wwPDB EM Validation Summary Report ⓘ

Nov 26, 2022 – 04:41 PM EST

PDB ID	:	5T0C
EMDB ID	:	EMD-8332
Title	:	Structural basis for dynamic regulation of the human 26S proteasome
Authors	:	Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on	:	2016-08-15
Resolution	:	3.80 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

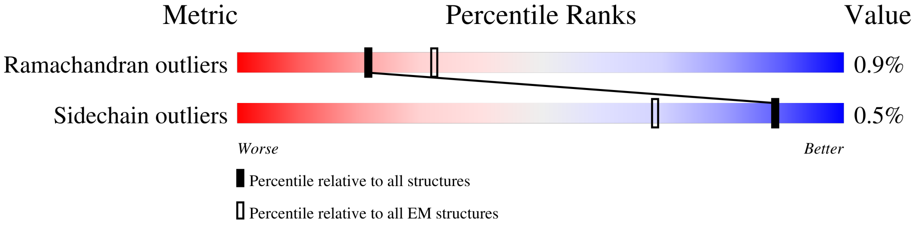
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

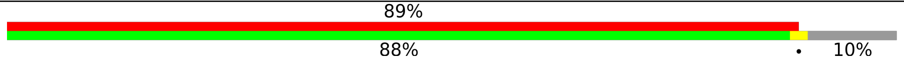
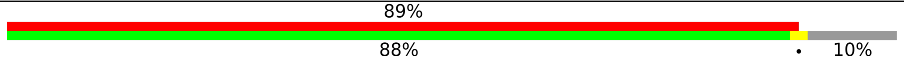
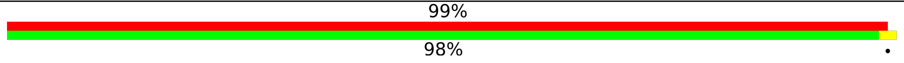
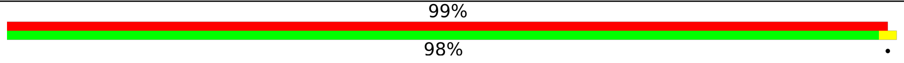
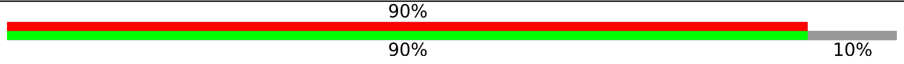
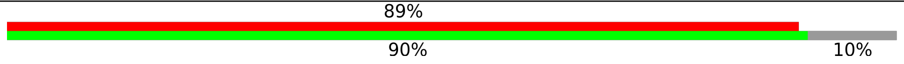
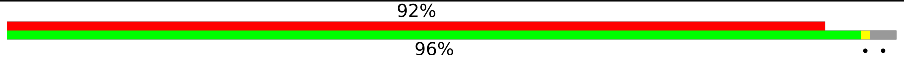
The reported resolution of this entry is 3.80 Å.

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	AU	953	
1	BU	953	
2	AV	533	
2	BV	533	
3	AW	456	
3	BW	456	
4	AX	422	
4	BX	422	
5	AY	389	

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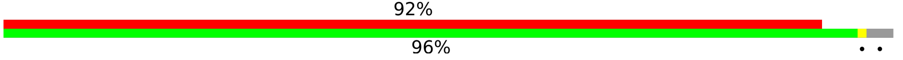
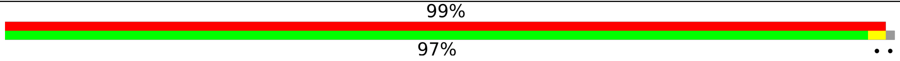
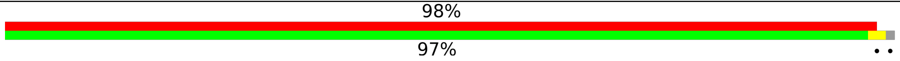
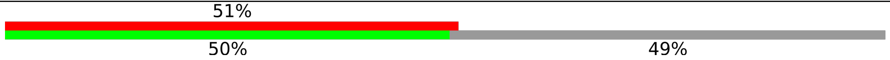
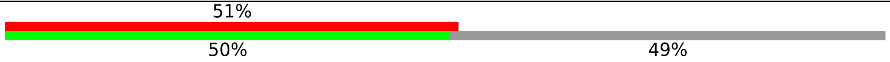
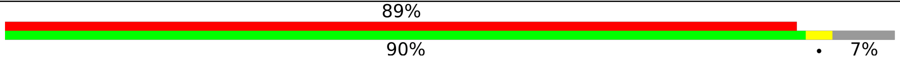
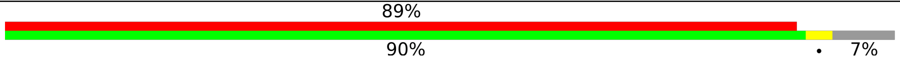
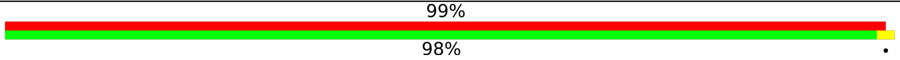
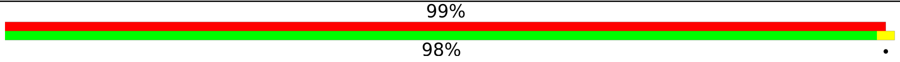
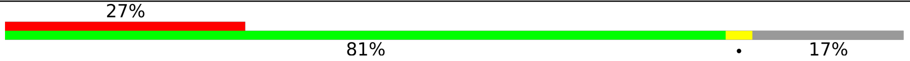
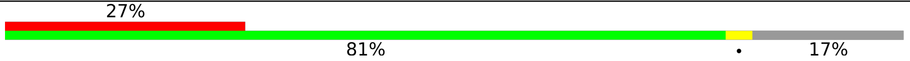
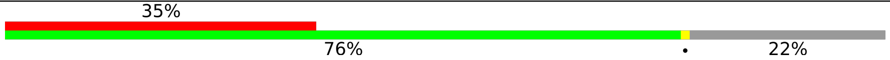
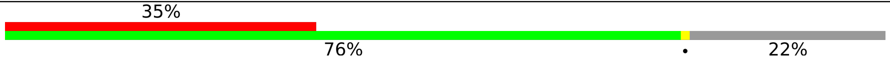
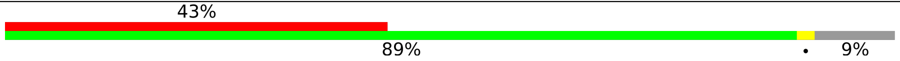
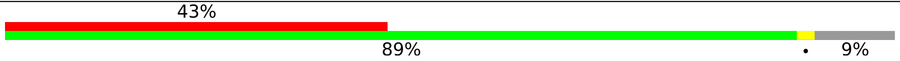
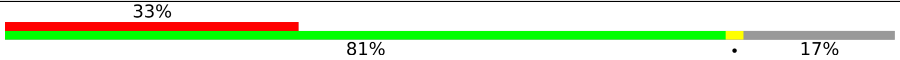
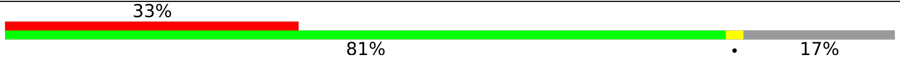
Mol	Chain	Length	Quality of chain
5	BY	389	
6	AZ	324	
6	BZ	324	
7	Aa	376	
7	Ba	376	
8	Ab	377	
8	Bb	377	
9	Ac	310	
9	Bc	310	
10	Ad	257	
10	Bd	257	
11	Ae	70	
11	Be	70	
12	Af	908	
12	Bf	908	
13	AA	433	
13	BA	433	
14	AB	440	
14	BB	440	
15	AD	418	
15	BD	418	
16	AE	389	
16	BE	389	
17	AF	439	
17	BF	439	

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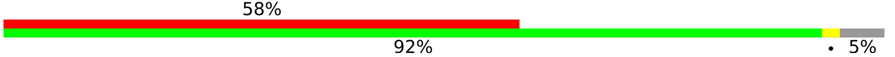
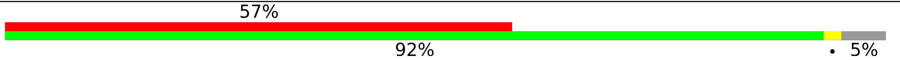
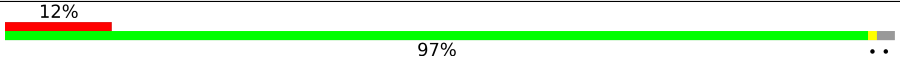
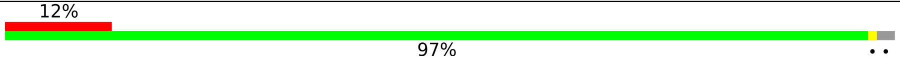
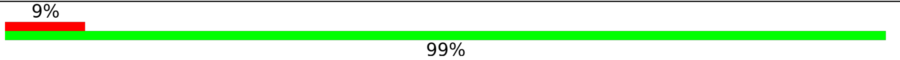
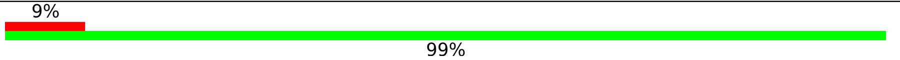
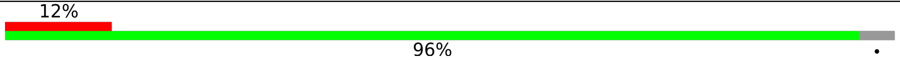
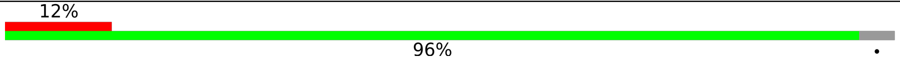
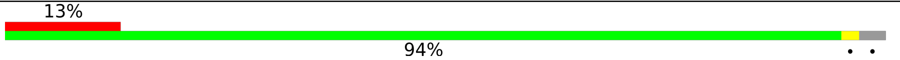
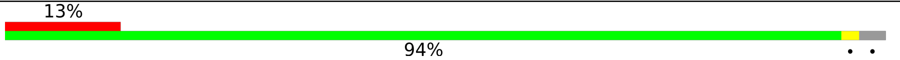
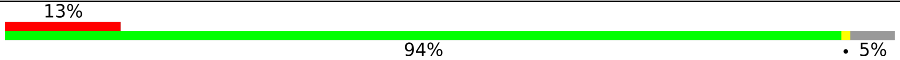
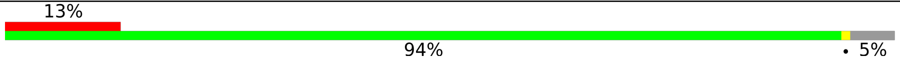
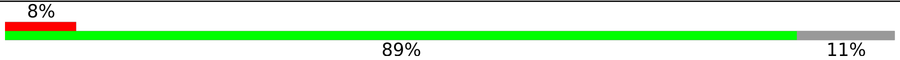
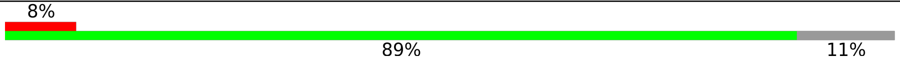
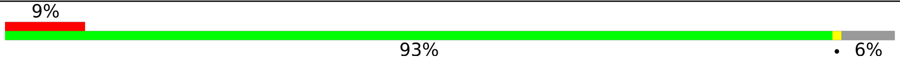
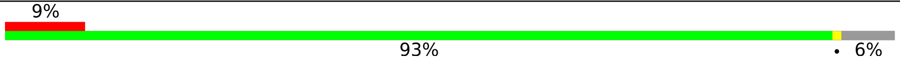
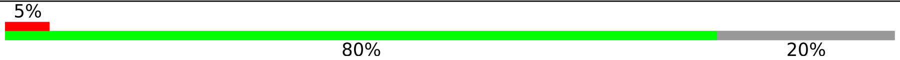
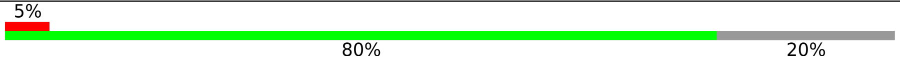
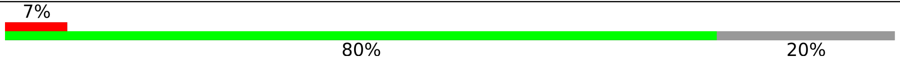
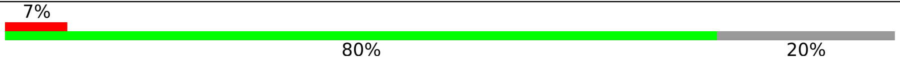
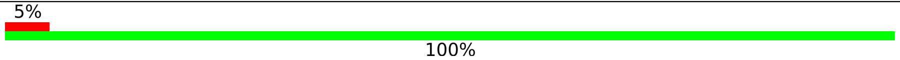
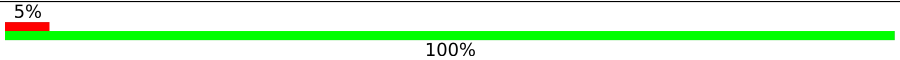
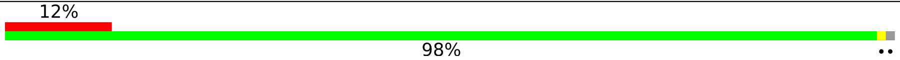
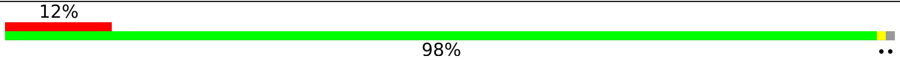
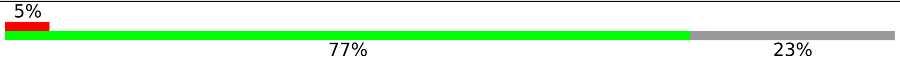
Mol	Chain	Length	Quality of chain
18	AC	406	 58% 92% • 5%
18	BC	406	 57% 92% • 5%
19	AG	245	 12% 97% • •
19	BG	245	 12% 97% • •
20	AH	233	 9% 99%
20	BH	233	 9% 99%
21	AI	260	 12% 96% •
21	BI	260	 12% 96% •
22	AJ	247	 13% 94% • •
22	BJ	247	 13% 94% • •
23	AK	240	 13% 94% • 5%
23	BK	240	 13% 94% • 5%
24	AL	268	 8% 89% 11%
24	BL	268	 8% 89% 11%
25	AM	254	 9% 93% • 6%
25	BM	254	 9% 93% • 6%
26	AN	238	 5% 80% 20%
26	BN	238	 5% 80% 20%
27	AO	276	 7% 80% 20%
27	BO	276	 7% 80% 20%
28	AP	204	 5% 100%
28	BP	204	 5% 100%
29	AQ	201	 12% 98% ••
29	BQ	201	 12% 98% ••
30	AR	262	 5% 77% 23%

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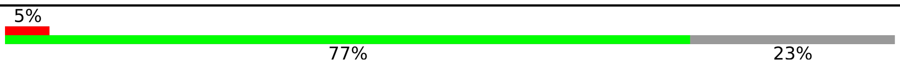
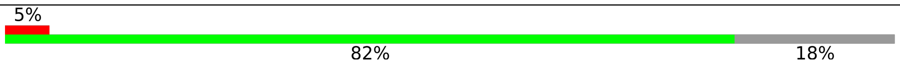
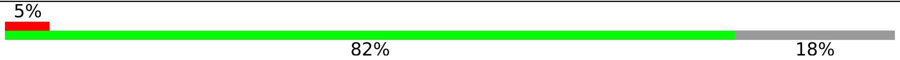
Mol	Chain	Length	Quality of chain
30	BR	262	
31	AS	240	
31	BS	240	
32	AT	263	
32	BT	263	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 155574 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	AU	806	6287	3990	1075	1178	44	0	0
1	BU	806	6287	3990	1075	1178	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	AV	480	3852	2444	684	710	14	0	0
2	BV	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	AW	456	3703	2339	635	704	25	0	0
3	BW	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	AX	380	3009	1918	509	570	12	0	0
4	BX	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	AY	378	3115	1987	533	578	17	0	0
5	BY	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	AZ	286	2281	1457	392	427	5	0	0
6	BZ	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	Aa	373	2995	1911	510	559	15	0	0
7	Ba	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	Ab	191	1458	910	261	279	8	0	0
8	Bb	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	Ac	287	2260	1430	389	422	19	0	0
9	Bc	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	Ad	257	2116	1371	346	390	9	0	0

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

- Molecule 11 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Ae	40	334	200	55	77	2	0	0
11	Be	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	Af	694	5331	3364	899	1027	41	0	0
12	Bf	694	5331	3364	899	1027	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AA	361	2835	1788	501	528	18	0	0
13	BA	361	2835	1788	501	528	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AB	341	2662	1671	453	526	12	0	0
14	BB	341	2662	1671	453	526	12	0	0

- Molecule 15 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AD	380	3040	1923	524	580	13	0	0
15	BD	380	3040	1923	524	580	13	0	0

- Molecule 16 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		
16	BE	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

- Molecule 17 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		
17	BF	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 18 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AC	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		
18	BC	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AG	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
19	BG	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AH	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
20	BH	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AI	250	Total 1912	C 1204	N 329	O 371	S 8	0	0
21	BI	250	Total 1912	C 1204	N 329	O 371	S 8	0	0

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AJ	239	Total 1704	C 1056	N 308	O 335	S 5	0	0
22	BJ	239	Total 1704	C 1056	N 308	O 335	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AK	228	Total 1722	C 1080	N 284	O 348	S 10	0	0
23	BK	228	Total 1722	C 1080	N 284	O 348	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AL	238	Total 1850	C 1159	N 334	O 346	S 11	0	0
24	BL	238	Total 1850	C 1159	N 334	O 346	S 11	0	0

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AM	240	Total 1856	C 1178	N 314	O 353	S 11	0	0
25	BM	240	Total 1856	C 1178	N 314	O 353	S 11	0	0

- Molecule 26 is a protein called Proteasome subunit beta type-6.

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

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

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	AO	220	Total C N O S 1643 1033 280 318 12	0	0
27	BO	220	Total C N O S 1643 1033 280 318 12	0	0

- Molecule 28 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	AP	204	Total C N O S 1585 1010 262 294 19	0	0
28	BP	204	Total C N O S 1585 1010 262 294 19	0	0

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	AQ	199	Total C N O S 1570 1006 265 290 9	0	0
29	BQ	199	Total C N O S 1570 1006 265 290 9	0	0

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	AR	201	Total C N O S 1548 974 273 292 9	0	0
30	BR	201	Total C N O S 1548 974 273 292 9	0	0

- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	AS	213	Total C N O S 1641 1036 282 313 10	0	0
31	BS	213	Total C N O S 1641 1036 282 313 10	0	0

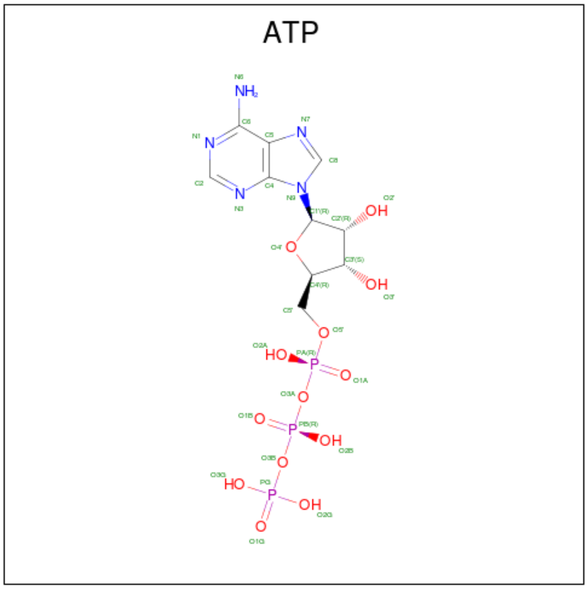
- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AT	215	Total 1667	C 1052	N 285	O 318	S 12	0	0
32	BT	215	Total 1667	C 1052	N 285	O 318	S 12	0	0

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

Mol	Chain	Residues	Atoms		AltConf
33	Ac	1	Total 1	Zn 1	0
33	Bc	1	Total 1	Zn 1	0

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
34	AA	1	Total 31	C 10	N 5	O 13	P 3	0
34	AD	1	Total 31	C 10	N 5	O 13	P 3	0
34	AE	1	Total 31	C 10	N 5	O 13	P 3	0
34	AF	1	Total 31	C 10	N 5	O 13	P 3	0

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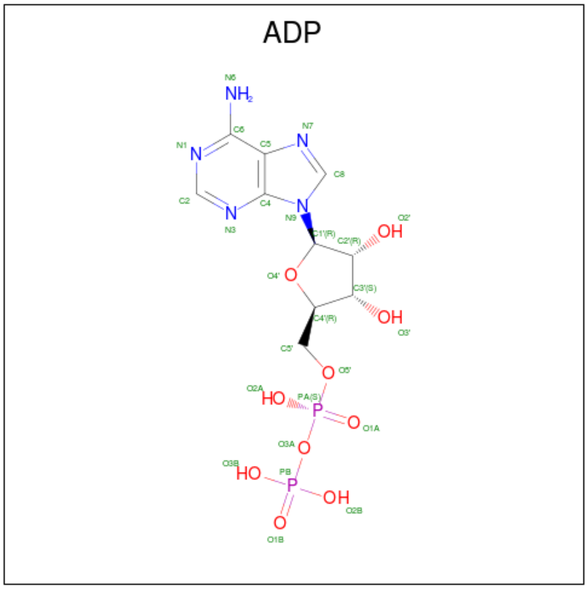
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	BA	1	31	10	5	13	3	0
34	BD	1	31	10	5	13	3	0
34	BE	1	31	10	5	13	3	0
34	BF	1	31	10	5	13	3	0

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



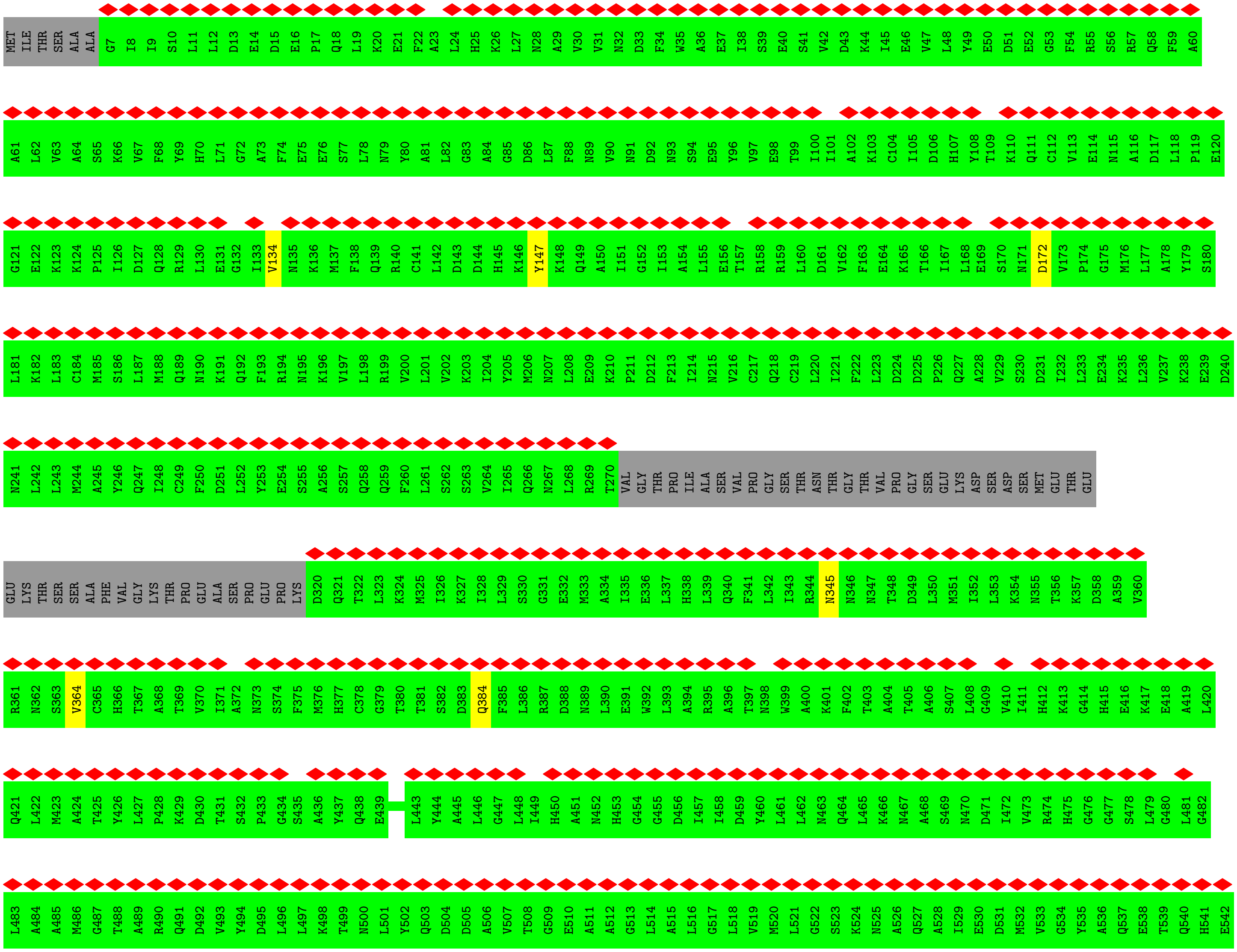
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	AB	1	27	10	5	10	2	0
35	AC	1	27	10	5	10	2	0
35	BB	1	27	10	5	10	2	0
35	BC	1	27	10	5	10	2	0

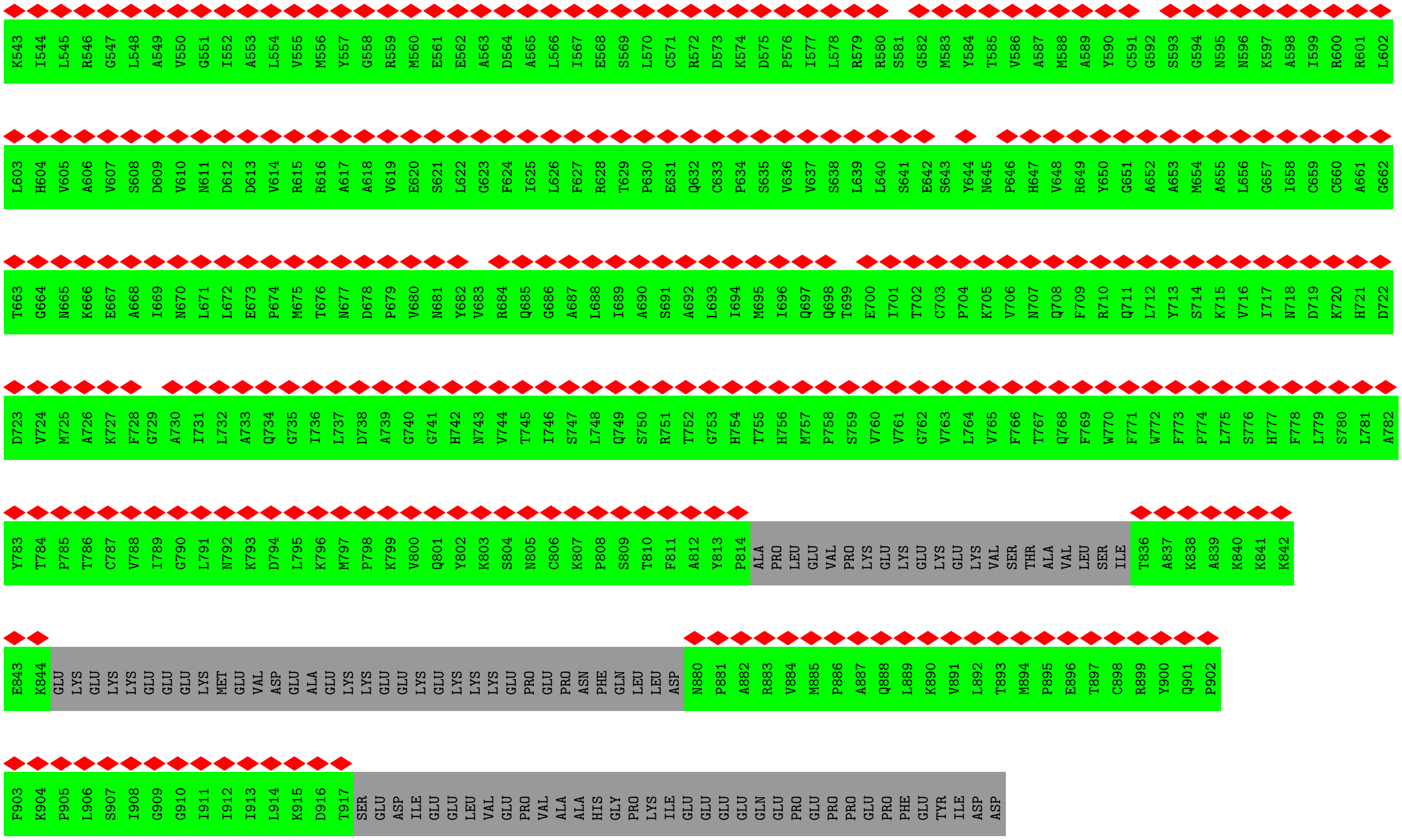
3 Residue-property plots ⓘ

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

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

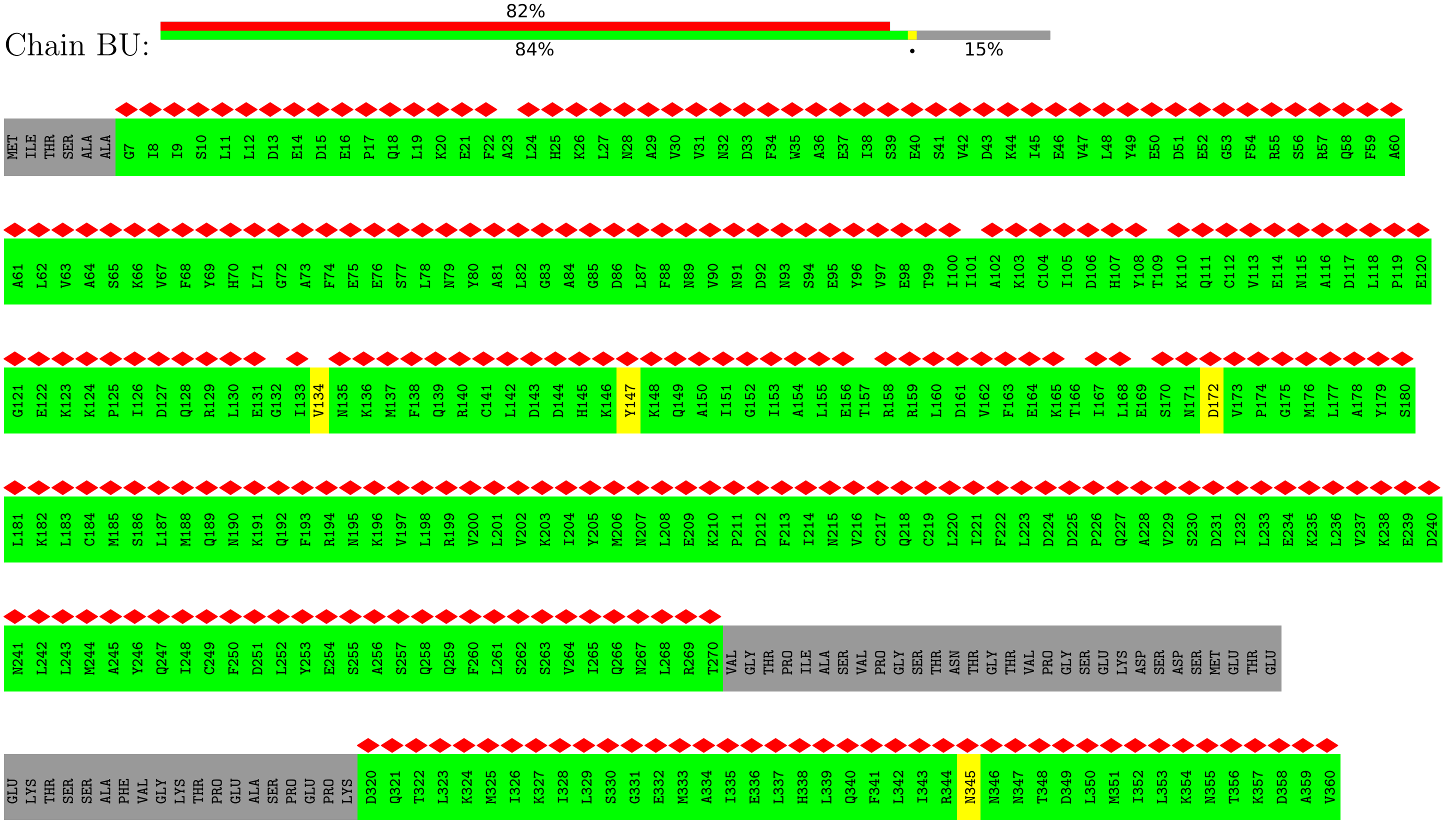
Chain AU:

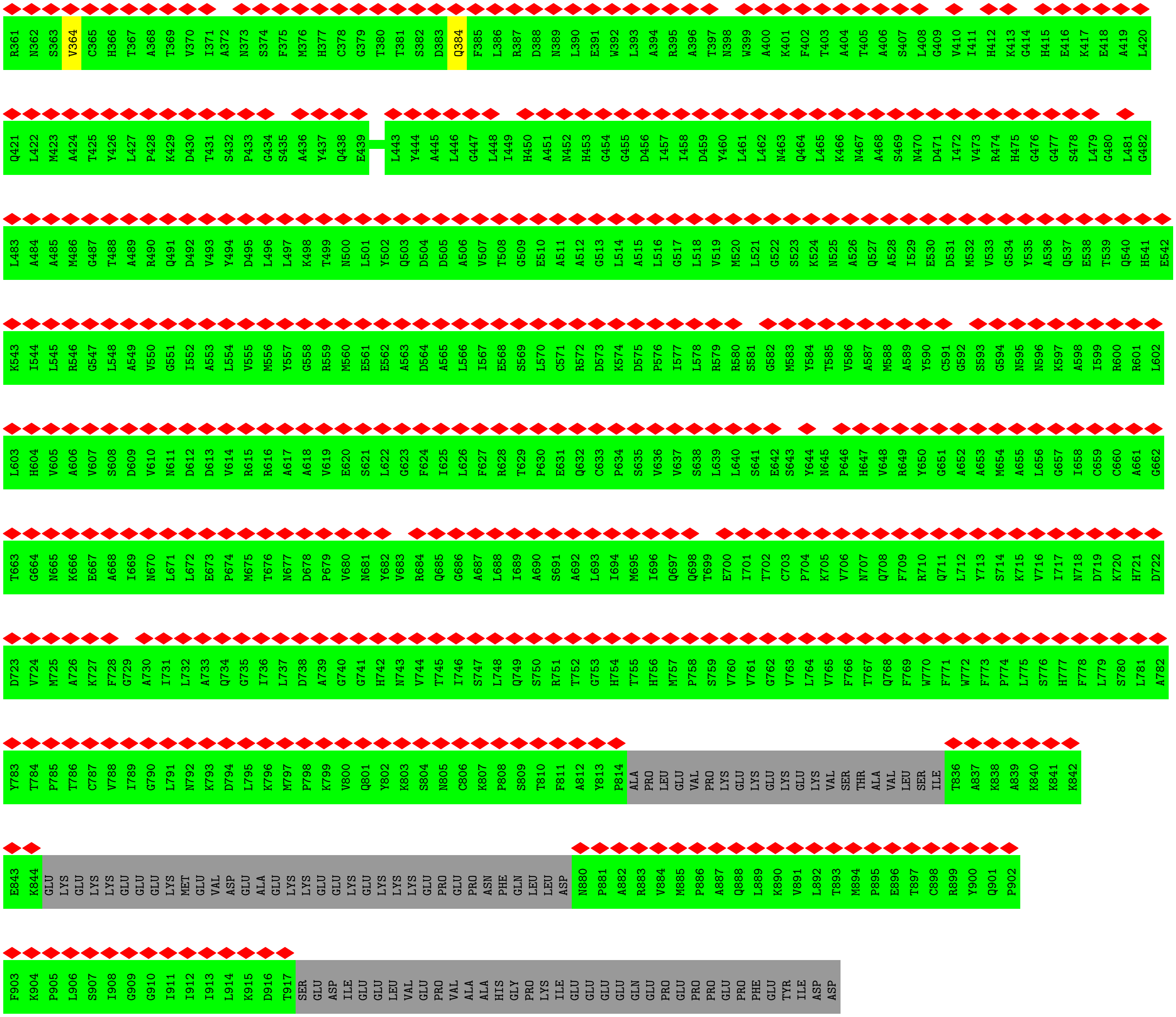




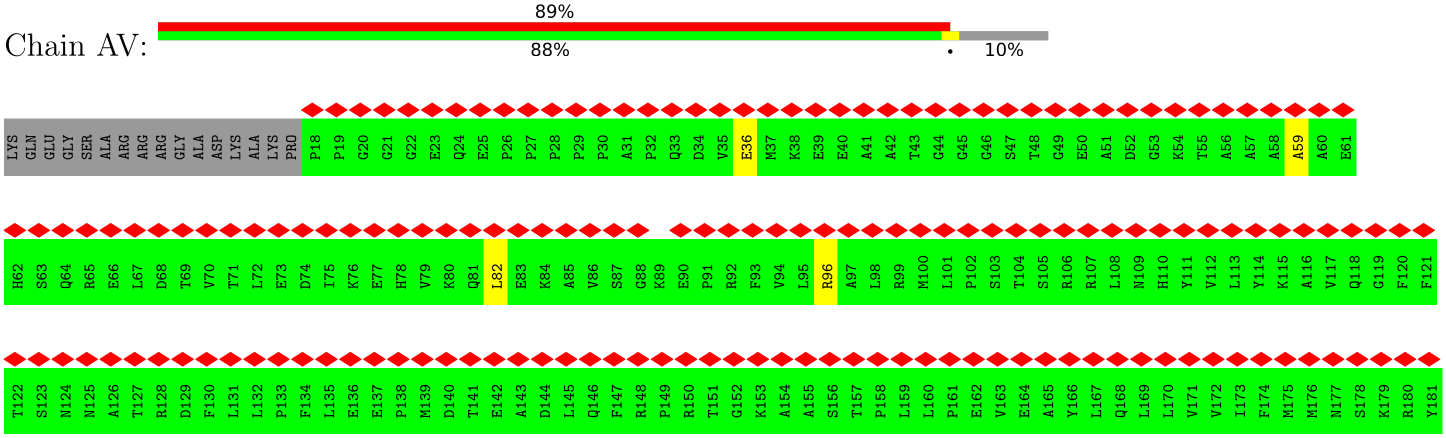
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

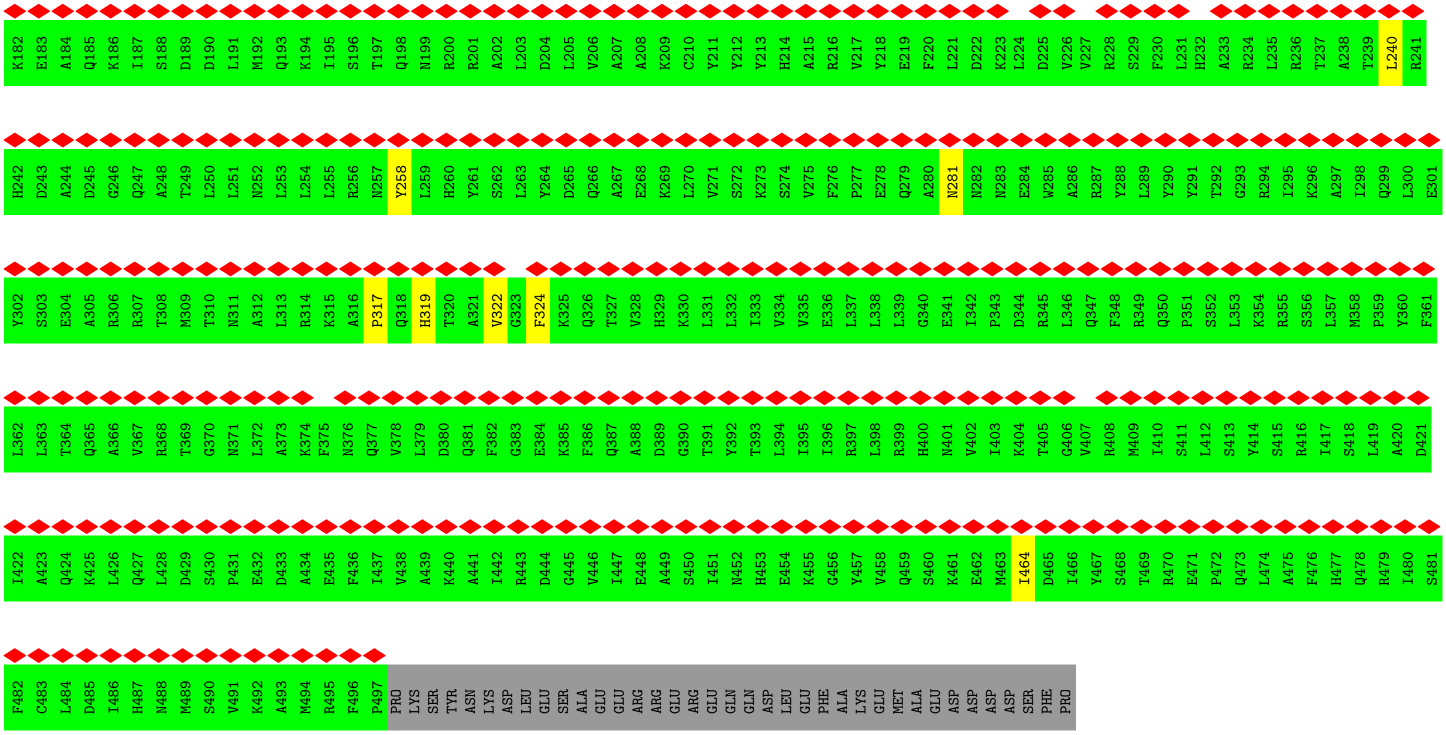
Chain BU:





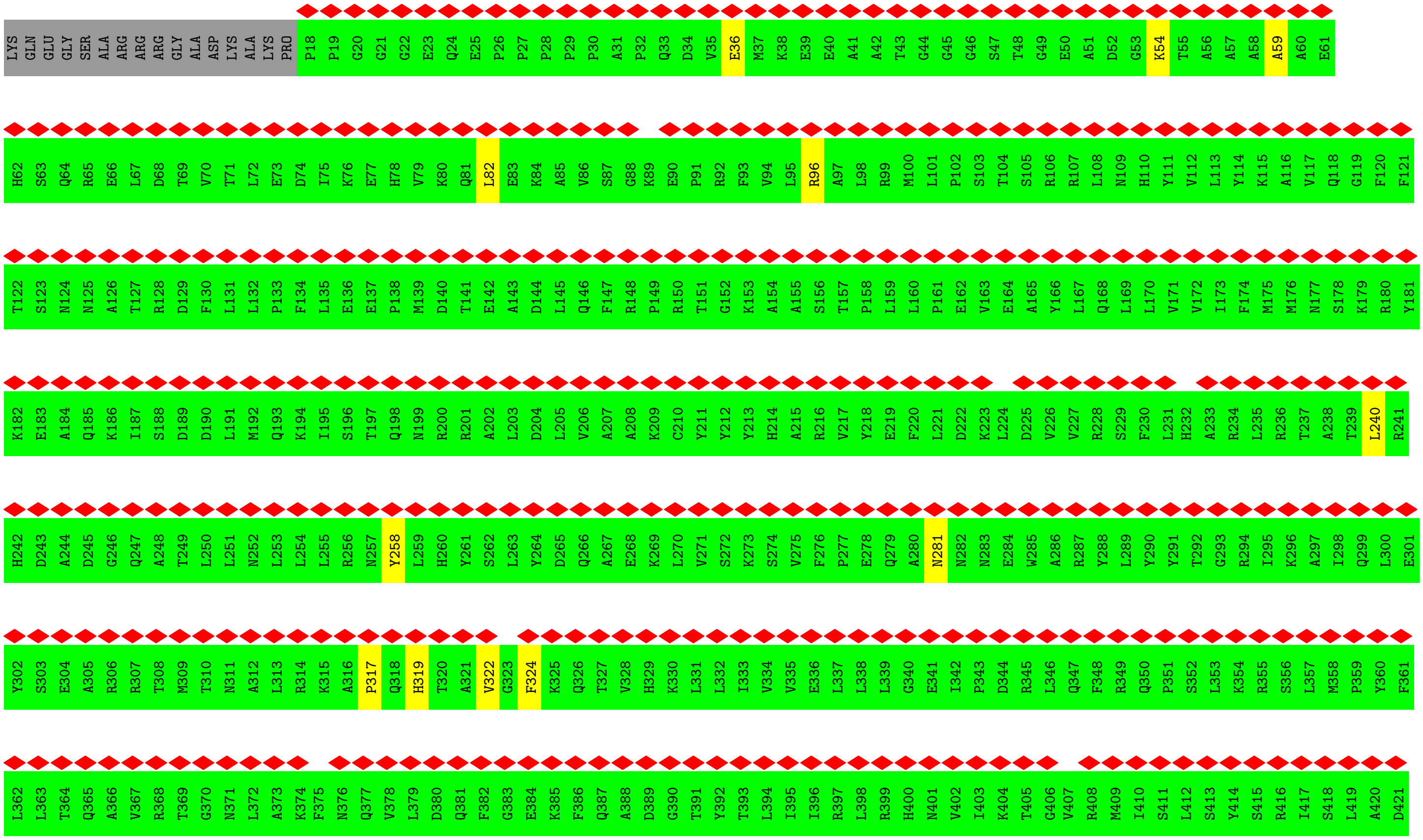
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

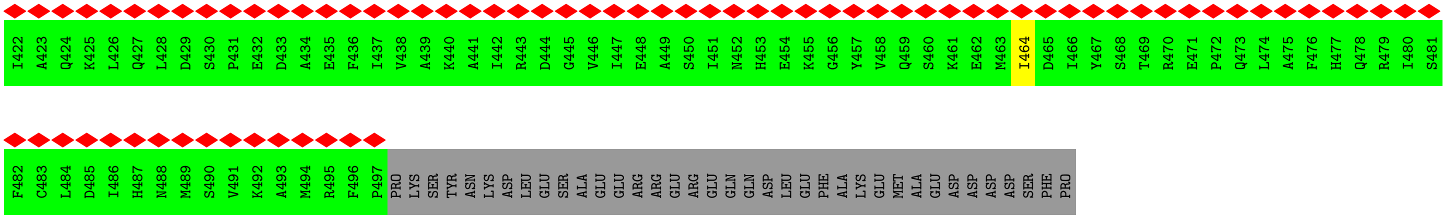




- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

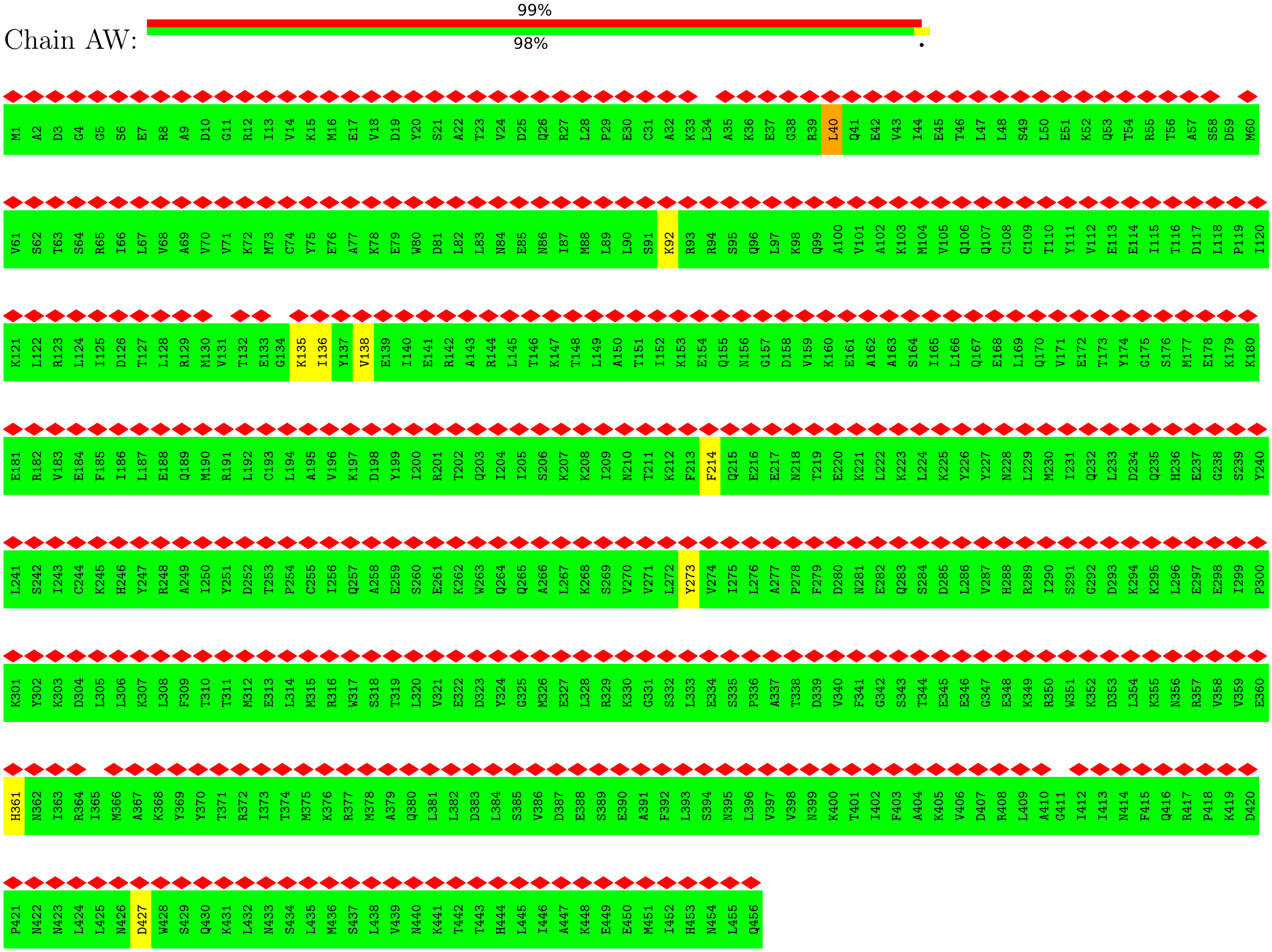
Chain BV:





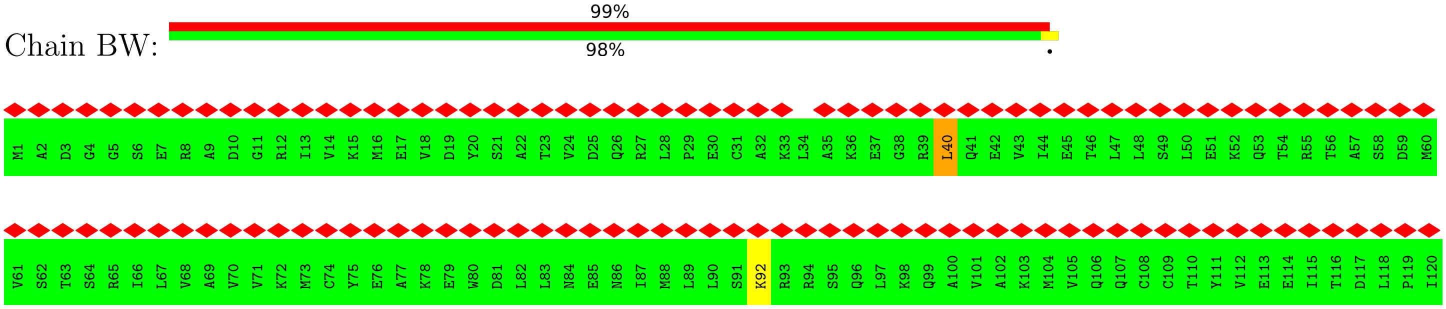
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

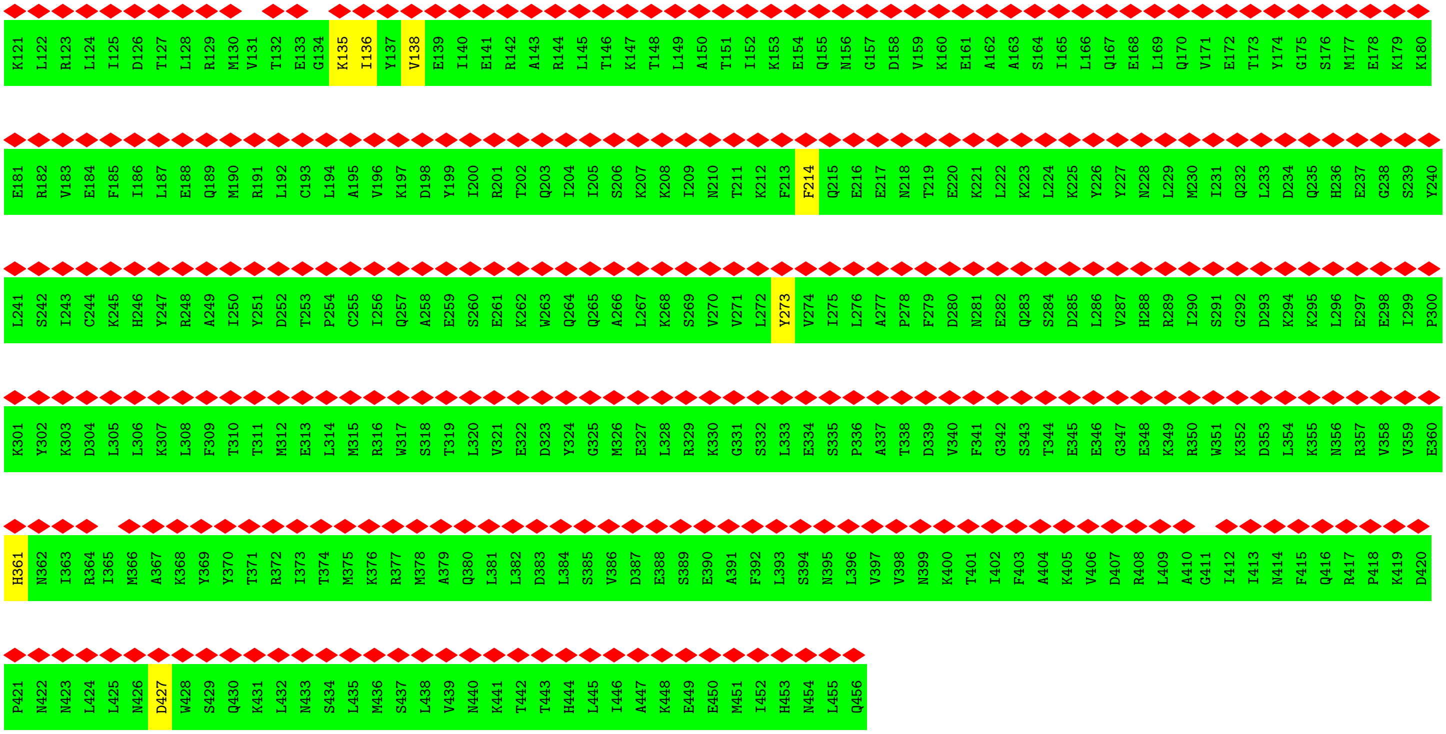
Chain AW:



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

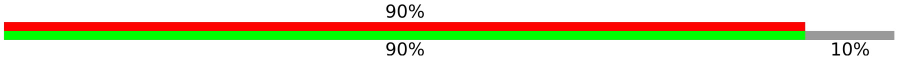
Chain BW:

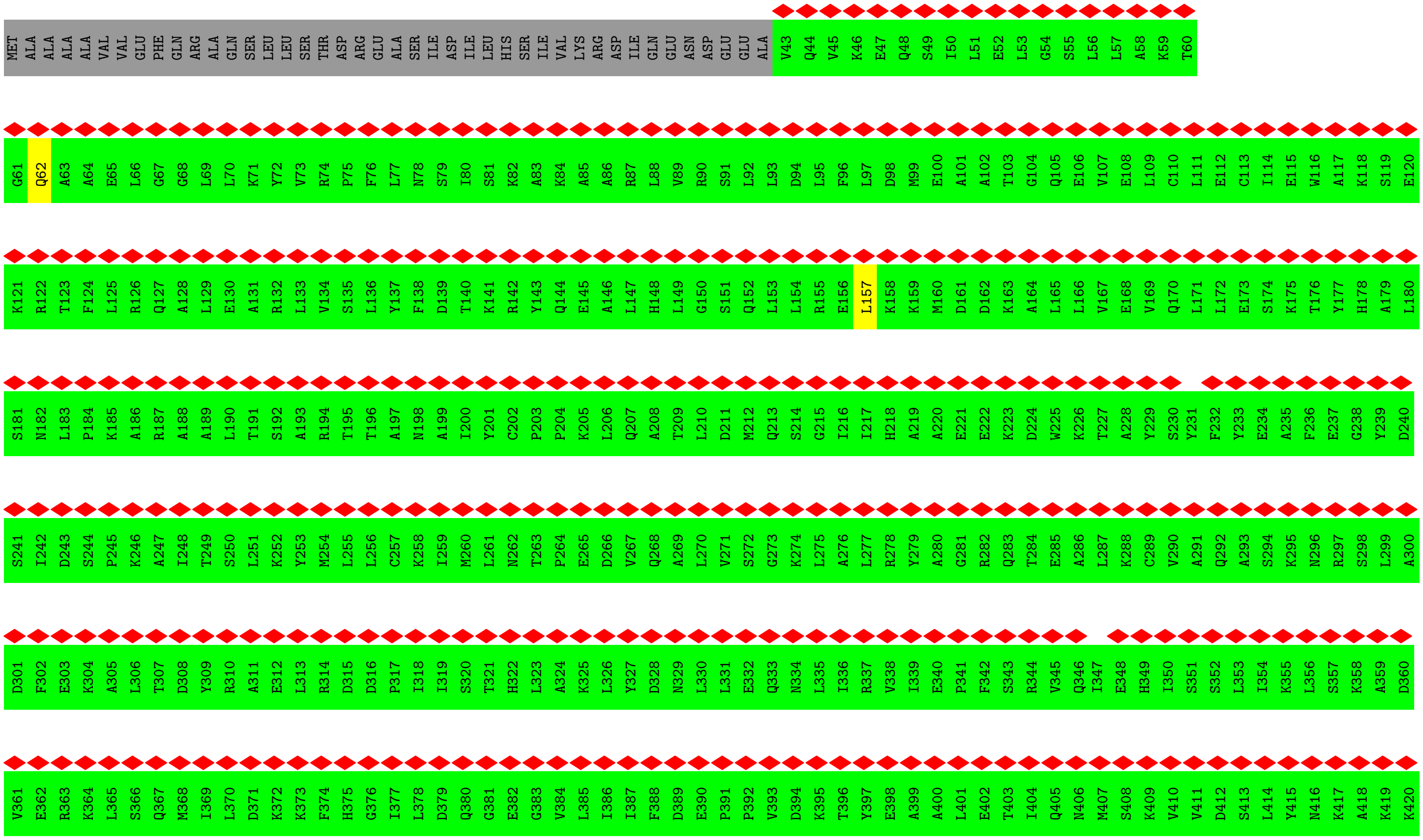


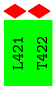


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain AX:

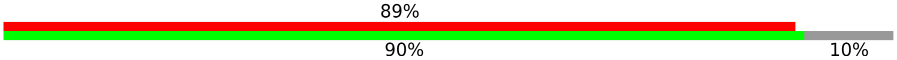


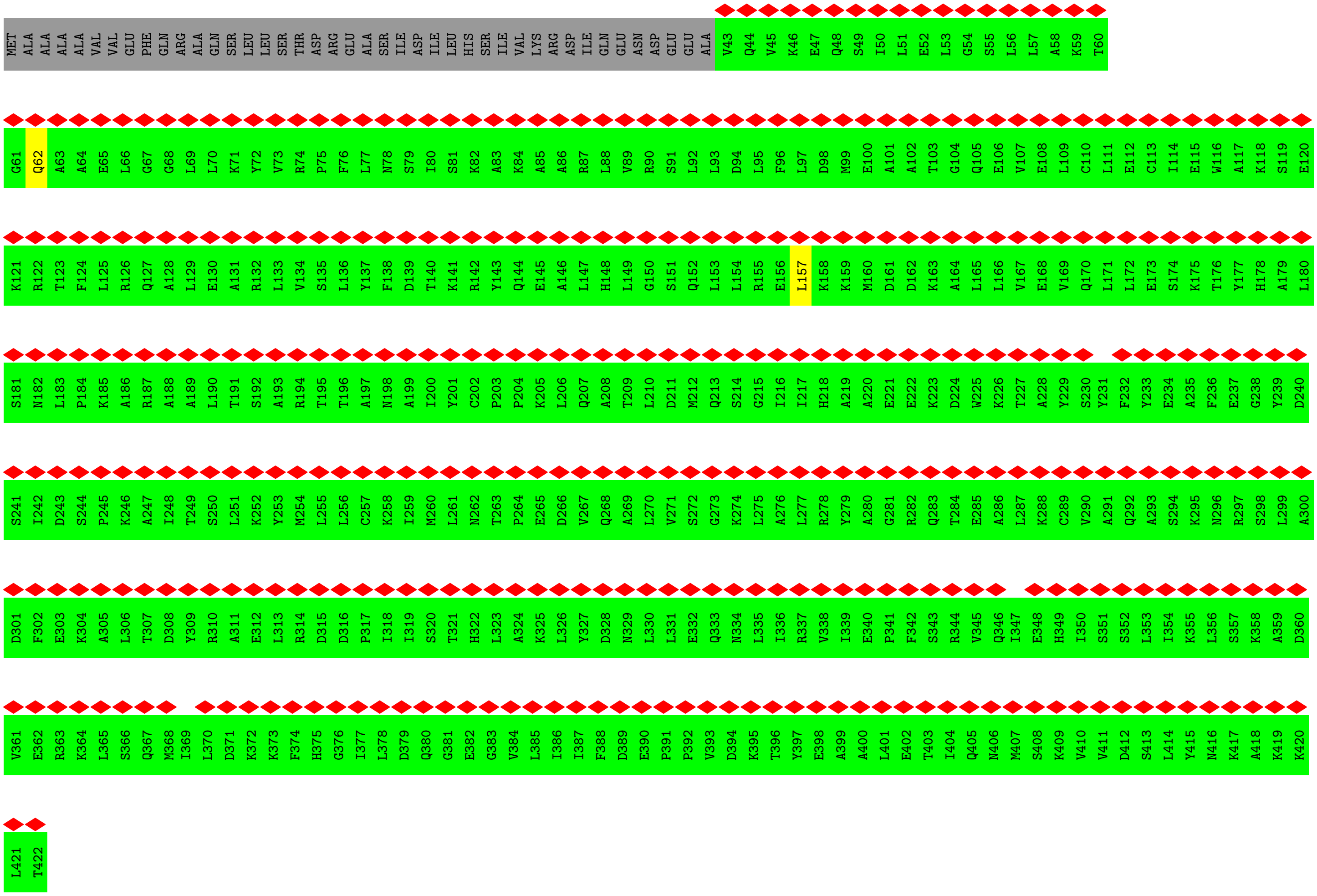




- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

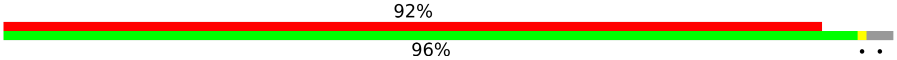
Chain BX:

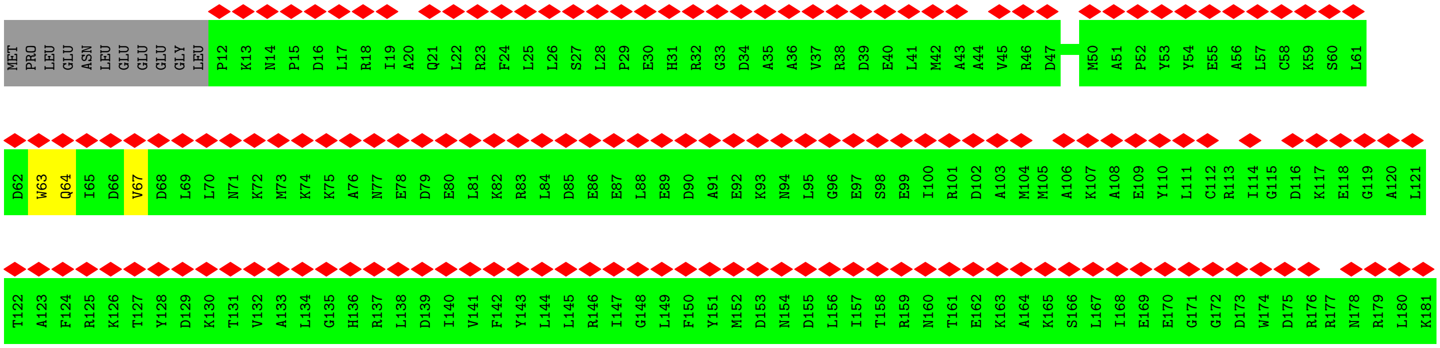


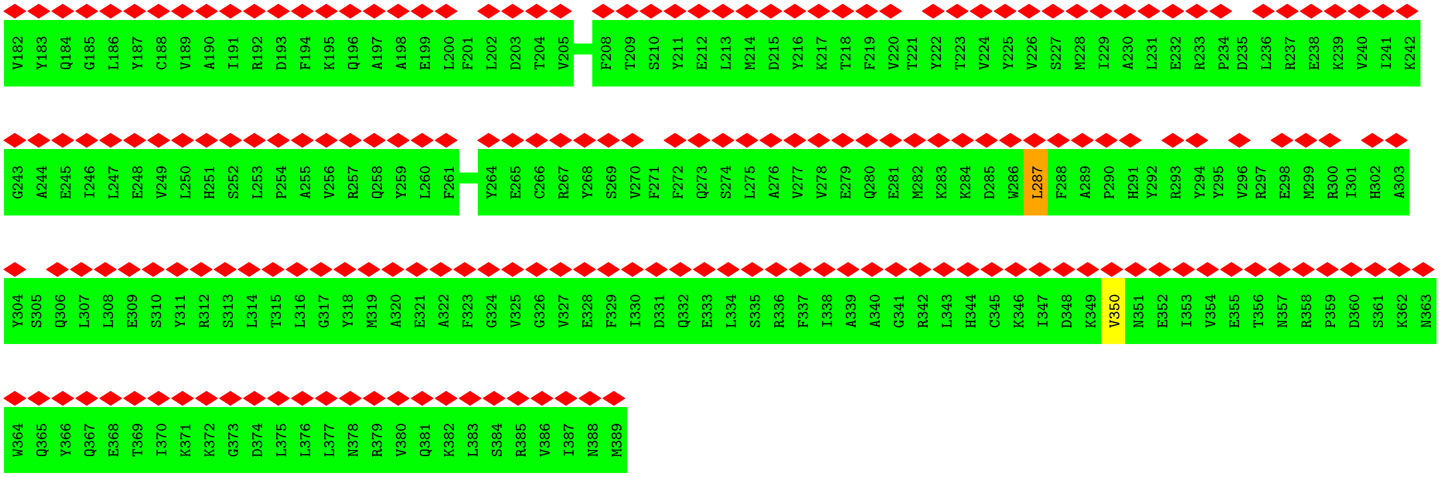


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain AY:

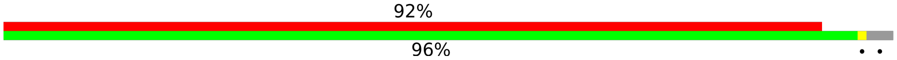


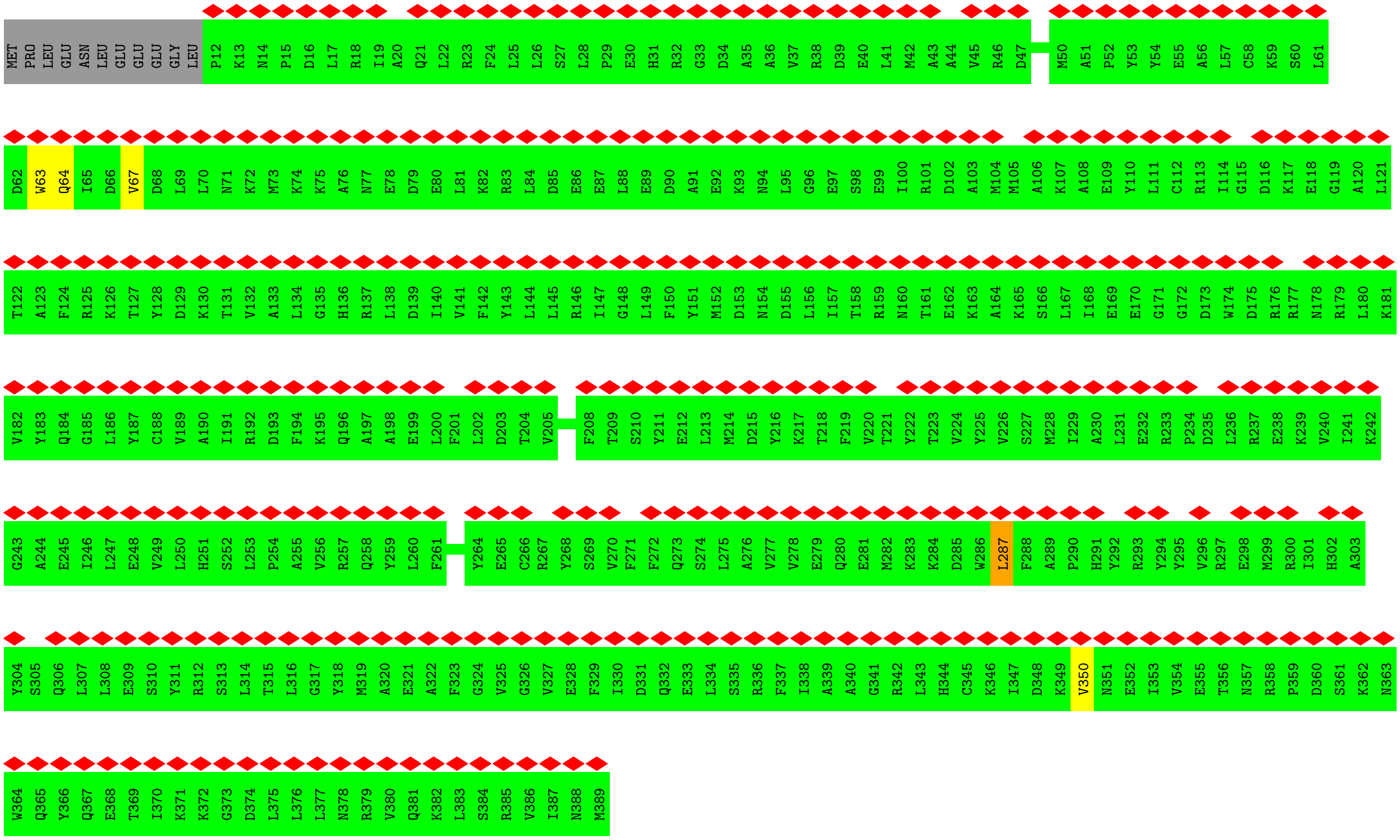




- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

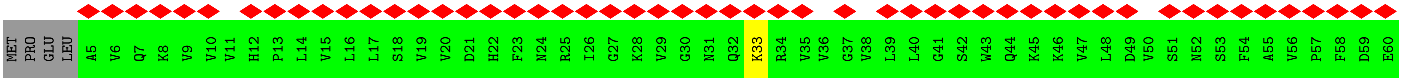
Chain BY:

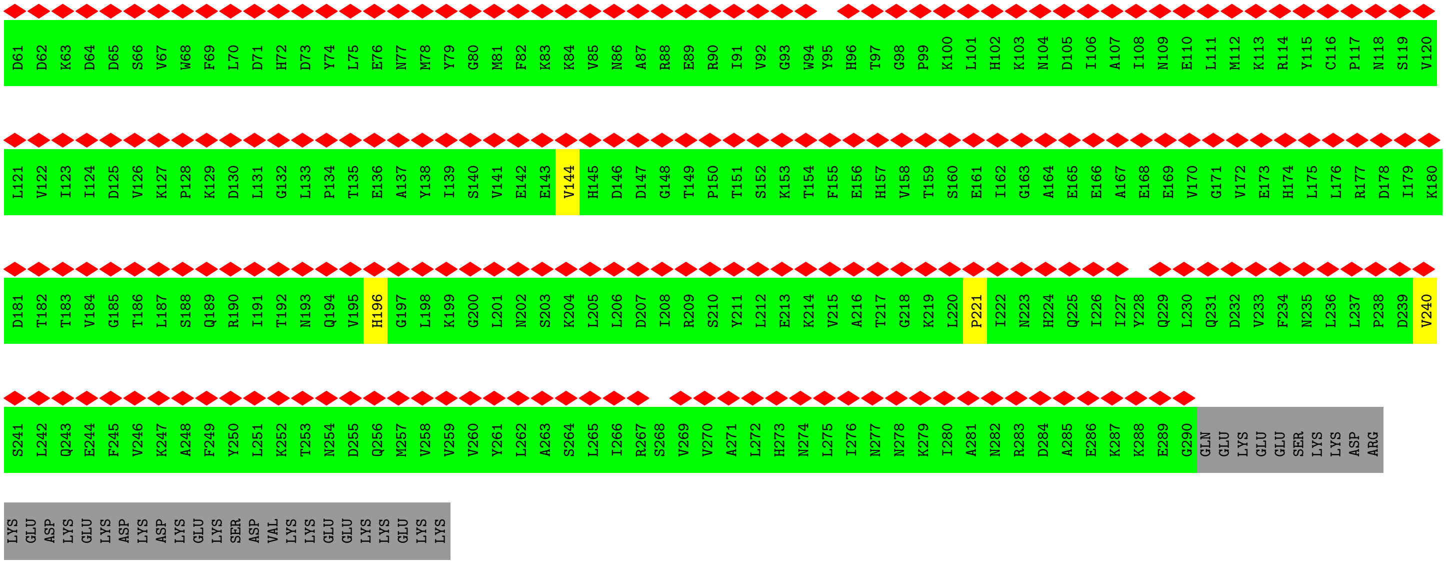




- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

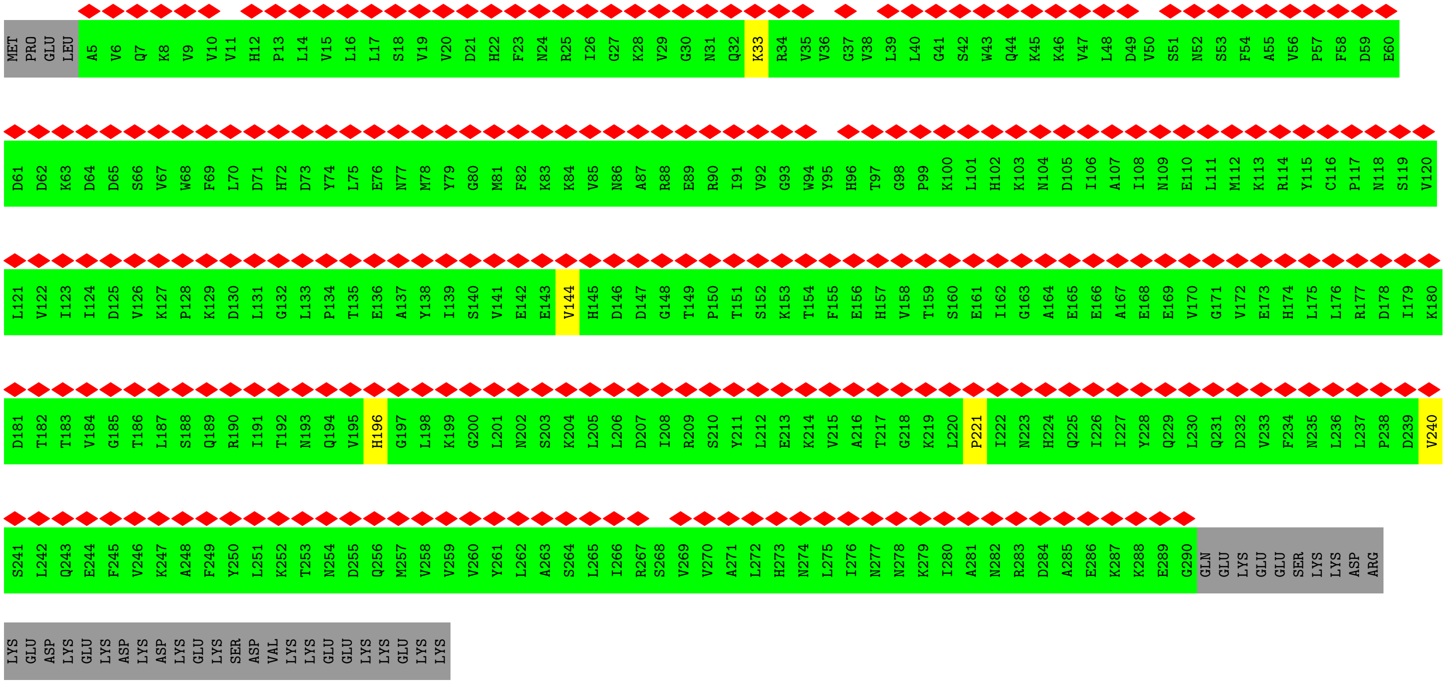
Chain AZ:





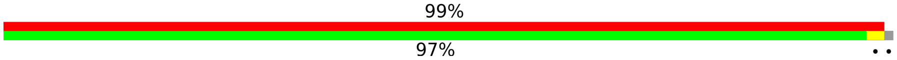
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

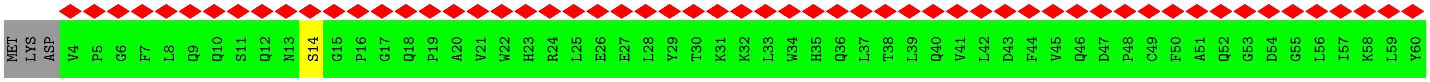
Chain BZ:

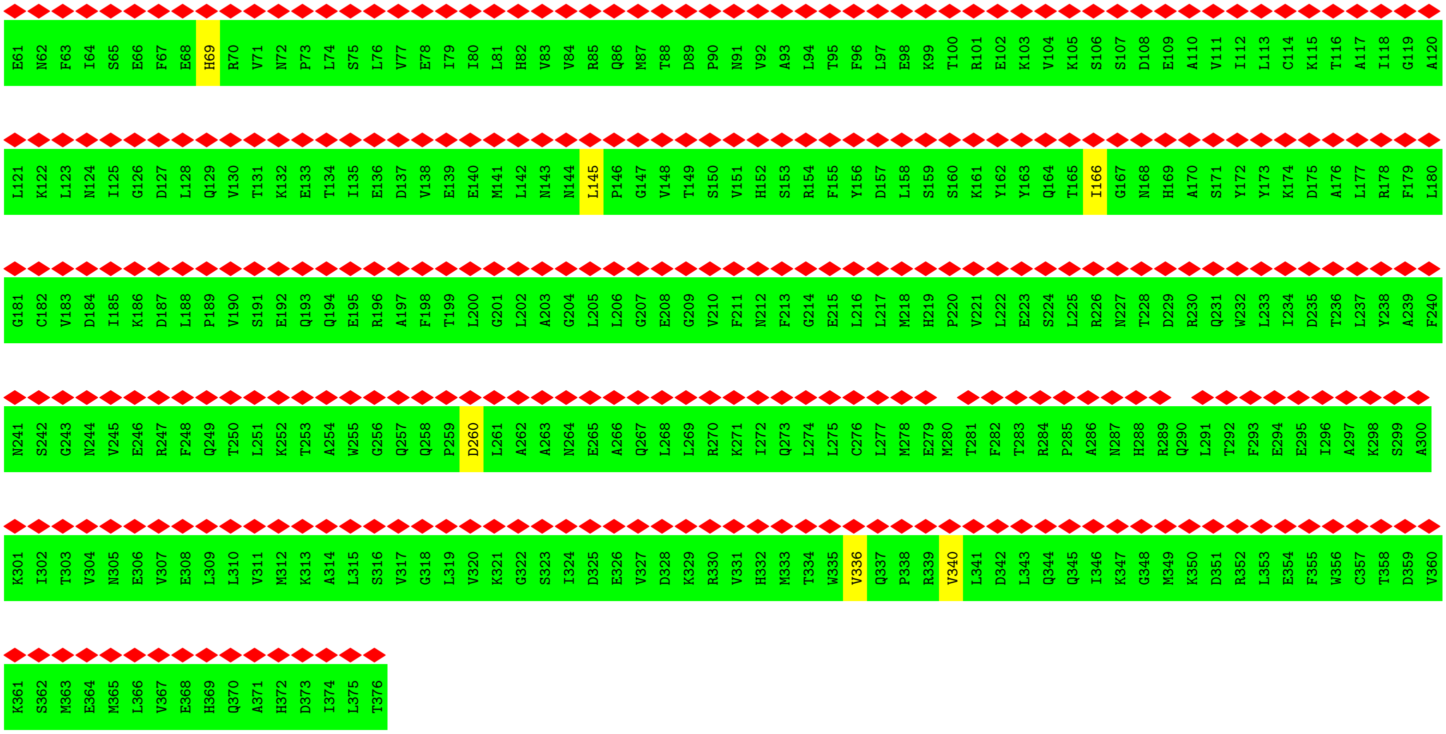


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain Aa:

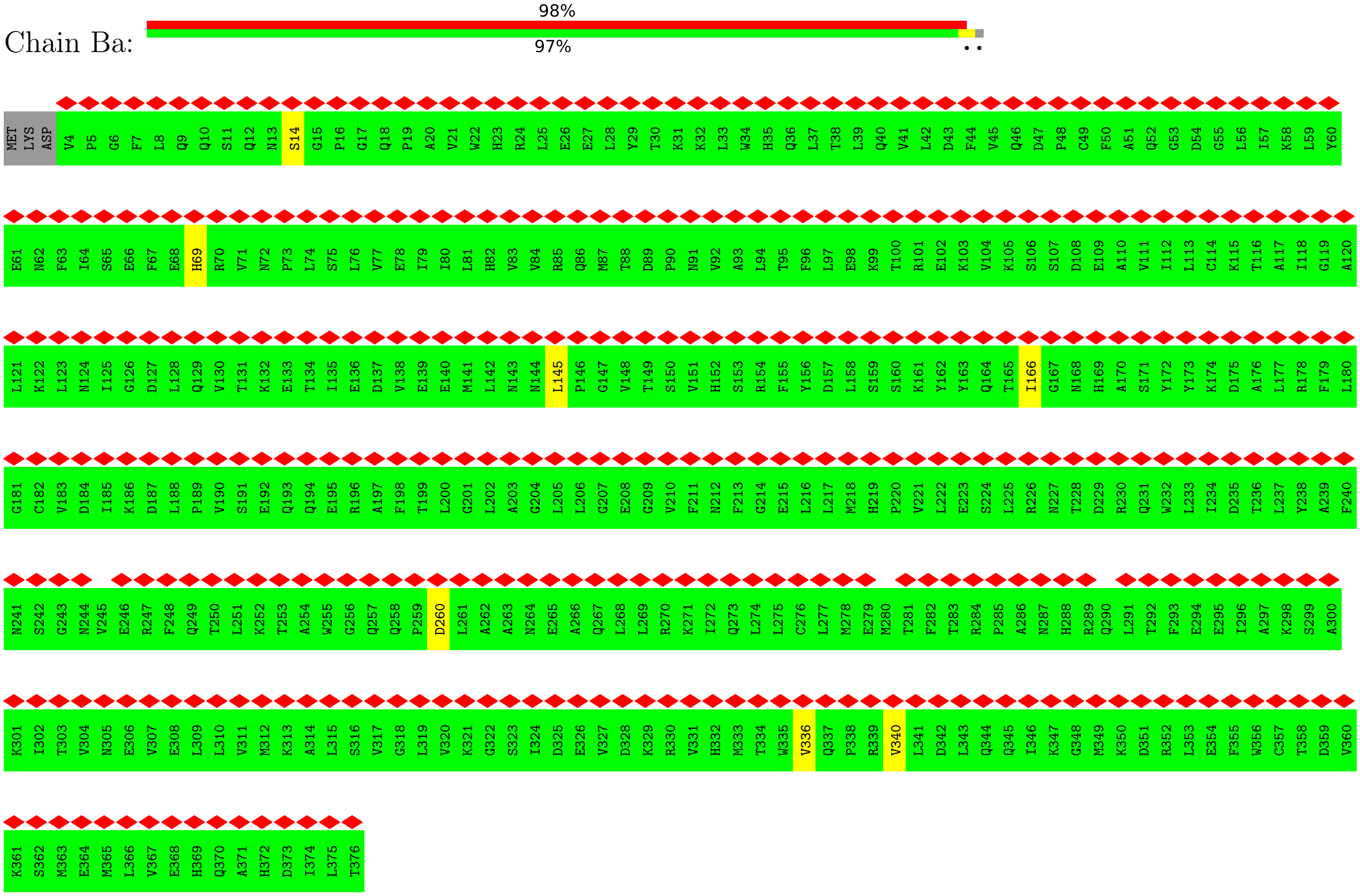




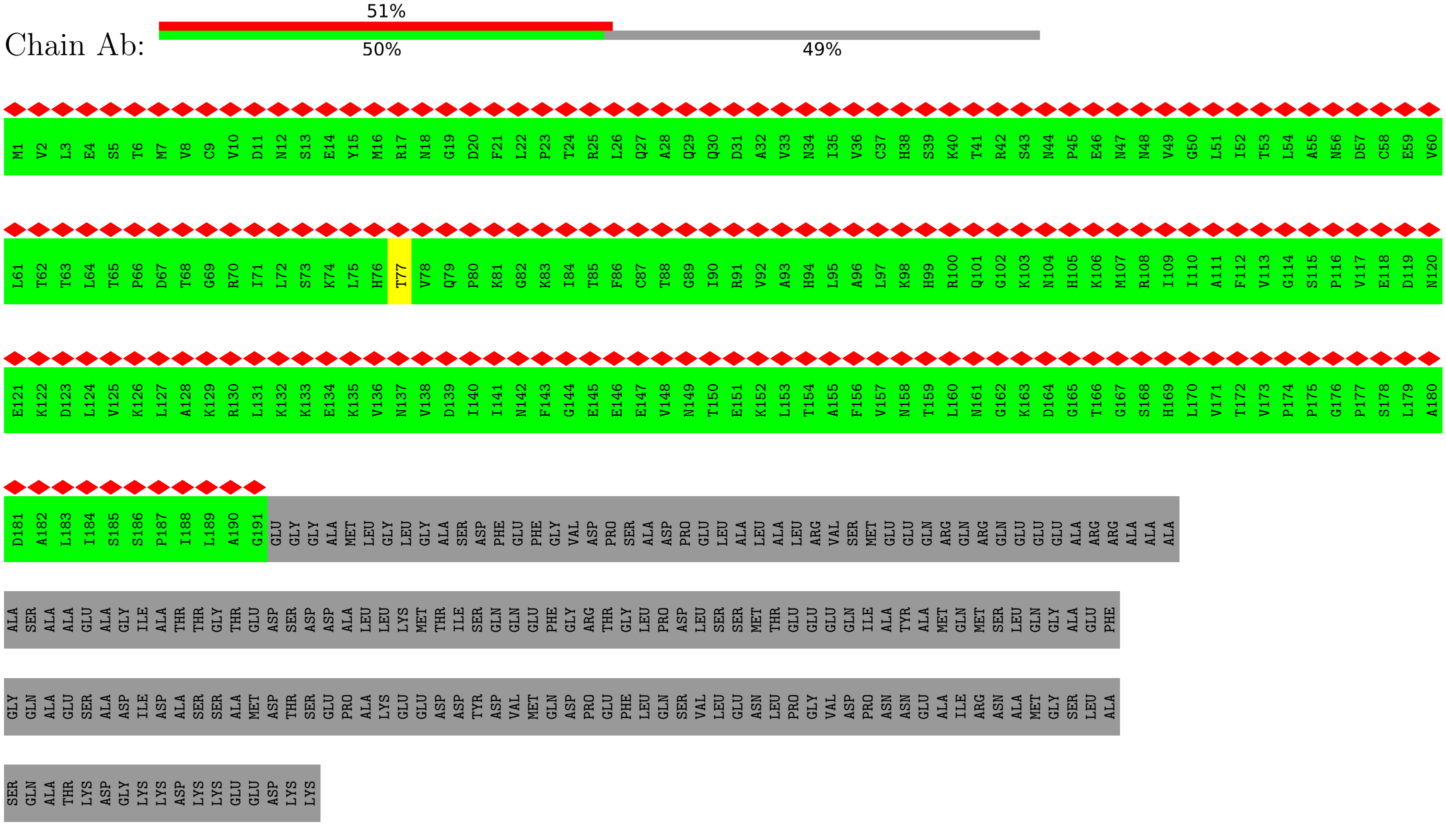


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain Ba:



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



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

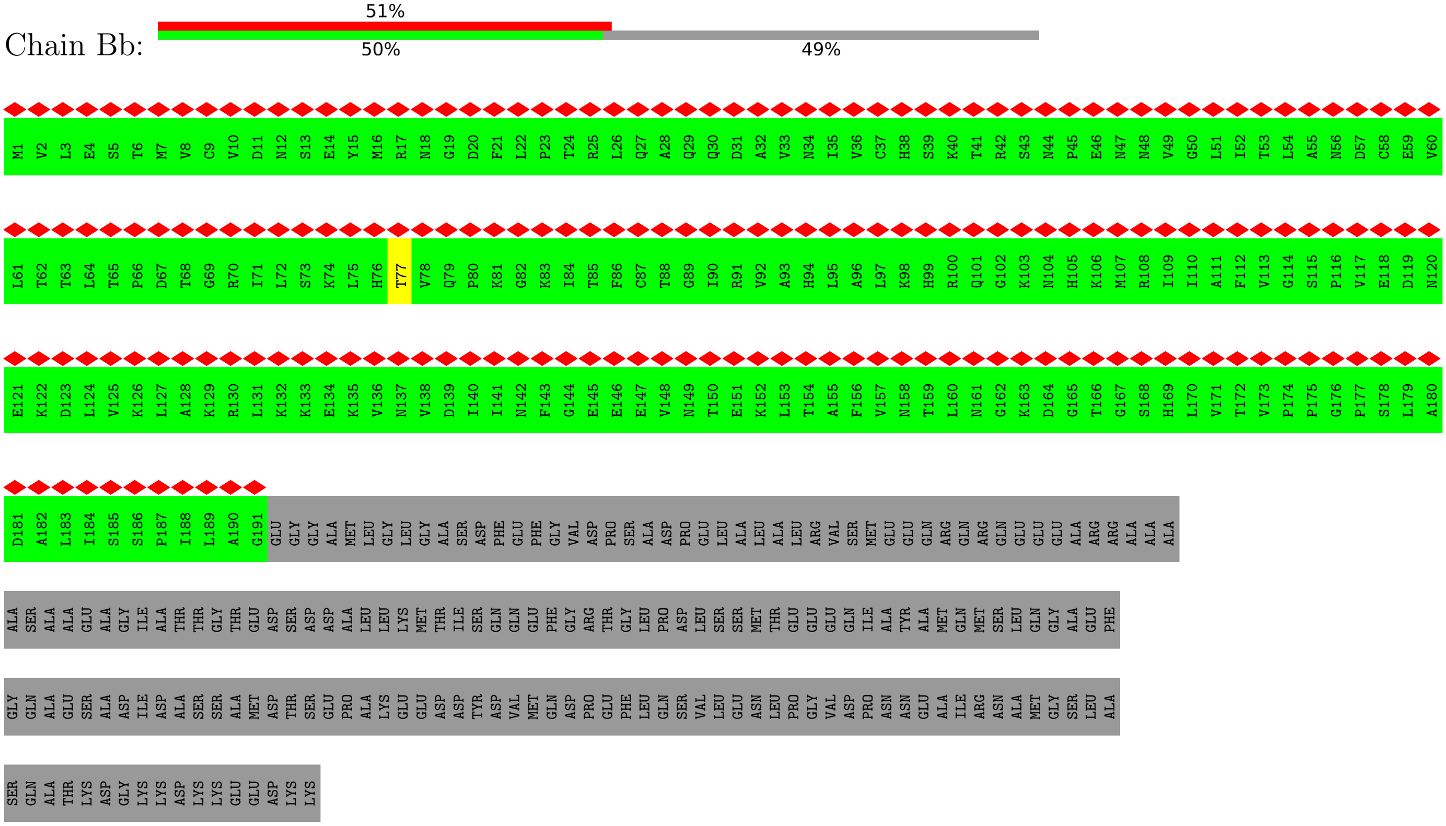
D181 A182 L183 I184 S185 S186 P187 I188 L189 A190 G191 GLU GLY GLY ALA MET LEU GLY LEU GLY ALA SER ASP PHE GLU PHE GLY VAL ASP PRO SER ALA ASP PRO GLU LEU ALA LEU ALA LEU ARG VAL SER MET GLU GLU GLN ARG GLN ARG GLN GLU GLU ALA ARG ARG ALA ALA ALA

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

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

SER GLN ALA THR LYS ASP GLY LYS LYS ASP LYS LYS GLU GLU ASP LYS LYS

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



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 GLU GLY GLY ALA MET LEU GLY LEU GLY ALA SER ASP PHE GLU PHE GLY VAL ASP PRO SER ALA ASP PRO GLU LEU ALA LEU ALA LEU ARG VAL SER MET GLU GLU GLN ARG GLN ARG GLN GLU GLU ALA ARG ARG ALA ALA ALA

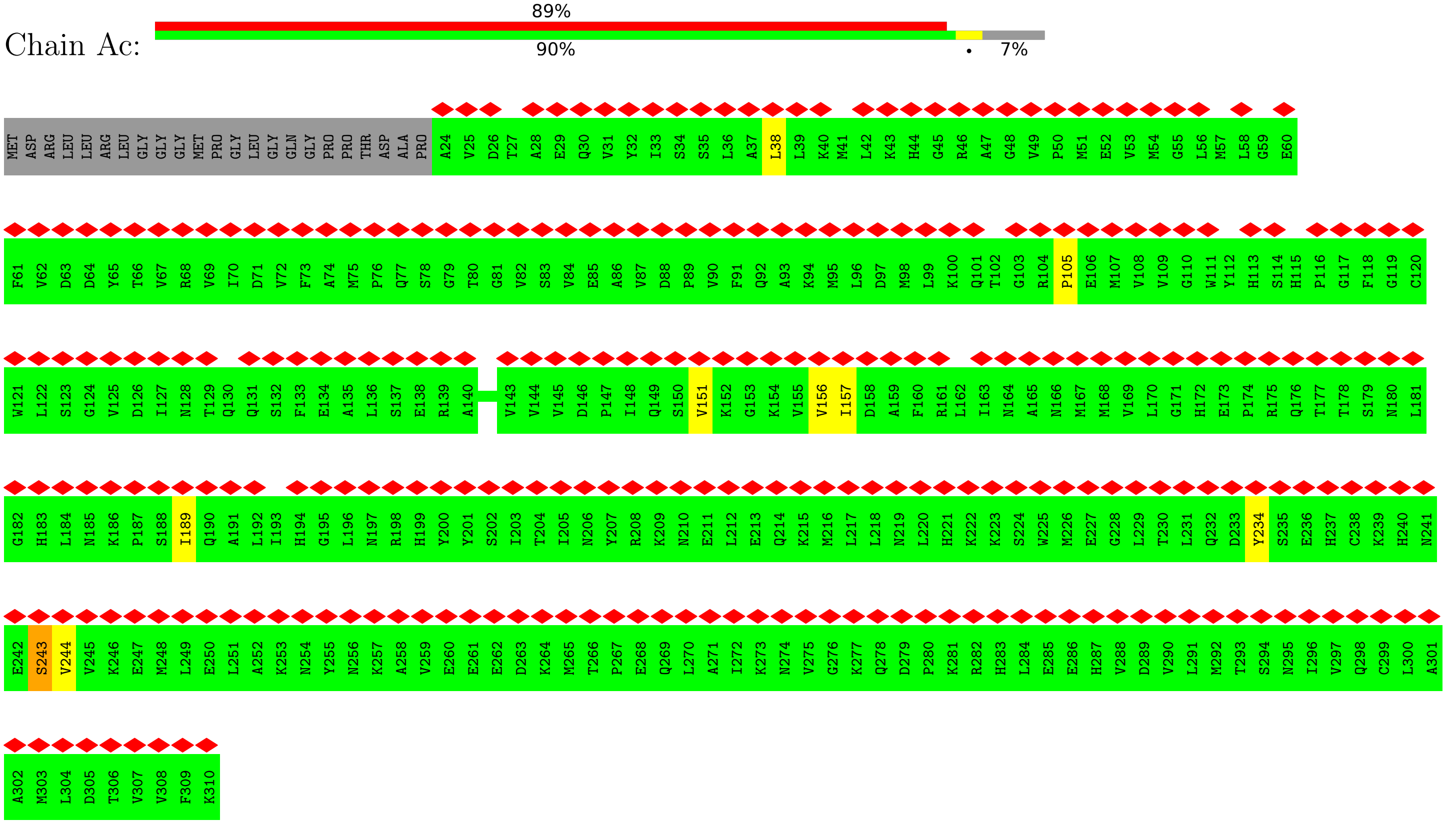
ALA SER ALA ALA GLU ALA GLY ILE ALA THR THR GLY THR GLU ASP SER ASP ASP ALA LEU LEU LYS MET THR ILE SER GLN GLN GLU PHE GLY ARG THR GLY LEU PRO ASP LEU SER SER MET THR GLU GLU GLU GLN ILE ALA TYR ALA MET GLN MET SER LEU GLN GLY ALA GLU PHE

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

SER GLN ALA THR LYS ASP GLY LYS LYS ASP LYS LYS GLU GLU ASP LYS LYS

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

Chain Ac:



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W121 L122 S123 G124 V125 D126 I127 N128 T129 Q130 Q131 S132 F133 E134 A135 L136 S137 E138 R139 A140 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 T178 S179 N180 L181

G182 H183 L184 N185 K186 P187 S188 I189 Q190 A191 L192 I193 H194 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 S235 E236 H237 C238 K239 H240 N241

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

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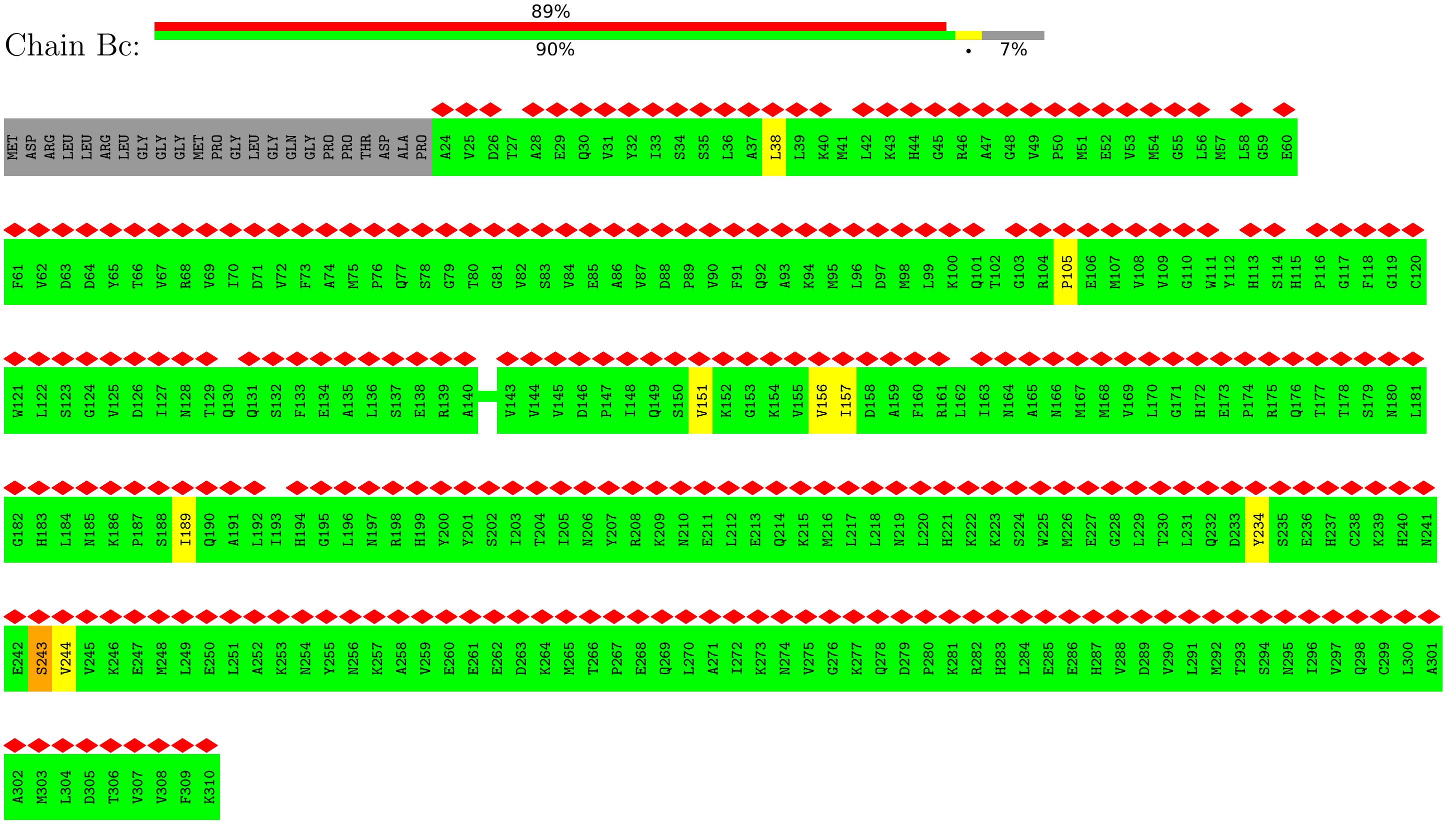

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G182 H183 L184 N185 K186 P187 S188 I189 Q190 A191 L192 I193 H194 G195 L196 N197 R198 H199 Y200 Y201 S202 I203 T204 I205 N206 Y207 R208 K209 N210 E211 L212 E213 Q214 K215 M216 L217 L218 N219 L220 H221 K222 K223 S224 W225 M226 E227 G228 L229 T230 L231 Q232 D233 Y234 S235 E236 H237 C238 K239 H240 N241

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

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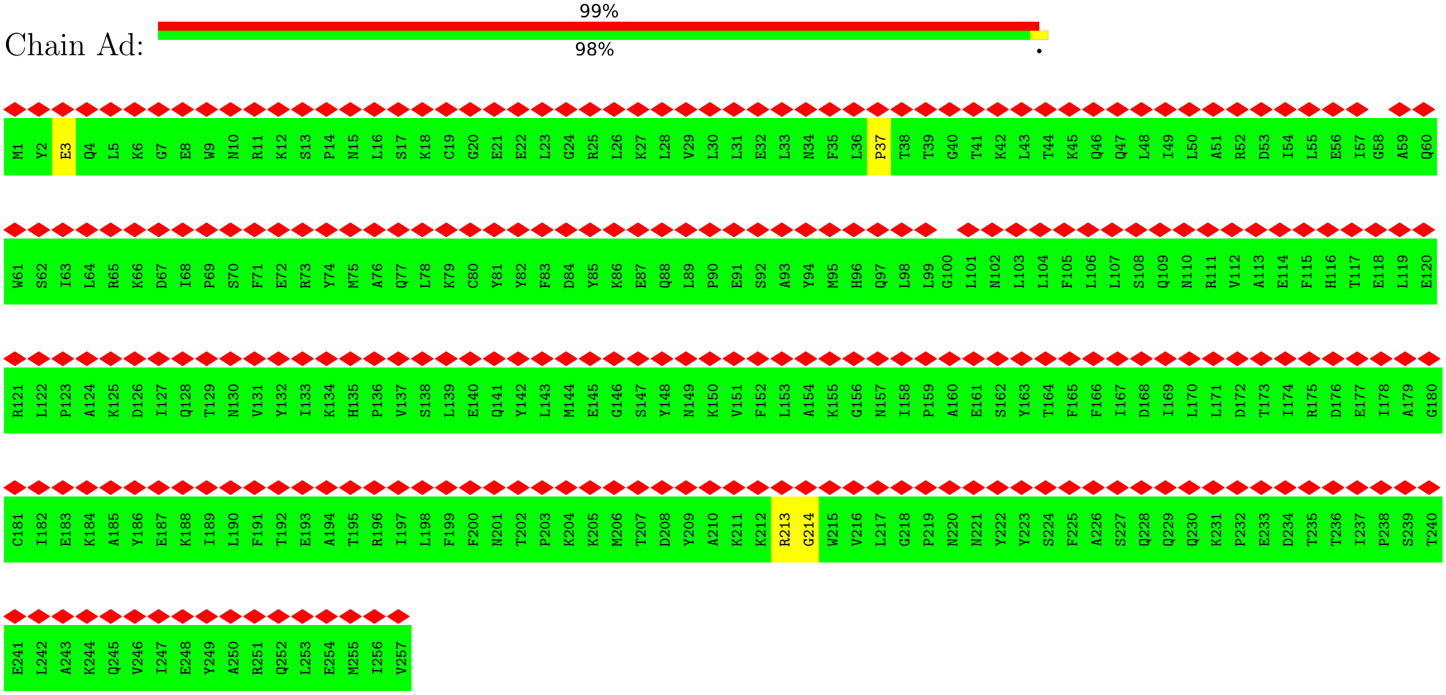

