wwPDB EM Validation Summary Report

Nov 7, 2022 – 10:04 AM JST

PDB ID	:	5GJR
EMDB ID	:	EMD-9512
Title	:	An atomic structure of the human 26S proteasome
Authors	:	Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G.
Deposited on	:	2016-07-01
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

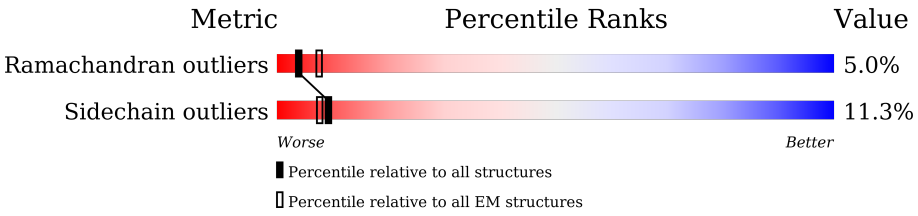
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	I	440	13% 62% 16% • 18%
1	w	440	13% 61% 18% • 18%
2	H	433	10% 64% 21% • 12%
2	v	433	10% 65% 20% • 12%
3	L	389	11% 73% 20% • •
3	z	389	11% 73% 19% • •
4	0	439	10% 64% 20% • 14%
4	M	439	10% 64% 20% • 14%
5	J	406	• 66% 19% • 12%

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Mol	Chain	Length	Quality of chain
5	x	406	66% 19% 12%
6	K	418	6% 67% 22% 9%
6	y	418	6% 67% 22% 9%
7	1	953	40% 80% 5% 14%
7	N	953	40% 80% 5% 14%
8	2	376	54% 89% 9%
8	O	376	54% 89% 9%
9	3	456	22% 83% 7% 9%
9	P	456	22% 83% 7% 9%
10	4	422	33% 83% 14%
10	Q	422	33% 83% 14%
11	5	389	11% 82% 13%
11	R	389	11% 83% 13%
12	6	525	31% 75% 5% 20%
12	S	525	30% 75% 5% 20%
13	7	350	48% 64% 8% 26%
13	T	350	48% 64% 8% 26%
14	8	324	21% 76% 10% 13%
14	U	324	21% 76% 10% 13%
15	9	310	20% 70% 11% 17%
15	V	310	20% 70% 11% 17%
16	AA	377	50% 45% 6% 49%
16	W	377	50% 44% 6% 49%
17	AB	70	51% 69% 16% 16%
17	Y	70	51% 69% 16% 16%

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Mol	Chain	Length	Quality of chain
18	AC	908	77% 75% 6% 19%
18	Z	908	77% 75% 6% 19%
19	B	246	92% 7%
19	h	246	94% 5%
20	C	234	95%
20	i	234	91% 7%
21	D	261	91% 5%
21	j	261	91%
22	E	248	91% 7%
22	k	248	92% 6%
23	F	241	94%
23	l	241	93%
24	G	263	87% 10%
24	m	263	85% 5% 10%
25	X	255	91% 5%
25	n	255	91% 5% 5%
26	a	239	82% 15%
26	o	239	82% 15%
27	b	277	75% 21%
27	p	277	76% 21%
28	c	205	94% 5%
28	q	205	94% 5%
29	d	201	96%
29	r	201	96%
30	e	263	75% 24%

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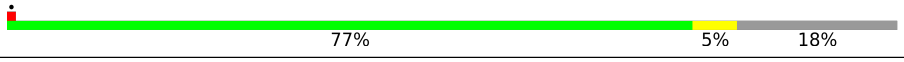
Mol	Chain	Length	Quality of chain
30	s	263	
31	f	241	
31	t	241	
32	g	264	
32	u	264	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 142753 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 protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	359	Total	C	N	O	S	0	0
			2720	1708	465	535	12		
1	w	359	Total	C	N	O	S	0	0
			2720	1708	465	535	12		

- Molecule 2 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		
2	v	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		

- Molecule 3 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		
3	z	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 4 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		
4	0	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 5 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	358	Total	C	N	O	S	0	0
			2820	1780	506	518	16		
5	x	358	Total	C	N	O	S	0	0
			2820	1780	506	518	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		
6	y	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	821	Total	C	N	O	S	0	0
			5449	3491	931	1009	18		
7	1	821	Total	C	N	O	S	0	0
			5449	3491	931	1009	18		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	372	Total	C	N	O	S	0	0
			2369	1515	405	438	11		
8	2	372	Total	C	N	O	S	0	0
			2375	1521	405	438	11		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	413	Total	C	N	O	S	0	0
			2832	1821	489	516	6		
9	3	413	Total	C	N	O	S	0	0
			2831	1820	489	516	6		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	421	Total	C	N	O	S	0	0
			2956	1866	512	569	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	421	Total	C	N	O	S	0	0
			2956	1866	512	569	9		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	376	Total	C	N	O	S	0	0
			2767	1794	461	504	8		
11	5	376	Total	C	N	O	S	0	0
			2770	1796	461	504	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	421	Total	C	N	O	S	0	0
			2723	1737	484	499	3		
12	6	421	Total	C	N	O	S	0	0
			2732	1741	487	501	3		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	258	Total	C	N	O	S	0	0
			1699	1099	280	315	5		
13	7	258	Total	C	N	O	S	0	0
			1699	1099	280	315	5		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		
14	8	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	257	Total	C	N	O	S	0	0
			2011	1276	341	377	17		
15	9	257	Total	C	N	O	S	0	0
			2009	1274	341	377	17		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		
16	AA	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		

- Molecule 17 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	59	Total	C	N	O	0	0
			316	191	60	65		
17	AB	59	Total	C	N	O	0	0
			316	191	60	65		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Z	732	Total	C	N	O	0	0
			3608	2144	732	732		
18	AC	732	Total	C	N	O	0	0
			3608	2144	732	732		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	244	Total	C	N	O	S	0	0
			1845	1171	309	352	13		
19	h	244	Total	C	N	O	S	0	0
			1853	1177	311	352	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	231	Total	C	N	O	S	0	0
			1737	1106	289	336	6		
20	i	231	Total	C	N	O	S	0	0
			1744	1112	290	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	250	Total	C	N	O	S	0	0
			1916	1206	330	372	8		
21	j	250	Total	C	N	O	S	0	0
			1913	1203	330	372	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	243	Total	C	N	O	S	0	0
			1724	1068	312	339	5		
22	k	243	Total	C	N	O	S	0	0
			1691	1051	309	327	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F	234	Total	C	N	O	S	0	0
			1766	1108	290	357	11		
23	l	234	Total	C	N	O	S	0	0
			1726	1107	291	317	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		
25	n	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
30	s	201	Total	C	N	O	S	0	0
			1551	977	273	292	9		

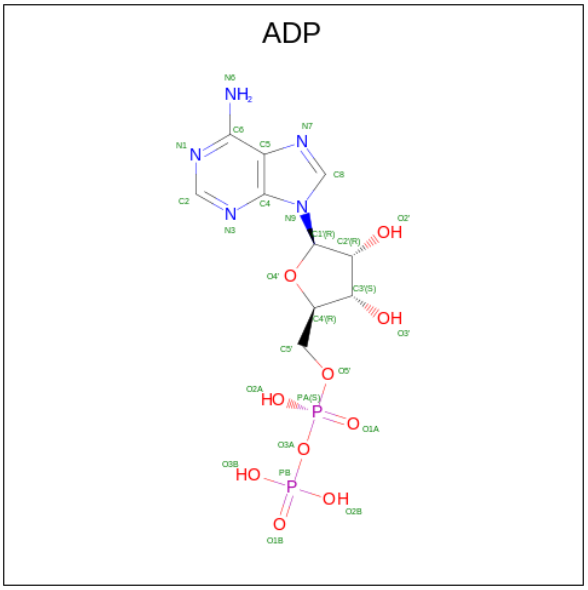
- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		
31	t	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	216	Total	C	N	O	S	0	0
			1672	1055	286	319	12		
32	u	217	Total	C	N	O	S	0	0
			1678	1058	290	318	12		

