



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:03 AM UTC

PDB ID : 6FVV / pdb_00006fvv
EMDB ID : EMD-4321
Title : 26S proteasome, s3 state
Authors : Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on : 2018-03-05
Resolution : 5.40 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:

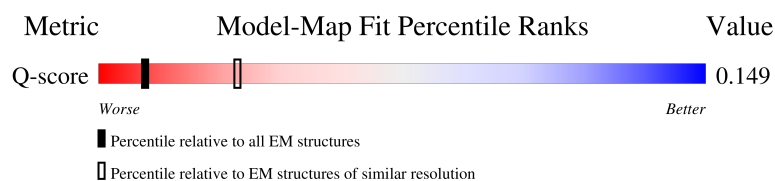
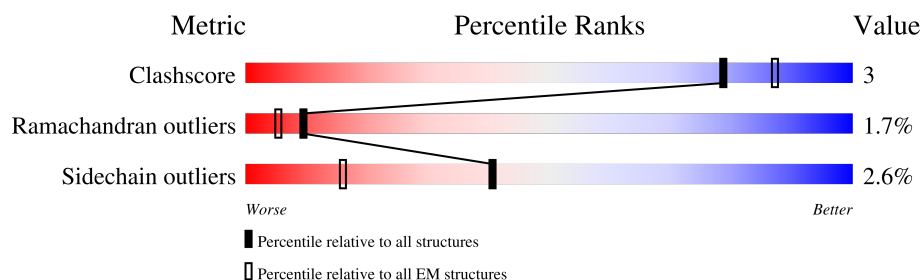
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

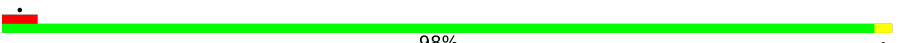
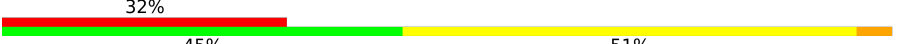
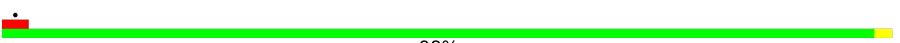
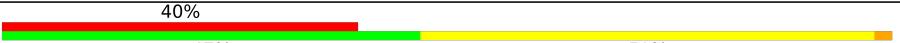
The reported resolution of this entry is 5.40 Å.

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.



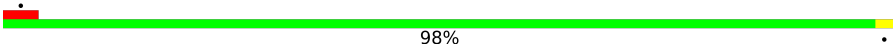
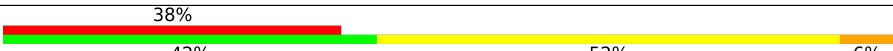
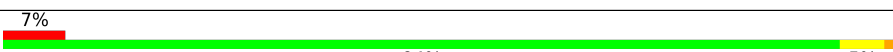
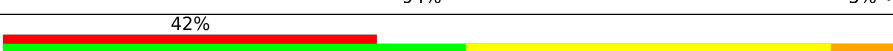
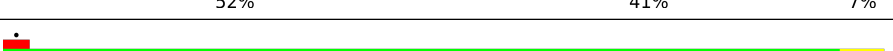
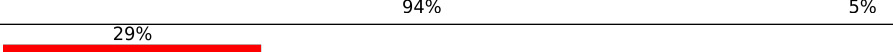
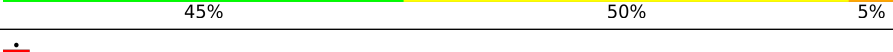
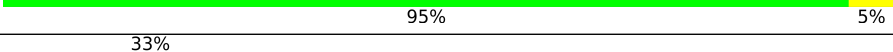
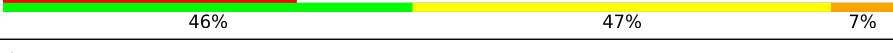
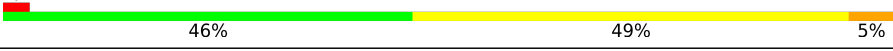
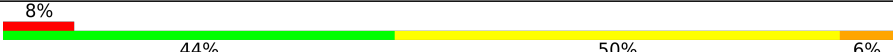
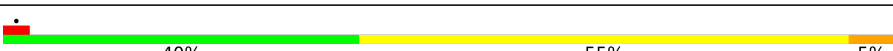
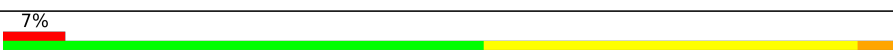
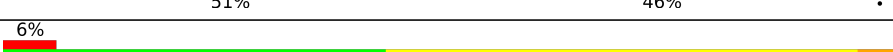
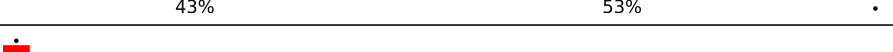
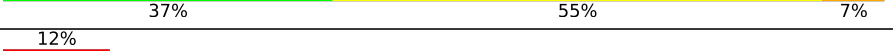
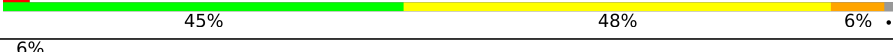
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	538 (4.90 - 5.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	 98% .
1	a	241	 32% 45% 51% .
2	B	249	 98% .
2	b	249	 40% 47% 51% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	244	
3	c	244	
4	D	251	
4	d	251	
5	E	244	
5	e	244	
6	F	231	
6	f	231	
7	G	242	
7	g	242	
8	1	196	
8	h	196	
9	2	226	
9	i	226	
10	3	204	
10	j	204	
11	4	195	
11	k	195	
12	5	212	
12	l	212	
13	6	222	
13	m	222	
14	7	232	
14	n	232	
15	W	197	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	289	
17	T	266	
18	X	127	
19	Y	89	
20	Z	970	
21	N	922	
22	S	475	
23	P	440	
24	Q	434	
25	R	405	
26	U	304	
27	O	388	
28	H	417	
29	I	385	
30	K	394	
31	L	388	
32	M	421	
33	J	405	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	ADP	H	501	-	-	X	-
36	ATP	I	501	-	-	X	-
36	ATP	K	501	-	-	X	-
36	ATP	L	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 110420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1908	1214	320	366	8		
1	A	241	Total	C	N	O	S	0	0
			1908	1214	320	366	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		
3	C	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	251	Total	C	N	O	S	0	0
			1982	1235	350	393	4		
4	D	237	Total	C	N	O	S	0	0
			1859	1164	325	366	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		
5	E	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1886	1199	328	355	4		
7	G	242	Total	C	N	O	S	0	0
			1886	1199	328	355	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1720	1082	298	333	7		
9	2	226	Total	C	N	O	S	0	0
			1720	1082	298	333	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1562	992	264	300	6		
11	4	195	Total	C	N	O	S	0	0
			1562	992	264	300	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	232	Total	C	N	O	S	0	0
			1816	1148	311	350	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1535	962	269	301	3		

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2193	1405	349	433	6		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	127	Total	C	N	O	S	0	0
			1033	664	169	196	4		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	89	Total	C	N	O	S	0	0
			731	447	119	164	1		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7006	4416	1150	1410	30		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	922	Total	C	N	O	S	0	0
			7158	4536	1205	1389	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3895	2488	653	739	15		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3609	2297	604	698	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

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

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3259	2077	535	637	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	304	Total	C	N	O	S	0	0
			2427	1529	414	477	7		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

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

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	417	Total	C	N	O	S	0	0
			3234	2008	578	632	16		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	394	Total	C	N	O	S	0	0
			3113	1951	548	604	10		

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	388	Total	C	N	O	S	0	0
			3083	1942	548	581	12		

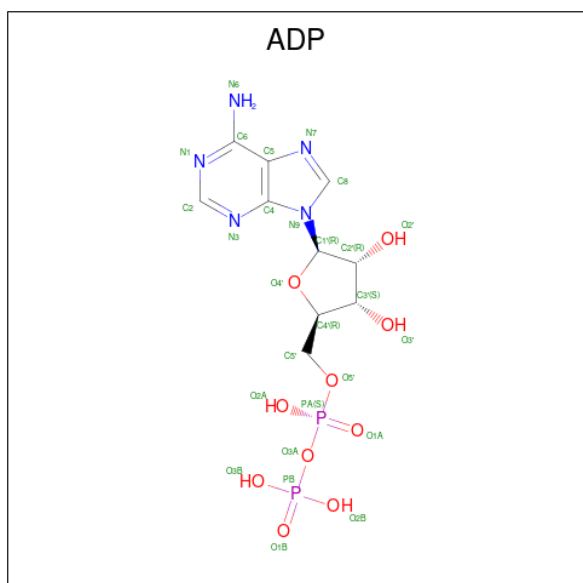
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	421	Total	C	N	O	S	0	0
			3285	2043	573	656	13		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	405	Total	C	N	O	S	0	0
			3171	1995	565	593	18		

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

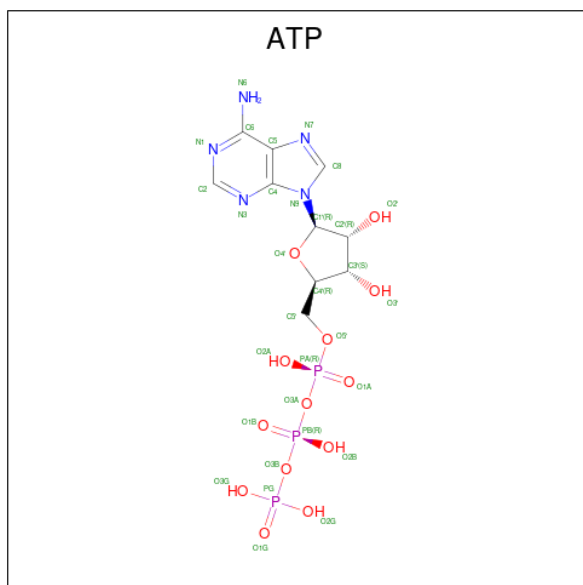
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
34	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	H	1	Total	Mg	0
			1	1	
35	I	1	Total	Mg	0
			1	1	
35	K	1	Total	Mg	0
			1	1	
35	L	1	Total	Mg	0
			1	1	
35	M	1	Total	Mg	0
			1	1	
35	J	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
36	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

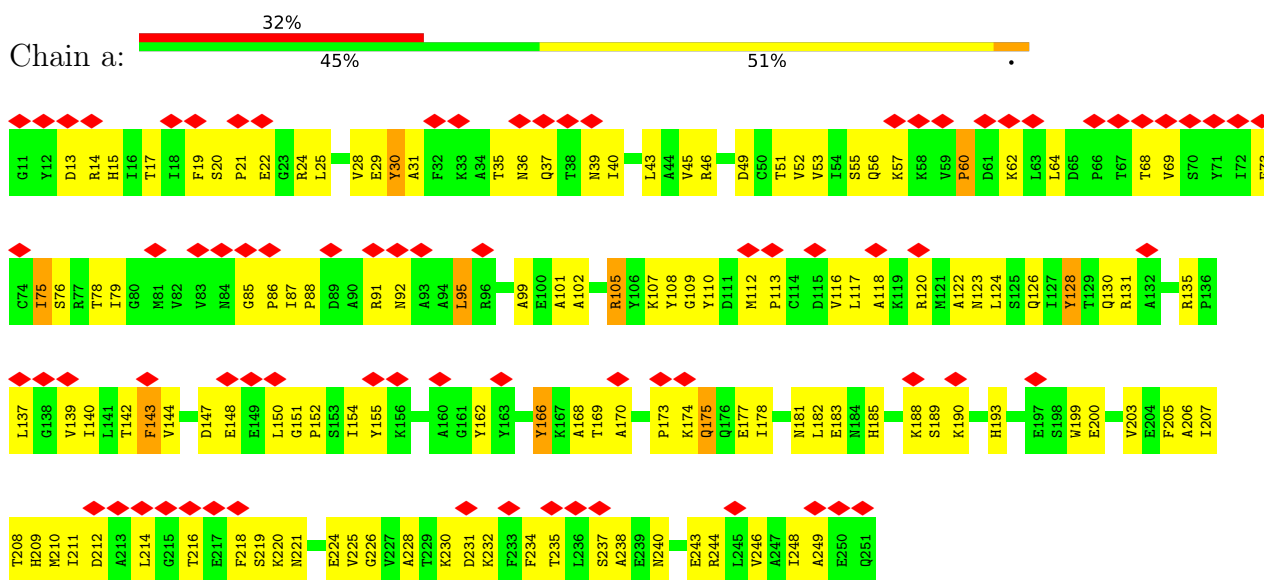
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

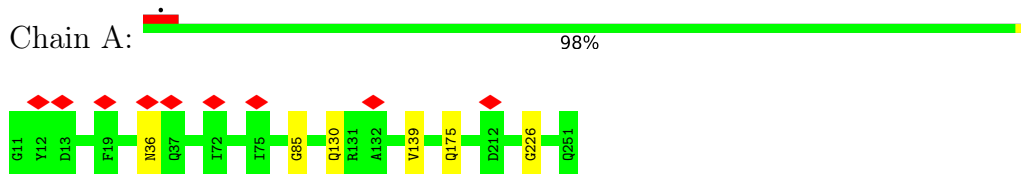
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

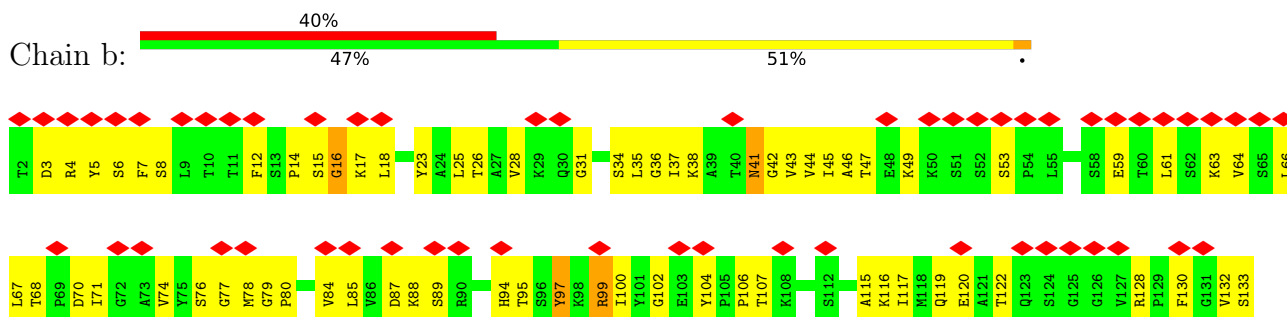
• Molecule 1: Proteasome subunit alpha type-1

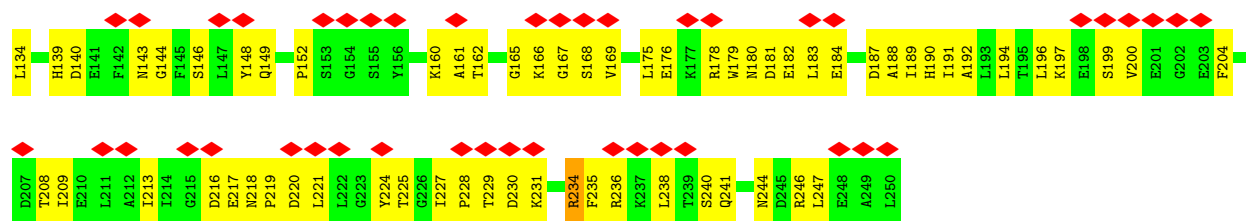


• Molecule 1: Proteasome subunit alpha type-1

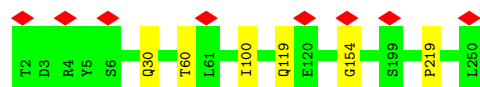


• Molecule 2: Proteasome subunit alpha type-2

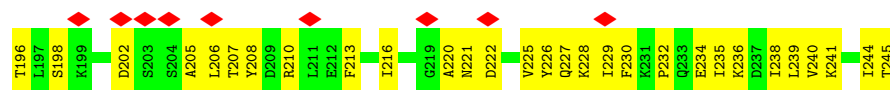
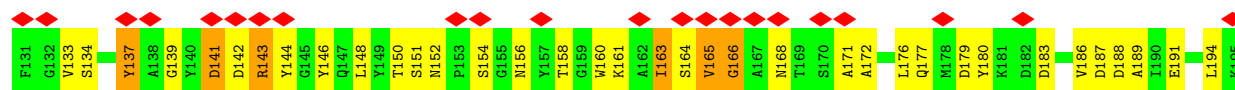
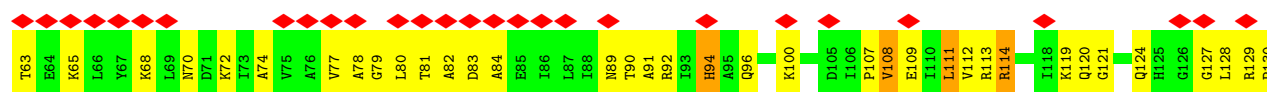




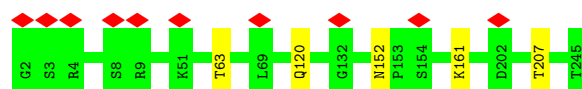
• Molecule 2: Proteasome subunit alpha type-2



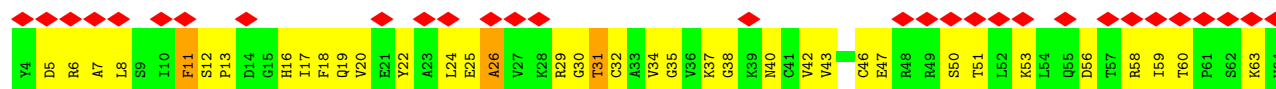
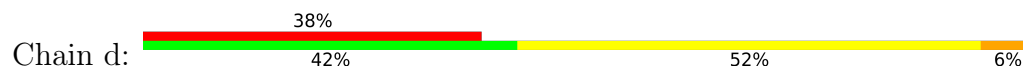
• Molecule 3: Proteasome subunit alpha type-3

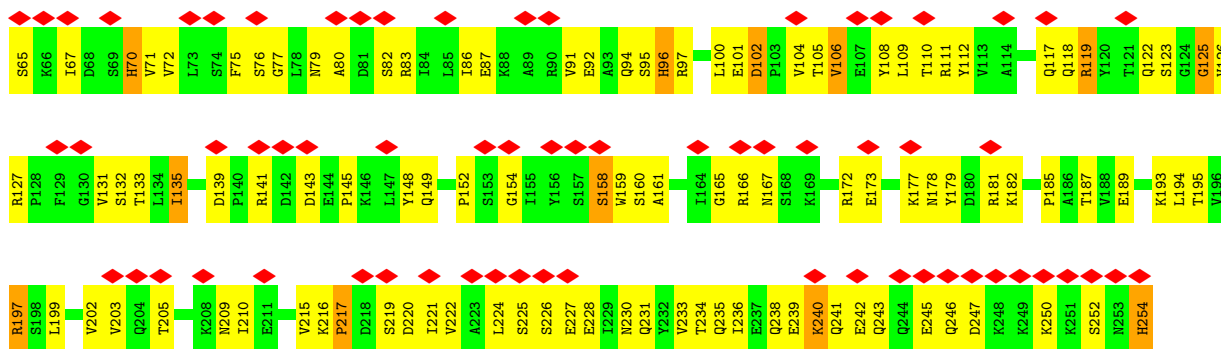


• Molecule 3: Proteasome subunit alpha type-3

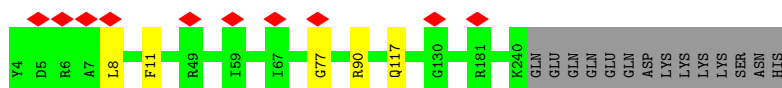
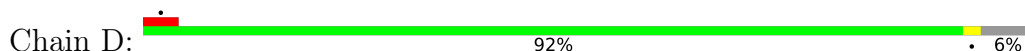


