wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 02:21 PM EST

PDB ID	:	6MSE
EMDB ID	:	EMD-9218
Title	:	Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors	:	Mao, Y.D.
Deposited on	:	2018-10-16
Resolution	:	3.30 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 (1)) were used in the production of this report:

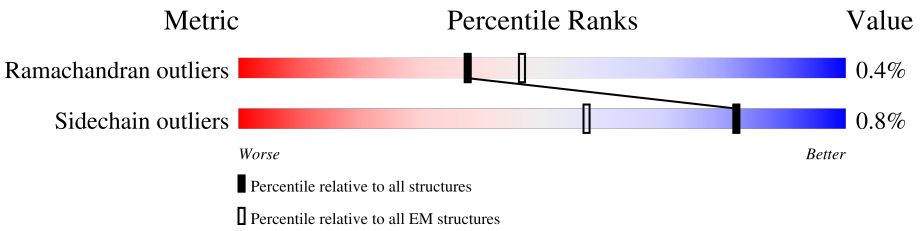
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	U	953	50% 85% • 15%
2	V	533	66% 88% • 10%
3	W	456	47% 98% •
4	X	422	50% 89% • 10%
5	Y	389	62% 89% 7% • •
6	Z	324	37% 86% • 12%
7	a	376	57% 97% • •
8	b	377	42% 50% • 49%
9	c	309	33% 90% • 7%

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Mol	Chain	Length	Quality of chain
10	d	349	65% 72% 26%
11	e	70	46% 36% 20% 43%
12	f	892	84% 95%
13	A	433	34% 88% 9%
14	B	440	40% 88% 10%
15	C	398	57% 92%
16	D	418	32% 88% 9%
17	E	403	28% 95%
18	F	439	32% 92% 5%
19	u	76	50% 99%
20	v	28	71% 100%
21	G	245	13% 98%
21	g	245	43% 98%
22	H	233	8% 100%
22	h	233	41% 100%
23	I	260	21% 96%
23	i	260	57% 96%
24	J	247	23% 96%
24	j	247	57% 96%
25	K	240	19% 94% 5%
25	k	240	53% 94% 5%
26	L	268	15% 89% 11%
26	l	268	32% 89% 11%
27	M	254	16% 94% 6%
27	m	254	38% 94% 6%

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Mol	Chain	Length	Quality of chain
28	N	238	8% 80% 20%
28	n	238	11% 80% 20%
29	O	276	10% 80% 20%
29	o	276	17% 80% 20%
30	P	204	14% 100%
30	p	204	16% 100%
31	Q	201	14% 98%
31	q	201	24% 98%
32	R	262	10% 77% 23%
32	r	262	12% 77% 23%
33	S	240	14% 89% 11%
33	s	240	15% 89% 11%
34	T	263	10% 81% 18%
34	t	263	11% 81% 18%

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 105062 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 non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	812	6334	4023	1078	1189	44	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	480	3852	2444	684	710	14	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	456	3703	2339	635	704	25	0	0

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	380	3009	1918	509	570	12	0	0

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	a	373	2995	1911	510	559	15	0	0

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d	257	2116	1371	346	390	9	0	0

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	40	334	200	55	77	2	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	f	889	6866	4315	1174	1331	46	0	0

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	393	3067	1930	539	581	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	395	3086	1946	523	602	15	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	381	2978	1872	536	554	16	0	0

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	D	380	3039	1923	524	579	13	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	E	389	3097	1947	552	581	17	0	0

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	415	3251	2038	561	634	18	0	0

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	76	603	378	107	117	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	v	28	143	86	29	28	0	0

- Molecule 21 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	240	1826	1160	305	348	13	0	0
			Total	C	N	O	S		
21	g	240	1826	1160	305	348	13	0	0

- Molecule 22 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	H	232	1708	1081	289	333	5	0	0
			Total	C	N	O	S		
22	h	232	1708	1081	289	333	5	0	0

- Molecule 23 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	I	250	1912	1204	329	371	8	0	0
			Total	C	N	O	S		
23	i	250	1912	1204	329	371	8	0	0

- Molecule 24 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	J	239	1704	1056	308	335	5	0	0
			Total	C	N	O	S		
24	j	239	1704	1056	308	335	5	0	0

- Molecule 25 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	K	228	1722	1080	284	348	10	0	0
			Total	C	N	O	S		
25	k	228	1722	1080	284	348	10	0	0

- Molecule 26 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	L	238	1850	1159	334	346	11	0	0
26	l	238	1850	1159	334	346	11	0	0

- Molecule 27 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	M	240	1856	1178	314	353	11	0	0
27	m	240	1856	1178	314	353	11	0	0

- Molecule 28 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	N	191	1430	893	245	280	12	0	0
28	n	191	1430	893	245	280	12	0	0

- Molecule 29 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	O	220	1643	1033	280	318	12	0	0
29	o	220	1643	1033	280	318	12	0	0

- Molecule 30 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	P	204	1585	1010	262	294	19	0	0
30	p	204	1585	1010	262	294	19	0	0

- Molecule 31 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Q	199	1570	1006	265	290	9	0	0
31	q	199	1570	1006	265	290	9	0	0

- Molecule 32 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	R	201	1548	974	273	292	9	0	0
32	r	201	1548	974	273	292	9	0	0

- Molecule 33 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	S	213	1641	1036	282	313	10	0	0
33	s	213	1641	1036	282	313	10	0	0

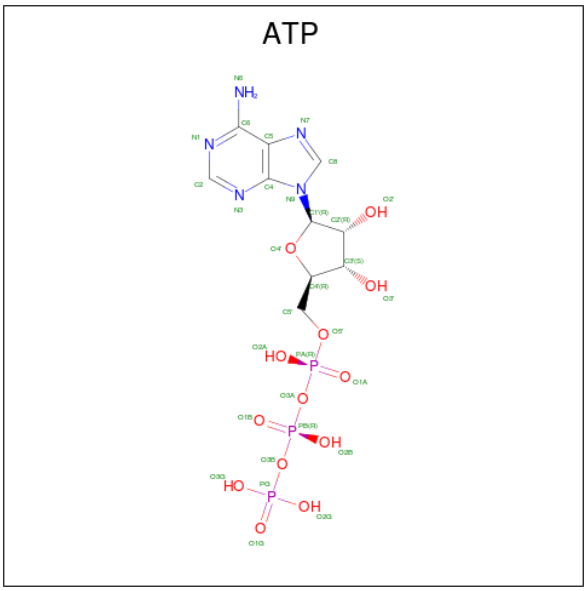
- Molecule 34 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	T	215	1667	1052	285	318	12	0	0
34	t	215	1667	1052	285	318	12	0	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

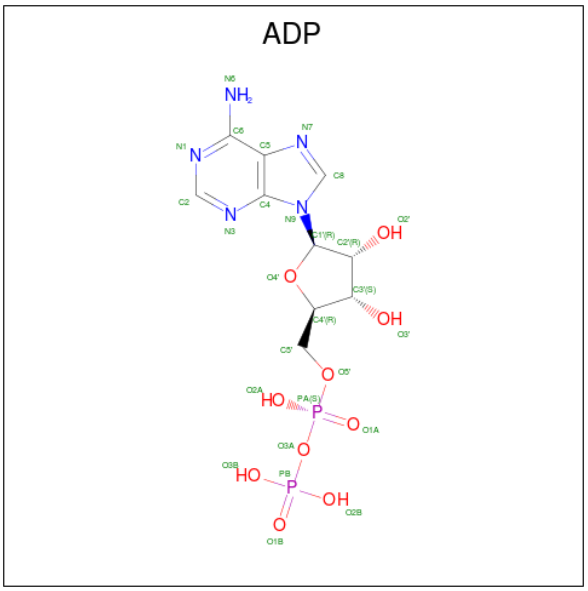


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	F	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



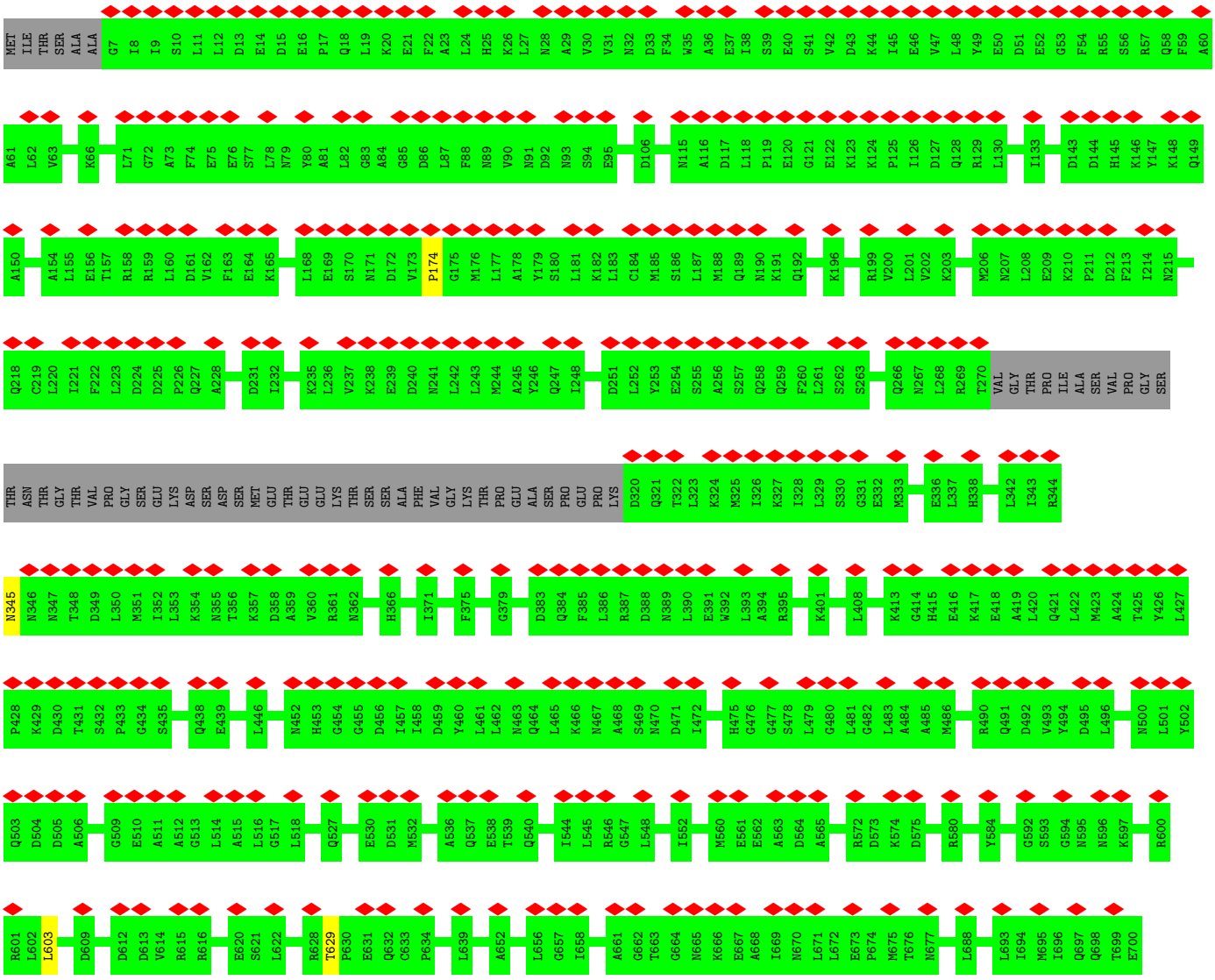
Mol	Chain	Residues	Atoms					AltConf
38	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
38	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

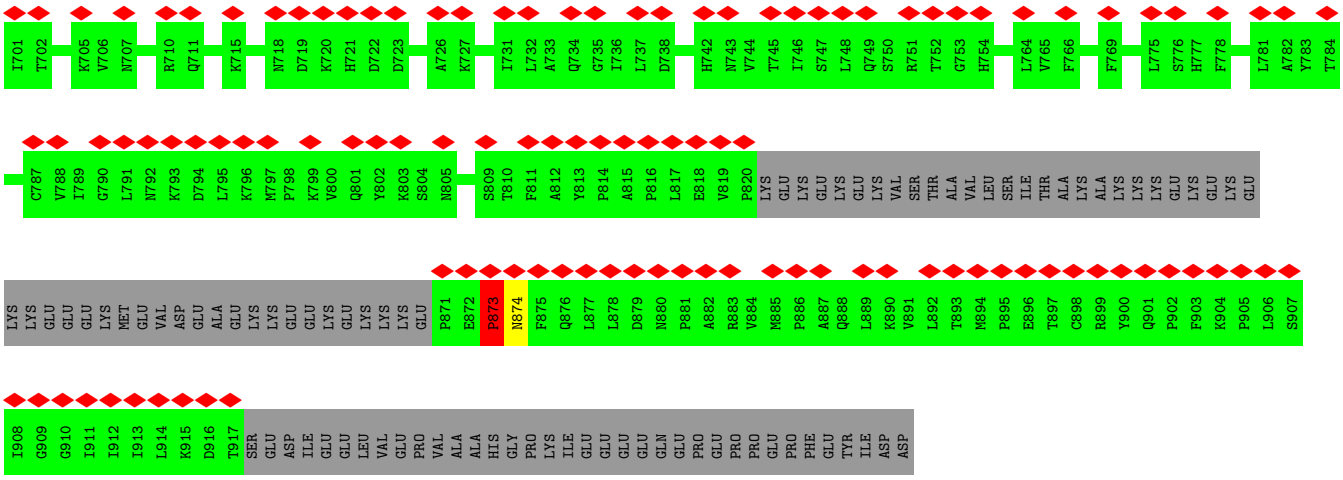
3 Residue-property plots (i)

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 non-ATPase regulatory subunit 1

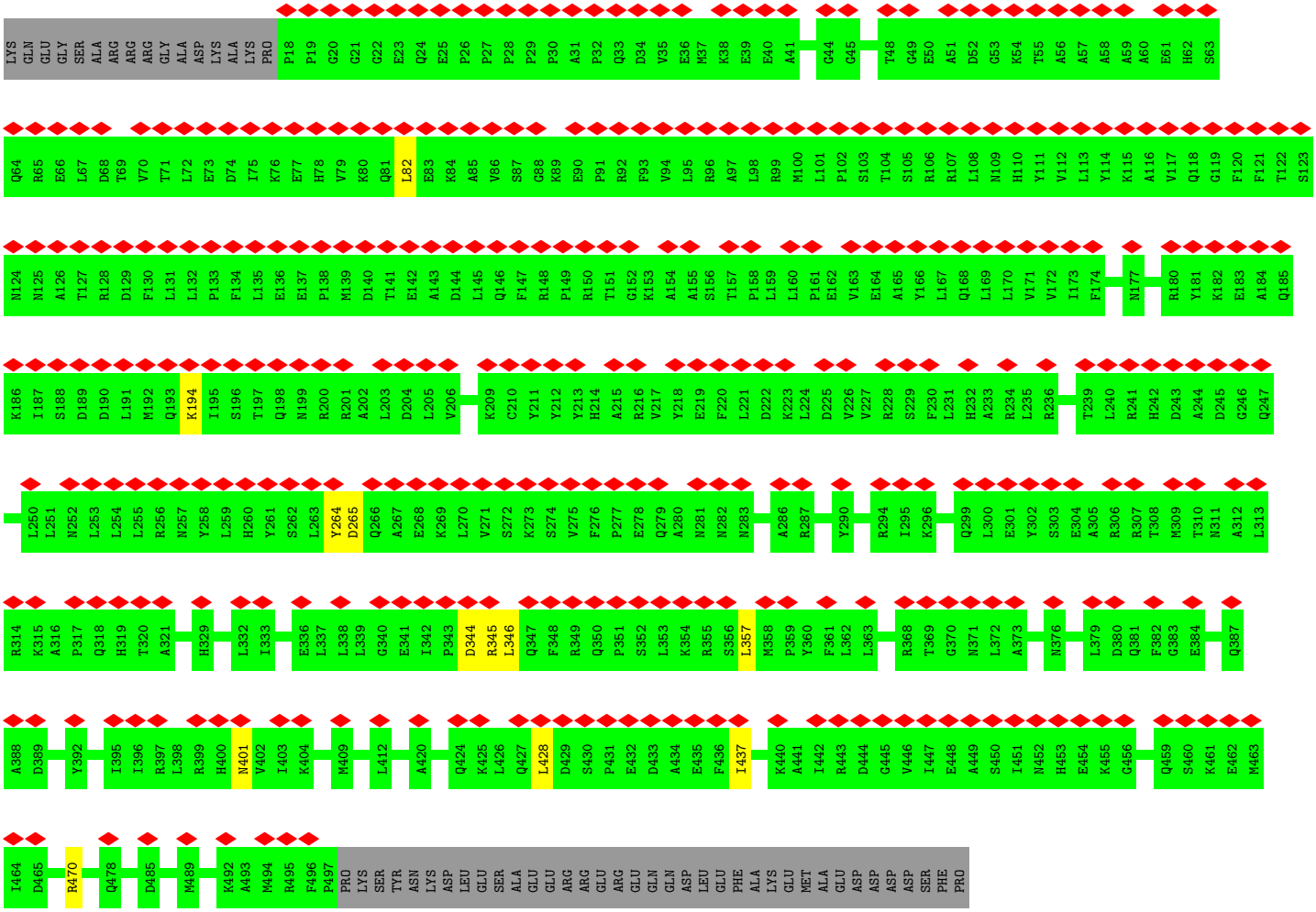
Chain U:





