wwPDB EM Validation Summary Report

Oct 26, 2024 – 08:41 AM EDT

PDB ID	:	5VFR
EMDB ID	:	EMD-8665
Title	:	Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors	:	Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on	:	2017-04-09
Resolution	:	4.90 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:

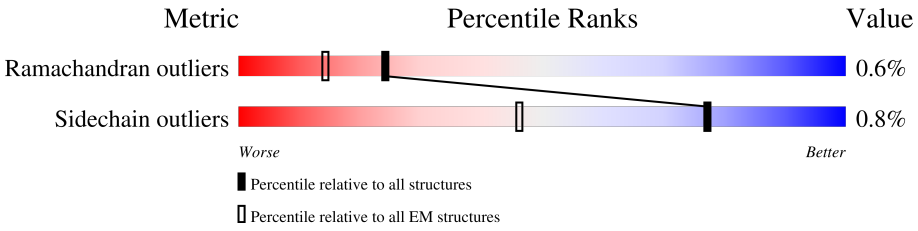
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.90 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	207382	16835
Sidechain outliers	206894	16415

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	911	83% 87% · 12%
2	V	480	95% 96% · ·
3	W	456	94% 98% ·
4	X	380	60% 63% 37%
5	Y	378	88% 99% ·
6	Z	286	89% 94% 6%
7	a	373	94% 98% ·
8	b	191	98% 99% ·
9	c	287	85% 93% · · ·

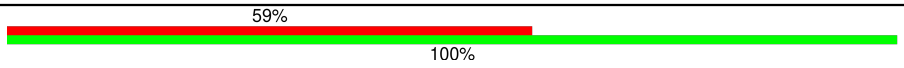
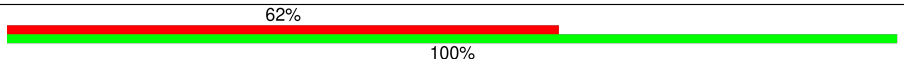
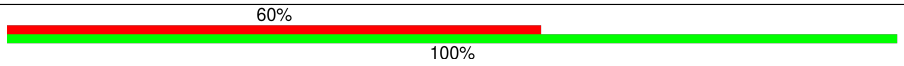
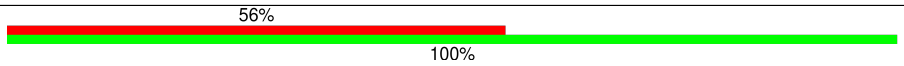
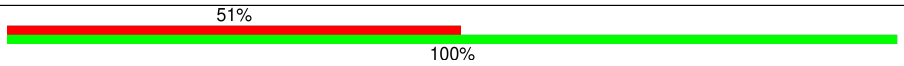
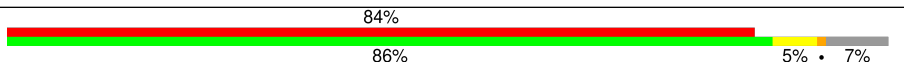
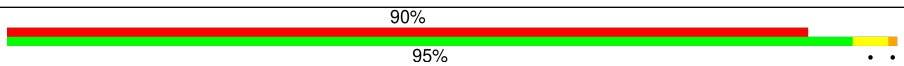
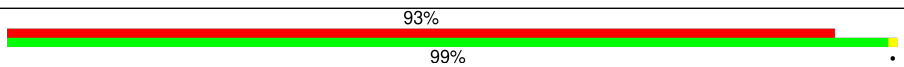
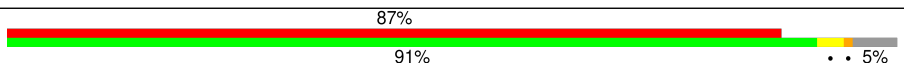
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	d	257	98% 99%
11	e	70	56% 54% 43%
12	G	240	77% 99%
12	g	240	78% 100%
13	H	232	84% 98%
13	h	232	79% 100%
14	I	250	76% 98%
14	i	250	84% 99%
15	J	243	76% 95%
15	j	243	76% 97%
16	K	234	63% 94%
16	k	234	62% 97%
17	L	238	60% 100%
17	l	238	67% 100%
18	M	245	69% 98%
18	m	245	74% 98%
19	N	191	61% 99%
19	n	191	55% 98%
20	O	220	69% 99%
20	o	220	66% 100%
21	P	204	63% 100%
21	p	204	63% 100%
22	Q	199	64% 99%
22	q	199	58% 97%
23	R	201	50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	r	201	
24	S	213	
24	s	213	
25	T	215	
25	t	215	
26	A	399	
27	B	389	
28	C	392	
29	D	380	
30	E	375	
31	F	396	
32	f	908	

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 99908 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
1	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	472	Total	C	N	O	S	0	0
			3799	2413	675	697	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

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

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

- Molecule 11 is a protein called Sem1.

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

- Molecule 12 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
12	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 13 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		

Continued on next page...

Continued from previous page...

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

- Molecule 14 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	248	Total 1895	C 1195	N 324	O 368	S 8	0	0
14	i	250	Total 1912	C 1204	N 329	O 371	S 8	0	0

- Molecule 15 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 16 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	228	Total 1729	C 1086	N 284	O 349	S 10	0	0
16	k	228	Total 1722	C 1080	N 284	O 348	S 10	0	0

- Molecule 17 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 18 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 19 is a protein called Proteasome subunit beta type-6.

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

- Molecule 20 is a protein called Proteasome subunit beta type-7.

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

- Molecule 21 is a protein called Proteasome subunit beta type-3.

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

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

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

- Molecule 23 is a protein called Proteasome subunit beta type-5.

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

- Molecule 24 is a protein called Proteasome subunit beta type-1.

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

- Molecule 25 is a protein called Proteasome subunit beta type-4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	342	Total	C	N	O	S	0	0
			2672	1684	475	497	16		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	350	Total	C	N	O	S	0	0
			2706	1703	458	533	12		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	363	Total	C	N	O	S	0	0
			2859	1804	513	525	17		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	F	376	2859	1802	496	546	15	0	0

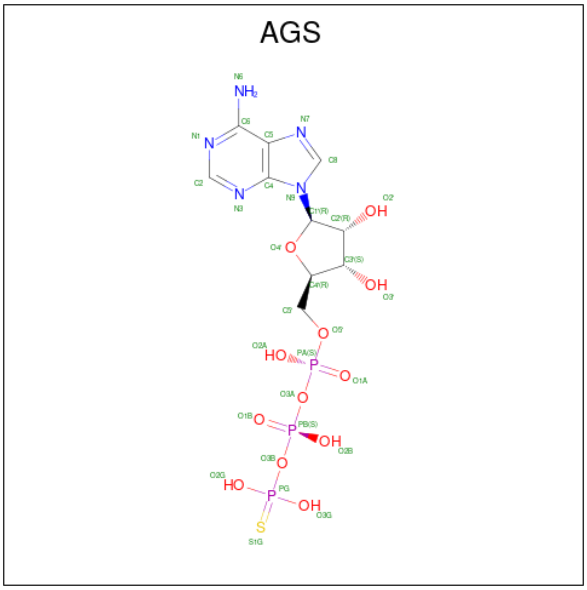
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	689	5319	3343	904	1037	35	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
34	A	1	31	10	5	12	3	1	0
34	B	1	31	10	5	12	3	1	0
34	D	1	31	10	5	12	3	1	0

Continued on next page...

Continued from previous page...

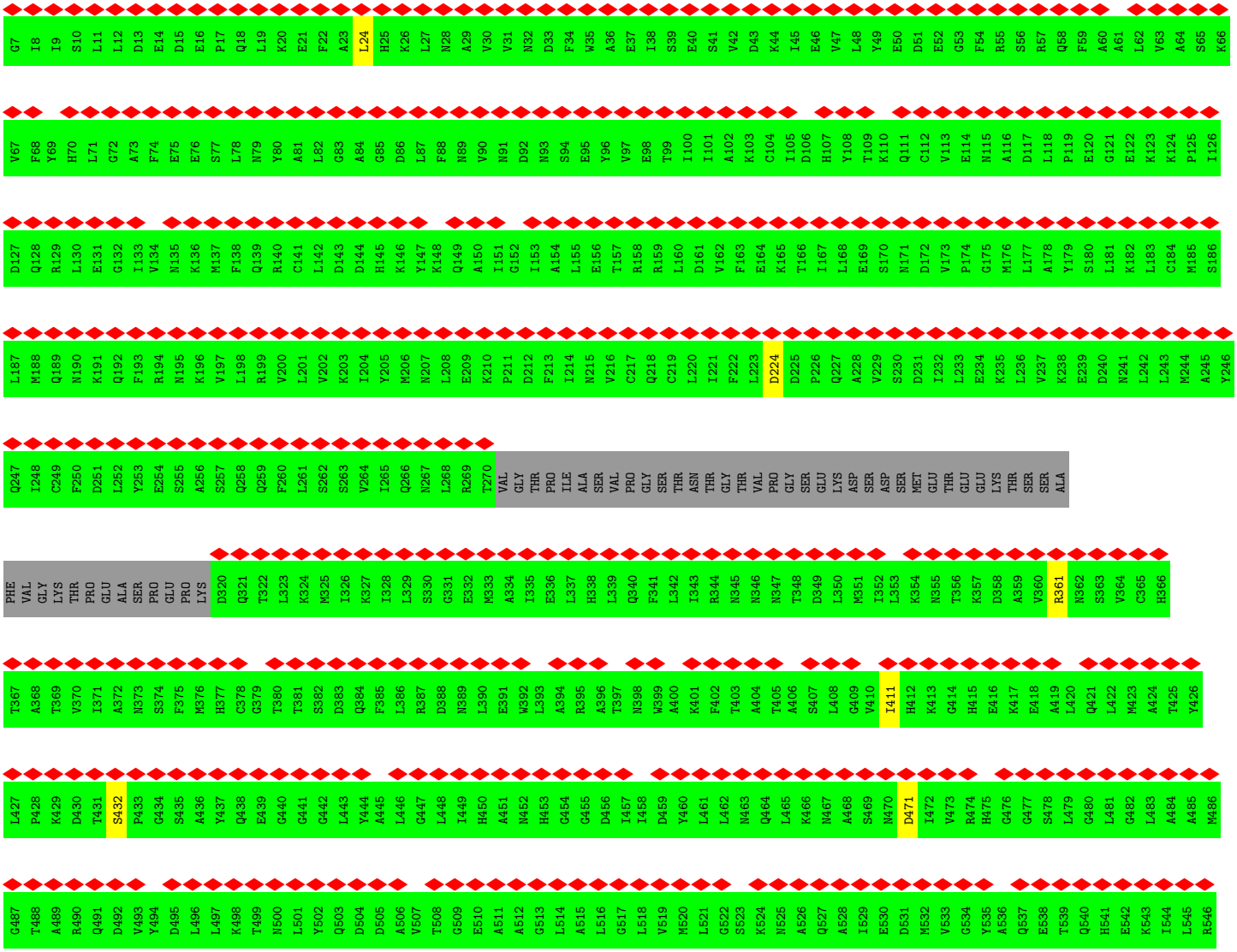
Mol	Chain	Residues	Atoms						AltConf
34	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

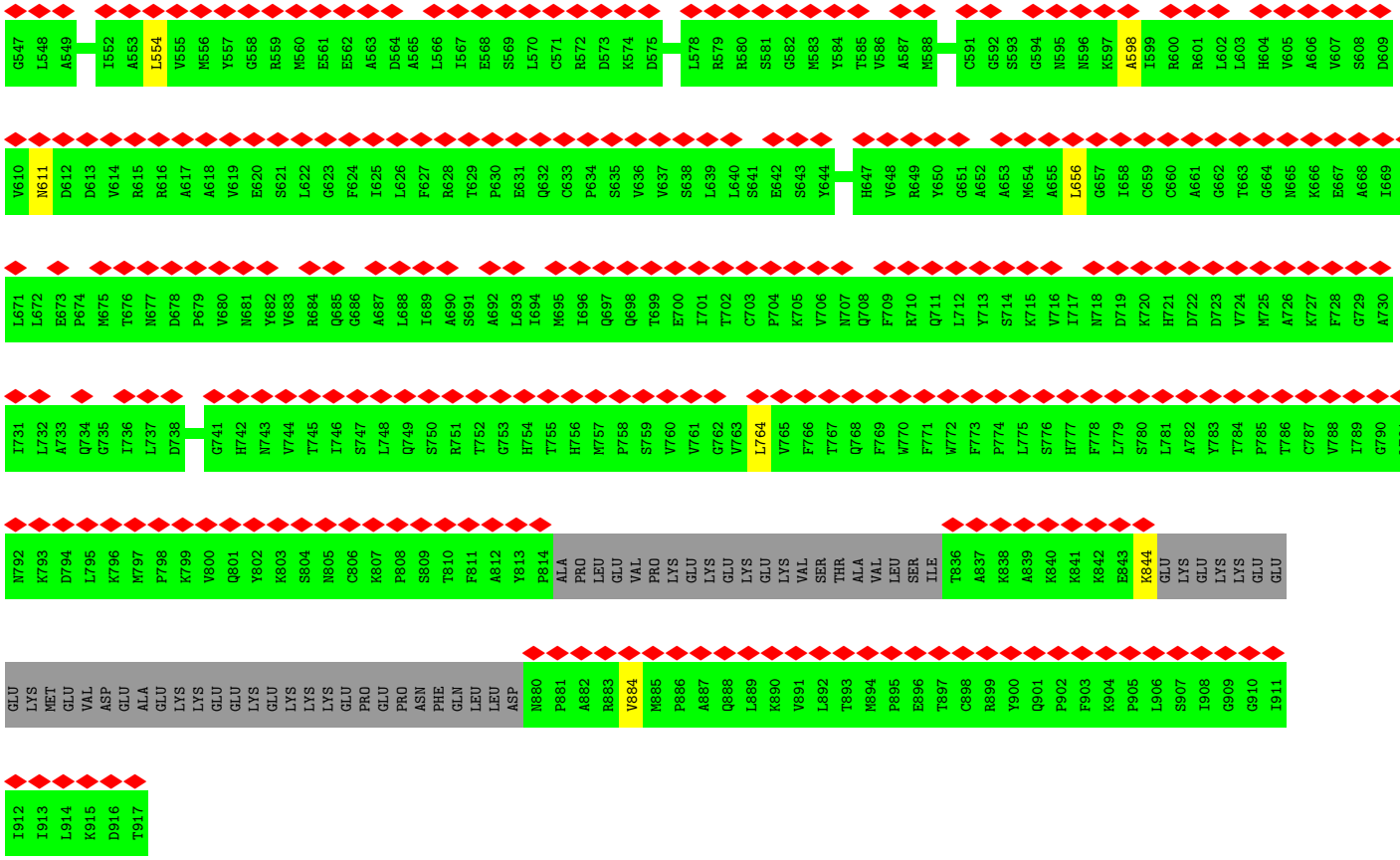
3 Residue-property plots (i)

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

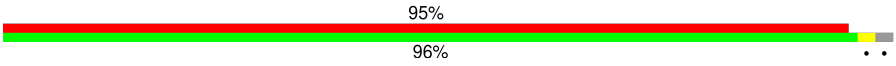
Chain U:

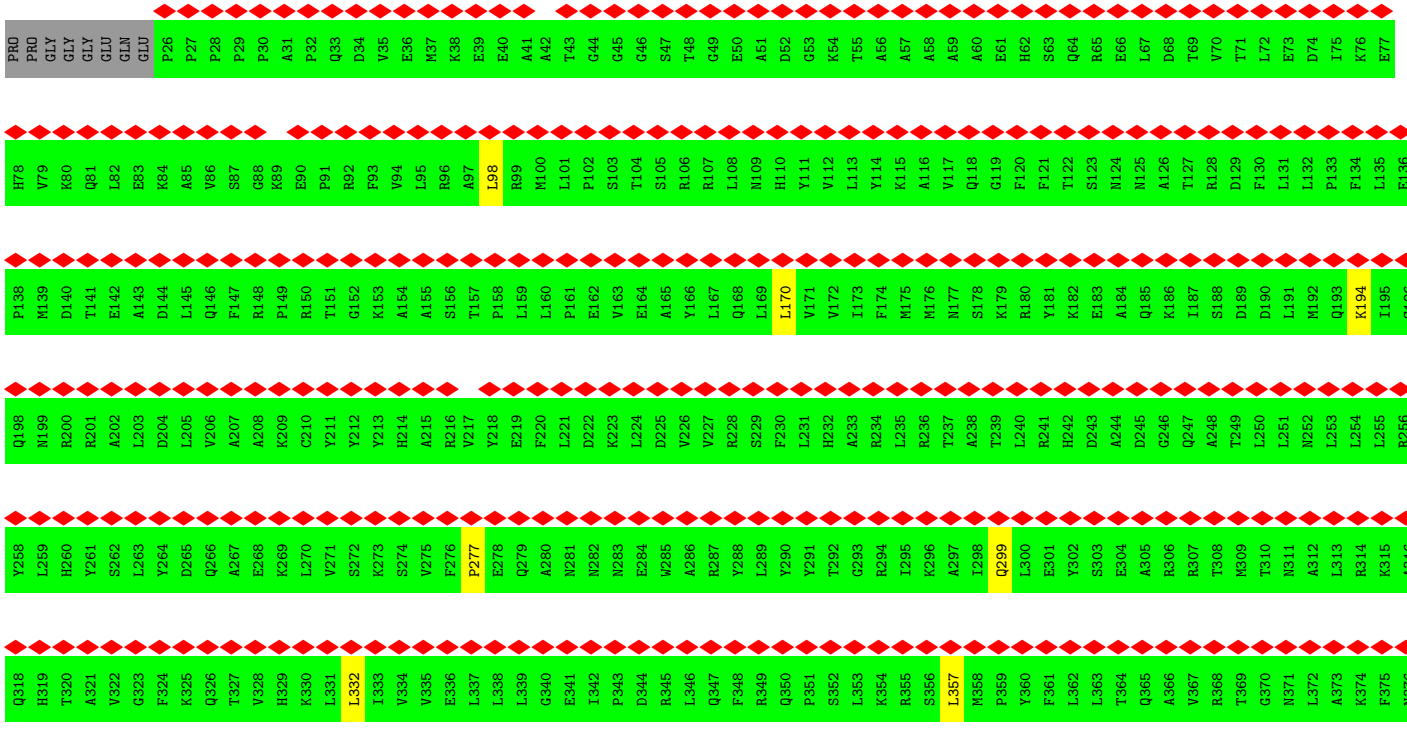




• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



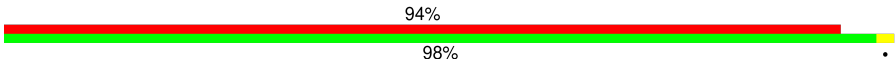


V378 L379 D380 Q381 F382 G383 E384 K385 F386 Q387 A388 D389 G390 T391 Y392 T393 L394 I395 I396 R397 L398 R399 H400 N401 V402 I403 K404 T405 G406 V407 R408 M409 I410 S411 L412 S413 R416 I417 S418 L419 A420 D421 I422 A423 Q424 K425 L426 Q427 L428 D429 S430 P431 E432 D433 A434 E435 F436 I437 V438

A439 K440 A441 I442 R443 D444 G445 V446 I447 E448 A449 S450 I451 N452 H453 E454 K455 G456 Y457 V458 Q459 S460 K461 E462 M463 I464 D465 I466 Y467 S468 T469 R470 E471 P472 Q473 L474 A475 F476 H477 Q478 R479 I480 S481 F482 C483 L484 D485 I486 H487 N488 M489 S490 V491 K492 A493 M494 R495 F496 P497

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

Chain W:



M1 A2 D3 G4 G5 S6 E7 R8 A9 D10 G11 R12 I13 V14 K15 M16 E17 V18 D19 Y20 S21 A22 T23 V24 D25 Q26 R27 L28 P29 E30 C31 A32 K33 L34 A35 K36 E37 G38 R39 L40 Q41 E42 V43 I44 E45 T46 L47 L48 S49 L50 E51 K52 Q53 T54 R55 T56 A57 S58 D59 M60

V61 S62 T63 S64 R65 I66 L67 V68 A69 V70 V71 K72 M73 C74 Y75 E76 A77 K78 E79 W80 D81 L82 L83 N84 E85 N86 I87 M88 L89 L90 S91 K92 R93 R94 S95 Q96 L97 K98 Q99 A100 V101 A102 K103 M104 V105 Q106 Q107 C108 C109 T110 Y111 V112 E113 E114 I115 T116 D117 L118 P119 I120

K121 L122 R123 L124 I125 D126 T127 L128 R129 M130 V131 T132 E133 G134 K135 I136 Y137 V138 E139 I140 E141 R142 A143 R144 L145 T146 K147 T148 L149 A150 T151 I152 K153 E154 Q155 N156 G157 D158 V159 K160 E161 A162 A163 S164 I165 L166 Q167 E168 L169 Q170 V171 E172 T173 Y174 G175 S176 M177 E178 K179 K180

E181 R182 V183 E184 F185 I186 L187 E188 Q189 M190 R191 L192 C193 L194 A195 V196 K197 D198 Y199 I200 R201 T202 Q203 I204 I205 S206 K207 K208 I209 N210 T211 K212 F213 F214 Q215 E216 E217 N218 T219 E220 K221 L222 K223 L224 K225 Y226 Y227 N228 L229 M230 I231 Q232 L233 D234 Q235 H236 E237 G238 S239 Y240

L241 S242 I243 C244 K245 H246 Y247 R248 Y251 D252 T253 P254 C255 I256 Q257 A258 E259 S260 E261 K262 W263 Q264 Q265 A266 L267 K268 S269 V270 V271 L272 Y273 V274 I275 L276 A277 P278 F279 D280 N281 E282 Q283 S284 D285 L286 V287 H288 R289 I290 S291 G292 D293 K294 K295 L296 E297 E298 I299 P300 K301

Y302 K303 D304 L305 L306 K307 L308 F309 T310 T311 M312 E313 L314 M315 R316 W317 S318 T319 L320 V321 E322 D323 Y324 G325 M326 E327 L328 R329 K330 G331 S332 L333 E334 S335 P336 A337 T338 D339 V340 F341 G342 S343 T344 E345 E346 G347 E348 K349 R350 W351 K352 D353 L354 K355 N356 R357 V358 H361 N362