• Molecule 4: Proteasome subunit alpha type-4

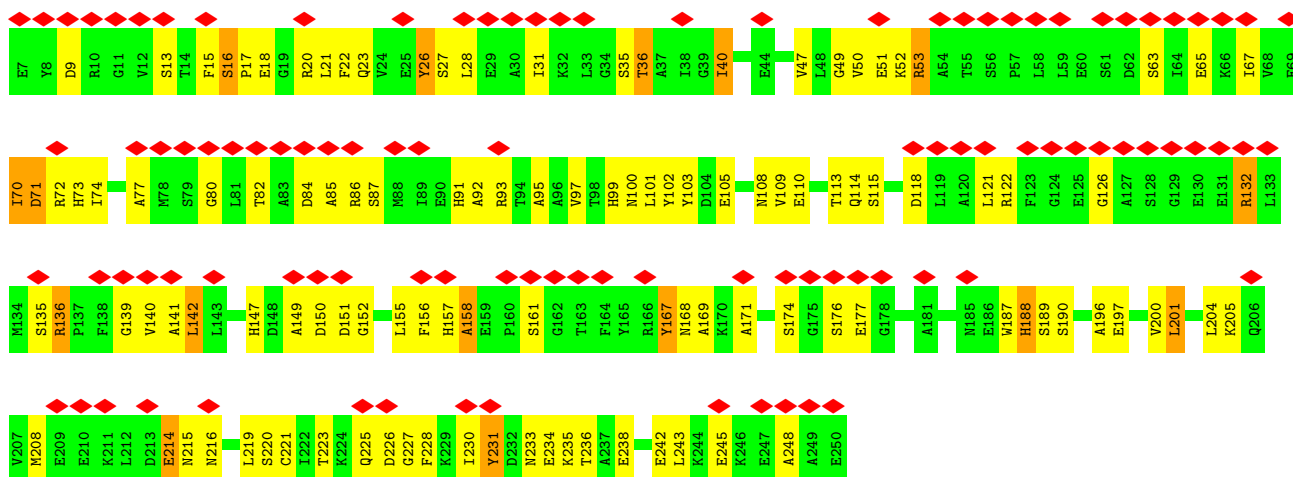
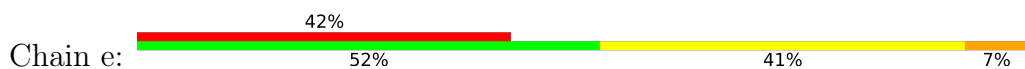




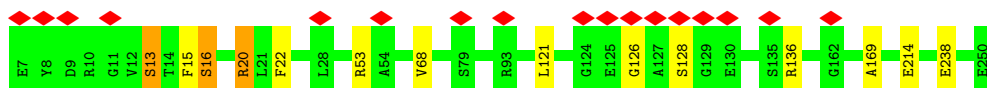
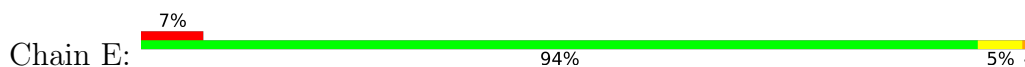
• Molecule 4: Proteasome subunit alpha type-4



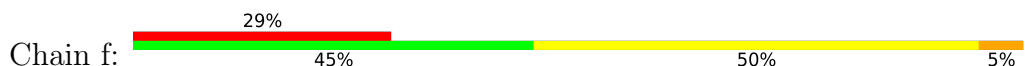
• Molecule 5: Proteasome subunit alpha type-5

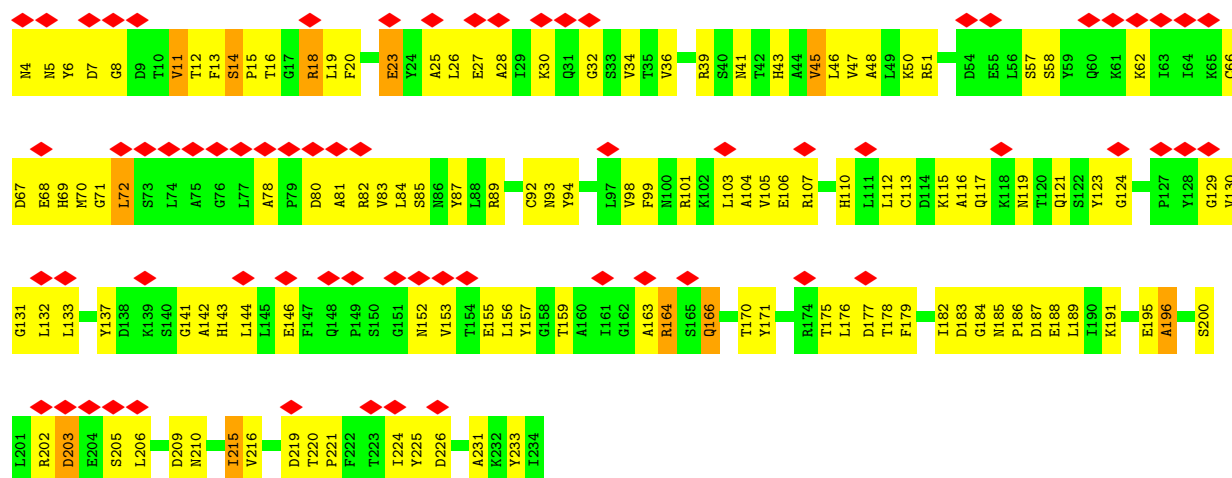


• Molecule 5: Proteasome subunit alpha type-5

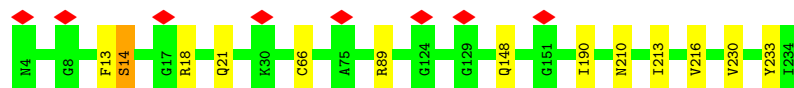


• Molecule 6: Proteasome subunit alpha type-6

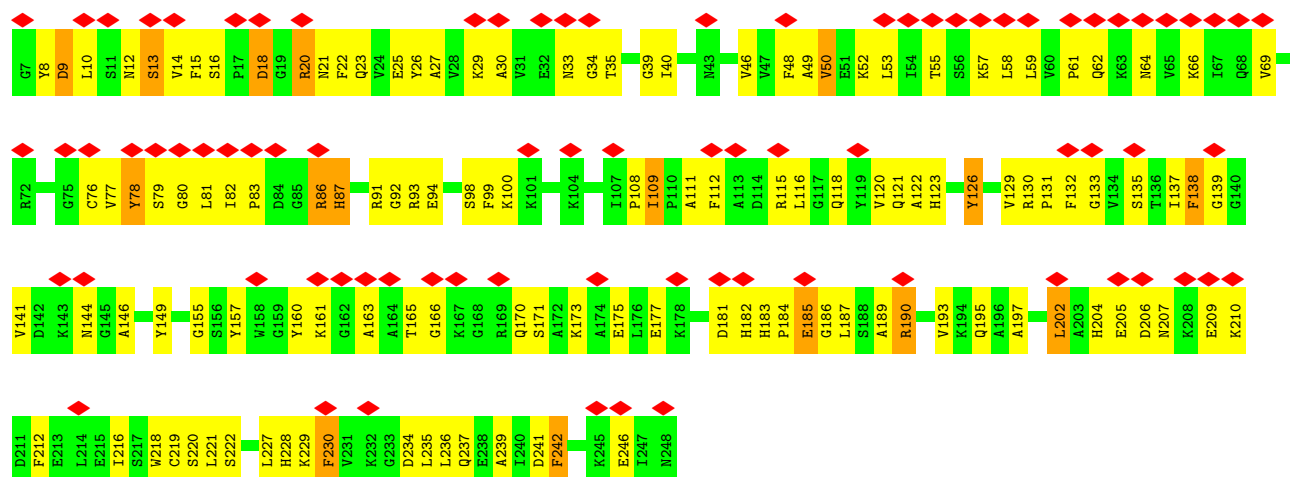




- Molecule 6: Proteasome subunit alpha type-6



- Molecule 7: Probable proteasome subunit alpha type-7

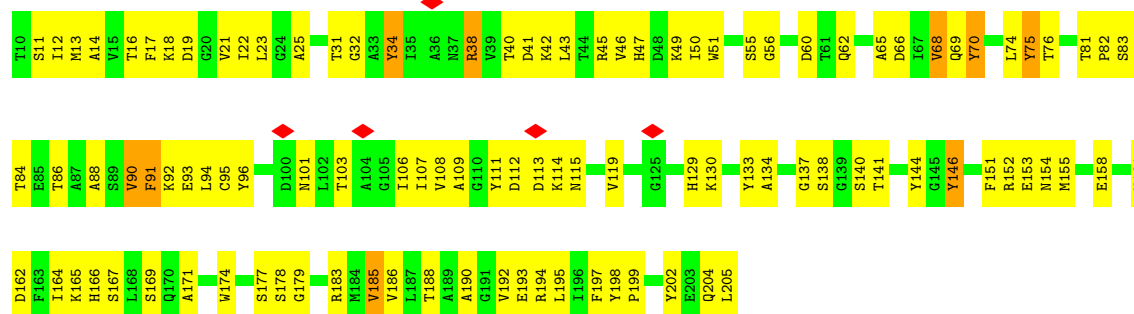


- Molecule 7: Probable proteasome subunit alpha type-7



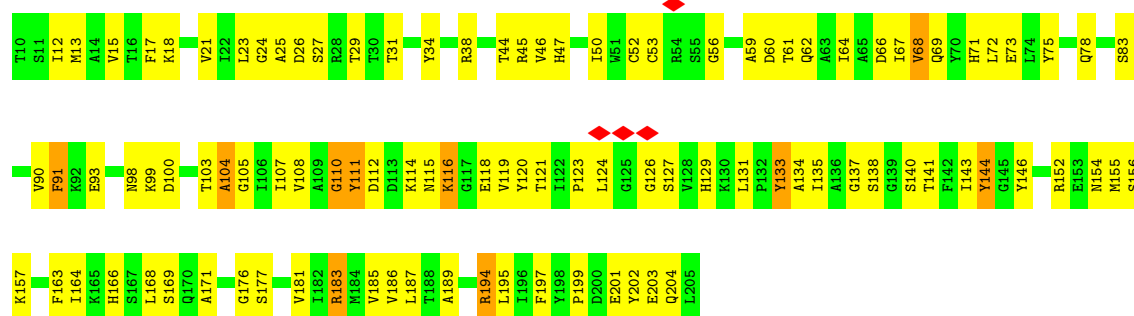
- Molecule 8: Proteasome subunit beta type-1

Chain h: 

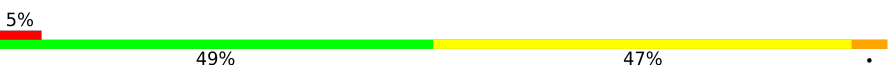


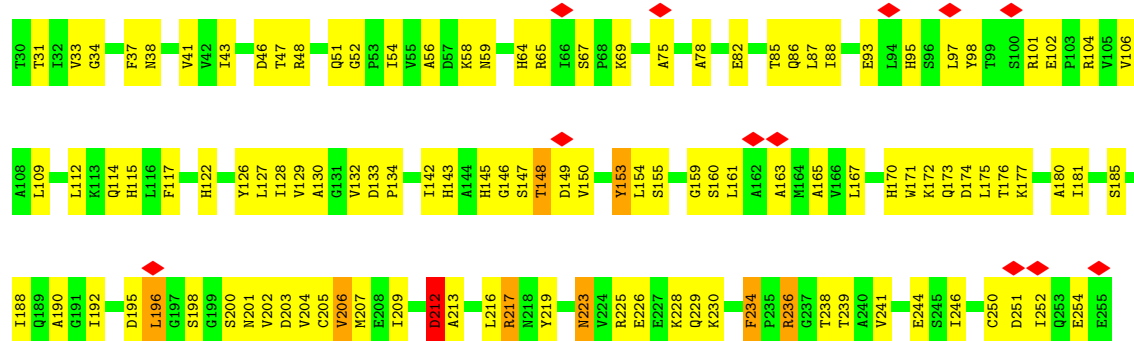
• Molecule 8: Proteasome subunit beta type-1

Chain 1: 



• Molecule 9: Proteasome subunit beta type-2

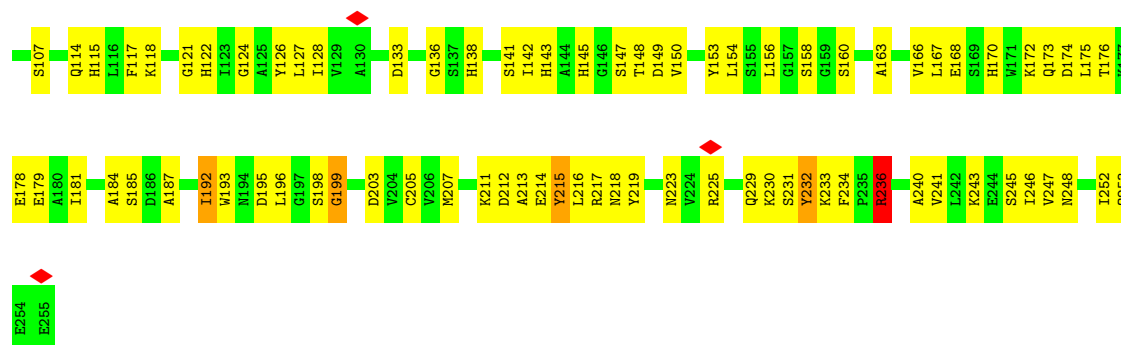
Chain i: 



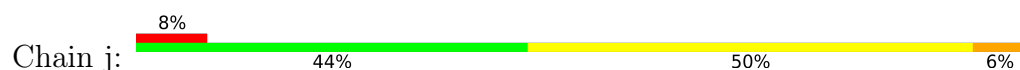
• Molecule 9: Proteasome subunit beta type-2

Chain 2: 





• Molecule 10: Proteasome subunit beta type-3

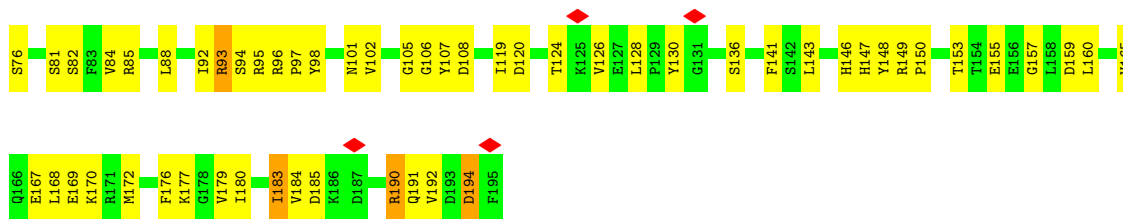


• Molecule 10: Proteasome subunit beta type-3

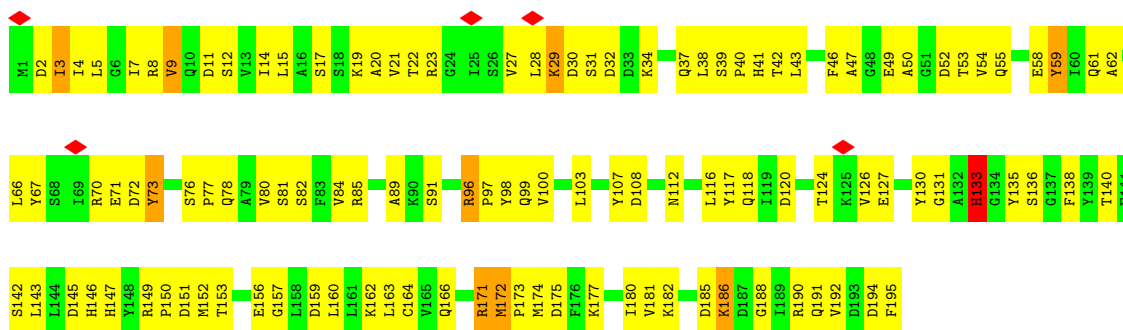


• Molecule 11: Proteasome subunit beta type-4

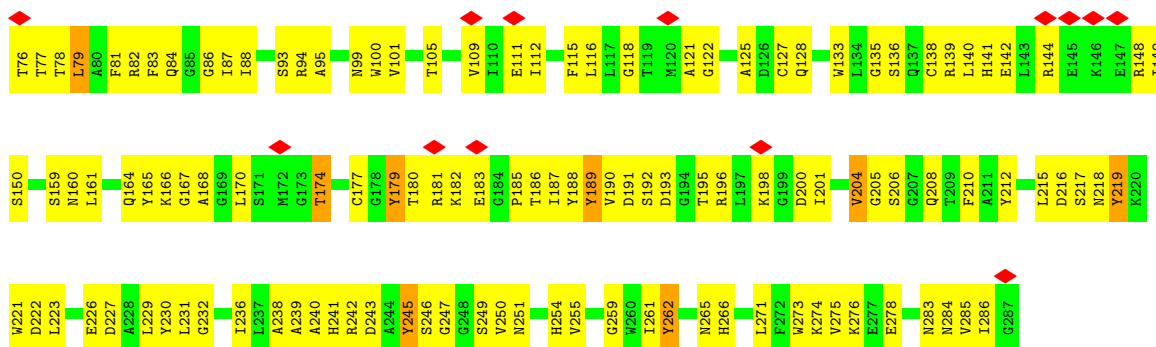




• Molecule 11: Proteasome subunit beta type-4



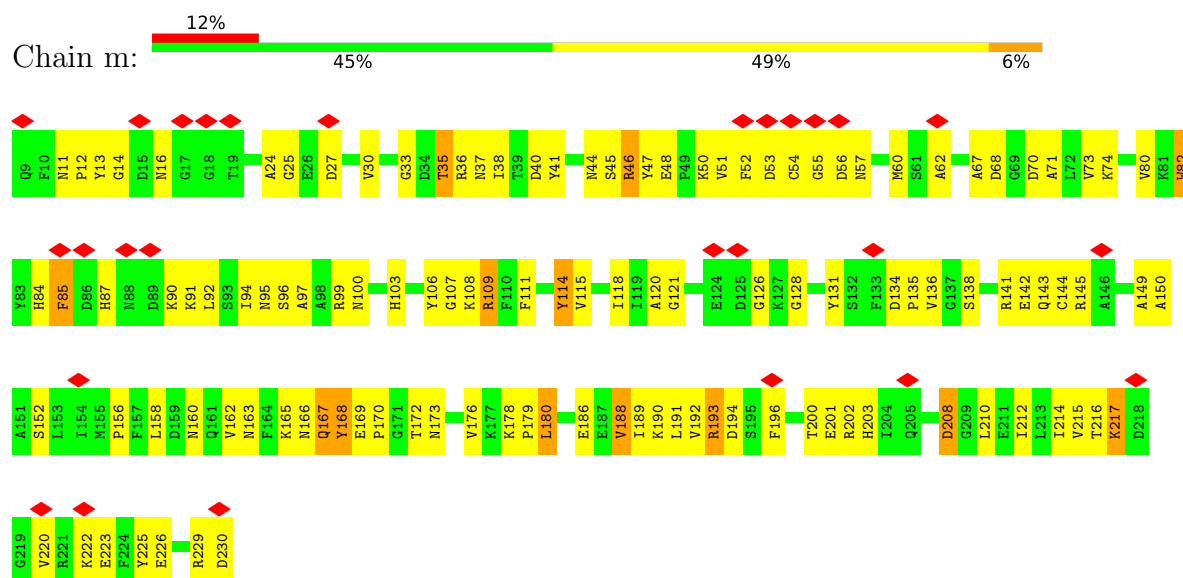
• Molecule 12: Proteasome subunit beta type-5