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- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

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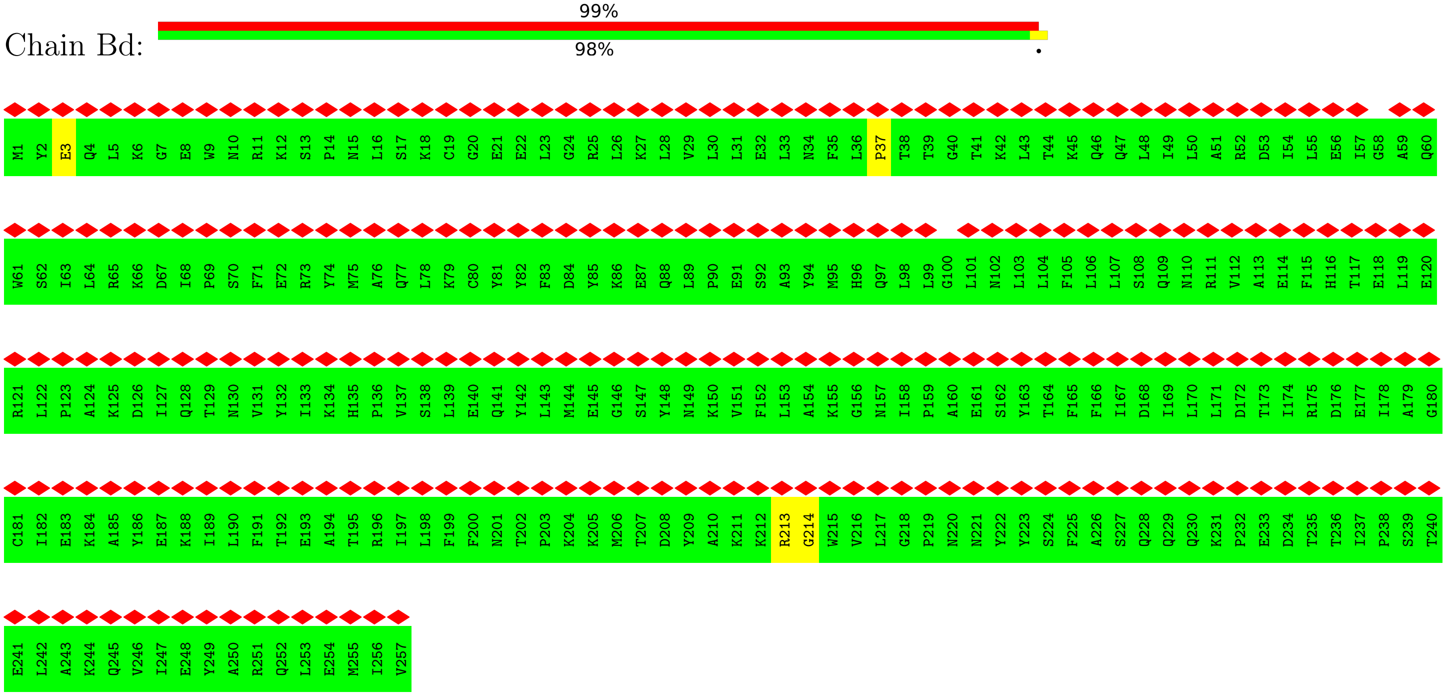

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W61 S62 I63 L64 R65 K66 D67 I68 P69 S70 F71 E72 R73 Y74 M75 A76 Q77 L78 K79 C80 Y81 Y82 F83 D84 Y85 K86 E87 Q88 L89 P90 E91 S92 A93 Y94 M95 H96 Q97 L98 L99 G100 L101 N102 L103 L104 F105 L106 L107 S108 Q109 N110 R111 V112 A113 E114 F115 H116 T117 E118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

C181 I182 E183 K184 A185 Y186 E187 K188 I189 L190 F191 T192 E193 A194 T195 R196 I197 L198 F199 F200 N201 T202 P203 K204 K205 M206 T207 D208 Y209 A210 K211 K212 R213 G214 W215 V216 L217 G218 P219 N220 N221 Y222 Y223 S224 F225 A226 S227 Q228 Q229 Q230 K231 P232 E233 D234 T235 T236 I237 P238 S239 T240

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- Molecule 11: 26S proteasome complex subunit DSS1

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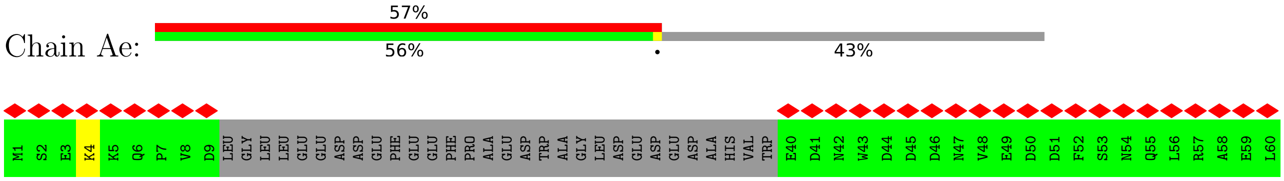

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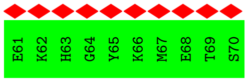
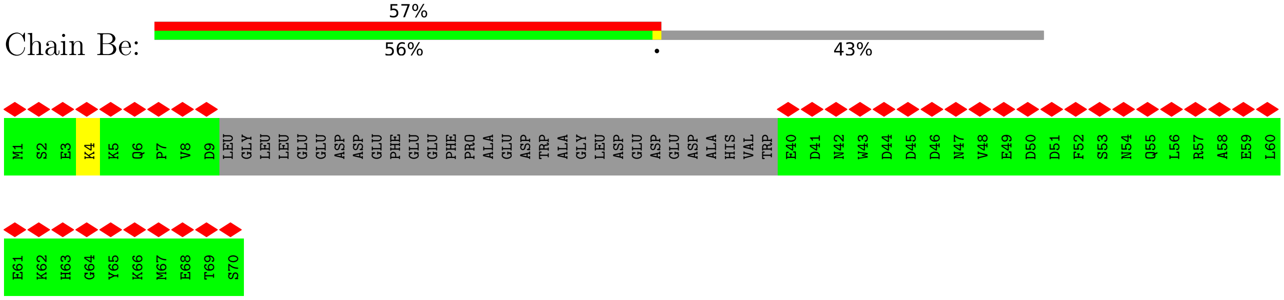
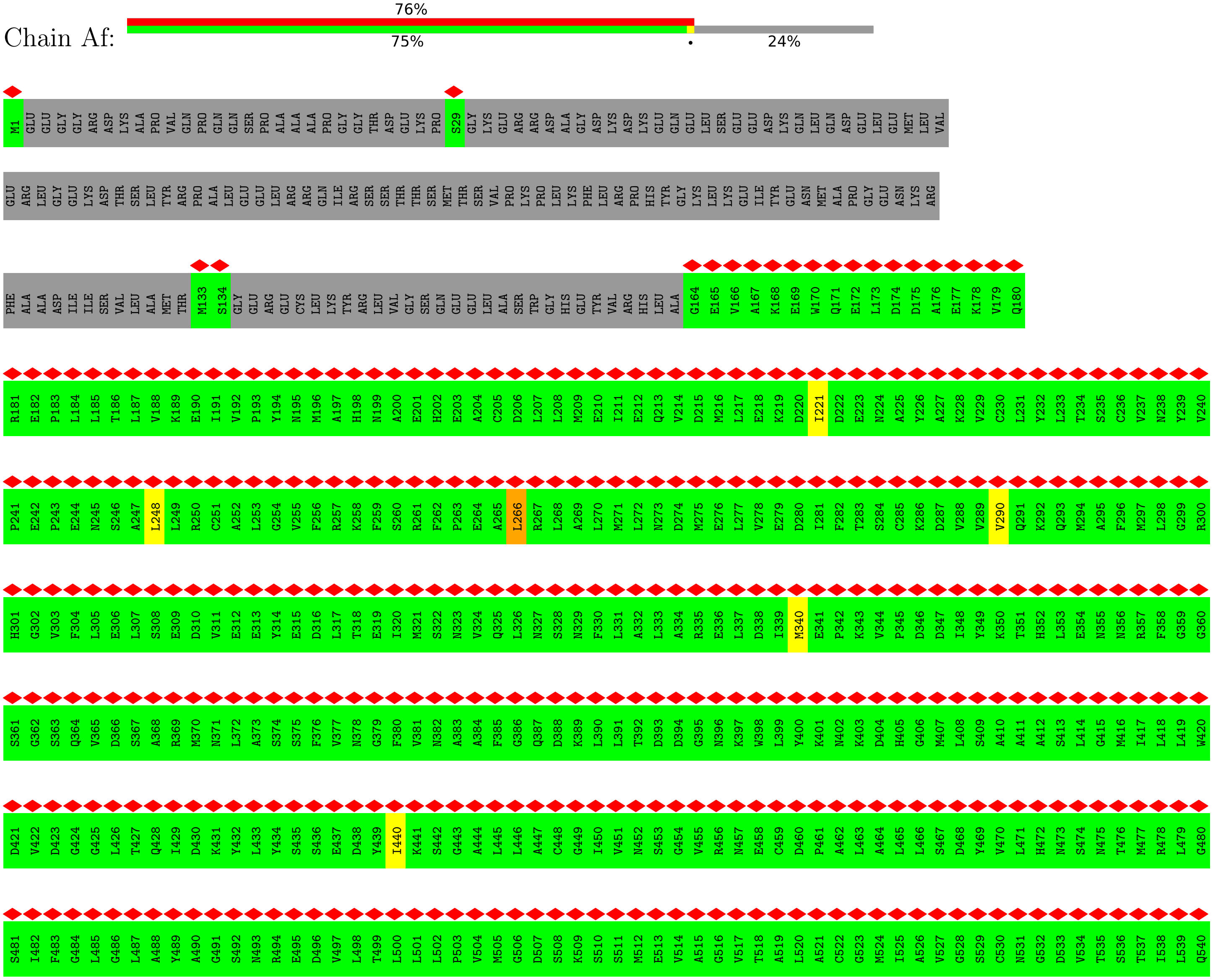
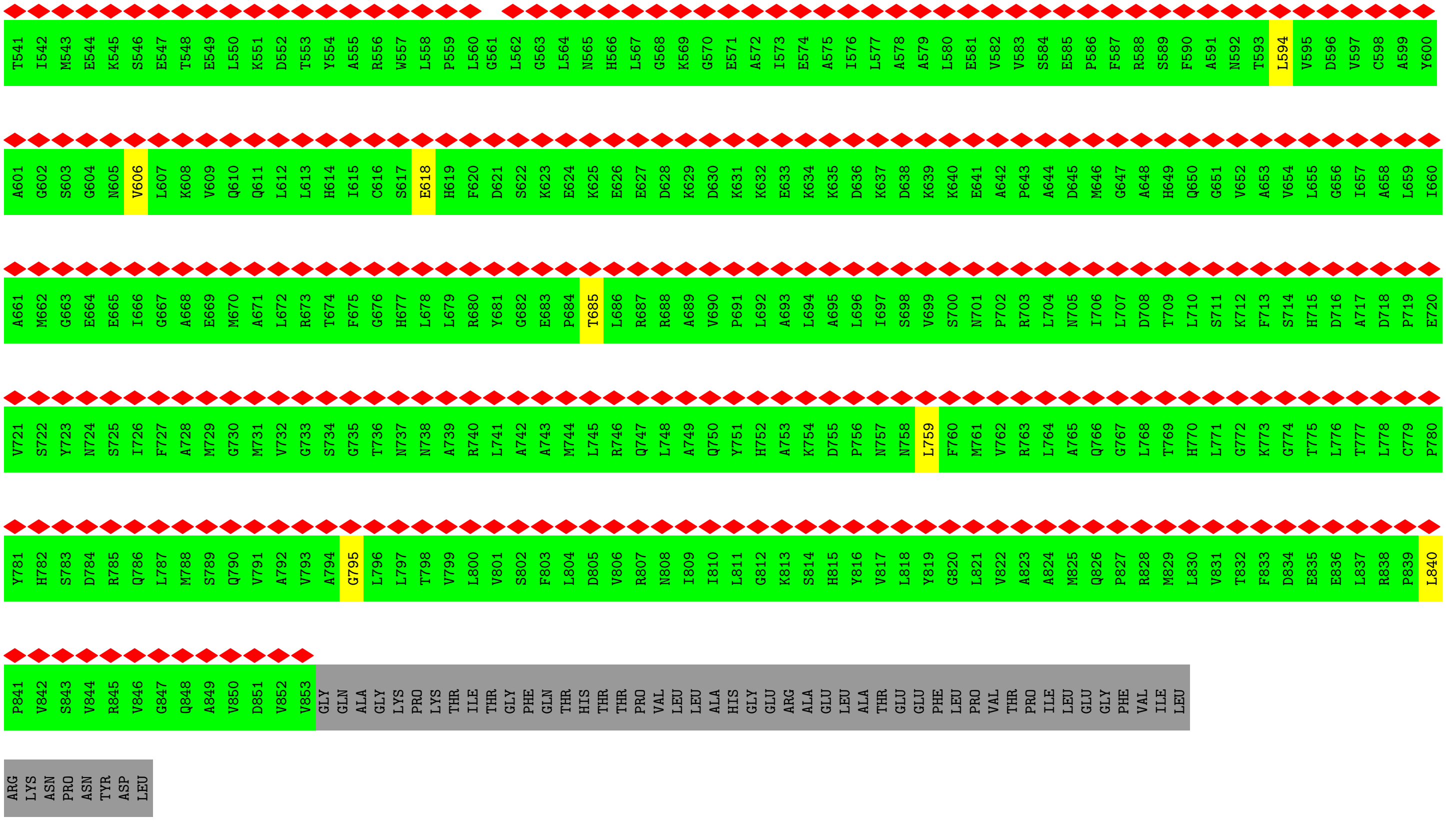


- Molecule 11: 26S proteasome complex subunit DSS1



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





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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

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V721 S722 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 H752 A753 K754 D755 P756 N757 N758 L759 F760 M761 V762 R763 L764 A765 Q766 G767 L768 T769 H770 L771 G772 K773 G774 T775 L776 T777 L778 C779 P780

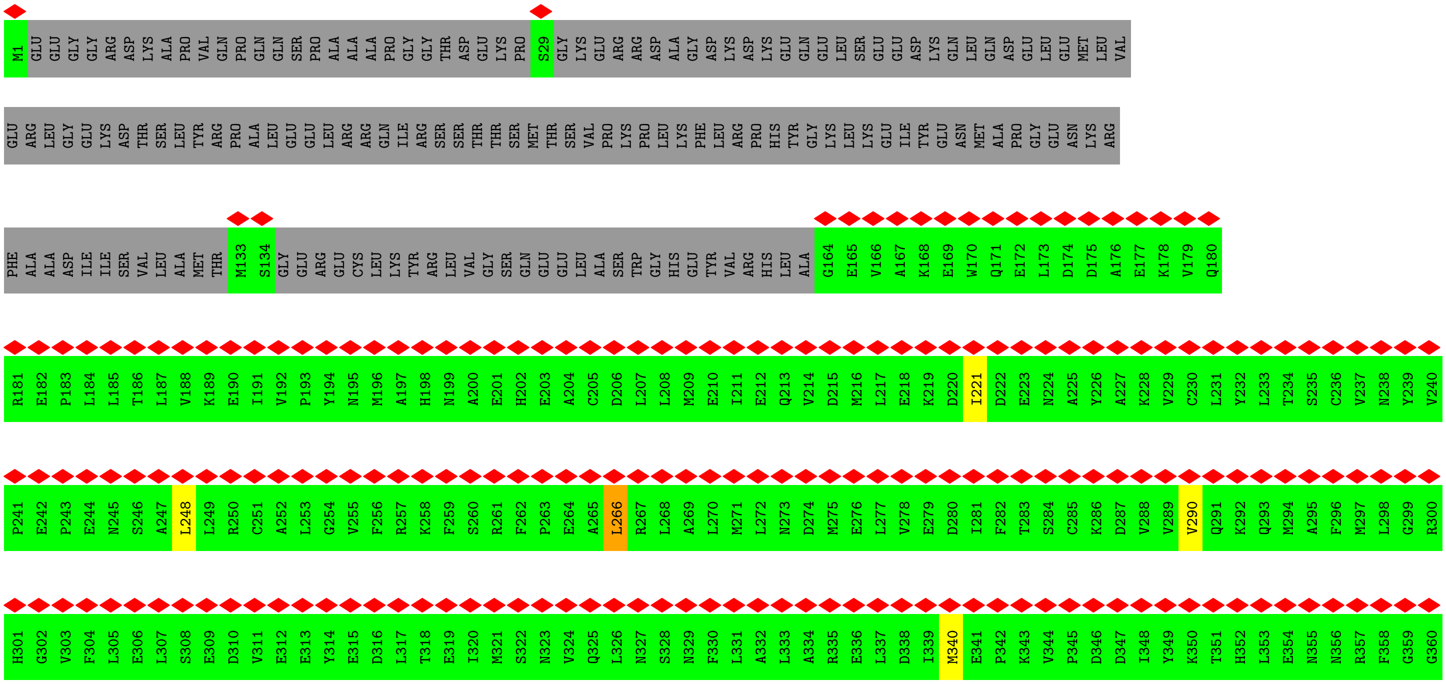
Y781 H782 S783 D784 R785 Q786 L787 M788 S789 Q790 V791 A792 V793 A794 G795 L796 L797 T798 V799 L800 V801 S802 F803 L804 D805 V806 R807 N808 I809 I810 L811 G812 K813 S814 H815 Y816 V817 L818 Y819 G820 L821 V822 A823 A824 M825 Q826 P827 R828 M829 L830 V831 T832 F833 D834 E835 E836 L837 R838 P839 L840

P841 V842 S843 V844 R845 V846 G847 Q848 A849 V850 D851 V852 V853 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 GLY PHE VAL ILE LEU

ARG LYS ASN PRO ASN TYR ASP LEU

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

Chain Bf:



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PHE ALA ALA ASP ILE ILE SER VAL LEU ALA MET THR M133 S134 GLY GLU ARG GLU CYS LEU LYS TYR ARG LEU VAL GLY SER GLN GLU GLU LEU ALA SER TRP GLY HIS GLU TYR VAL ARG HIS LEU ALA G164 E165 V166 A167 K168 E169 W170 Q171 E172 L173 D174 D175 A176 E177 K178 V179 Q180

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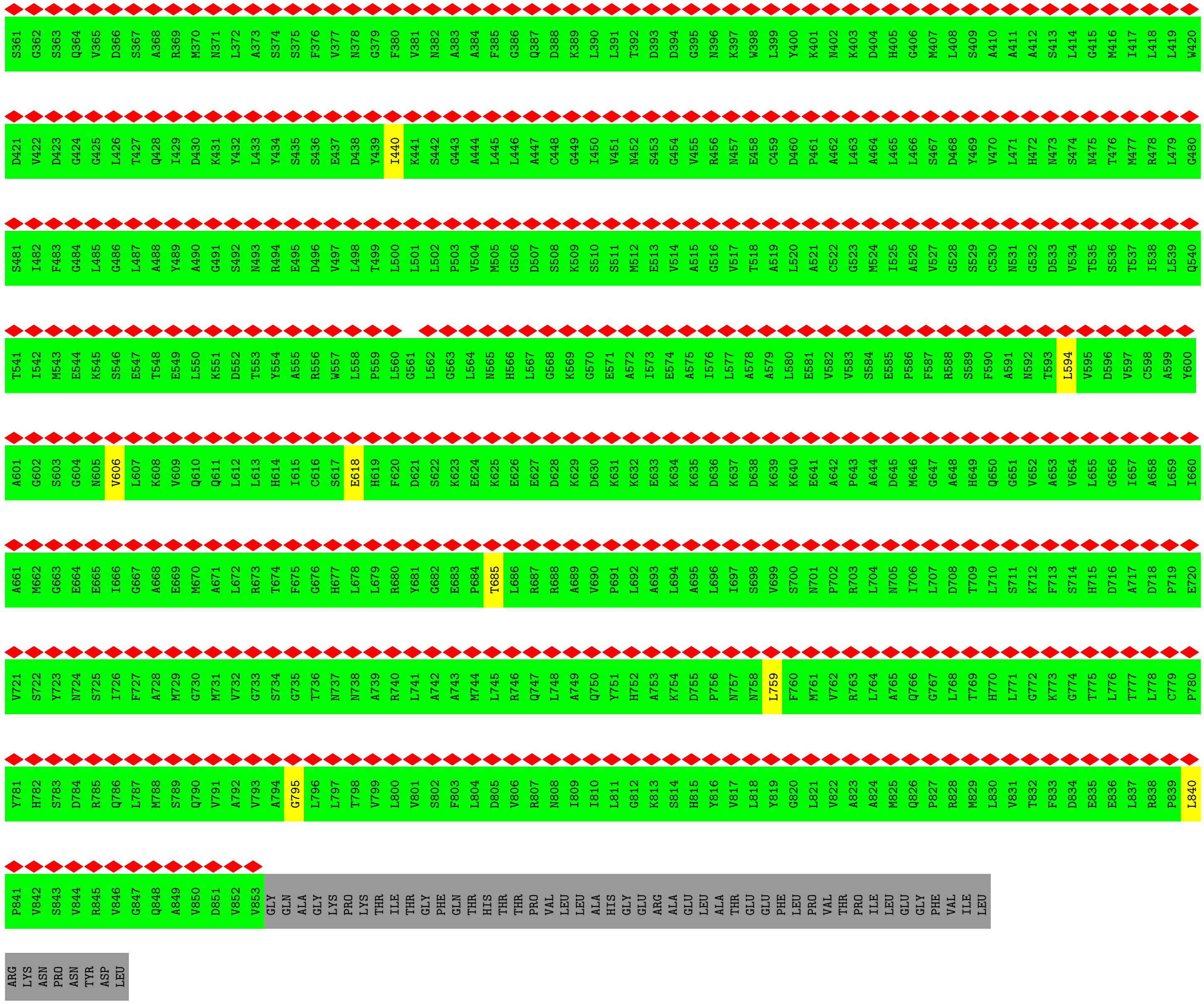
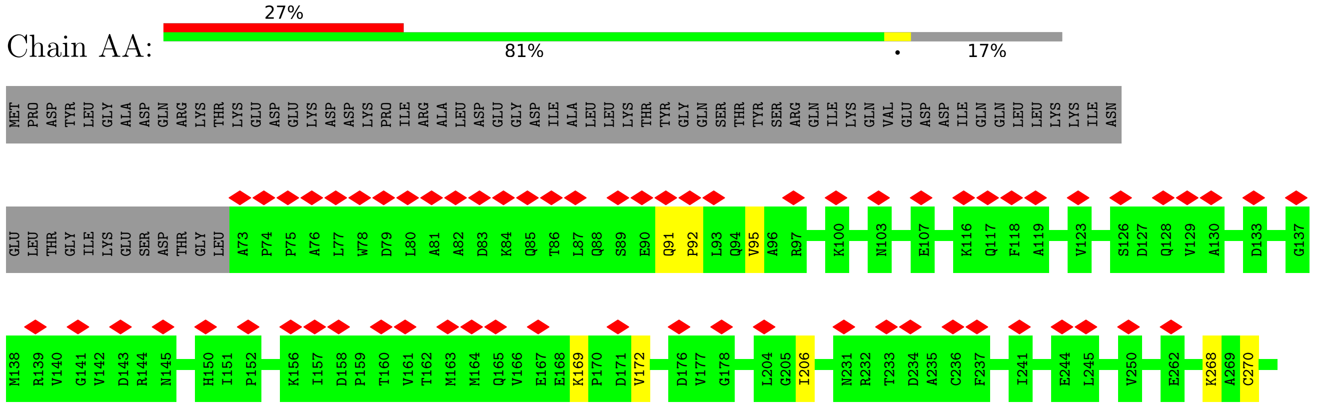
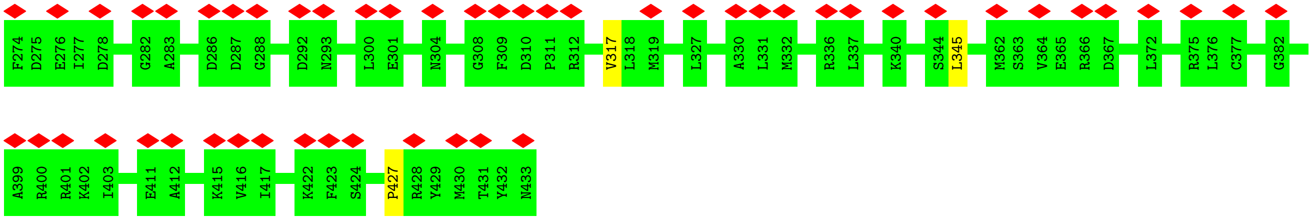
H301 G302 V303 F304 L305 E306 L307 S308 E309 D310 V311 E312 E313 Y314 E315 D316 L317 T318 E319 I320 M321 S322 N323 V324 Q325 L326 N327 S328 N329 F330 L331 A332 L333 A334 R335 E336 L337 D338 I339 M340 E341 P342 K343 V344 P345 D346 D347 I348 Y349 K350 T351 H352 L353 E354 N355 N356 R357 F358 G359 G360



- Molecule 13: 26S protease regulatory subunit 7





- Molecule 13: 26S protease regulatory subunit 7

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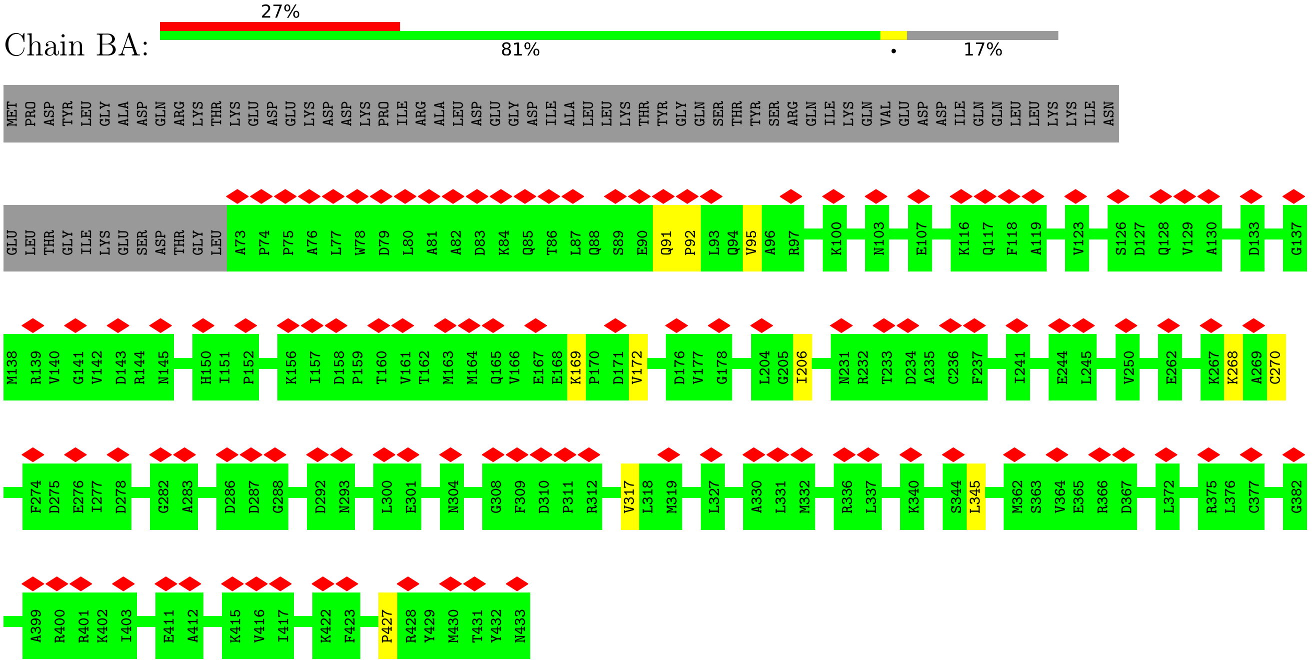

- Molecule 14: 26S protease regulatory subunit 4

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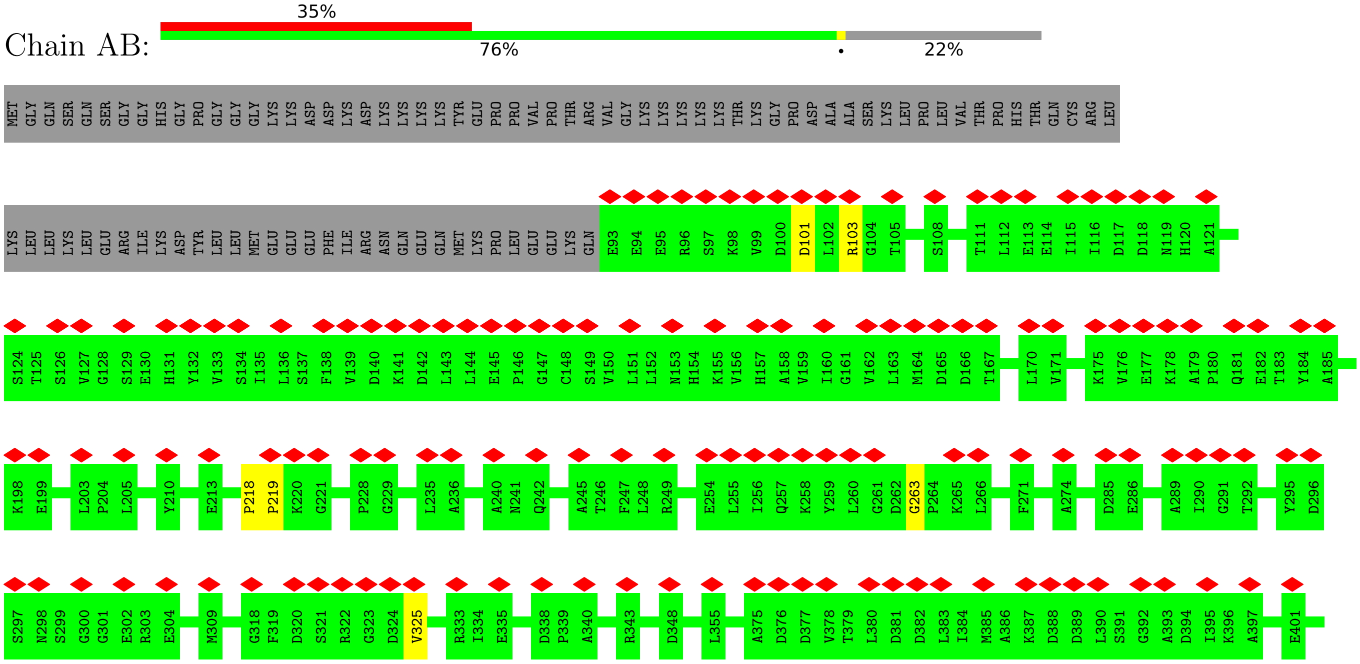