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
33	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	v	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

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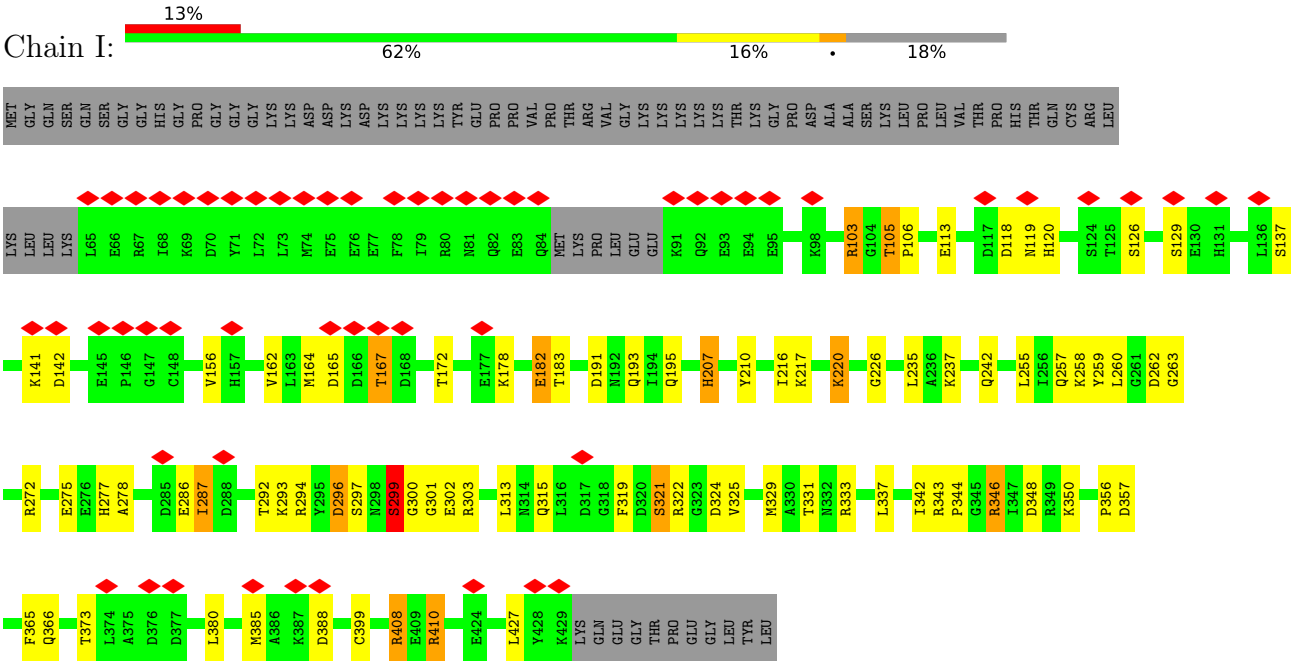
Mol	Chain	Residues	Atoms					AltConf
33	x	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	y	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	z	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	0	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

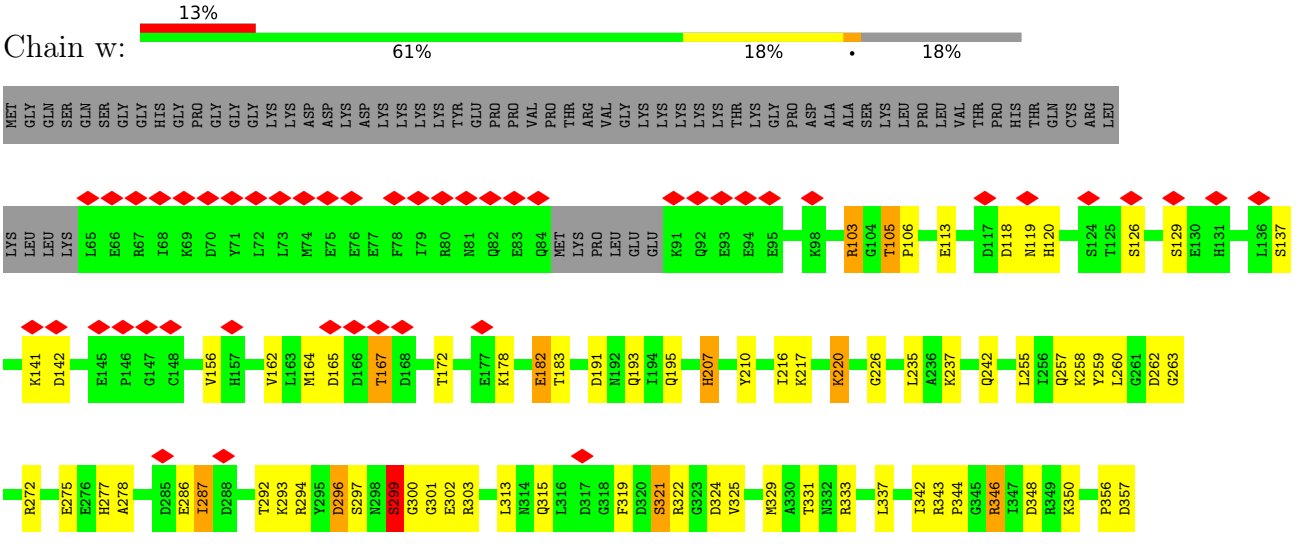
• Molecule 1: 26S protease regulatory subunit 4

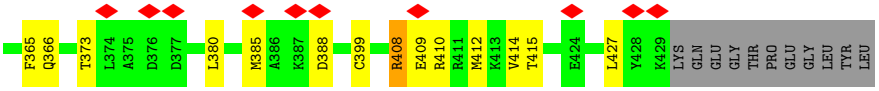
Chain I:



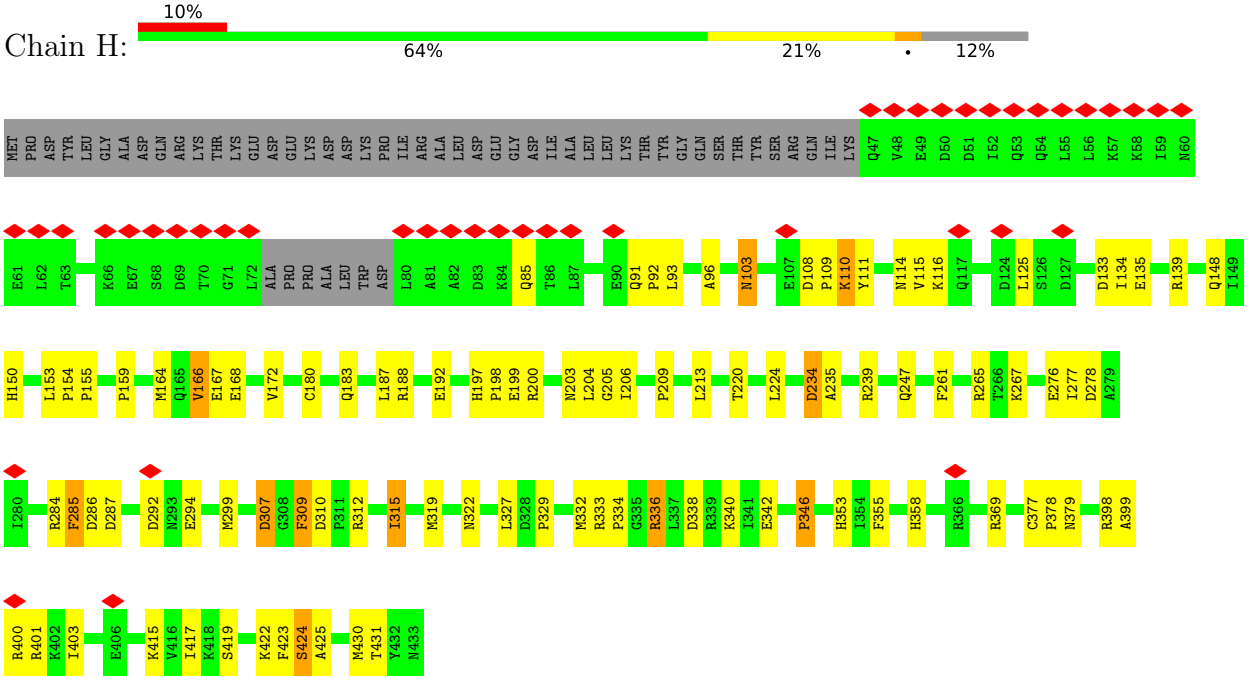
• Molecule 1: 26S protease regulatory subunit 4