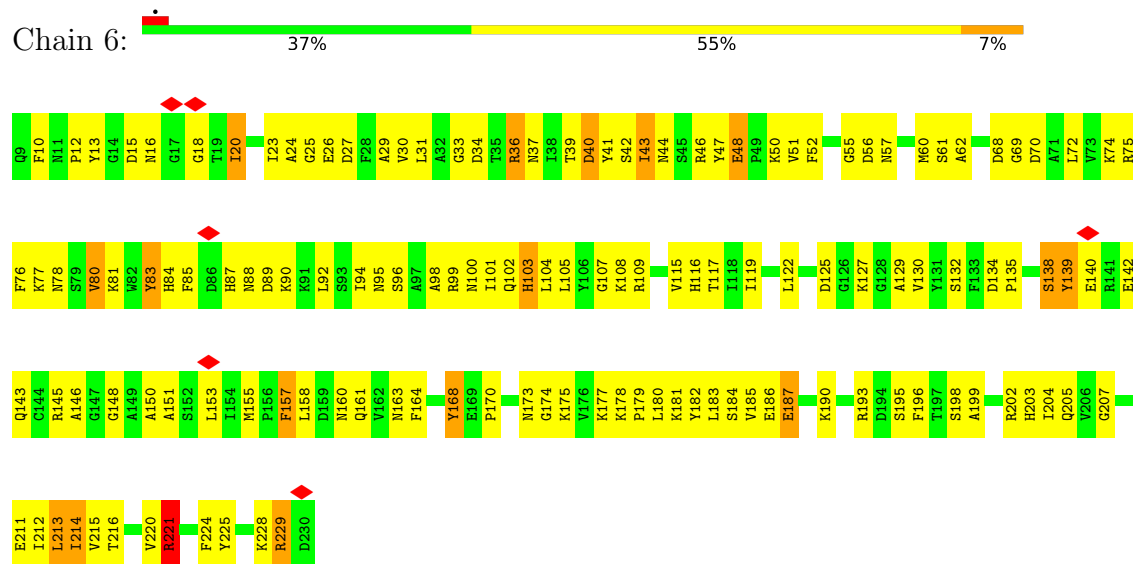
• Molecule 12: Proteasome subunit beta type-5



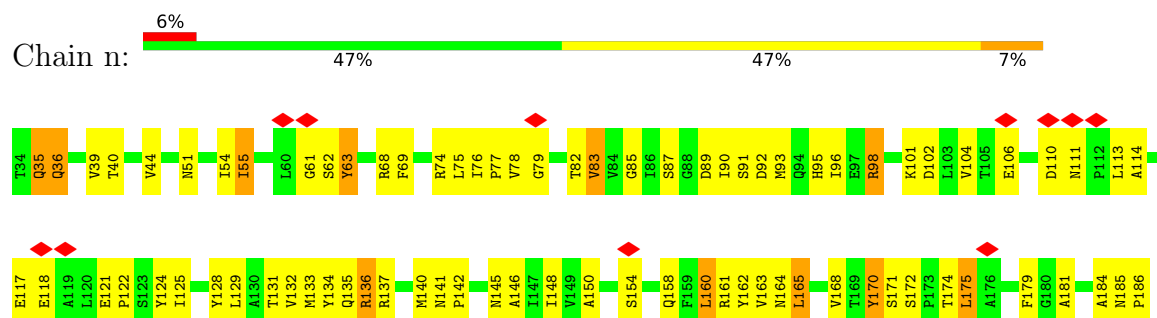
- Molecule 13: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-6

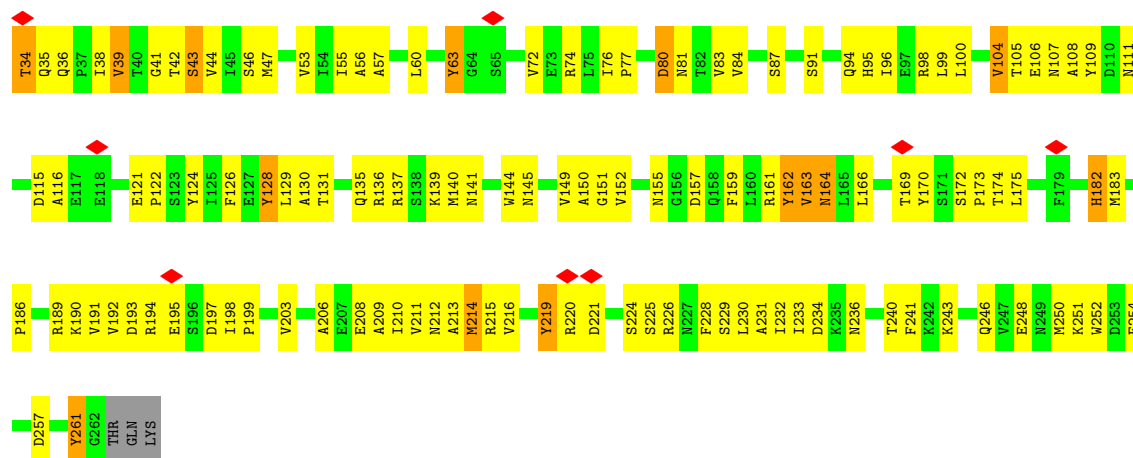


- Molecule 14: Proteasome subunit beta type-7

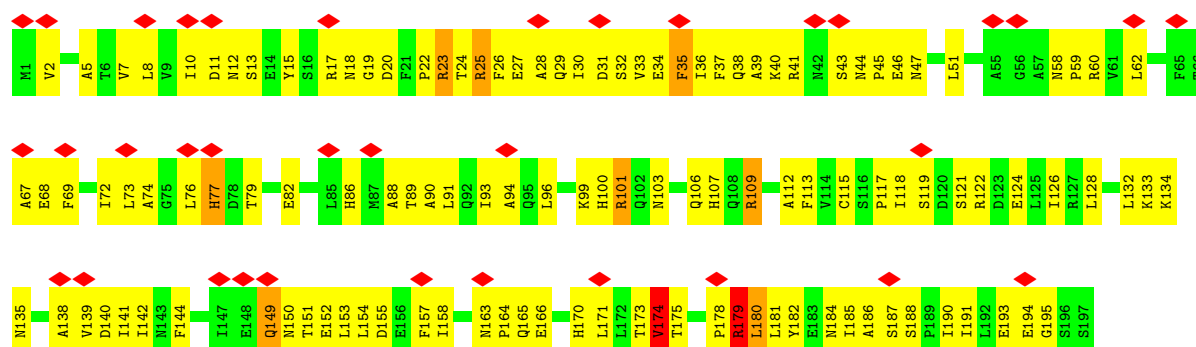




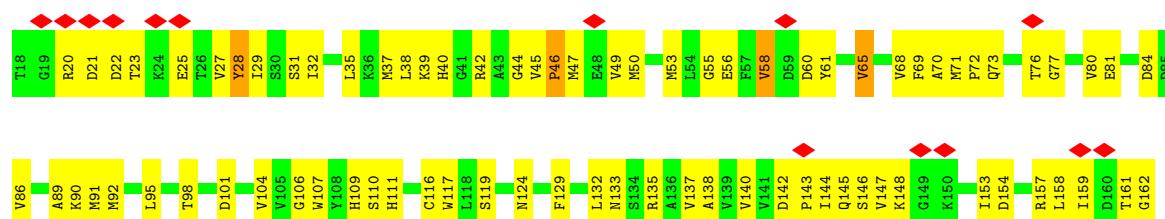
• Molecule 14: Proteasome subunit beta type-7

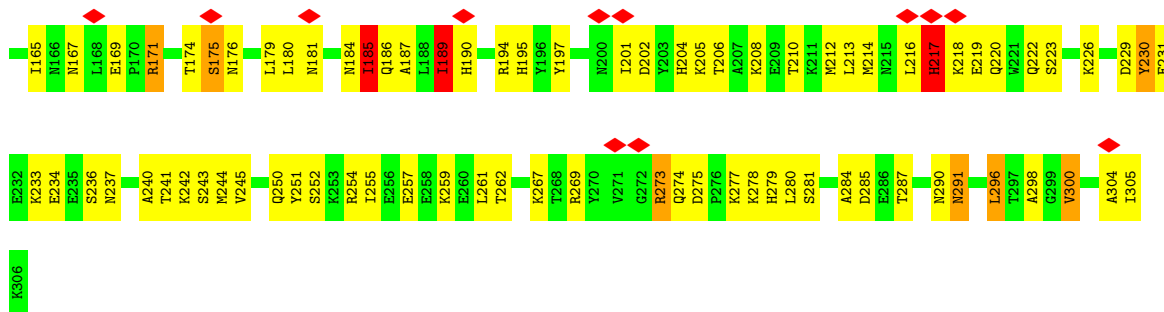


• Molecule 15: 26S proteasome regulatory subunit RPN10

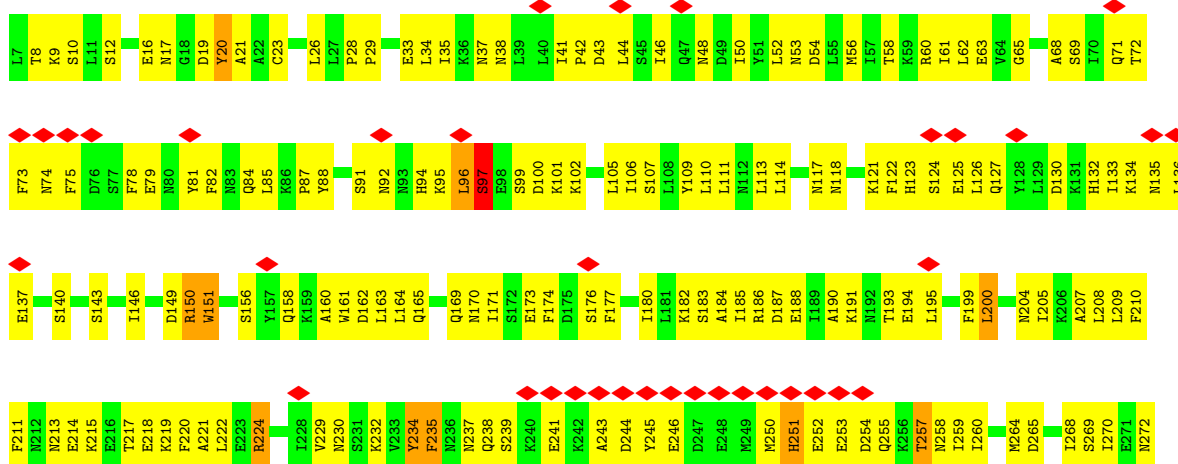


• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

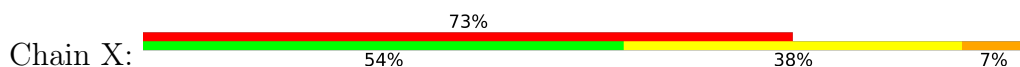




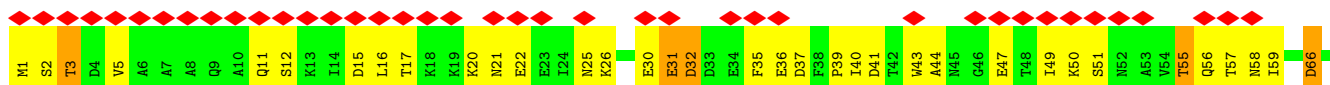
- Molecule 17: 26S proteasome regulatory subunit RPN12

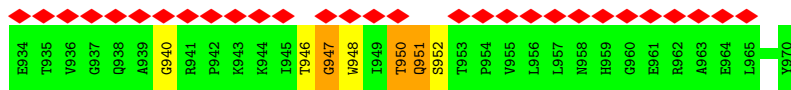
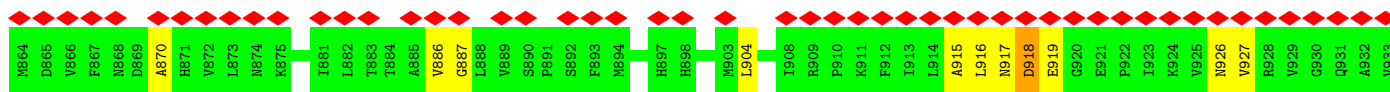


- Molecule 18: 26S proteasome regulatory subunit RPN13

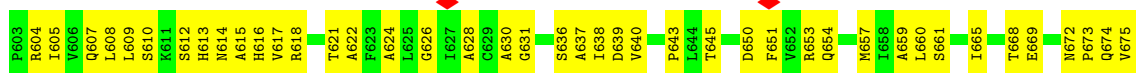
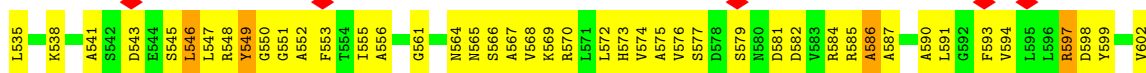
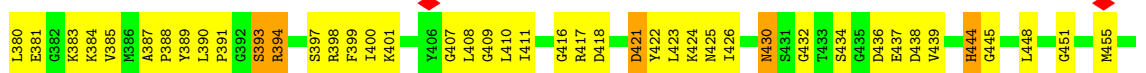
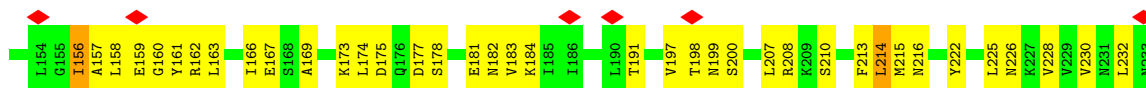
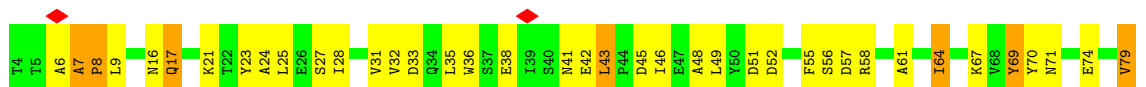


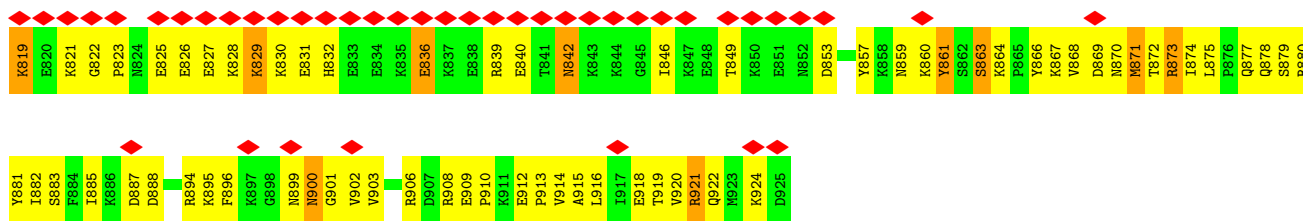
- Molecule 19: 26S proteasome complex subunit SEM1



