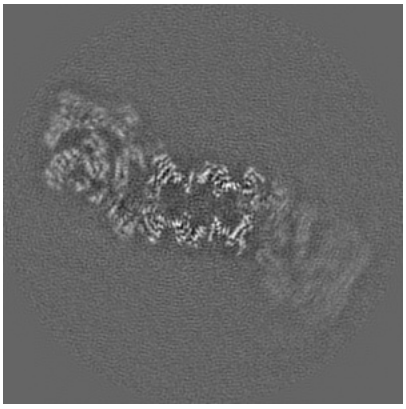
6.2.1 Primary map



X Index: 192



Y Index: 192

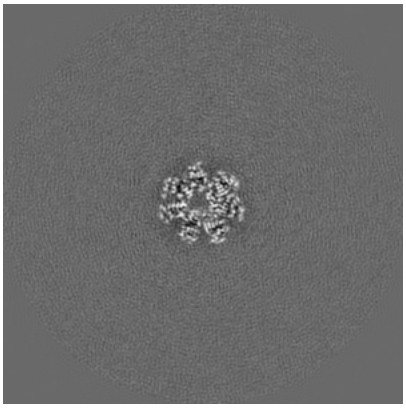


Z Index: 192

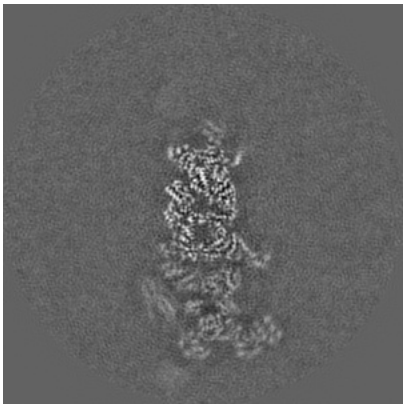
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

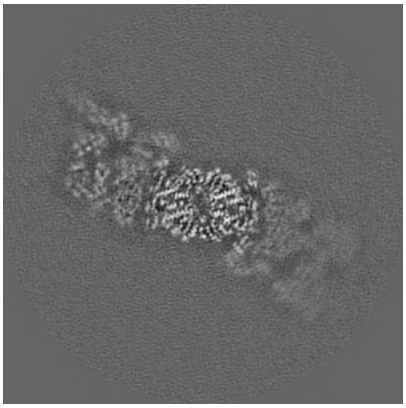
6.3.1 Primary map



X Index: 206



Y Index: 210



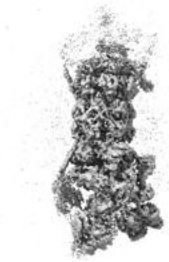
Z Index: 210

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.