Chain w:

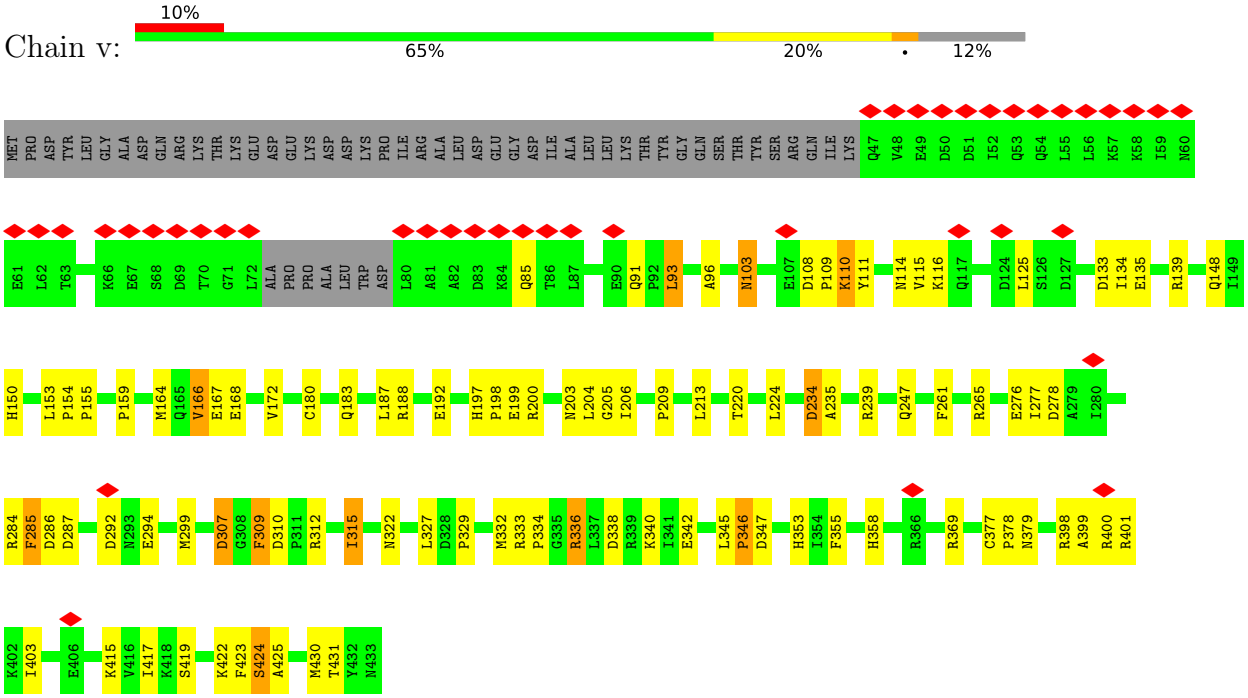




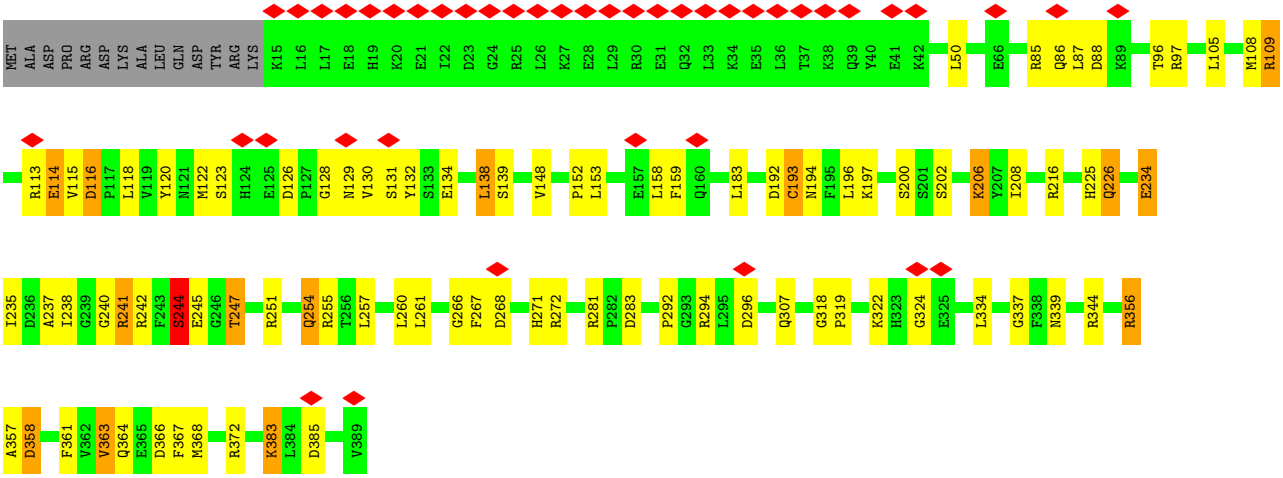
• Molecule 2: 26S protease regulatory subunit 7