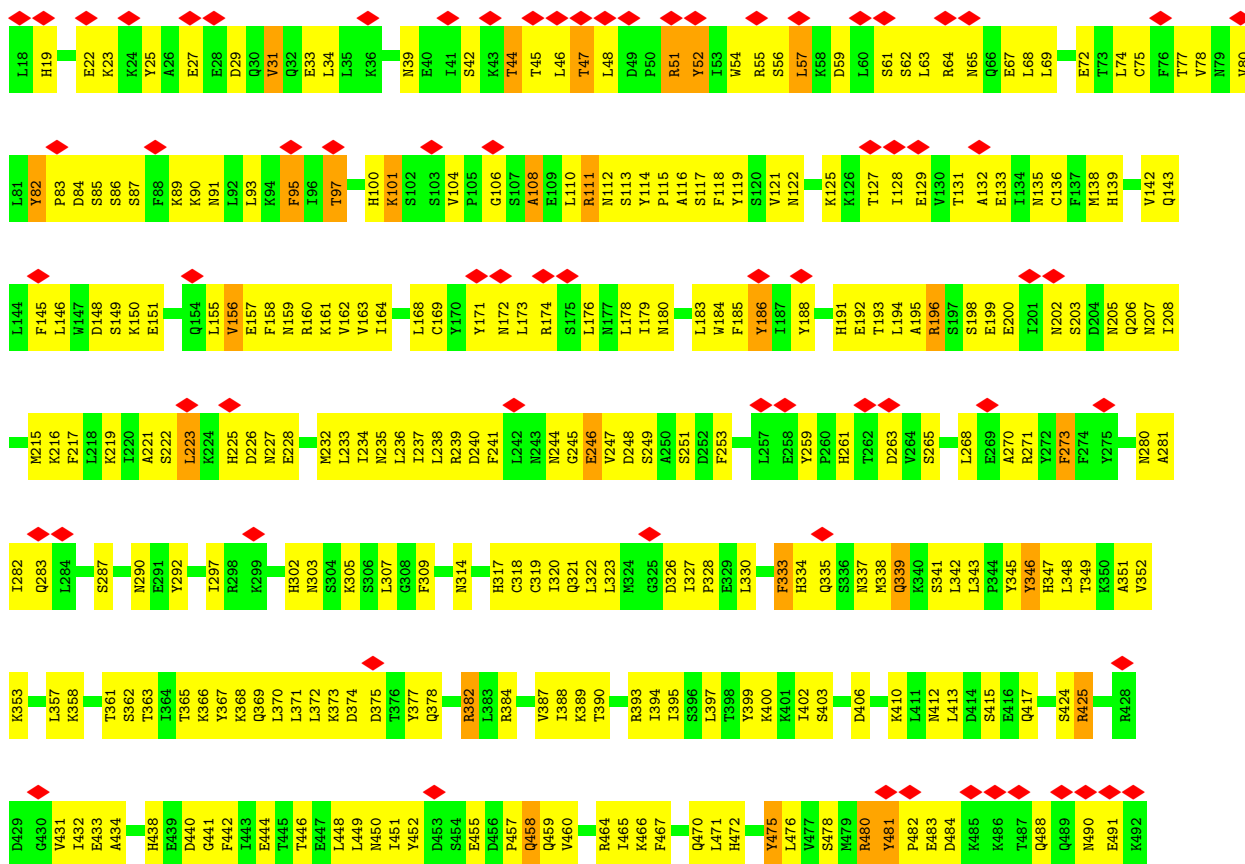


• Molecule 21: 26S proteasome regulatory subunit RPN2

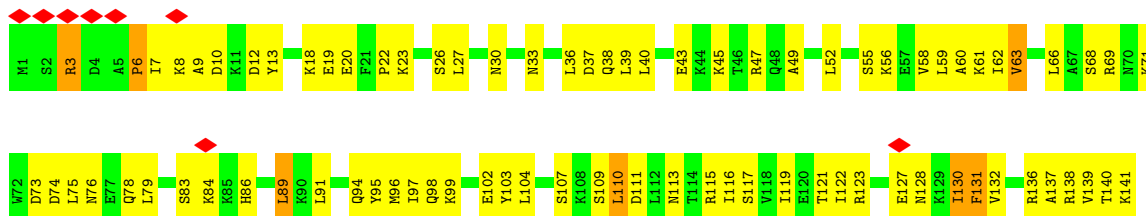


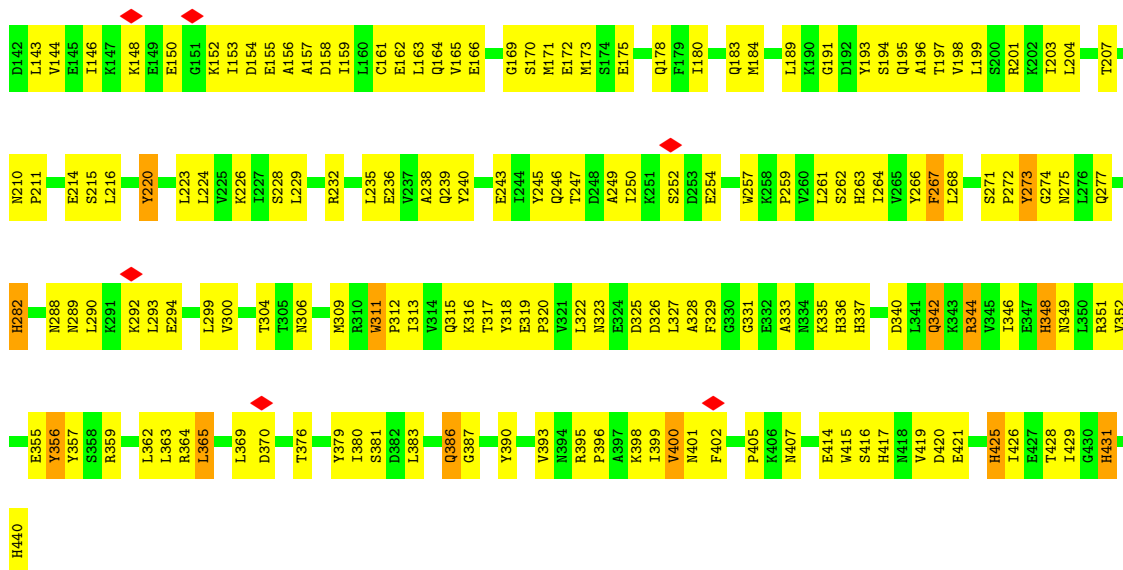


• Molecule 22: 26S proteasome regulatory subunit RPN3

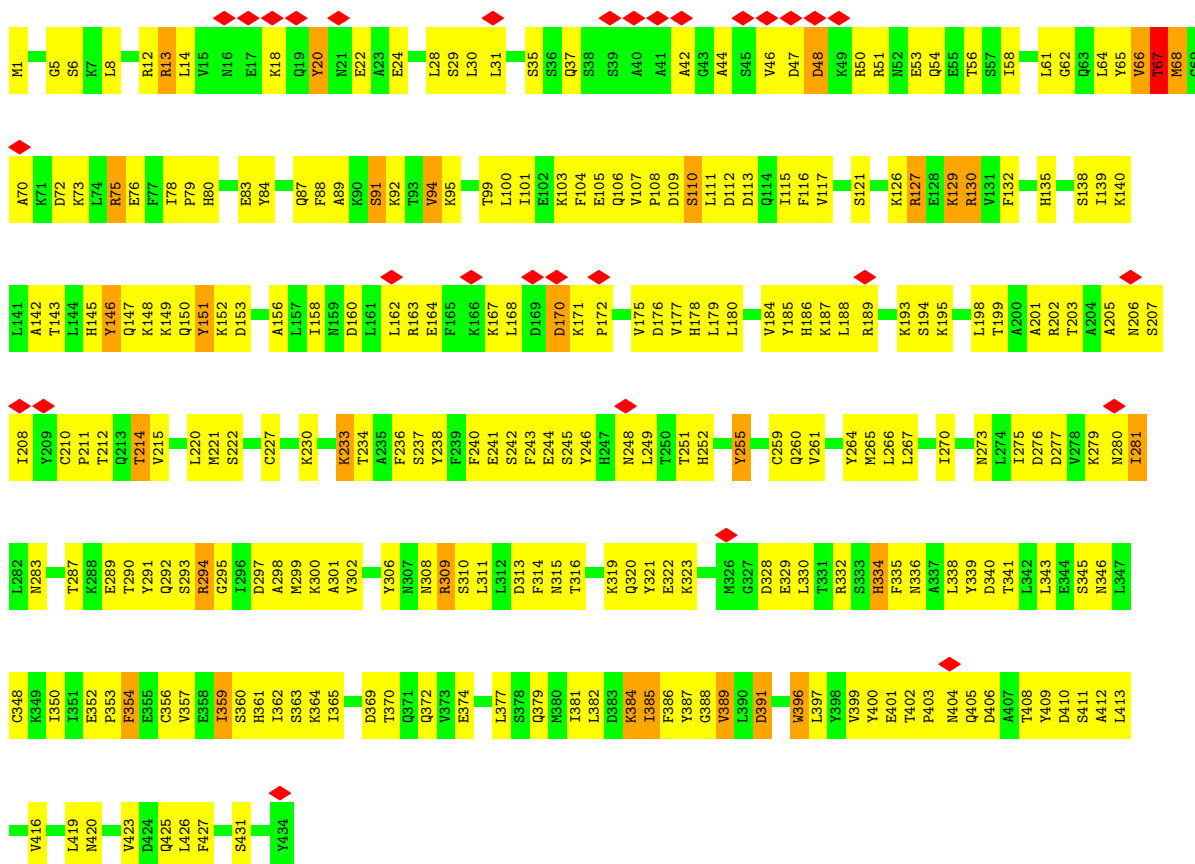


• Molecule 23: 26S proteasome regulatory subunit RPN5

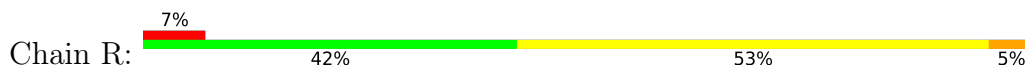


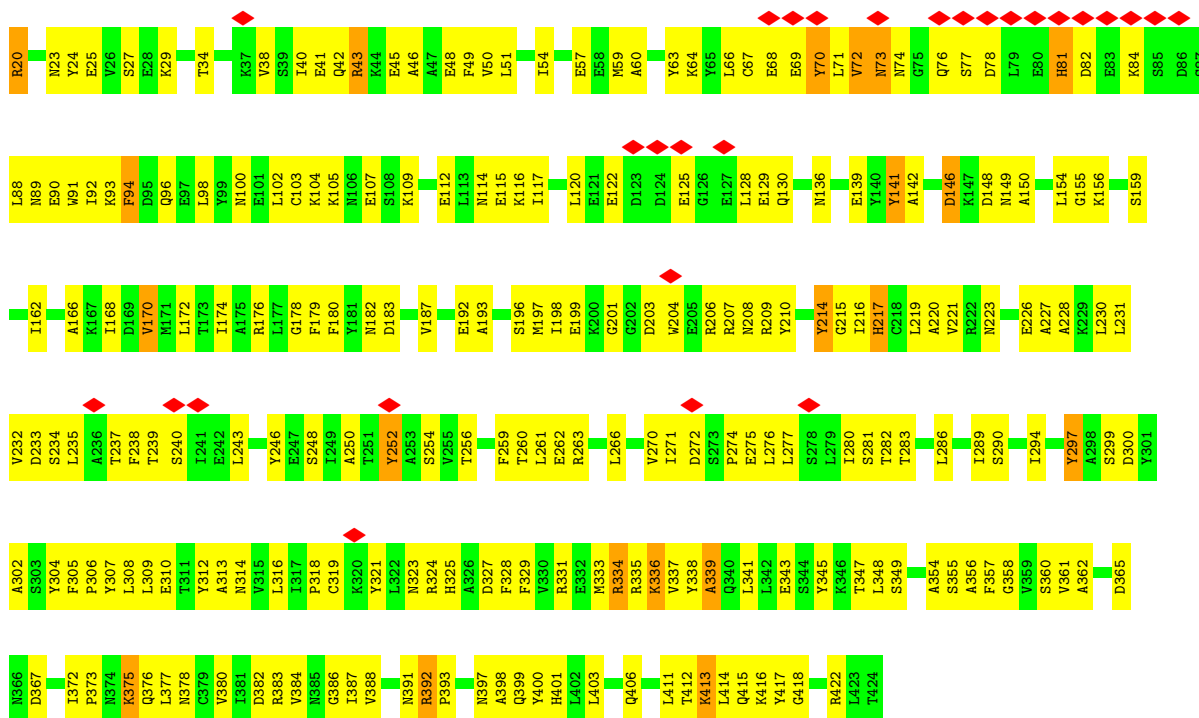


• Molecule 24: 26S proteasome regulatory subunit RPN6

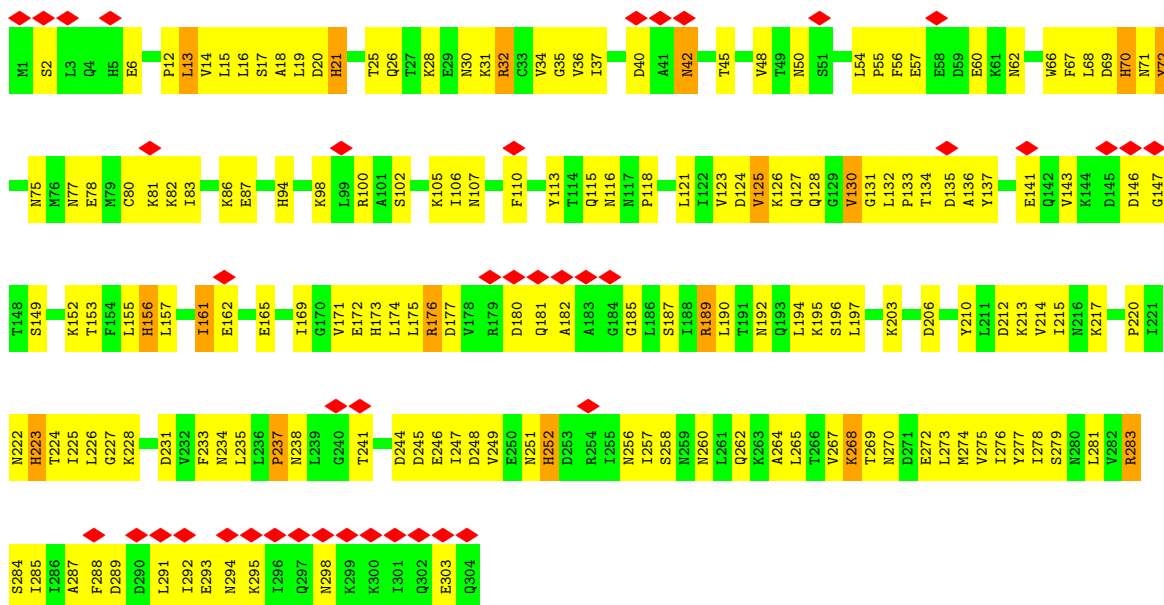
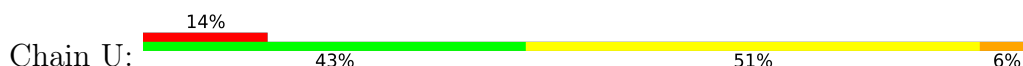


• Molecule 25: 26S proteasome regulatory subunit RPN7

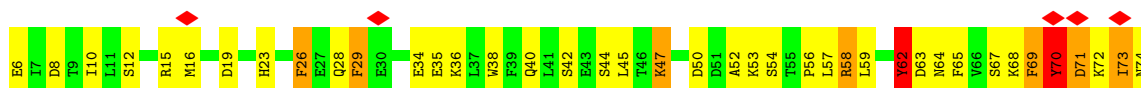
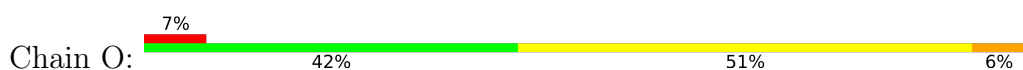


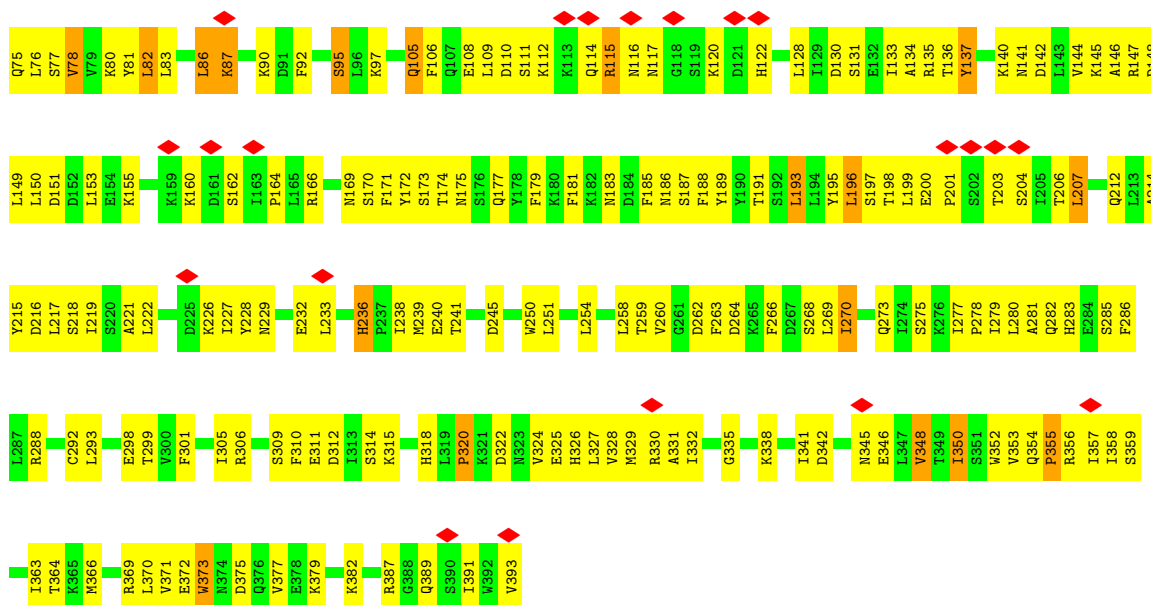


• Molecule 26: 26S proteasome regulatory subunit RPN8



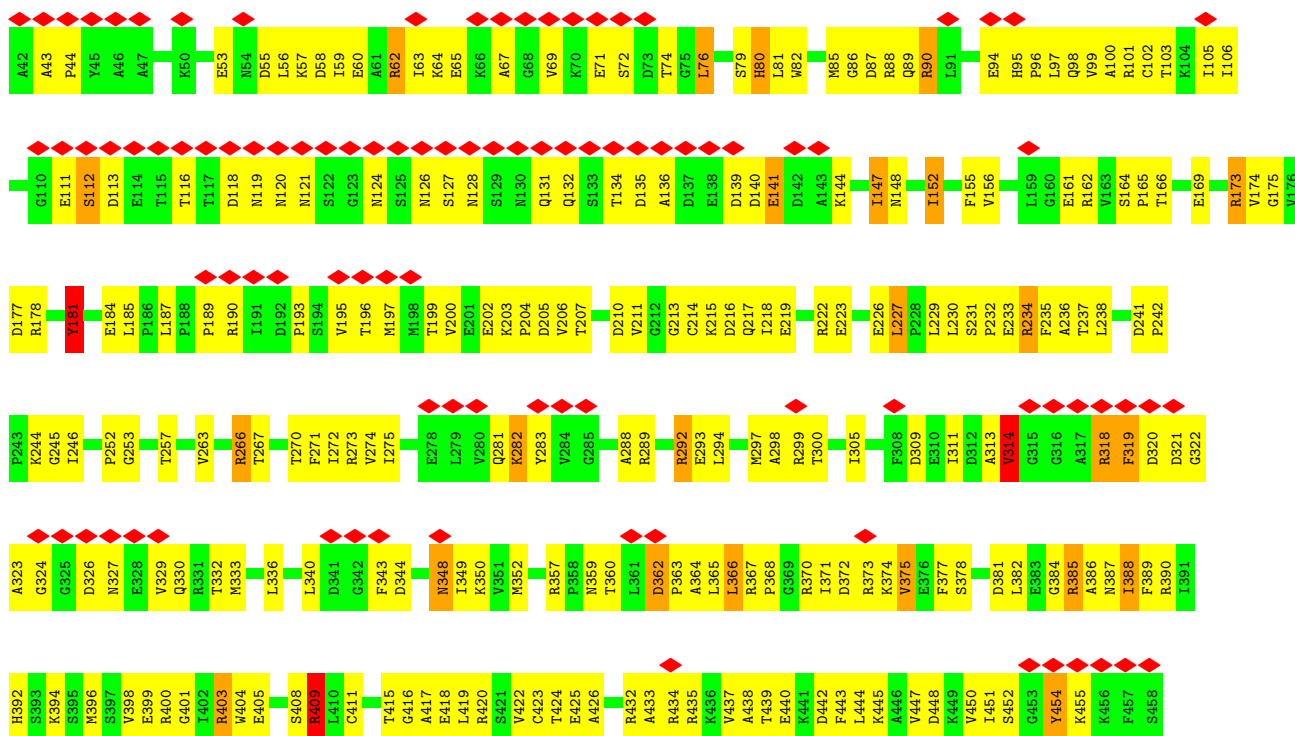
• Molecule 27: 26S proteasome regulatory subunit RPN9





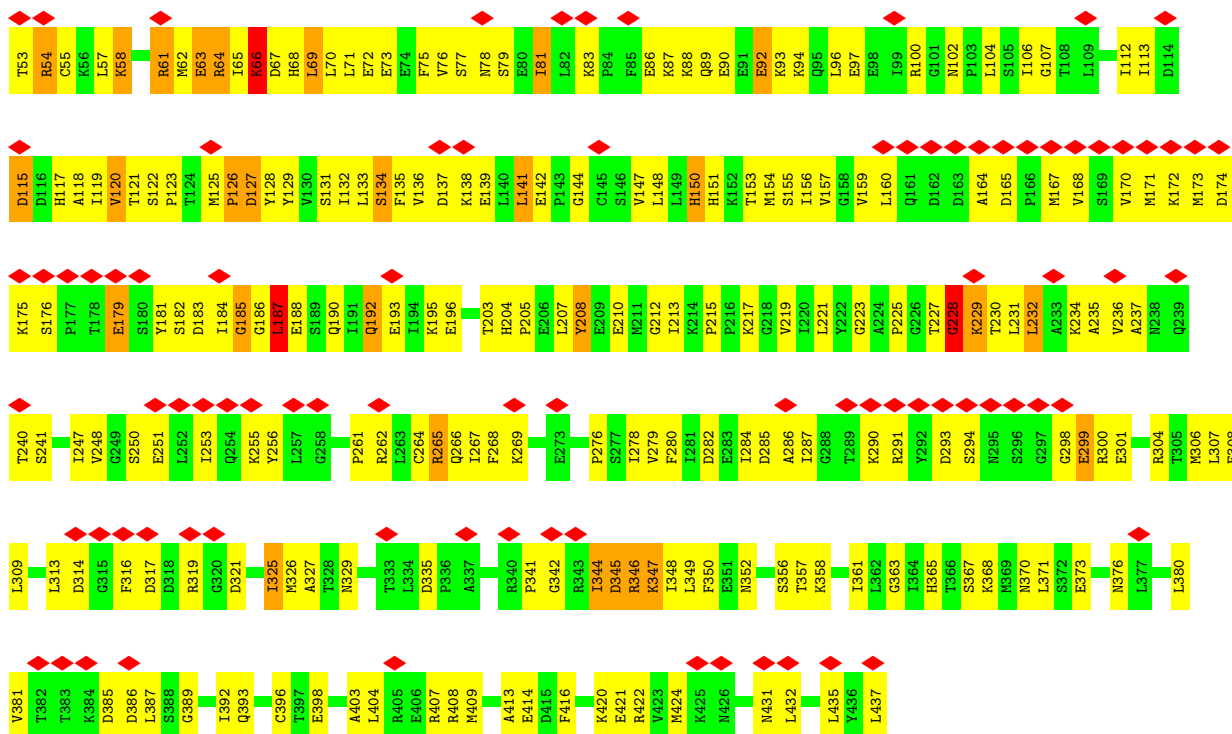
• Molecule 28: 26S proteasome regulatory subunit 7 homolog

Chain H: 23% 41% 52% 6% .