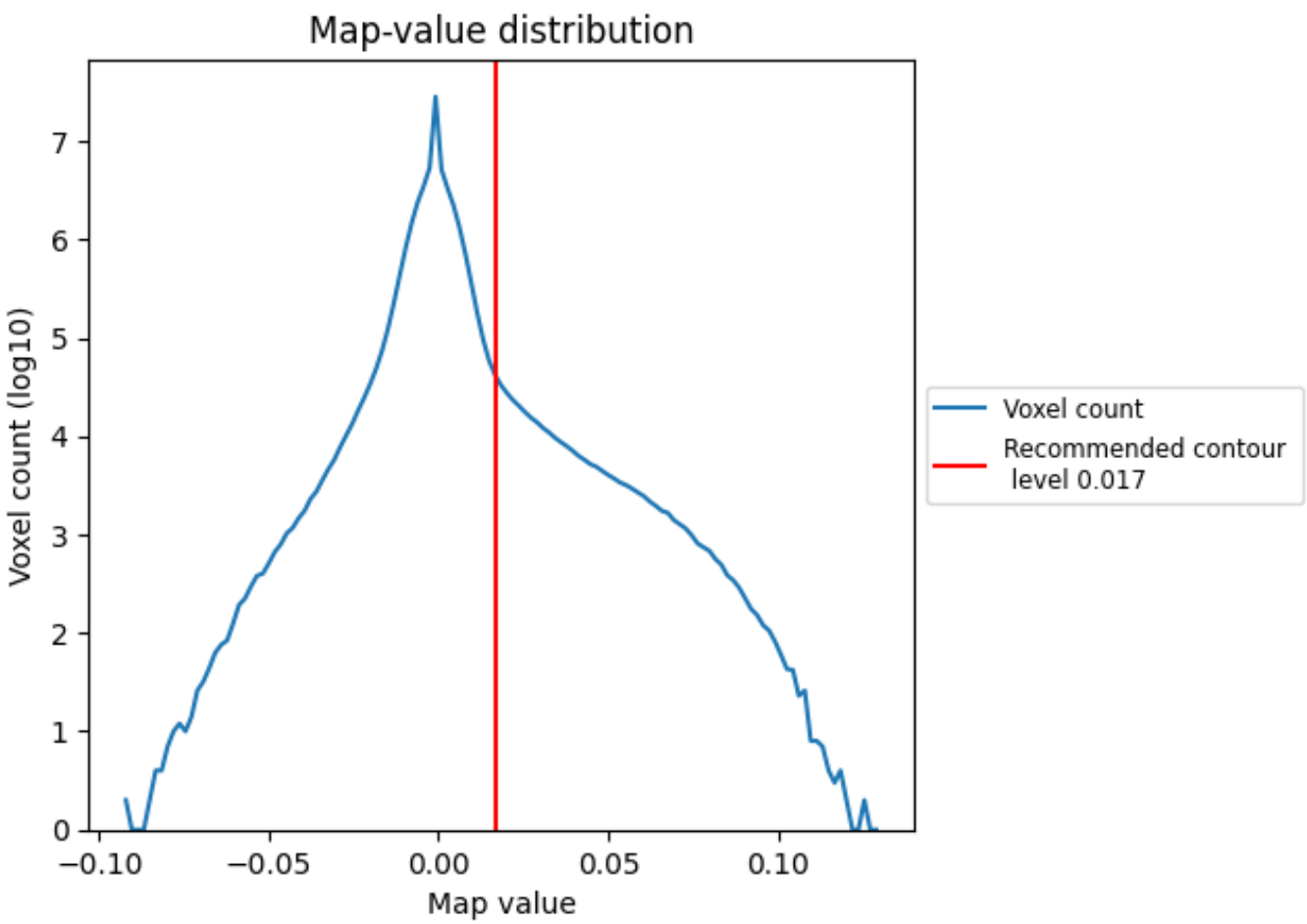
6.5 Mask visualisation (i)

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

7 Map analysis (i)

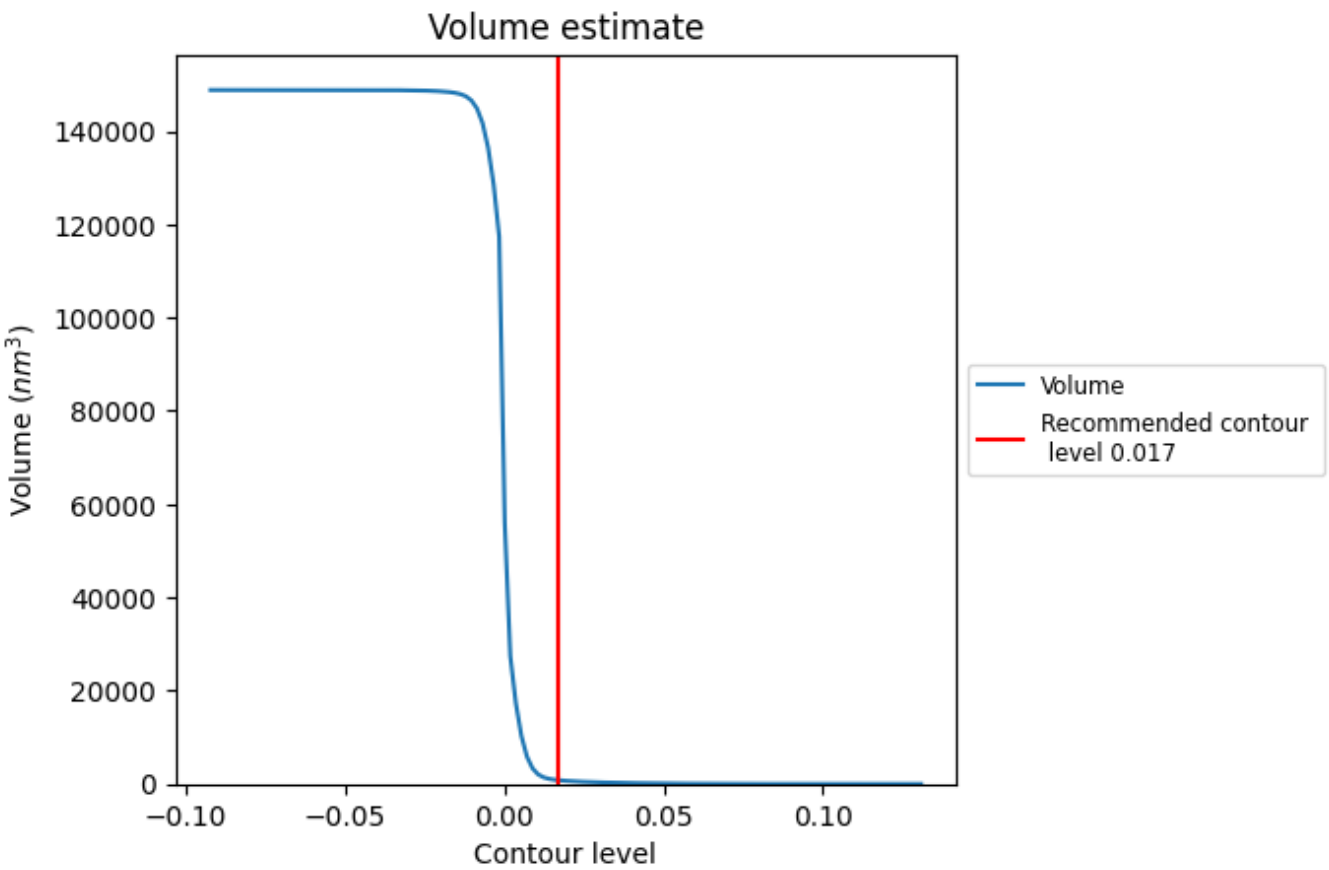
This section contains the results of statistical analysis of the map.