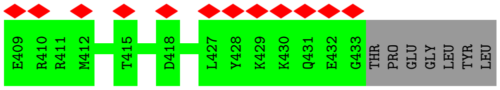

- Molecule 14: 26S protease regulatory subunit 4

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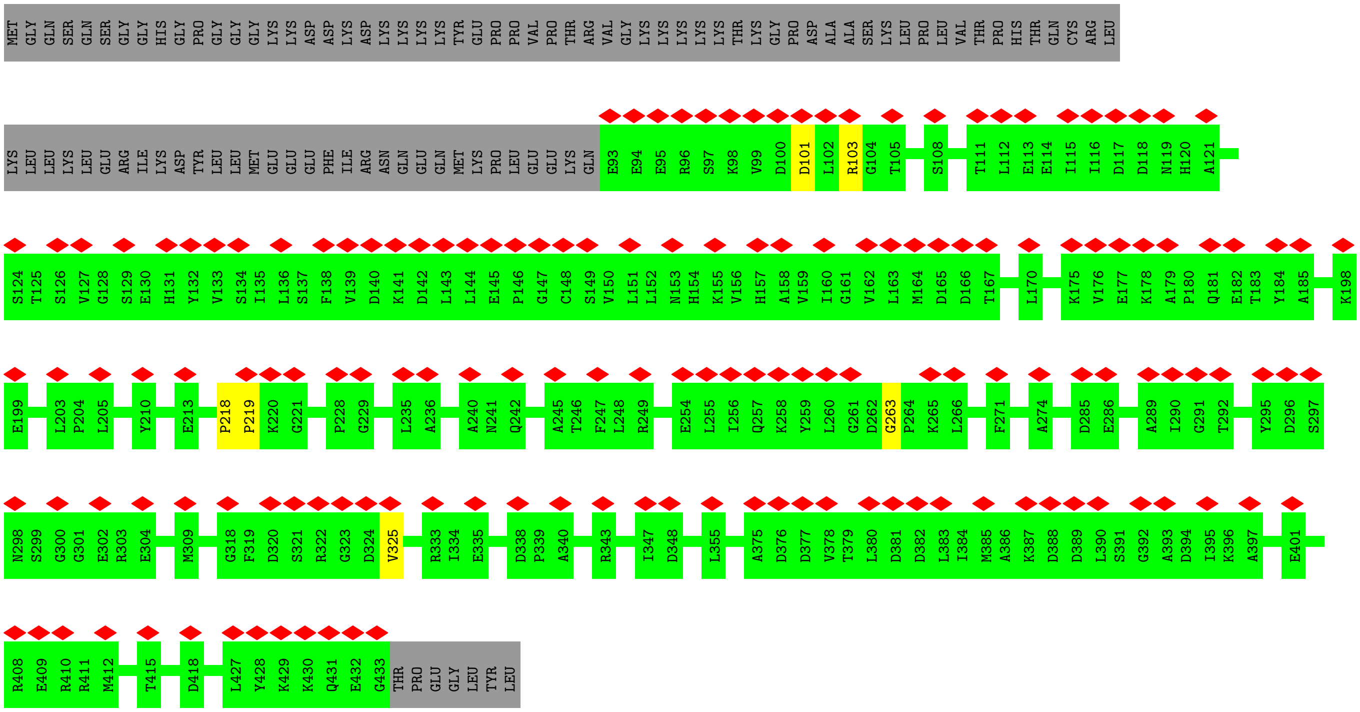
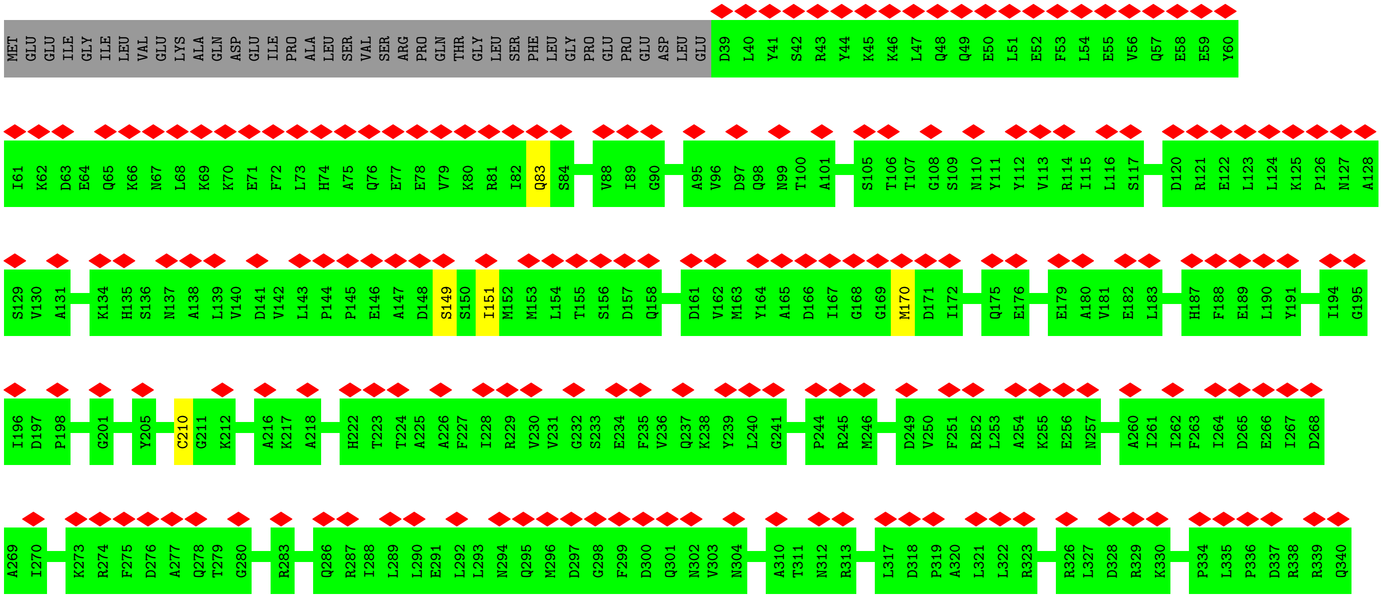
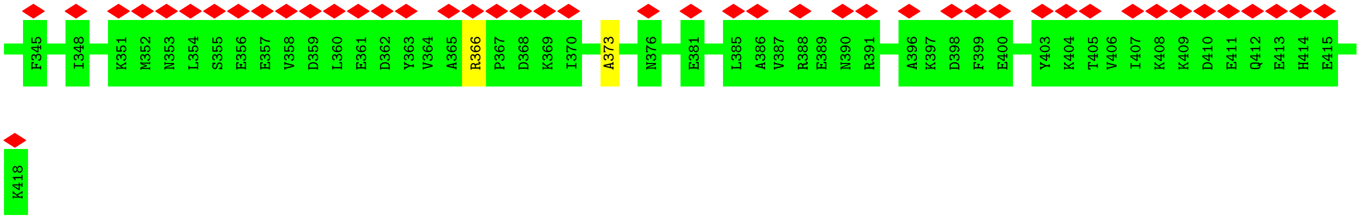


- Molecule 15: 26S protease regulatory subunit 6B

Chain AD:





- Molecule 15: 26S protease regulatory subunit 6B

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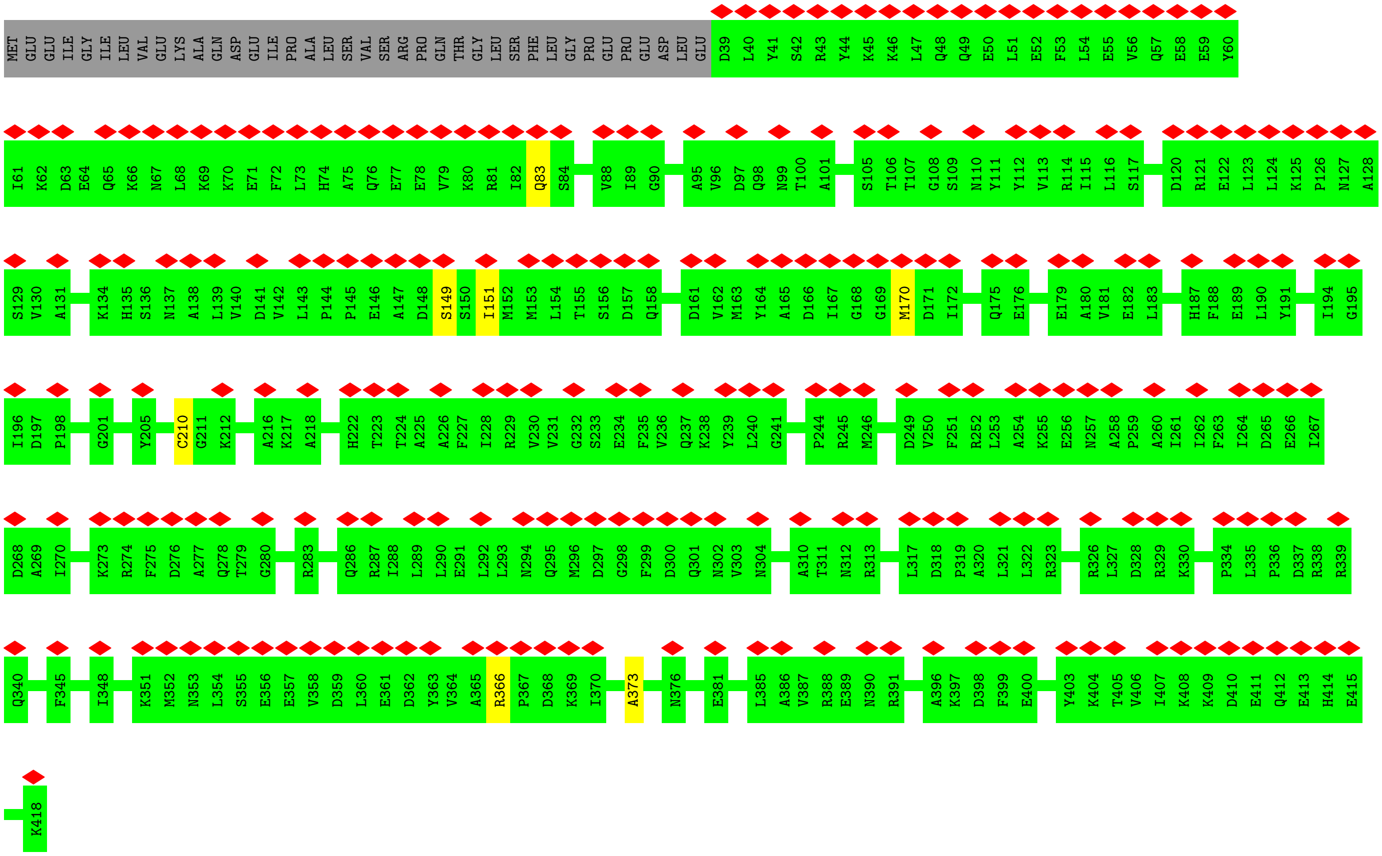

- Molecule 16: 26S protease regulatory subunit 10B

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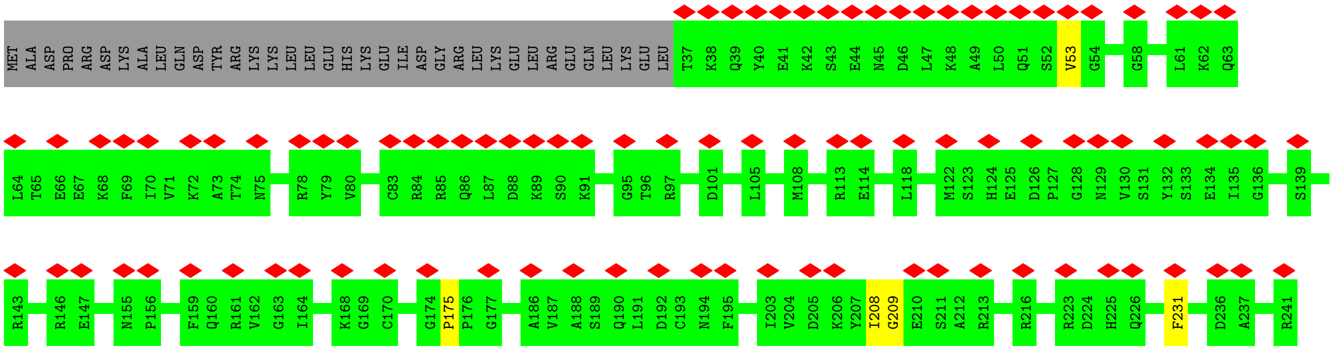
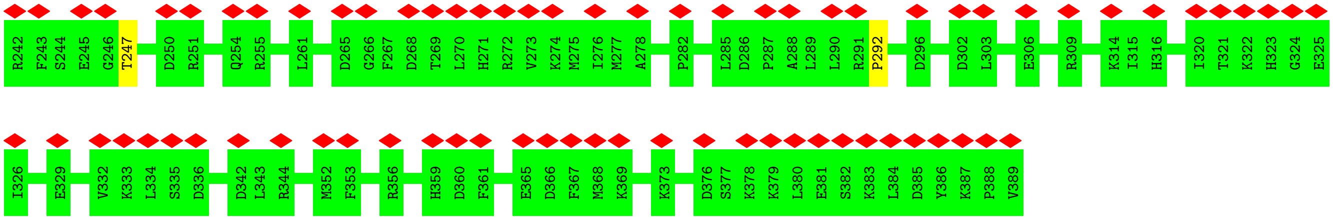
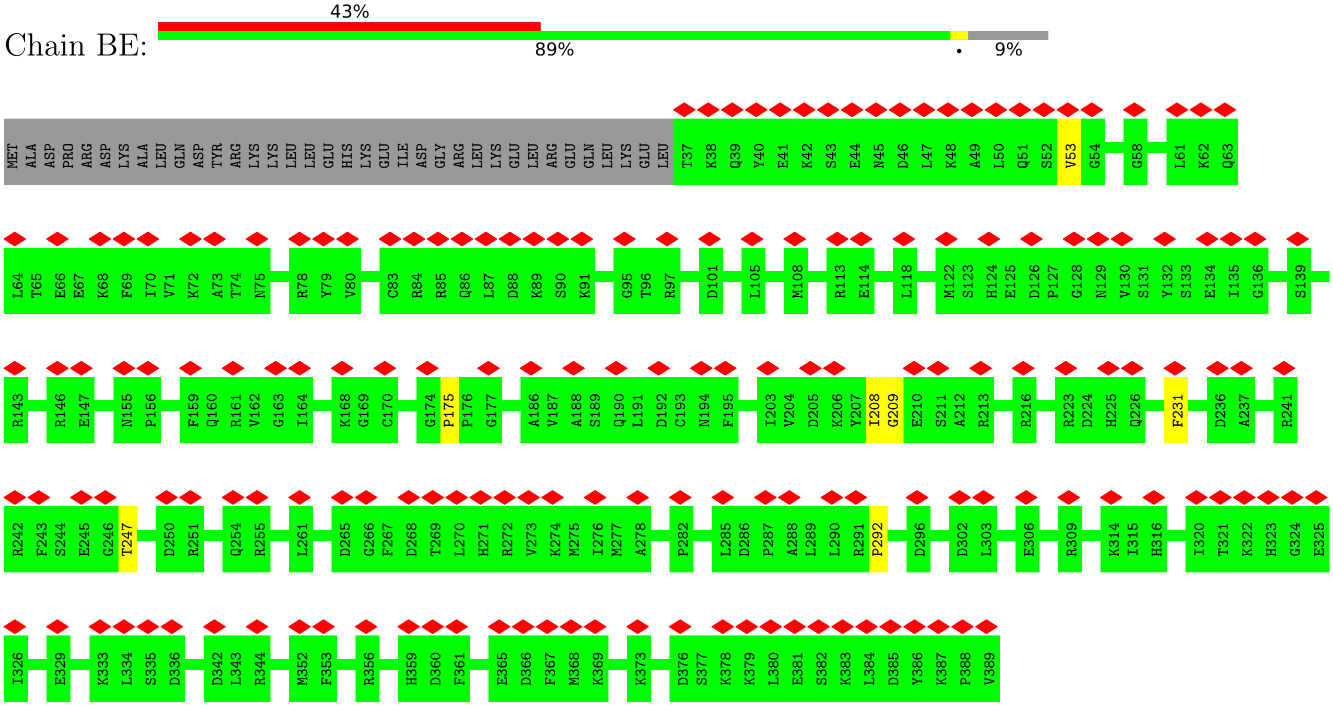
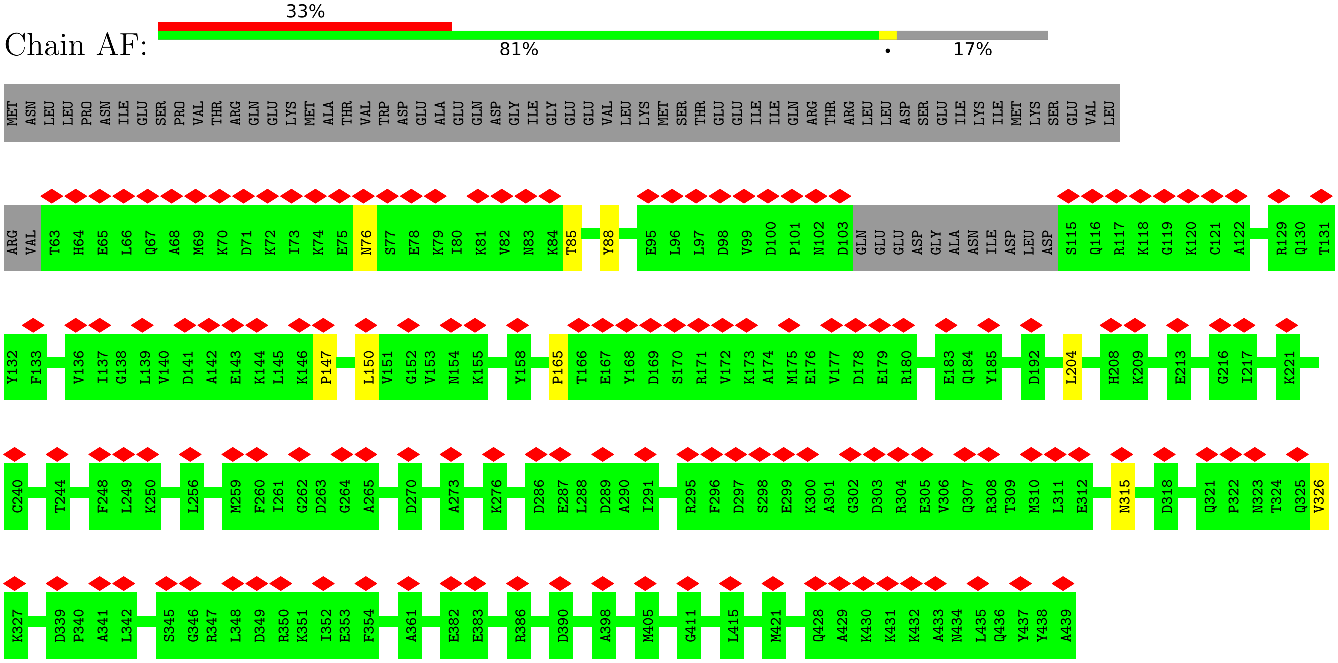




- Molecule 16: 26S protease regulatory subunit 10B



- Molecule 17: 26S protease regulatory subunit 6A



- Molecule 17: 26S protease regulatory subunit 6A

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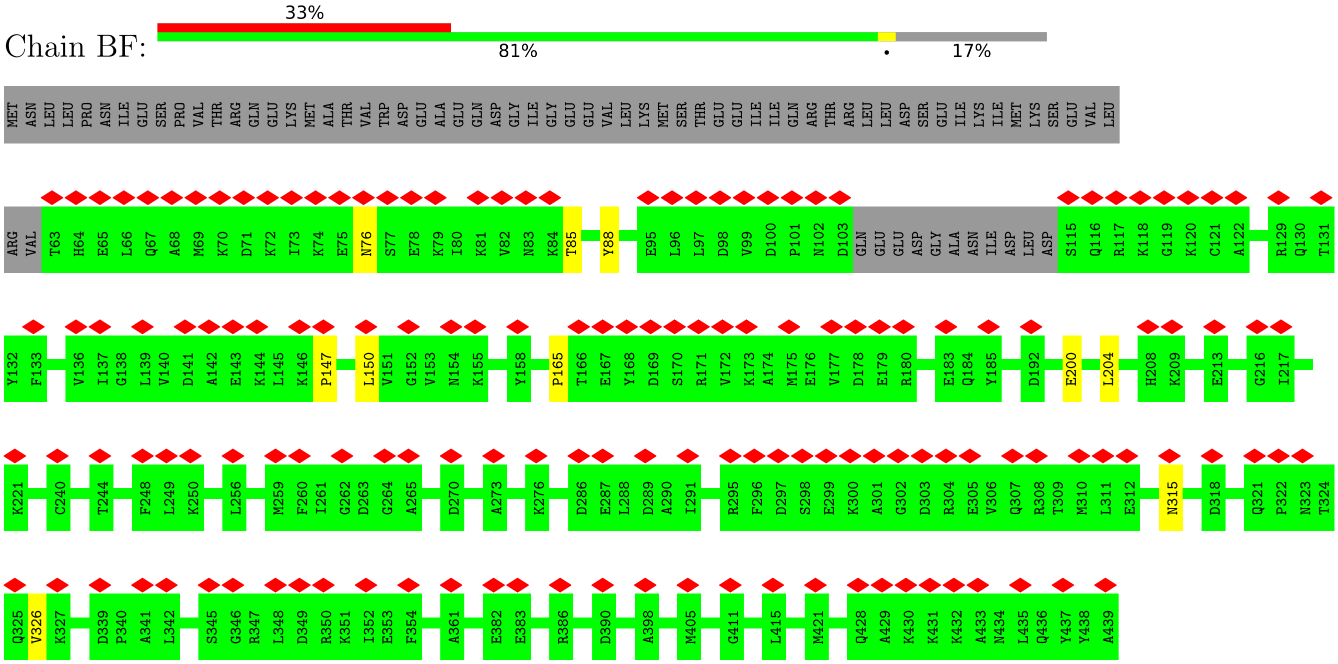
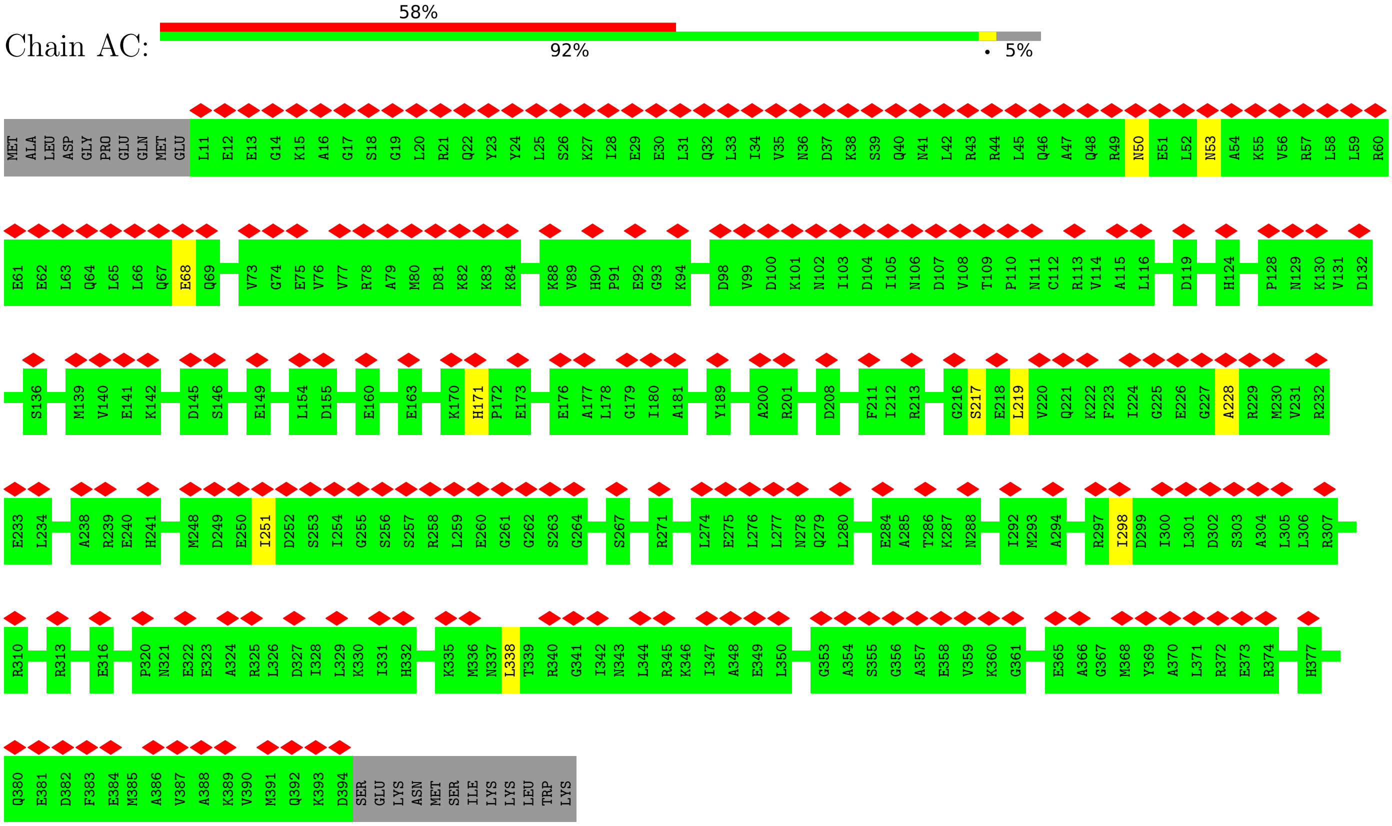


- Molecule 18: 26S protease regulatory subunit 8

Chain AC:



- Molecule 18: 26S protease regulatory subunit 8

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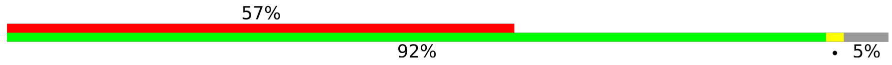
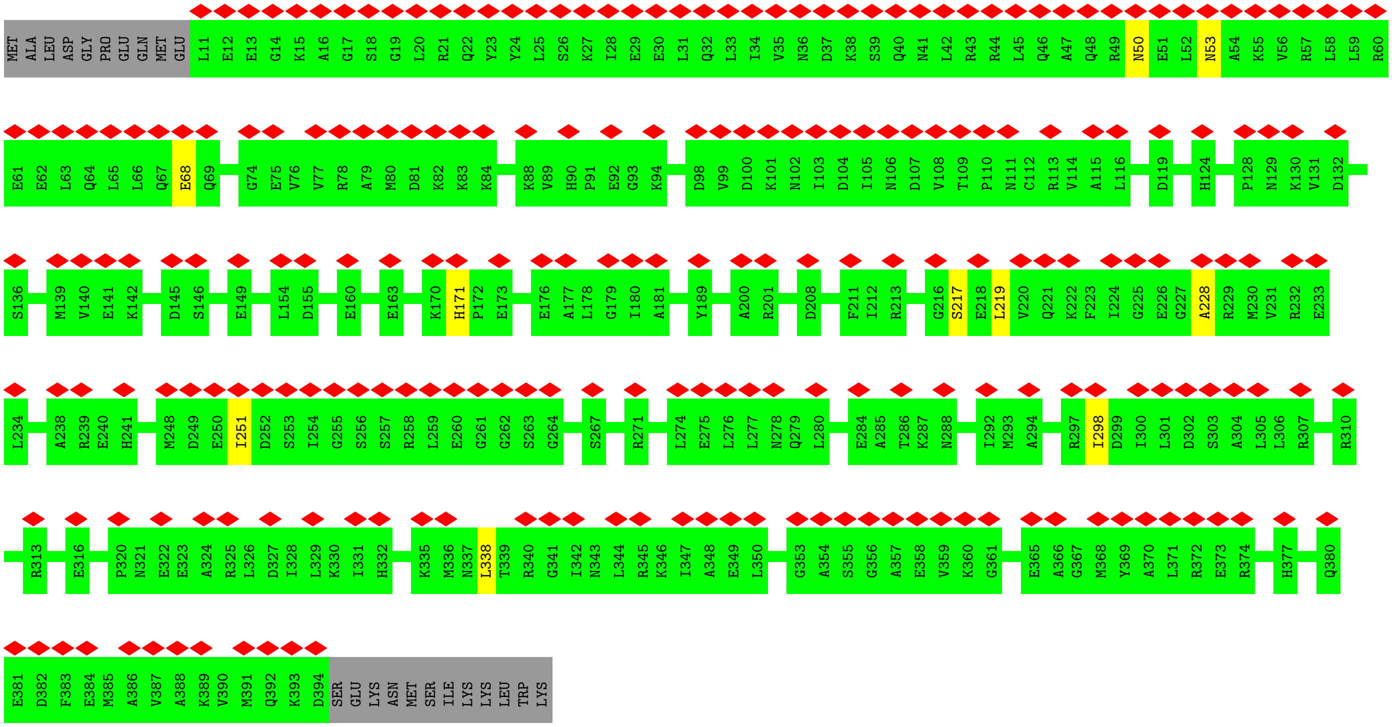
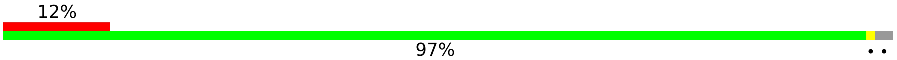
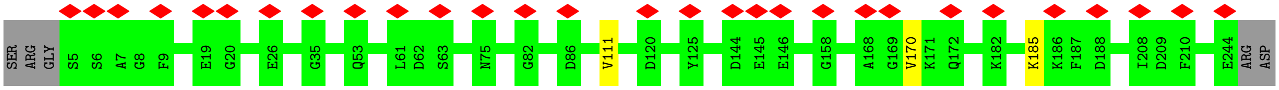




- Molecule 19: Proteasome subunit alpha type-6

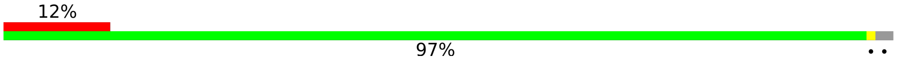
Chain AG:

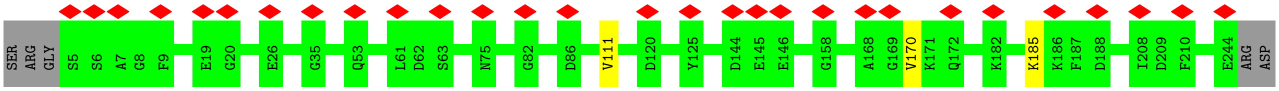




- Molecule 19: Proteasome subunit alpha type-6

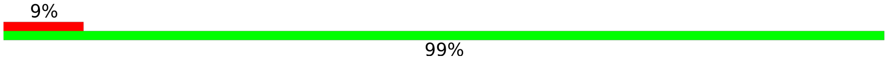
Chain BG:

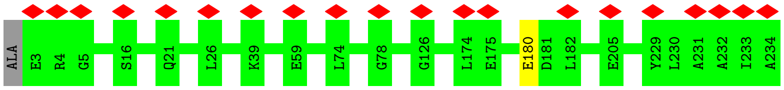




- Molecule 20: Proteasome subunit alpha type-2

Chain AH:





- Molecule 20: Proteasome subunit alpha type-2

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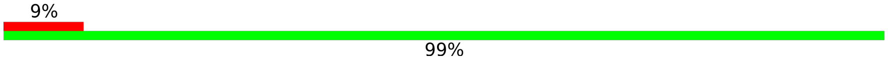
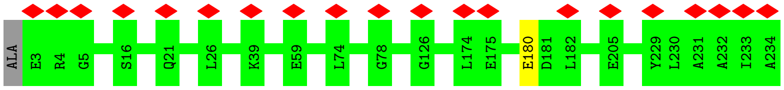
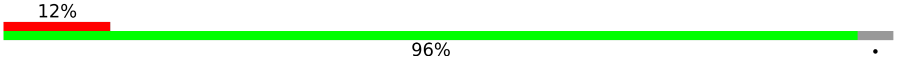
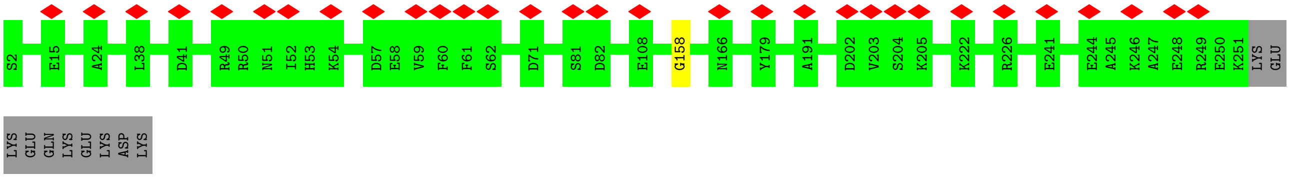




- Molecule 21: Proteasome subunit alpha type-4

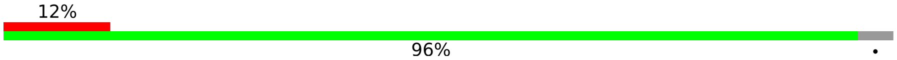
Chain AI:

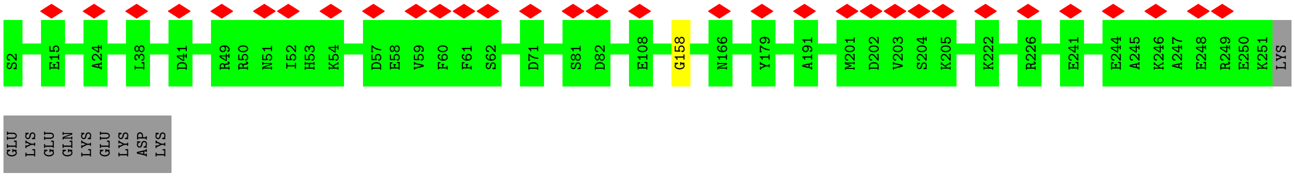




- Molecule 21: Proteasome subunit alpha type-4

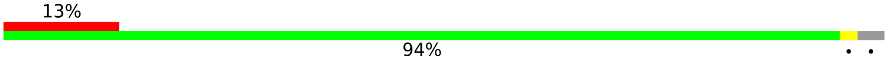
Chain BI:

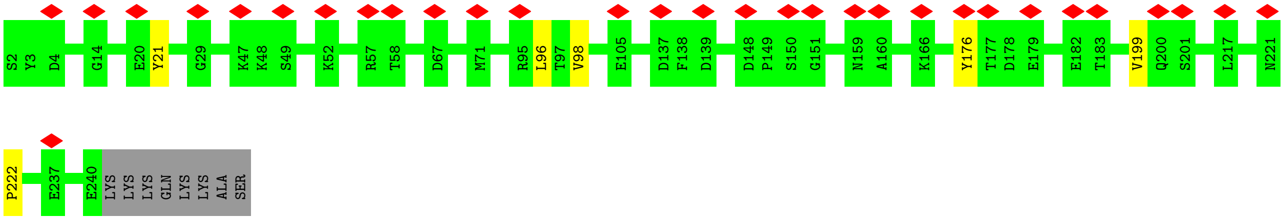




- Molecule 22: Proteasome subunit alpha type-7

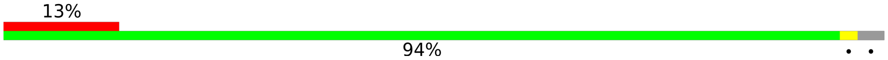
Chain AJ:

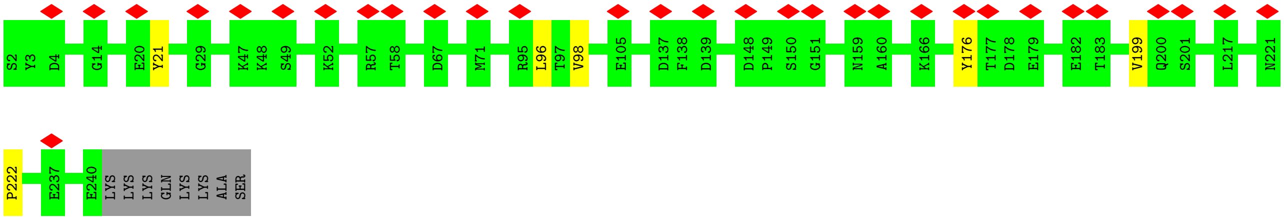




- Molecule 22: Proteasome subunit alpha type-7

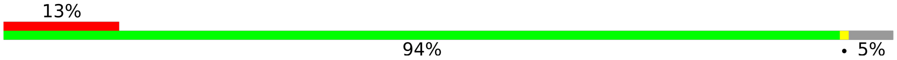
Chain BJ:

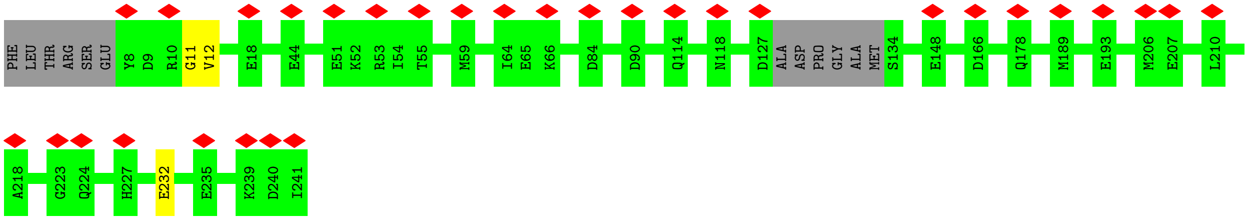




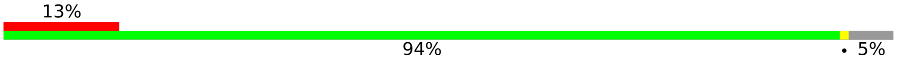
- Molecule 23: Proteasome subunit alpha type-5