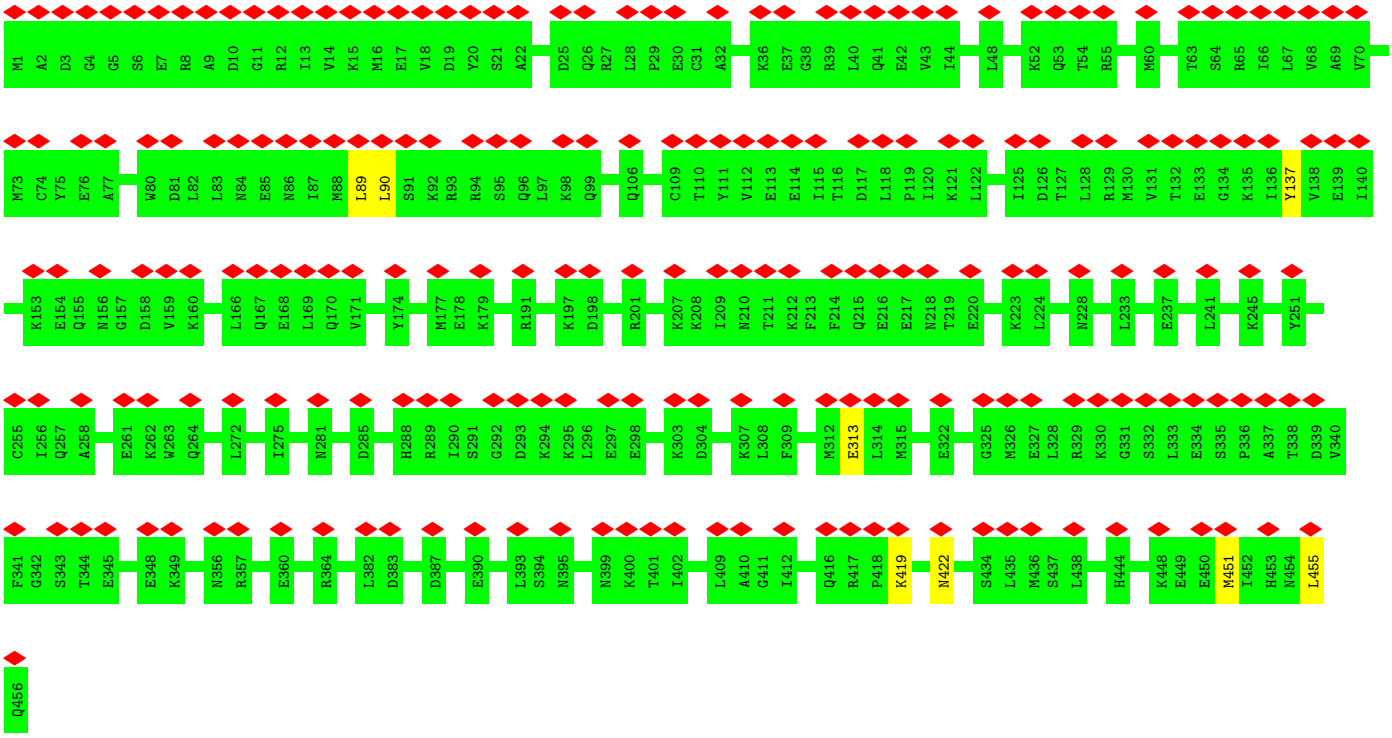
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 47% 98%

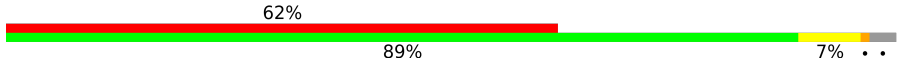


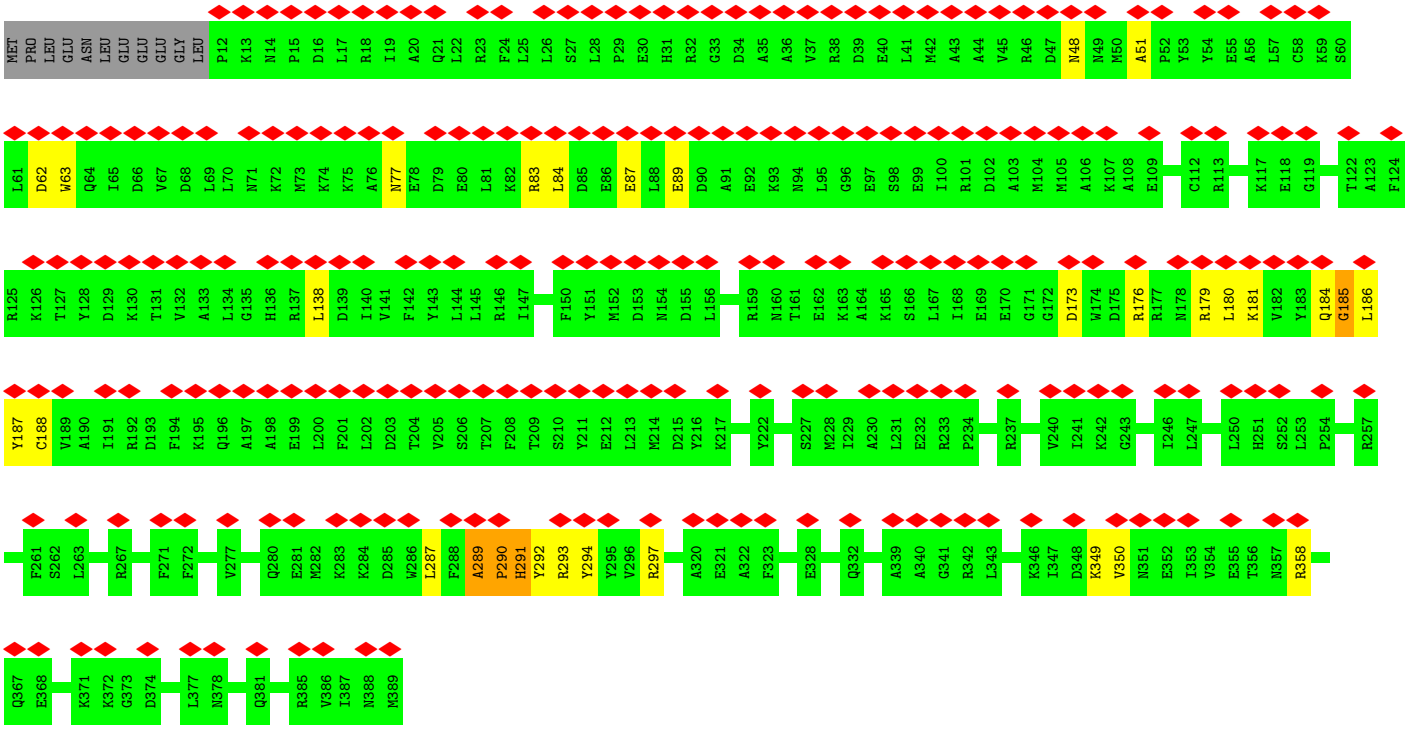
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 50% 89% 10%

- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

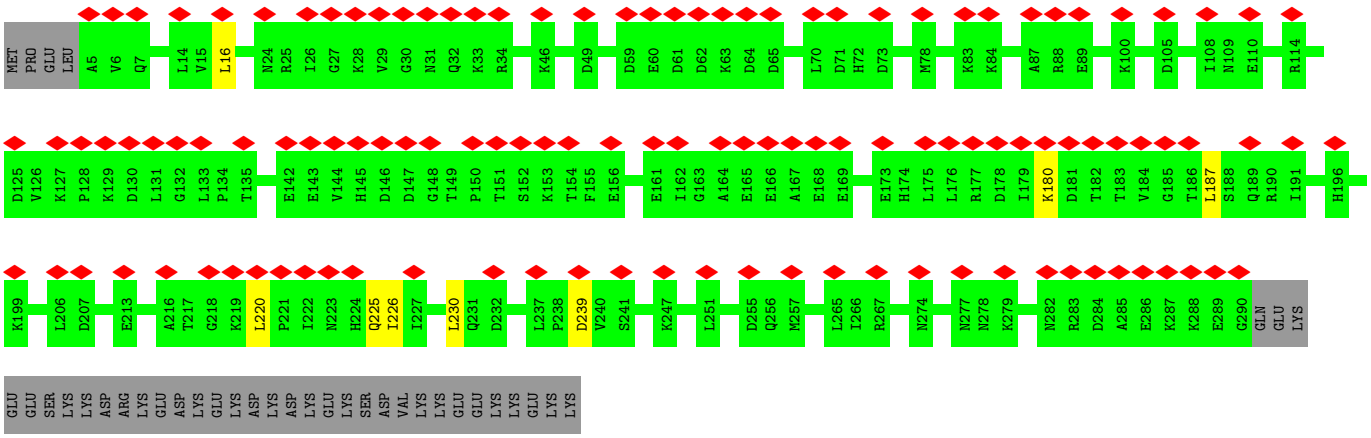
Chain Y:





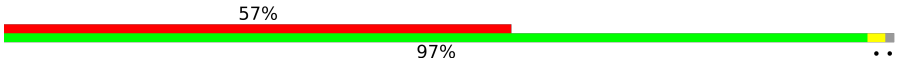
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

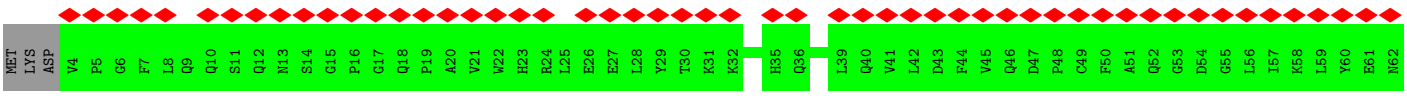
Chain Z:

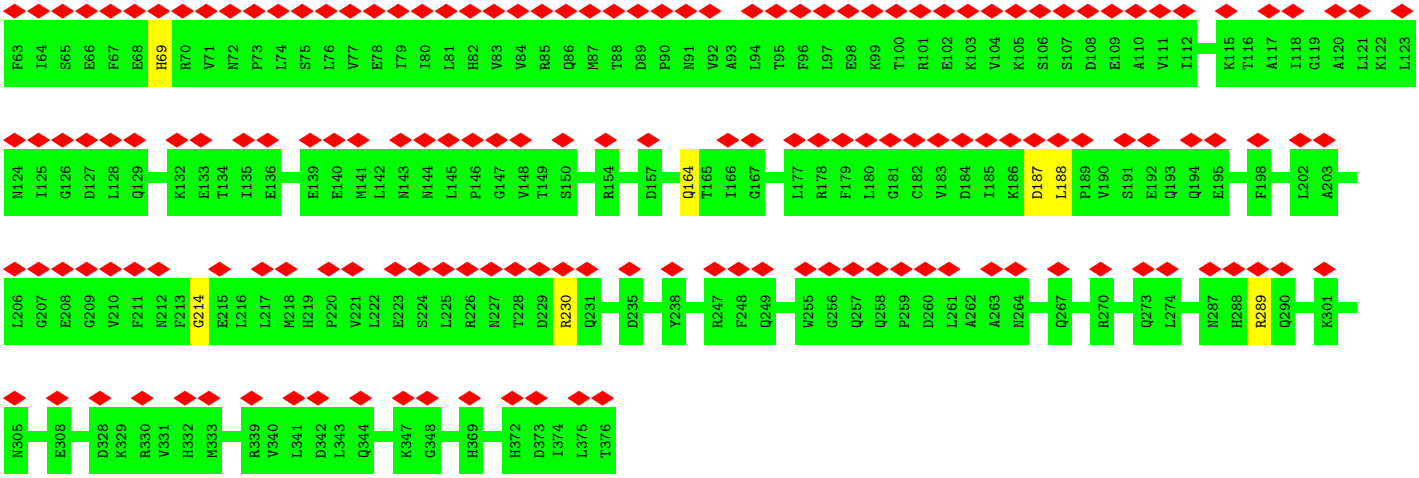


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a:

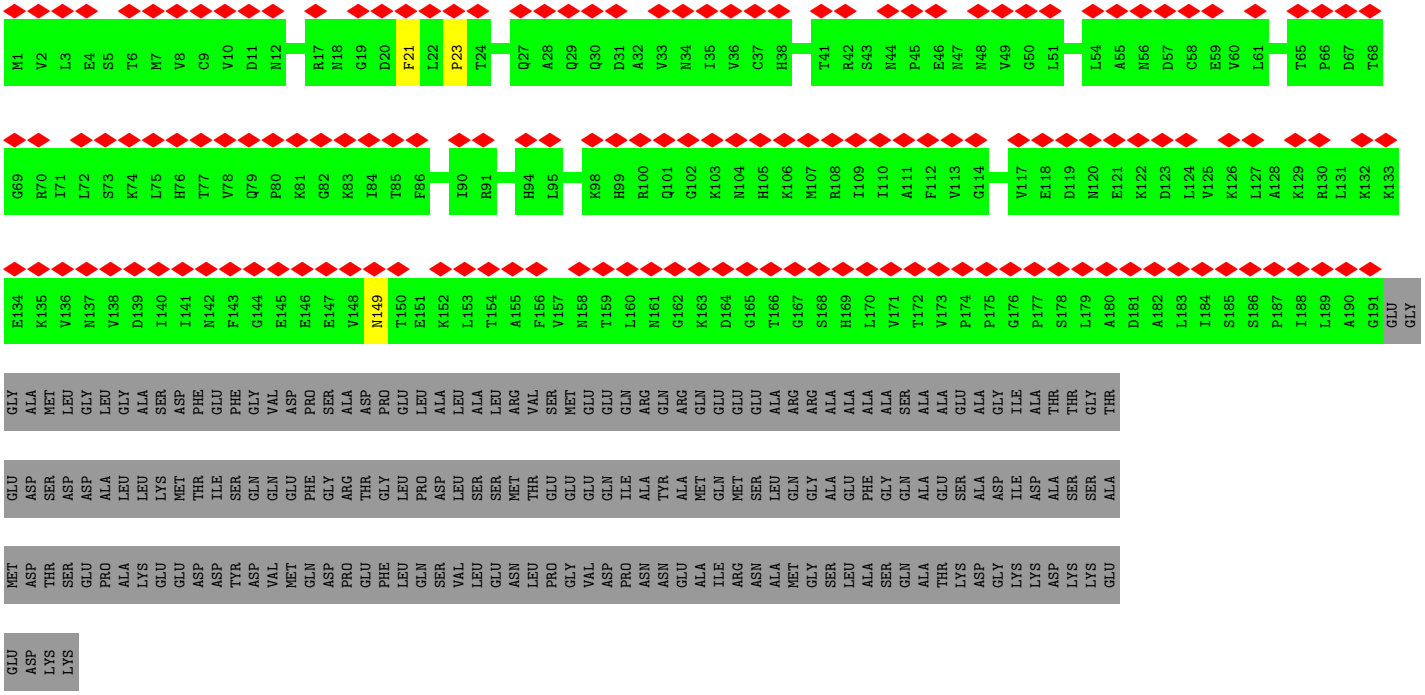






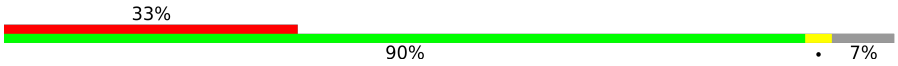
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

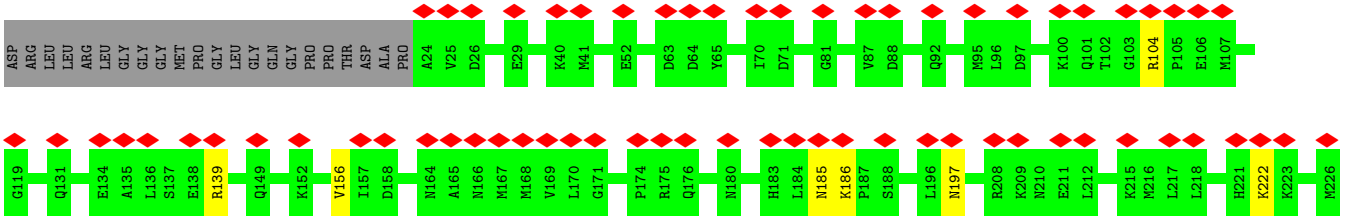
Chain b:

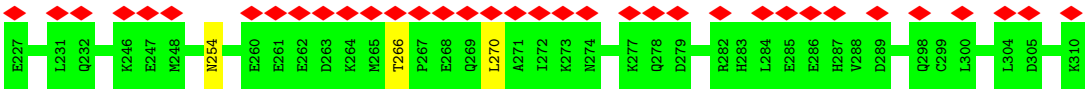


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c:

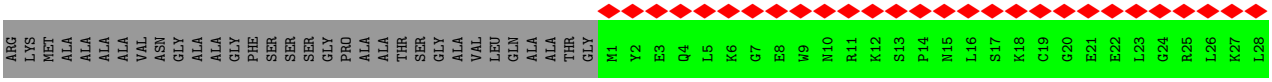


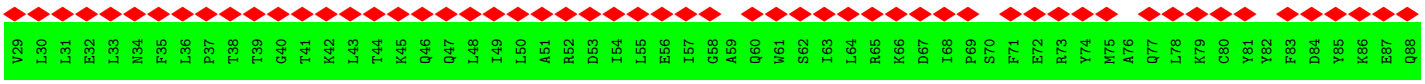


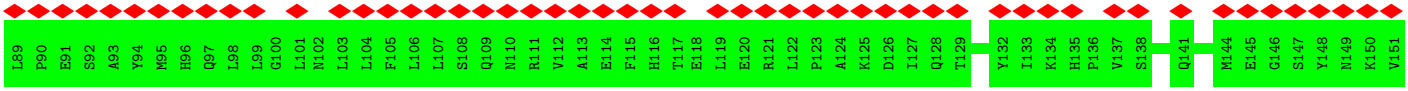


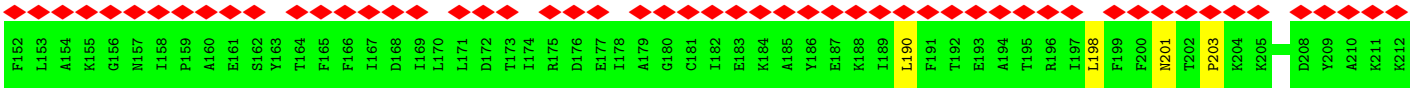
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

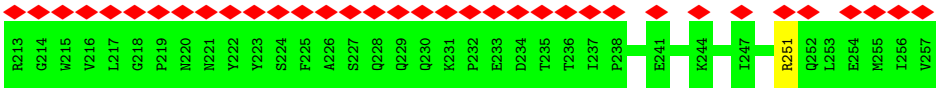
Chain d:





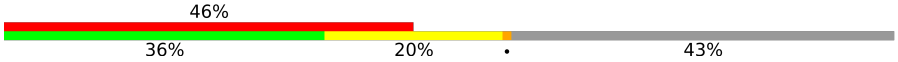


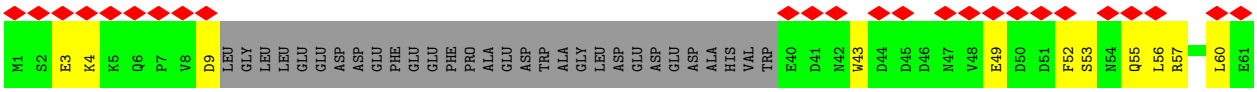




- Molecule 11: 26S proteasome complex subunit SEM1

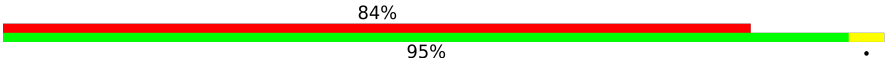
Chain e:

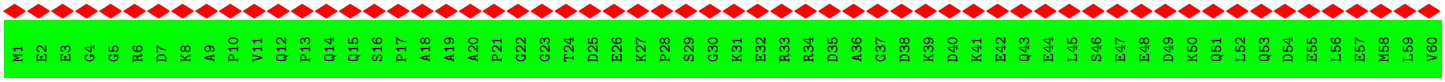


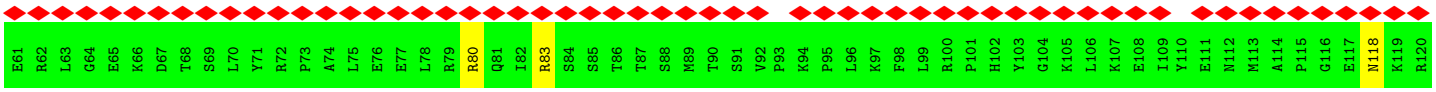


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f:







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E182 P183 L184 L185 T186 L187 V188 K189 E190 I191 V192 P193 Y194 N195 M196 N199 A200 E201 H202 E203 A204 C205 D206 L207 L208 M209 E210 I211 E212 Q213 V214 D215 M216 L217 E218 I221 D222 E223 N224 A225 Y226 A227 K228 V229 C230 L231 Y232 S235 C236 Y239 P243 E244 N245 S246 A247

L248 L249 G254 V255 F256 R257 K258 F259 S260 R261 F262 P263 E264 A265 L266 R267 L268 A269 L270 M271 L272 N273 L277 V278 E279 D280 I281 F282 T283 S284 C285 V290 Q293 M294 A295 F296 M297 L298 G299 R300 H301 G302 V303 F304 L305 E306 L307 S308 E309 D310 V311 E312 E313 Y314 E315 D316

L317 T318 E319 S322 N323 V324 Q325 L326 N327 S328 N329 F330 L331 A332 L333 A334 R335 E336 L337 D338 I339 M340 E341 P342 K343 V344 P345 D346 D347 I348 Y349 K350 T351 H352 L353 E354 N355 N356 R357 F358 G359 G360 S361 G362 S363 Q364 V365 D366 S367 A368 R369 M370 N371 L372 A373 S374 S375 F376 V377

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L498 T499 L500 L501 L502 P503 V504 M505 G506 D507 S508 K509 S510 S511 M512 E513 V514 A515 G516 V517 T518 A519 L520 G523 M524 V527 G528 S529 C530 N531 G532 D533 V534 T535 S536 T537 I538 L539 Q540 T541 I542 M543 E544 K545 S546 E547 T548 E549 L550 K551 D552 T553 Y554 A555 R556 W557 L558 P559

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R688 L692 A695 L696 I697 S698 V699 S700 N701 P702 R703 L704 N705 I706 L707 D708 S711 K712 F713 S714 H715 D716 A717 D718 P719 E720 Y723 N724 S725 I726 F727 A728 M729 G730 M731 V732 G733 S734 G735 T736 N737 N738 A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751

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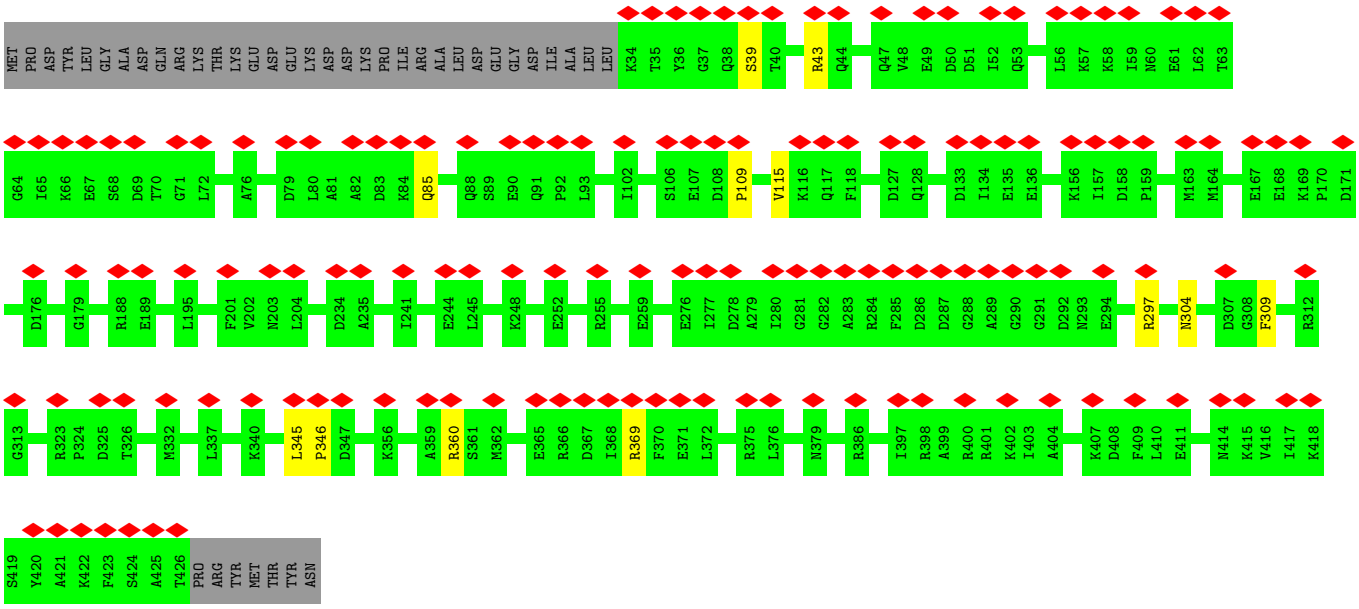
A883 T884 E885 E886 F887 L888 P889 VAL THR PRO

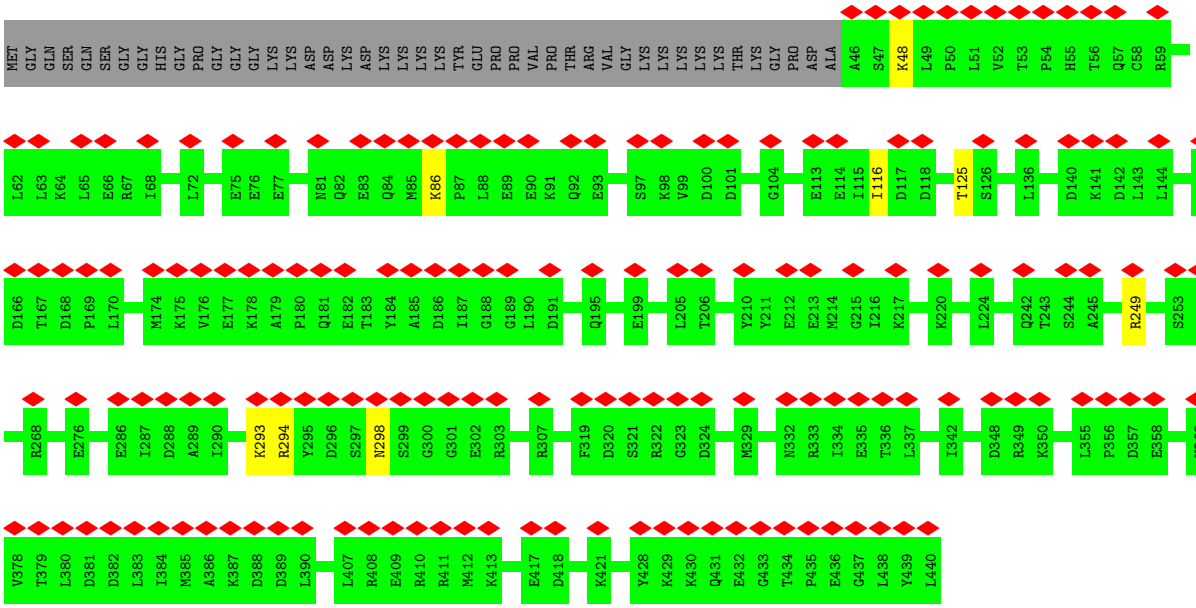
- Molecule 13: 26S proteasome regulatory subunit 7

Chain A: 34% 88% • 9%



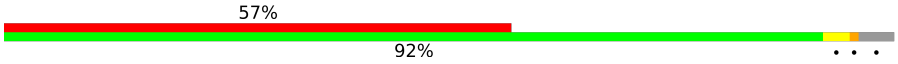
- Molecule 14: 26S proteasome regulatory subunit 4

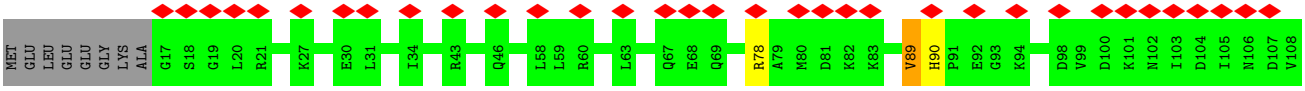
Chain B:

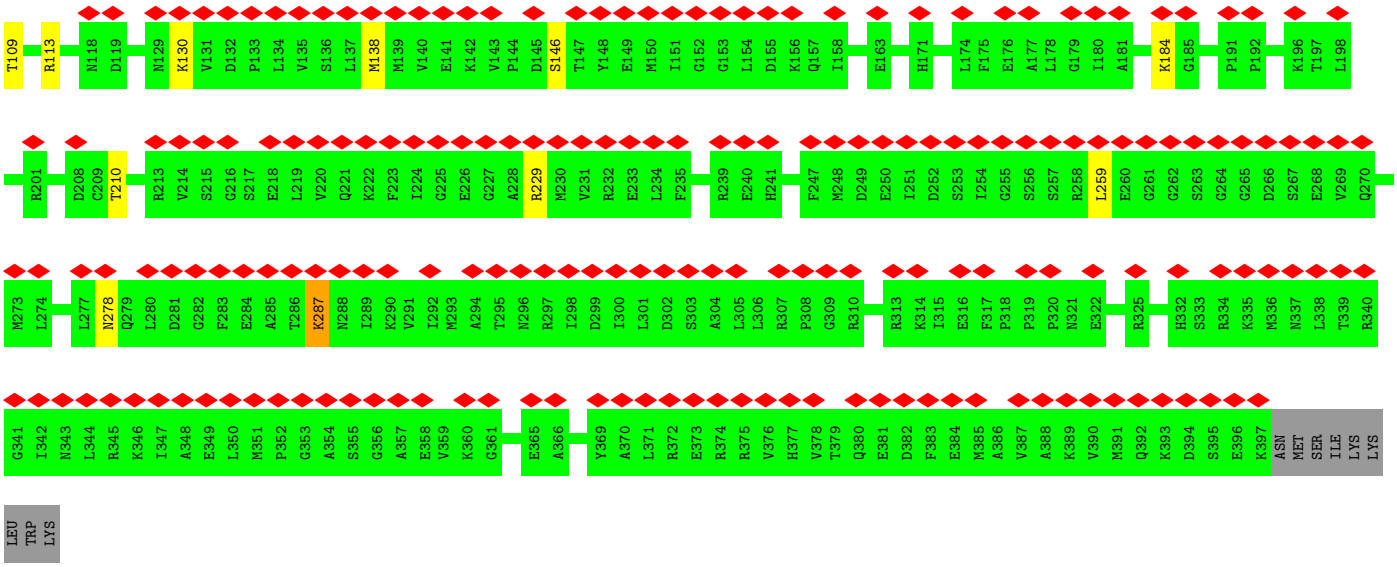


- Molecule 15: 26S proteasome regulatory subunit 8

Chain C:

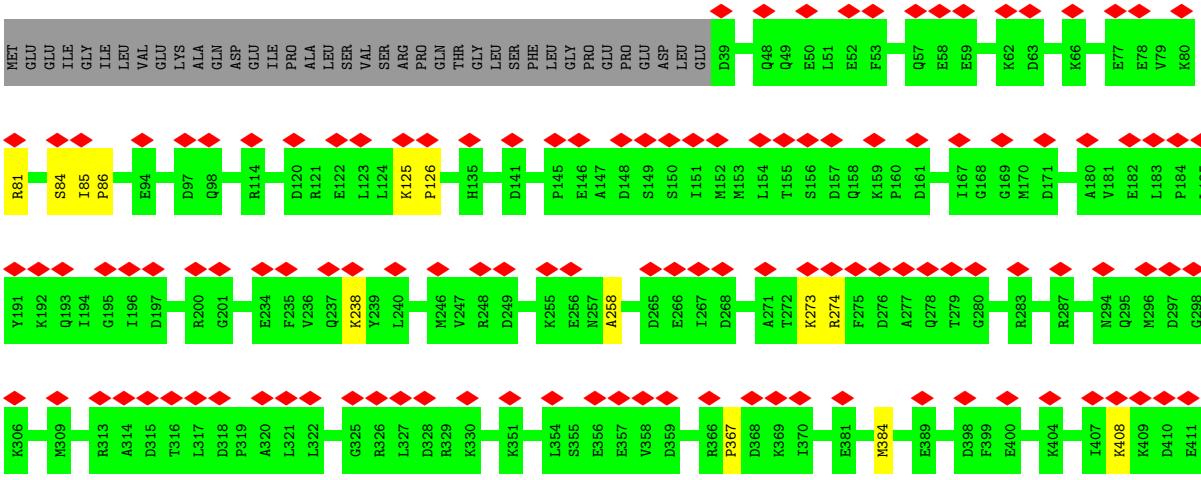






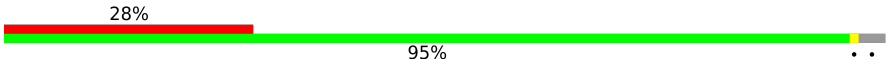
- Molecule 16: 26S proteasome regulatory subunit 6B

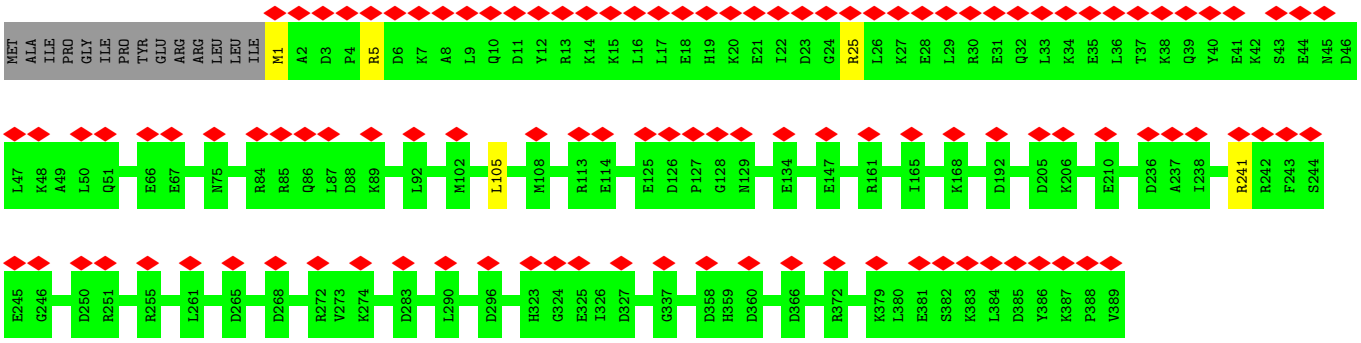
Chain D:



- Molecule 17: 26S proteasome regulatory subunit 10B

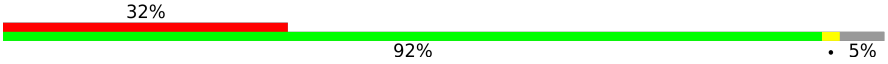
Chain E:

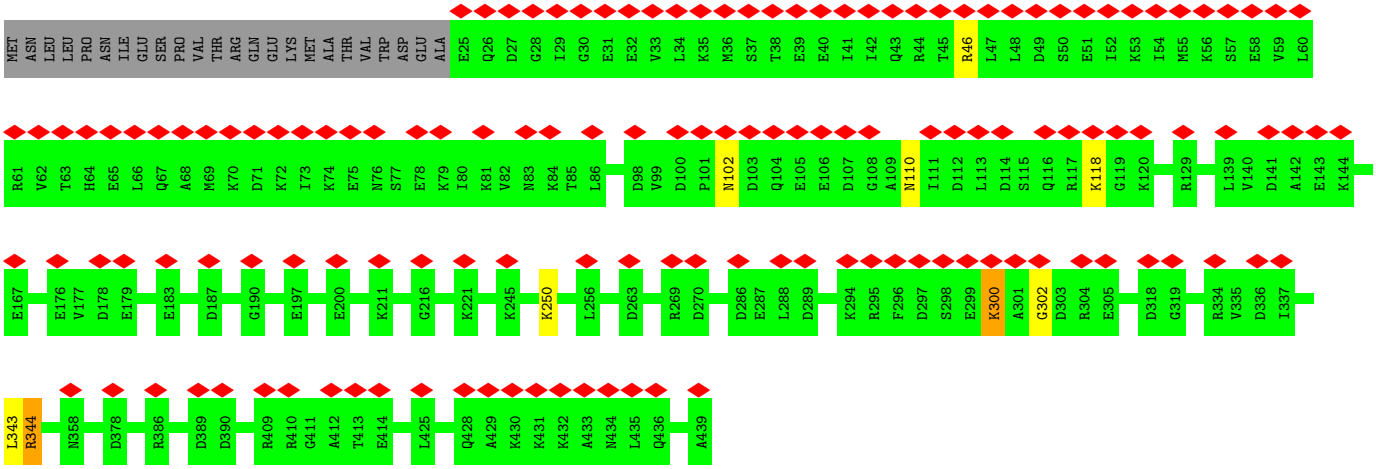




- Molecule 18: 26S proteasome regulatory subunit 6A

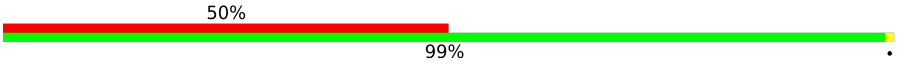
Chain F:

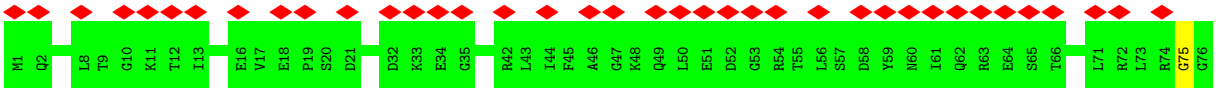




- Molecule 19: Ubiquitin

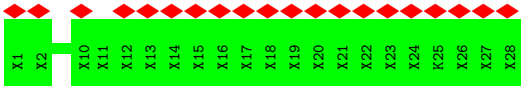
Chain u:





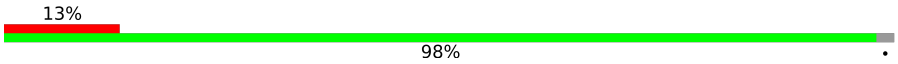
- Molecule 20: substrate

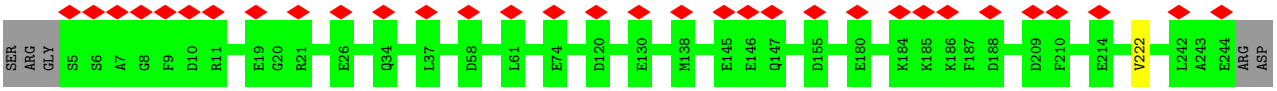
Chain v:



- Molecule 21: Proteasome subunit alpha type-6

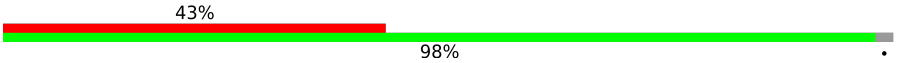
Chain G:

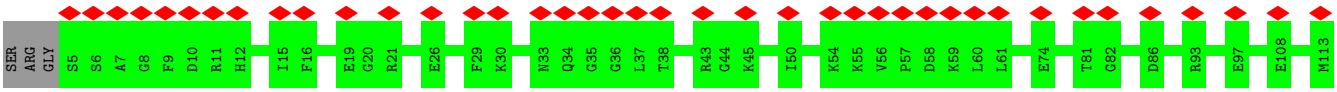


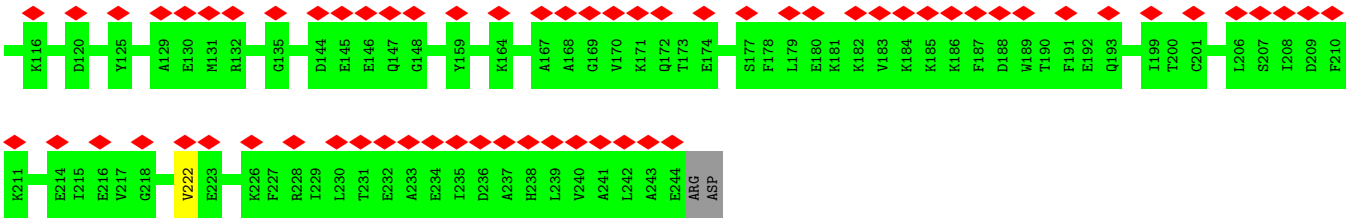


- Molecule 21: Proteasome subunit alpha type-6

Chain g:

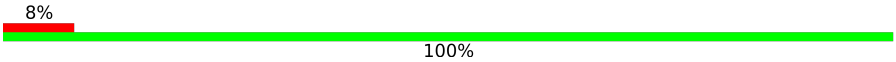


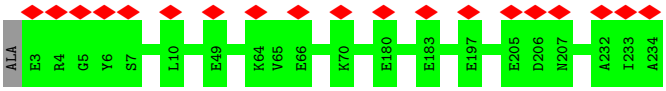




• Molecule 22: Proteasome subunit alpha type-2

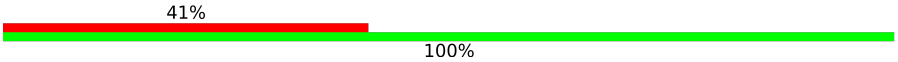
Chain H:

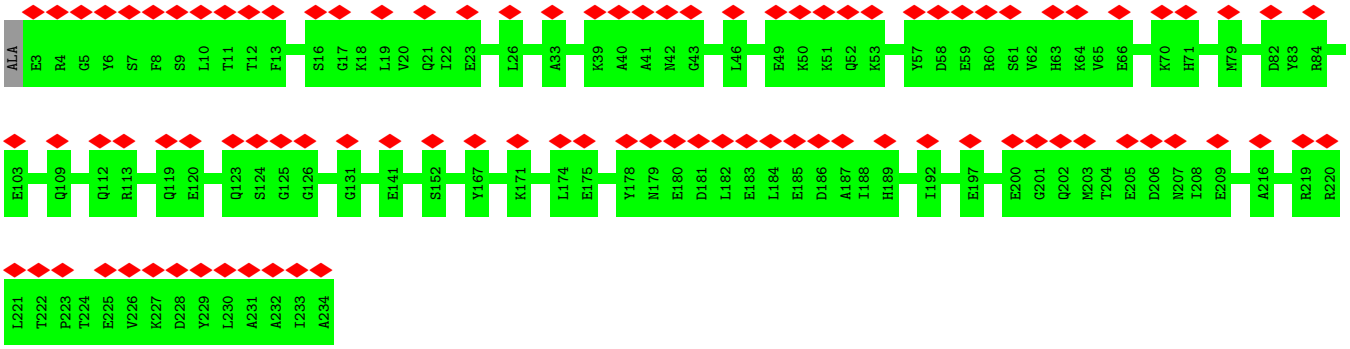




• Molecule 22: Proteasome subunit alpha type-2

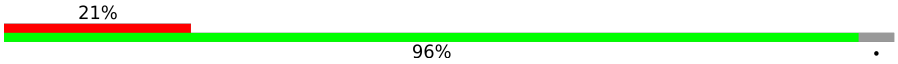
Chain h:

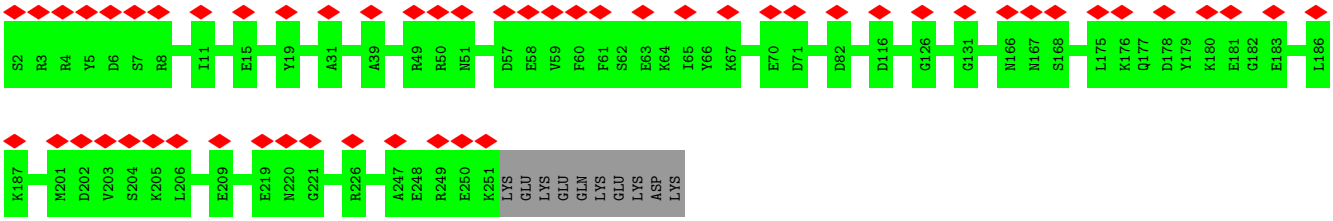




• Molecule 23: Proteasome subunit alpha type-4

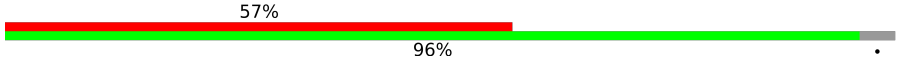
Chain I:

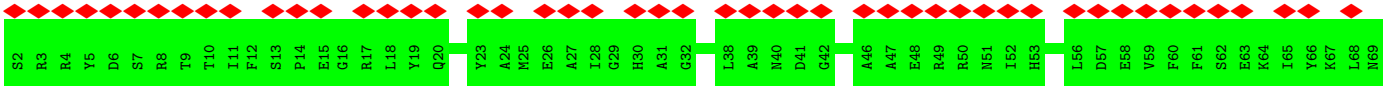


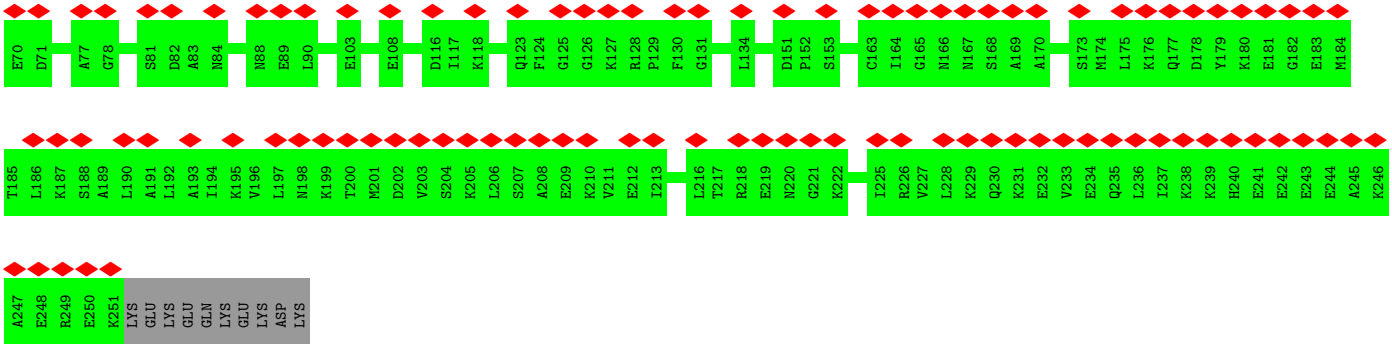


• Molecule 23: Proteasome subunit alpha type-4

Chain i:

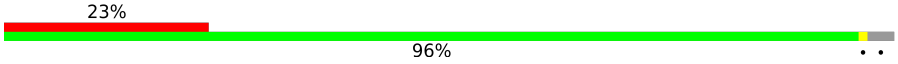


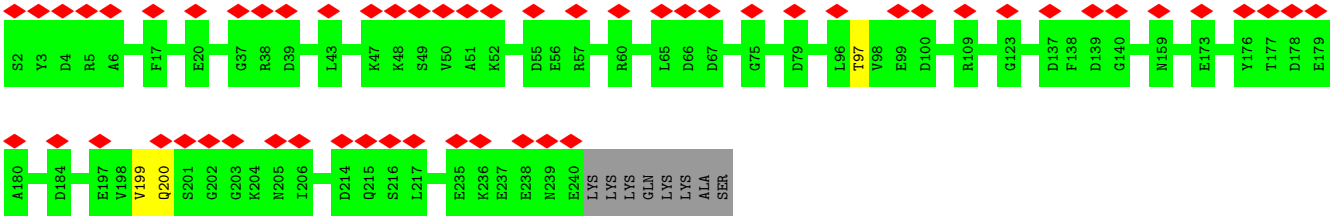




- Molecule 24: Proteasome subunit alpha type-7

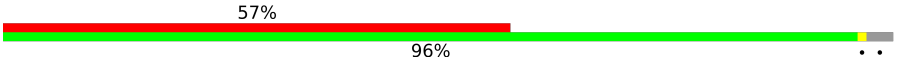
Chain J:

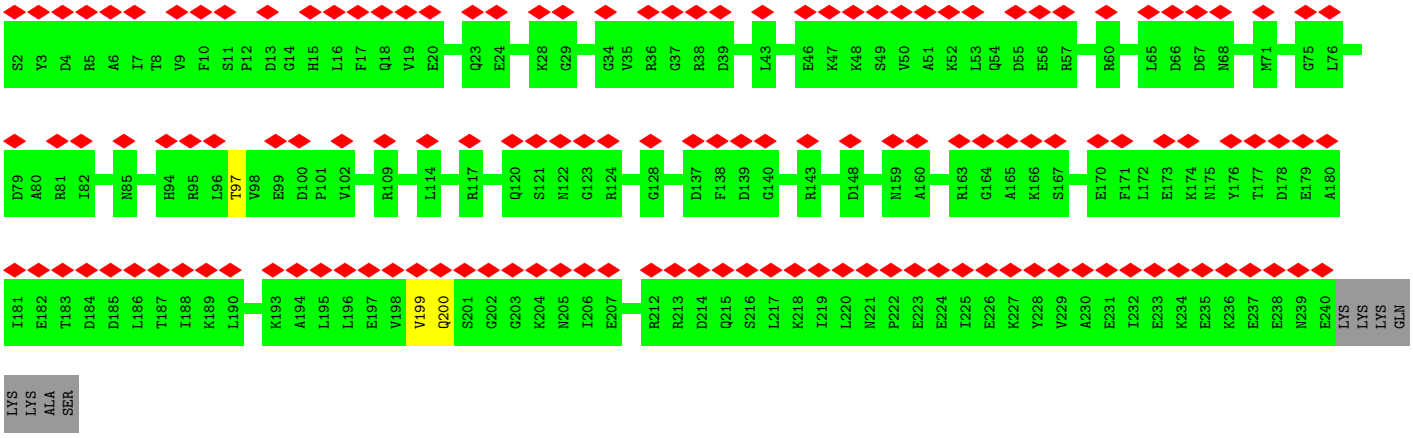




- Molecule 24: Proteasome subunit alpha type-7

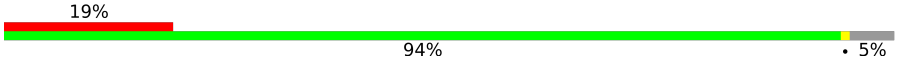
Chain j:

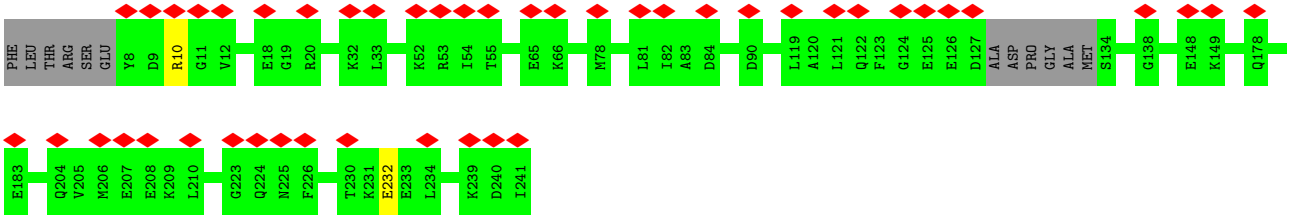




- Molecule 25: Proteasome subunit alpha type-5

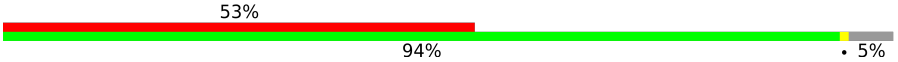
Chain K:

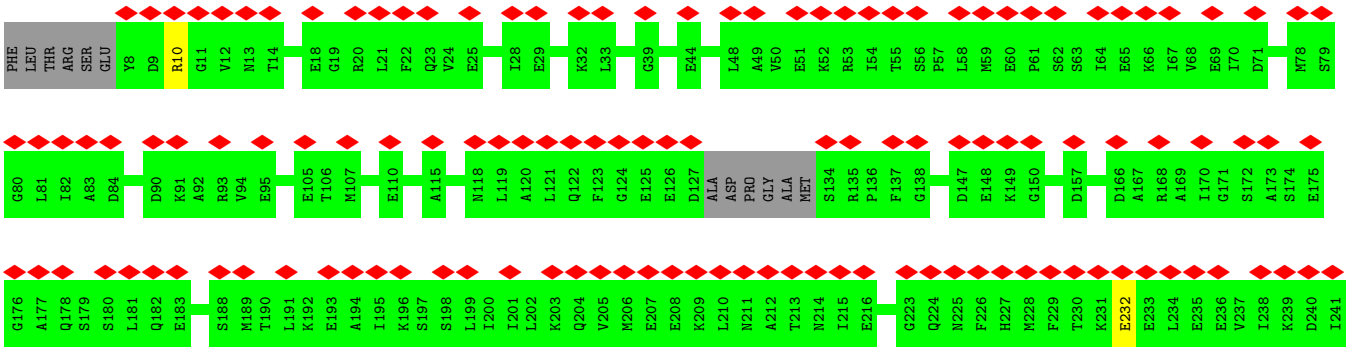




- Molecule 25: Proteasome subunit alpha type-5

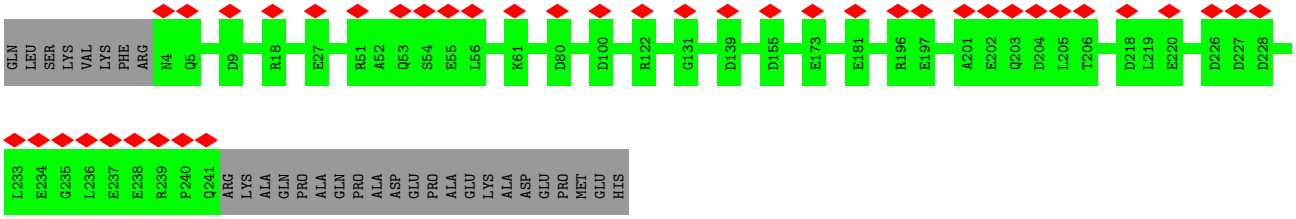
Chain k:





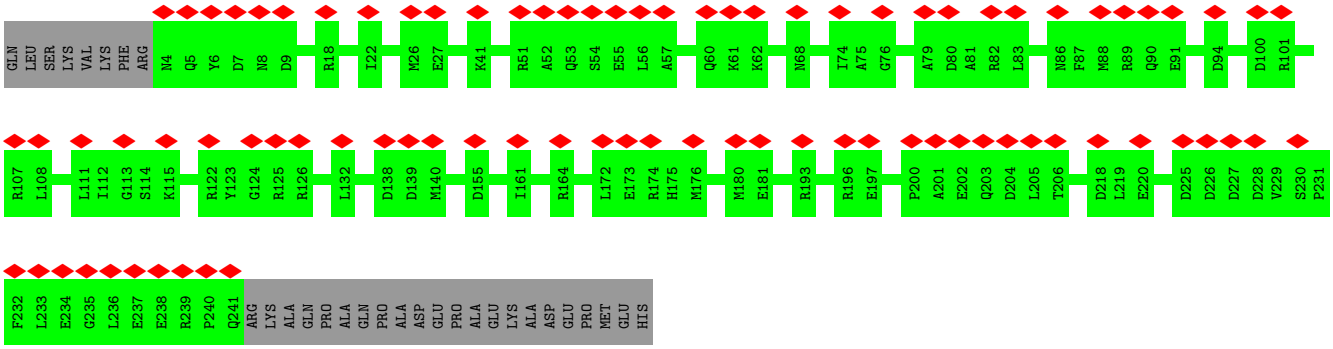
- Molecule 26: Proteasome subunit alpha type-1

Chain L:



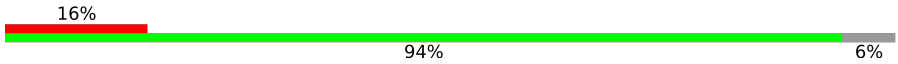
- Molecule 26: Proteasome subunit alpha type-1

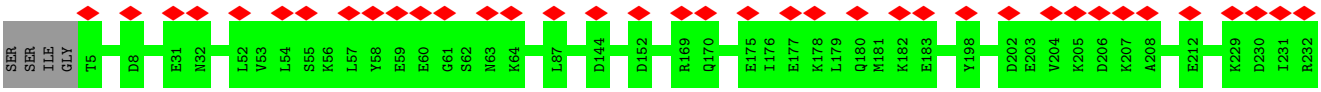
Chain l:

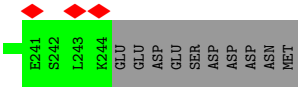


- Molecule 27: Proteasome subunit alpha type-3

Chain M:

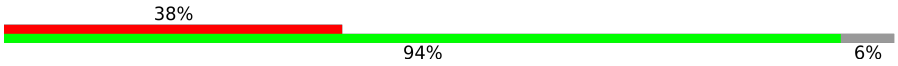


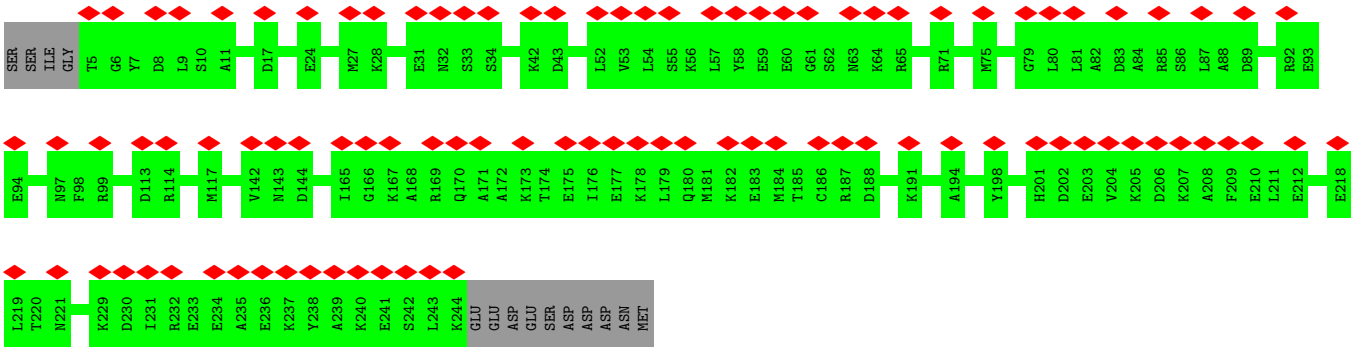




• Molecule 27: Proteasome subunit alpha type-3

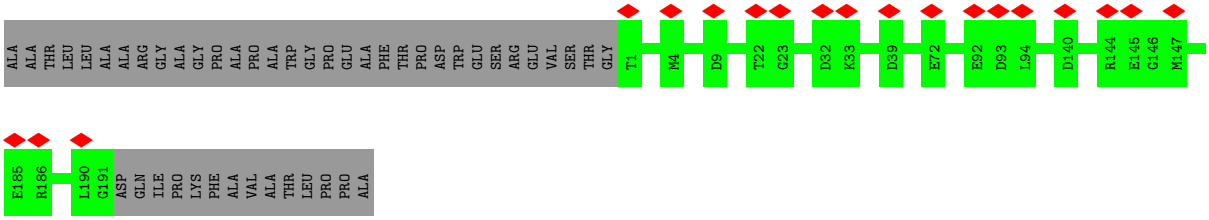
Chain m:





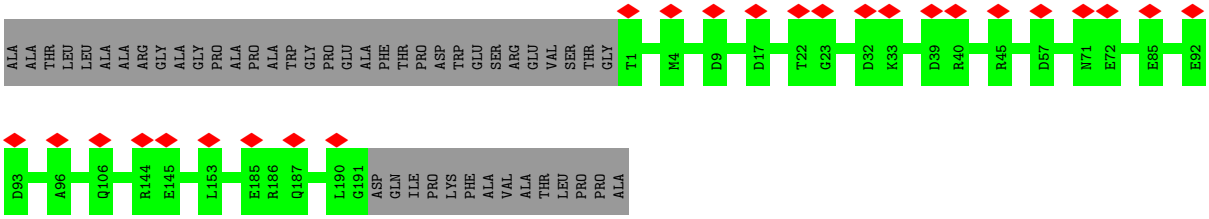
• Molecule 28: Proteasome subunit beta type-6

Chain N:



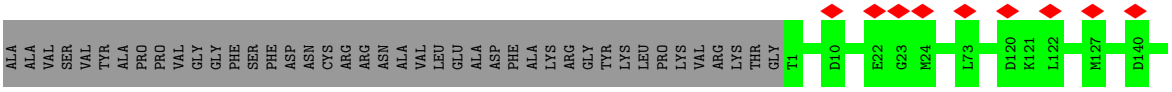
• Molecule 28: Proteasome subunit beta type-6

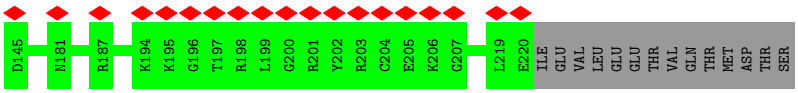
Chain n:



• Molecule 29: Proteasome subunit beta type-7

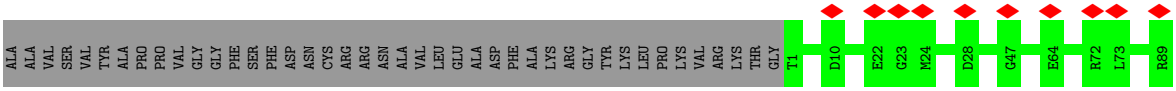
Chain O:

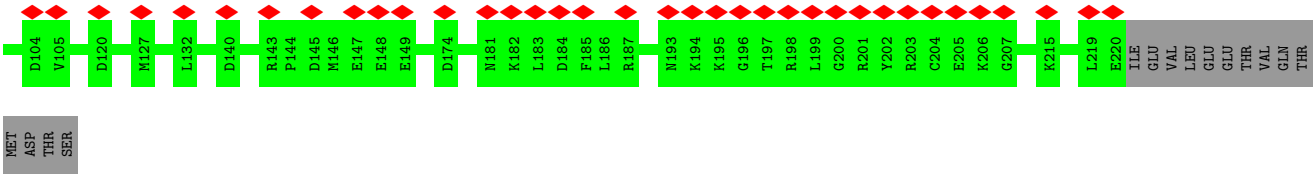




• Molecule 29: Proteasome subunit beta type-7

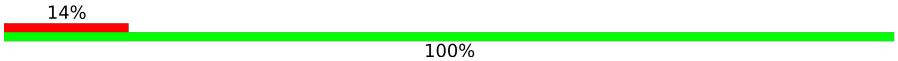
Chain o:





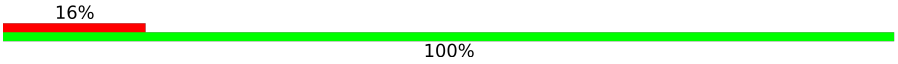
• Molecule 30: Proteasome subunit beta type-3

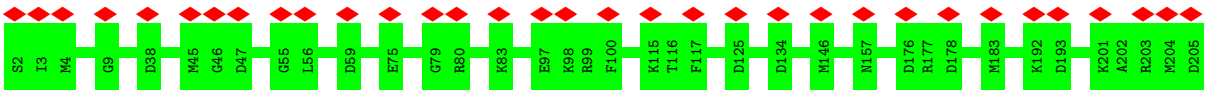
Chain P:



• Molecule 30: Proteasome subunit beta type-3

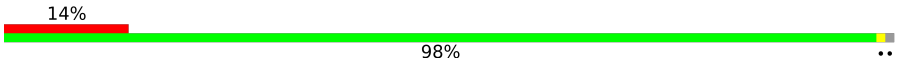
Chain p:

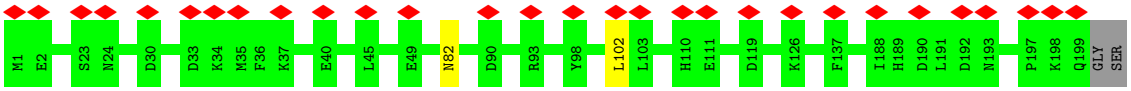




• Molecule 31: Proteasome subunit beta type-2

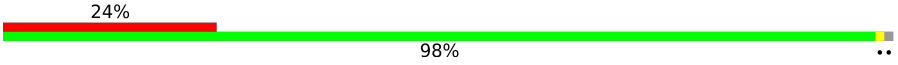
Chain Q:

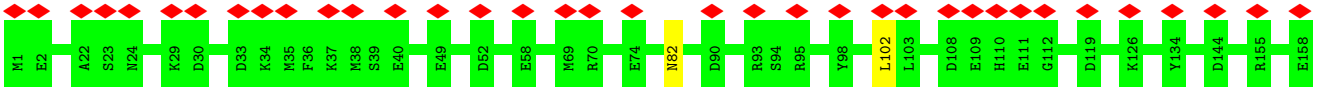


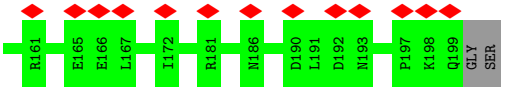


• Molecule 31: Proteasome subunit beta type-2

Chain q:

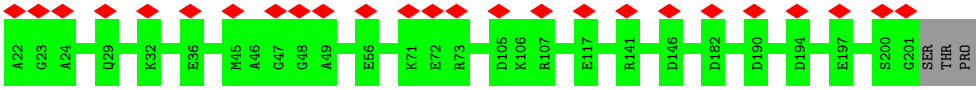






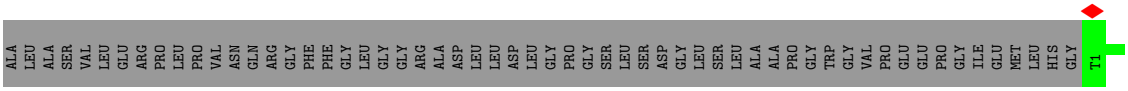
• Molecule 32: Proteasome subunit beta type-5

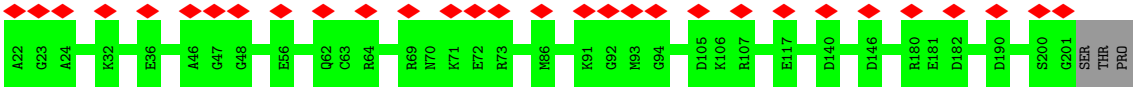
Chain R:



• Molecule 32: Proteasome subunit beta type-5

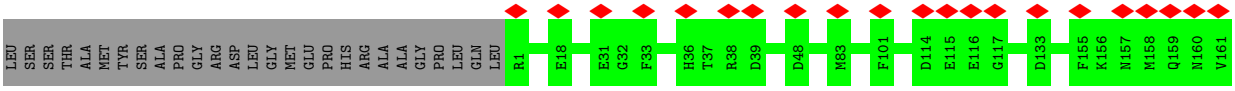
Chain r:

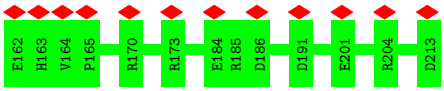




• Molecule 33: Proteasome subunit beta type-1

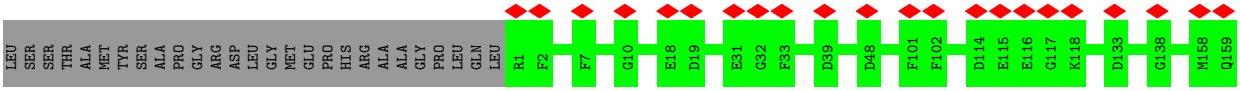
Chain S:

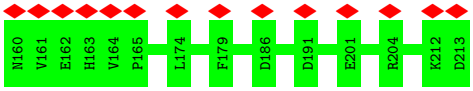




• Molecule 33: Proteasome subunit beta type-1

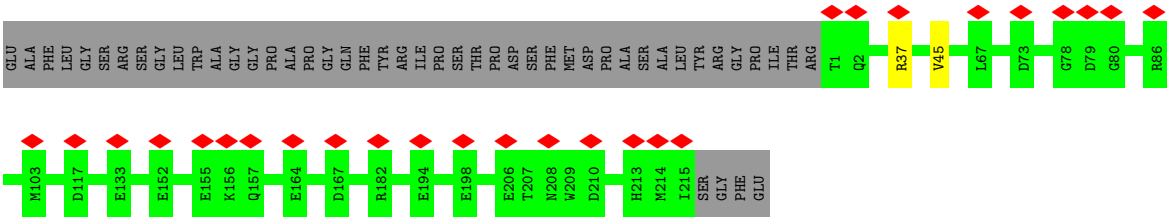
Chain s:





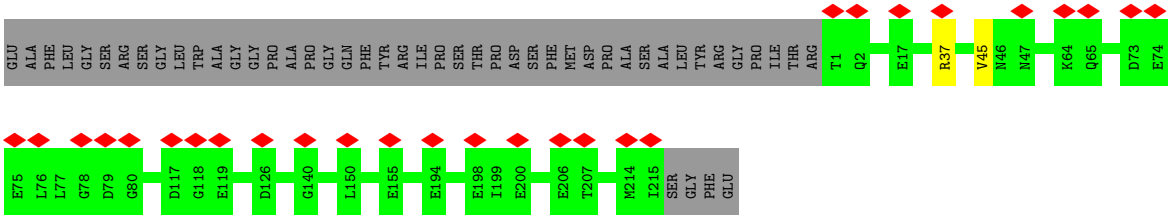
• Molecule 34: Proteasome subunit beta type-4

Chain T:



- Molecule 34: Proteasome subunit beta type-4

Chain t:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	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	0.016	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	U	0.30	0/6449	0.56	3/8729 (0.0%)
2	V	0.34	0/3929	0.68	4/5309 (0.1%)
3	W	0.31	0/3751	0.65	2/5042 (0.0%)
4	X	0.28	0/3053	0.54	0/4115
5	Y	0.49	4/3173 (0.1%)	0.85	11/4273 (0.3%)
6	Z	0.32	0/2324	0.68	4/3150 (0.1%)
7	a	0.31	0/3053	0.60	2/4133 (0.0%)
8	b	0.30	0/1478	0.61	0/2001
9	c	0.32	0/2302	0.63	1/3110 (0.0%)
10	d	0.31	0/2162	0.59	1/2919 (0.0%)
11	e	0.91	2/338 (0.6%)	1.98	17/450 (3.8%)
12	f	0.33	1/6980 (0.0%)	0.71	7/9433 (0.1%)
13	A	0.32	0/3117	0.61	1/4207 (0.0%)
14	B	0.32	0/3131	0.60	0/4227
15	C	0.31	0/3017	0.62	1/4058 (0.0%)
16	D	0.32	0/3089	0.57	0/4168
17	E	0.32	0/3145	0.56	1/4233 (0.0%)
18	F	0.34	0/3292	0.56	0/4435
19	u	0.30	0/609	0.60	1/819 (0.1%)
20	v	0.20	0/8	0.18	0/8
21	G	0.31	0/1859	0.54	0/2523
21	g	0.31	0/1859	0.54	0/2523
22	H	0.34	0/1743	0.53	0/2372
22	h	0.34	0/1743	0.53	0/2372
23	I	0.31	0/1942	0.55	0/2628
23	i	0.31	0/1942	0.55	0/2628
24	J	0.30	0/1728	0.56	0/2358
24	j	0.30	0/1728	0.56	0/2358
25	K	0.30	0/1747	0.54	0/2364
25	k	0.30	0/1747	0.54	0/2364
26	L	0.32	0/1885	0.56	0/2552
26	l	0.32	0/1885	0.56	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	M	0.33	0/1891	0.54	0/2552
27	m	0.33	0/1891	0.54	0/2552
28	N	0.30	0/1454	0.51	0/1967
28	n	0.30	0/1454	0.51	0/1967
29	O	0.30	0/1670	0.49	0/2265
29	o	0.30	0/1670	0.49	0/2265
30	P	0.30	0/1614	0.49	0/2177
30	p	0.30	0/1614	0.49	0/2177
31	Q	0.33	0/1603	0.56	0/2174
31	q	0.33	0/1603	0.56	0/2174
32	R	0.32	0/1579	0.45	0/2134
32	r	0.32	0/1579	0.46	0/2134
33	S	0.31	0/1671	0.49	0/2253
33	s	0.31	0/1671	0.49	0/2253
34	T	0.31	0/1700	0.50	0/2305
34	t	0.31	0/1700	0.50	0/2305
All	All	0.33	7/106572 (0.0%)	0.59	56/144067 (0.0%)