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.

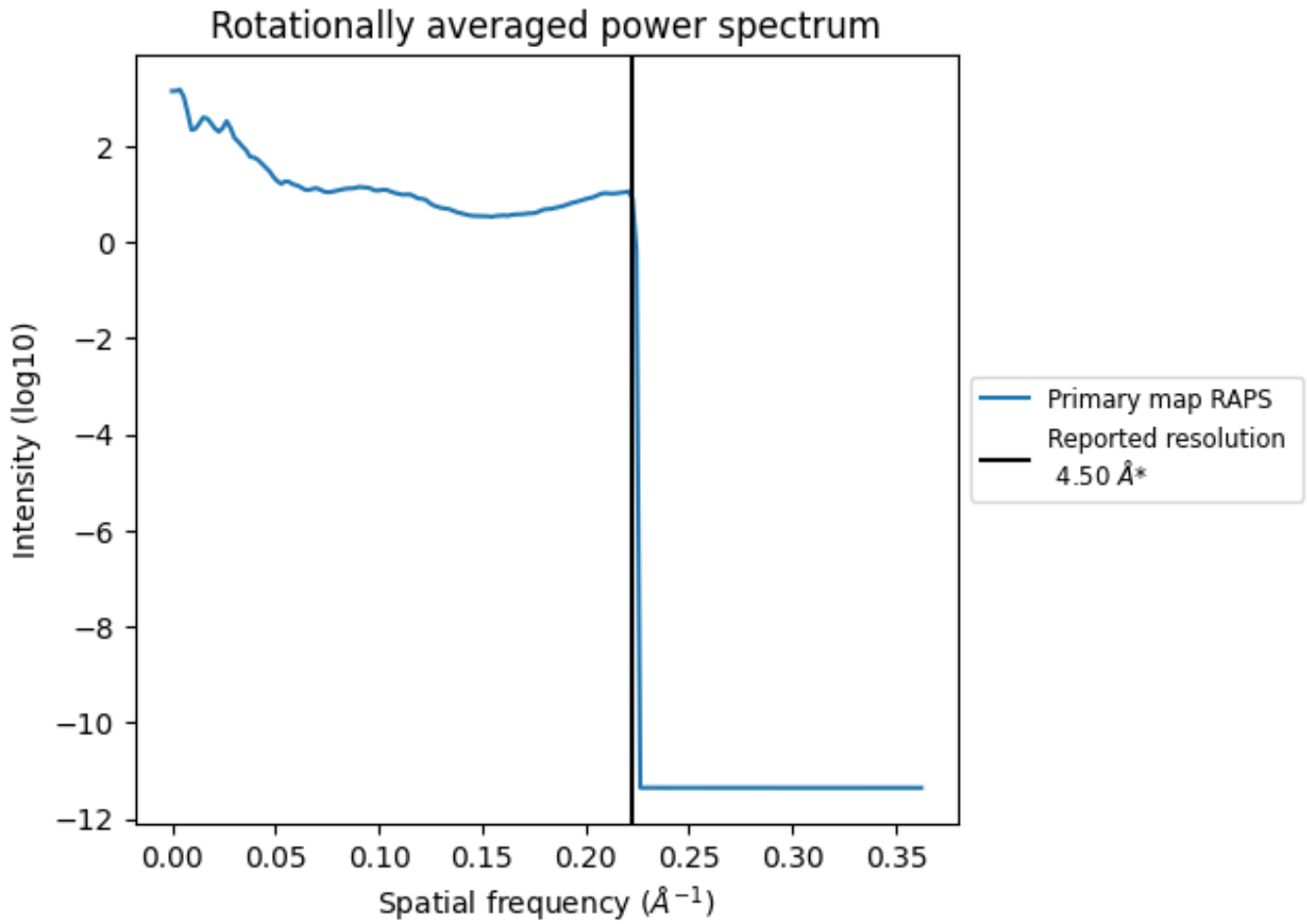
7.2 Volume estimate (i)