• Molecule 2: 26S protease regulatory subunit 7

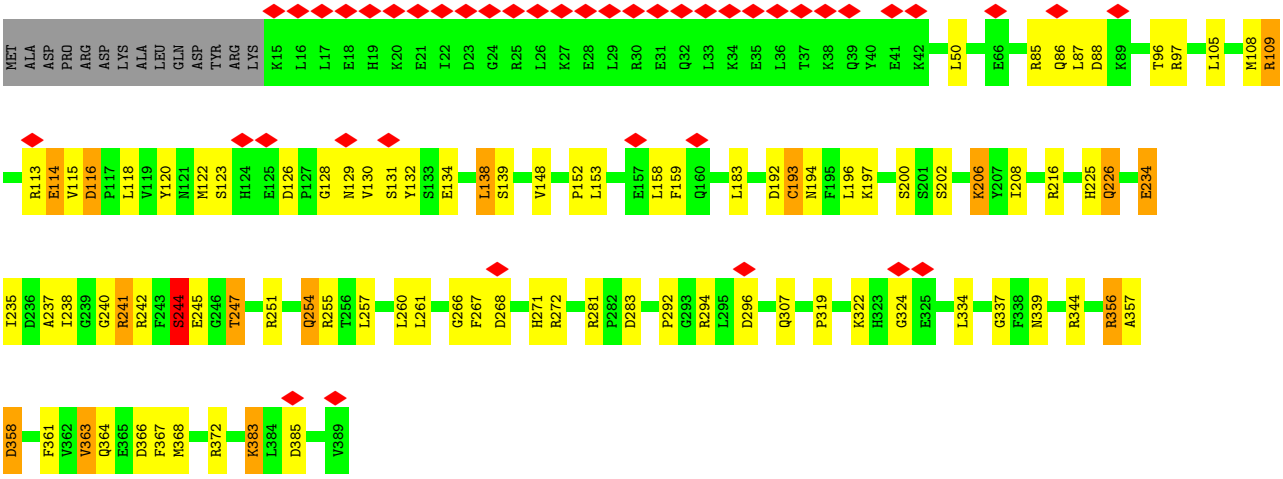


• Molecule 3: 26S protease regulatory subunit 10B



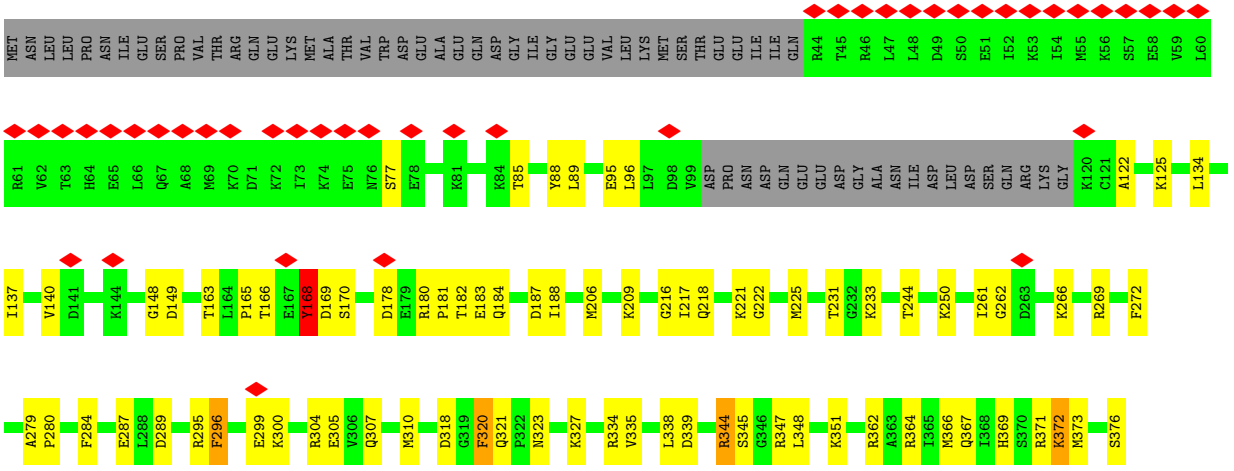
• Molecule 3: 26S protease regulatory subunit 10B

Chain z:

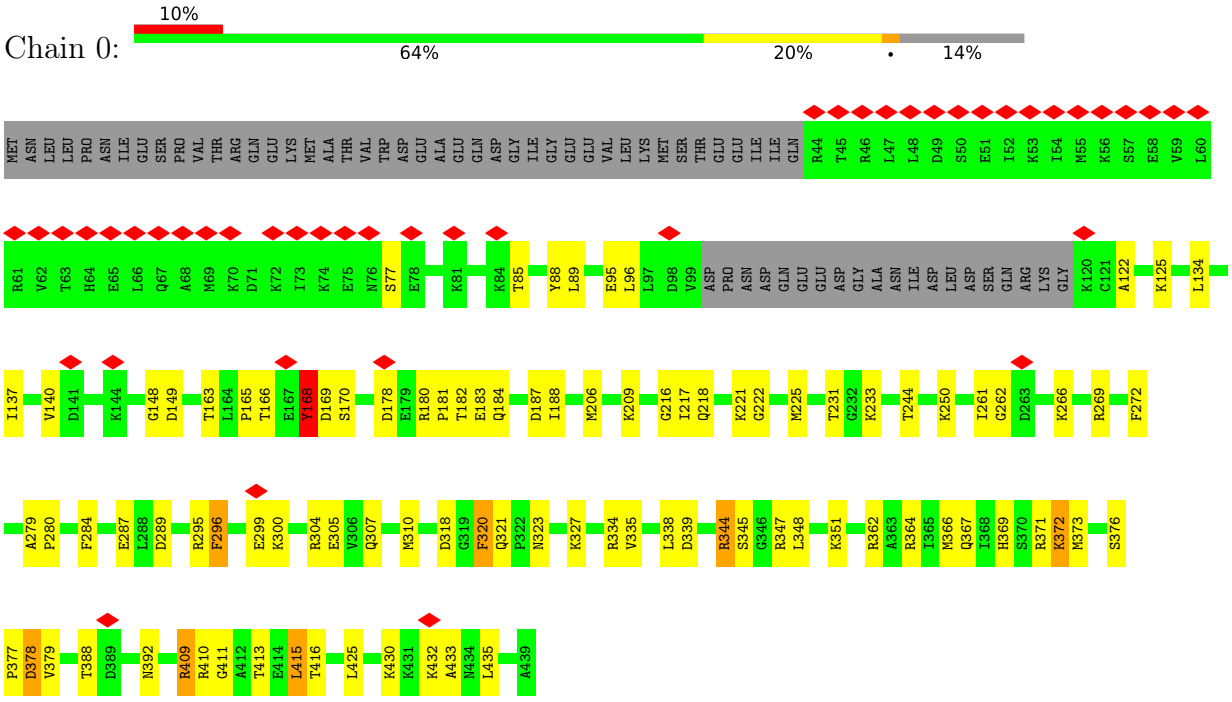


• Molecule 4: 26S protease regulatory subunit 6A

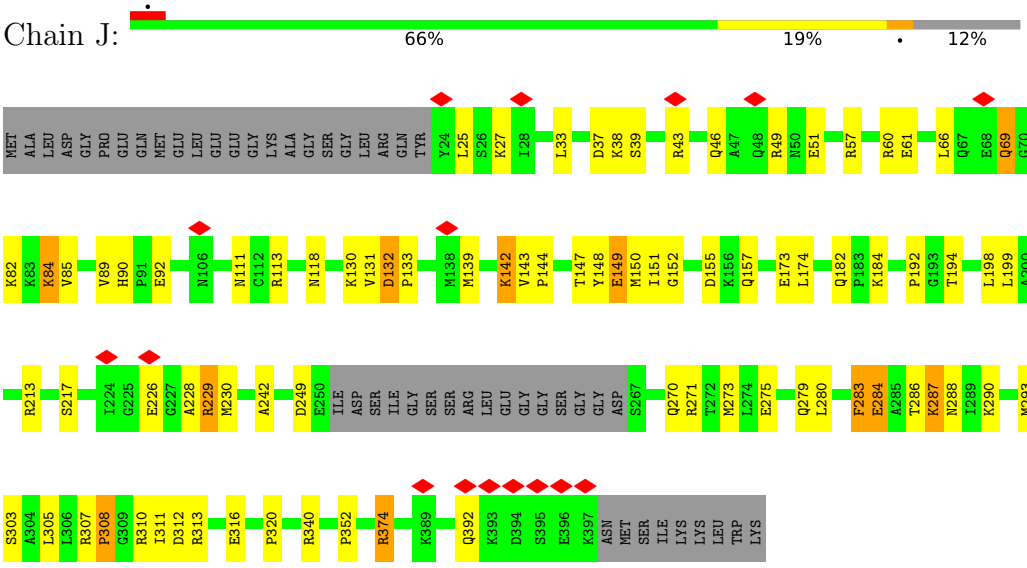
Chain M:



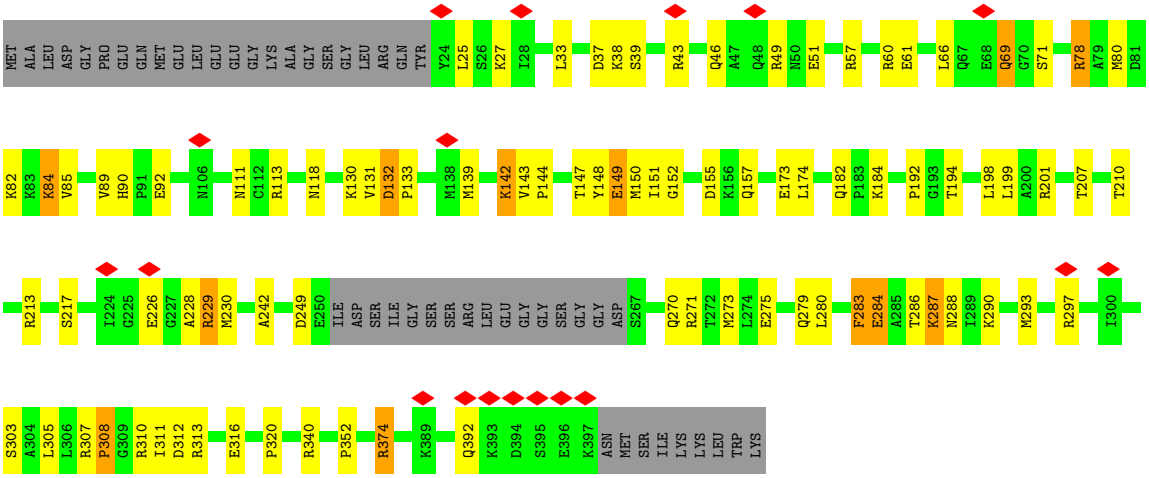
• Molecule 4: 26S protease regulatory subunit 6A



• Molecule 5: 26S protease regulatory subunit 8

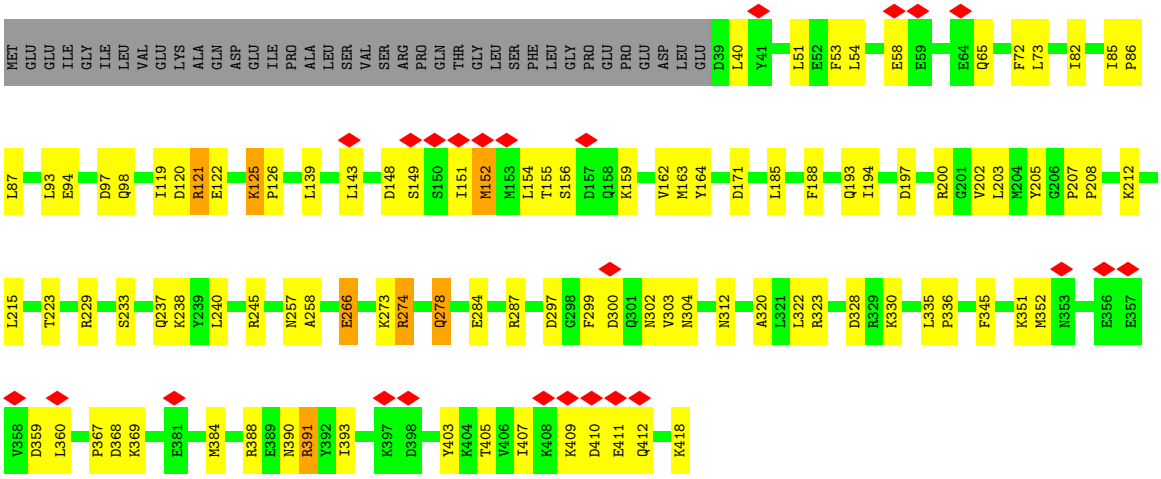


• Molecule 5: 26S protease regulatory subunit 8



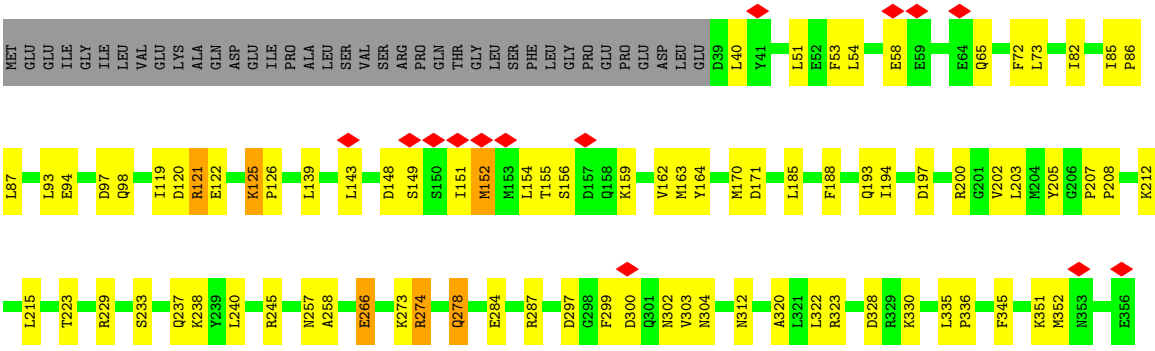
• Molecule 6: 26S protease regulatory subunit 6B

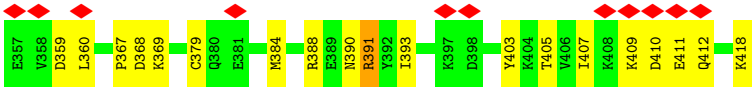
Chain K:



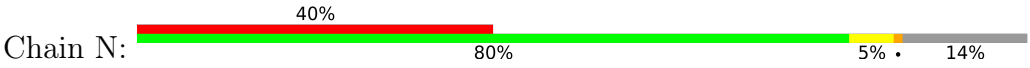
• Molecule 6: 26S protease regulatory subunit 6B

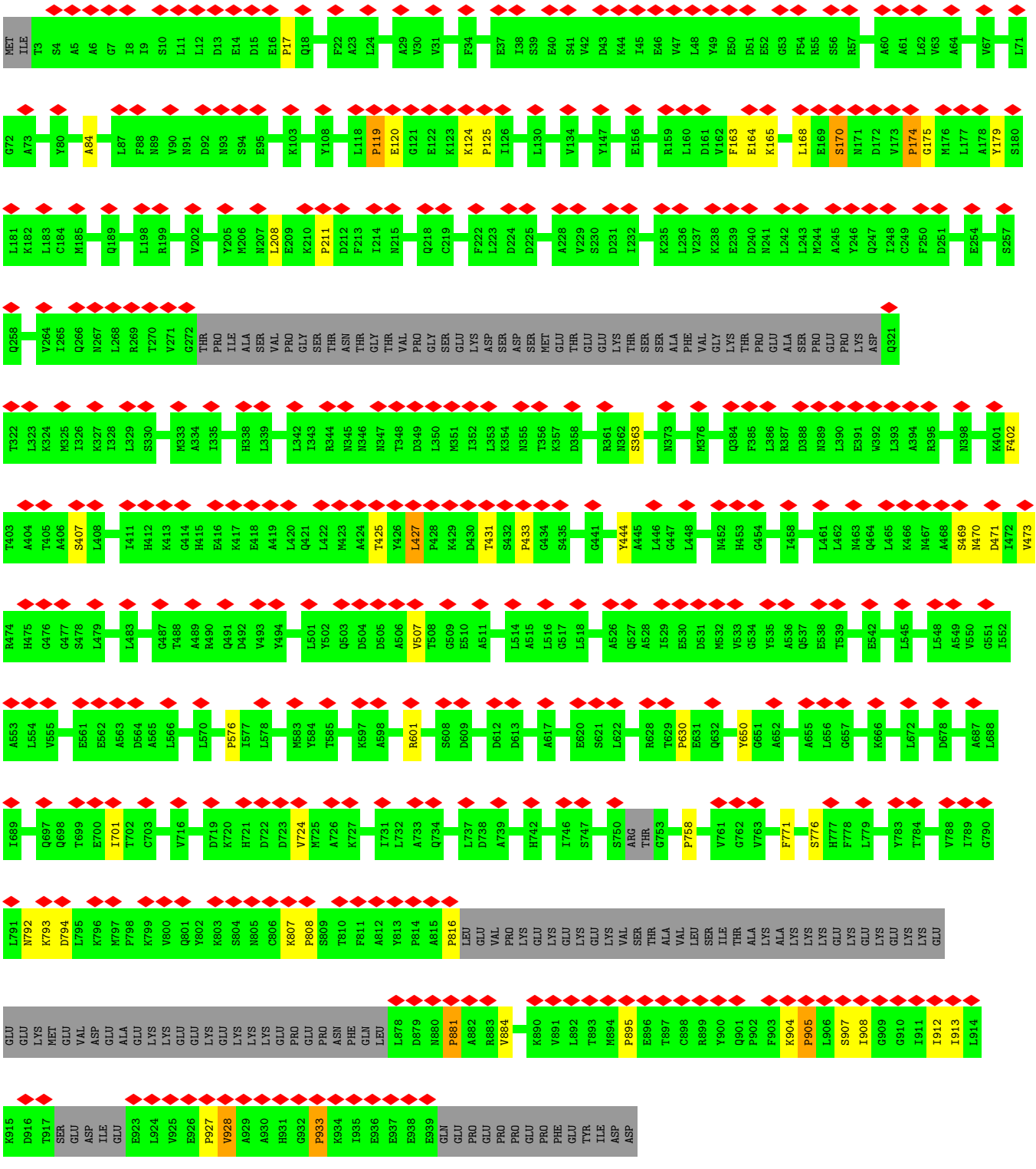
Chain y:





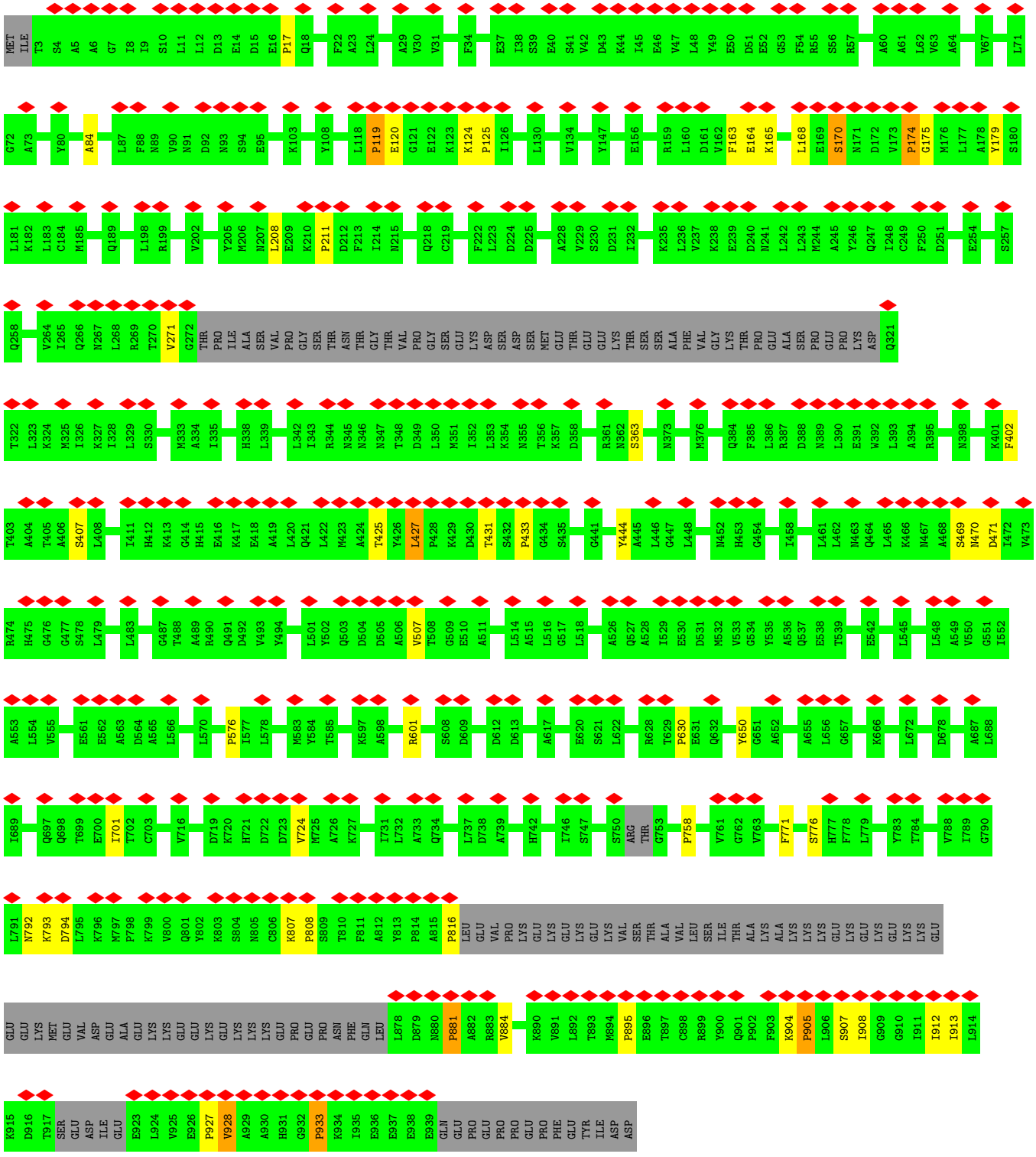
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1





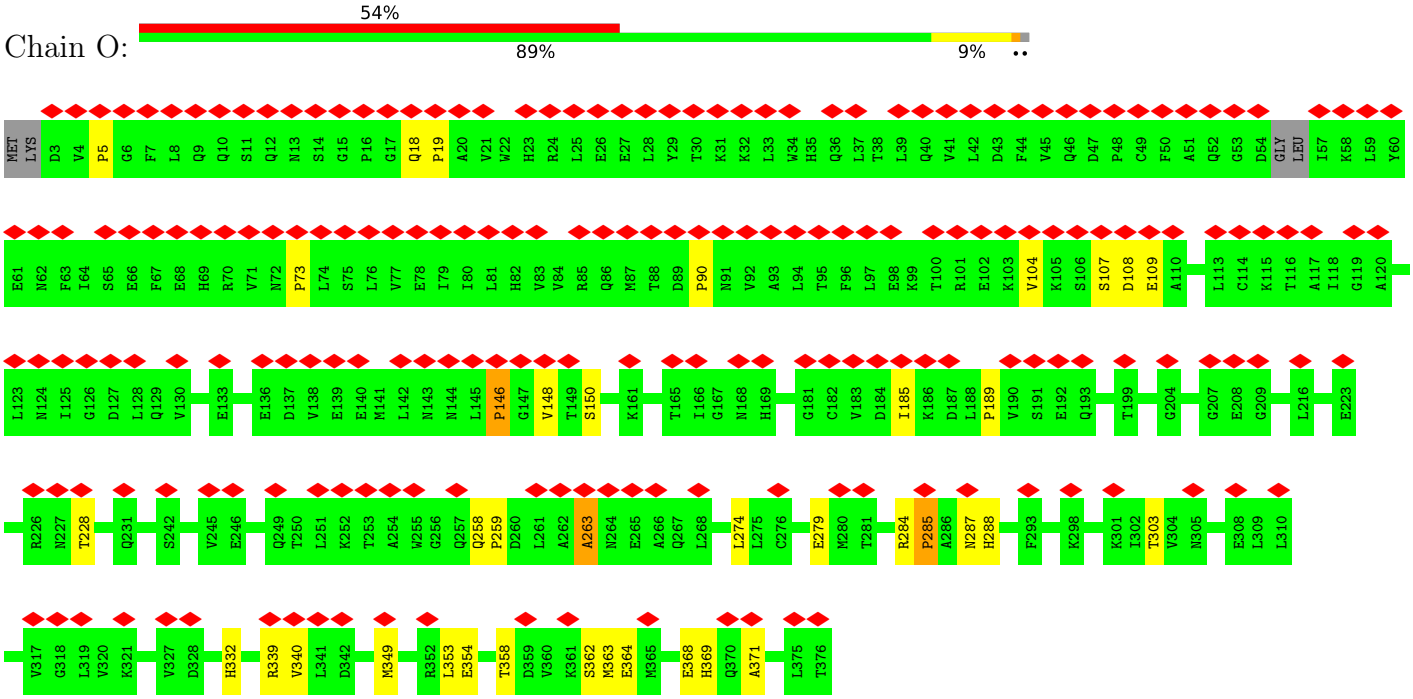
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1