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	U	0	1
2	V	0	3
3	W	0	2
5	Y	0	12
6	Z	0	2
7	a	0	1
8	b	0	2
9	c	0	2
10	d	0	2
11	e	0	5
12	f	0	11
13	A	0	3
14	B	0	1
15	C	0	3
16	D	0	6
18	F	0	2
21	G	0	1
21	g	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	J	0	1
24	j	0	1
25	K	0	1
25	k	0	1
34	T	0	1
34	t	0	1
All	All	0	66

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	289	ALA	C-N	7.22	1.48	1.34
5	Y	185	GLY	CA-C	6.97	1.62	1.51
11	e	64	GLY	CA-C	5.80	1.61	1.51
12	f	192	VAL	C-N	5.75	1.45	1.34
5	Y	292	TYR	CB-CG	5.62	1.60	1.51

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	e	63	HIS	CB-CA-C	12.60	135.61	110.40
11	e	63	HIS	C-N-CA	12.17	147.86	122.30
5	Y	292	TYR	CA-CB-CG	10.89	134.09	113.40
11	e	57	ARG	CG-CD-NE	10.77	134.41	111.80
11	e	63	HIS	N-CA-CB	-10.55	91.61	110.60

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
2	V	344	ASP	Peptide
2	V	82	LEU	Peptide
3	W	137	TYR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	748 (93%)	55 (7%)	3 (0%)	34	66
2	V	478/533 (90%)	412 (86%)	65 (14%)	1 (0%)	47	77
3	W	454/456 (100%)	409 (90%)	45 (10%)	0	100	100
4	X	378/422 (90%)	362 (96%)	15 (4%)	1 (0%)	41	71
5	Y	376/389 (97%)	317 (84%)	51 (14%)	8 (2%)	7	31
6	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	34	66
7	a	371/376 (99%)	334 (90%)	35 (9%)	2 (0%)	29	61
8	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	29	61
9	c	285/309 (92%)	256 (90%)	29 (10%)	0	100	100
10	d	255/349 (73%)	213 (84%)	41 (16%)	1 (0%)	34	66
11	e	36/70 (51%)	16 (44%)	18 (50%)	2 (6%)	2	11
12	f	887/892 (99%)	714 (80%)	164 (18%)	9 (1%)	15	46
13	A	391/433 (90%)	335 (86%)	53 (14%)	3 (1%)	19	51
14	B	393/440 (89%)	343 (87%)	50 (13%)	0	100	100
15	C	379/398 (95%)	334 (88%)	42 (11%)	3 (1%)	19	51
16	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	12	40
17	E	387/403 (96%)	349 (90%)	38 (10%)	0	100	100
18	F	413/439 (94%)	374 (91%)	36 (9%)	3 (1%)	22	54
19	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
20	v	1/28 (4%)	0	1 (100%)	0	100	100
21	G	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
21	g	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
22	H	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
22	h	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
23	I	248/260 (95%)	228 (92%)	20 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	i	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
24	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	19	51
24	j	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	19	51
25	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
25	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
26	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
26	l	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
27	M	238/254 (94%)	216 (91%)	22 (9%)	0	100	100
27	m	238/254 (94%)	215 (90%)	23 (10%)	0	100	100
28	N	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
28	n	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
29	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
30	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
31	Q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
31	q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
32	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
32	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
33	S	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
33	s	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
34	T	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
34	t	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
All	All	13375/14947 (90%)	12160 (91%)	1168 (9%)	47 (0%)	38	66

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	e	65	TYR
12	f	808	ASN
12	f	853	VAL
1	U	874	ASN
5	Y	89	GLU

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	U	692/816 (85%)	690 (100%)	2 (0%)	92	96
2	V	414/459 (90%)	410 (99%)	4 (1%)	76	86
3	W	416/416 (100%)	412 (99%)	4 (1%)	76	86
4	X	327/362 (90%)	325 (99%)	2 (1%)	86	91
5	Y	334/344 (97%)	329 (98%)	5 (2%)	65	81
6	Z	257/295 (87%)	256 (100%)	1 (0%)	91	95
7	a	333/336 (99%)	331 (99%)	2 (1%)	86	91
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	245 (97%)	7 (3%)	43	70
10	d	231/293 (79%)	230 (100%)	1 (0%)	91	95
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	729 (98%)	16 (2%)	53	75
13	A	332/372 (89%)	327 (98%)	5 (2%)	65	81
14	B	344/385 (89%)	336 (98%)	8 (2%)	50	73
15	C	326/346 (94%)	317 (97%)	9 (3%)	43	70
16	D	333/366 (91%)	330 (99%)	3 (1%)	78	87
17	E	341/353 (97%)	337 (99%)	4 (1%)	71	83
18	F	357/379 (94%)	351 (98%)	6 (2%)	60	78
19	u	68/68 (100%)	68 (100%)	0	100	100
20	v	1/1 (100%)	1 (100%)	0	100	100
21	G	193/209 (92%)	193 (100%)	0	100	100
21	g	193/209 (92%)	193 (100%)	0	100	100
22	H	164/190 (86%)	164 (100%)	0	100	100
22	h	164/190 (86%)	164 (100%)	0	100	100
23	I	193/220 (88%)	193 (100%)	0	100	100
23	i	193/220 (88%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	J	152/210 (72%)	152 (100%)	0	100	100
24	j	152/210 (72%)	152 (100%)	0	100	100
25	K	186/202 (92%)	185 (100%)	1 (0%)	88	93
25	k	186/202 (92%)	185 (100%)	1 (0%)	88	93
26	L	198/229 (86%)	198 (100%)	0	100	100
26	l	198/229 (86%)	198 (100%)	0	100	100
27	M	192/211 (91%)	192 (100%)	0	100	100
27	m	192/211 (91%)	192 (100%)	0	100	100
28	N	148/180 (82%)	148 (100%)	0	100	100
28	n	148/180 (82%)	148 (100%)	0	100	100
29	O	177/227 (78%)	177 (100%)	0	100	100
29	o	177/227 (78%)	177 (100%)	0	100	100
30	P	172/173 (99%)	172 (100%)	0	100	100
30	p	172/173 (99%)	172 (100%)	0	100	100
31	Q	164/171 (96%)	162 (99%)	2 (1%)	71	83
31	q	164/171 (96%)	162 (99%)	2 (1%)	71	83
32	R	153/201 (76%)	153 (100%)	0	100	100
32	r	153/201 (76%)	153 (100%)	0	100	100
33	S	174/198 (88%)	174 (100%)	0	100	100
33	s	174/198 (88%)	174 (100%)	0	100	100
34	T	175/214 (82%)	174 (99%)	1 (1%)	86	91
34	t	175/214 (82%)	174 (99%)	1 (1%)	86	91
All	All	11190/12651 (88%)	11103 (99%)	87 (1%)	82	89

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	C	78	ARG
17	E	25	ARG
15	C	113	ARG
15	C	278	ASN
18	F	110	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
12	f	382	ASN
34	T	81	HIS
14	B	241	ASN
32	R	38	ASN
25	k	164	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)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	A	501	37	26,33,33	0.89	1 (3%)	31,52,52	1.67	5 (16%)
36	ATP	F	501	37	26,33,33	0.94	1 (3%)	31,52,52	1.64	5 (16%)
38	ADP	B	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.57	4 (13%)
38	ADP	E	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.60	4 (13%)
36	ATP	D	501	37	26,33,33	0.94	1 (3%)	31,52,52	1.71	5 (16%)

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	A	501	37	-	0/18/38/38	0/3/3/3
36	ATP	F	501	37	-	3/18/38/38	0/3/3/3
38	ADP	B	501	-	-	4/12/32/32	0/3/3/3
38	ADP	E	401	-	-	3/12/32/32	0/3/3/3
36	ATP	D	501	37	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ATP	C5-C4	2.47	1.47	1.40
36	F	501	ATP	C5-C4	2.39	1.47	1.40
38	B	501	ADP	C5-C4	2.37	1.47	1.40
38	E	401	ADP	C5-C4	2.30	1.47	1.40
36	A	501	ATP	C5-C4	2.26	1.46	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	501	ATP	PA-O3A-PB	-4.66	116.84	132.83
36	F	501	ATP	PA-O3A-PB	-4.59	117.08	132.83
38	E	401	ADP	PA-O3A-PB	-4.26	118.20	132.83
36	D	501	ATP	C3'-C2'-C1'	4.17	107.25	100.98
38	B	501	ADP	C3'-C2'-C1'	4.12	107.18	100.98

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	D	501	ATP	C5'-O5'-PA-O3A
36	D	501	ATP	C3'-C4'-C5'-O5'
36	F	501	ATP	C5'-O5'-PA-O1A
36	F	501	ATP	C5'-O5'-PA-O2A
38	B	501	ADP	C5'-O5'-PA-O1A

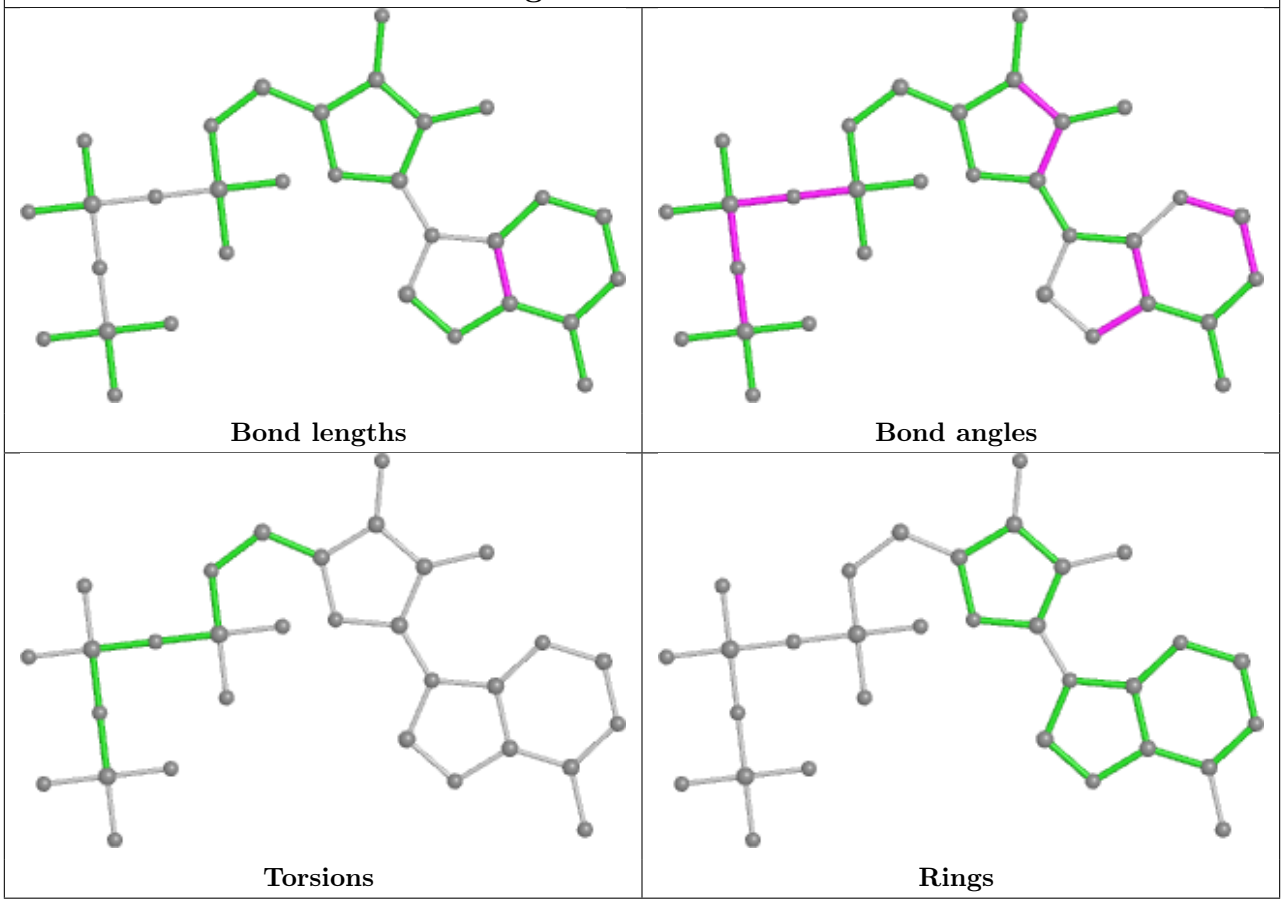
There are no ring outliers.

No monomer is involved in short contacts.

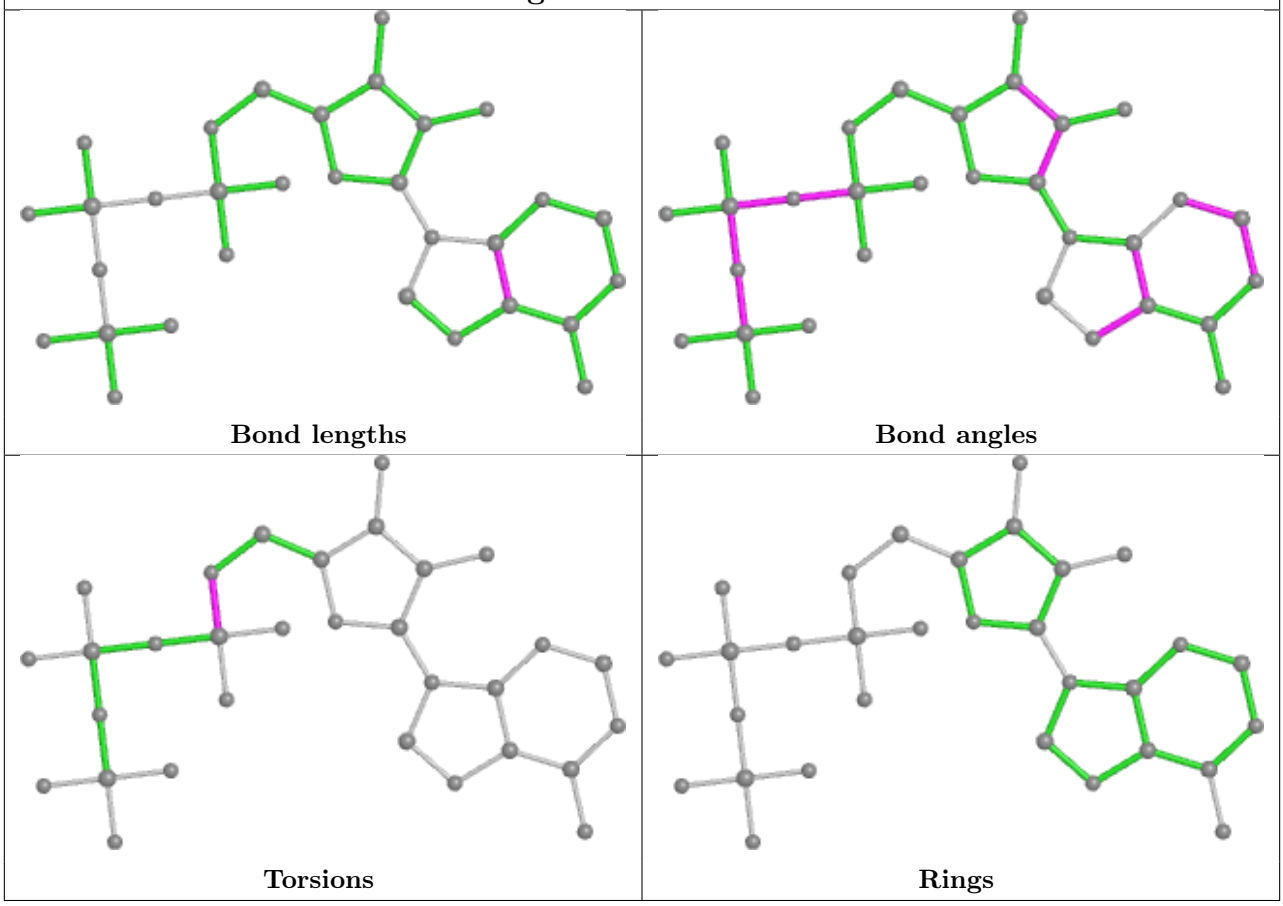
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