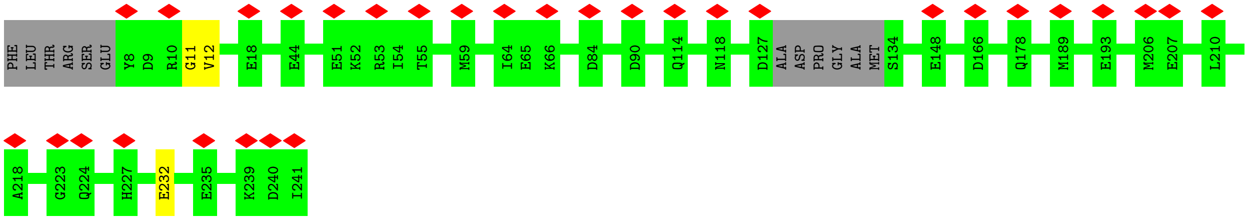
Chain AK:





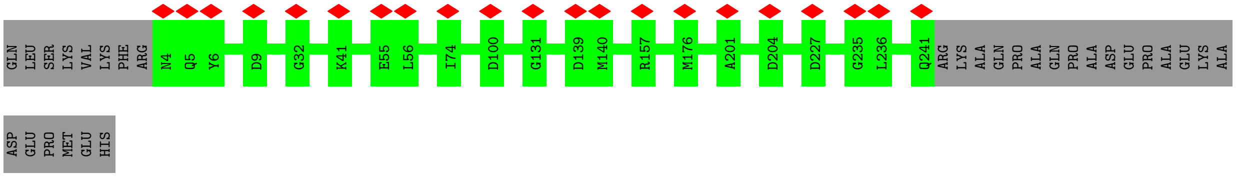
- Molecule 23: Proteasome subunit alpha type-5

Chain BK:




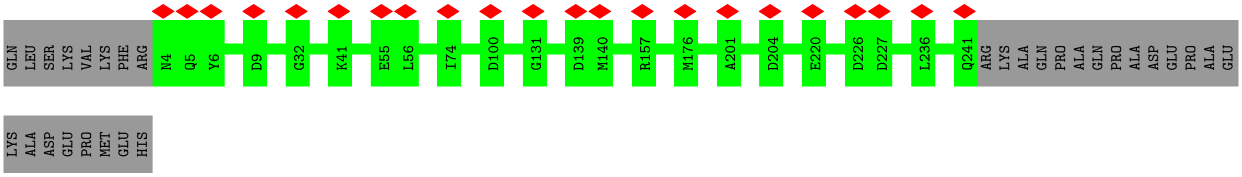
- Molecule 24: Proteasome subunit alpha type-1

Chain AL:

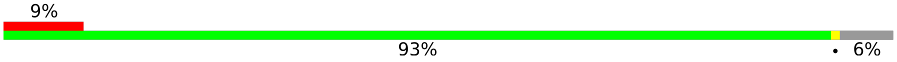



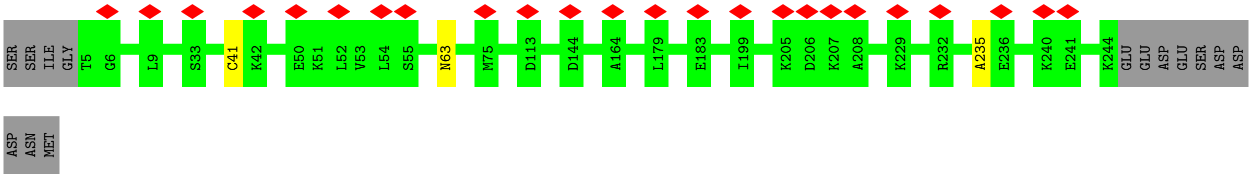
- Molecule 24: Proteasome subunit alpha type-1

Chain BL:

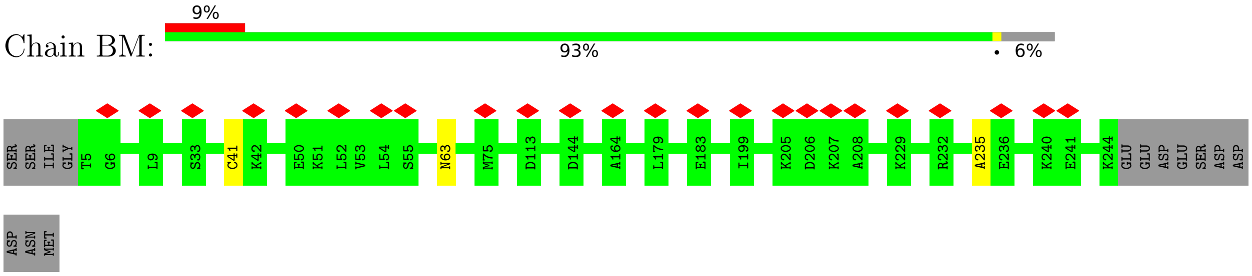



- Molecule 25: Proteasome subunit alpha type-3

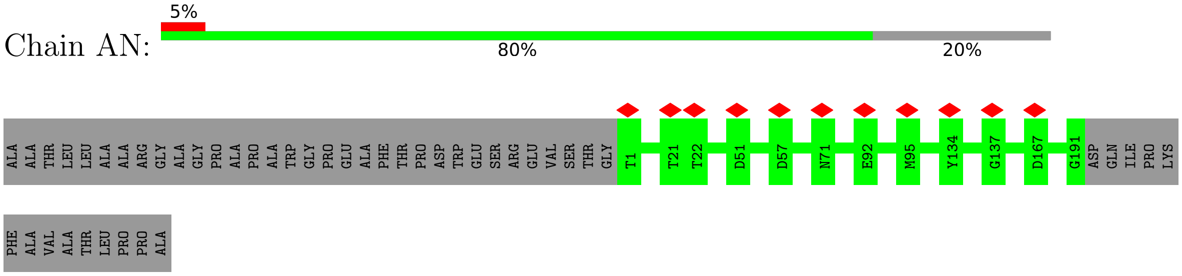
Chain AM:




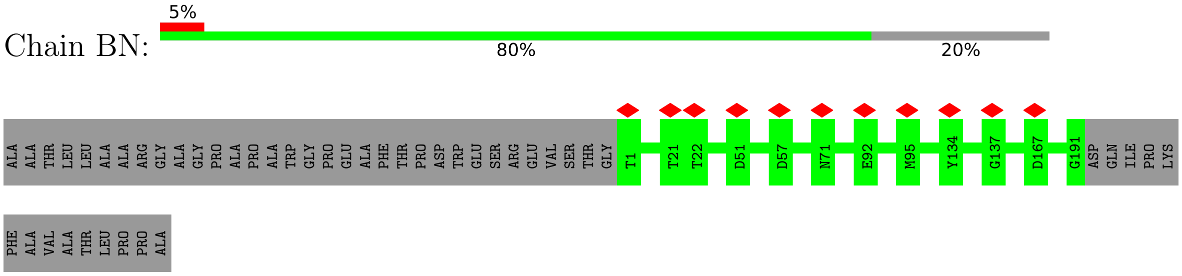
- Molecule 25: Proteasome subunit alpha type-3



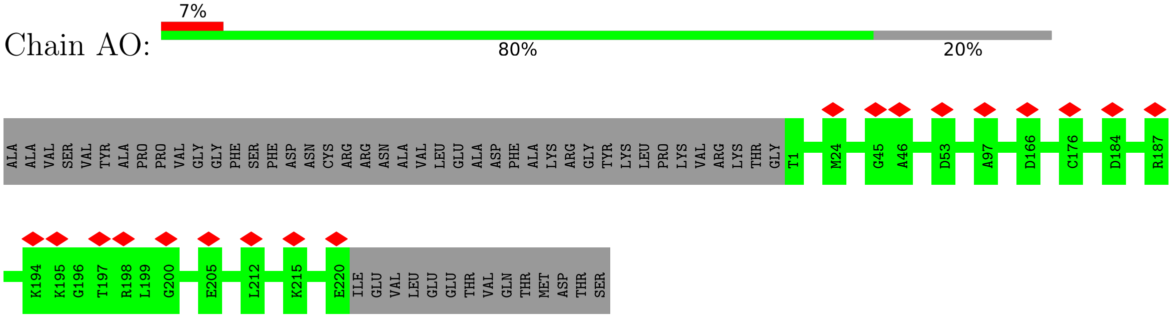
- Molecule 26: Proteasome subunit beta type-6



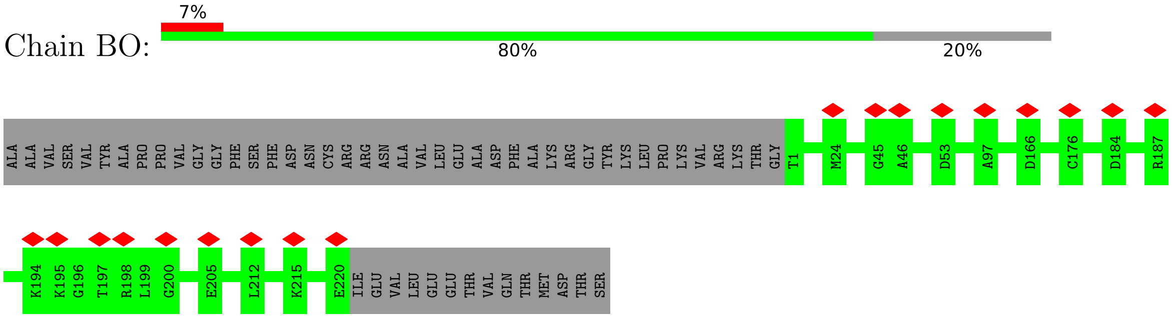
- Molecule 26: Proteasome subunit beta type-6



- Molecule 27: Proteasome subunit beta type-7

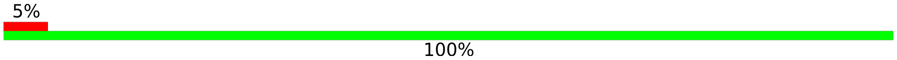


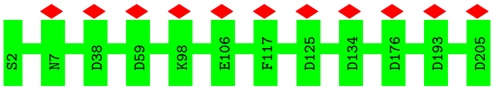
- Molecule 27: Proteasome subunit beta type-7



- Molecule 28: Proteasome subunit beta type-3

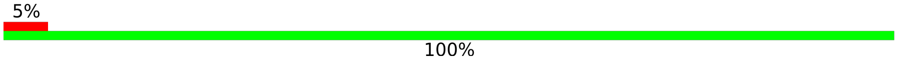
Chain AP:

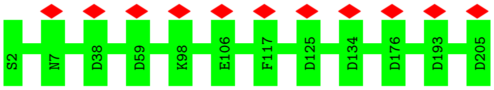




- Molecule 28: Proteasome subunit beta type-3

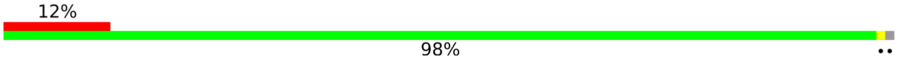
Chain BP:

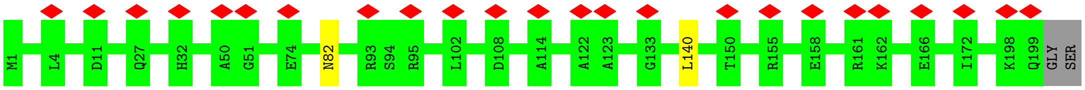




- Molecule 29: Proteasome subunit beta type-2

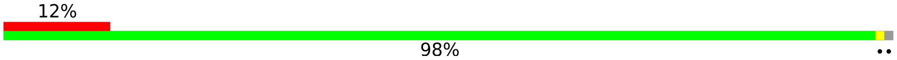
Chain AQ:

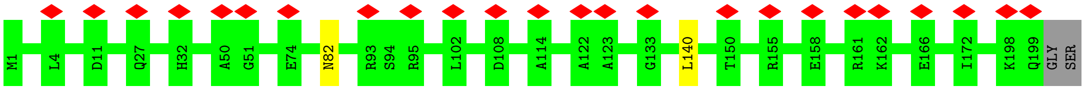




- Molecule 29: Proteasome subunit beta type-2

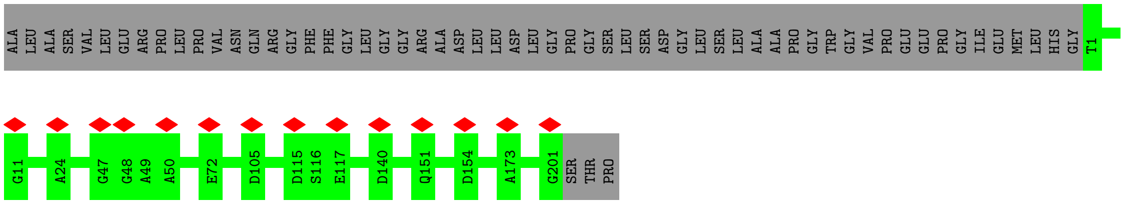
Chain BQ:





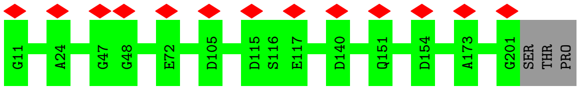
- Molecule 30: Proteasome subunit beta type-5

Chain AR:



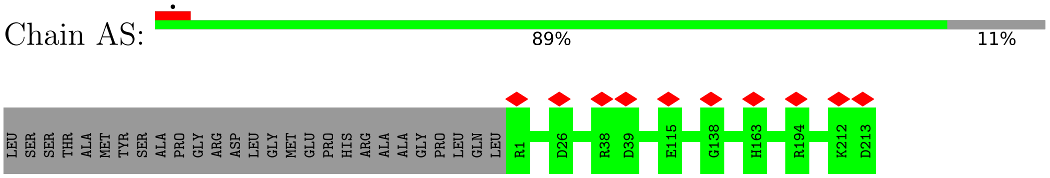
- Molecule 30: Proteasome subunit beta type-5

Chain BR:



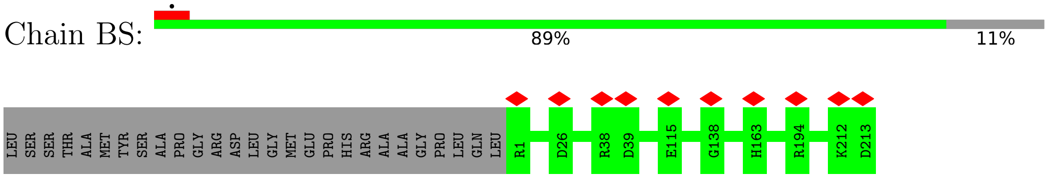
- Molecule 31: Proteasome subunit beta type-1

Chain AS:



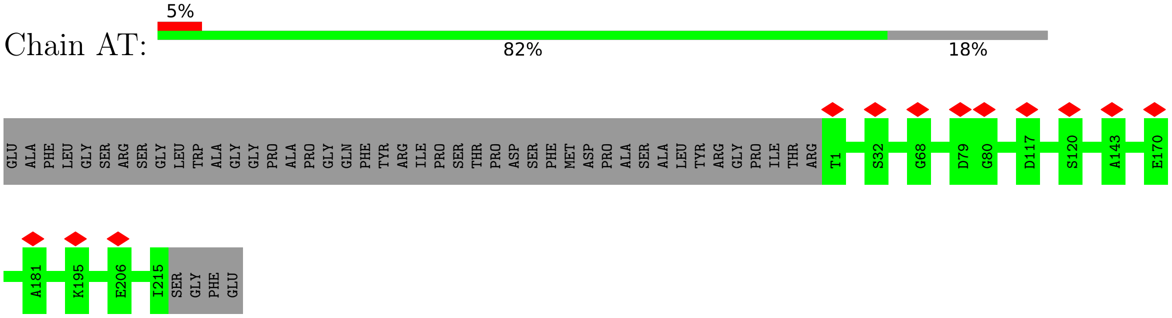
- Molecule 31: Proteasome subunit beta type-1

Chain BS:



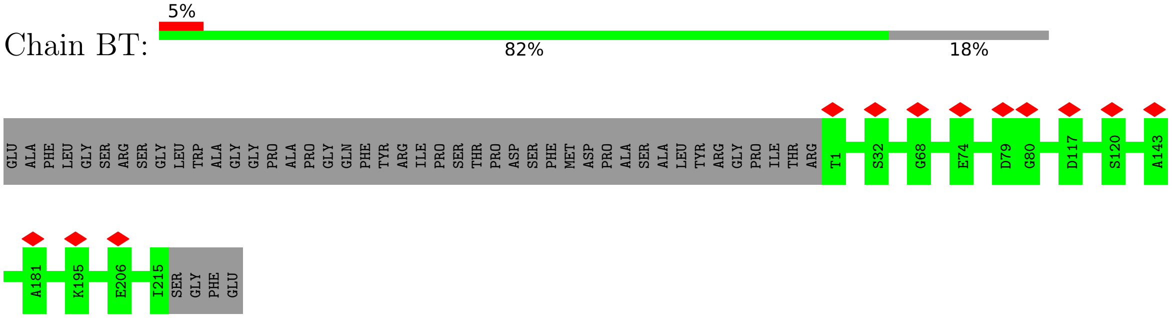
- Molecule 32: Proteasome subunit beta type-4

Chain AT:



- Molecule 32: Proteasome subunit beta type-4

Chain BT:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	86420	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 ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	28736	Depositor
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	0.006	Depositor
Map size (Å)	550.4, 550.4, 550.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AU	0.29	0/6396	0.49	0/8646
1	BU	0.29	0/6396	0.49	0/8646
2	AV	0.31	0/3929	0.57	0/5309
2	BV	0.31	0/3929	0.57	0/5309
3	AW	0.29	0/3751	0.54	3/5042 (0.1%)
3	BW	0.29	0/3751	0.54	3/5042 (0.1%)
4	AX	0.27	0/3053	0.45	0/4115
4	BX	0.27	0/3053	0.45	0/4115
5	AY	0.30	0/3173	0.53	2/4273 (0.0%)
5	BY	0.30	0/3173	0.53	2/4273 (0.0%)
6	AZ	0.28	0/2324	0.55	0/3150
6	BZ	0.28	0/2324	0.55	0/3150
7	Aa	0.36	1/3053 (0.0%)	0.52	0/4133
7	Ba	0.36	1/3053 (0.0%)	0.52	0/4133
8	Ab	0.27	0/1478	0.48	0/2001
8	Bb	0.27	0/1478	0.48	0/2001
9	Ac	0.33	0/2302	0.60	1/3110 (0.0%)
9	Bc	0.33	0/2302	0.60	1/3110 (0.0%)
10	Ad	0.30	0/2162	0.57	0/2919
10	Bd	0.30	0/2162	0.57	0/2919
11	Ae	0.28	0/338	0.56	0/450
11	Be	0.28	0/338	0.56	0/450
12	Af	0.33	2/5413 (0.0%)	0.63	3/7317 (0.0%)
12	Bf	0.33	2/5413 (0.0%)	0.63	3/7317 (0.0%)
13	AA	0.31	0/2886	0.56	1/3899 (0.0%)
13	BA	0.31	0/2886	0.56	1/3899 (0.0%)
14	AB	0.29	0/2700	0.54	0/3645
14	BB	0.29	0/2700	0.54	0/3645
15	AD	0.29	0/3090	0.58	1/4168 (0.0%)
15	BD	0.29	0/3090	0.58	1/4168 (0.0%)
16	AE	0.29	0/2835	0.54	0/3821
16	BE	0.29	0/2835	0.54	0/3821

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AF	0.32	0/2903	0.59	2/3912 (0.1%)
17	BF	0.32	0/2903	0.59	2/3912 (0.1%)
18	AC	0.29	0/3054	0.57	2/4107 (0.0%)
18	BC	0.29	0/3054	0.57	2/4107 (0.0%)
19	AG	0.30	0/1859	0.51	0/2523
19	BG	0.30	0/1859	0.51	0/2523
20	AH	0.30	0/1743	0.50	0/2372
20	BH	0.30	0/1743	0.50	0/2372
21	AI	0.31	0/1942	0.53	0/2628
21	BI	0.31	0/1942	0.53	0/2628
22	AJ	0.30	0/1728	0.48	0/2358
22	BJ	0.30	0/1728	0.48	0/2358
23	AK	0.30	0/1747	0.53	0/2364
23	BK	0.30	0/1747	0.53	0/2364
24	AL	0.28	0/1885	0.49	0/2552
24	BL	0.28	0/1885	0.49	0/2552
25	AM	0.31	0/1891	0.49	0/2552
25	BM	0.31	0/1891	0.49	0/2552
26	AN	0.29	0/1454	0.48	0/1967
26	BN	0.29	0/1454	0.48	0/1967
27	AO	0.28	0/1670	0.48	0/2265
27	BO	0.28	0/1670	0.48	0/2265
28	AP	0.31	0/1614	0.49	0/2177
28	BP	0.31	0/1614	0.49	0/2177
29	AQ	0.31	0/1603	0.51	1/2174 (0.0%)
29	BQ	0.31	0/1603	0.51	1/2174 (0.0%)
30	AR	0.30	0/1579	0.46	0/2134
30	BR	0.30	0/1579	0.46	0/2134
31	AS	0.29	0/1671	0.48	0/2253
31	BS	0.29	0/1671	0.48	0/2253
32	AT	0.30	0/1700	0.49	0/2305
32	BT	0.30	0/1700	0.49	0/2305
All	All	0.30	6/157852 (0.0%)	0.54	32/213282 (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
9	Ac	0	1
9	Bc	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	AE	0	1
16	BE	0	1
18	AC	0	1
18	BC	0	1
23	AK	0	1
23	BK	0	1
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Aa	145	LEU	C-N	11.88	1.56	1.34
7	Ba	145	LEU	C-N	11.88	1.56	1.34
12	Af	840	LEU	C-N	6.42	1.46	1.34
12	Bf	840	LEU	C-N	6.42	1.46	1.34
12	Af	340	MET	C-N	-5.33	1.21	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BF	150	LEU	CB-CG-CD2	8.79	125.95	111.00
17	AF	150	LEU	CB-CG-CD2	8.76	125.90	111.00
17	BF	204	LEU	CA-CB-CG	6.02	129.15	115.30
17	AF	204	LEU	CA-CB-CG	6.02	129.15	115.30
12	Af	618	GLU	N-CA-C	6.00	127.21	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	AC	171	HIS	Peptide
16	AE	175	PRO	Peptide
23	AK	232	GLU	Peptide
9	Ac	243	SER	Peptide
9	Bc	243	SER	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AU	798/953 (84%)	762 (96%)	34 (4%)	2 (0%)	41	74
1	BU	798/953 (84%)	762 (96%)	34 (4%)	2 (0%)	41	74
2	AV	478/533 (90%)	431 (90%)	40 (8%)	7 (2%)	10	46
2	BV	478/533 (90%)	431 (90%)	39 (8%)	8 (2%)	9	43
3	AW	454/456 (100%)	412 (91%)	38 (8%)	4 (1%)	17	54
3	BW	454/456 (100%)	412 (91%)	38 (8%)	4 (1%)	17	54
4	AX	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
4	BX	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
5	AY	376/389 (97%)	342 (91%)	30 (8%)	4 (1%)	14	51
5	BY	376/389 (97%)	342 (91%)	30 (8%)	4 (1%)	14	51
6	AZ	284/324 (88%)	257 (90%)	23 (8%)	4 (1%)	11	46
6	BZ	284/324 (88%)	257 (90%)	23 (8%)	4 (1%)	11	46
7	Aa	371/376 (99%)	343 (92%)	23 (6%)	5 (1%)	12	48
7	Ba	371/376 (99%)	343 (92%)	23 (6%)	5 (1%)	12	48
8	Ab	189/377 (50%)	180 (95%)	8 (4%)	1 (0%)	29	66
8	Bb	189/377 (50%)	180 (95%)	8 (4%)	1 (0%)	29	66
9	Ac	285/310 (92%)	252 (88%)	27 (10%)	6 (2%)	7	40
9	Bc	285/310 (92%)	252 (88%)	27 (10%)	6 (2%)	7	40
10	Ad	255/257 (99%)	227 (89%)	25 (10%)	3 (1%)	13	50
10	Bd	255/257 (99%)	227 (89%)	25 (10%)	3 (1%)	13	50
11	Ae	36/70 (51%)	32 (89%)	3 (8%)	1 (3%)	5	35
11	Be	36/70 (51%)	32 (89%)	3 (8%)	1 (3%)	5	35
12	Af	686/908 (76%)	571 (83%)	110 (16%)	5 (1%)	22	60
12	Bf	686/908 (76%)	571 (83%)	110 (16%)	5 (1%)	22	60
13	AA	359/433 (83%)	317 (88%)	33 (9%)	9 (2%)	5	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BA	359/433 (83%)	317 (88%)	33 (9%)	9 (2%)	5	36
14	AB	339/440 (77%)	303 (89%)	32 (9%)	4 (1%)	13	50
14	BB	339/440 (77%)	303 (89%)	32 (9%)	4 (1%)	13	50
15	AD	378/418 (90%)	330 (87%)	44 (12%)	4 (1%)	14	51
15	BD	378/418 (90%)	330 (87%)	44 (12%)	4 (1%)	14	51
16	AE	351/389 (90%)	307 (88%)	40 (11%)	4 (1%)	14	51
16	BE	351/389 (90%)	307 (88%)	40 (11%)	4 (1%)	14	51
17	AF	362/439 (82%)	326 (90%)	32 (9%)	4 (1%)	14	51
17	BF	362/439 (82%)	326 (90%)	31 (9%)	5 (1%)	11	46
18	AC	382/406 (94%)	341 (89%)	37 (10%)	4 (1%)	15	52
18	BC	382/406 (94%)	341 (89%)	37 (10%)	4 (1%)	15	52
19	AG	238/245 (97%)	221 (93%)	14 (6%)	3 (1%)	12	48
19	BG	238/245 (97%)	221 (93%)	14 (6%)	3 (1%)	12	48
20	AH	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
20	BH	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
21	AI	248/260 (95%)	226 (91%)	21 (8%)	1 (0%)	34	70
21	BI	248/260 (95%)	226 (91%)	21 (8%)	1 (0%)	34	70
22	AJ	237/247 (96%)	226 (95%)	7 (3%)	4 (2%)	9	43
22	BJ	237/247 (96%)	226 (95%)	7 (3%)	4 (2%)	9	43
23	AK	224/240 (93%)	201 (90%)	21 (9%)	2 (1%)	17	54
23	BK	224/240 (93%)	202 (90%)	20 (9%)	2 (1%)	17	54
24	AL	236/268 (88%)	214 (91%)	22 (9%)	0	100	100
24	BL	236/268 (88%)	214 (91%)	22 (9%)	0	100	100
25	AM	238/254 (94%)	219 (92%)	17 (7%)	2 (1%)	19	57
25	BM	238/254 (94%)	219 (92%)	17 (7%)	2 (1%)	19	57
26	AN	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
26	BN	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
27	AO	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
27	BO	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
28	AP	202/204 (99%)	181 (90%)	21 (10%)	0	100	100
28	BP	202/204 (99%)	181 (90%)	21 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AQ	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
29	BQ	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
30	AR	199/262 (76%)	192 (96%)	7 (4%)	0	100	100
30	BR	199/262 (76%)	192 (96%)	7 (4%)	0	100	100
31	AS	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
31	BS	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
32	AT	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
32	BT	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
All	All	19682/22662 (87%)	17947 (91%)	1567 (8%)	168 (1%)	21	54

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AU	364	VAL
3	AW	136	ILE
5	AY	350	VAL
9	Ac	157	ILE
9	Ac	244	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AU	685/816 (84%)	681 (99%)	4 (1%)	86	92
1	BU	685/816 (84%)	681 (99%)	4 (1%)	86	92
2	AV	414/459 (90%)	409 (99%)	5 (1%)	71	84
2	BV	414/459 (90%)	409 (99%)	5 (1%)	71	84
3	AW	416/416 (100%)	413 (99%)	3 (1%)	84	91
3	BW	416/416 (100%)	413 (99%)	3 (1%)	84	91
4	AX	327/362 (90%)	325 (99%)	2 (1%)	86	92
4	BX	327/362 (90%)	325 (99%)	2 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AY	334/344 (97%)	334 (100%)	0	100	100
5	BY	334/344 (97%)	334 (100%)	0	100	100
6	AZ	257/295 (87%)	256 (100%)	1 (0%)	91	95
6	BZ	257/295 (87%)	256 (100%)	1 (0%)	91	95
7	Aa	333/336 (99%)	332 (100%)	1 (0%)	92	96
7	Ba	333/336 (99%)	332 (100%)	1 (0%)	92	96
8	Ab	167/312 (54%)	167 (100%)	0	100	100
8	Bb	167/312 (54%)	167 (100%)	0	100	100
9	Ac	252/268 (94%)	250 (99%)	2 (1%)	81	89
9	Bc	252/268 (94%)	250 (99%)	2 (1%)	81	89
10	Ad	231/231 (100%)	230 (100%)	1 (0%)	91	95
10	Bd	231/231 (100%)	230 (100%)	1 (0%)	91	95
11	Ae	38/63 (60%)	38 (100%)	0	100	100
11	Be	38/63 (60%)	38 (100%)	0	100	100
12	Af	582/763 (76%)	578 (99%)	4 (1%)	84	91
12	Bf	582/763 (76%)	578 (99%)	4 (1%)	84	91
13	AA	308/372 (83%)	307 (100%)	1 (0%)	92	96
13	BA	308/372 (83%)	307 (100%)	1 (0%)	92	96
14	AB	298/385 (77%)	296 (99%)	2 (1%)	84	91
14	BB	298/385 (77%)	296 (99%)	2 (1%)	84	91
15	AD	333/366 (91%)	331 (99%)	2 (1%)	86	92
15	BD	333/366 (91%)	331 (99%)	2 (1%)	86	92
16	AE	308/341 (90%)	306 (99%)	2 (1%)	86	92
16	BE	308/341 (90%)	306 (99%)	2 (1%)	86	92
17	AF	312/379 (82%)	309 (99%)	3 (1%)	76	86
17	BF	312/379 (82%)	309 (99%)	3 (1%)	76	86
18	AC	332/352 (94%)	329 (99%)	3 (1%)	78	88
18	BC	332/352 (94%)	329 (99%)	3 (1%)	78	88
19	AG	193/209 (92%)	193 (100%)	0	100	100
19	BG	193/209 (92%)	193 (100%)	0	100	100
20	AH	164/190 (86%)	163 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BH	164/190 (86%)	163 (99%)	1 (1%)	86	92
21	AI	193/220 (88%)	193 (100%)	0	100	100
21	BI	193/220 (88%)	193 (100%)	0	100	100
22	AJ	152/210 (72%)	150 (99%)	2 (1%)	69	82
22	BJ	152/210 (72%)	150 (99%)	2 (1%)	69	82
23	AK	186/202 (92%)	186 (100%)	0	100	100
23	BK	186/202 (92%)	186 (100%)	0	100	100
24	AL	198/229 (86%)	198 (100%)	0	100	100
24	BL	198/229 (86%)	198 (100%)	0	100	100
25	AM	192/211 (91%)	191 (100%)	1 (0%)	88	94
25	BM	192/211 (91%)	191 (100%)	1 (0%)	88	94
26	AN	148/180 (82%)	148 (100%)	0	100	100
26	BN	148/180 (82%)	148 (100%)	0	100	100
27	AO	177/227 (78%)	177 (100%)	0	100	100
27	BO	177/227 (78%)	177 (100%)	0	100	100
28	AP	172/173 (99%)	172 (100%)	0	100	100
28	BP	172/173 (99%)	172 (100%)	0	100	100
29	AQ	164/171 (96%)	163 (99%)	1 (1%)	86	92
29	BQ	164/171 (96%)	163 (99%)	1 (1%)	86	92
30	AR	153/201 (76%)	153 (100%)	0	100	100
30	BR	153/201 (76%)	153 (100%)	0	100	100
31	AS	174/198 (88%)	174 (100%)	0	100	100
31	BS	174/198 (88%)	174 (100%)	0	100	100
32	AT	175/214 (82%)	175 (100%)	0	100	100
32	BT	175/214 (82%)	175 (100%)	0	100	100
All	All	16736/19390 (86%)	16654 (100%)	82 (0%)	89	94

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Bc	38	LEU
17	BF	76	ASN
10	Bd	3	GLU

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Mol	Chain	Res	Type
14	BB	101	ASP
18	BC	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
7	Ba	244	ASN
12	Bf	650	GLN
28	BP	169	GLN
9	Bc	298	GLN
12	Bf	396	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	ATP	AA	501	-	26,33,33	0.89	1 (3%)	31,52,52	1.75	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
35	ADP	BC	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.37	4 (13%)
34	ATP	BF	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
35	ADP	AC	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.36	4 (13%)
34	ATP	AE	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
35	ADP	AB	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.36	5 (17%)
34	ATP	BE	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
34	ATP	BA	501	-	26,33,33	0.89	1 (3%)	31,52,52	1.75	5 (16%)
34	ATP	AF	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
34	ATP	AD	501	-	26,33,33	0.88	1 (3%)	31,52,52	1.42	5 (16%)
34	ATP	BD	501	-	26,33,33	0.89	1 (3%)	31,52,52	1.42	5 (16%)
35	ADP	BB	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.36	5 (17%)

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	ATP	AA	501	-	-	4/18/38/38	0/3/3/3
35	ADP	BC	501	-	-	5/12/32/32	0/3/3/3
34	ATP	BF	501	-	-	1/18/38/38	0/3/3/3
35	ADP	AC	501	-	-	5/12/32/32	0/3/3/3
34	ATP	AE	401	-	-	3/18/38/38	0/3/3/3
35	ADP	AB	501	-	-	6/12/32/32	0/3/3/3
34	ATP	BE	401	-	-	3/18/38/38	0/3/3/3
34	ATP	BA	501	-	-	4/18/38/38	0/3/3/3
34	ATP	AF	501	-	-	1/18/38/38	0/3/3/3
34	ATP	AD	501	-	-	2/18/38/38	0/3/3/3
34	ATP	BD	501	-	-	2/18/38/38	0/3/3/3
35	ADP	BB	501	-	-	6/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BC	501	ADP	C5-C4	2.58	1.47	1.40
35	AC	501	ADP	C5-C4	2.55	1.47	1.40
34	AE	401	ATP	C5-C4	2.53	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BE	401	ATP	C5-C4	2.52	1.47	1.40
34	AF	501	ATP	C5-C4	2.47	1.47	1.40

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	501	ATP	PA-O3A-PB	-4.97	115.77	132.83
34	AA	501	ATP	PA-O3A-PB	-4.96	115.80	132.83
34	BF	501	ATP	PB-O3B-PG	-4.57	117.15	132.83
34	AF	501	ATP	PB-O3B-PG	-4.57	117.16	132.83
34	AA	501	ATP	PB-O3B-PG	-4.27	118.18	132.83