The volume at the recommended contour level is 813 nm^3; 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}

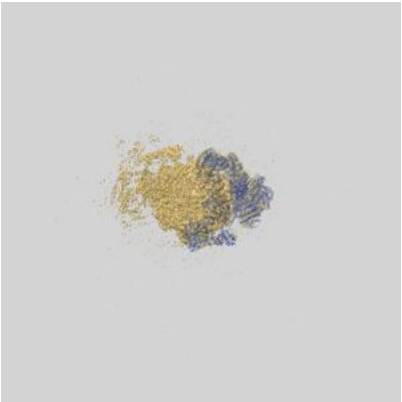
8 Fourier-Shell correlation (i)

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

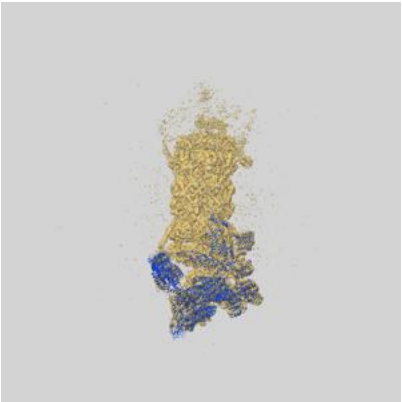
9 Map-model fit (i)

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.

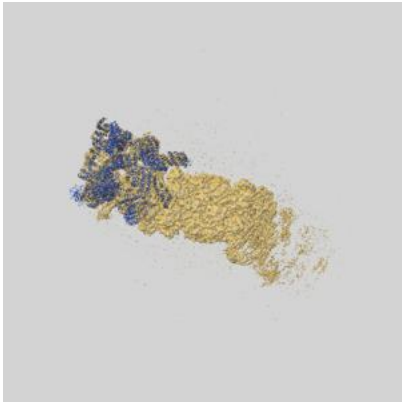
9.1 Map-model overlay (i)



X



Y



Z

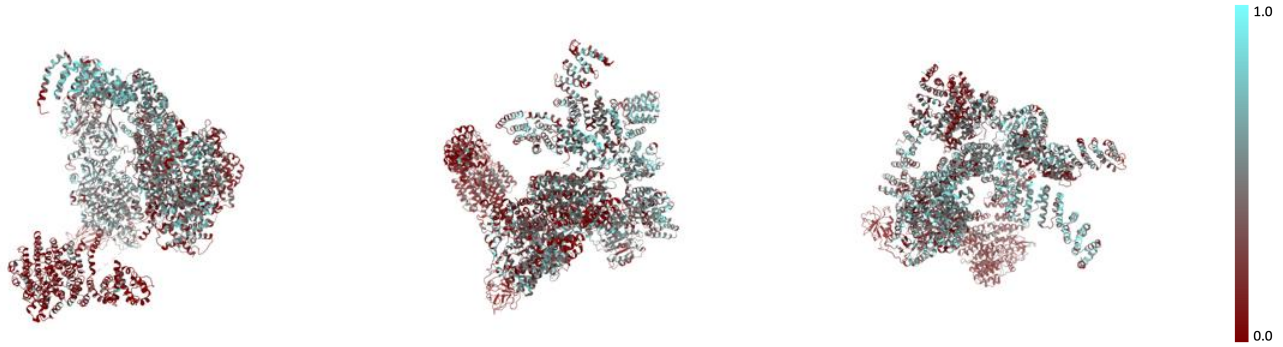
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according 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.