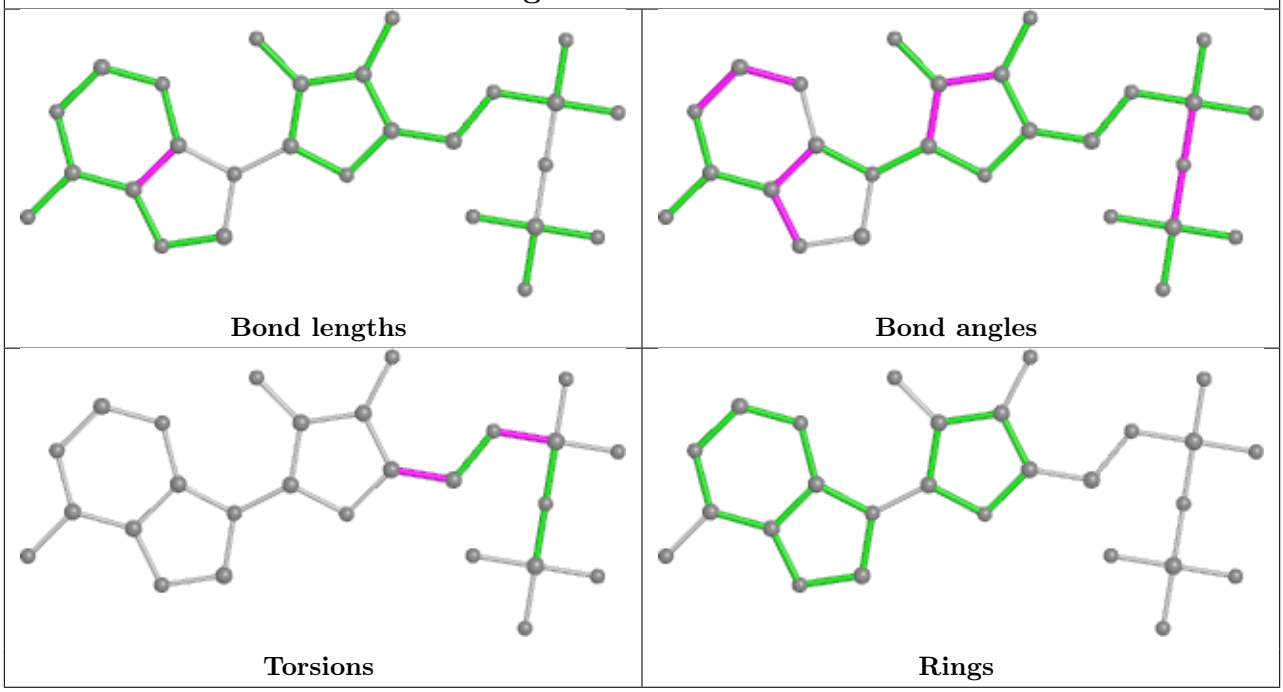
Ligand ATP A 501



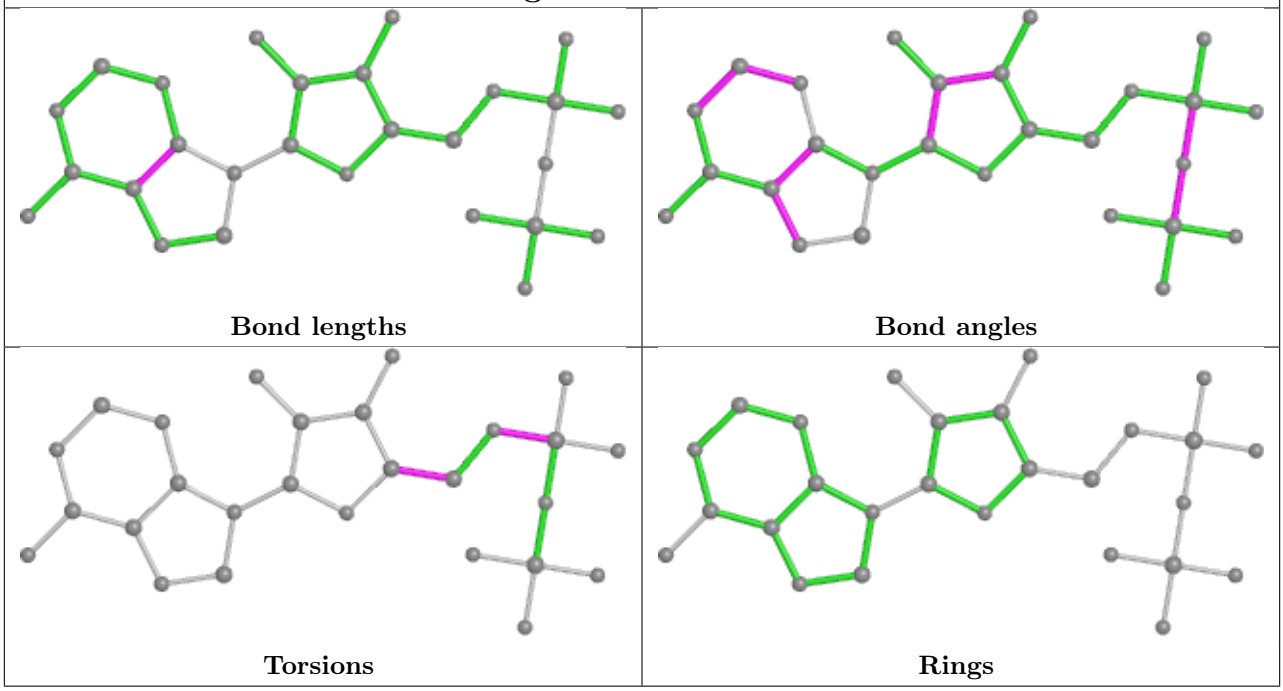
Ligand ATP F 501



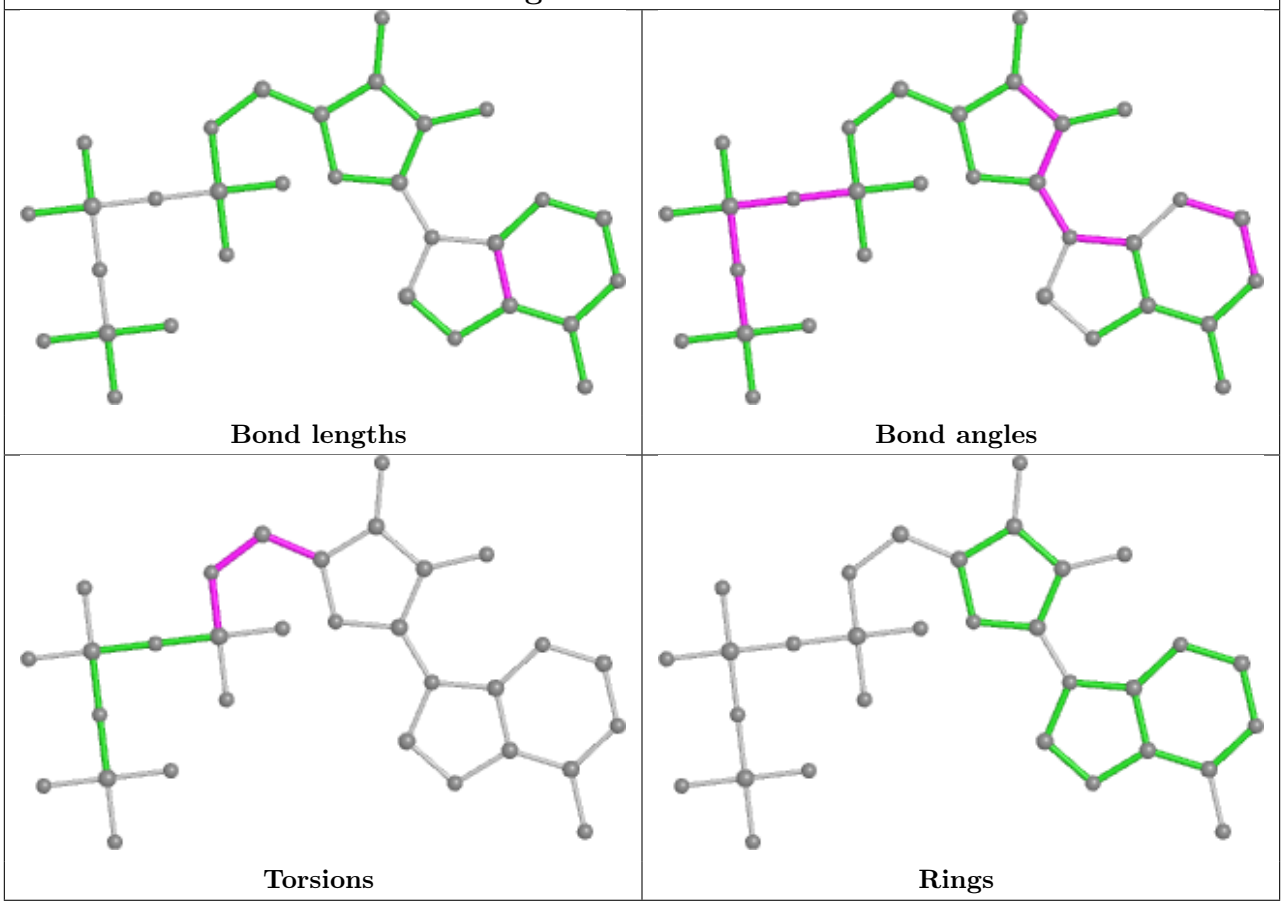
Ligand ADP B 501



Ligand ADP E 401



Ligand ATP D 501



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.

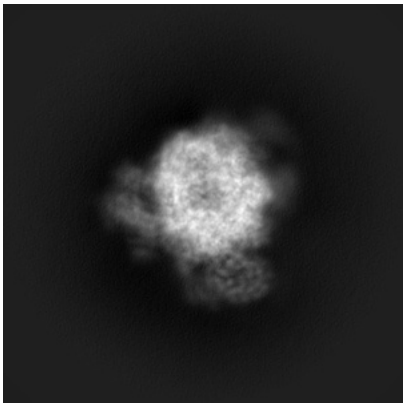
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9218. These allow visual inspection of the internal detail of the map and identification of artifacts.

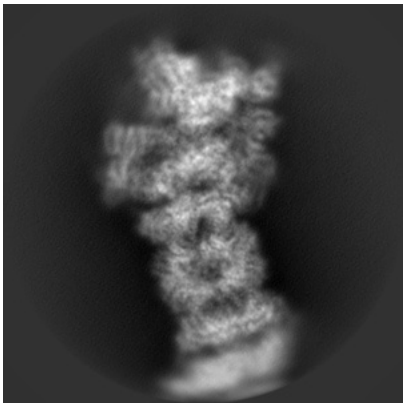
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

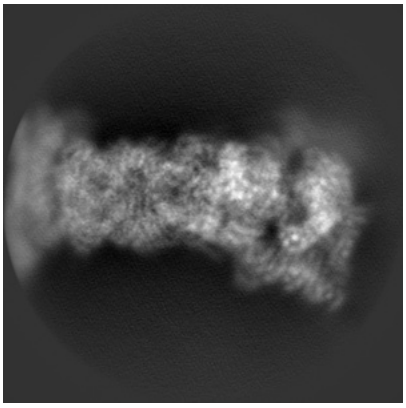
6.1.1 Primary map



X



Y

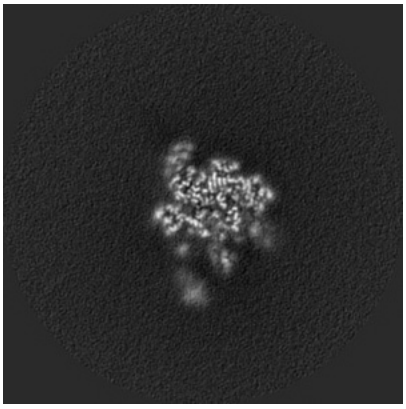


Z

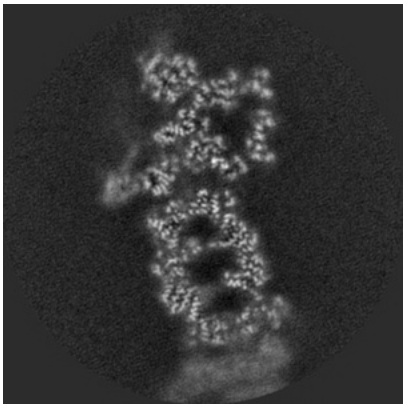
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

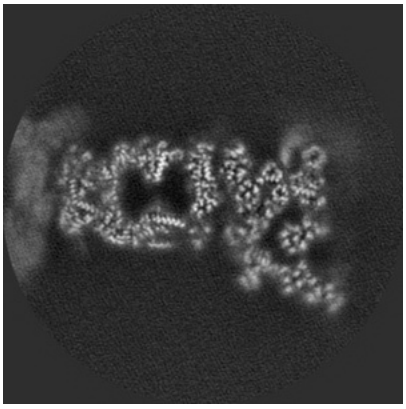
6.2.1 Primary map



X Index: 300



Y Index: 300

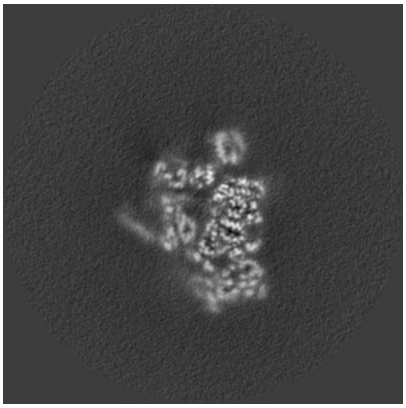


Z Index: 300

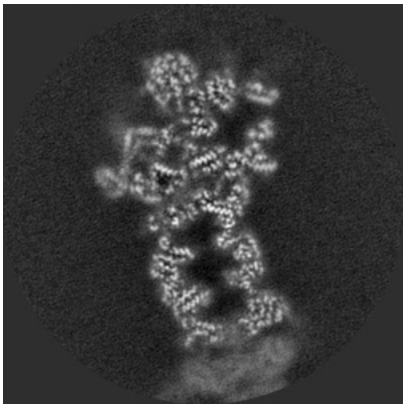
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

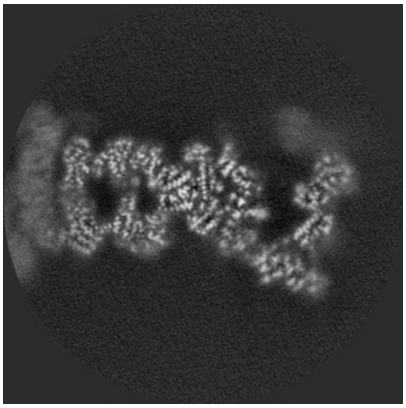
6.3.1 Primary map



X Index: 344



Y Index: 313

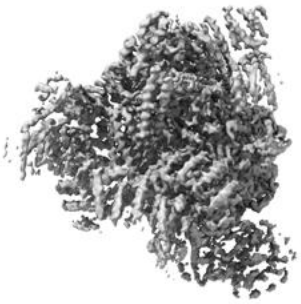


Z Index: 335

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

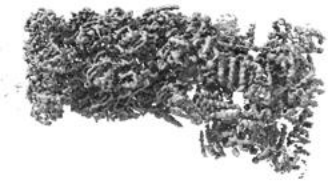
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

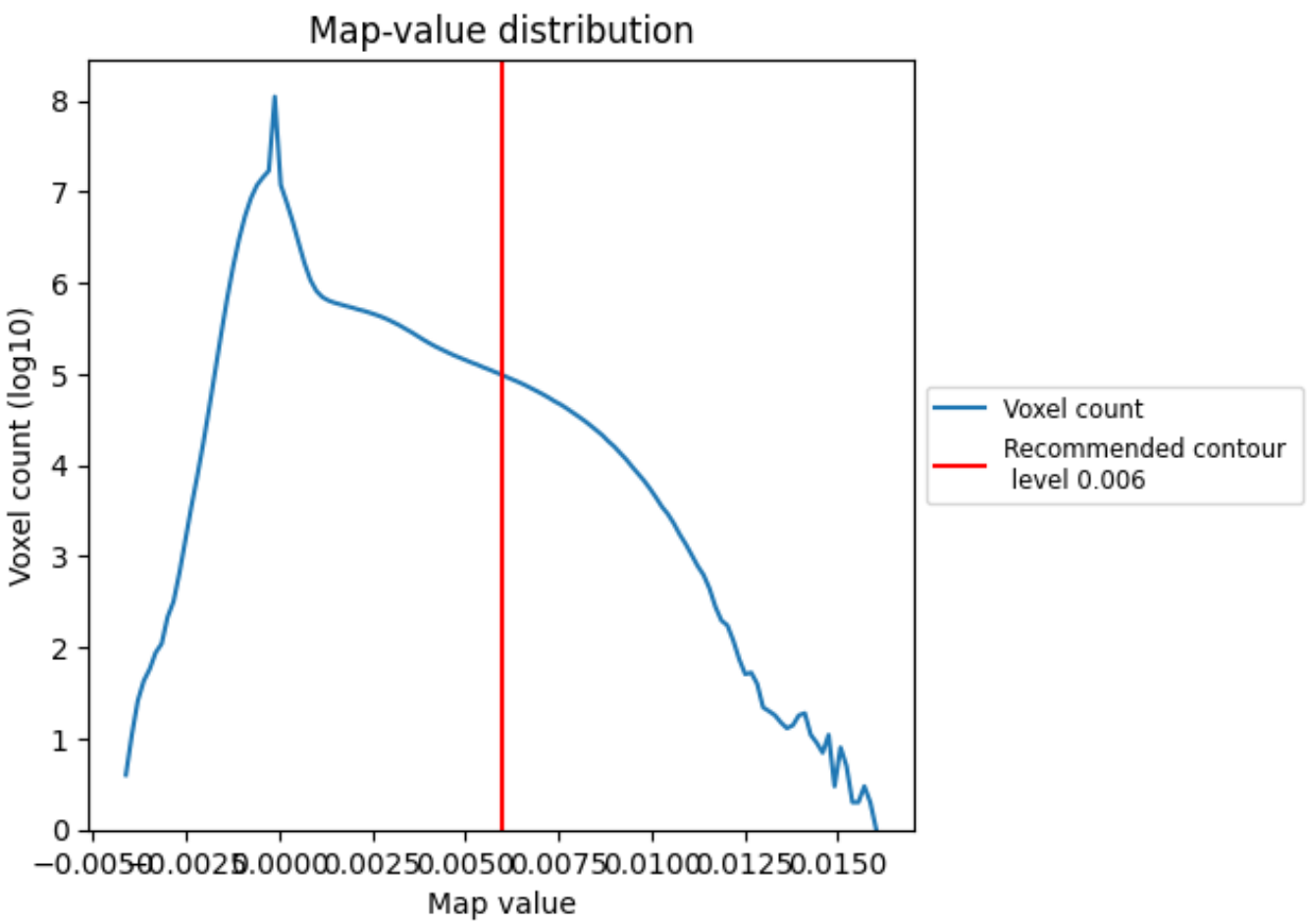
6.5 Mask visualisation (i)