I363 R364 I365 M366 A367 K368 Y369 Y370 T371 R372 I373 T374 M375 K376 R377 M378 A379 Q380 L381 L382 D383 L384 S385 V386 D387 E388 S389 E390 A391 F392 L393 S394 N395 L396 V397 V398 N399 K400 T401 I402 F403 A404 K405 V406 D407 R408 L409 A410 G411 I412 I413 N414 F415 Q416 R417 P418 K419 D420 P421 N422

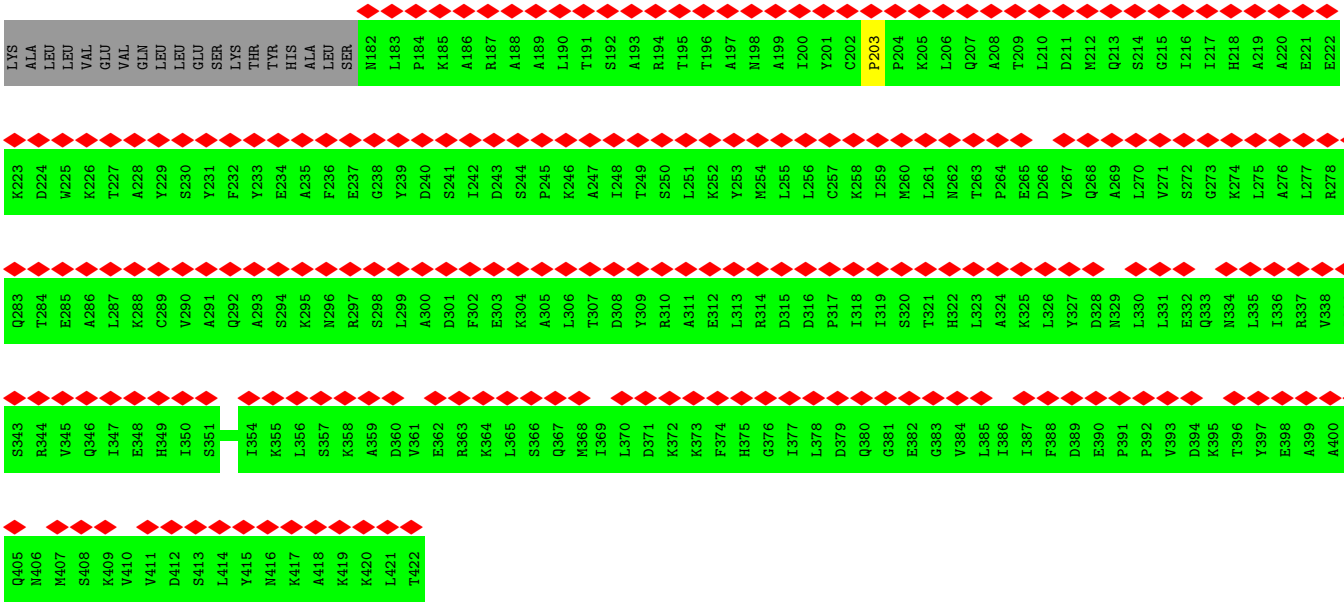
N423 L424 L425 N426 D427 W428 S429 Q430 K431 L432 N433 S434 S437 L438 V439 T443 H444 L445 I446 A447 K448 E449 E450 M451 I452 H453 N454 L455 Q456

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

Chain X:

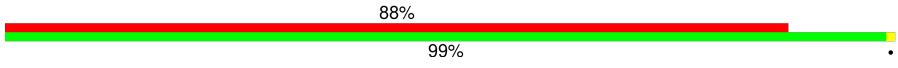
VAL GLN VAL LYS GLU GLN SER ILE LEU GLU LEU GLY SER LEU LEU ALA LYS THR GLY GLN ALA ALA GLU LEU GLY GLY LEU LEU LYS TYR VAL ARG PRO PHE LEU ASN SER ILE SER LYS ALA LYS ALA ALA ARG LEU VAL ARG SER LEU LEU ASP LEU PHE LEU ASP MET GLU ALA ALA

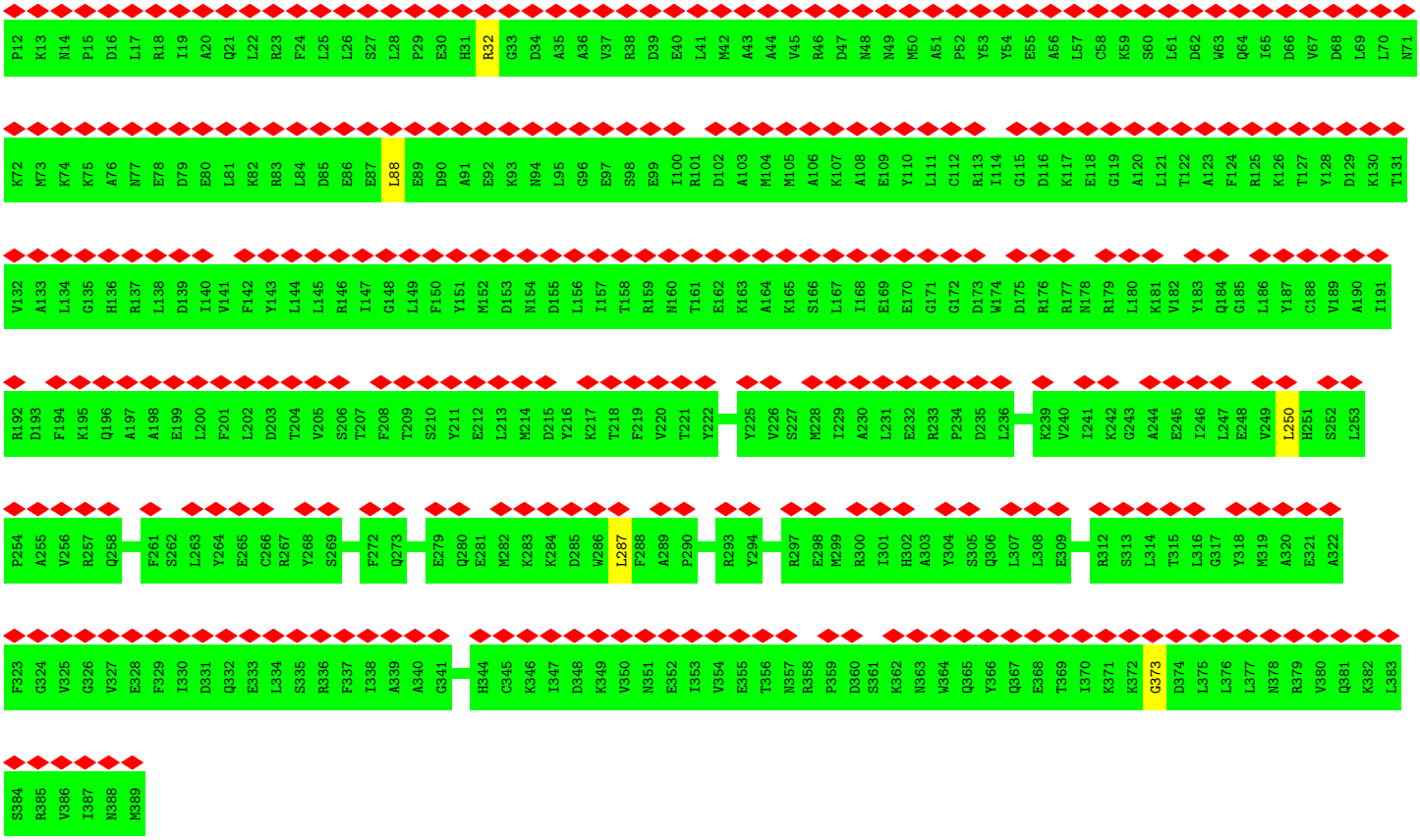
THR GLY GLN GLU VAL GLU LEU CYS LEU GLU CYS ILE GLU TRP ALA LYS SER GLU LYS ARG THR PHE LEU ARG GLN ALA LEU GLU ALA ARG LEU VAL SER LEU TYR PHE ASP THR LYS ARG TYR GLN GLU ALA LEU HIS LEU GLY SER GLN LEU LEU ARG GLU LEU LYS LYS MET ASP ASP



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

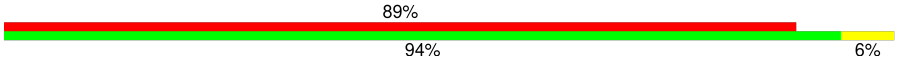
Chain Y:

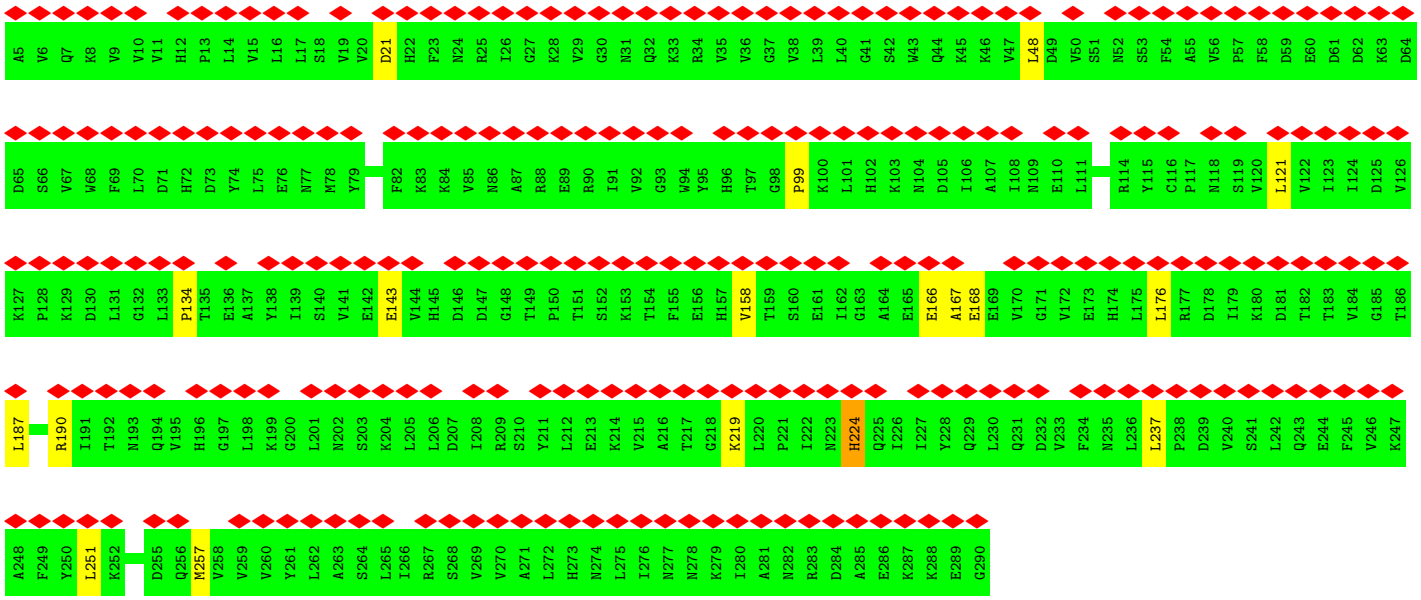




• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

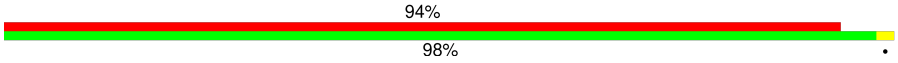
Chain Z:

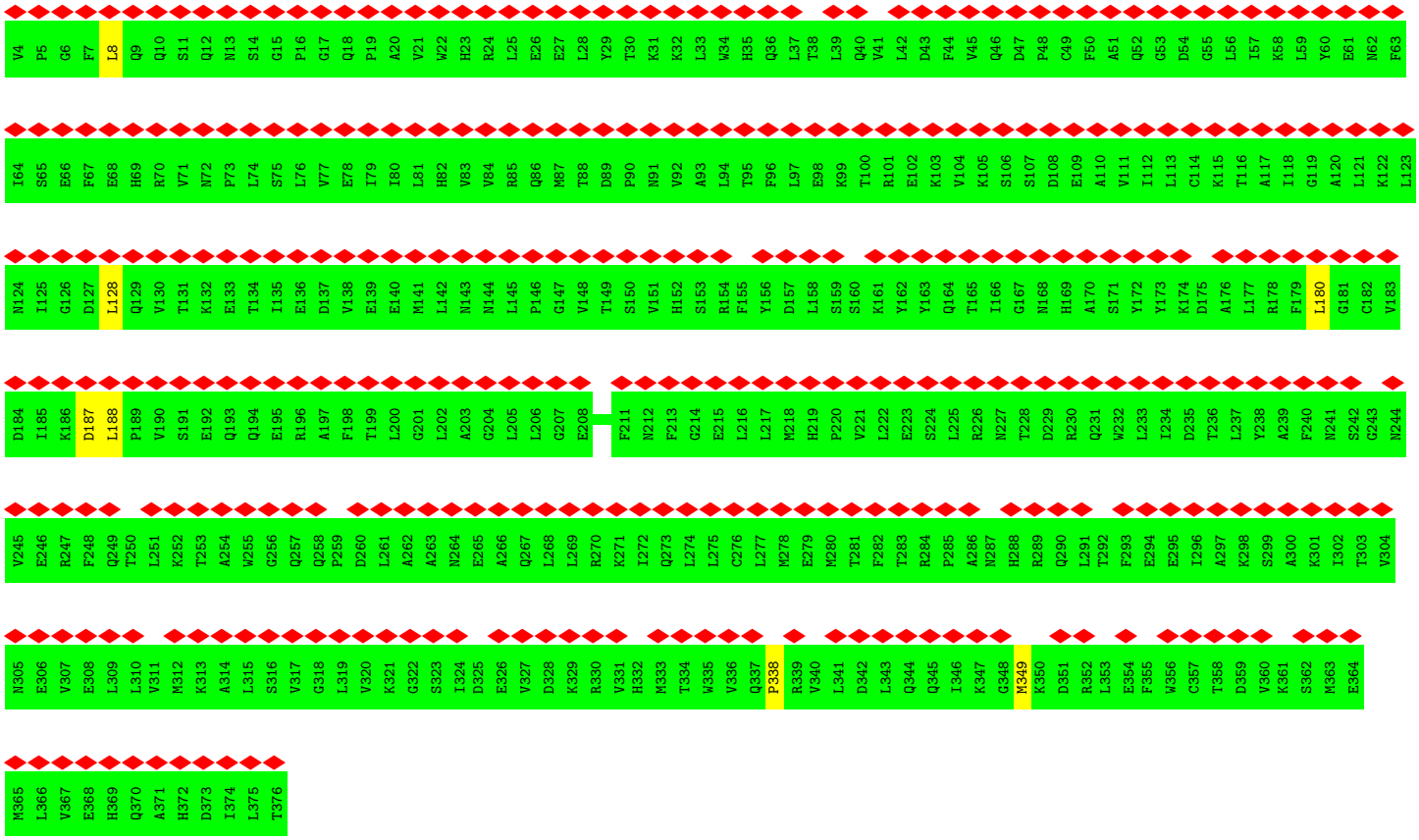




• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

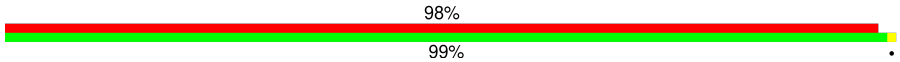
Chain a:





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

Chain b:



M1 V2 L3 E4 S5 T6 M7 V8 C9 V10 D11 N12 S13 E14 Y15 M16 R17 N18 G19 D20 F21 L22 P23 T24 R25 L26 Q27 A28 Q29 Q30 D31 A32 V33 N34 I35 V36 C37 H38 S39 K40 T41 R42 S43 N44 P45 E46 N47 N48 V49 G50 L51 I52 T53 L54 A55 N56 D57 C58 E59 V60

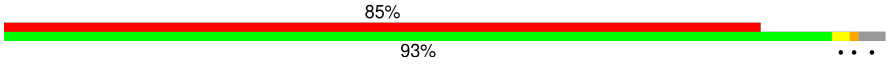
L61 T62 T63 L64 T65 P66 D67 T68 G69 R70 I71 L72 S73 K74 L75 H76 T77 V78 Q79 P80 K81 G82 K83 I84 T85 F86 C87 T88 G89 I90 R91 V92 A93 H94 L95 A96 L97 K98 H99 R100 Q101 G102 K103 N104 H105 K106 M107 R108 I109 I110 A111 F112 V113 G114 S115 P116 V117 E118 D119 N120

E121 K122 D123 L124 V125 K126 L127 A128 K129 R130 L131 K132 K133 E134 K135 V136 N137 V138 D139 I140 I141 N142 F143 G144 E145 E146 E147 V148 N149 T150 E151 K152 L153 T154 A155 F156 V157 N158 T159 L160 N161 G162 K163 D164 G165 T166 G167 S168 H169 L170 V171 T172 V173 P174 P175 G176 P177 S178 L179 A180

D181 A182 L183 I184 S185 S186 P187 I188 L189 A190 G191

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

Chain c:



A24 V25 D26 T27 A28 E29 Q30 V31 Y32 I33 S34 S35 L36 A37 L38 L39 K40 M41 L42 K43 H44 G45 R46 A47 G48 V49 P50 M51 E52 V53 M54 G55 L56 M57 L58 G59 E60 F61 V62 D63 D64 Y65 T66 V67 R68 V69 I70 D71 V72 F73 A74 M75 P76 Q77 S78 G79 T80 G81 V82 S83

V84 E85 A86 V87 V90 F91 Q92 A93 K94 M95 L96 D97 M98 L99 K100 Q101 T102 G103 R104 P105 E106 M107 V108 V109 G110 W111 Y112 H113 S114 H115 P116 G117 F118 G119 C120 G124 V125 D126 Q130 Q131 S132 F133 E134 A135 L136 S137 E138 R139 A140 V141 A142 V143 V144 V145 D146 P147 I148

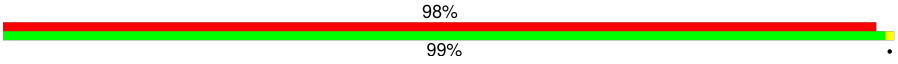
Q149 S150 V151 K152 G153 K154 V155 V156 I157 D158 A159 F160 R161 L162 I163 N164 A165 N166 M167 M168 V169 L170 G171 H172 E173 P174 R175 Q176 T177 N180 L181 G182 H183 L184 N185 K186 P187 S188 I189 Q190 A191 L192 G195 L196 N197 R198 H199 Y200 Y201 S202 I203 T204 I205 N206 Y207 R208 K209 N210

E211 L212 E213 Q214 K215 M216 L217 L218 N219 L220 H221 K222 K223 S224 W225 M226 E227 G228 L229 T230 L231 Q232 D233 Y234 SER GLU HIS CYS LYS HIS ASN GLU SER V244 V245 K246 E247 M248 L249 E250 L251 A252 K253 N254 Y255 N256 K257 A258 E262 D263 K264 M265 T266 P267 E268 Q269 L270 A271 I272

K273 N274 V275 G276 K277 Q278 D279 P280 K281 R282 H283 L284 E285 E286 H287 V288 D289 V290 L291 M292 T293 S294 N295 I296 V297 Q298 A301 A302 M303 L304 D305 T306 V307 V308 F309 K310

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

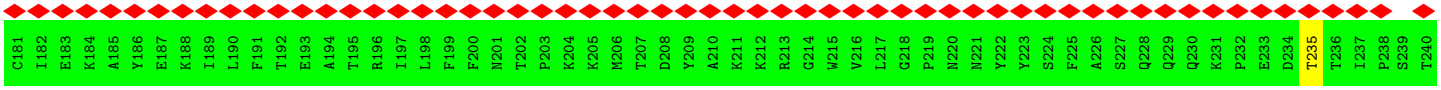
Chain d:

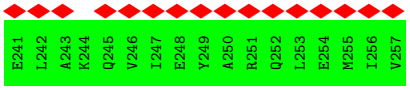


M1 Y2 E3 Q4 L5 K6 G7 E8 W9 N10 R11 K12 S13 P14 N15 L16 S17 K18 C19 G20 E21 E22 L23 G24 R25 L26 K27 L28 V29 L30 L31 E32 L33 N34 F35 L36 P37 T38 T39 G40 T41 K42 L43 T44 K45 Q46 Q47 L48 I49 L50 A51 R52 D53 I54 L55 E56 I57 G58 A59 Q60

W61 S62 I63 L64 R65 K66 D67 I68 P69 S70 F71 E72 R73 Y74 M75 A76 Q77 L78 K79 C80 Y81 Y82 F83 D84 Y85 K86 E87 Q88 L89 P90 E91 S92 A93 Y94 M95 H96 Q97 L98 L99 G100 L101 N102 L103 L104 F105 L106 L107 S108 Q109 N110 R111 V112 A113 E114 F115 H116 T117 E118 L119 E120

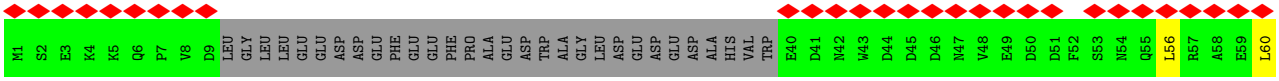
R121 L122 P123 A124 K125 D126 I127 Q128 T129 N130 V131 Y132 I133 K134 H135 P136 V137 S138 L139 E140 Q141 Y142 L143 M144 E145 G146 S147 Y148 N149 K150 V151 F152 L153 A154 K155 G156 N157 I158 P159 A160 E161 S162 Y163 T164 F165 F166 I167 D168 I169 L170 L171 D172 T173 I174 R175 D176 E177 I178 A179 G180

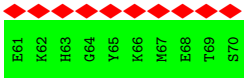




• Molecule 11: Sem1

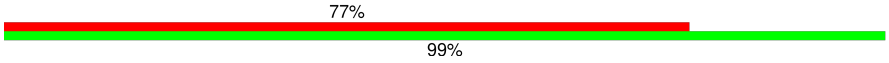
Chain e:

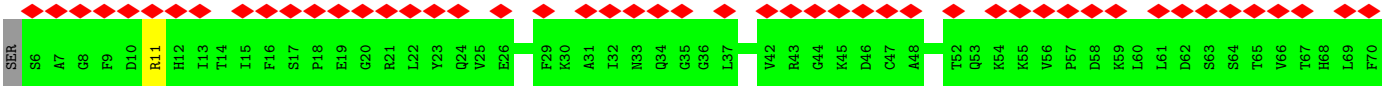


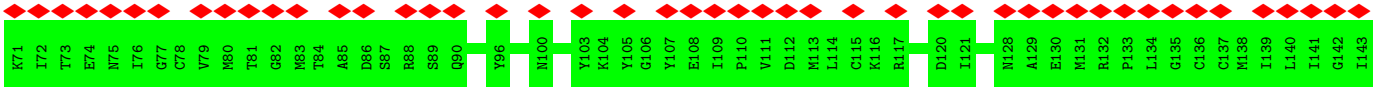


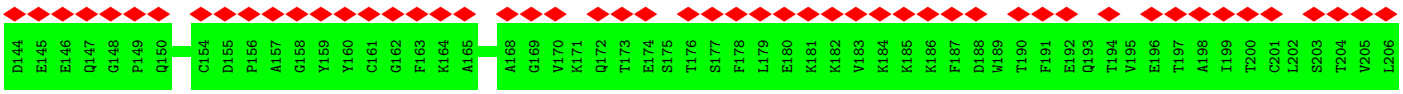
• Molecule 12: Proteasome subunit alpha type-6

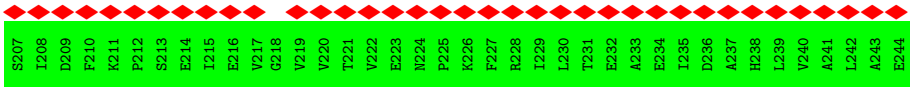
Chain G:





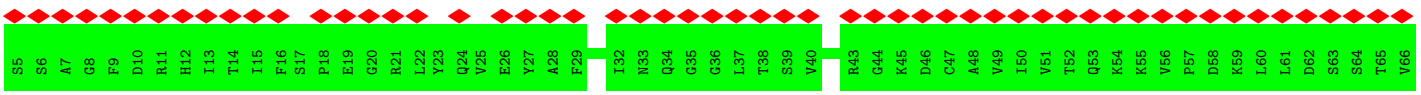


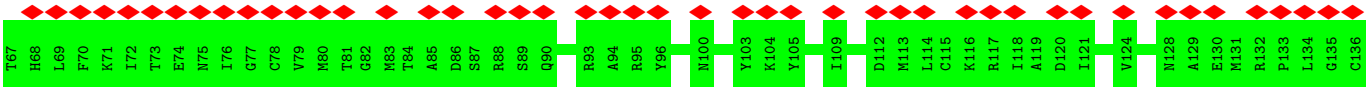


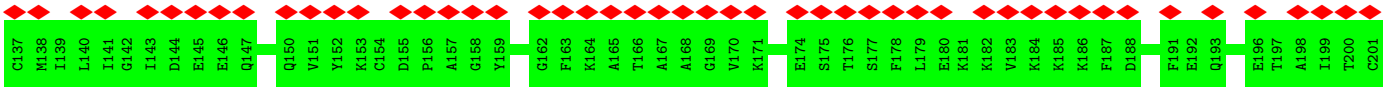


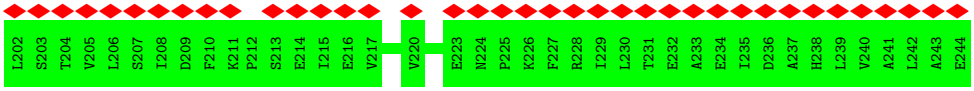
• Molecule 12: Proteasome subunit alpha type-6

Chain g:



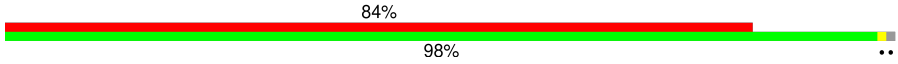


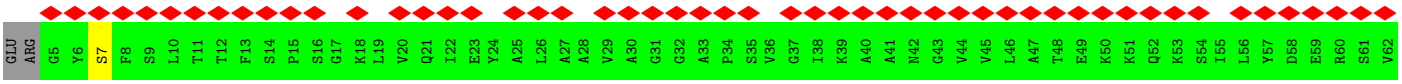


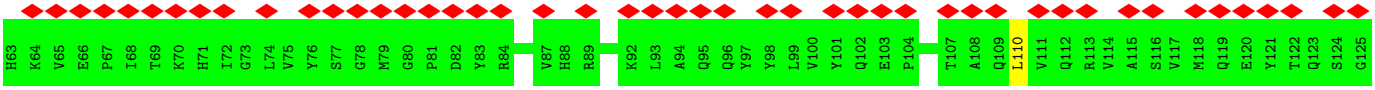


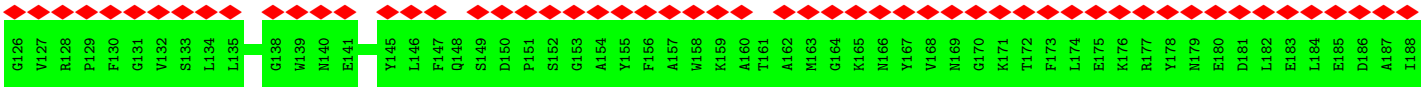
• Molecule 13: Proteasome subunit alpha type-2

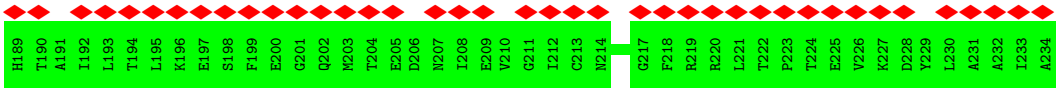
Chain H:





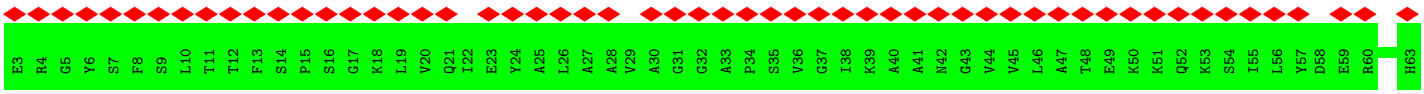


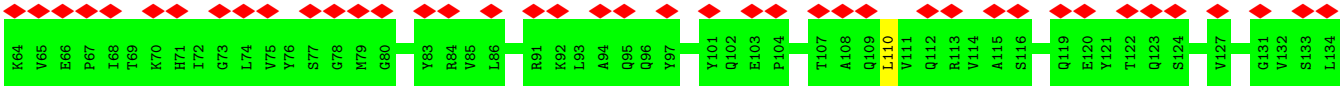


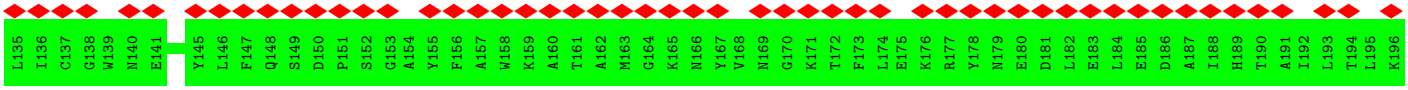


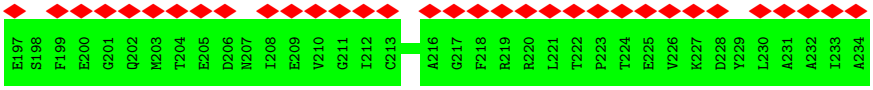
• Molecule 13: Proteasome subunit alpha type-2

Chain h:



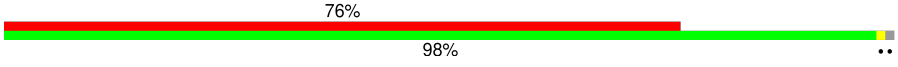


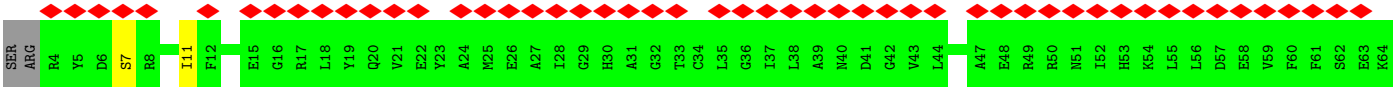


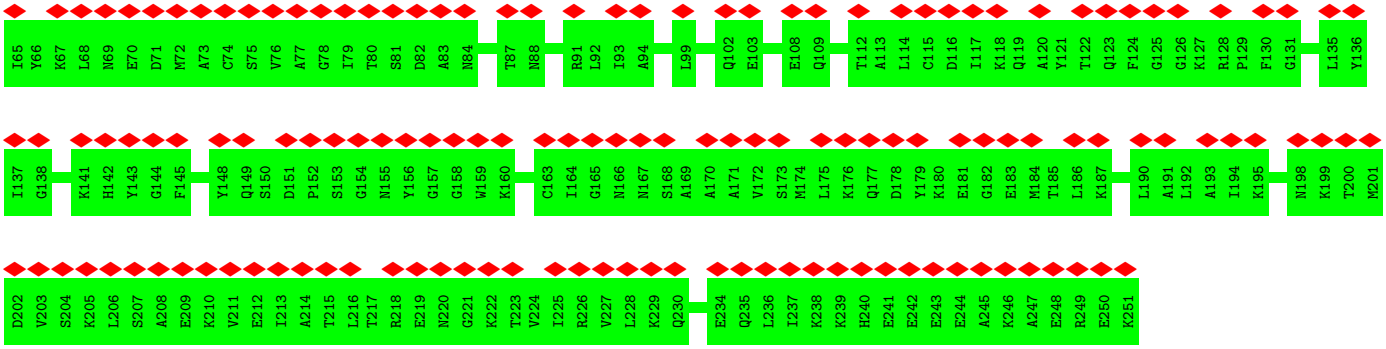


• Molecule 14: Proteasome subunit alpha type-4

Chain I:

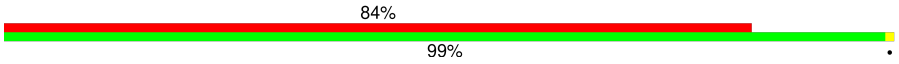


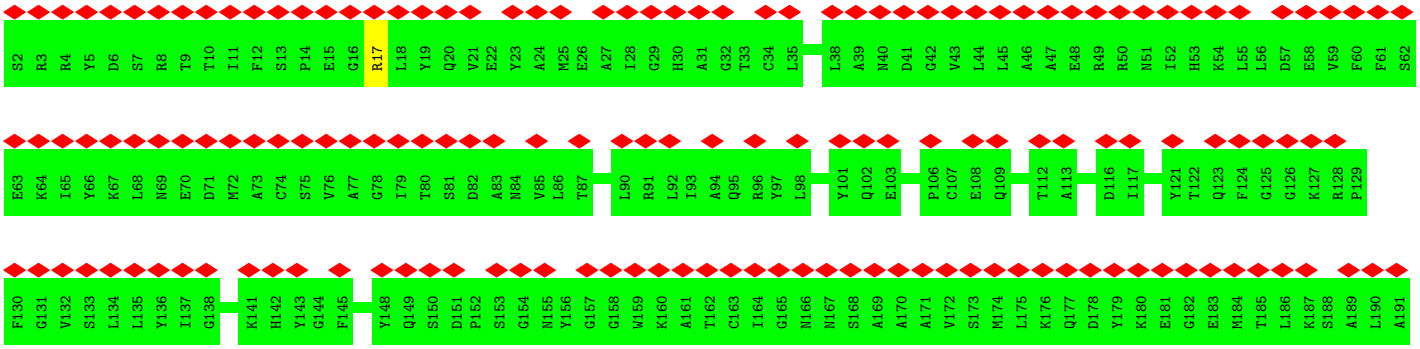




• Molecule 14: Proteasome subunit alpha type-4

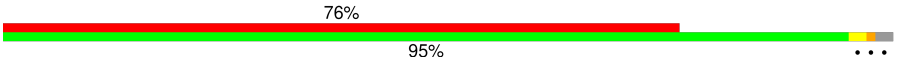
Chain i:

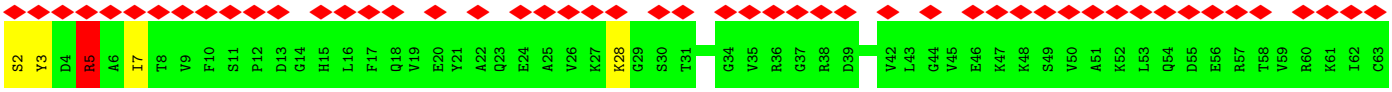




• Molecule 15: Proteasome subunit alpha type-7

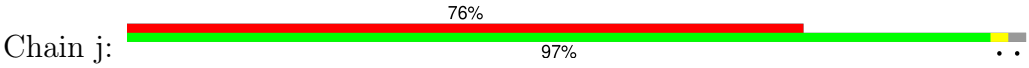
Chain J:

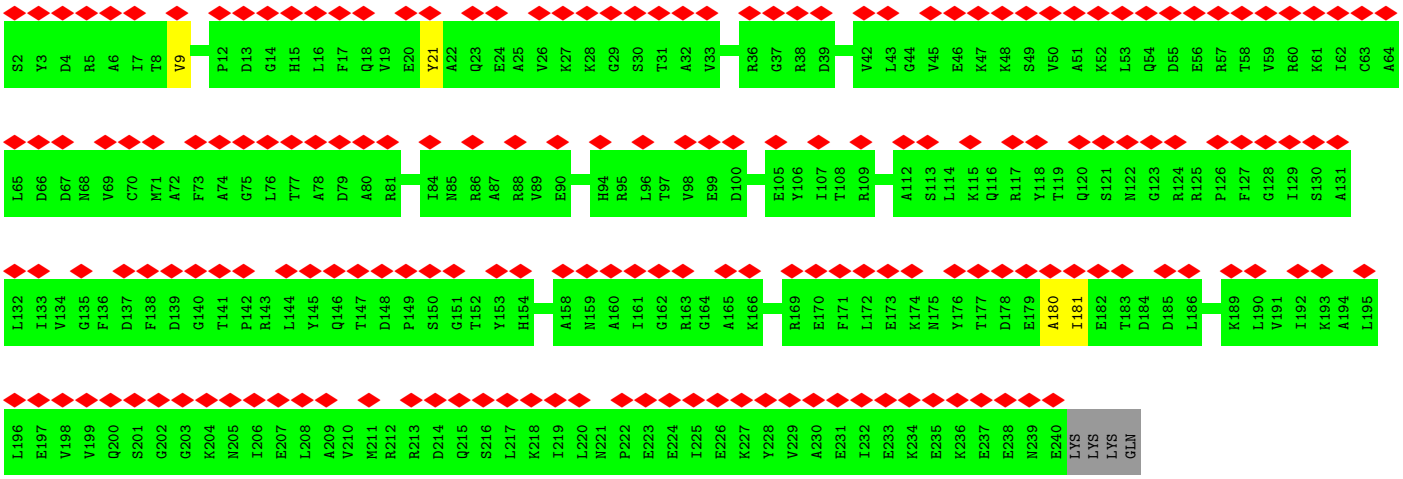




• Molecule 15: Proteasome subunit alpha type-7

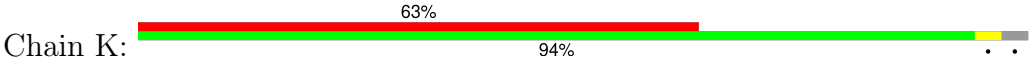
Chain j:

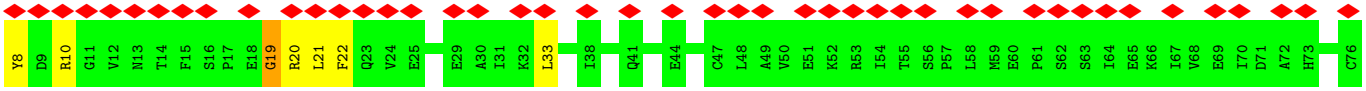




• Molecule 16: Proteasome subunit alpha type-5

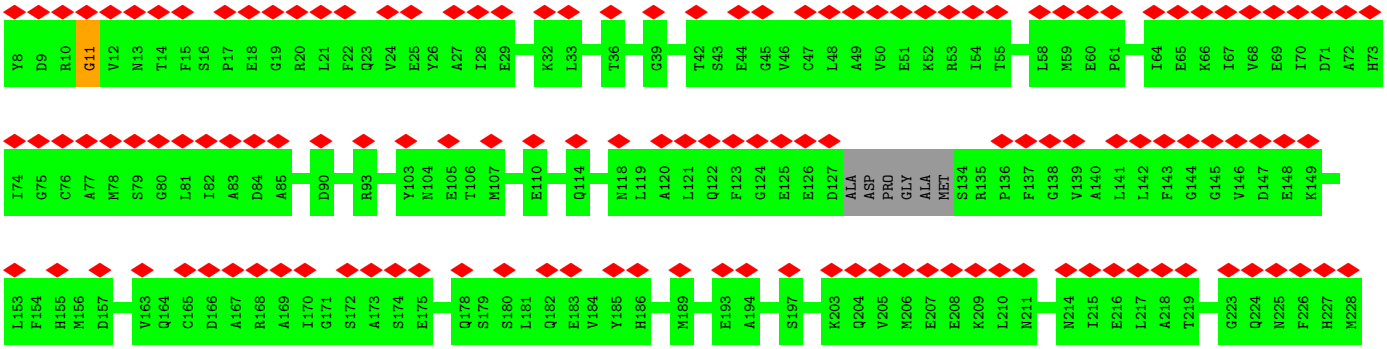
Chain K:

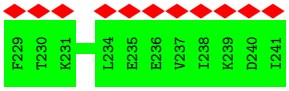




• Molecule 16: Proteasome subunit alpha type-5

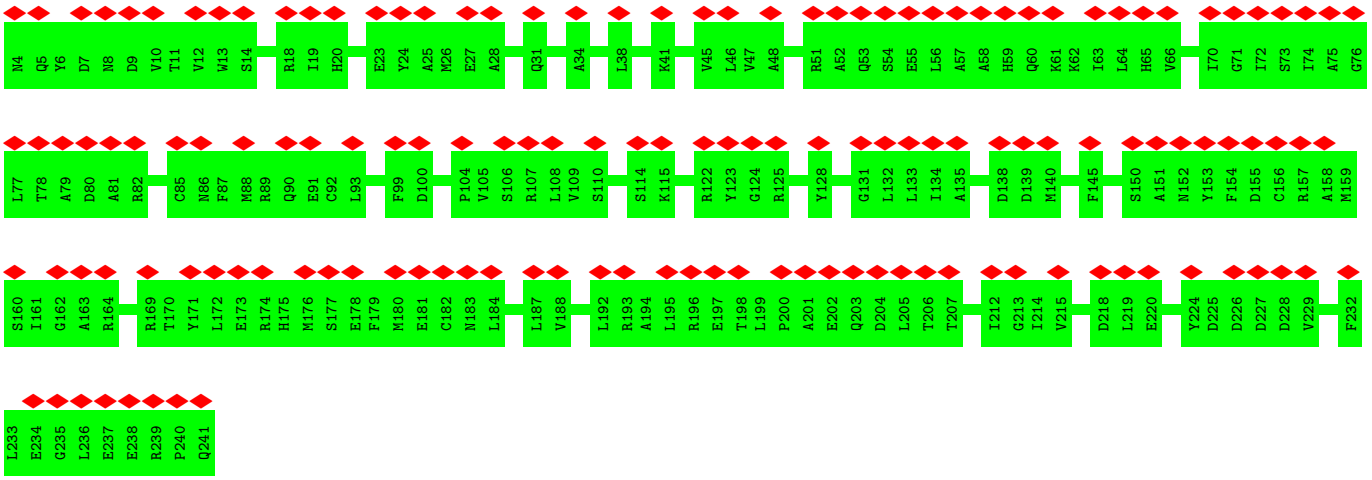
Chain k:





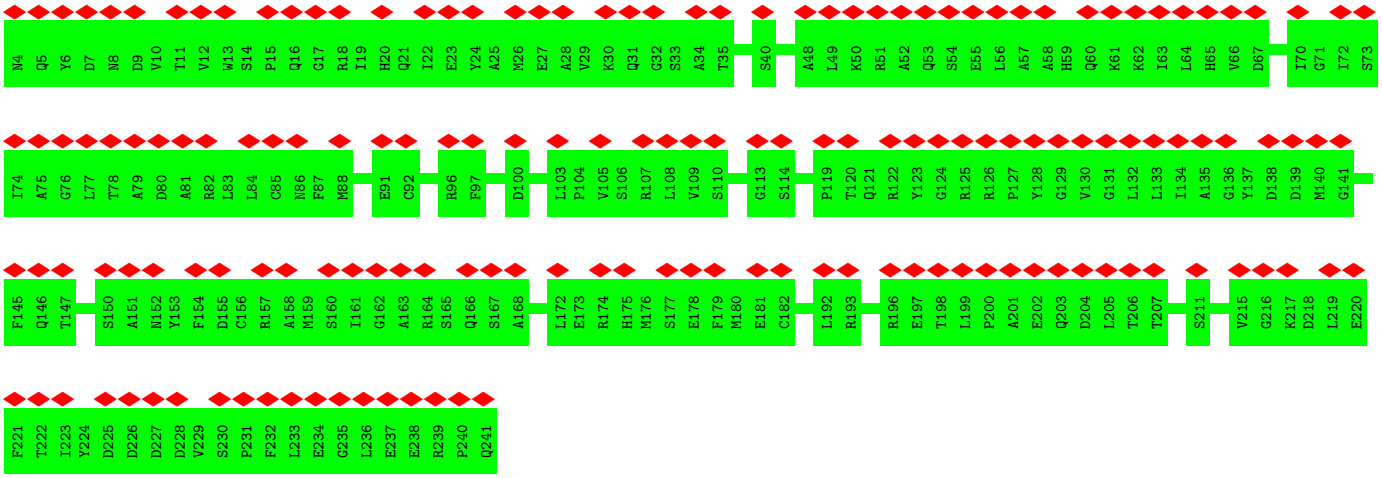
• Molecule 17: Proteasome subunit alpha type-1

Chain L:



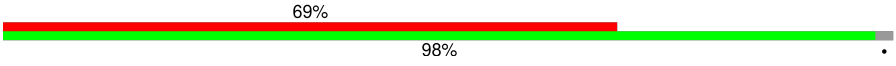
• Molecule 17: Proteasome subunit alpha type-1

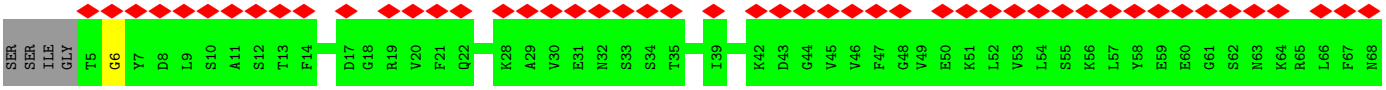
Chain l:

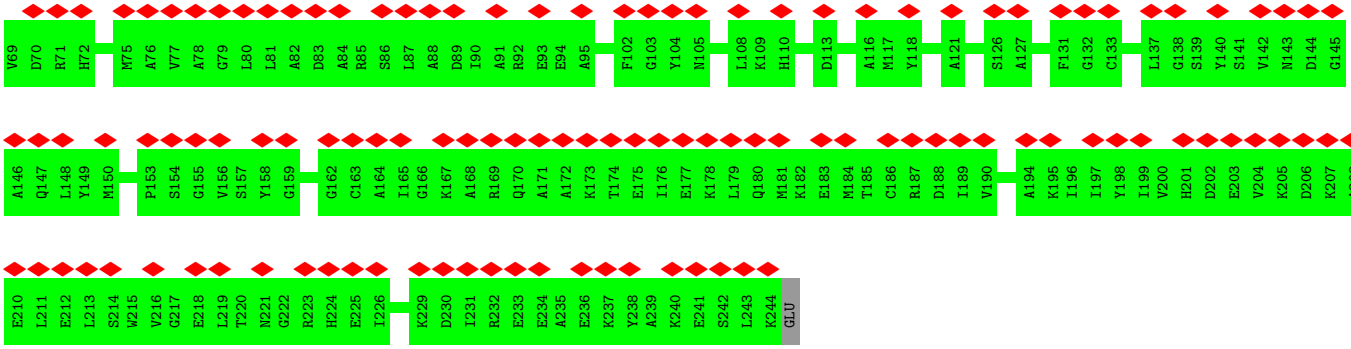


• Molecule 18: Proteasome subunit alpha type-3

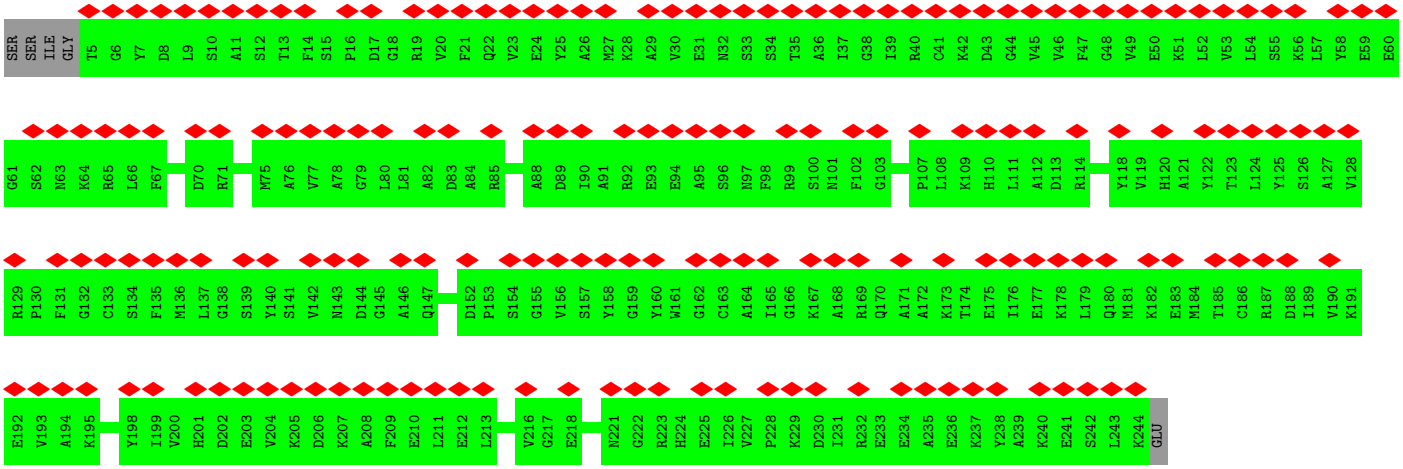
Chain M:



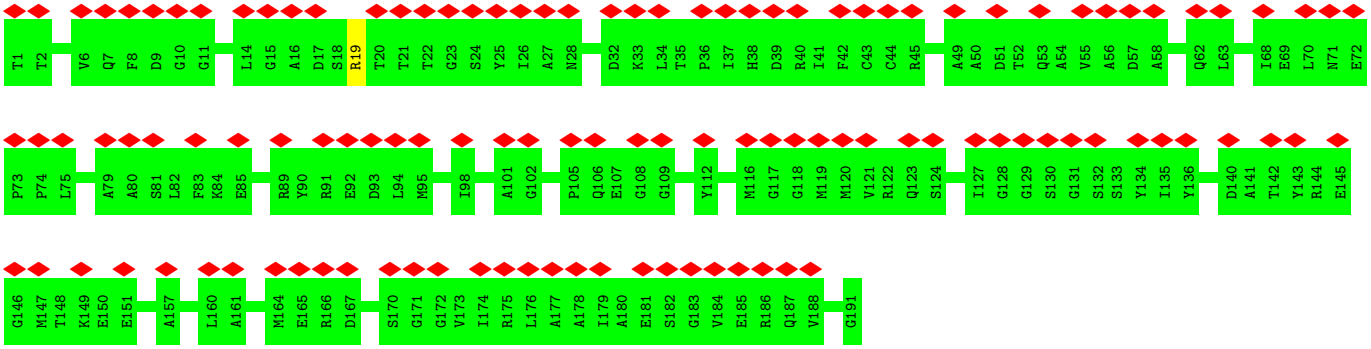




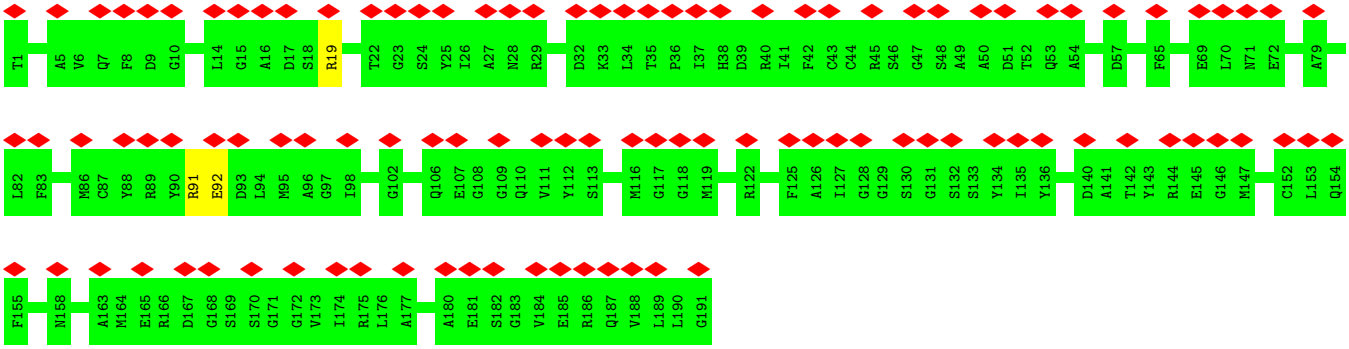
• Molecule 18: Proteasome subunit alpha type-3



• Molecule 19: Proteasome subunit beta type-6

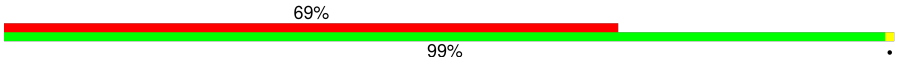


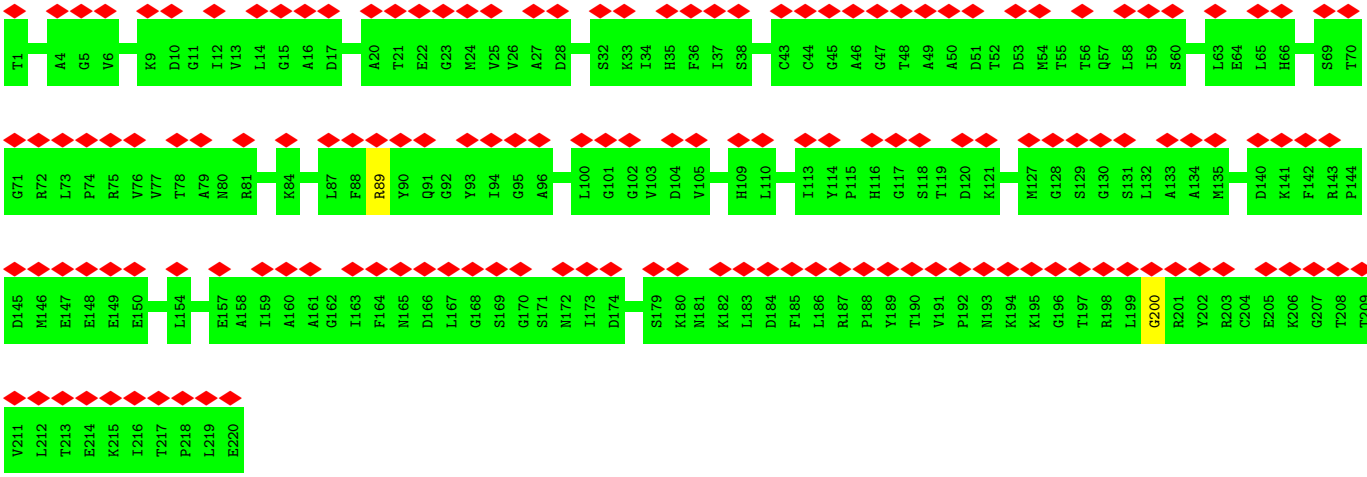
• Molecule 19: Proteasome subunit beta type-6



• Molecule 20: Proteasome subunit beta type-7

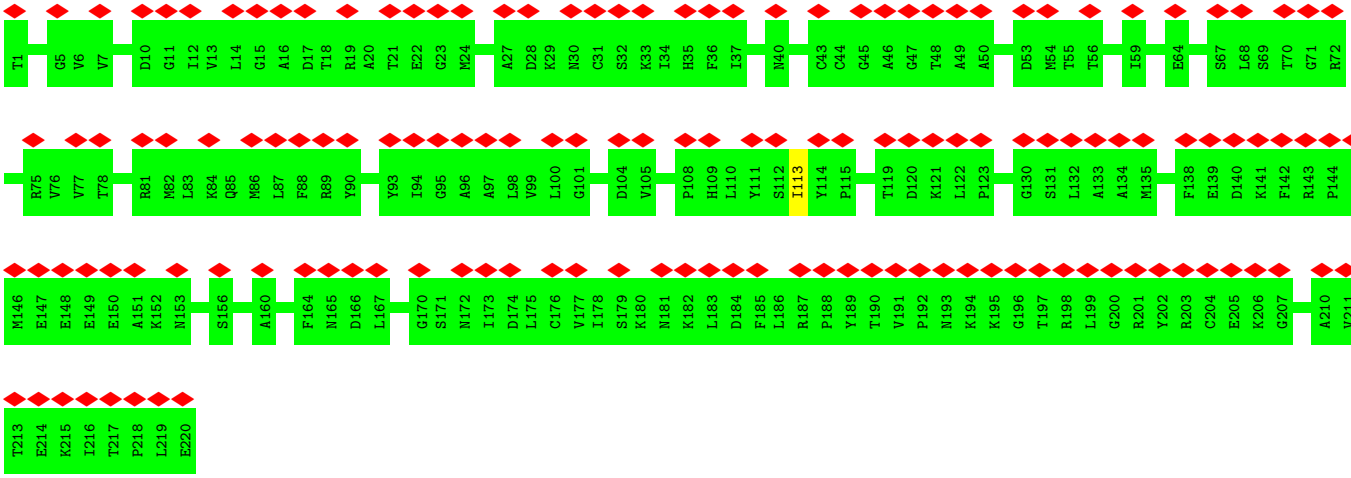
Chain O:





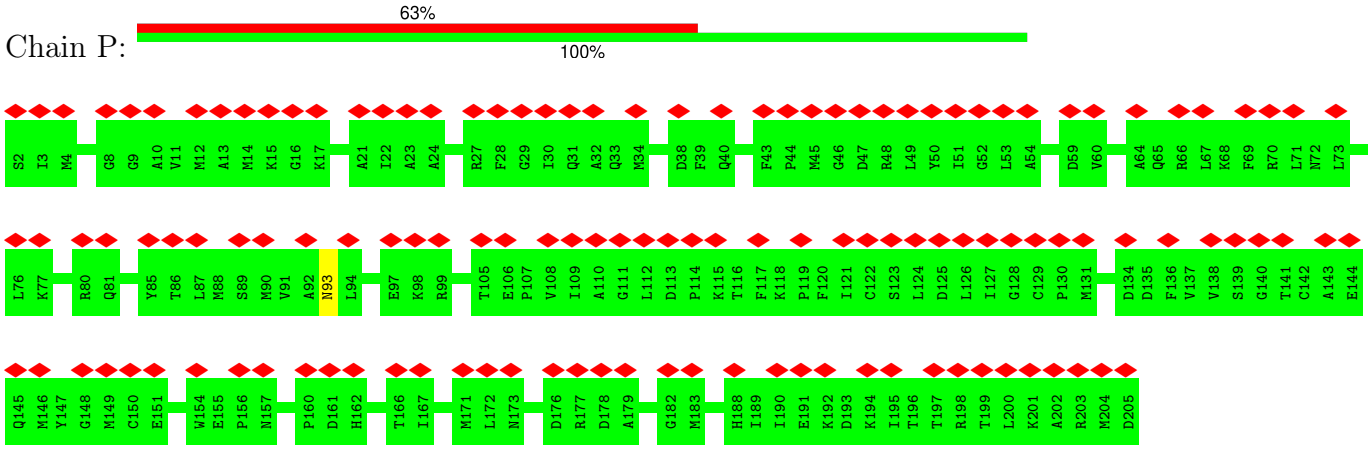
• Molecule 20: Proteasome subunit beta type-7

Chain o:



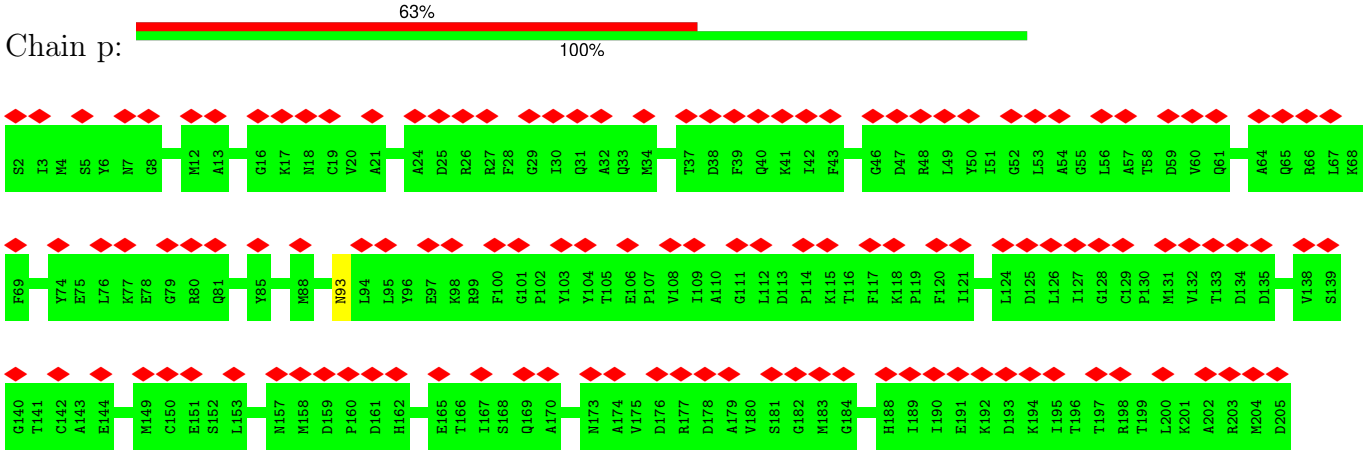
• Molecule 21: Proteasome subunit beta type-3

Chain P:



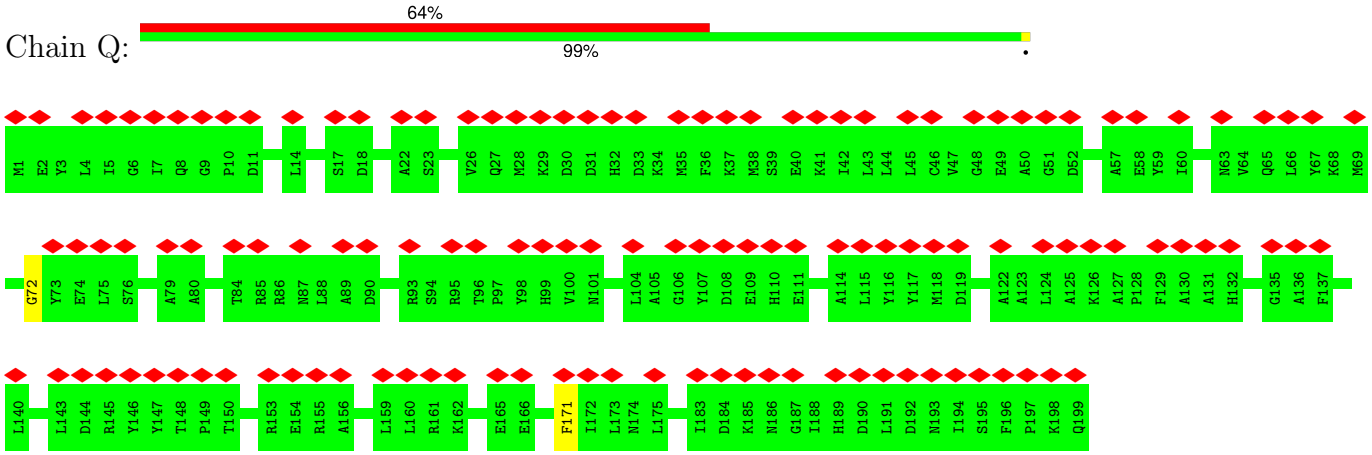
• Molecule 21: Proteasome subunit beta type-3

Chain p:



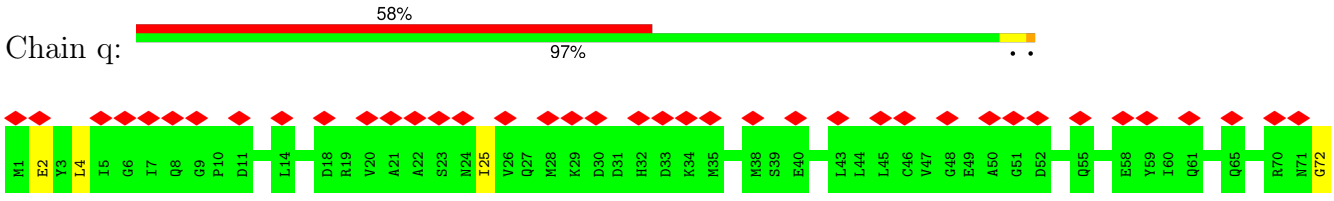
• Molecule 22: Proteasome subunit beta type-2

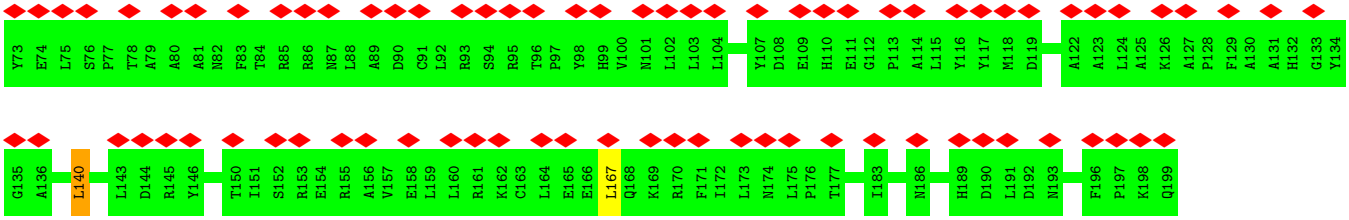
Chain Q:



• Molecule 22: Proteasome subunit beta type-2

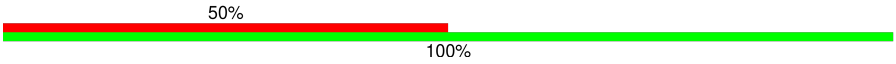
Chain q:

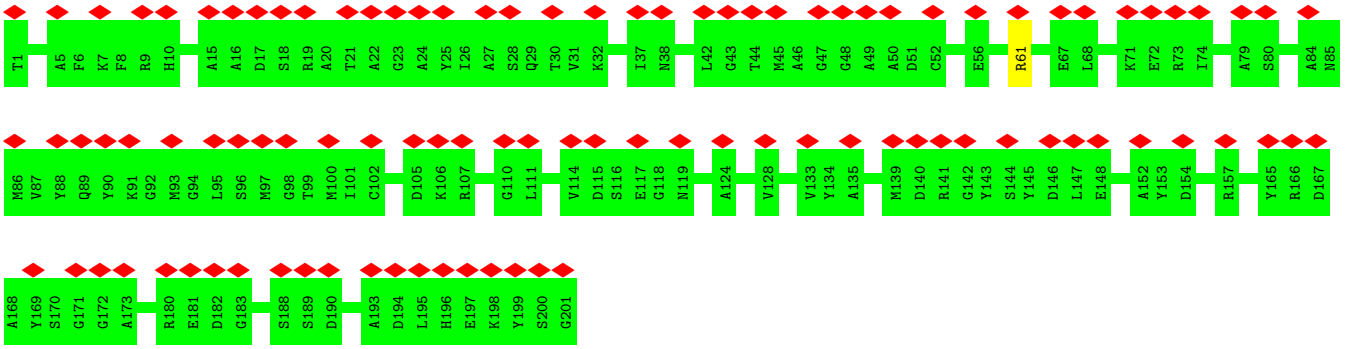




• Molecule 23: Proteasome subunit beta type-5

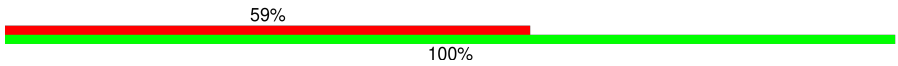
Chain R:

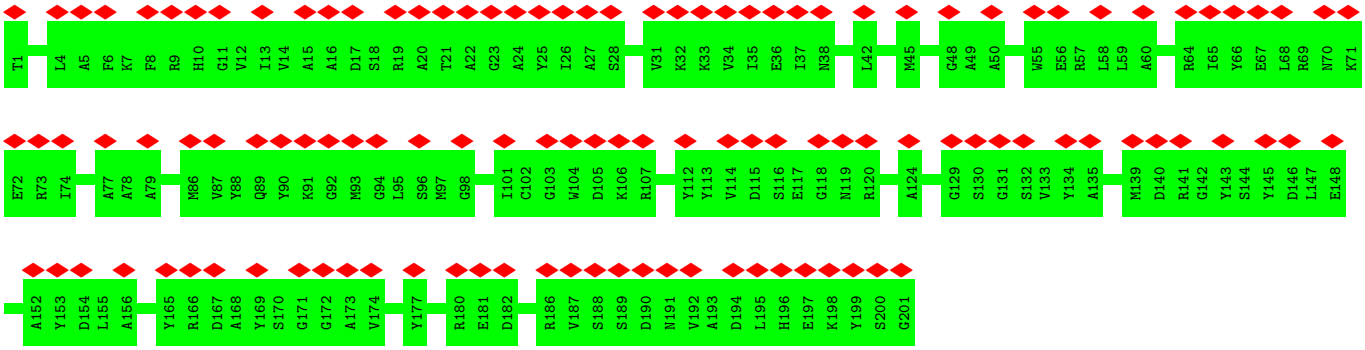




• Molecule 23: Proteasome subunit beta type-5

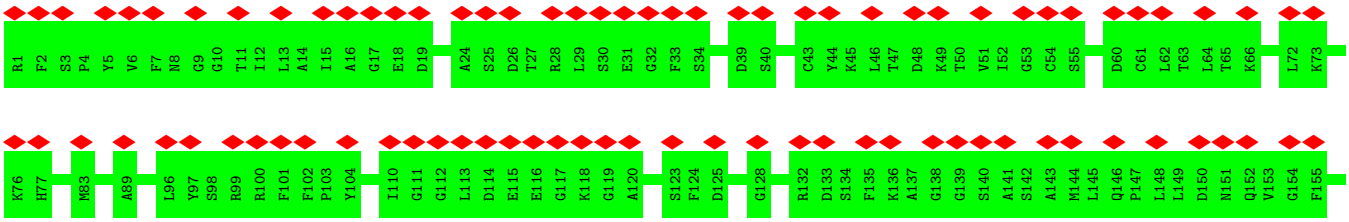
Chain r:

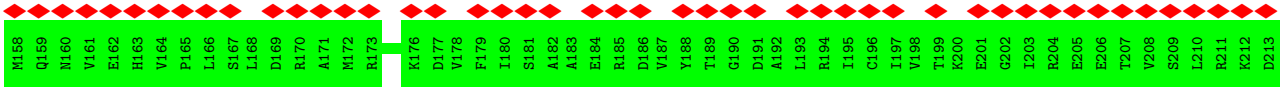




• Molecule 24: Proteasome subunit beta type-1

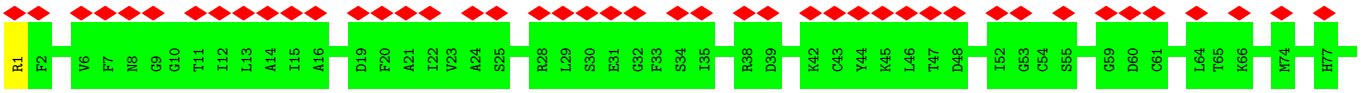
Chain S:





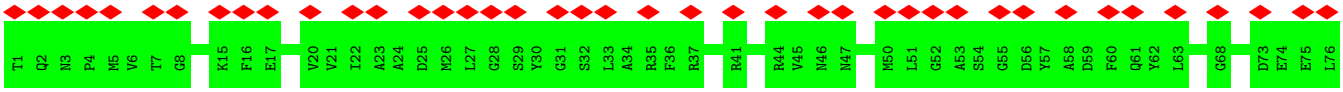
• Molecule 24: Proteasome subunit beta type-1

Chain s:



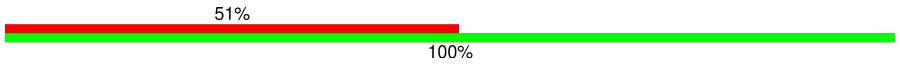
• Molecule 25: Proteasome subunit beta type-4

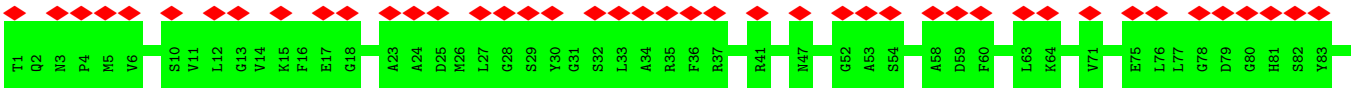
Chain T:



• Molecule 25: Proteasome subunit beta type-4

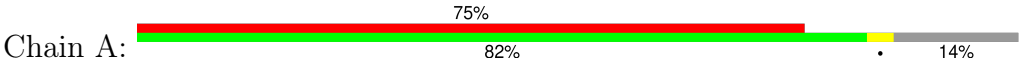
Chain t:

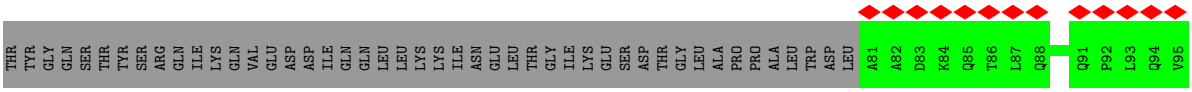


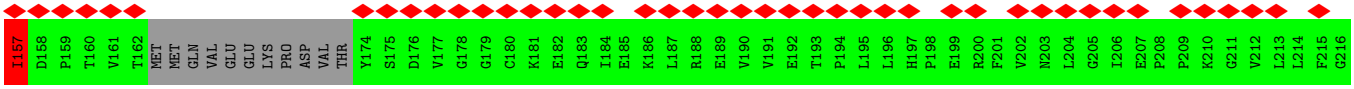


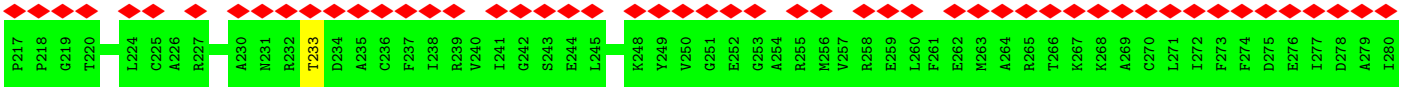
• Molecule 26: 26S proteasome regulatory subunit 7

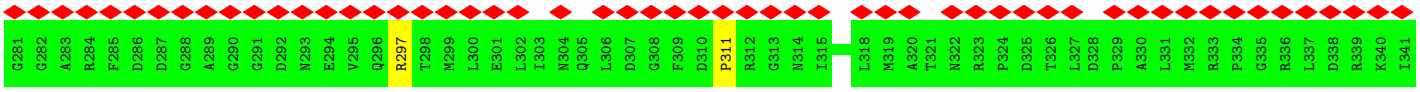
Chain A:

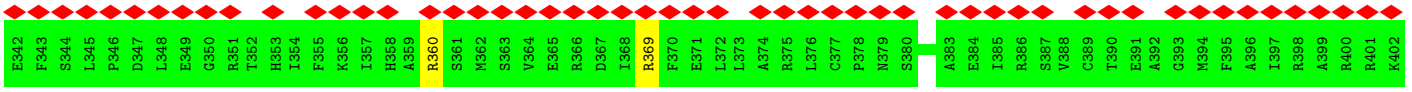


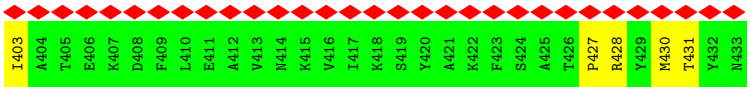






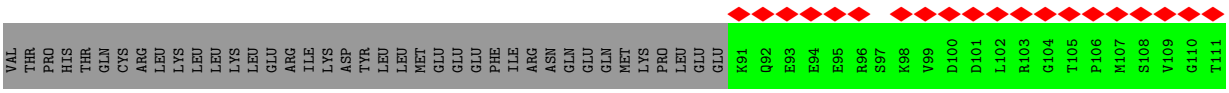


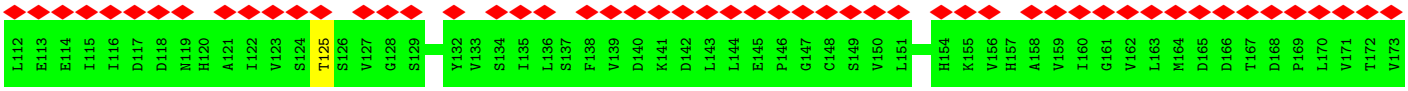


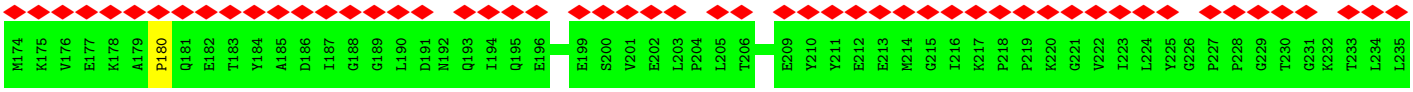


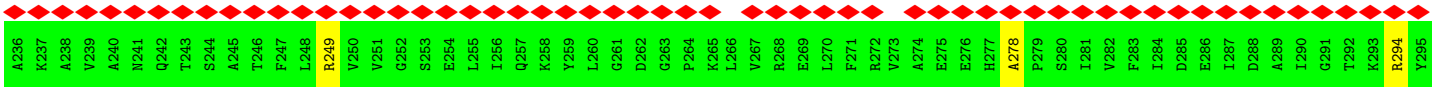
• Molecule 27: 26S proteasome regulatory subunit 4

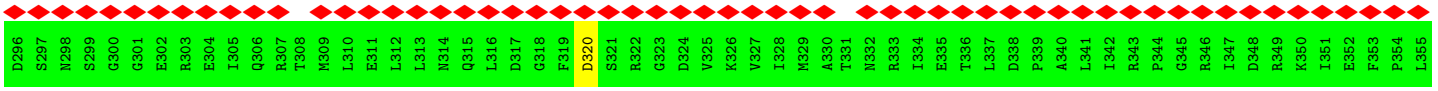
Chain B:











P356 D357 E358 K359 T360 K361 K362 R363 I364 F365 Q366 I367 H368 T369 S370 R371 M372 T373 L374 A375 D376 D377 V378 T379 L380 D381 D382 L383 I384 M385 A386 K387 D388 D389 L390 S391 G392 A393 D394 I395 K396 A397 I398 C399 T400 E401 A402 G403 L404 M405 A406 L407 R408 E409 R410 R411 M412 K413 V414 T415

N416 E417 D418 F419 K420 K421 S422 K423 E424 N425 V426 L427 Y428 K429 K430 Q431 E432 G433 T434 P435 E436 G437 L438 Y439 L440

- Molecule 28: 26S proteasome regulatory subunit 8

Chain C:

LEU GLU GLU GLY LYS ALA GLY SER GLY LEU ARG GLN TYR Y24 L25 S26 K27 I28 E29 E30 L31 Q32 L33 I34 V35 N36 D37 K38 S39 Q40 N41 L42 R43 R44 L45 Q46 A47 Q48 R49 N50 E51 L52 N53 A54 K55 V56 R57 L58 L59 R60 E61 E62 L63 Q64 L65 L66 Q67 E68 Q69 G70

S71 Y72 V73 G74 E75 V76 V77 R78 A79 M80 D81 K82 K83 K84 V85 L86 V87 K88 V89 H90 P91 E92 G93 K94 F95 V96 V97 D98 V99 D100 K101 N102 I103 D104 I105 N106 D107 V108 T109 P110 N111 C112 R113 V114 A115 L116 R117 N118 D119 S120 Y121 T122 L123 H124 K125 I126 L127 P128 N129 K130

V131 D132 P133 L134 V135 S136 L137 M138 M139 V140 E141 K142 V143 P144 D145 S146 T147 Y148 E149 M150 I151 G152 G153 L154 D155 K156 Q157 I158 K159 E160 I161 K162 E163 V164 I165 E166 L167 P168 V169 K170 H171 P172 E173 L174 F175 E176 A177 L178 G179 I180 A181 Q182 P183 K184 G185 V186 L187 L188 Y189 G190

P191 T194 T197 L198 L199 A200 R201 A202 V203 A204 H205 H206 T207 D208 C209 T210 F211 I212 R213 V214 S215 G216 S217 E218 L219 V220 Q221 K222 F223 I224 G225 E226 G227 A228 R229 M230 V231 R232 E233 L234 F235 V236 M237 A238 R239 E240 H241 A242 P243 S244 I245 I246 F247 M248 D249 E250 ILE ASP

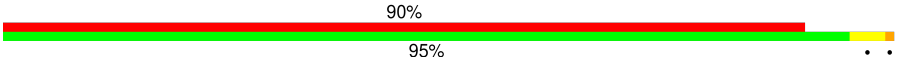
SER ILE GLY SER SER ARG LEU GLU GLY GLY SER GLY GLY ASP S267 E268 V269 Q270 R271 T272 M273 L274 E275 L276 L277 N278 Q279 L280 D281 G282 F283 E284 A285 T286 K287 N288 I289 K290 V291 I292 M293 A294 T295 M296 R297 I298 D299 I300 L301 D302 S303 A304 L305 L306 R307 P308 G309 R310 I311 D312

R313 K314 I315 E316 F317 P318 P319 P320 N321 E322 E323 A324 R325 L326 D327 I328 L329 K330 I331 H332 S333 R334 K335 M336 N337 L338 T339 R340 G341 I342 N343 L344 R345 K346 I347 A348 E349 L350 M351 P352 G353 A354 S355 G356 A357 E358 V359 K360 G361 V362 C363 T364 E365 A366 G367 M368 Y369 A370 L371 R372

E373 R374 R375 V376 H377 V378 T379 Q380 E381 D382 F383 E384 M385 A386 V387 A388 K389 V390 M391 Q392 K393 D394 S395 E396 K397 N398 M399 S400 I401 K402

- Molecule 29: 26S proteasome regulatory subunit 6B

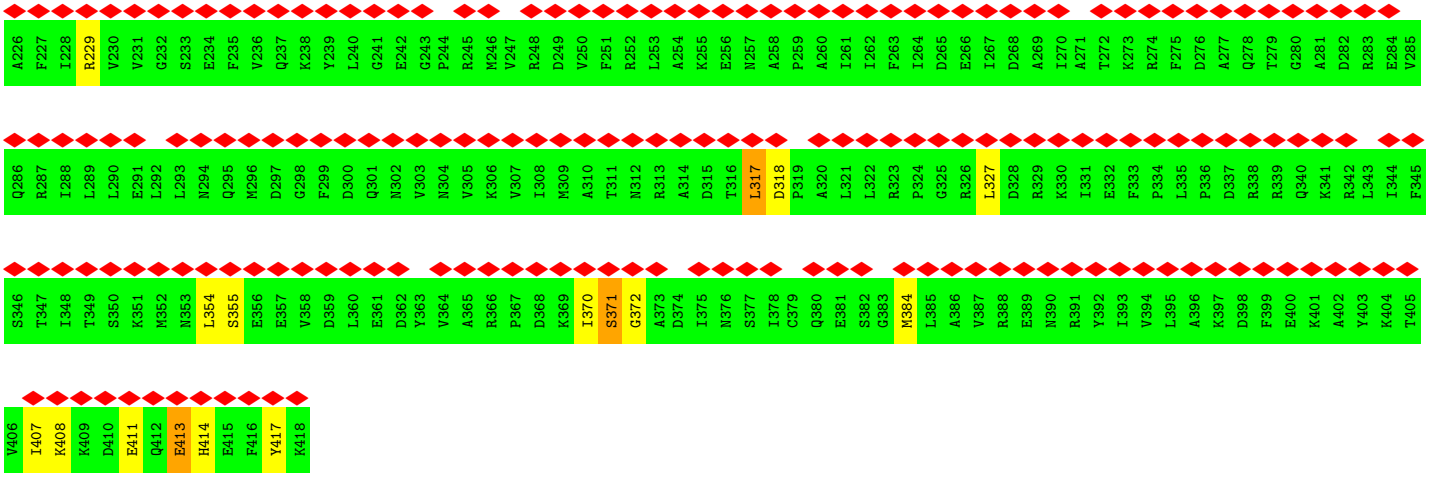
Chain D:



D39 L40 Y41 S42 R43 Y44 K45 K46 L47 Q48 Q49 E50 L51 E52 F53 L54 E55 V56 Q57 E58 E59 K62 D63 E64 Q65 K66 K70 E71 F72 L73 H74 E77 E78 R81 I82 Q83 S84 I85 P86 L87 V88 I89 G90 Q91 F92 L93 E94 A95 V96 D97 Q98 N99 T100 A101 I102 V103

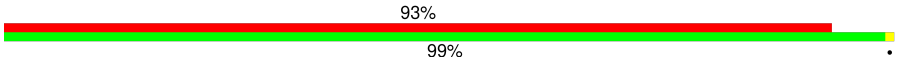
G104 S105 T106 T107 G108 S109 N110 Y111 Y112 V113 R114 I115 L116 S117 T118 I119 D120 R121 E122 L123 L124 K125 P126 N127 A128 S129 V130 A131 L132 H133 K134 H135 S136 N137 A138 L139 V140 D141 V142 L143 P144 P145 E146 A147 D148 S149 S150 I151 M152 M153 L154 T155 S156 D157 Q158 K159 P160 D161 V162 M163

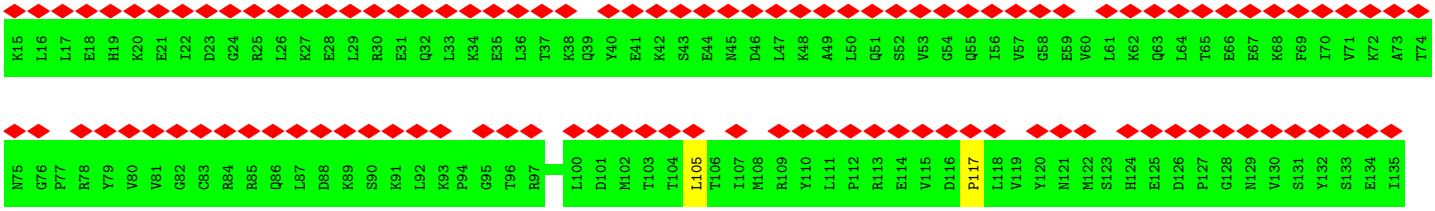
Y164 A165 D166 I167 G168 G169 M170 D171 I172 Q173 K174 Q175 E176 V177 R178 E179 A180 V181 E182 L183 P184 L185 T186 H187 F188 E189 L190 Y191 K192 Q193 I194 G195 I196 D197 P198 P199 R200 G201 V202 L203 M204 Y205 G206 P207 P208 G209 T213 M214 L215 A216 K217 A218 V219 A220 H221 H222 T223 T224 A226



• Molecule 30: 26S proteasome regulatory subunit 10B

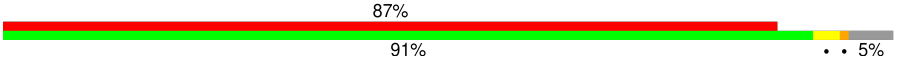
Chain E:

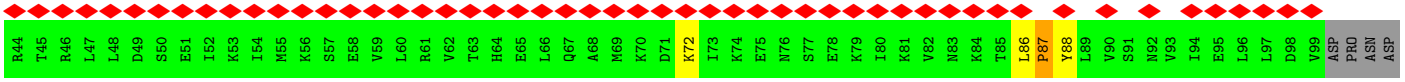


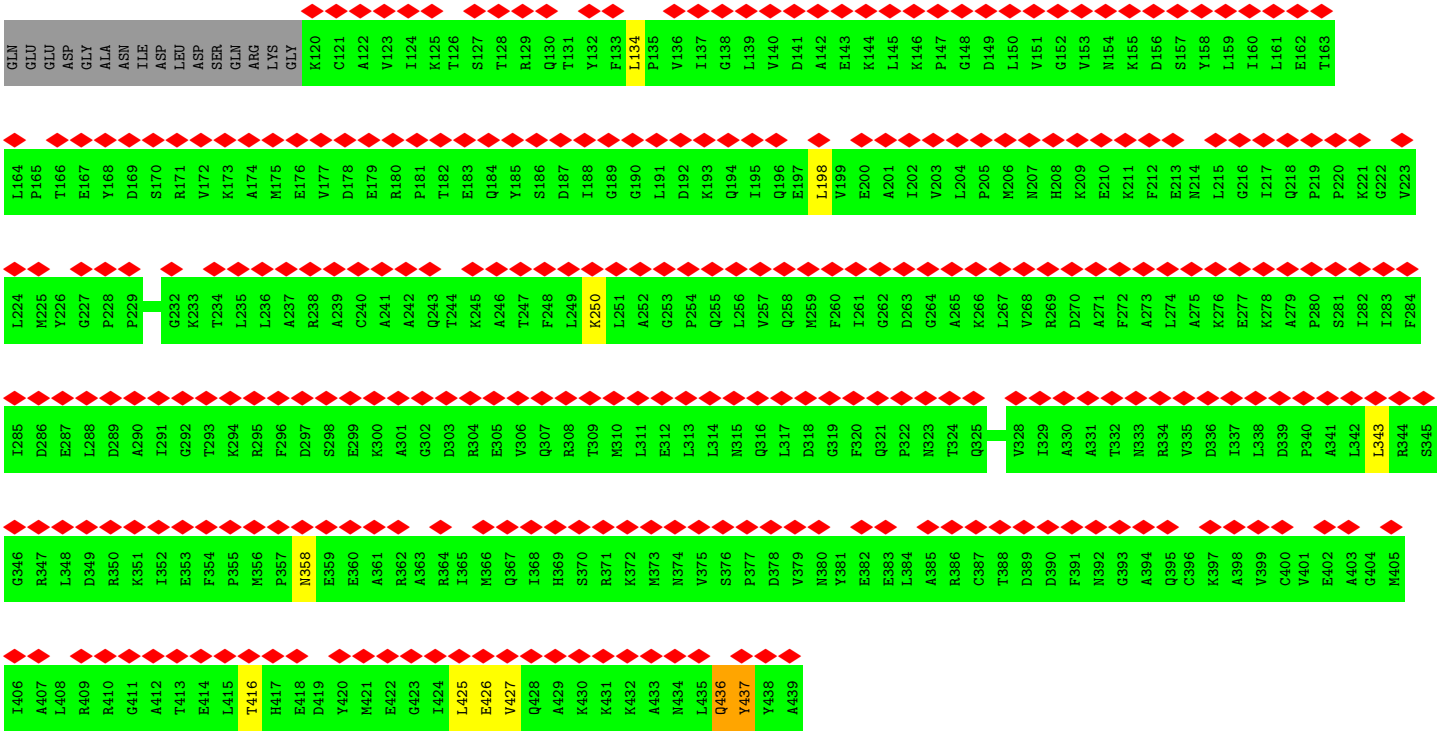


• Molecule 31: 26S proteasome regulatory subunit 6A

Chain F:

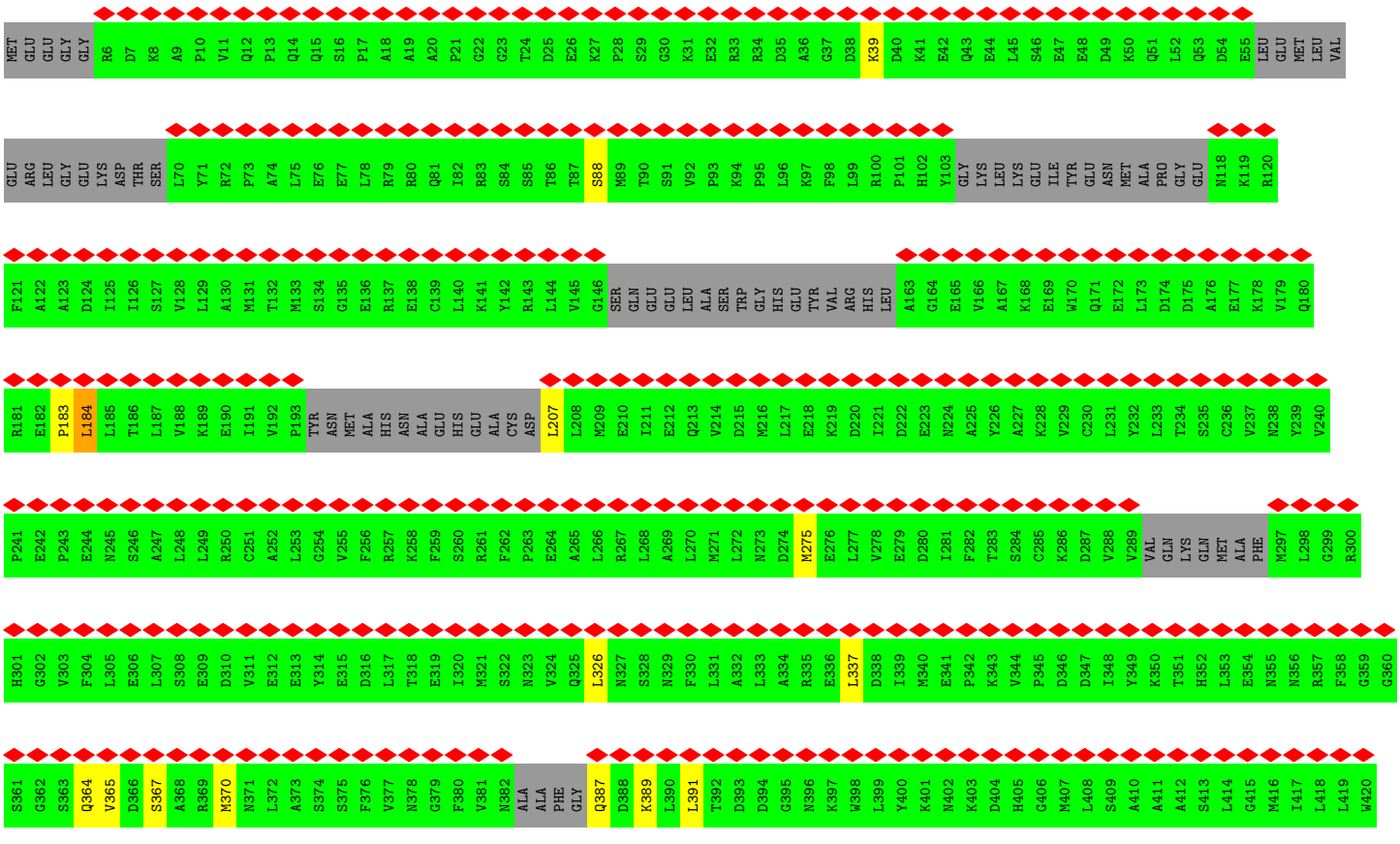


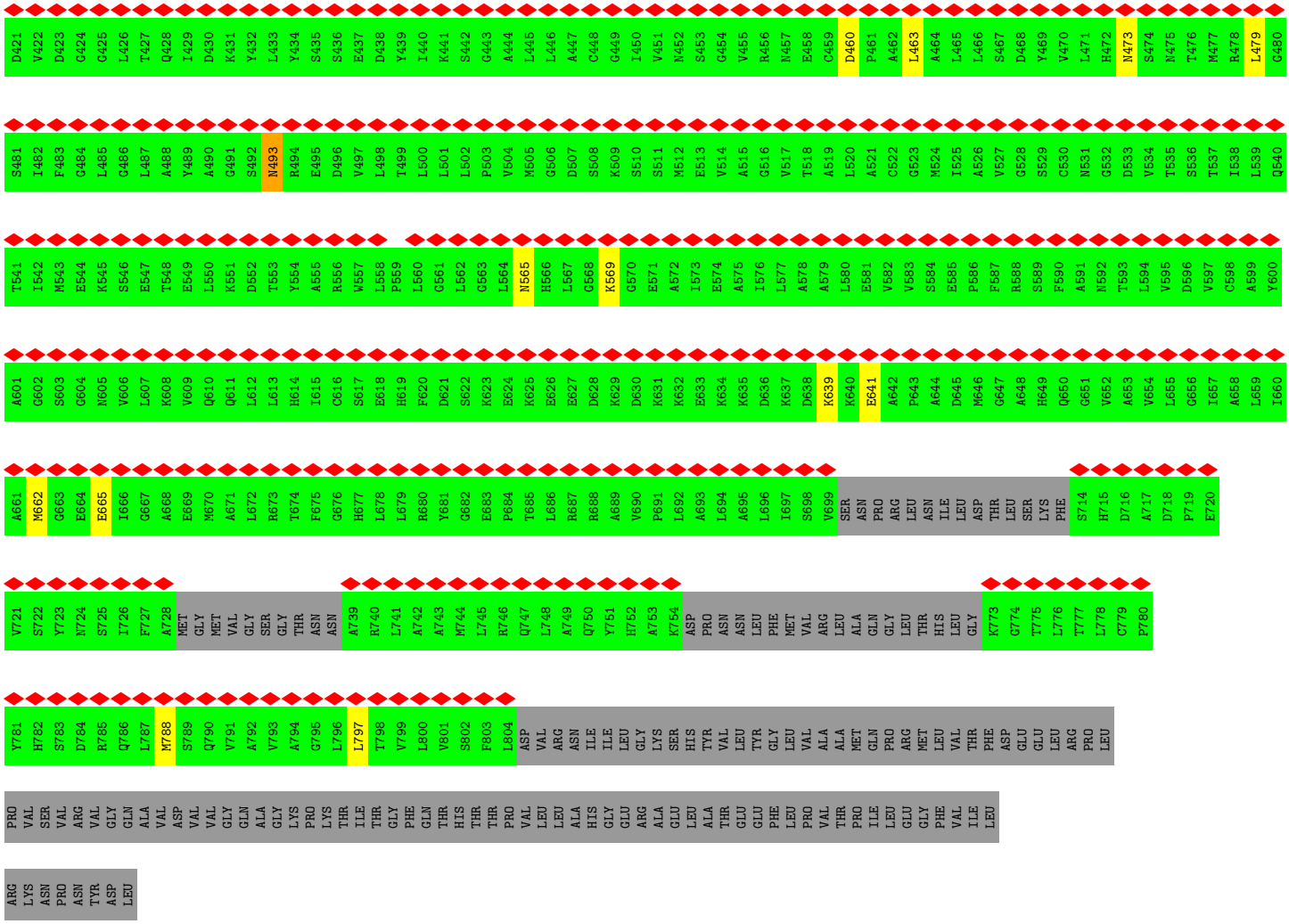




• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f:




D421 V422 D423 G424 G425 L426 T427 Q428 I429 D430 K431 Y432 L433 Y434 S435 S436 E437 D438 Y439 I440 K441 S442 G443 A444 L445 L446 A447 C448 G449 I450 V451 N452 S453 G454 V455 R456 N457 E458 C459 D460 P461 A462 L463 A464 L465 L466 S467 D468 Y469 V470 L471 H472 N473 S474 N475 T476 M477 R478 L479 G480
S481 I482 F483 G484 L485 G486 L487 A488 Y489 A490 G491 S492 N493 R494 E495 D496 V497 L498 T499 L500 L501 L502 P503 V504 M505 G506 D507 S508 K509 S510 S511 M512 E513 V514 A515 G516 V517 T518 A519 L520 A521 C522 G523 M524 I525 A526 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 L560 G561 L562 G563 L564 N565 H566 L567 G568 K569 G570 E571 A572 I573 E574 A575 I576 L577 A578 A579 L580 E581 V582 V583 S584 E585 P586 F587 R588 S589 F590 A591 N592 T593 L594 V595 D596 V597 C598 A599 Y600
A601 G602 S603 G604 N605 V606 L607 K608 V609 Q610 Q611 L612 L613 H614 I615 C616 S617 E618 H619 F620 D621 S622 K623 E624 K625 E626 E627 D628 K629 D630 K631 K632 E633 K634 K635 D636 K637 D638 K639 K640 E641 A642 P643 A644 D645 M646 G647 A648 H649 Q650 G651 V652 A653 V654 L655 G656 I657 A658 L659 I660
A661 M662 G663 E664 E665 I666 G667 A668 E669 M670 A671 L672 R673 T674 F675 G676 H677 L678 L679 R680 Y681 G682 E683 P684 T685 L686 R687 R688 A689 V690 P691 L692 A693 L694 A695 L696 I697 S698 V699 SER ASN PRO ARG LEU ASN ILE LEU ASP THR LEU SER LYS PHE S714 H715 D716 A717 D718 P719 E720
V721 S722 Y723 N724 S725 I726 F727 A728 MET GLY MET VAL GLY SER GLY THR ASN ASN A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751 H752 A753 K754 ASP PRO ASN ASN LEU PHE MET VAL ARG LEU ALA GLN GLY LEU THR HIS LEU GLY K773 G774 T775 L776 T777 L778 C779 P780
Y781 H782 S783 D784 R785 Q786 L787 M788 S789 Q790 V791 A792 V793 A794 G795 L796 L797 T798 V799 L800 V801 S802 F803 L804 ASP VAL ARG ASN ILE ILE LEU GLY LYS SER HIS TYR VAL LEU TYR GLY LEU VAL ALA ALA MET GLN PRO ARG MET LEU VAL THR PHE ASP GLU GLU LEU ARG PRO LEU
PRO VAL SER VAL ARG VAL GLY GLN ALA VAL ASP VAL VAL GLY GLN ALA GLY LYS PRO LYS THR ILE THR GLY PHE GLN THR HIS THR THR PRO VAL LEU LEU ALA HIS GLY GLU ARG ALA GLU LEU ALA THR GLU GLU PHE LEU PRO VAL THR PRO ILE LEU GLU GLU GLY PHE VAL ILE LEU
ARG LYS ASN PRO ASN TYR ASP LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33278	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	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	0.017	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	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: ZN, AGS

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	0.33	0/6396	0.66	7/8646 (0.1%)
2	V	0.35	0/3874	0.71	4/5234 (0.1%)
3	W	0.32	0/3751	0.71	3/5042 (0.1%)
4	X	0.31	0/1936	0.62	0/2614
5	Y	0.35	0/3173	0.70	3/4273 (0.1%)
6	Z	0.33	0/2324	0.77	7/3150 (0.2%)
7	a	0.32	0/3053	0.71	5/4133 (0.1%)
8	b	0.32	0/1478	0.69	0/2001
9	c	0.35	0/2226	0.75	2/3007 (0.1%)
10	d	0.33	0/2162	0.71	1/2919 (0.0%)
11	e	0.37	0/338	0.84	1/450 (0.2%)
12	G	0.35	0/1853	0.65	0/2515
12	g	0.34	0/1859	0.61	0/2523
13	H	0.35	0/1723	0.62	2/2346 (0.1%)
13	h	0.34	0/1743	0.60	1/2372 (0.0%)
14	I	0.35	0/1925	0.72	1/2606 (0.0%)
14	i	0.34	0/1942	0.67	0/2628
15	J	0.39	0/1728	0.75	2/2358 (0.1%)
15	j	0.41	1/1728 (0.1%)	0.69	0/2358
16	K	0.34	0/1755	0.69	5/2375 (0.2%)
16	k	0.33	0/1747	0.60	0/2364
17	L	0.36	0/1885	0.63	0/2552
17	l	0.34	0/1885	0.63	0/2552
18	M	0.36	0/1891	0.61	1/2552 (0.0%)
18	m	0.35	0/1891	0.59	0/2552
19	N	0.34	0/1454	0.60	0/1967
19	n	0.36	0/1454	0.62	0/1967
20	O	0.34	0/1670	0.59	0/2265
20	o	0.35	0/1670	0.66	1/2265 (0.0%)
21	P	0.33	0/1614	0.56	0/2177
21	p	0.34	0/1614	0.57	0/2177
22	Q	0.40	0/1603	0.70	0/2174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
22	q	0.40	0/1603	0.72	1/2174 (0.0%)
23	R	0.36	0/1579	0.56	0/2134
23	r	0.34	0/1579	0.55	0/2134
24	S	0.35	0/1671	0.59	0/2253
24	s	0.35	0/1671	0.59	0/2253
25	T	0.35	0/1700	0.57	0/2305
25	t	0.34	0/1700	0.57	0/2305
26	A	0.34	0/2717	0.68	2/3665 (0.1%)
27	B	0.31	0/2745	0.67	1/3709 (0.0%)
28	C	0.34	0/2896	0.79	4/3895 (0.1%)
29	D	0.39	0/3090	0.77	3/4168 (0.1%)
30	E	0.31	0/2904	0.60	0/3924
31	F	0.33	0/2897	0.66	3/3912 (0.1%)
32	f	0.31	0/5393	0.68	1/7271 (0.0%)
All	All	0.34	1/101490 (0.0%)	0.67	61/137216 (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	2
2	V	0	1
3	W	0	1
5	Y	0	1
6	Z	0	5
8	b	0	1
9	c	0	5
15	J	0	2
15	j	0	1
16	K	0	3
16	k	0	1
20	O	0	1
26	A	0	3
27	B	0	1
28	C	0	10
29	D	0	8
31	F	0	5
All	All	0	51

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	21	TYR	CD2-CE2	-5.53	1.31	1.39

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	320	ASP	CB-CG-OD1	9.52	126.87	118.30
22	q	140	LEU	CA-CB-CG	8.52	134.90	115.30
9	c	278	GLN	C-N-CA	8.51	142.97	121.70
6	Z	176	LEU	CA-CB-CG	8.23	134.23	115.30
6	Z	251	LEU	CA-CB-CG	7.49	132.53	115.30

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	432	SER	Peptide
1	U	598	ALA	Peptide
2	V	194	LYS	Peptide
3	W	313	GLU	Peptide
5	Y	373	GLY	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	798/911 (88%)	735 (92%)	63 (8%)	0	100	100
2	V	470/480 (98%)	400 (85%)	68 (14%)	2 (0%)	30	68
3	W	454/456 (100%)	394 (87%)	58 (13%)	2 (0%)	30	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	X	239/380 (63%)	222 (93%)	16 (7%)	1 (0%)	30 68
5	Y	376/378 (100%)	336 (89%)	40 (11%)	0	100 100
6	Z	284/286 (99%)	240 (84%)	39 (14%)	5 (2%)	7 34
7	a	371/373 (100%)	339 (91%)	31 (8%)	1 (0%)	37 72
8	b	189/191 (99%)	160 (85%)	29 (15%)	0	100 100
9	c	274/287 (96%)	237 (86%)	33 (12%)	4 (2%)	8 39
10	d	255/257 (99%)	219 (86%)	34 (13%)	2 (1%)	16 54
11	e	36/70 (51%)	26 (72%)	9 (25%)	1 (3%)	4 24
12	G	237/240 (99%)	215 (91%)	22 (9%)	0	100 100
12	g	238/240 (99%)	220 (92%)	18 (8%)	0	100 100
13	H	228/232 (98%)	210 (92%)	18 (8%)	0	100 100
13	h	230/232 (99%)	219 (95%)	11 (5%)	0	100 100
14	I	246/250 (98%)	222 (90%)	23 (9%)	1 (0%)	30 68
14	i	248/250 (99%)	218 (88%)	29 (12%)	1 (0%)	30 68
15	J	237/243 (98%)	222 (94%)	12 (5%)	3 (1%)	10 42
15	j	237/243 (98%)	220 (93%)	15 (6%)	2 (1%)	16 54
16	K	224/234 (96%)	205 (92%)	18 (8%)	1 (0%)	30 68
16	k	224/234 (96%)	203 (91%)	20 (9%)	1 (0%)	30 68
17	L	236/238 (99%)	221 (94%)	15 (6%)	0	100 100
17	l	236/238 (99%)	221 (94%)	15 (6%)	0	100 100
18	M	238/245 (97%)	216 (91%)	22 (9%)	0	100 100
18	m	238/245 (97%)	219 (92%)	19 (8%)	0	100 100
19	N	189/191 (99%)	179 (95%)	9 (5%)	1 (0%)	25 64
19	n	189/191 (99%)	179 (95%)	7 (4%)	3 (2%)	8 37
20	O	218/220 (99%)	204 (94%)	14 (6%)	0	100 100
20	o	218/220 (99%)	209 (96%)	9 (4%)	0	100 100
21	P	202/204 (99%)	190 (94%)	12 (6%)	0	100 100
21	p	202/204 (99%)	190 (94%)	12 (6%)	0	100 100
22	Q	197/199 (99%)	181 (92%)	15 (8%)	1 (0%)	25 64
22	q	197/199 (99%)	179 (91%)	16 (8%)	2 (1%)	13 48
23	R	199/201 (99%)	190 (96%)	9 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	r	199/201 (99%)	190 (96%)	9 (4%)	0	100 100
24	S	211/213 (99%)	198 (94%)	13 (6%)	0	100 100
24	s	211/213 (99%)	198 (94%)	13 (6%)	0	100 100
25	T	213/215 (99%)	203 (95%)	10 (5%)	0	100 100
25	t	213/215 (99%)	203 (95%)	10 (5%)	0	100 100
26	A	338/399 (85%)	269 (80%)	64 (19%)	5 (2%)	8 39
27	B	348/389 (90%)	300 (86%)	46 (13%)	2 (1%)	22 59
28	C	359/392 (92%)	290 (81%)	59 (16%)	10 (3%)	4 24
29	D	378/380 (100%)	298 (79%)	74 (20%)	6 (2%)	8 37
30	E	373/375 (100%)	343 (92%)	29 (8%)	1 (0%)	37 72
31	F	372/396 (94%)	334 (90%)	33 (9%)	5 (1%)	10 42
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	11 44
All	All	12738/13558 (94%)	11445 (90%)	1222 (10%)	71 (1%)	24 59

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	424	LEU
9	c	279	ASP
11	e	60	LEU
15	J	184	ASP
16	K	10	ARG

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	685/779 (88%)	681 (99%)	4 (1%)	84 88
2	V	409/414 (99%)	407 (100%)	2 (0%)	86 89
3	W	416/416 (100%)	414 (100%)	2 (0%)	86 89
4	X	208/327 (64%)	208 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	Y	334/334 (100%)	333 (100%)	1 (0%)	91 92
6	Z	257/257 (100%)	254 (99%)	3 (1%)	67 79
7	a	333/333 (100%)	332 (100%)	1 (0%)	91 92
8	b	167/167 (100%)	167 (100%)	0	100 100
9	c	243/252 (96%)	241 (99%)	2 (1%)	79 85
10	d	231/231 (100%)	231 (100%)	0	100 100
11	e	38/63 (60%)	38 (100%)	0	100 100
12	G	192/205 (94%)	191 (100%)	1 (0%)	86 89
12	g	193/205 (94%)	193 (100%)	0	100 100
13	H	162/190 (85%)	162 (100%)	0	100 100
13	h	164/190 (86%)	164 (100%)	0	100 100
14	I	191/210 (91%)	191 (100%)	0	100 100
14	i	193/210 (92%)	192 (100%)	1 (0%)	86 89
15	J	152/207 (73%)	147 (97%)	5 (3%)	33 53
15	j	152/207 (73%)	152 (100%)	0	100 100
16	K	187/196 (95%)	187 (100%)	0	100 100
16	k	186/196 (95%)	186 (100%)	0	100 100
17	L	198/204 (97%)	198 (100%)	0	100 100
17	l	198/204 (97%)	198 (100%)	0	100 100
18	M	192/202 (95%)	192 (100%)	0	100 100
18	m	192/202 (95%)	192 (100%)	0	100 100
19	N	148/148 (100%)	148 (100%)	0	100 100
19	n	148/148 (100%)	148 (100%)	0	100 100
20	O	177/181 (98%)	176 (99%)	1 (1%)	84 88
20	o	177/181 (98%)	177 (100%)	0	100 100
21	P	172/173 (99%)	171 (99%)	1 (1%)	84 88
21	p	172/173 (99%)	171 (99%)	1 (1%)	84 88
22	Q	164/170 (96%)	163 (99%)	1 (1%)	84 88
22	q	164/170 (96%)	160 (98%)	4 (2%)	44 63
23	R	153/156 (98%)	152 (99%)	1 (1%)	81 87
23	r	153/156 (98%)	153 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	S	174/178 (98%)	174 (100%)	0	100	100
24	s	174/178 (98%)	173 (99%)	1 (1%)	84	88
25	T	175/178 (98%)	174 (99%)	1 (1%)	84	88
25	t	175/178 (98%)	174 (99%)	1 (1%)	84	88
26	A	286/343 (83%)	281 (98%)	5 (2%)	56	72
27	B	300/345 (87%)	296 (99%)	4 (1%)	65	77
28	C	315/340 (93%)	310 (98%)	5 (2%)	58	74
29	D	333/333 (100%)	328 (98%)	5 (2%)	60	75
30	E	298/329 (91%)	294 (99%)	4 (1%)	65	77
31	F	296/340 (87%)	291 (98%)	5 (2%)	56	72
32	f	580/763 (76%)	559 (96%)	21 (4%)	30	51
All	All	10607/11562 (92%)	10524 (99%)	83 (1%)	77	85