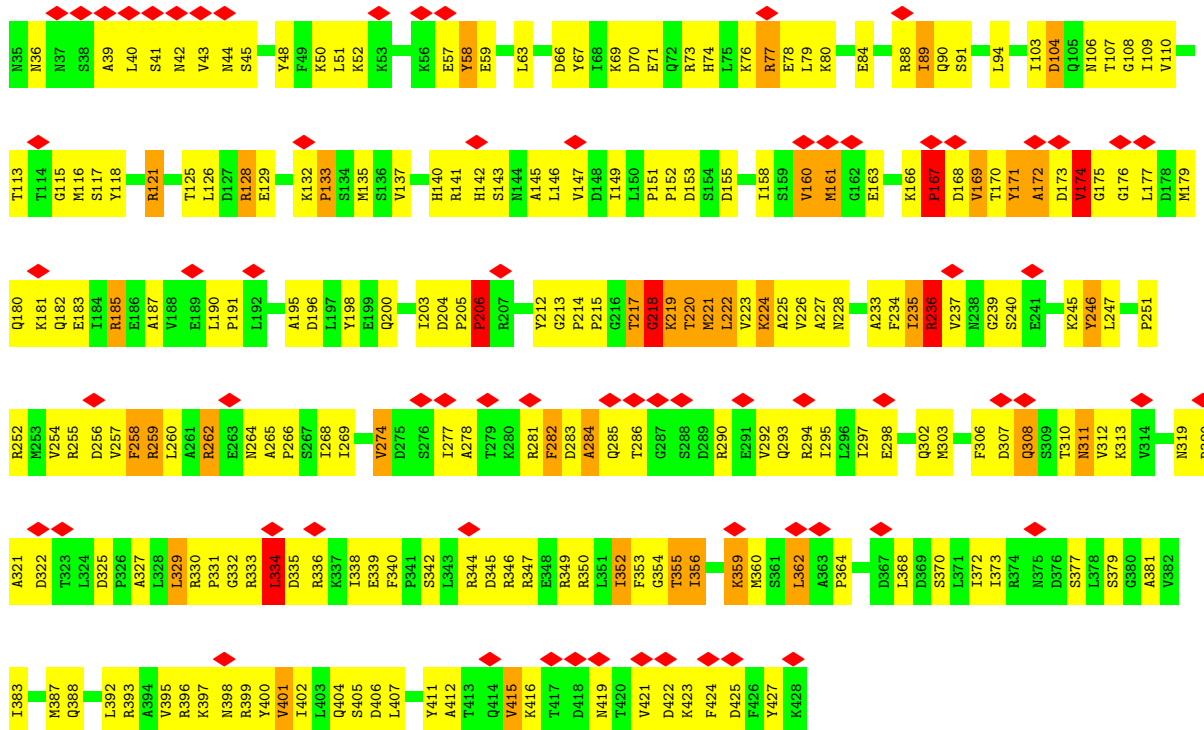


• Molecule 29: 26S proteasome regulatory subunit 4 homolog

Chain I: 23% 42% 50% 7% .

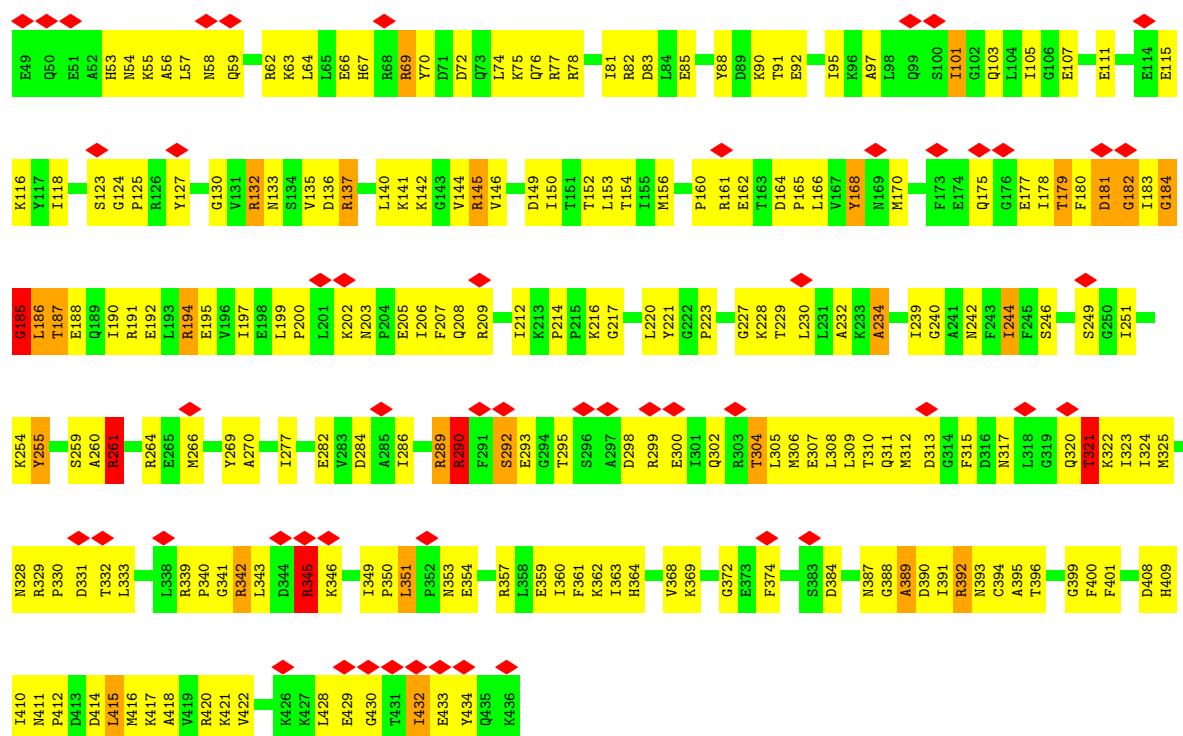


• Molecule 30: 26S proteasome regulatory subunit 6B homolog



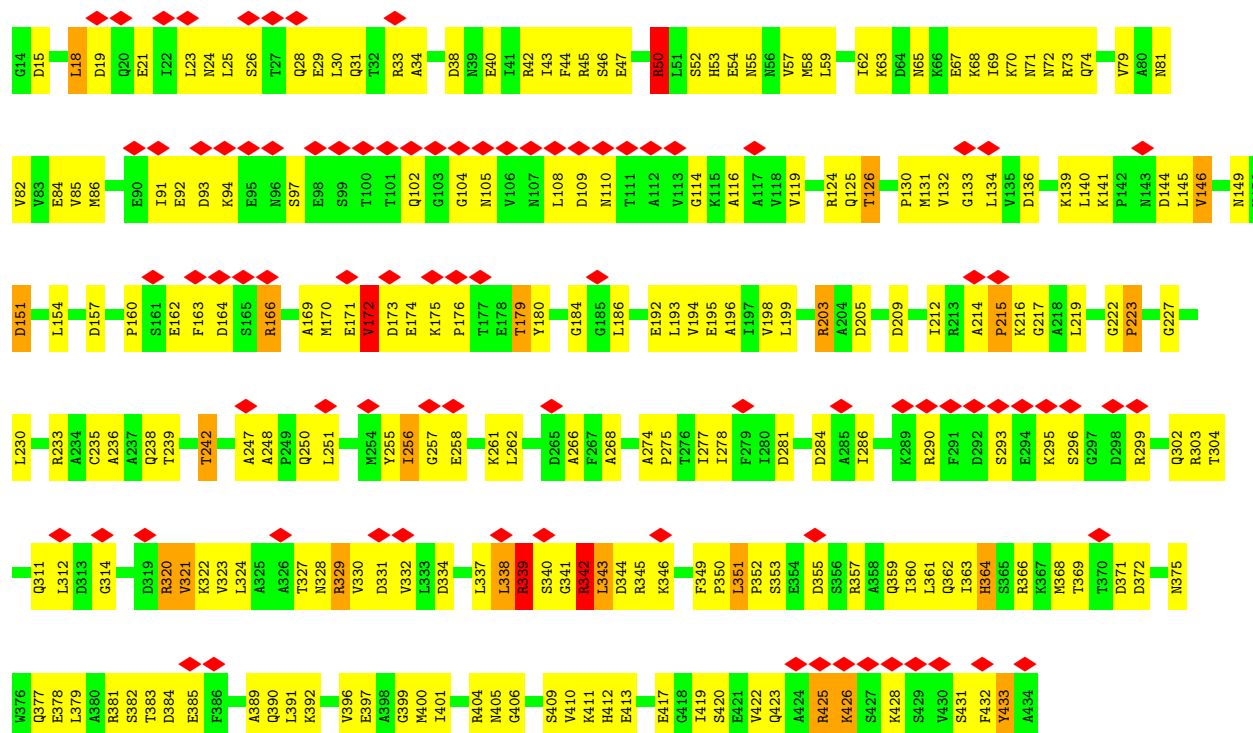
• Molecule 31: 26S proteasome subunit RPT4

Chain L: 13% 44% 48% 6%

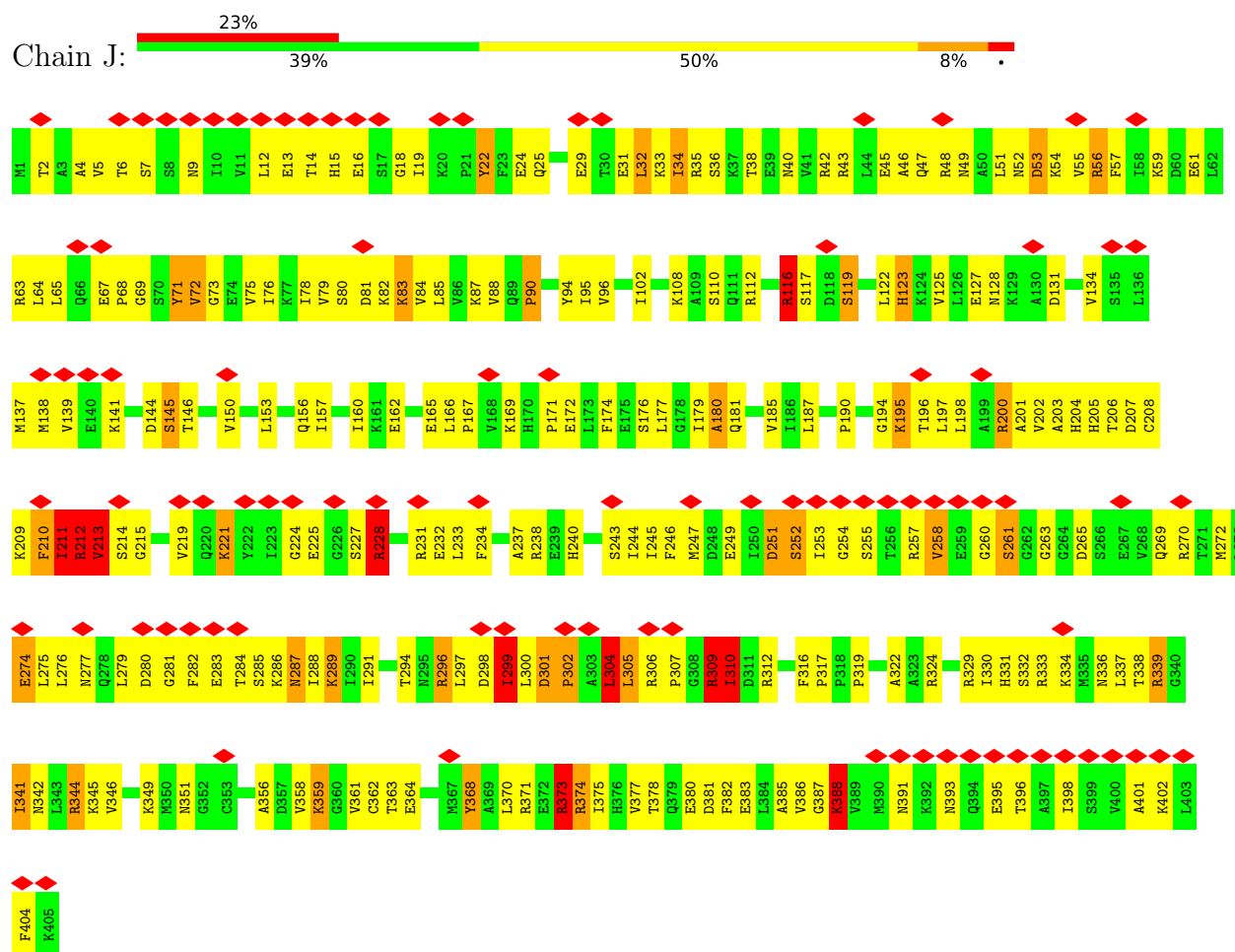


• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M: 21% 45% 49% 5%



● Molecule 33: 26S proteasome regulatory subunit 8 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292279	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.19	0/1946	1.44	5/2634 (0.2%)
1	a	2.26	74/1946 (3.8%)	2.38	119/2634 (4.5%)
2	B	1.16	0/1944	1.41	5/2632 (0.2%)
2	b	2.29	77/1944 (4.0%)	2.36	114/2632 (4.3%)
3	C	1.20	0/1935	1.41	6/2618 (0.2%)
3	c	2.32	79/1935 (4.1%)	2.47	127/2618 (4.9%)
4	D	1.23	0/1888	1.45	4/2557 (0.2%)
4	d	2.34	87/2012 (4.3%)	2.44	128/2718 (4.7%)
5	E	2.07	2/1909 (0.1%)	1.60	10/2571 (0.4%)
5	e	2.24	64/1909 (3.4%)	2.36	96/2571 (3.7%)
6	F	1.22	0/1800	1.44	10/2433 (0.4%)
6	f	2.29	72/1800 (4.0%)	2.41	108/2433 (4.4%)
7	G	1.21	1/1926 (0.1%)	1.70	5/2599 (0.2%)
7	g	2.25	71/1926 (3.7%)	2.60	123/2599 (4.7%)
8	1	2.27	64/1541 (4.2%)	2.31	81/2087 (3.9%)
8	h	2.26	60/1541 (3.9%)	2.34	84/2087 (4.0%)
9	2	2.30	69/1751 (3.9%)	2.39	112/2373 (4.7%)
9	i	2.36	80/1751 (4.6%)	2.46	107/2373 (4.5%)
10	3	2.30	66/1611 (4.1%)	2.34	84/2174 (3.9%)
10	j	2.25	59/1611 (3.7%)	2.34	104/2174 (4.8%)
11	4	2.33	63/1590 (4.0%)	2.41	98/2142 (4.6%)
11	k	2.31	53/1590 (3.3%)	2.40	77/2142 (3.6%)
12	5	2.25	63/1681 (3.7%)	2.39	98/2274 (4.3%)
12	l	2.29	66/1681 (3.9%)	2.46	138/2274 (6.1%)
13	6	2.29	83/1795 (4.6%)	2.42	115/2420 (4.8%)
13	m	2.26	60/1795 (3.3%)	2.41	103/2420 (4.3%)
14	7	2.29	75/1821 (4.1%)	2.46	121/2470 (4.9%)
14	n	2.29	74/1847 (4.0%)	2.46	126/2503 (5.0%)
15	W	2.34	63/1558 (4.0%)	2.45	111/2111 (5.3%)
16	V	2.25	91/2309 (3.9%)	2.53	158/3115 (5.1%)
17	T	2.22	81/2236 (3.6%)	2.53	173/3017 (5.7%)
18	X	2.22	31/1059 (2.9%)	2.38	51/1432 (3.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	2.08	18/741 (2.4%)	2.53	57/1000 (5.7%)
20	Z	1.65	23/7123 (0.3%)	1.98	176/9645 (1.8%)
21	N	2.27	270/7273 (3.7%)	2.50	489/9822 (5.0%)
22	S	2.26	144/3967 (3.6%)	2.51	302/5355 (5.6%)
23	P	2.18	113/3664 (3.1%)	2.53	278/4940 (5.6%)
24	Q	2.28	136/3556 (3.8%)	2.56	286/4787 (6.0%)
25	R	2.25	120/3314 (3.6%)	2.51	250/4469 (5.6%)
26	U	2.23	88/2461 (3.6%)	2.42	160/3327 (4.8%)
27	O	2.26	119/3247 (3.7%)	2.50	228/4380 (5.2%)
28	H	2.30	136/3282 (4.1%)	2.48	223/4423 (5.0%)
29	I	2.25	102/3059 (3.3%)	2.48	219/4115 (5.3%)
30	K	2.33	125/3156 (4.0%)	2.76	232/4261 (5.4%)
31	L	2.28	116/3128 (3.7%)	2.86	221/4201 (5.3%)
32	M	2.57	119/3323 (3.6%)	2.70	232/4478 (5.2%)
33	J	2.63	147/3212 (4.6%)	2.77	251/4316 (5.8%)
All	All	2.17	3504/112094 (3.1%)	2.38	6405/151356 (4.2%)

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	a	0	9
2	b	0	3
3	c	0	5
4	D	0	1
4	d	0	5
5	e	0	3
6	F	0	1
6	f	0	6
7	G	0	2
7	g	0	12
8	1	0	6
8	h	0	8
9	2	0	4
9	i	0	6
10	3	0	4
10	j	0	4
11	4	0	6
11	k	0	4
12	5	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
12	l	0	5
13	6	0	9
13	m	0	6
14	7	0	5
14	n	0	12
15	W	0	7
16	V	0	6
17	T	0	10
18	X	0	2
19	Y	0	1
20	Z	0	9
21	N	0	24
22	S	0	18
23	P	0	16
24	Q	0	13
25	R	0	11
26	U	0	6
27	O	0	9
28	H	0	13
29	I	0	9
30	K	0	19
31	L	0	18
32	M	0	13
33	J	0	15
All	All	0	351

The worst 5 of 3504 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	20	ARG	NE-CZ	73.61	2.14	1.33
33	J	211	ILE	C-N	-58.03	0.52	1.33
20	Z	728	LYS	CG-CD	52.64	3.10	1.52
20	Z	728	LYS	CA-CB	35.97	2.14	1.53
20	Z	738	TYR	CZ-OH	35.14	2.11	1.38

The worst 5 of 6405 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	185	GLY	O-C-N	-86.19	16.00	122.87
33	J	211	ILE	O-C-N	-64.49	47.31	122.12
30	K	167	PRO	O-C-N	-55.87	47.21	122.64
32	M	338	LEU	O-C-N	-39.48	69.00	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	728	LYS	CG-CD-CE	-38.20	23.45	111.30

There are no chirality outliers.