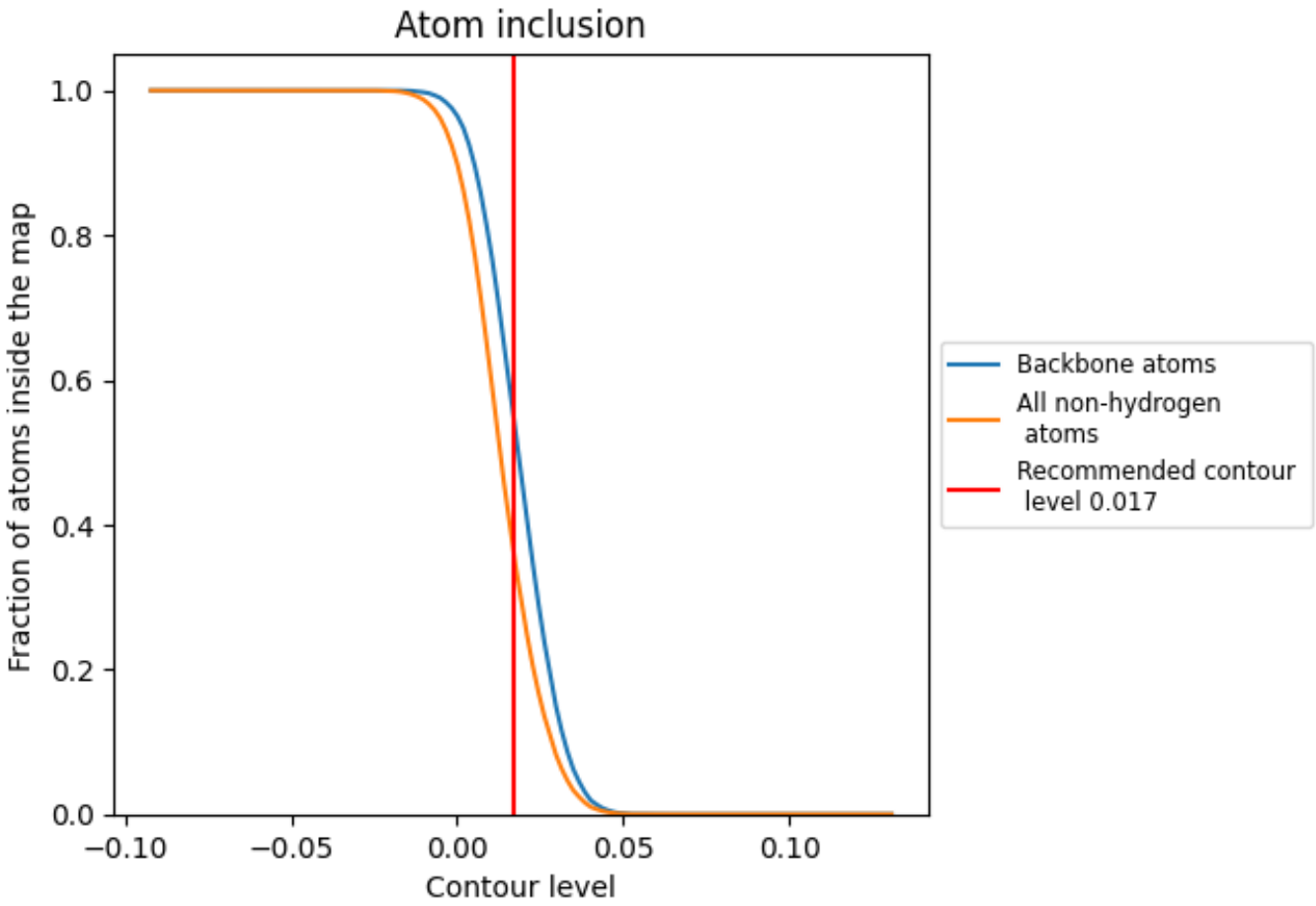
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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