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	F	72	LYS
32	f	460	ASP
31	F	250	LYS
32	f	207	LEU
32	f	493	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
19	N	154	GLN
14	i	146	GLN
32	f	752	HIS
32	f	387	GLN
19	N	187	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
34	AGS	A	501	-	28,33,33	0.95	1 (3%)	31,52,52	1.07	2 (6%)
34	AGS	D	501	-	28,33,33	0.80	1 (3%)	31,52,52	1.10	1 (3%)
34	AGS	B	501	-	28,33,33	1.04	2 (7%)	31,52,52	1.37	2 (6%)
34	AGS	F	501	-	28,33,33	0.79	0	31,52,52	1.06	2 (6%)

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
34	AGS	A	501	-	-	8/17/38/38	0/3/3/3
34	AGS	D	501	-	-	2/17/38/38	0/3/3/3
34	AGS	B	501	-	-	2/17/38/38	0/3/3/3
34	AGS	F	501	-	-	5/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	AGS	PA-O3A	-2.26	1.57	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	501	AGS	PB-O3A	-2.15	1.57	1.59
34	A	501	AGS	PA-O3A	-2.09	1.57	1.59
34	D	501	AGS	PG-S1G	2.06	1.95	1.90

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	501	AGS	PB-O3B-PG	-5.16	114.27	133.17
34	A	501	AGS	PB-O3B-PG	-4.41	117.01	133.17
34	D	501	AGS	PB-O3B-PG	-4.22	117.73	133.17
34	F	501	AGS	PB-O3B-PG	-2.87	122.65	133.17
34	B	501	AGS	C5-C6-N6	2.64	124.33	120.31

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

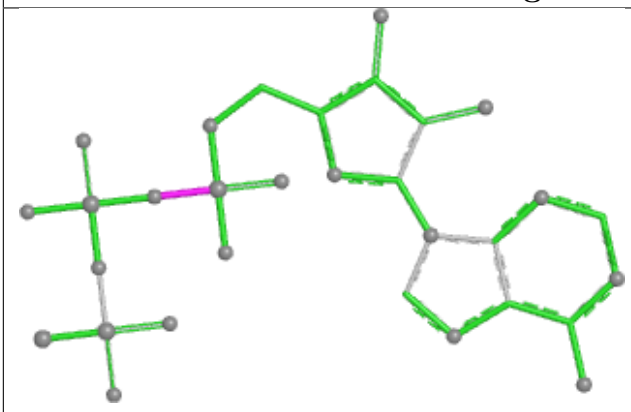
Mol	Chain	Res	Type	Atoms
34	A	501	AGS	C5'-O5'-PA-O1A
34	A	501	AGS	C5'-O5'-PA-O2A
34	A	501	AGS	C5'-O5'-PA-O3A
34	B	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

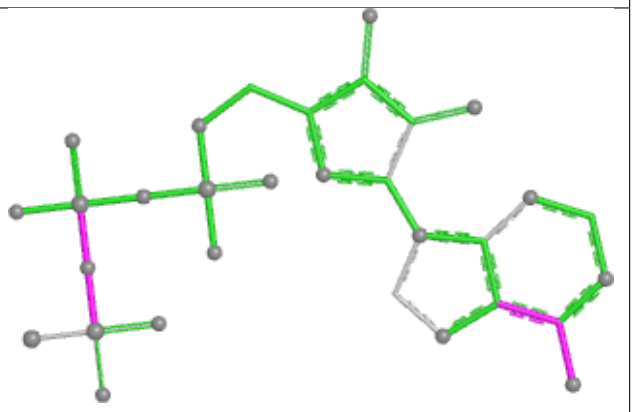
No monomer is involved in short contacts.

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.

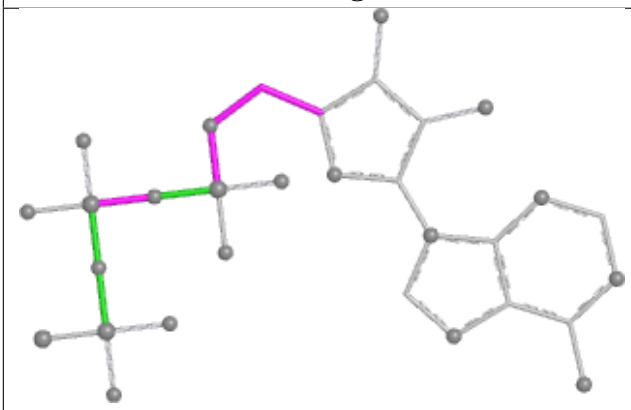
Ligand AGS A 501



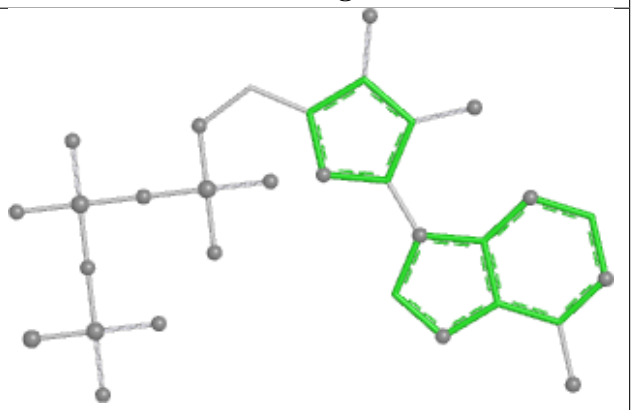
Bond lengths



Bond angles

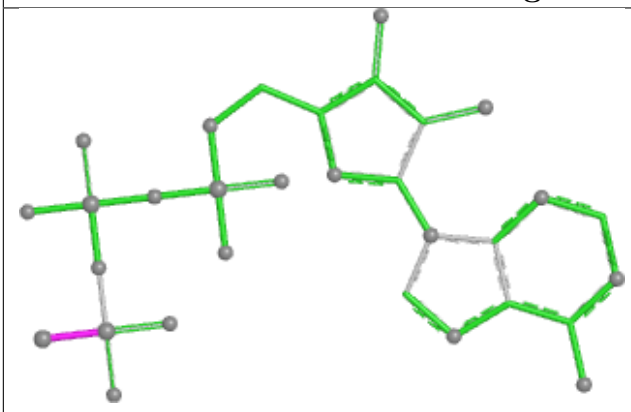


Torsions

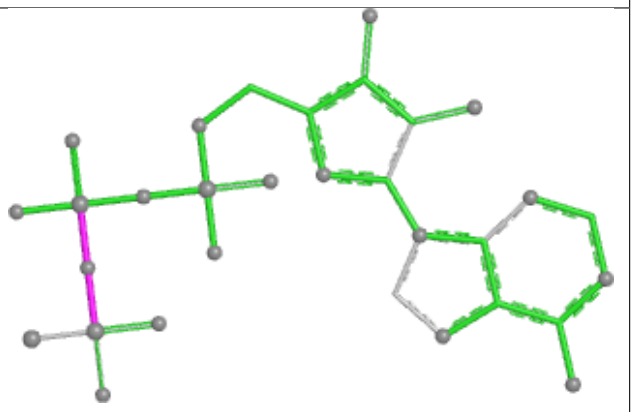


Rings

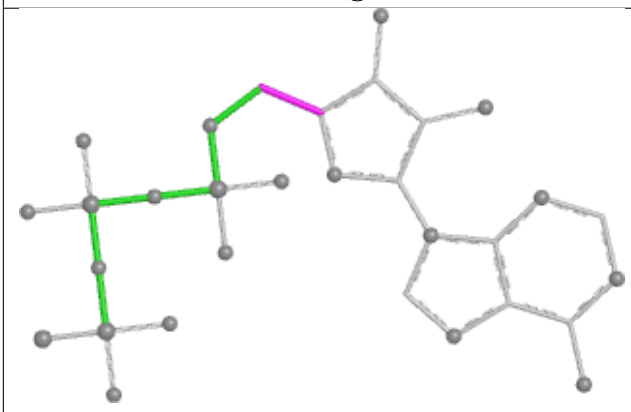
Ligand AGS D 501



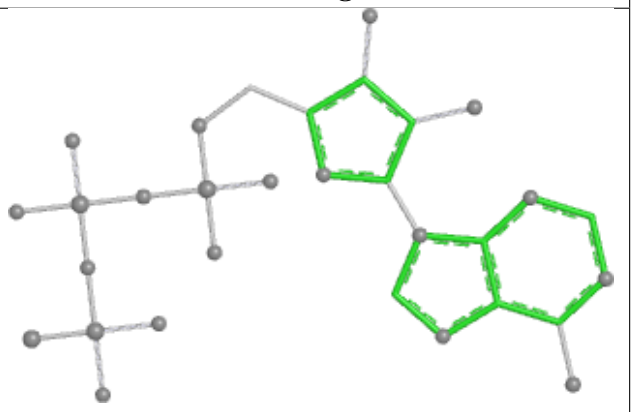
Bond lengths



Bond angles

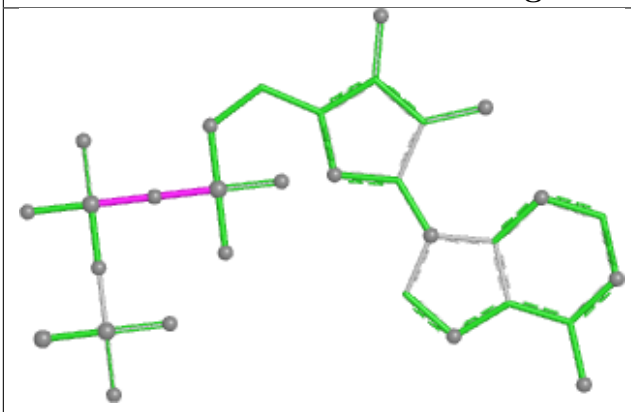


Torsions

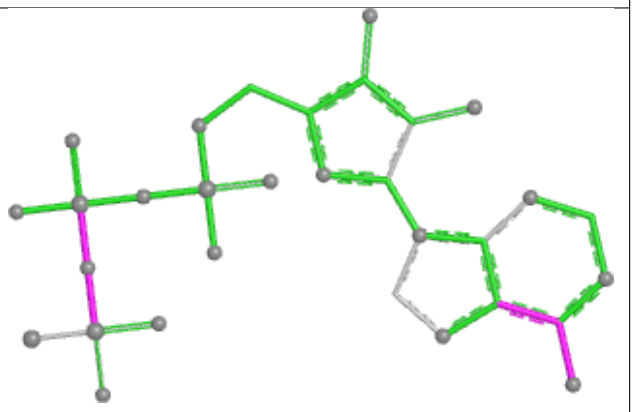


Rings

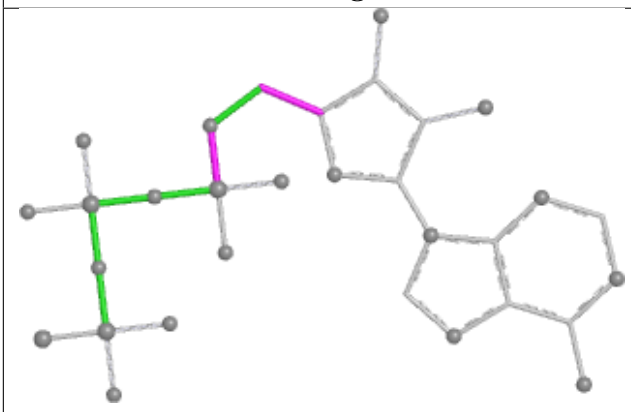
Ligand AGS B 501



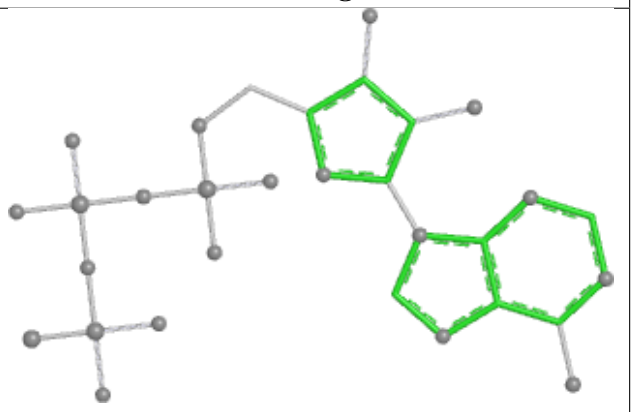
Bond lengths



Bond angles

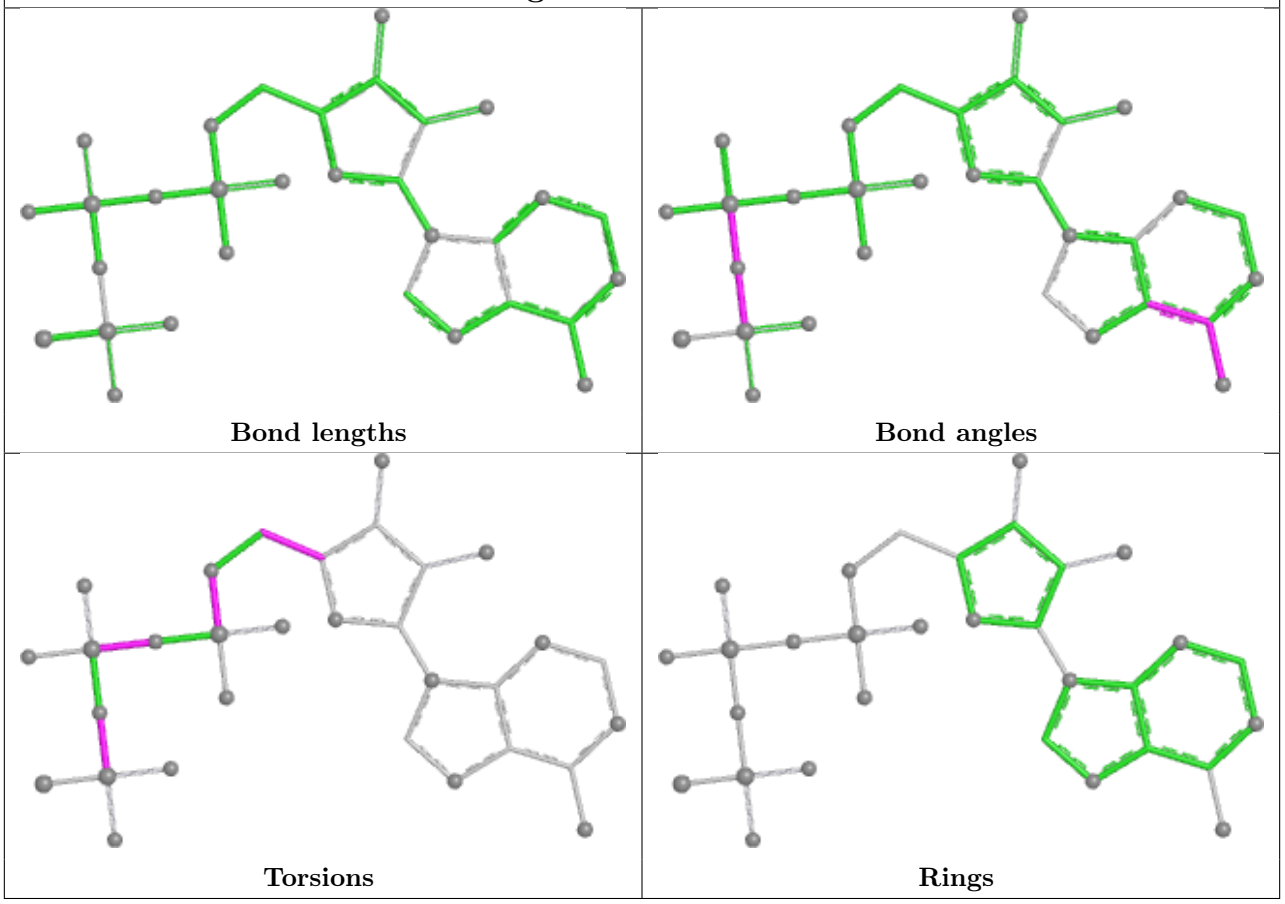


Torsions



Rings

Ligand AGS F 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.

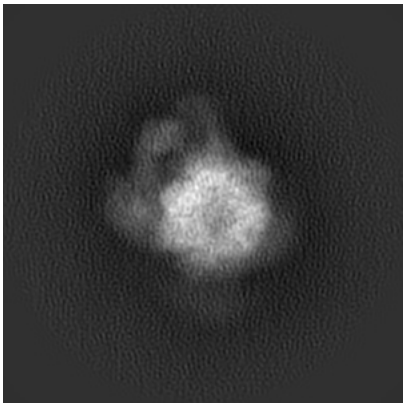
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8665. These allow visual inspection of the internal detail of the map and identification of artifacts.

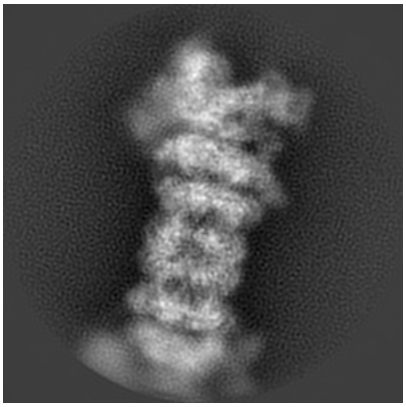
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

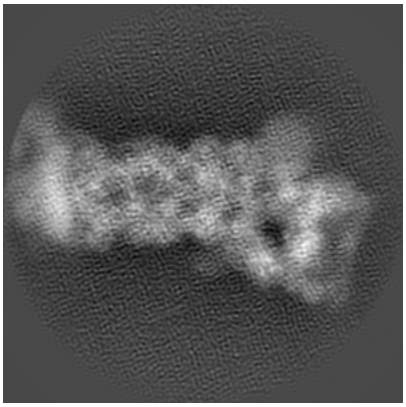
6.1.1 Primary map



X



Y

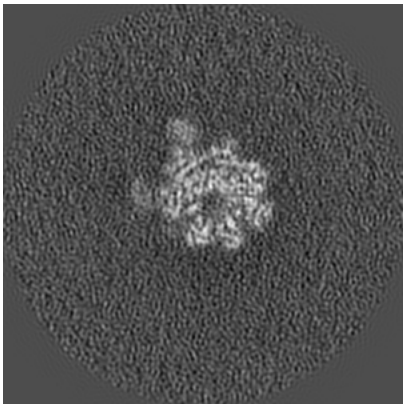


Z

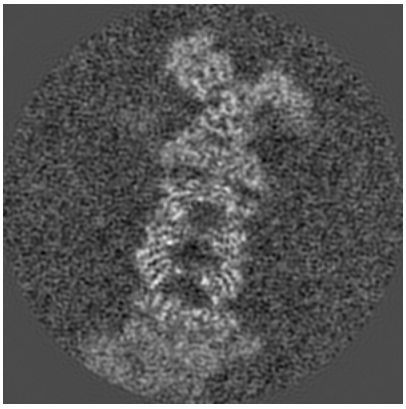
The images above show the map projected in three orthogonal directions.