5 of 351 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	105	ARG	Sidechain
1	a	128	TYR	Sidechain
1	a	131	ARG	Sidechain
1	a	30	TYR	Sidechain
1	a	46	ARG	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	A	1908	0	1901	0	0
1	a	1908	0	1901	0	0
2	B	1907	0	1917	0	0
2	b	1907	0	1917	2	0
3	C	1905	0	1901	0	0
3	c	1905	0	1901	6	0
4	D	1859	0	1875	0	0
4	d	1982	0	1993	8	0
5	E	1883	0	1851	21	0
5	e	1883	0	1851	10	0
6	F	1773	0	1775	2	0
6	f	1773	0	1775	5	0
7	G	1886	0	1876	1	0
7	g	1886	0	1876	3	0
8	l	1512	0	1478	4	0
8	h	1512	0	1478	3	0
9	2	1720	0	1716	2	0
9	i	1720	0	1716	3	0
10	3	1581	0	1571	2	0
10	j	1581	0	1571	5	0
11	4	1562	0	1569	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	k	1562	0	1569	4	0
12	5	1644	0	1592	1	0
12	l	1644	0	1592	5	0
13	6	1757	0	1708	8	0
13	m	1757	0	1708	5	0
14	7	1790	0	1790	5	0
14	n	1816	0	1818	4	0
15	W	1535	0	1542	5	0
16	V	2274	0	2273	9	0
17	T	2193	0	2161	5	0
18	X	1033	0	1017	2	0
19	Y	731	0	675	1	0
20	Z	7006	0	6932	194	0
21	N	7158	0	7226	49	0
22	S	3895	0	3938	9	0
23	P	3609	0	3694	11	0
24	Q	3499	0	3524	6	0
25	R	3259	0	3263	8	0
26	U	2427	0	2462	11	0
27	O	3186	0	3213	10	0
28	H	3234	0	3250	29	0
29	I	3022	0	3088	180	0
30	K	3113	0	3164	67	0
31	L	3083	0	3155	45	0
32	M	3285	0	3322	38	0
33	J	3171	0	3311	46	0
34	H	27	0	12	14	0
34	M	27	0	12	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
36	I	31	0	12	10	0
36	J	31	0	12	4	0
36	K	31	0	12	10	0
36	L	31	0	12	13	0
All	All	110420	0	110468	626	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 3.

The worst 5 of 626 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)
30:K:173:ASP:C	30:K:355:THR:HG21	1.30	1.51
30:K:173:ASP:C	30:K:355:THR:CG2	1.80	1.49
33:J:212:ARG:C	33:J:213:VAL:N	1.68	1.48
32:M:338:LEU:C	32:M:339:ARG:N	1.69	1.48
32:M:433:TYR:CZ	32:M:433:TYR:CE1	2.01	1.46

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	A	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
1	a	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	16	53
2	B	247/249 (99%)	232 (94%)	15 (6%)	0	100	100
2	b	247/249 (99%)	231 (94%)	14 (6%)	2 (1%)	16	53
3	C	242/244 (99%)	232 (96%)	10 (4%)	0	100	100
3	c	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
4	D	235/251 (94%)	222 (94%)	13 (6%)	0	100	100
4	d	249/251 (99%)	229 (92%)	14 (6%)	6 (2%)	4	26
5	E	242/244 (99%)	225 (93%)	11 (4%)	6 (2%)	4	25
5	e	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	10	43
6	F	229/231 (99%)	219 (96%)	9 (4%)	1 (0%)	30	67
6	f	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	5	28
7	G	240/242 (99%)	229 (95%)	11 (5%)	0	100	100
7	g	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	30	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1	194/196 (99%)	185 (95%)	8 (4%)	1 (0%)	24	63
8	h	194/196 (99%)	177 (91%)	12 (6%)	5 (3%)	4	24
9	2	224/226 (99%)	215 (96%)	7 (3%)	2 (1%)	14	50
9	i	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	9	40
10	3	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	24	63
10	j	202/204 (99%)	185 (92%)	11 (5%)	6 (3%)	3	22
11	4	193/195 (99%)	183 (95%)	7 (4%)	3 (2%)	7	36
11	k	193/195 (99%)	176 (91%)	13 (7%)	4 (2%)	5	28
12	5	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	24	63
12	l	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
13	6	220/222 (99%)	204 (93%)	12 (6%)	4 (2%)	6	33
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	9	38
14	7	227/232 (98%)	205 (90%)	18 (8%)	4 (2%)	6	33
14	n	230/232 (99%)	214 (93%)	14 (6%)	2 (1%)	14	50
15	W	195/197 (99%)	178 (91%)	11 (6%)	6 (3%)	3	21
16	V	287/289 (99%)	260 (91%)	20 (7%)	7 (2%)	4	26
17	T	264/266 (99%)	248 (94%)	14 (5%)	2 (1%)	16	53
18	X	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	2	17
19	Y	87/89 (98%)	72 (83%)	10 (12%)	5 (6%)	1	13
20	Z	902/970 (93%)	820 (91%)	59 (6%)	23 (2%)	4	25
21	N	920/922 (100%)	865 (94%)	41 (4%)	14 (2%)	8	38
22	S	473/475 (100%)	445 (94%)	19 (4%)	9 (2%)	6	31
23	P	438/440 (100%)	415 (95%)	16 (4%)	7 (2%)	7	36
24	Q	432/434 (100%)	394 (91%)	26 (6%)	12 (3%)	4	23
25	R	403/405 (100%)	388 (96%)	10 (2%)	5 (1%)	10	43
26	U	302/304 (99%)	288 (95%)	13 (4%)	1 (0%)	36	71
27	O	386/388 (100%)	371 (96%)	10 (3%)	5 (1%)	9	40
28	H	415/417 (100%)	364 (88%)	39 (9%)	12 (3%)	3	23
29	I	379/385 (98%)	353 (93%)	18 (5%)	8 (2%)	5	28
30	K	392/394 (100%)	353 (90%)	28 (7%)	11 (3%)	4	23
31	L	384/388 (99%)	360 (94%)	18 (5%)	6 (2%)	7	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	M	419/421 (100%)	376 (90%)	30 (7%)	13 (3%)	3	21
33	J	403/405 (100%)	362 (90%)	22 (6%)	19 (5%)	2	16
All	All	13911/14094 (99%)	12913 (93%)	763 (6%)	235 (2%)	9	34

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	31	THR
4	d	50	SER
6	f	14	SER
5	E	16	SER
13	6	27	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/206 (100%)	204 (99%)	2 (1%)	68	76
1	a	206/206 (100%)	201 (98%)	5 (2%)	43	62
2	B	208/208 (100%)	207 (100%)	1 (0%)	81	82
2	b	208/208 (100%)	204 (98%)	4 (2%)	50	66
3	C	203/203 (100%)	202 (100%)	1 (0%)	81	82
3	c	203/203 (100%)	197 (97%)	6 (3%)	36	56
4	D	210/224 (94%)	209 (100%)	1 (0%)	81	82
4	d	224/224 (100%)	216 (96%)	8 (4%)	31	52
5	E	200/200 (100%)	196 (98%)	4 (2%)	48	65
5	e	200/200 (100%)	190 (95%)	10 (5%)	22	42
6	F	190/190 (100%)	189 (100%)	1 (0%)	81	82
6	f	190/190 (100%)	182 (96%)	8 (4%)	26	47
7	G	200/200 (100%)	196 (98%)	4 (2%)	48	65
7	g	200/200 (100%)	189 (94%)	11 (6%)	19	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1	162/162 (100%)	157 (97%)	5 (3%)	35	55
8	h	162/162 (100%)	155 (96%)	7 (4%)	26	47
9	2	185/185 (100%)	181 (98%)	4 (2%)	45	63
9	i	185/185 (100%)	179 (97%)	6 (3%)	34	55
10	3	172/172 (100%)	168 (98%)	4 (2%)	44	63
10	j	172/172 (100%)	167 (97%)	5 (3%)	37	57
11	4	173/173 (100%)	169 (98%)	4 (2%)	44	63
11	k	173/173 (100%)	170 (98%)	3 (2%)	53	67
12	5	169/169 (100%)	165 (98%)	4 (2%)	43	62
12	l	169/169 (100%)	165 (98%)	4 (2%)	43	62
13	6	185/185 (100%)	182 (98%)	3 (2%)	55	69
13	m	185/185 (100%)	178 (96%)	7 (4%)	29	50
14	7	195/198 (98%)	187 (96%)	8 (4%)	27	48
14	n	198/198 (100%)	192 (97%)	6 (3%)	36	56
15	W	171/171 (100%)	163 (95%)	8 (5%)	23	44
16	V	253/253 (100%)	251 (99%)	2 (1%)	73	78
17	T	249/249 (100%)	241 (97%)	8 (3%)	34	55
18	X	116/116 (100%)	111 (96%)	5 (4%)	26	47
19	Y	81/81 (100%)	79 (98%)	2 (2%)	42	61
20	Z	773/828 (93%)	754 (98%)	19 (2%)	42	61
21	N	776/776 (100%)	760 (98%)	16 (2%)	47	64
22	S	447/447 (100%)	436 (98%)	11 (2%)	42	61
23	P	412/412 (100%)	407 (99%)	5 (1%)	63	74
24	Q	391/391 (100%)	378 (97%)	13 (3%)	33	54
25	R	356/356 (100%)	348 (98%)	8 (2%)	45	63
26	U	277/277 (100%)	268 (97%)	9 (3%)	34	55
27	O	363/363 (100%)	349 (96%)	14 (4%)	28	49
28	H	352/352 (100%)	345 (98%)	7 (2%)	48	65
29	I	342/342 (100%)	331 (97%)	11 (3%)	34	55
30	K	346/346 (100%)	333 (96%)	13 (4%)	29	50
31	L	332/332 (100%)	321 (97%)	11 (3%)	33	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	M	364/364 (100%)	357 (98%)	7 (2%)	50	66
33	J	352/352 (100%)	337 (96%)	15 (4%)	26	47
All	All	12086/12158 (99%)	11766 (97%)	320 (3%)	41	60

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	R	375	LYS
30	K	401	VAL
26	U	212	ASP
28	H	267	THR
32	M	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 336 such sidechains are listed below:

Mol	Chain	Res	Type
22	S	378	GLN
27	O	282	GLN
23	P	277	GLN
25	R	325	HIS
29	I	151	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
36	ATP	K	501	35	32,33,33	4.47	5 (15%)	48,52,52	1.75	12 (25%)
34	ADP	H	501	35	28,29,29	1.52	4 (14%)	43,45,45	1.66	7 (16%)
36	ATP	J	501	35	32,33,33	3.77	6 (18%)	48,52,52	1.37	6 (12%)
36	ATP	I	501	35	32,33,33	4.48	6 (18%)	48,52,52	1.72	11 (22%)
34	ADP	M	501	35	28,29,29	2.34	8 (28%)	43,45,45	1.53	6 (13%)
36	ATP	L	501	35	32,33,33	4.45	6 (18%)	48,52,52	1.70	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	K	501	35	-	4/22/38/38	0/3/3/3
34	ADP	H	501	35	-	4/16/32/32	0/3/3/3
36	ATP	J	501	35	-	5/22/38/38	0/3/3/3
36	ATP	I	501	35	-	5/22/38/38	0/3/3/3
34	ADP	M	501	35	-	4/16/32/32	0/3/3/3
36	ATP	L	501	35	-	6/22/38/38	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	501	ATP	PB-O3B	19.33	1.80	1.59
36	L	501	ATP	PB-O3B	19.22	1.80	1.59
36	K	501	ATP	PB-O3B	19.17	1.80	1.59
36	J	501	ATP	PB-O3A	14.78	1.75	1.59
36	J	501	ATP	PB-O3B	13.00	1.73	1.59

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	M	501	ADP	C4-N9-C8	-5.80	99.65	105.74
34	H	501	ADP	N3-C2-N1	5.17	136.41	128.58
36	K	501	ATP	O4'-C1'-N9	4.70	117.11	108.09
36	I	501	ATP	O4'-C1'-N9	4.69	117.09	108.09
36	L	501	ATP	O4'-C1'-N9	4.66	117.04	108.09

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

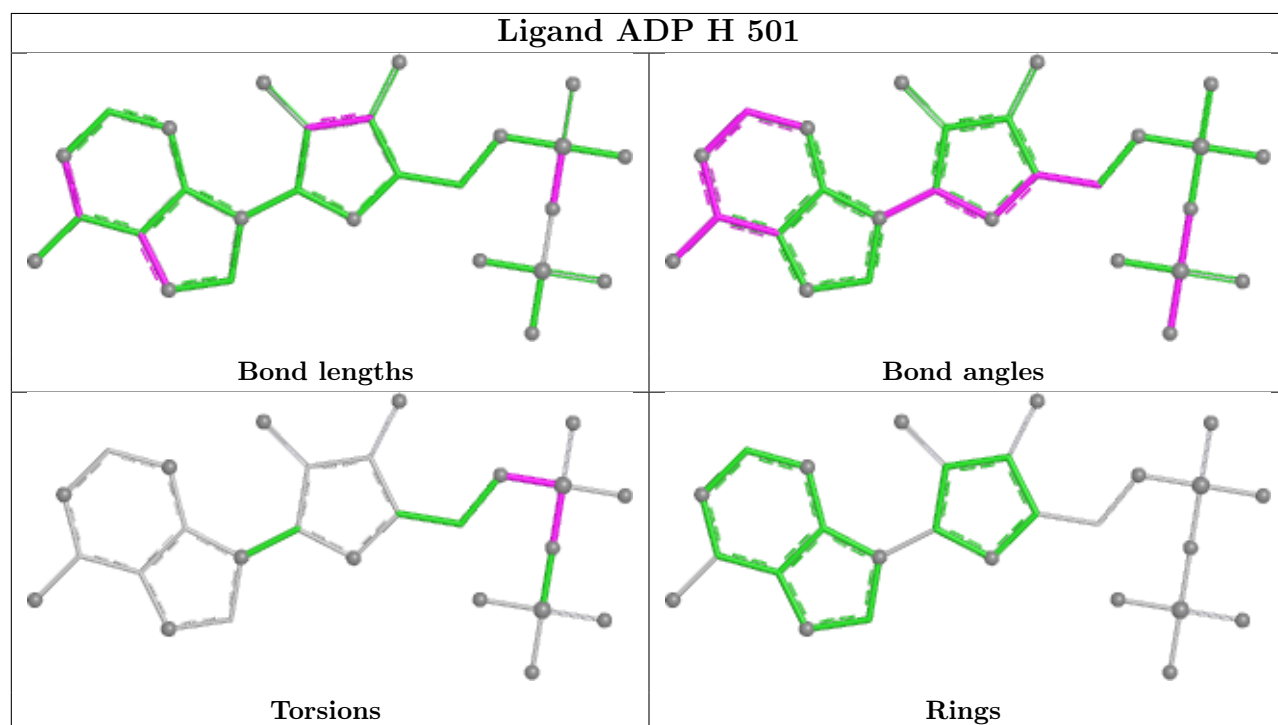
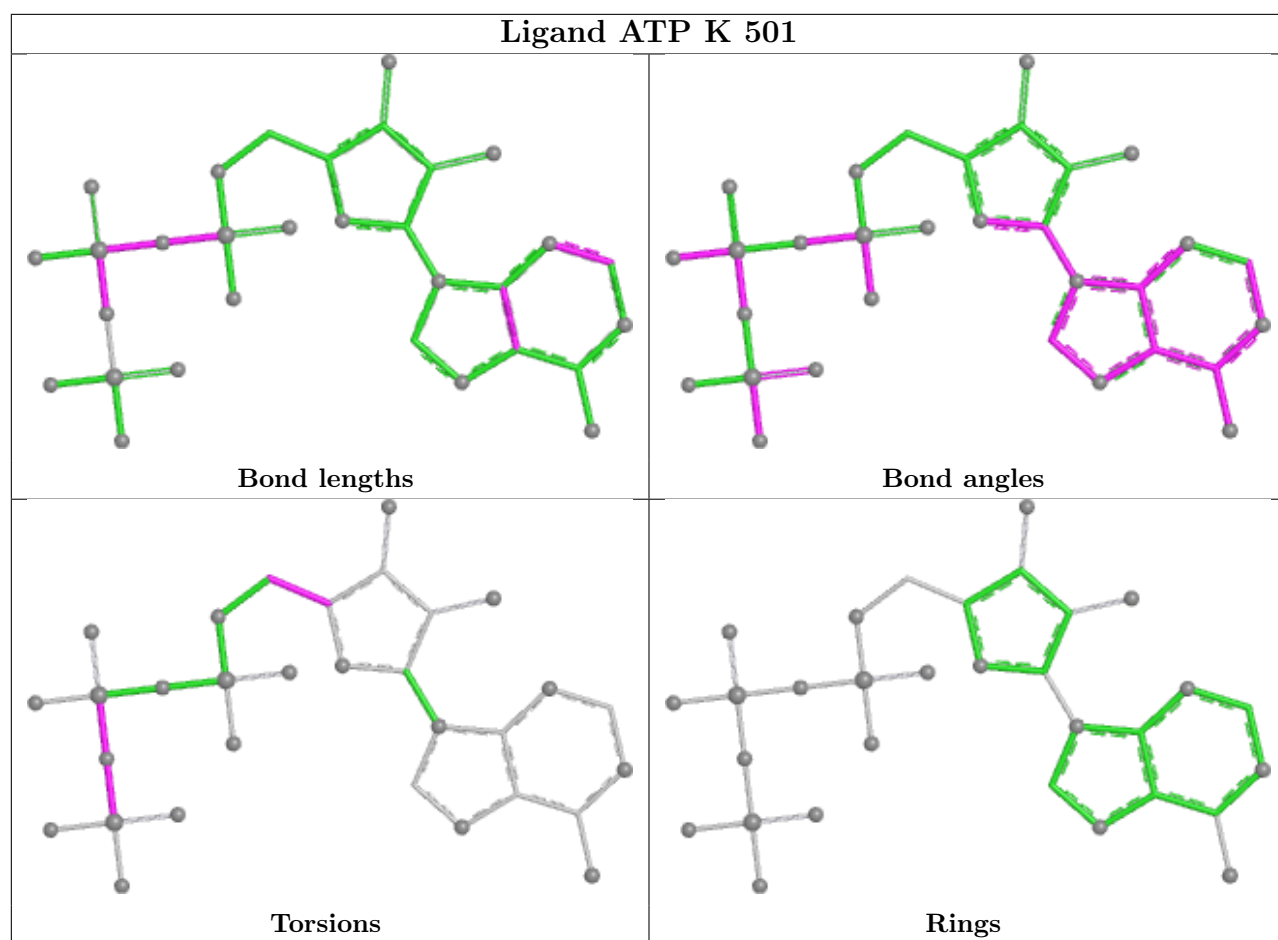
Mol	Chain	Res	Type	Atoms
34	H	501	ADP	C5'-O5'-PA-O2A
34	H	501	ADP	C5'-O5'-PA-O3A
34	M	501	ADP	C5'-O5'-PA-O1A
34	M	501	ADP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3B-PG-O2G

There are no ring outliers.