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

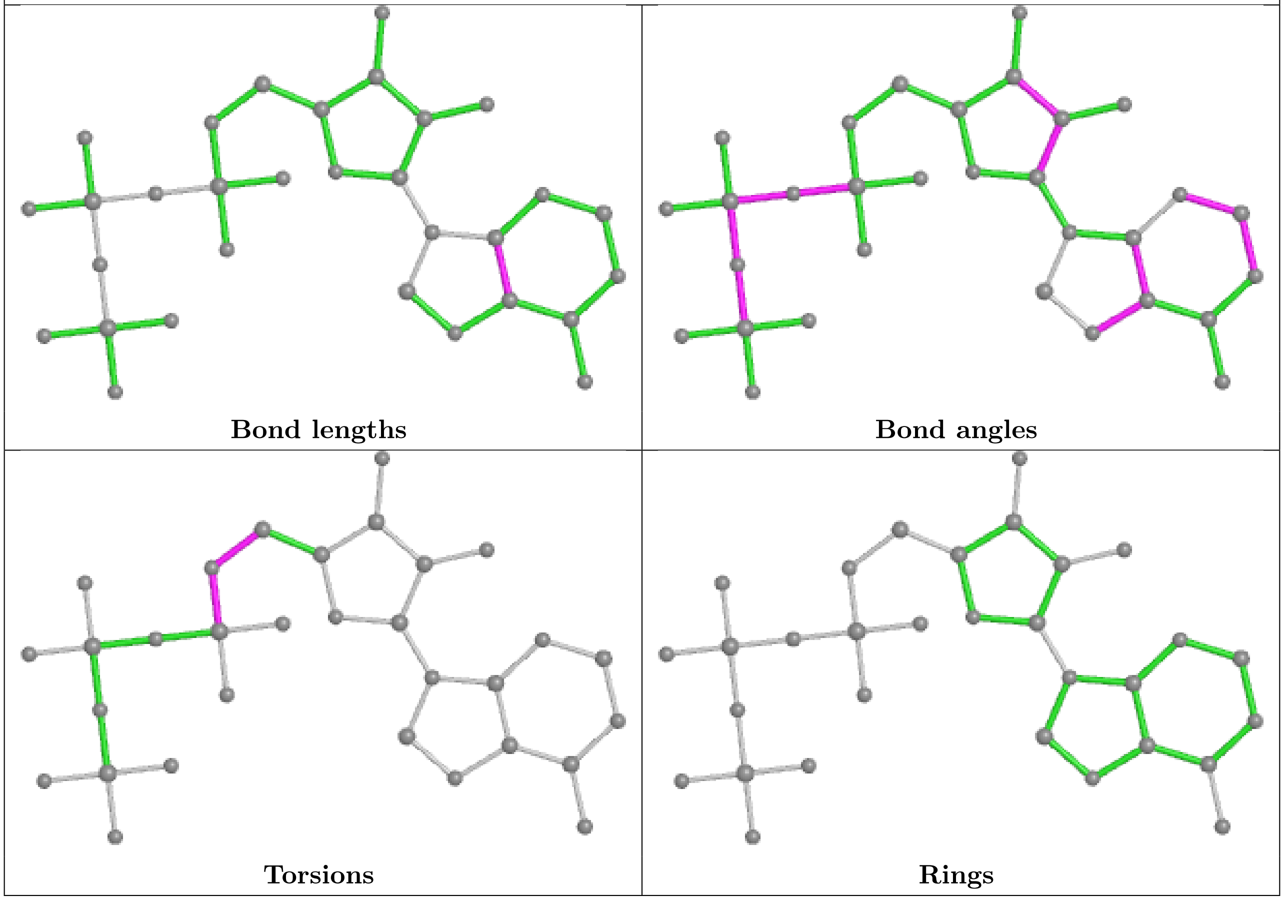
Mol	Chain	Res	Type	Atoms
34	AA	501	ATP	C5'-O5'-PA-O2A
34	AA	501	ATP	C5'-O5'-PA-O3A
34	AD	501	ATP	PB-O3B-PG-O2G
34	AE	401	ATP	C5'-O5'-PA-O3A
34	BA	501	ATP	C5'-O5'-PA-O2A

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 AA 501



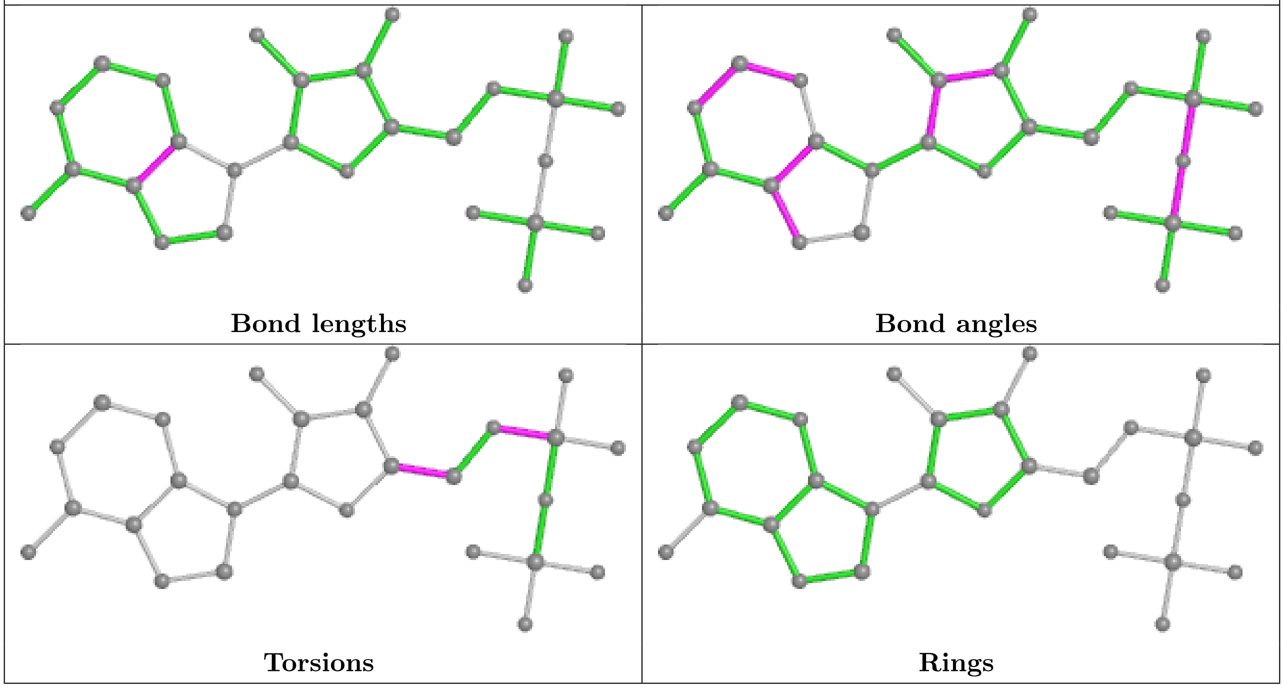
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP BC 501



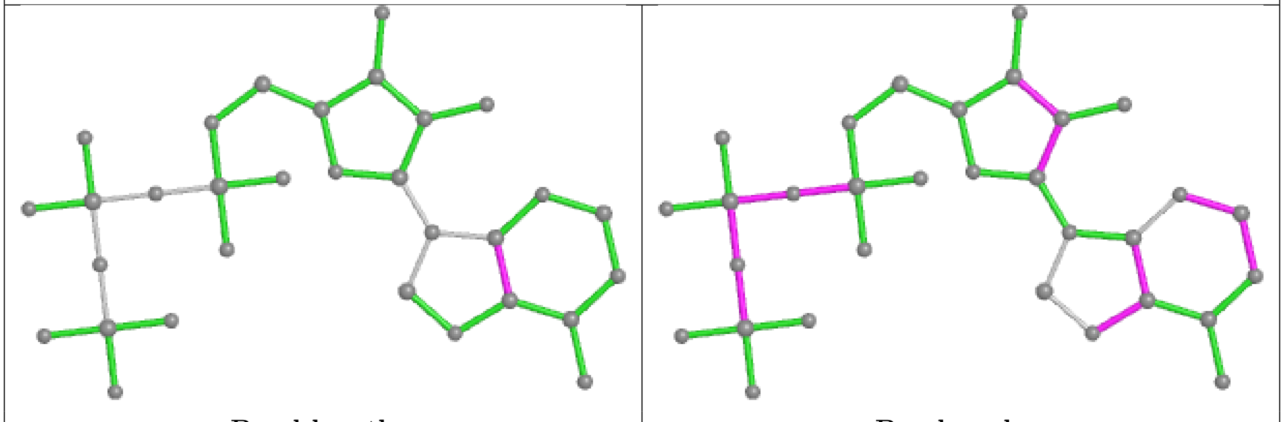
Bond lengths

Bond angles

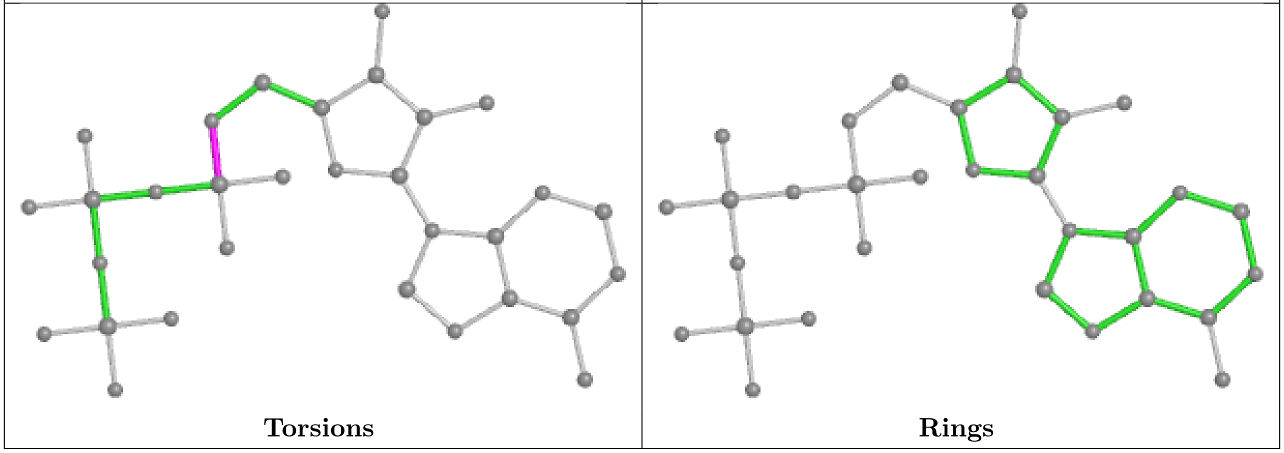
Torsions

Rings

Ligand ATP BF 501

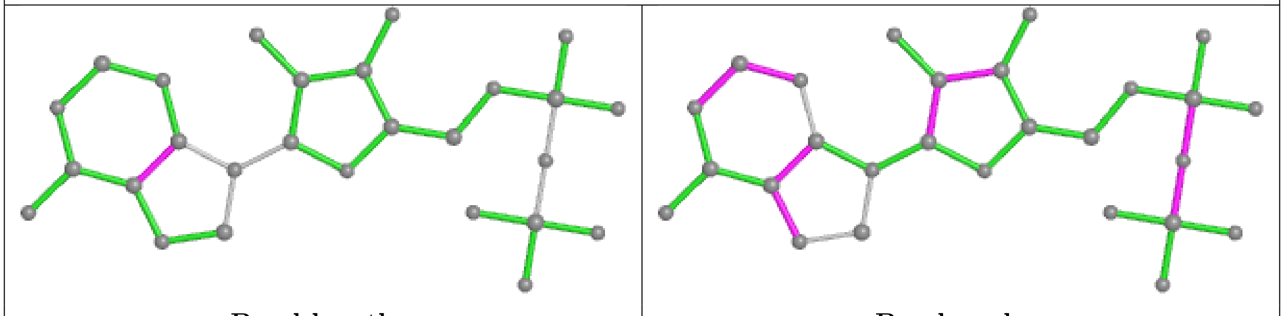


Bond lengths Bond angles

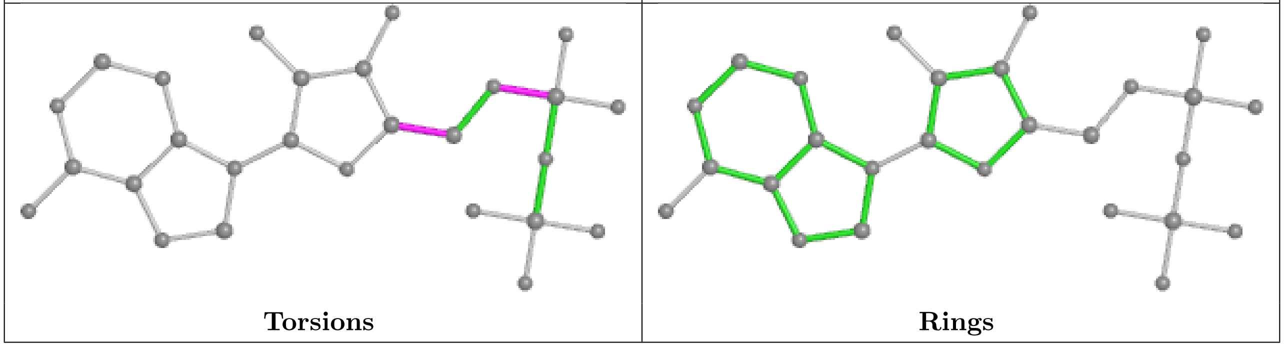


Torsions Rings

Ligand ADP AC 501

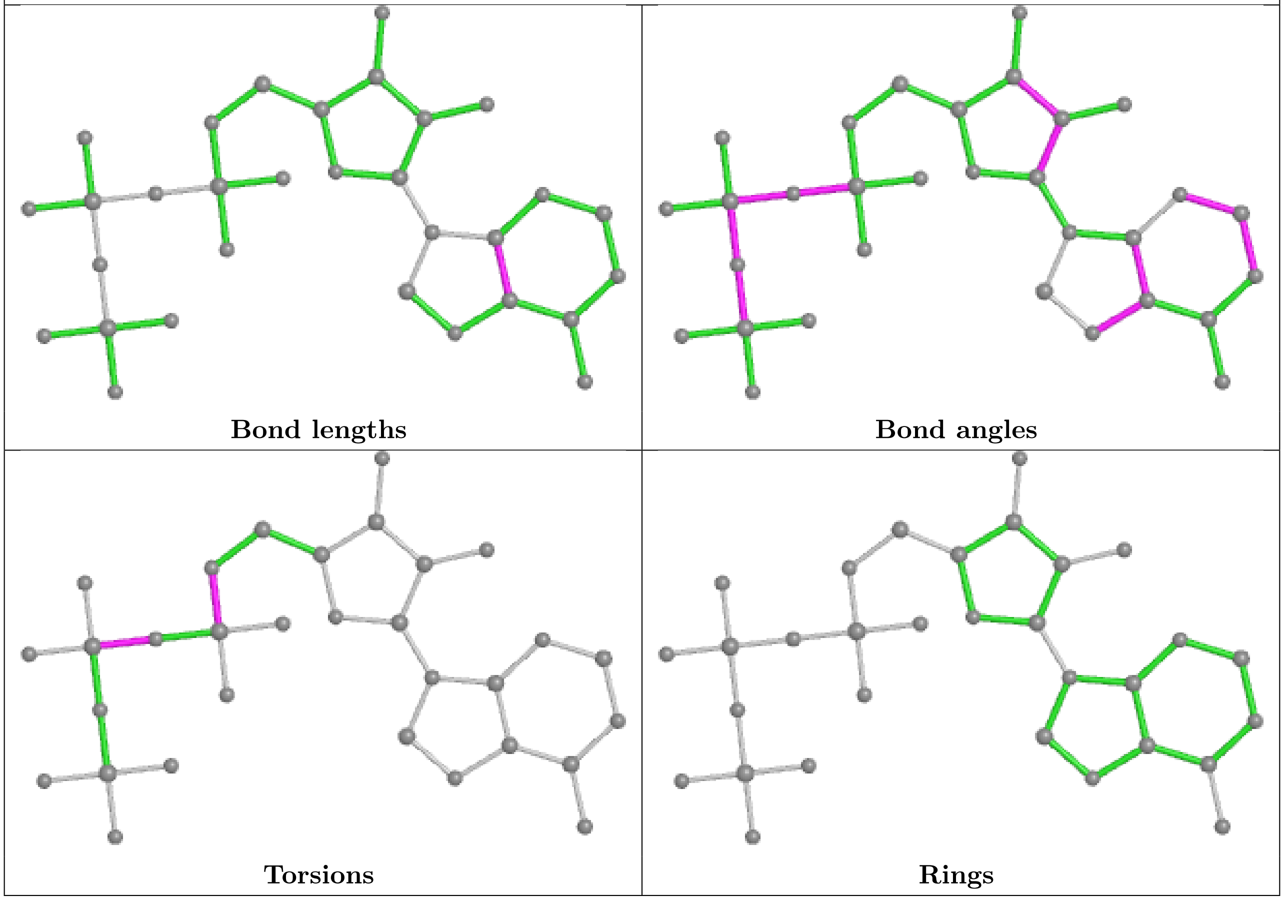


Bond lengths Bond angles



Torsions Rings

Ligand ATP AE 401



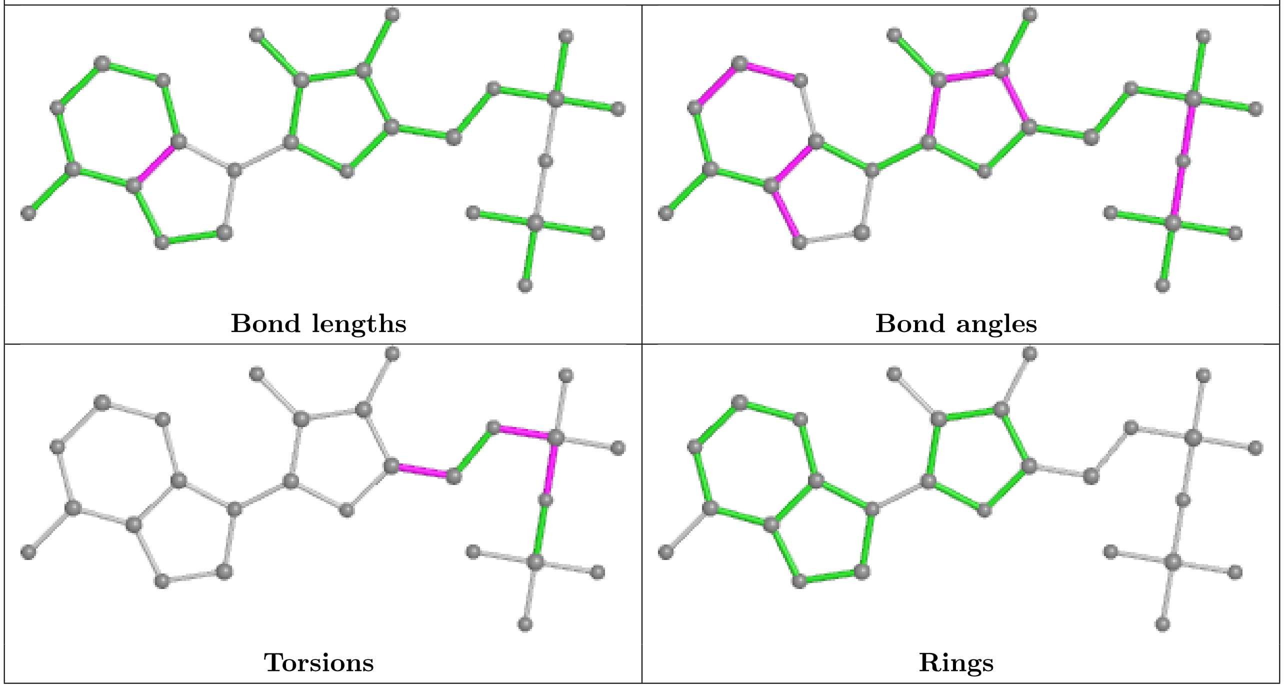
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP AB 501