6.2 Central slices

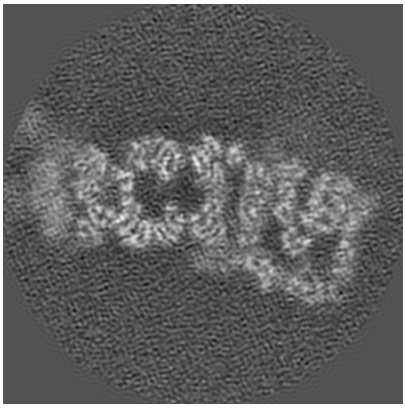
6.2.1 Primary map



X Index: 280



Y Index: 280

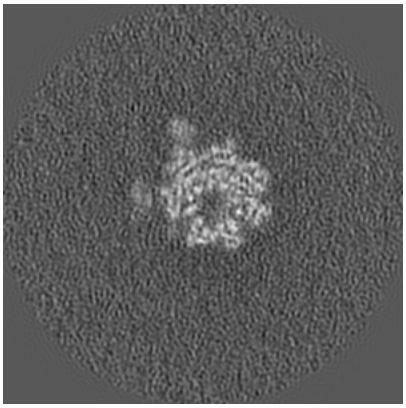


Z Index: 280

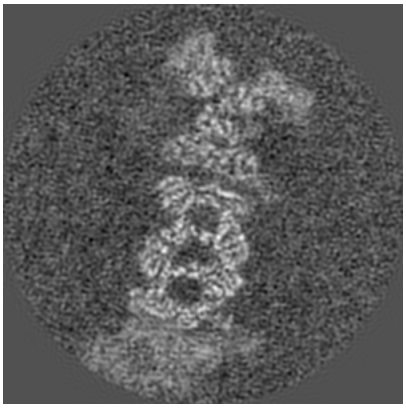
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

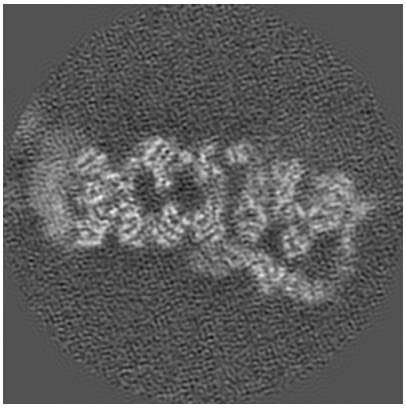
6.3.1 Primary map



X Index: 278



Y Index: 273

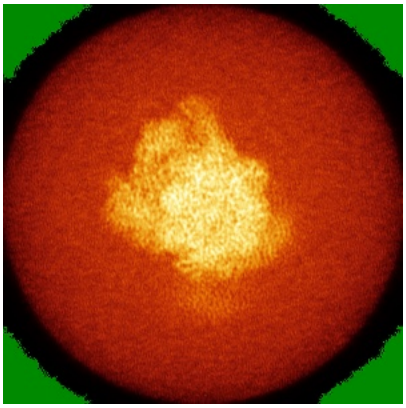


Z Index: 286

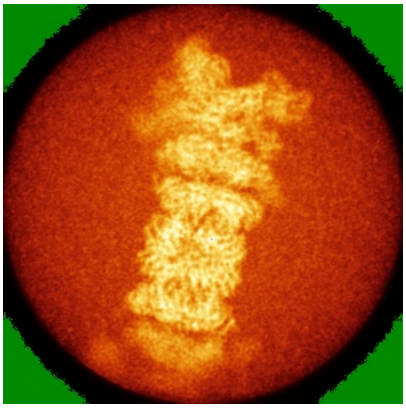
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

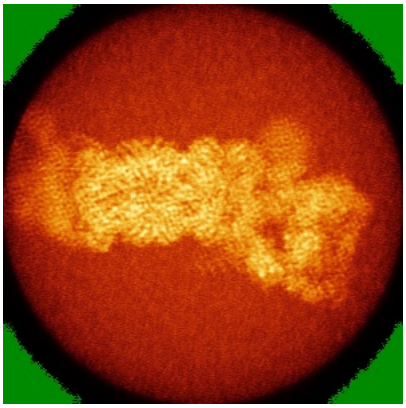
6.4.1 Primary map



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 (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

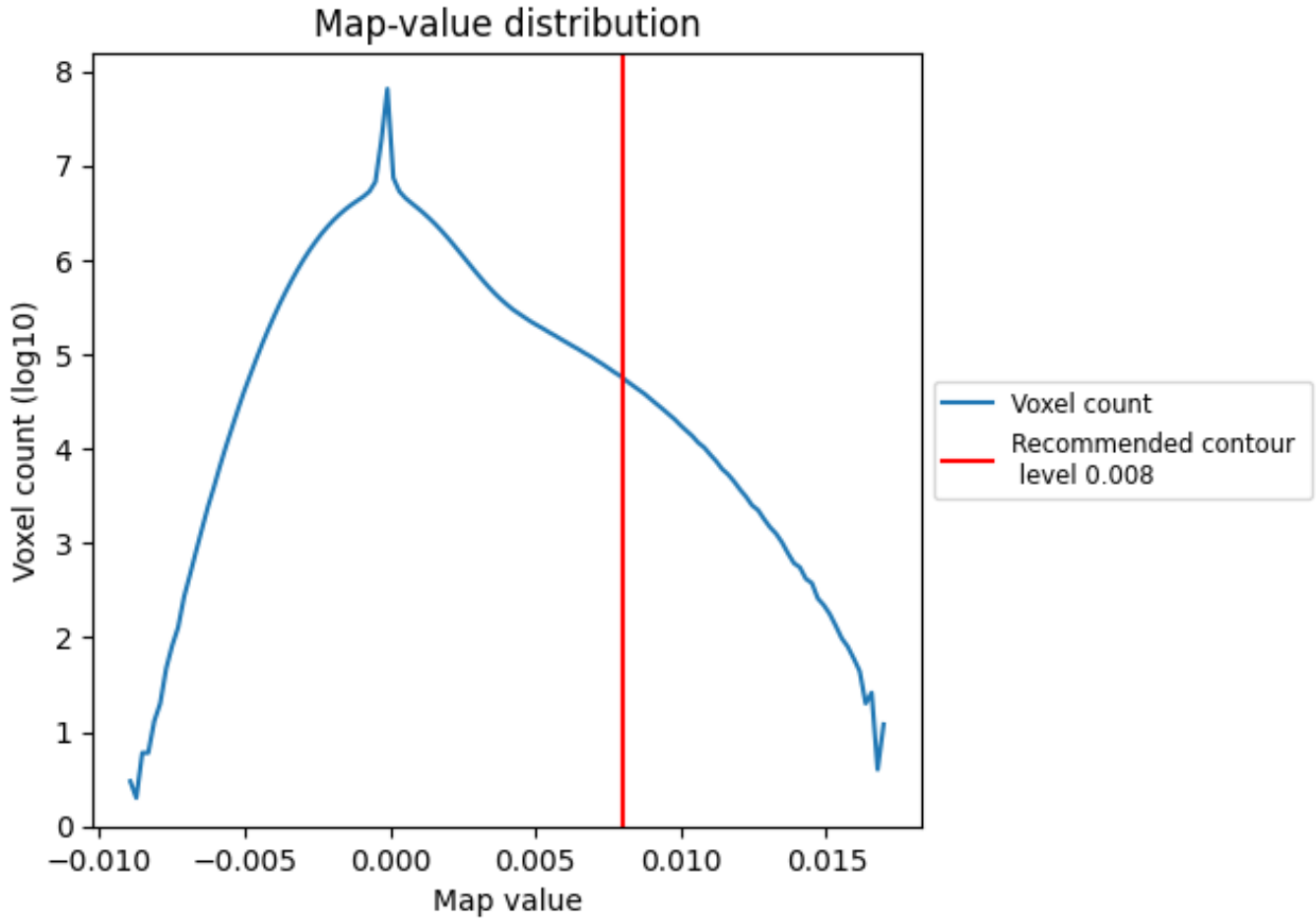
6.6 Mask visualisation (i)

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

7 Map analysis

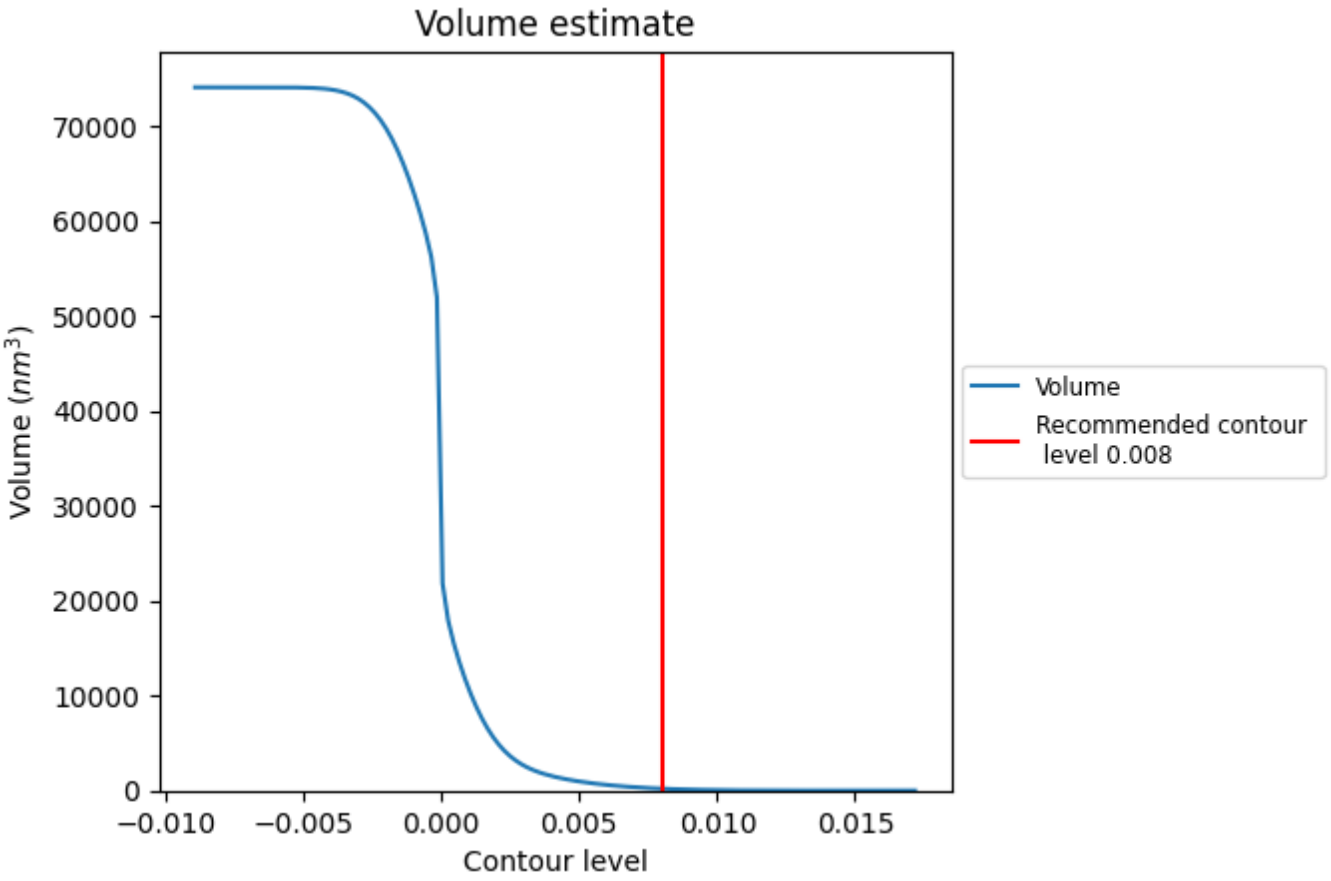
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

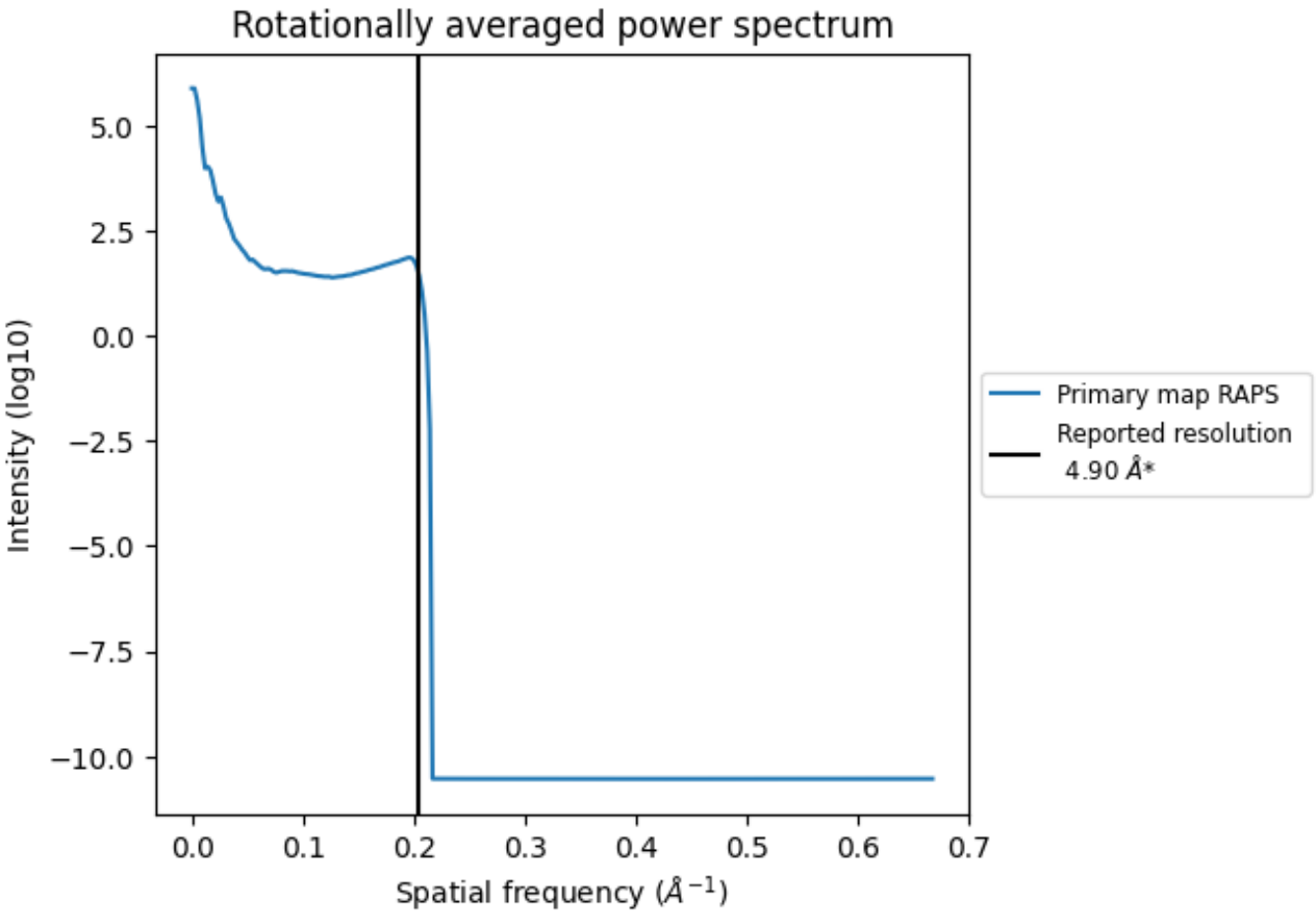
7.2 Volume estimate (i)



The volume at the recommended contour level is 199 nm^3; this corresponds to an approximate mass of 180 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 0.204 $Å^{-1}$

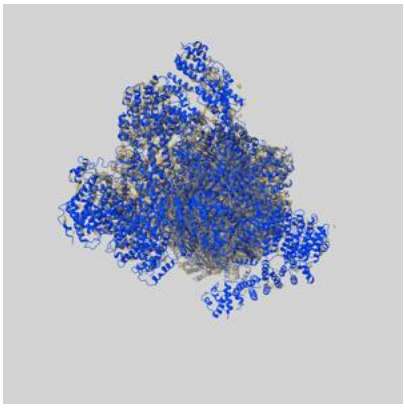
8 Fourier-Shell correlation (i)

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

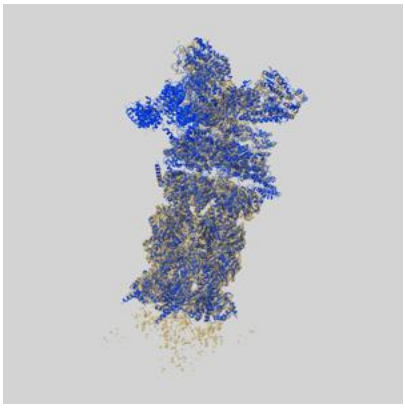
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8665 and PDB model 5VFR. Per-residue inclusion information can be found in section 3 on page 12.

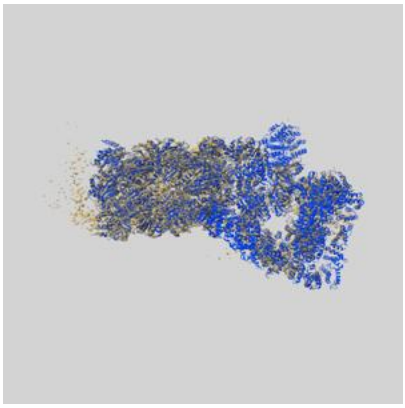
9.1 Map-model overlay



X



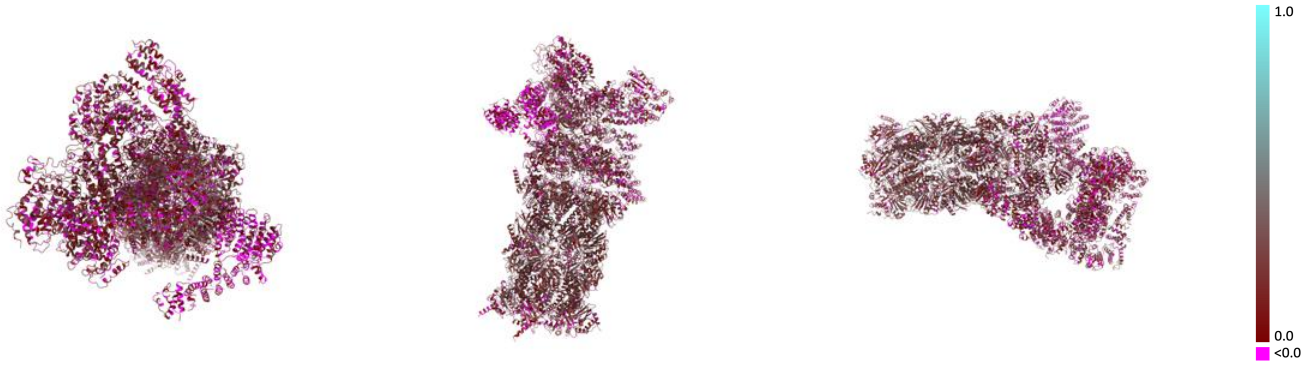
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

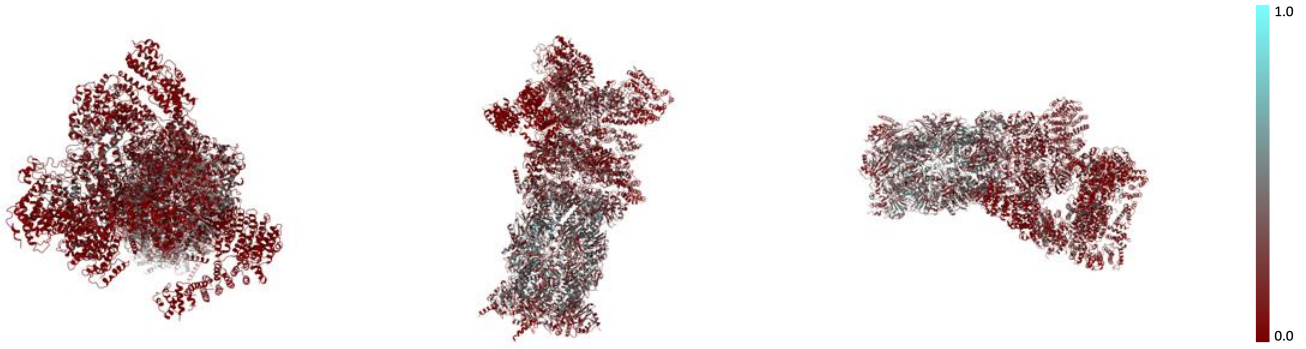
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

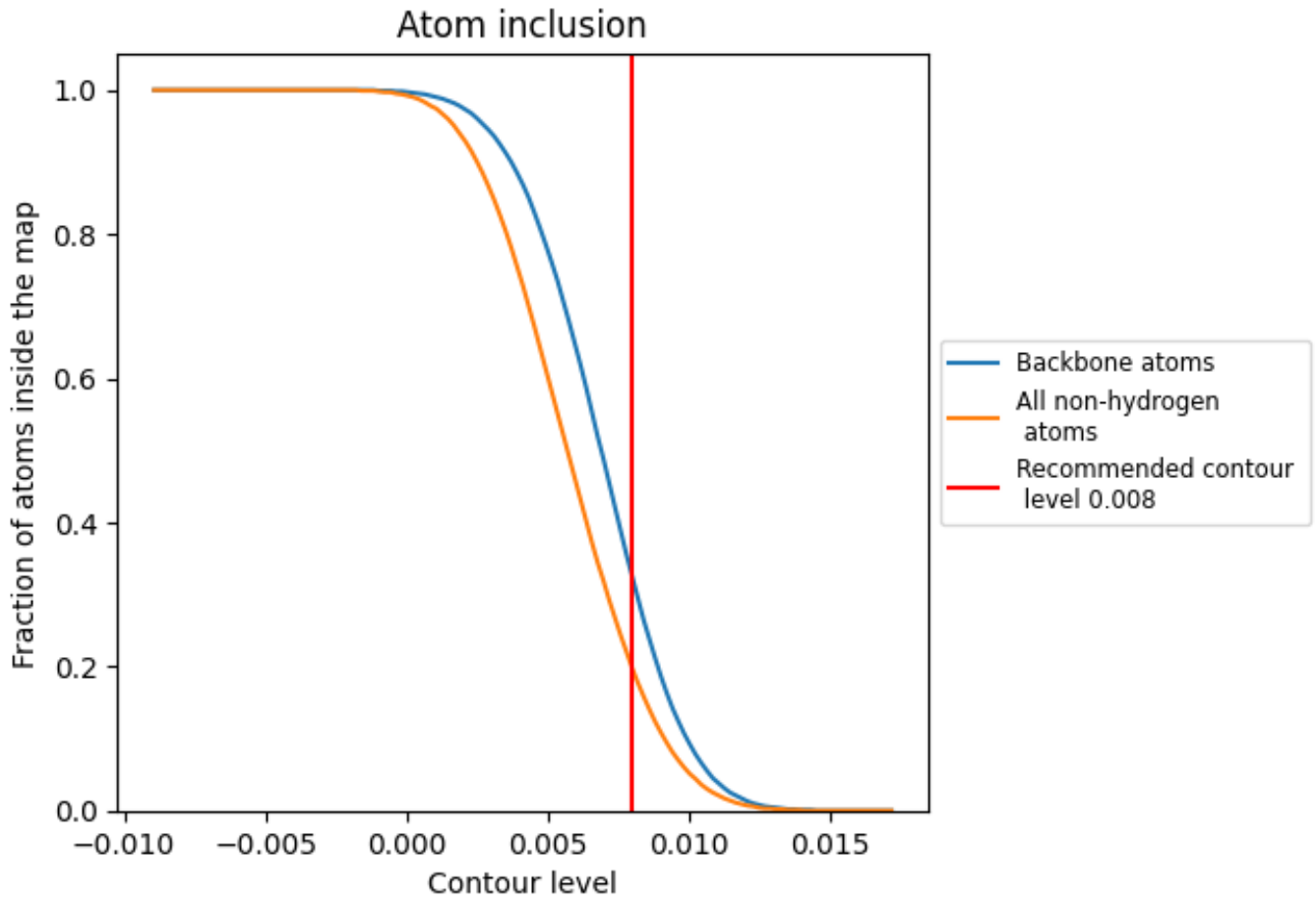
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 32% of all backbone atoms, 20% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1970	0.1860
A	0.1520	0.1910
B	0.1050	0.1900
C	0.1190	0.1960
D	0.1460	0.1980
E	0.1200	0.2070
F	0.1280	0.2010
G	0.2490	0.2070
H	0.2100	0.2030
I	0.2340	0.2090
J	0.2470	0.2200
K	0.3090	0.2120
L	0.3360	0.2280
M	0.2830	0.2150
N	0.3350	0.2540
O	0.2910	0.2390
P	0.3380	0.2470
Q	0.3400	0.2390
R	0.4270	0.2710
S	0.3460	0.2450
T	0.3900	0.2640
U	0.1060	0.1580
V	0.0700	0.1380
W	0.0870	0.1360
X	0.0740	0.1310
Y	0.1580	0.1480
Z	0.1580	0.1450
a	0.0980	0.1480
b	0.0490	0.0980
c	0.1770	0.1640
d	0.0480	0.1520
e	0.0700	0.1860
f	0.0040	0.0220
g	0.2400	0.2120
h	0.2190	0.2030

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.1970	0.1760
j	0.2430	0.1990
k	0.2920	0.2100
l	0.3080	0.2060
m	0.2660	0.2030
n	0.3570	0.2410
o	0.3190	0.2460
p	0.3480	0.2360
q	0.3720	0.2570
r	0.3810	0.2470
s	0.3510	0.2470
t	0.3820	0.2450