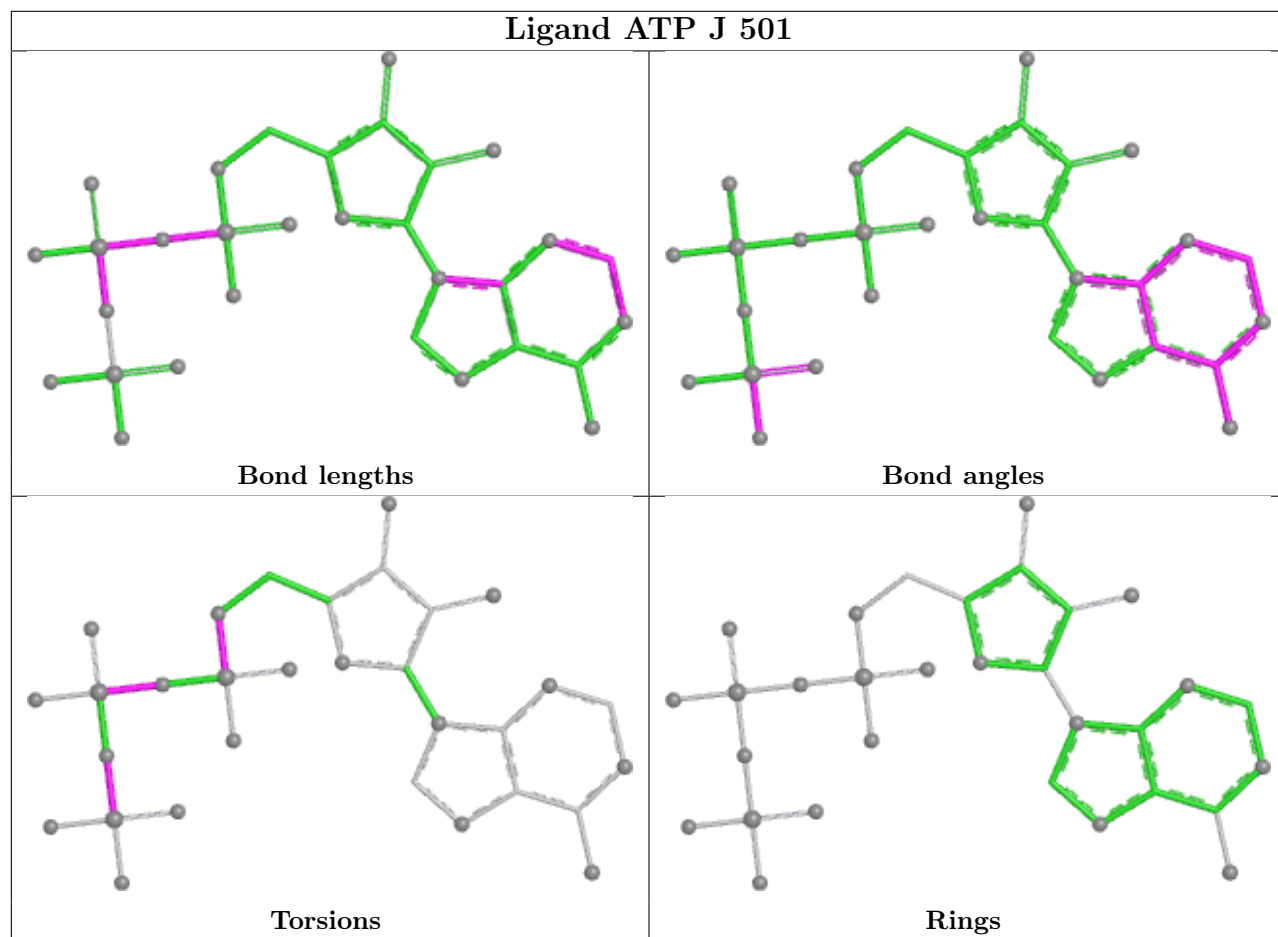
5 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	K	501	ATP	10	0
34	H	501	ADP	14	0
36	J	501	ATP	4	0
36	I	501	ATP	10	0
36	L	501	ATP	13	0

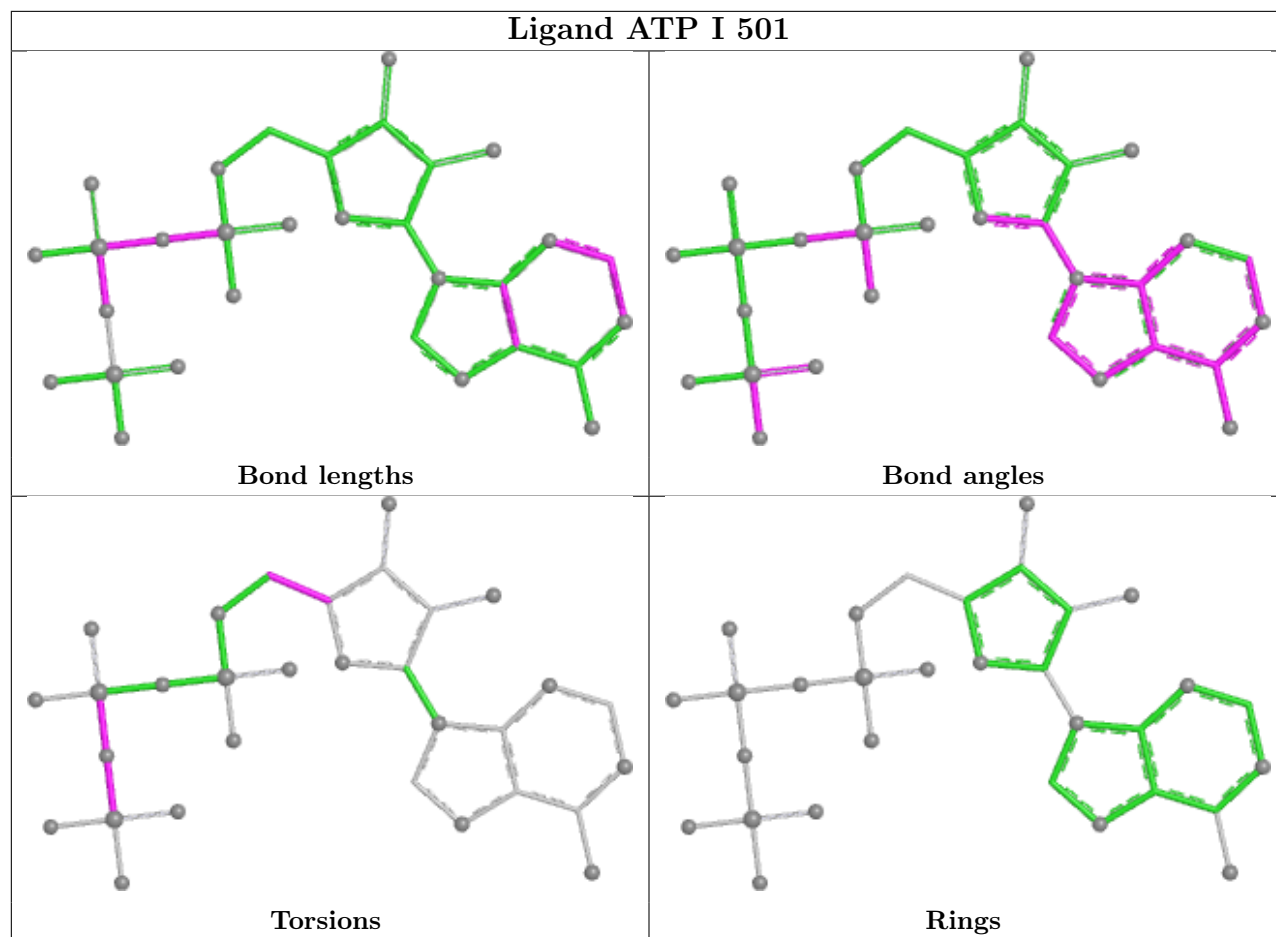
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



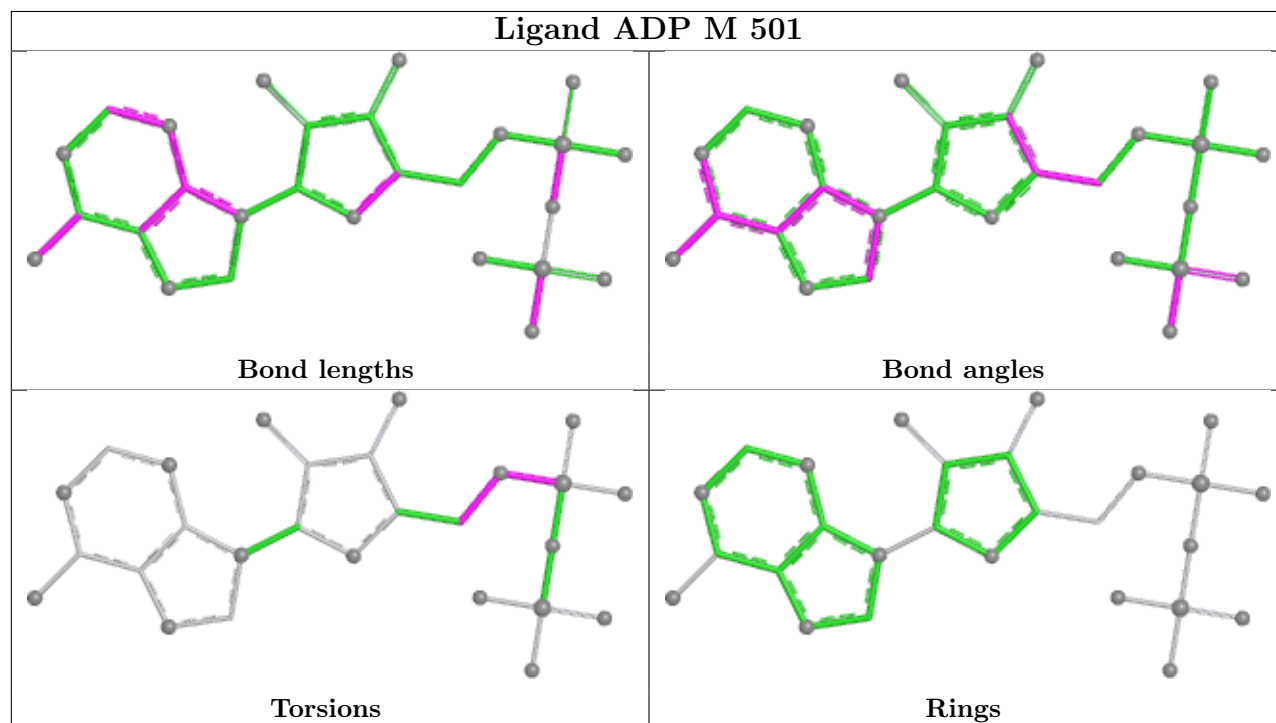
Ligand ATP J 501

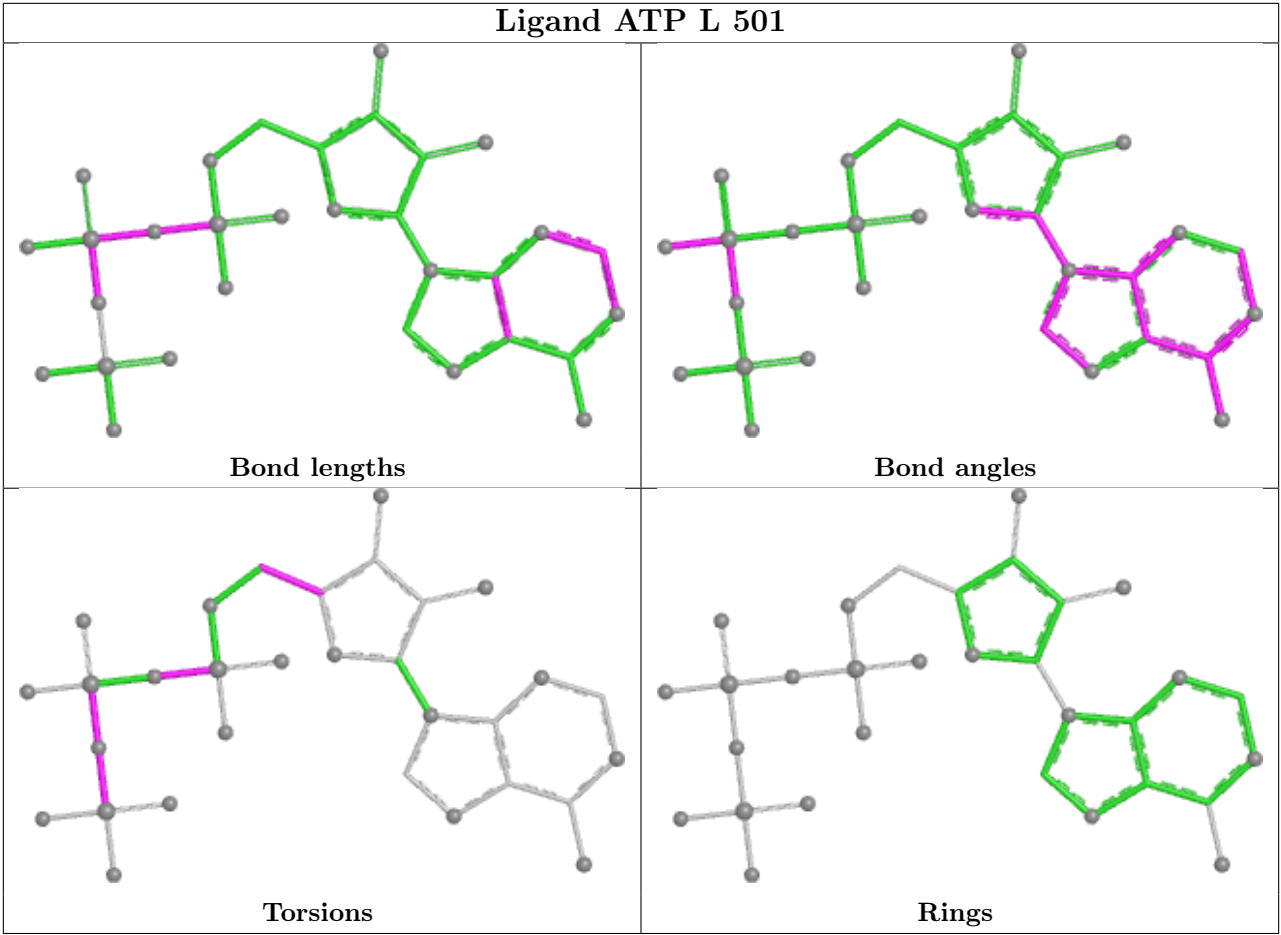


Ligand ATP I 501



Ligand ADP M 501





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
29	I	2
32	M	2
33	J	2
31	L	1
30	K	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	180:PHE	C	181:ASP	N	2.67

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	183:ASP	C	184:ILE	N	2.58
1	I	186:GLY	C	187:LEU	N	2.56
1	M	338:LEU	C	339:ARG	N	1.69
1	J	212:ARG	C	213:VAL	N	1.68

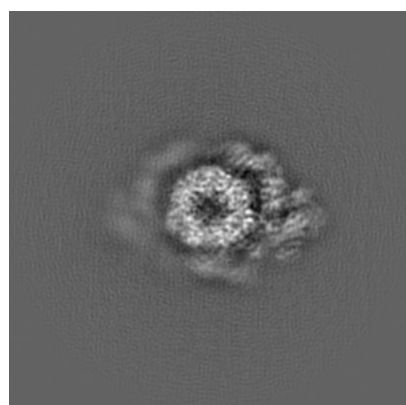
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4321. These allow visual inspection of the internal detail of the map and identification of artifacts.

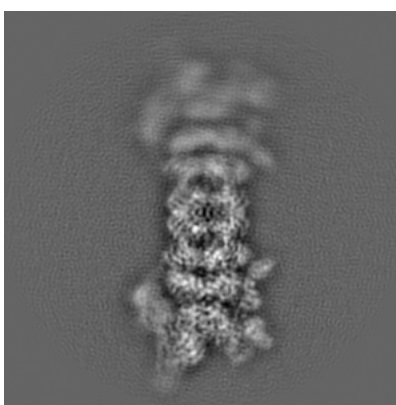
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

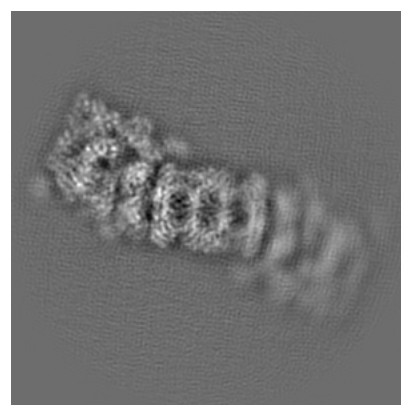
6.1.1 Primary map



X



Y

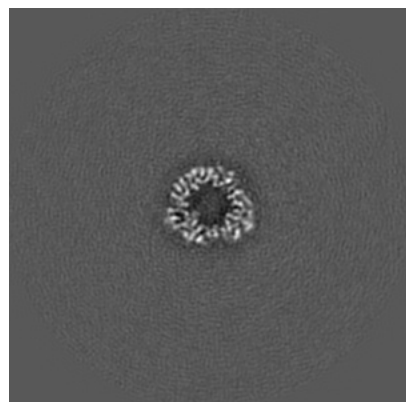


Z

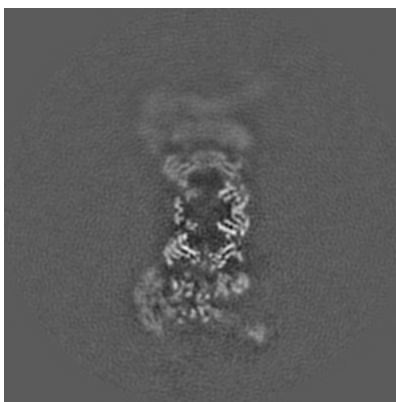
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

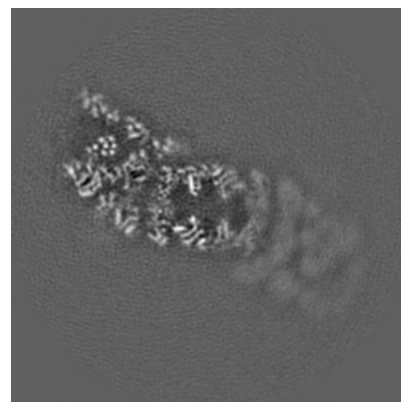
6.2.1 Primary map



X Index: 192



Y Index: 192

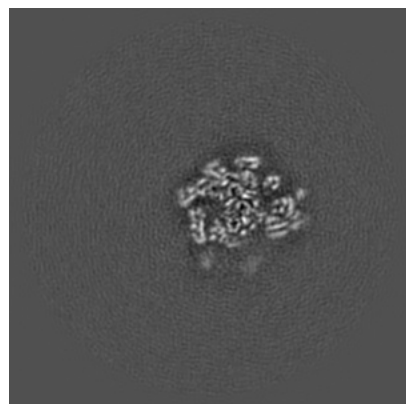


Z Index: 192

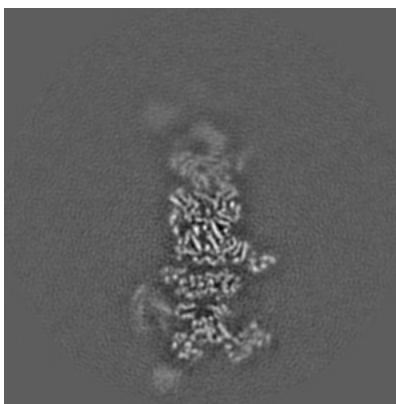
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

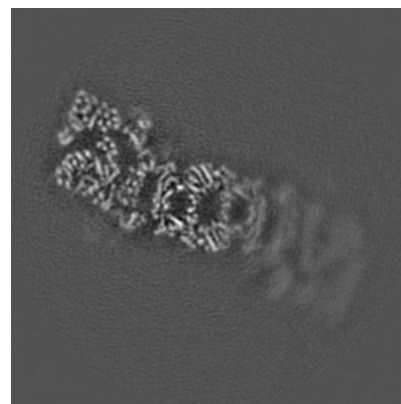
6.3.1 Primary map



X Index: 122



Y Index: 213

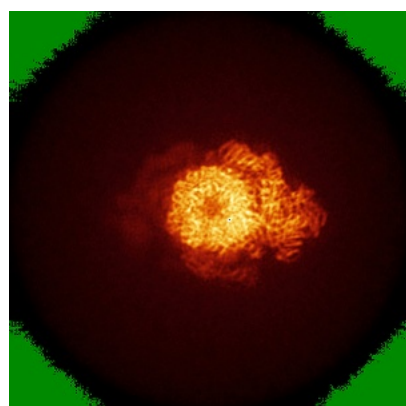


Z Index: 182

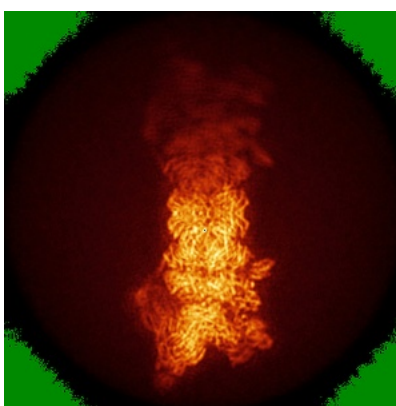
The images above show the largest variance slices of the map in three orthogonal directions.