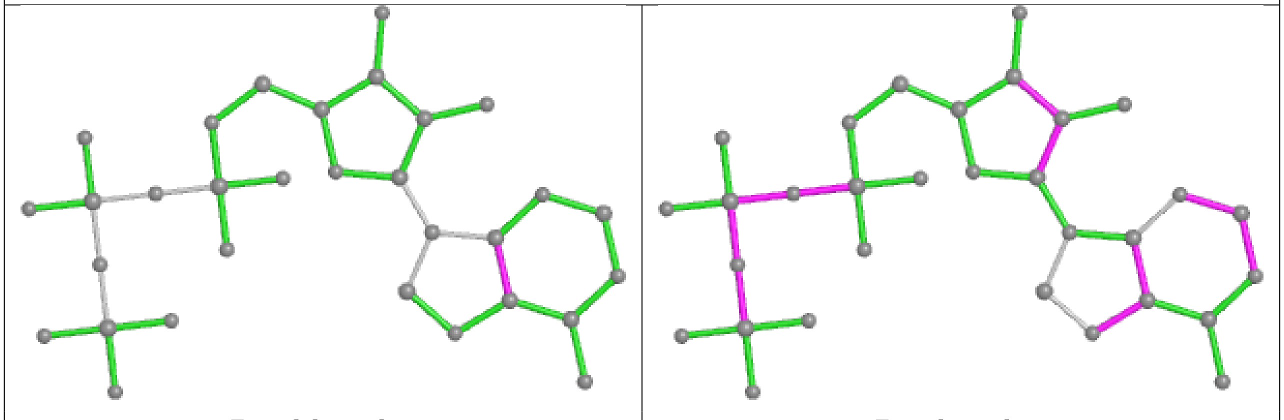
Bond lengths

Bond angles

Torsions

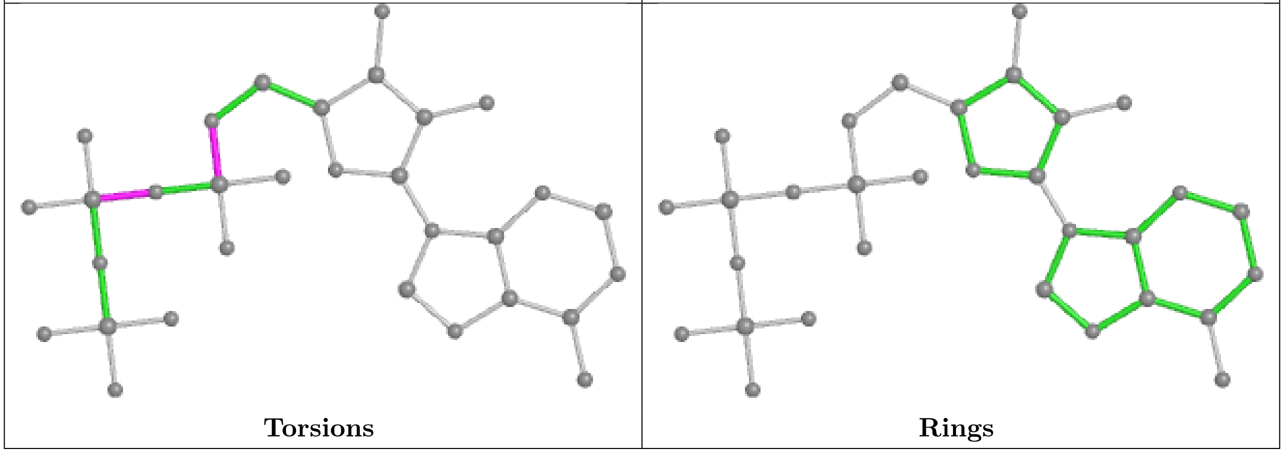
Rings

Ligand ATP BE 401



Bond lengths

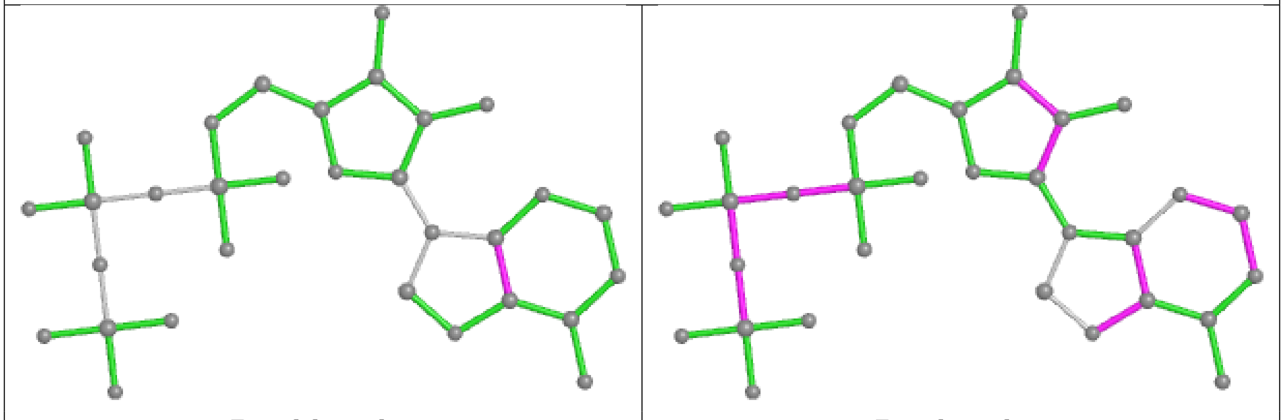
Bond angles



Torsions

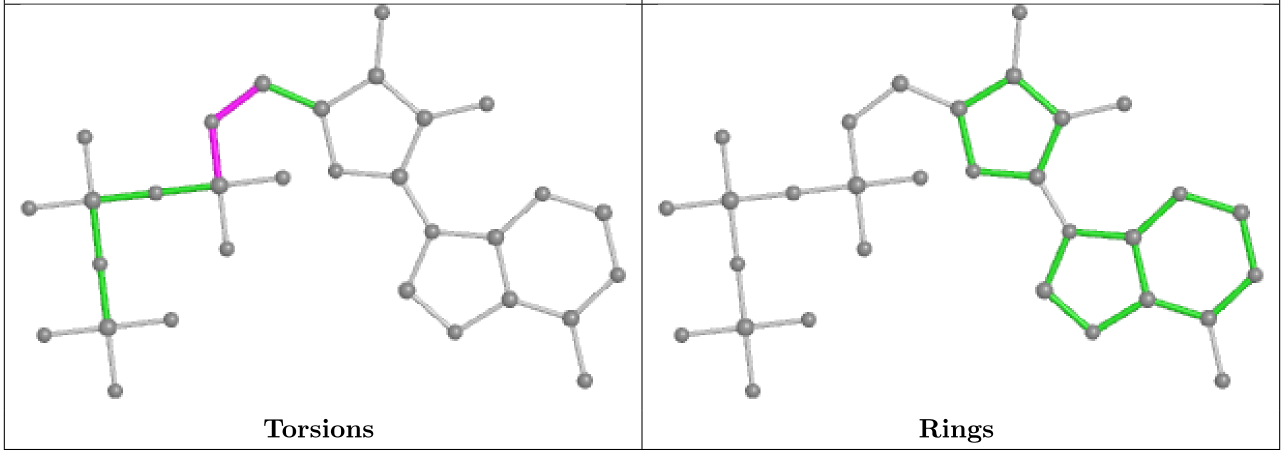
Rings

Ligand ATP BA 501



Bond lengths

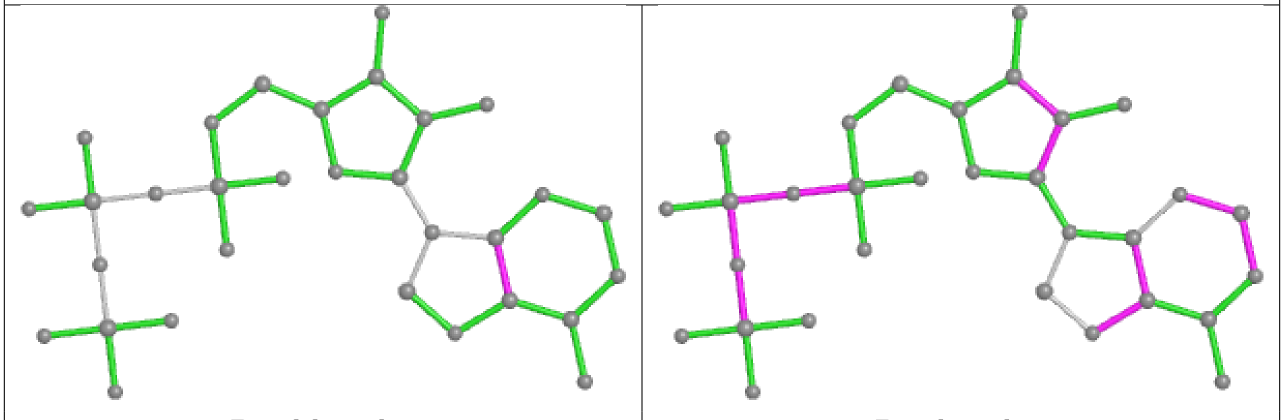
Bond angles



Torsions

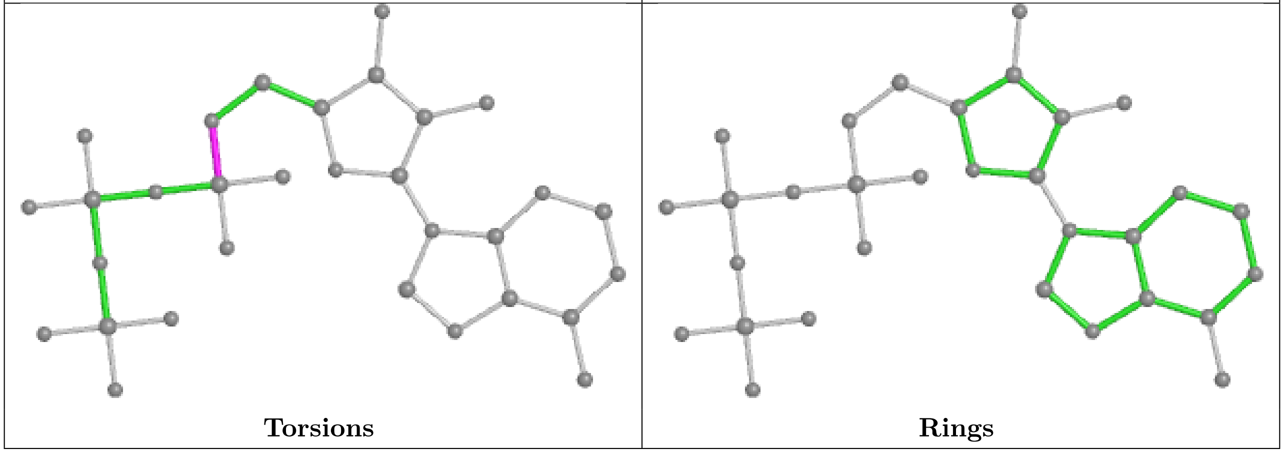
Rings

Ligand ATP AF 501



Bond lengths

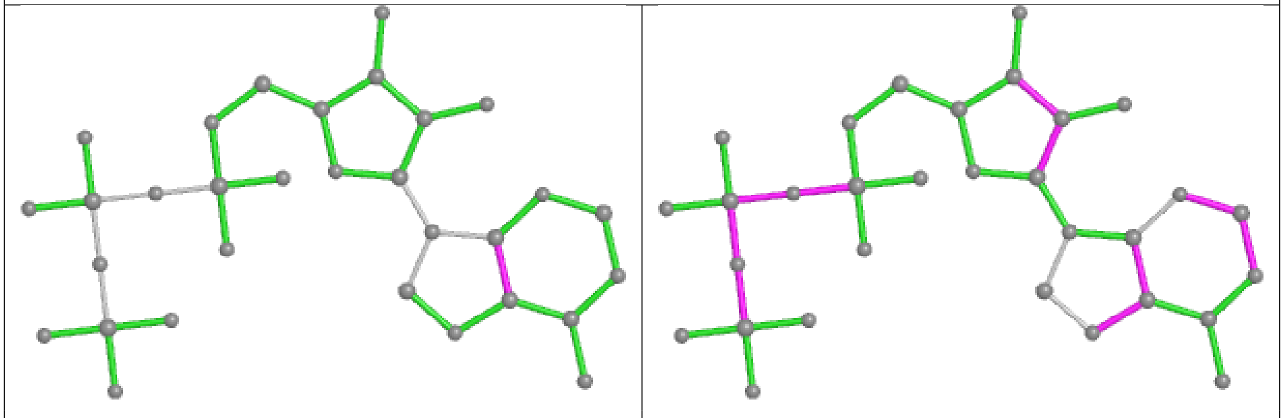
Bond angles



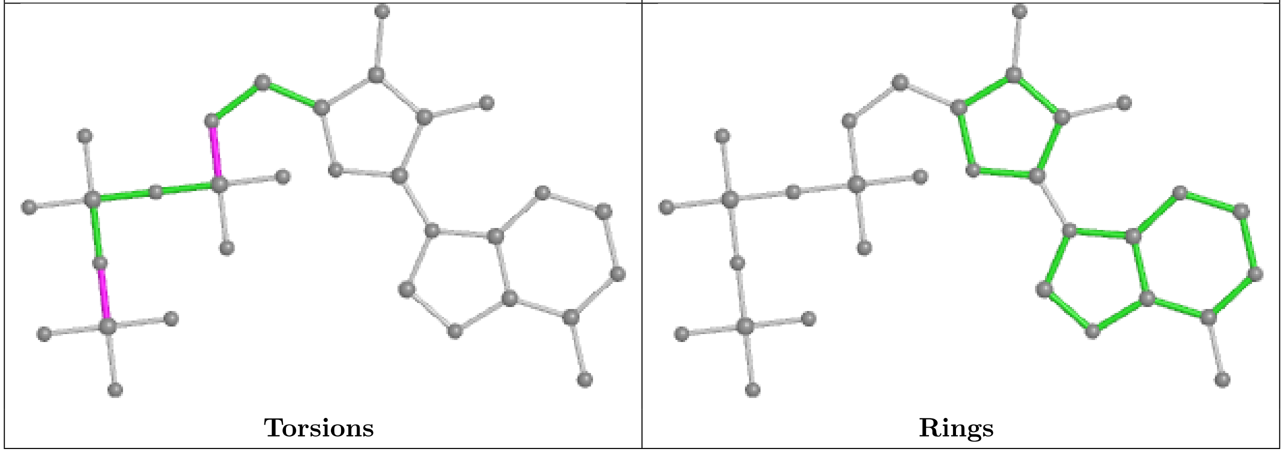
Torsions

Rings

Ligand ATP AD 501

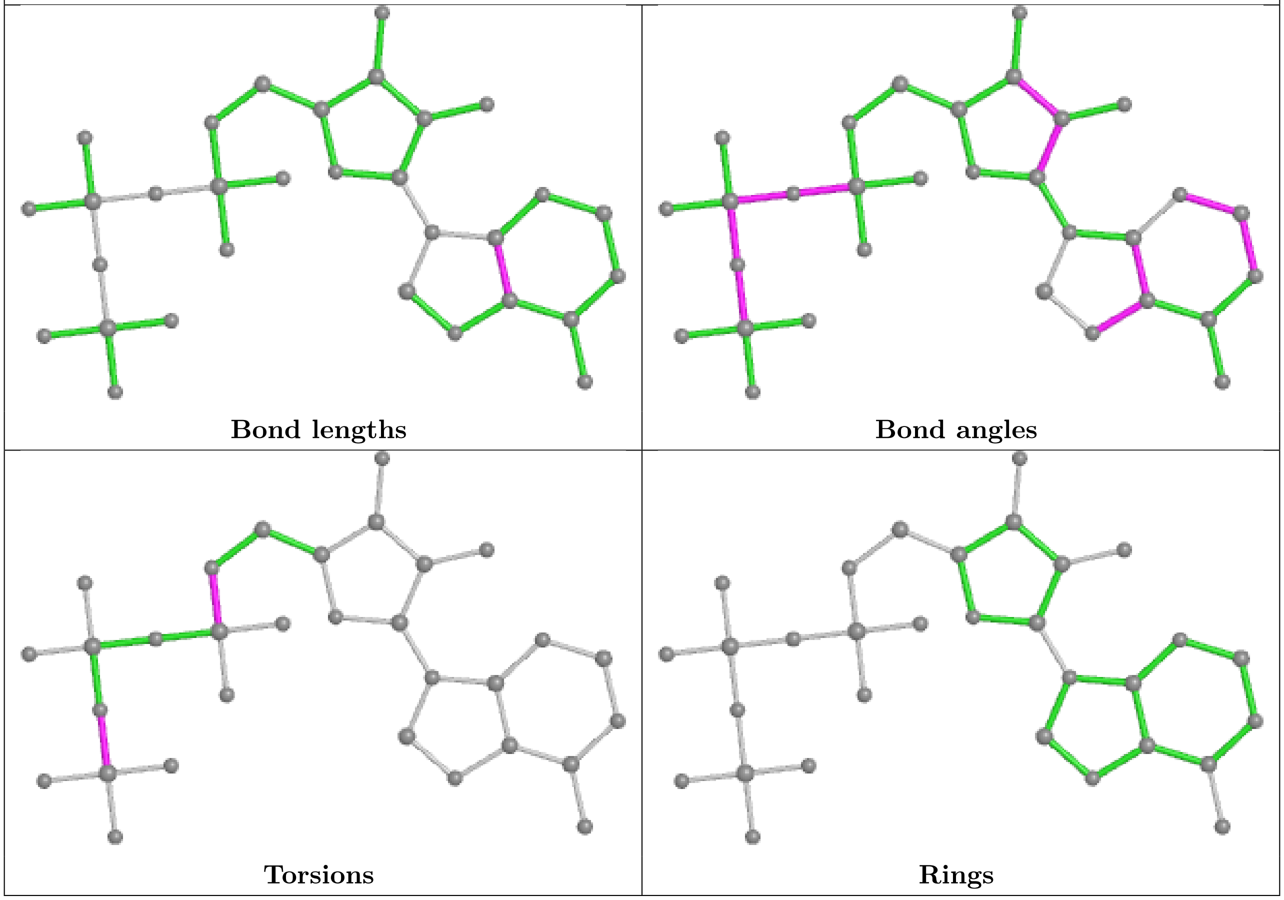


Bond lengths **Bond angles**

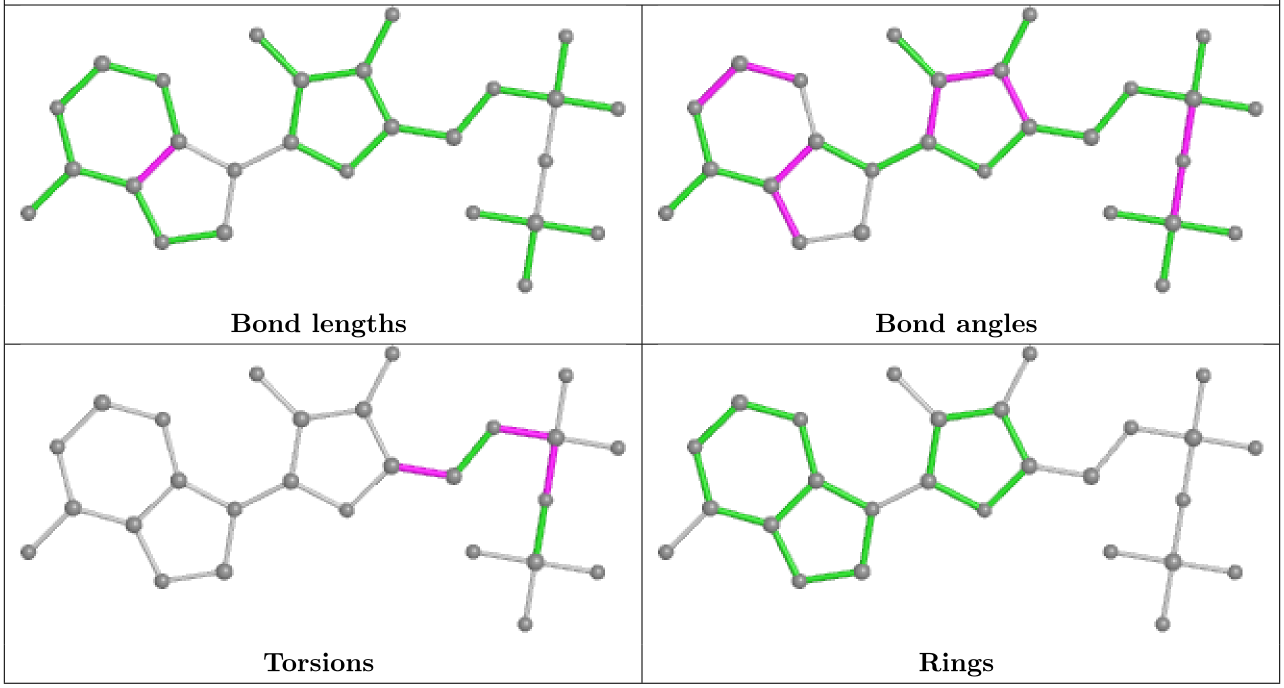


Torsions **Rings**

Ligand ATP BD 501


Bond lengths
Bond angles
Torsions
Rings

Ligand ADP BB 501


Bond lengths
Bond angles
Torsions
Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Bf	3
12	Af	3

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bf	269:ALA	C	270:LEU	N	9.72
1	Af	269:ALA	C	270:LEU	N	9.71
1	Af	238:ASN	C	239:TYR	N	7.22
1	Bf	238:ASN	C	239:TYR	N	7.22
1	Af	507:ASP	C	508:SER	N	5.88

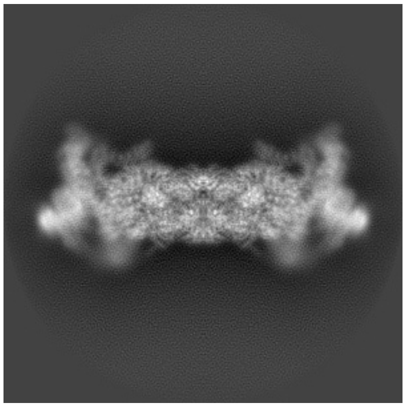
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8332. These allow visual inspection of the internal detail of the map and identification of artifacts.

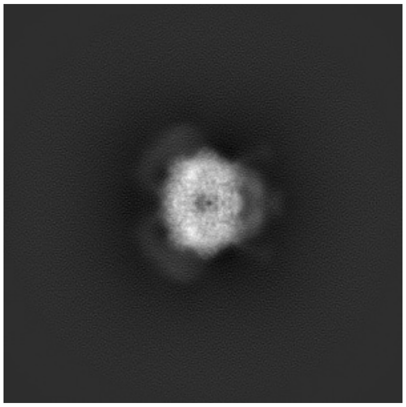
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

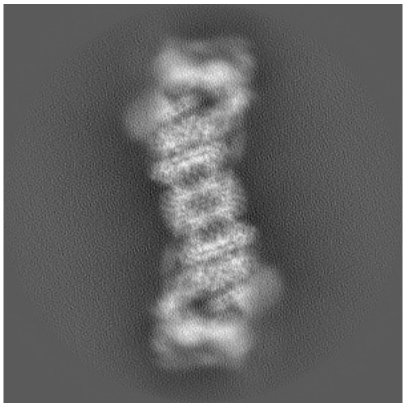
6.1.1 Primary map



X



Y

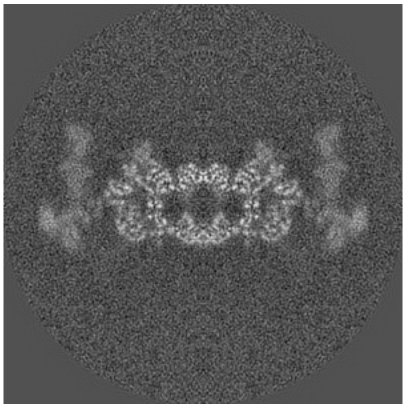


Z

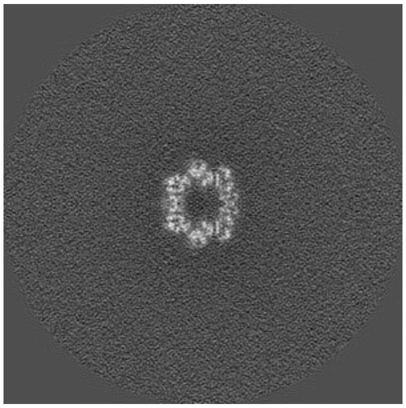
The images above show the map projected in three orthogonal directions.

6.2 Central slices

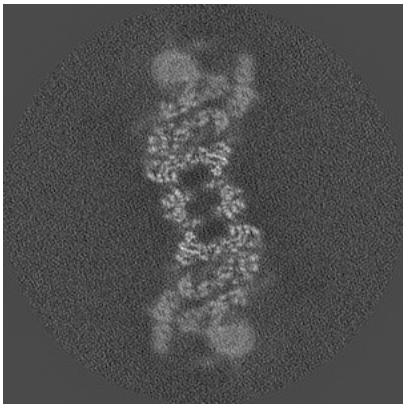
6.2.1 Primary map



X Index: 320



Y Index: 320

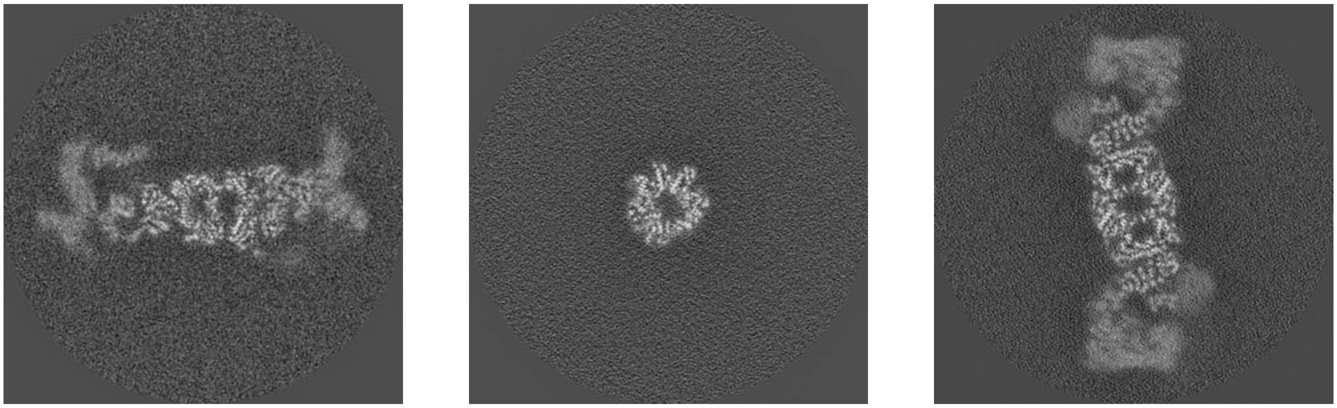


Z Index: 320

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

6.3 Largest variance slices

6.3.1 Primary map



X Index: 294

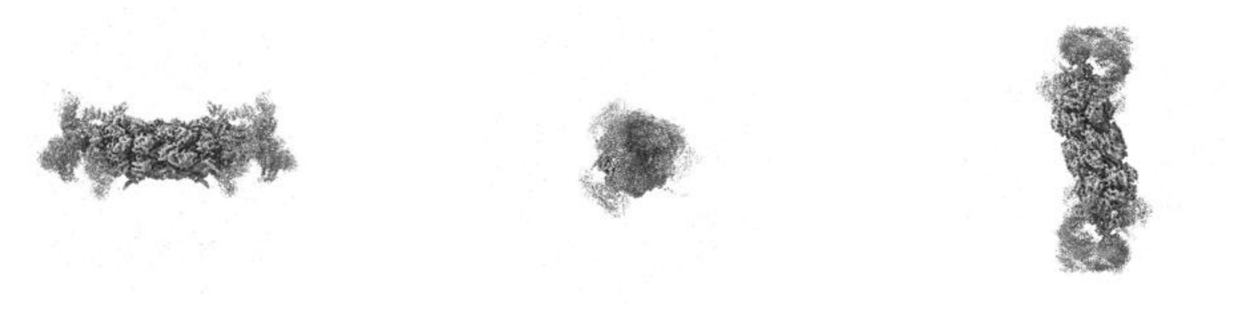
Y Index: 302

Z Index: 297

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

6.4 Orthogonal surface views

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.

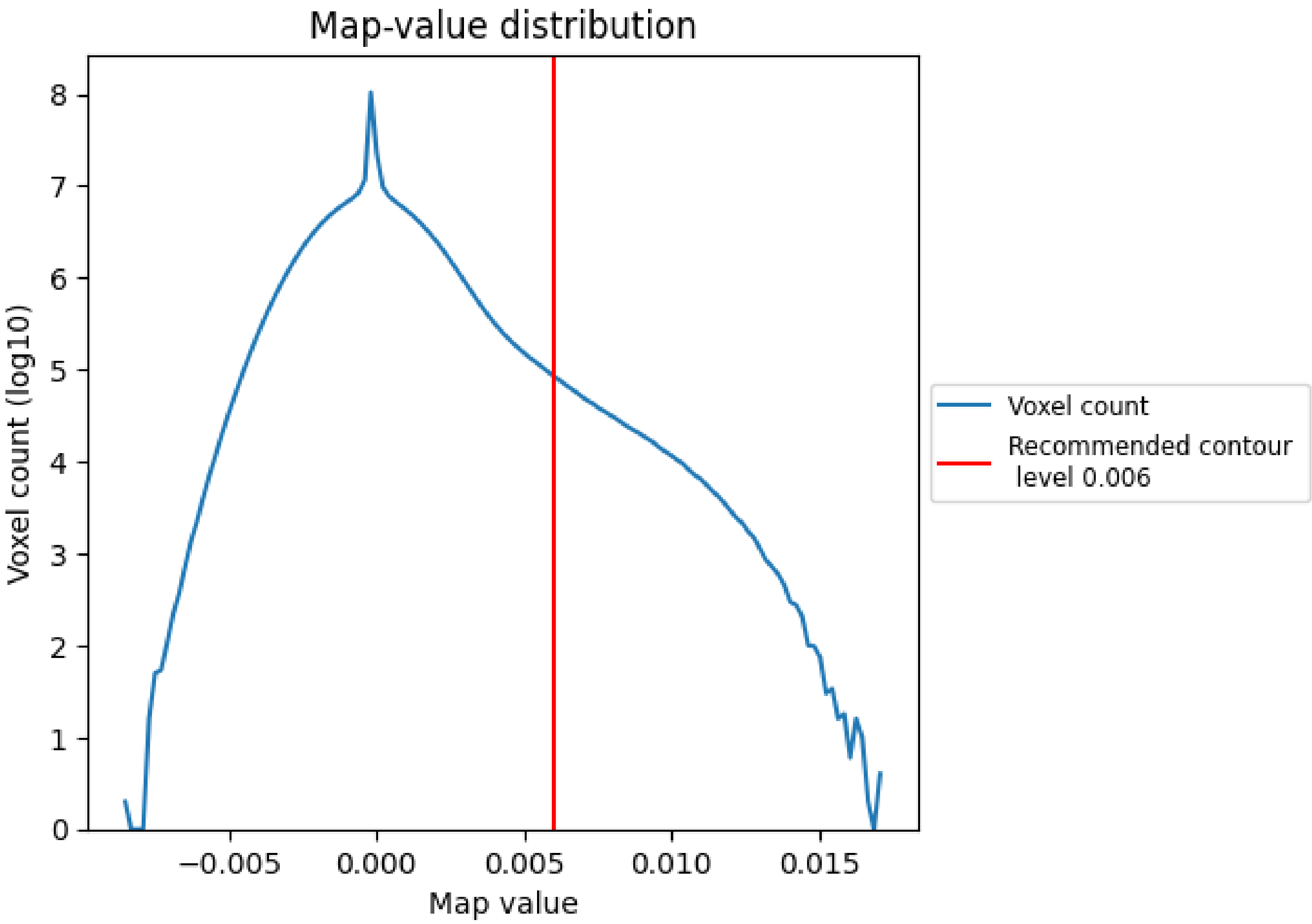
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

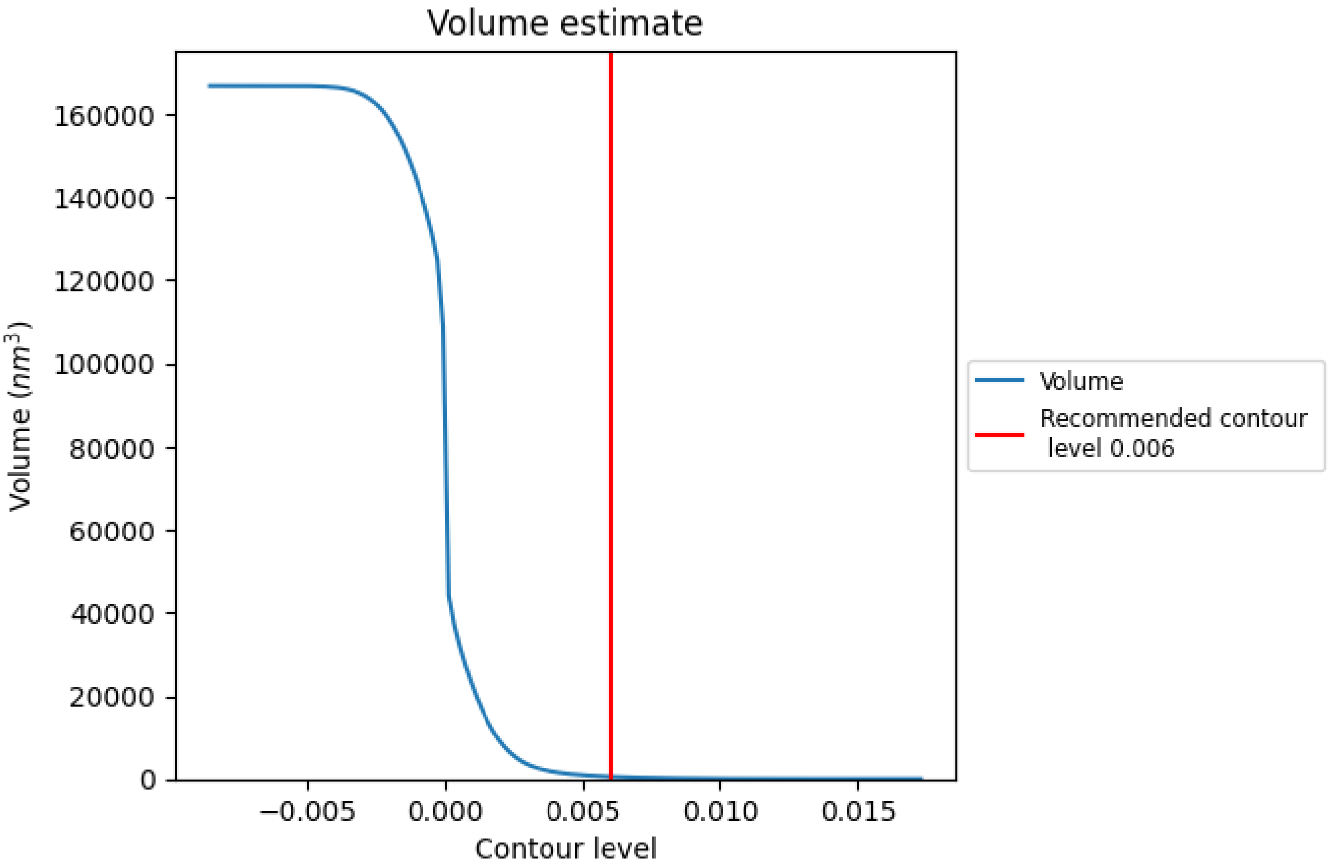
This section contains the results of statistical analysis of the map.

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.

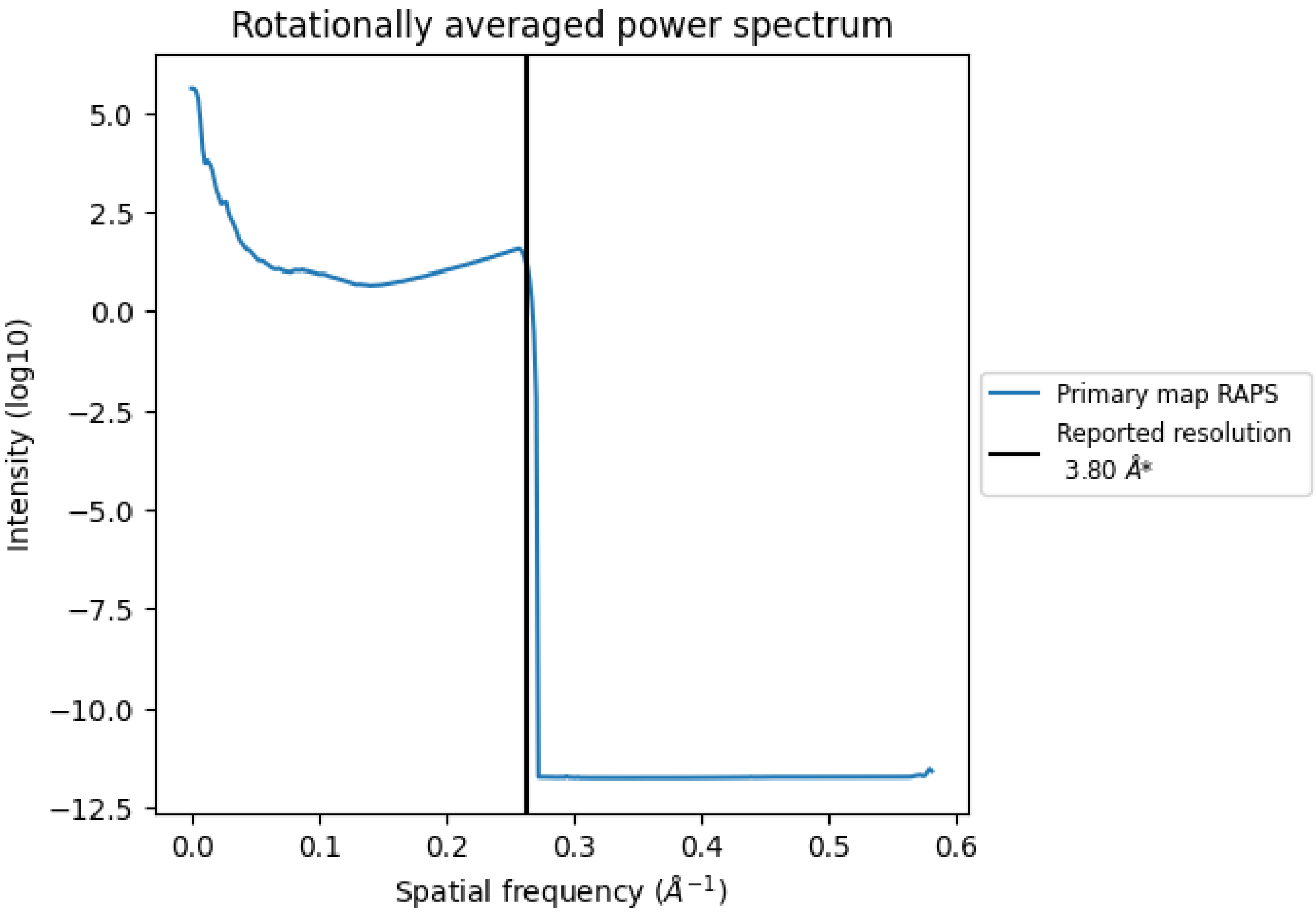
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 538 nm^3; this corresponds to an approximate mass of 486 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 $Å^{-1}$

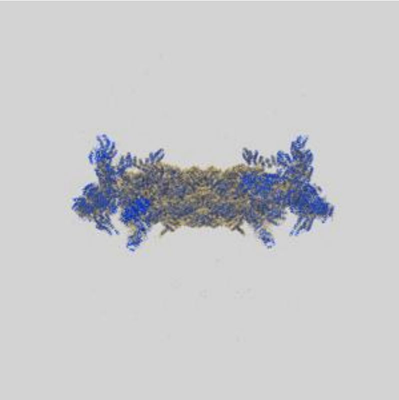
8 Fourier-Shell correlation

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

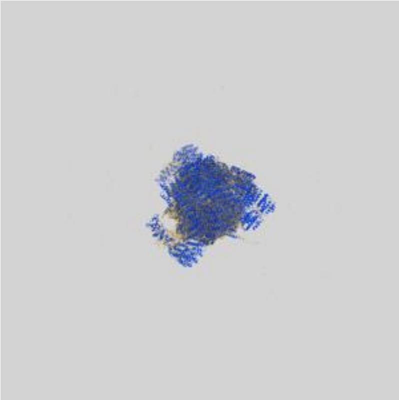
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8332 and PDB model 5T0C. Per-residue inclusion information can be found in section 3 on page 14.

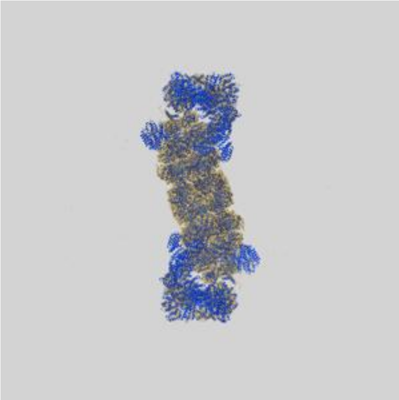
9.1 Map-model overlay (i)



X



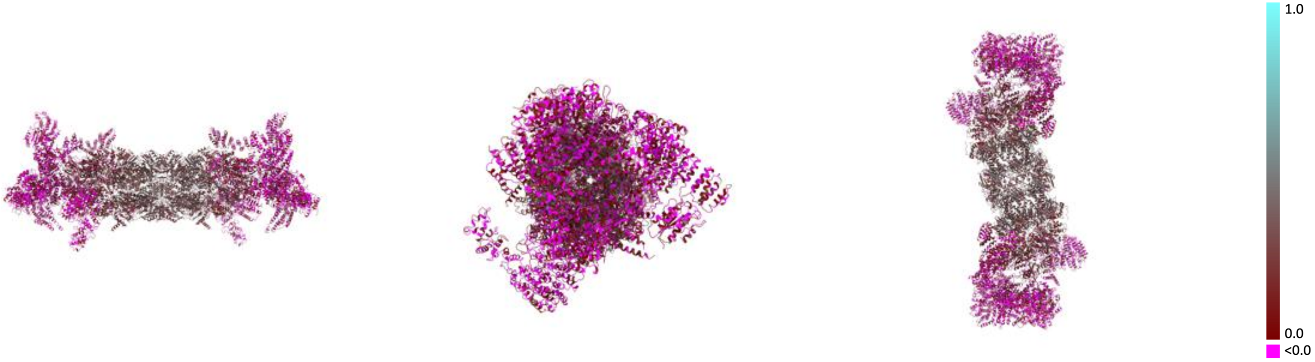
Y



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.

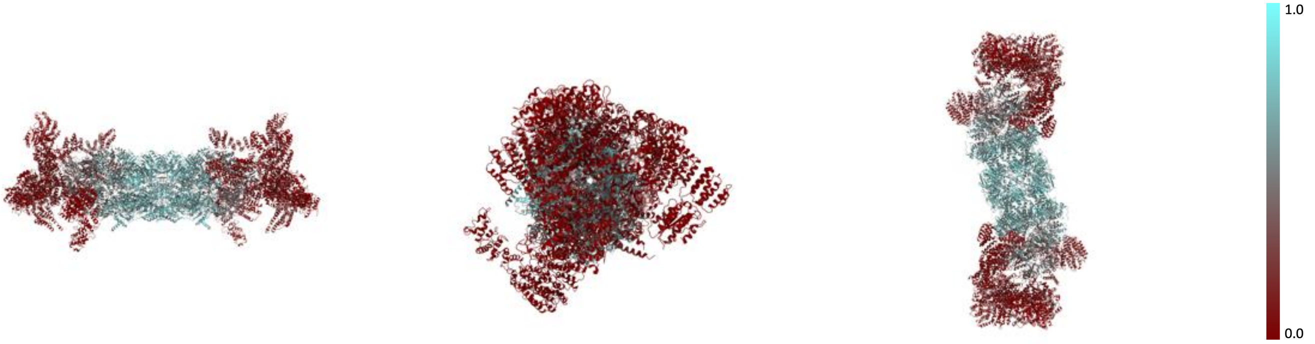
9.2 Q-score mapped to coordinate model ⓘ



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.

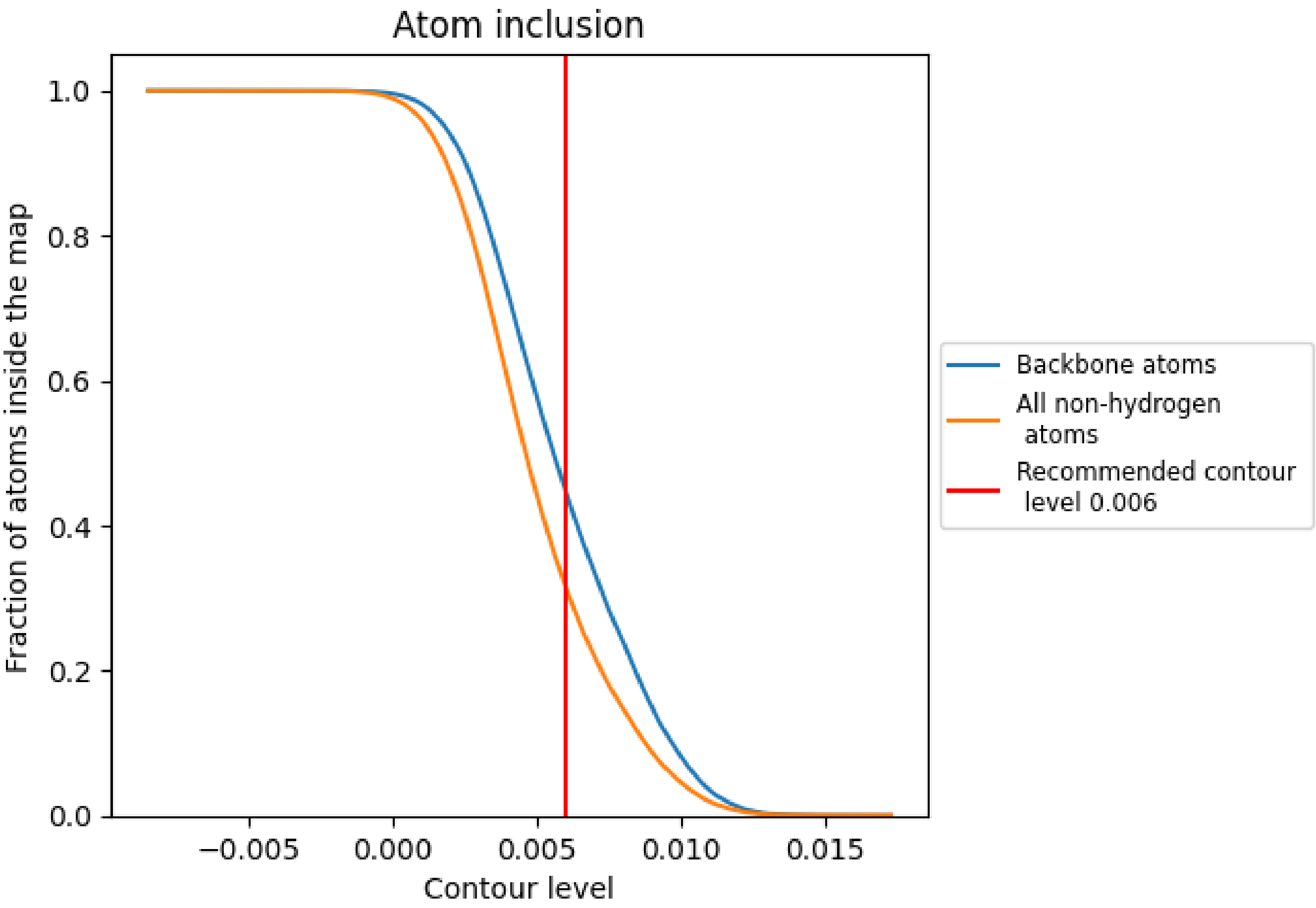
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 45% of all backbone atoms, 31% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3144	0.1560
AA	0.4868	0.2160
AB	0.4117	0.2020
AC	0.3345	0.1930
AD	0.3420	0.1850
AE	0.4168	0.2020
AF	0.4547	0.2150
AG	0.6041	0.3040
AH	0.6406	0.3170
AI	0.6142	0.2940
AJ	0.6441	0.2840
AK	0.5932	0.2860
AL	0.6419	0.3090
AM	0.6197	0.3060
AN	0.6667	0.3370
AO	0.6654	0.3340
AP	0.6836	0.3460
AQ	0.6450	0.3060
AR	0.6996	0.3400
AS	0.6542	0.3350
AT	0.6969	0.3370
AU	0.0778	0.0220
AV	0.0572	0.0280
AW	0.0573	0.0460
AX	0.0504	0.0730
AY	0.1303	0.0580
AZ	0.0551	0.0370
Aa	0.0492	0.0150
Ab	0.0187	0.0250
Ac	0.0923	0.0470
Ad	0.0279	0.0240
Ae	0.0364	0.0240
Af	0.0147	0.0040
BA	0.4857	0.2190
BB	0.4121	0.2050

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Chain	Atom inclusion	Q-score
BC	0.3358	0.1920
BD	0.3413	0.1850
BE	0.4168	0.2030
BF	0.4550	0.2140
BG	0.6024	0.3020
BH	0.6395	0.3200
BI	0.6142	0.2940
BJ	0.6453	0.2830
BK	0.5914	0.2870
BL	0.6414	0.3090
BM	0.6203	0.3050
BN	0.6688	0.3370
BO	0.6654	0.3360
BP	0.6842	0.3430
BQ	0.6436	0.3060
BR	0.7003	0.3400
BS	0.6548	0.3330
BT	0.6987	0.3370
BU	0.0783	0.0220
BV	0.0564	0.0290
BW	0.0556	0.0450
BX	0.0514	0.0730
BY	0.1313	0.0590
BZ	0.0542	0.0340
Ba	0.0512	0.0170
Bb	0.0187	0.0270
Bc	0.0914	0.0470
Bd	0.0275	0.0250
Be	0.0364	0.0180
Bf	0.0150	0.0040