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

7 Map analysis (i)

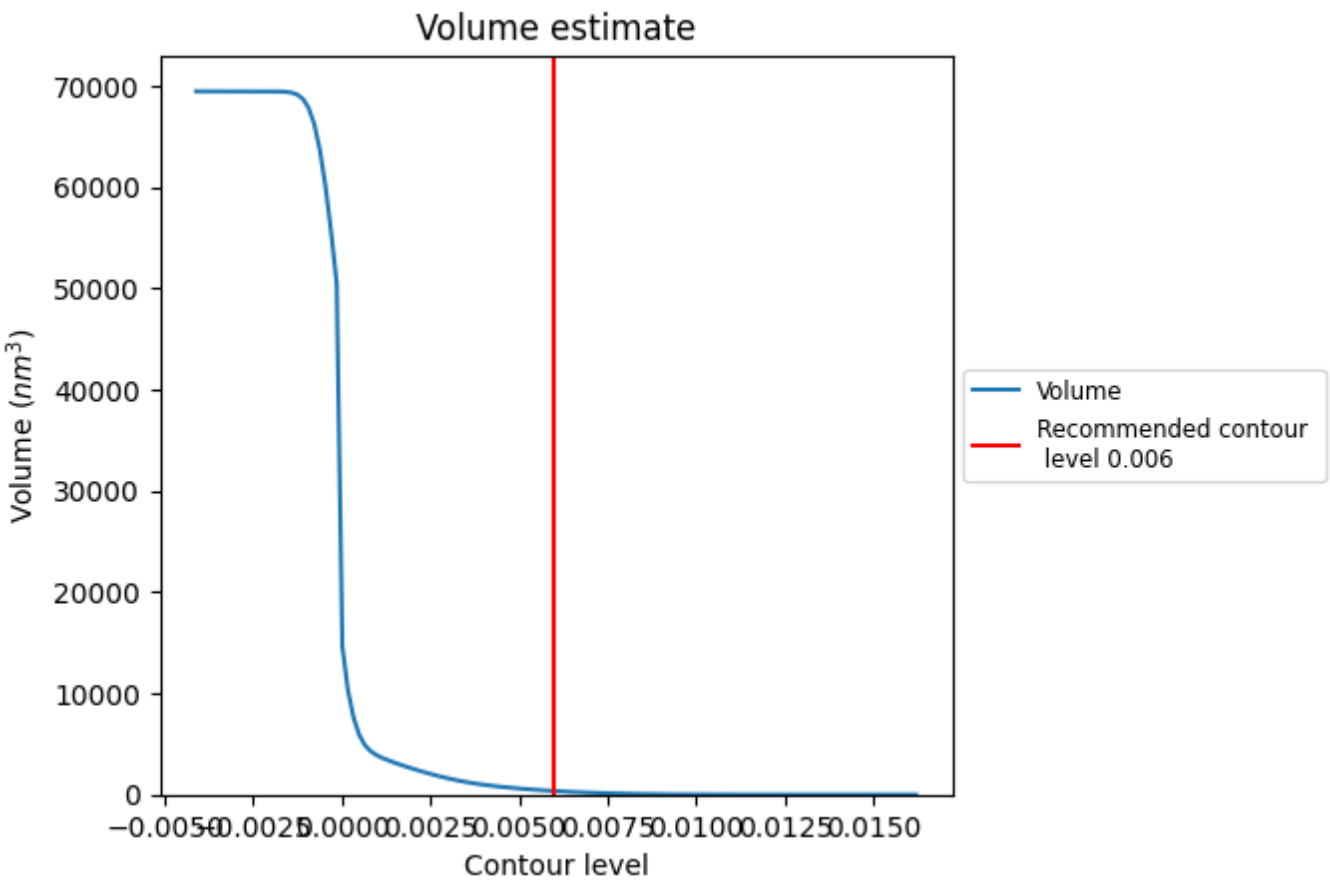
This section contains the results of statistical analysis of the map.

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.

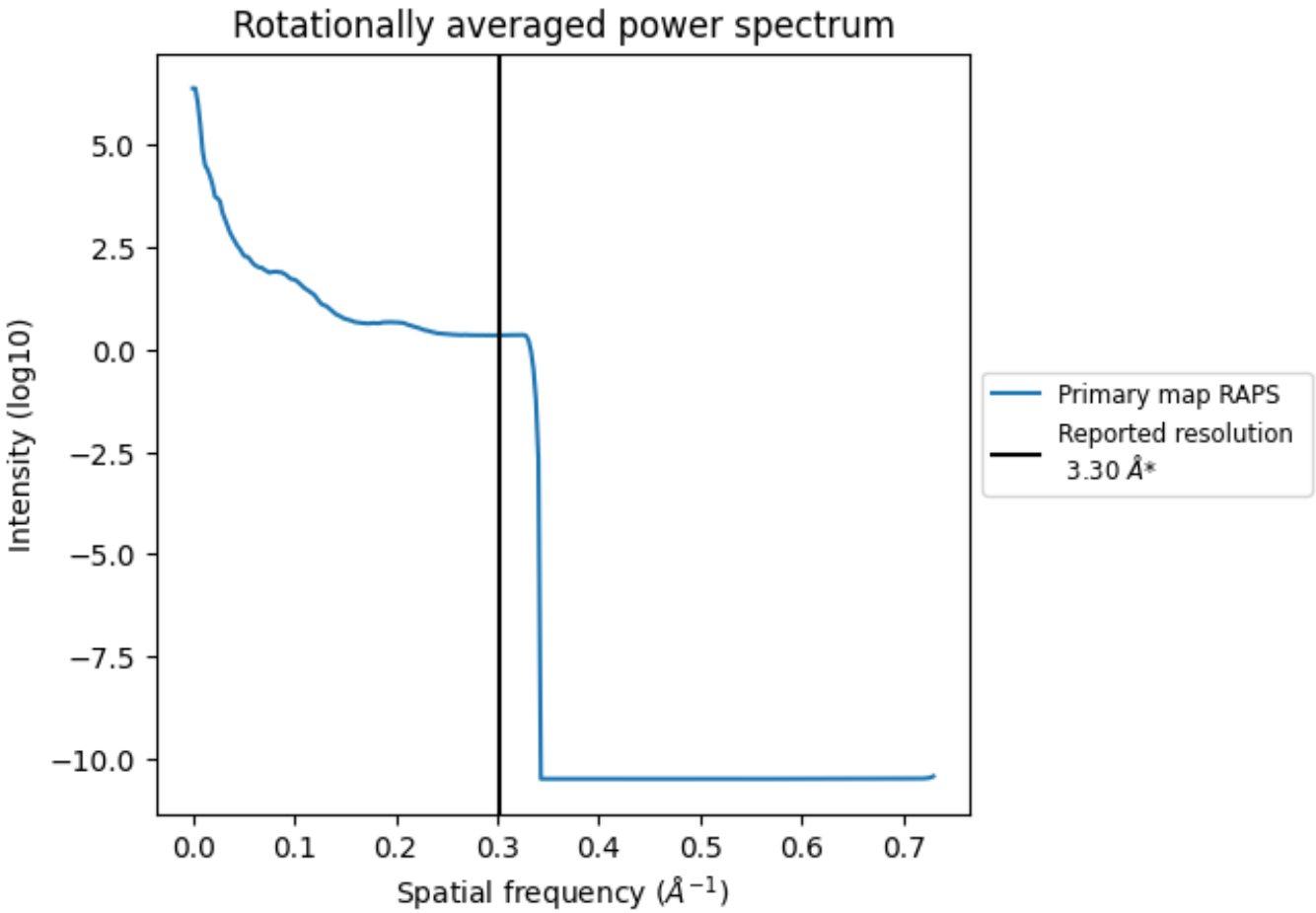
7.2 Volume estimate (i)



The volume at the recommended contour level is 350 nm^3; this corresponds to an approximate mass of 316 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 0.303 Å^{-1}

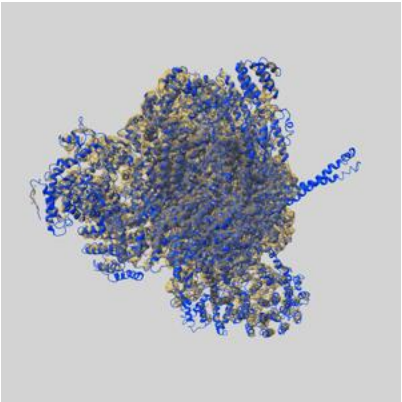
8 Fourier-Shell correlation (i)

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

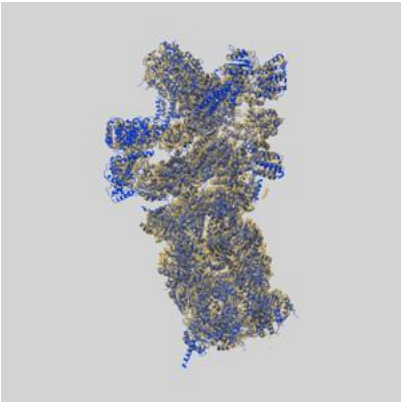
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9218 and PDB model 6MSE. Per-residue inclusion information can be found in section 3 on page 13.

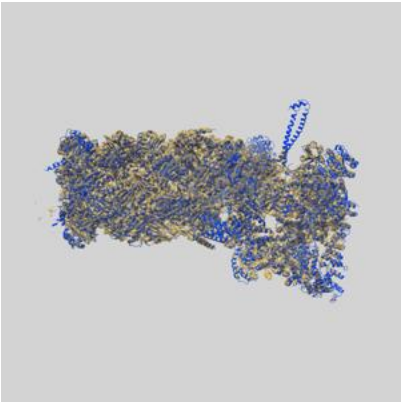
9.1 Map-model overlay (i)



X



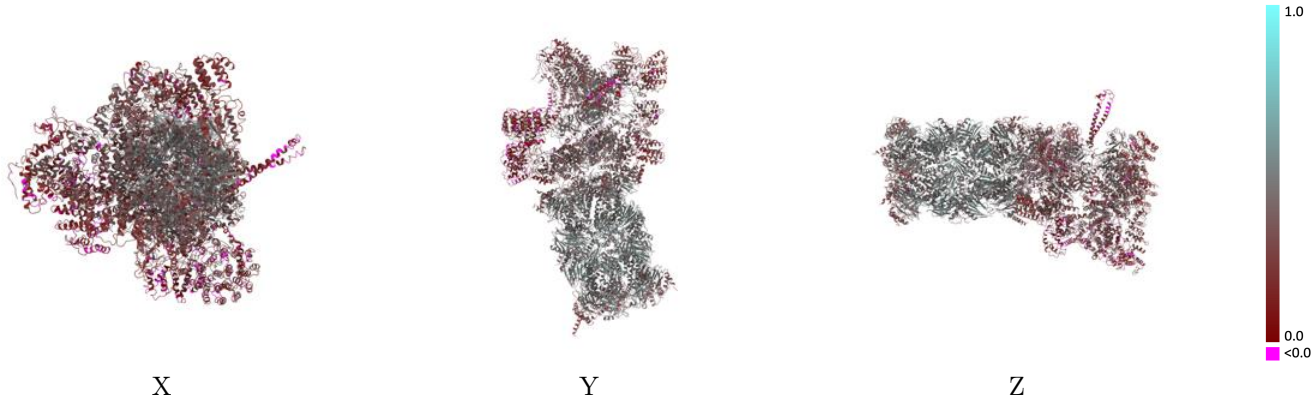
Y



Z

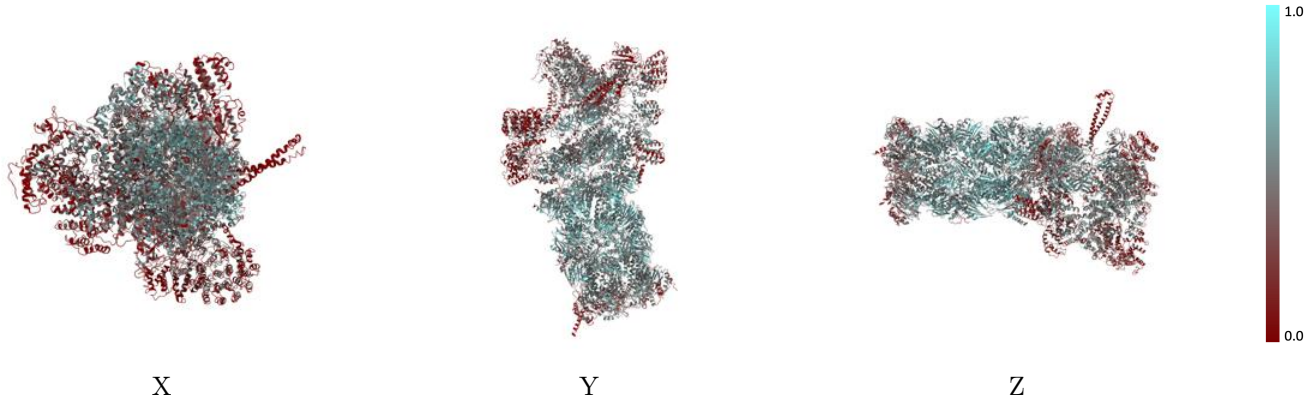
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



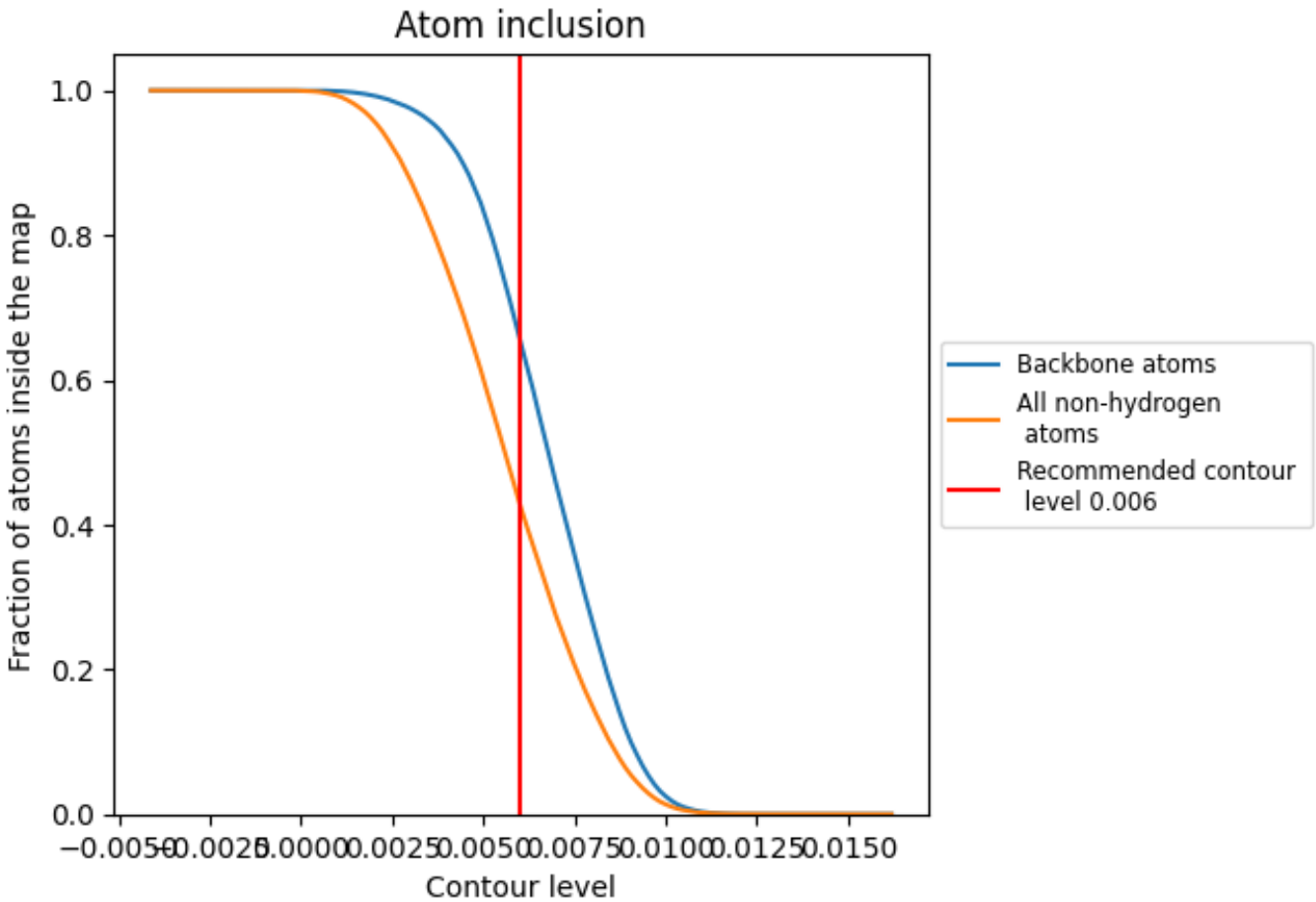
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 43% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4288	0.3550
A	0.4580	0.3390
B	0.4143	0.3210
C	0.3404	0.2970
D	0.4814	0.3710
E	0.4874	0.3650
F	0.4562	0.3530
G	0.5958	0.4380
H	0.6251	0.4410
I	0.5587	0.4010
J	0.5318	0.4010
K	0.5252	0.4120
L	0.5833	0.4330
M	0.5597	0.4060
N	0.6295	0.4730
O	0.5979	0.4690
P	0.6033	0.4800
Q	0.5883	0.4490
R	0.6262	0.4810
S	0.5676	0.4790
T	0.6254	0.4790
U	0.3494	0.2980
V	0.2465	0.2070
W	0.3923	0.2490
X	0.3599	0.3020
Y	0.2943	0.2070
Z	0.4291	0.3590
a	0.3337	0.2620
b	0.2137	0.2880
c	0.4646	0.3730
d	0.1508	0.2060
e	0.1758	0.0300
f	0.1609	0.1760
g	0.4237	0.4320
h	0.4279	0.4300

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Chain	Atom inclusion	Q-score
i	0.3426	0.3770
j	0.3259	0.3800
k	0.3775	0.3940
l	0.4726	0.4310
m	0.4414	0.4120
n	0.5844	0.4840
o	0.5273	0.4760
p	0.5520	0.4810
q	0.5322	0.4560
r	0.5854	0.4920
s	0.5458	0.4780
t	0.6075	0.4860
u	0.3834	0.3900
v	0.2517	0.3740