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

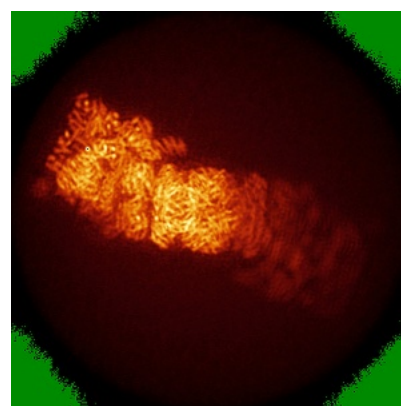
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

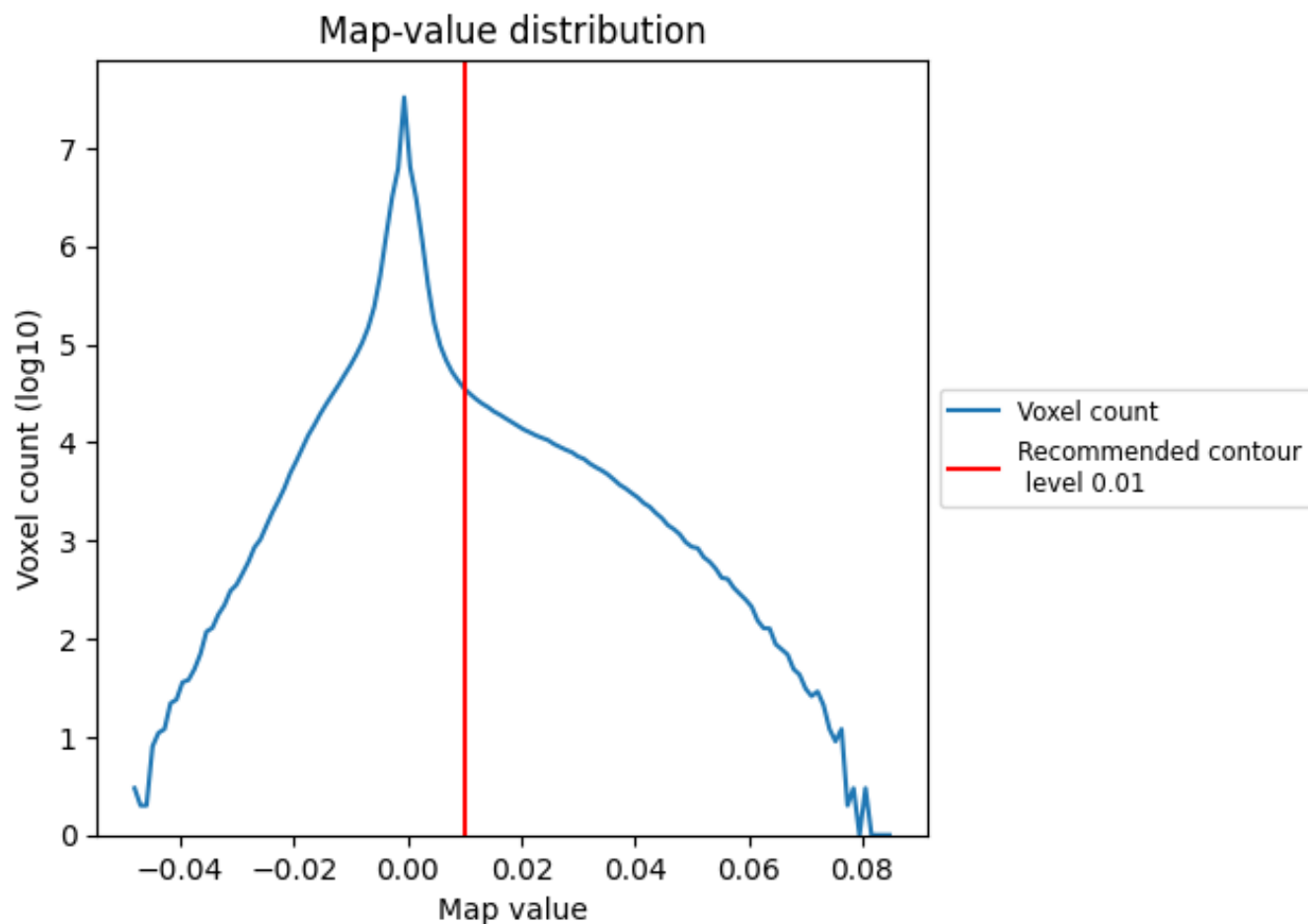
6.6 Mask visualisation

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

7 Map analysis [i](#)

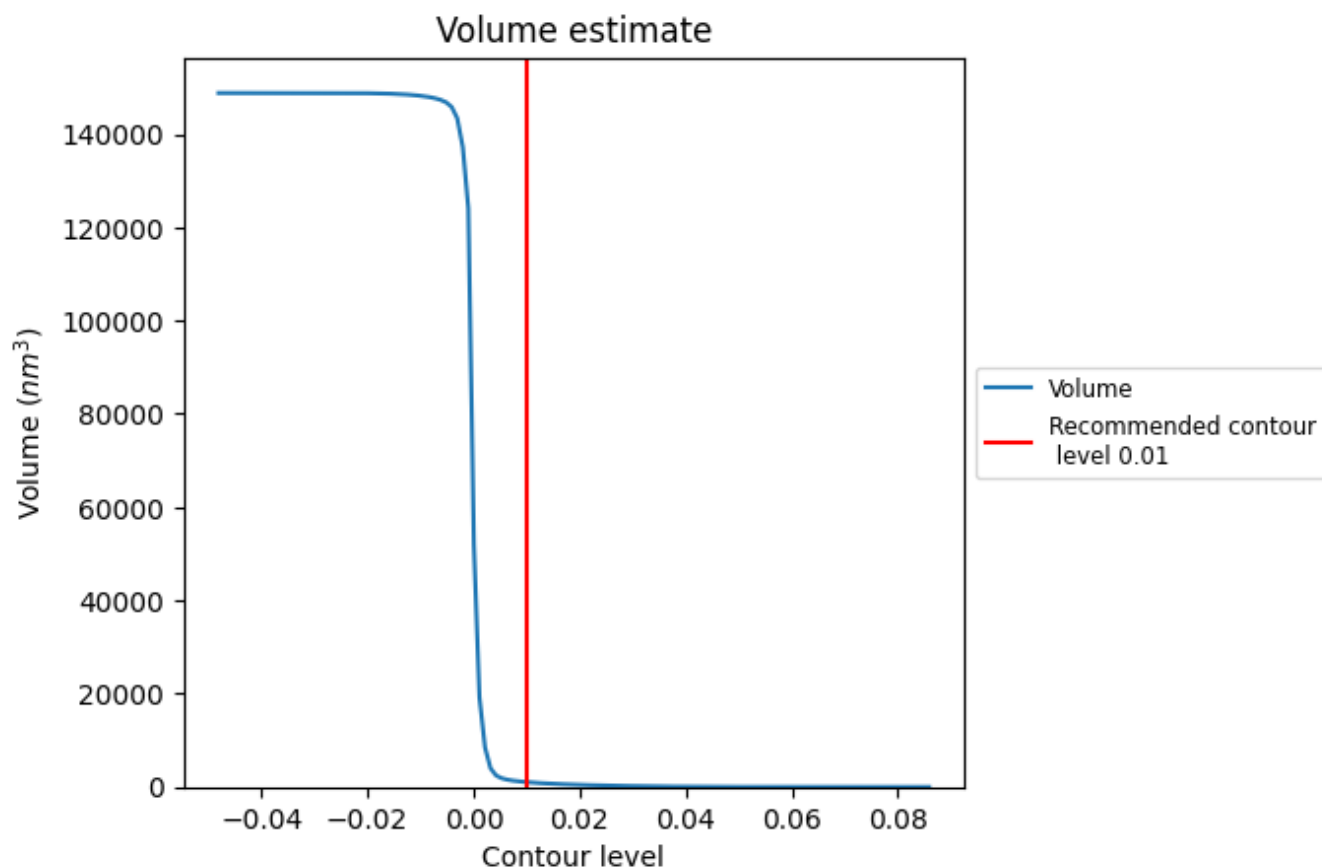
This section contains the results of statistical analysis of the map.

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.

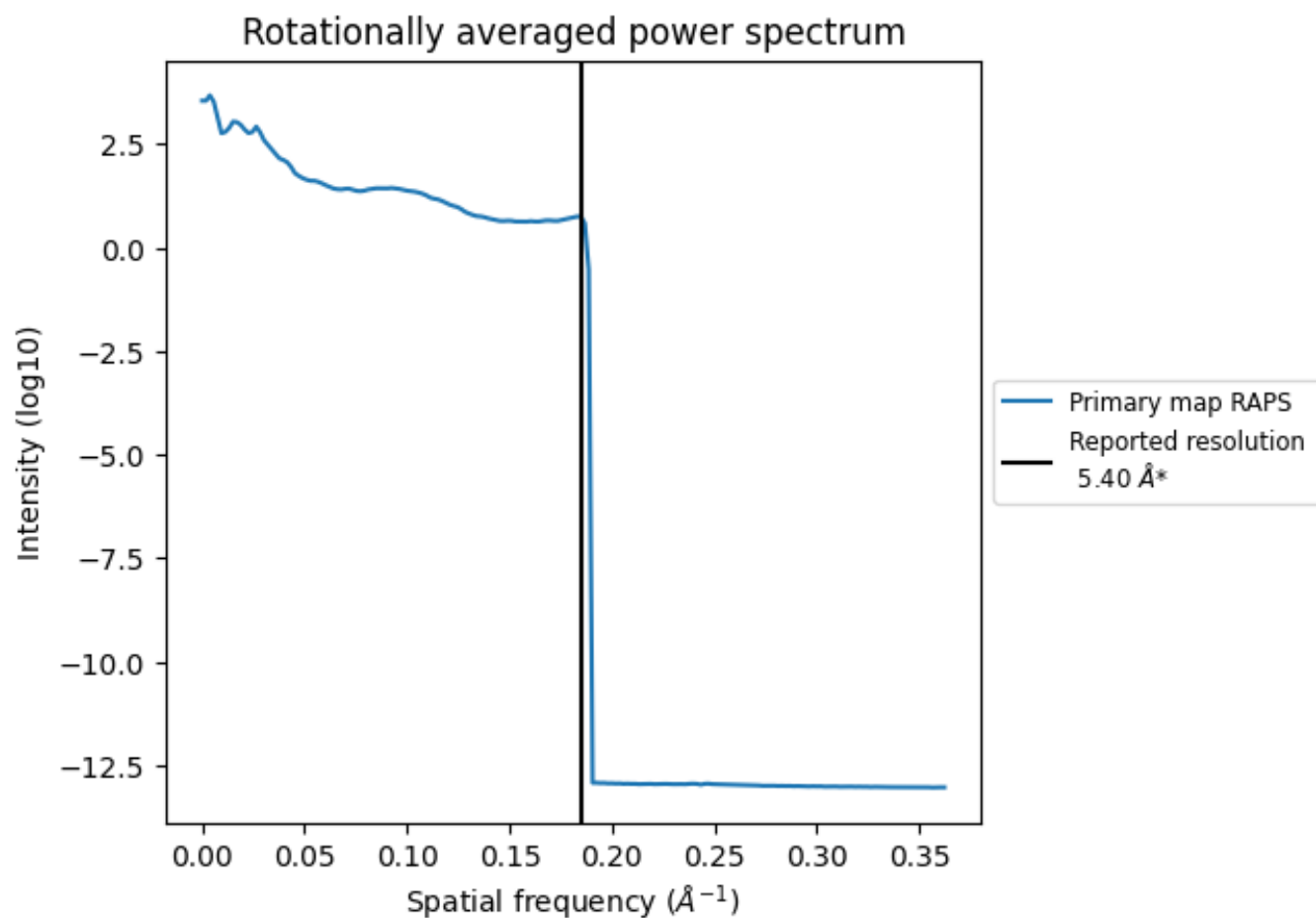
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1039 nm^3 ; this corresponds to an approximate mass of 938 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.185 $\text{\AA}^{-1}$

8 Fourier-Shell correlation ⓘ

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

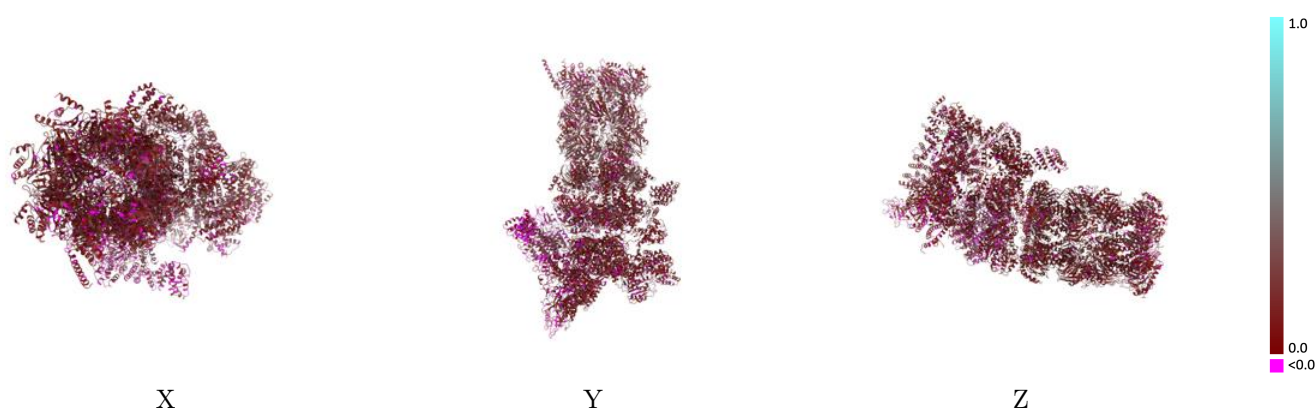
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4321 and PDB model 6FVV. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

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

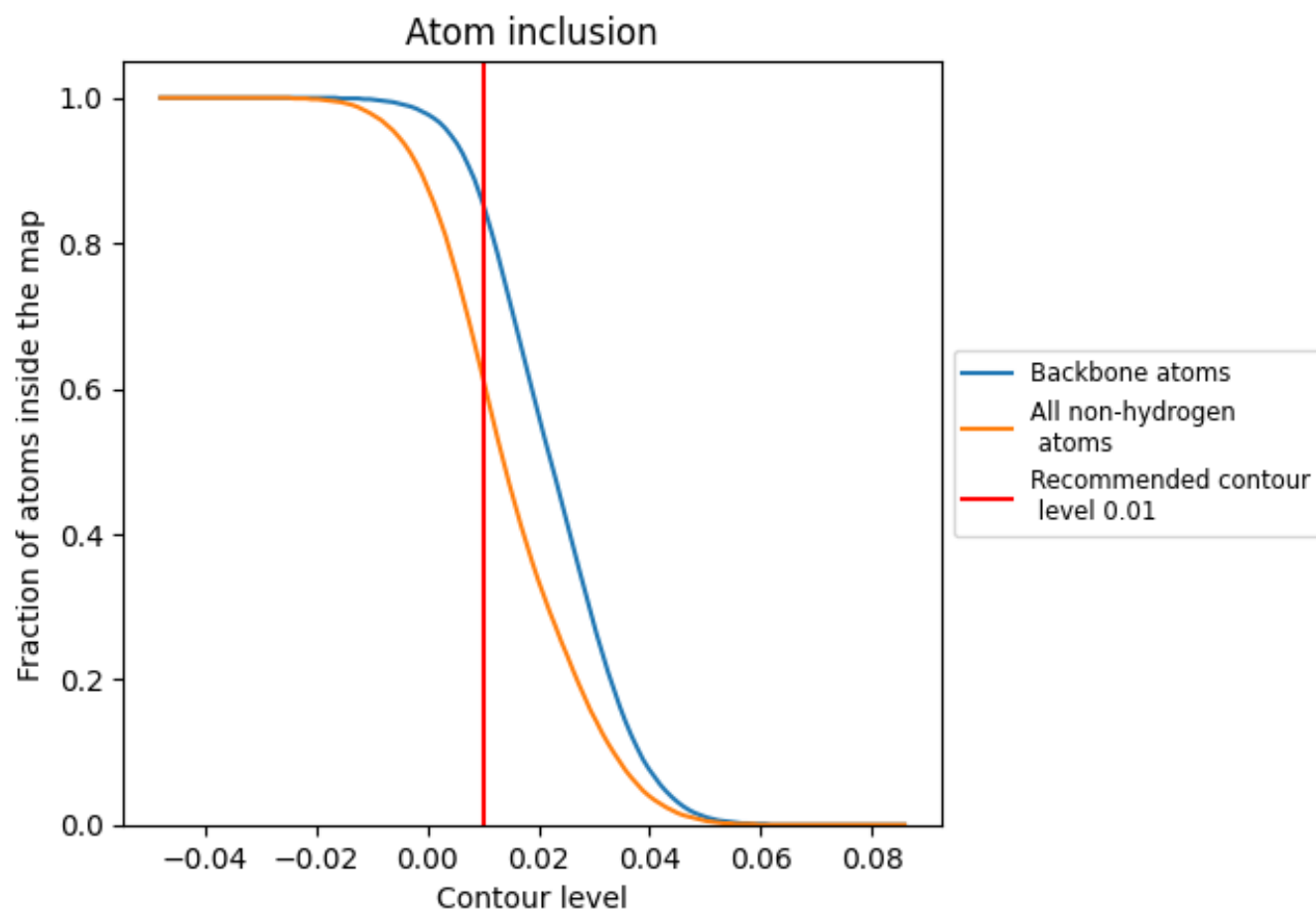


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 61% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.1490
1	 0.7310	 0.1860
2	 0.7210	 0.1970
3	 0.6850	 0.1880
4	 0.7140	 0.1830
5	 0.7400	 0.1850
6	 0.7100	 0.1840
7	 0.7230	 0.1830
A	 0.7000	 0.1800
B	 0.6810	 0.1950
C	 0.6880	 0.1850
D	 0.7000	 0.1870
E	 0.6740	 0.1750
F	 0.7100	 0.1830
G	 0.7100	 0.1820
H	 0.5850	 0.1240
I	 0.5760	 0.1380
J	 0.5790	 0.1250
K	 0.5990	 0.1410
L	 0.6450	 0.1490
M	 0.5990	 0.1300
N	 0.6510	 0.1540
O	 0.6890	 0.1520
P	 0.7390	 0.1520
Q	 0.6930	 0.1450
R	 0.6900	 0.1450
S	 0.6220	 0.1380
T	 0.6380	 0.1340
U	 0.6130	 0.1490
V	 0.6500	 0.1610
W	 0.6020	 0.1360
X	 0.2610	 0.0510
Y	 0.4140	 0.0670
Z	 0.3350	 0.0590
a	 0.5000	 0.1460



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.4420	 0.1550
c	 0.4700	 0.1370
d	 0.4520	 0.1300
e	 0.4500	 0.1420
f	 0.5230	 0.1570
g	 0.5170	 0.1430
h	 0.6950	 0.1650
i	 0.6780	 0.1790
j	 0.6600	 0.1750
k	 0.6760	 0.1760
l	 0.6870	 0.1680
m	 0.6530	 0.1690
n	 0.6640	 0.1710