Chain 1:



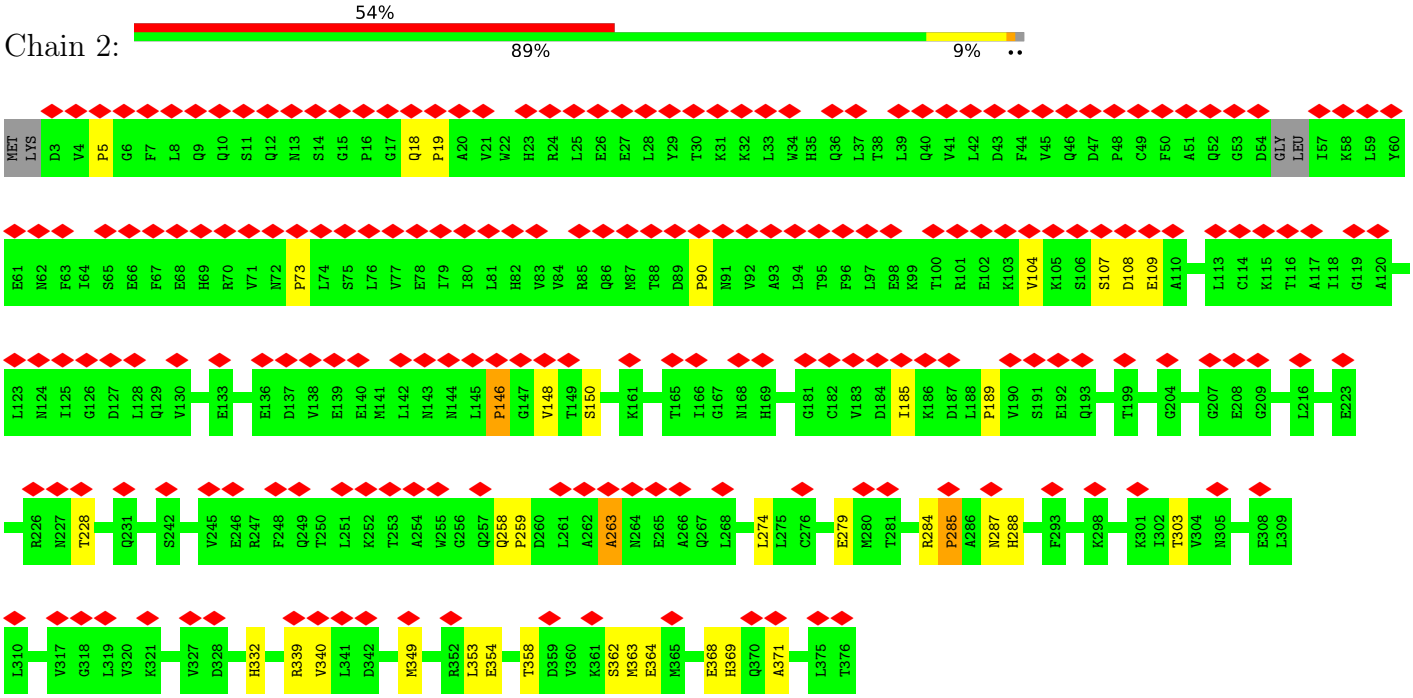
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

Chain O:



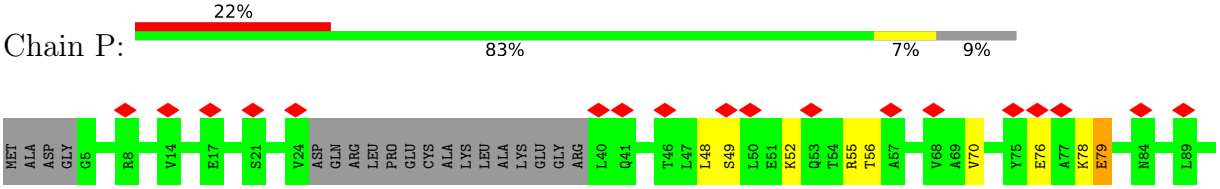
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

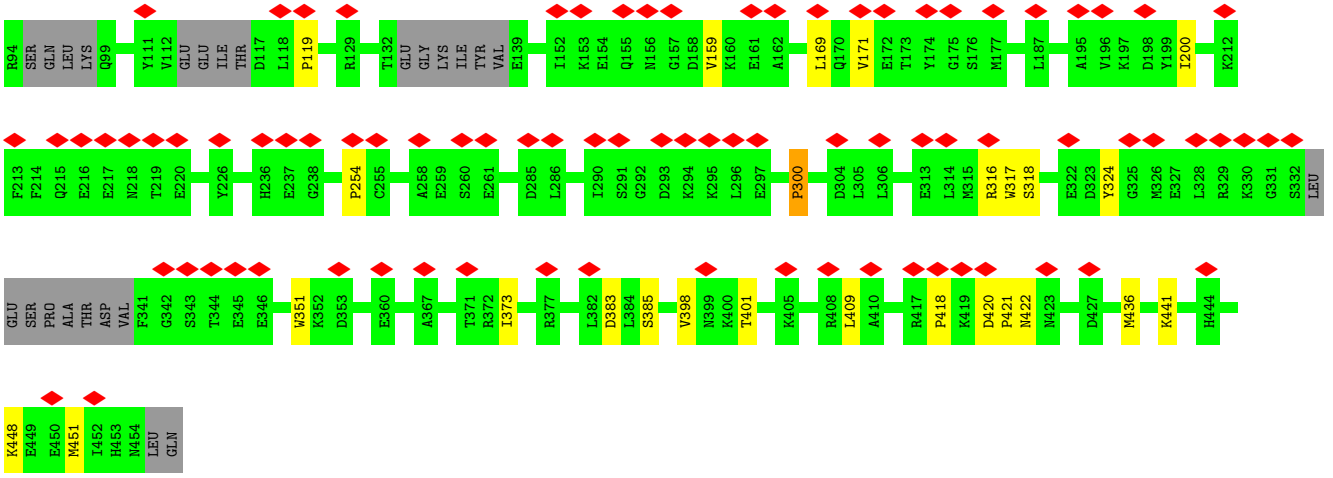
Chain 2:



• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

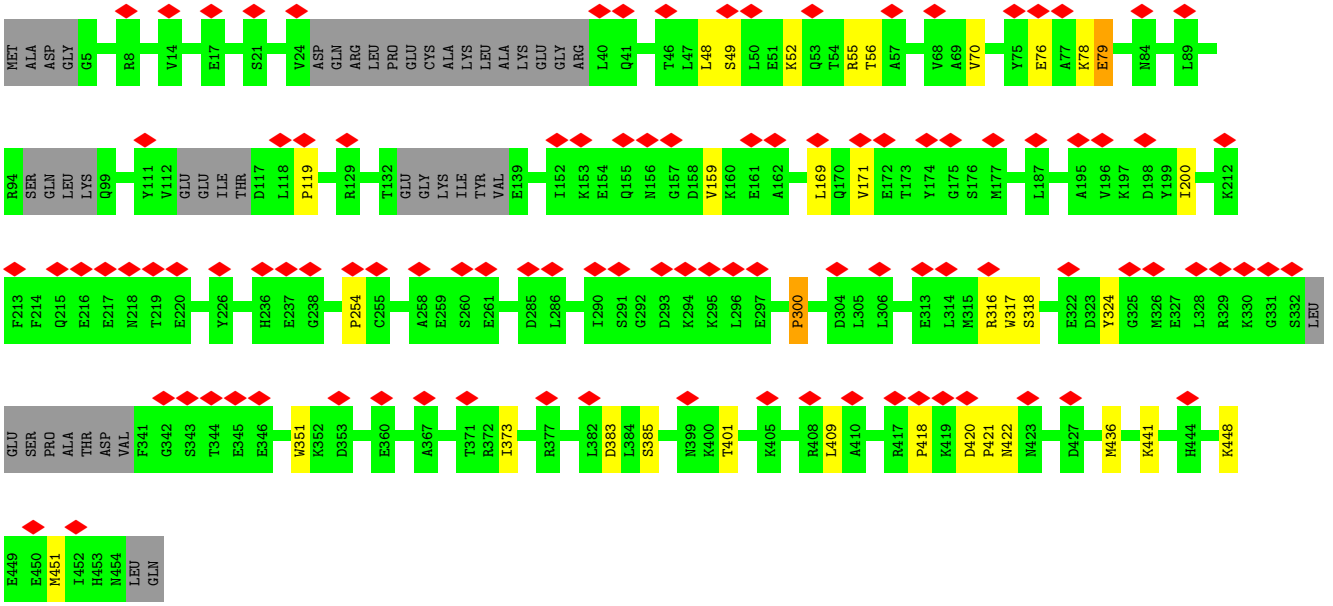
Chain P:





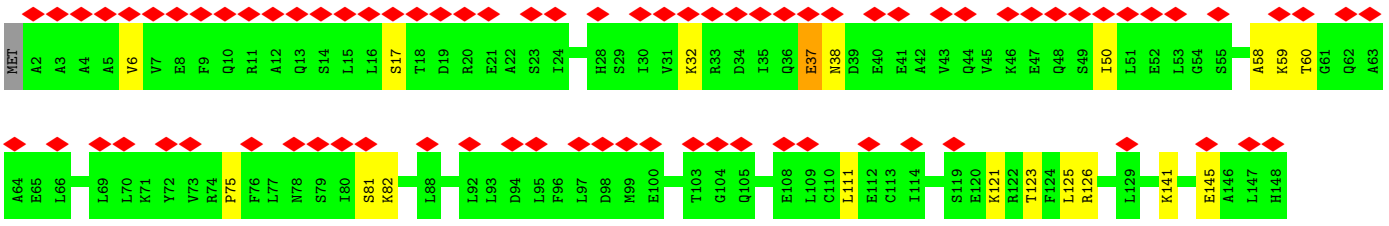
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

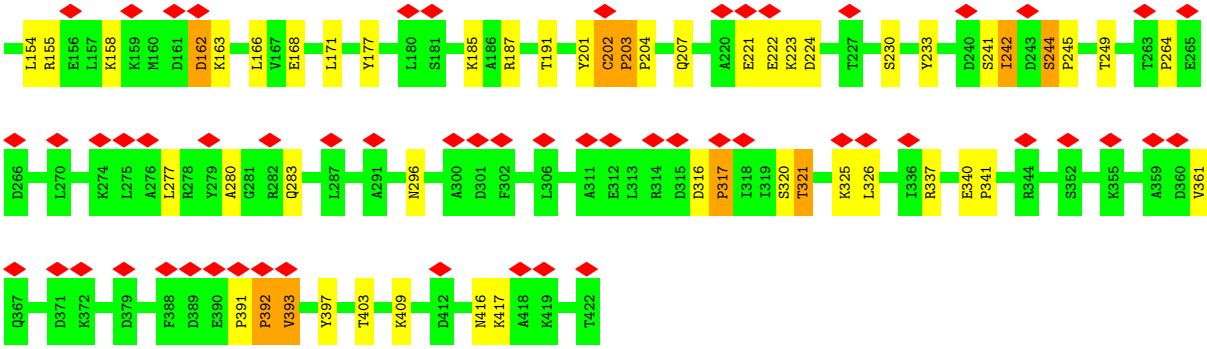
Chain 3:



• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

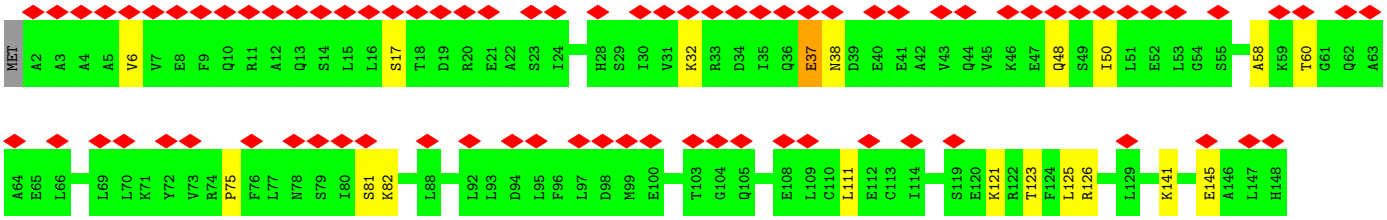
Chain Q:





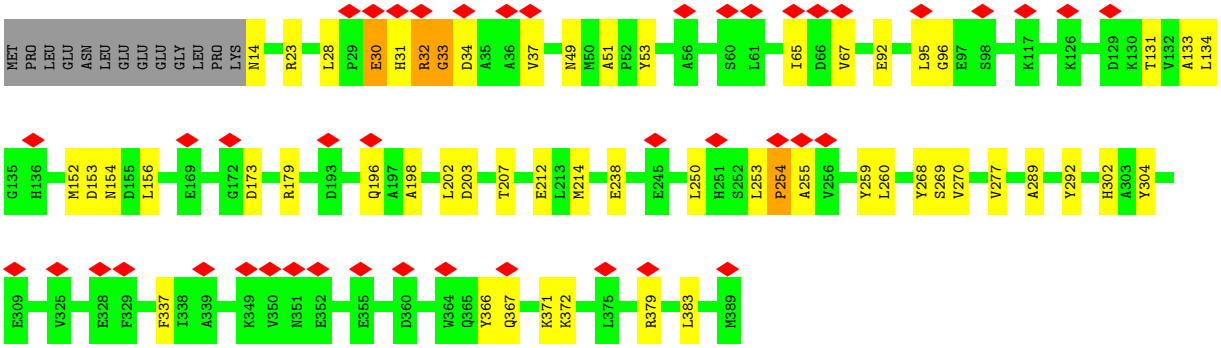
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

Chain 4:



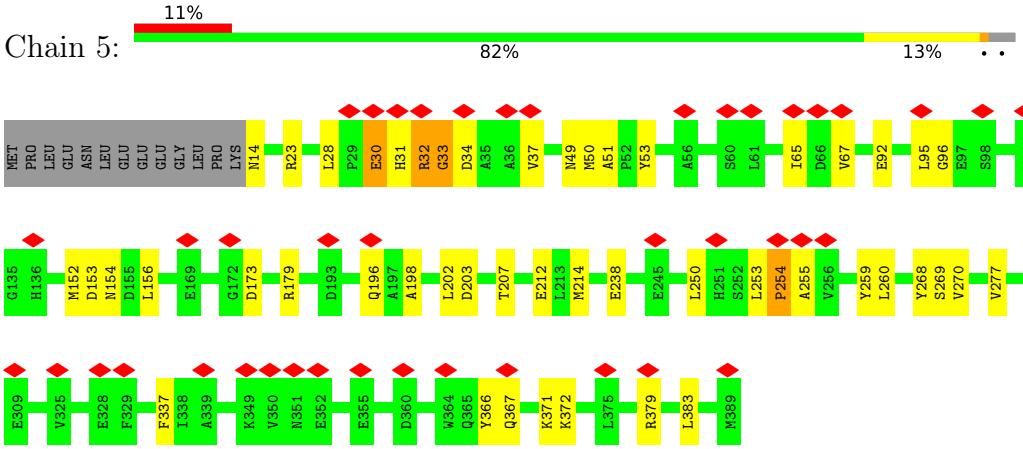
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

Chain R:



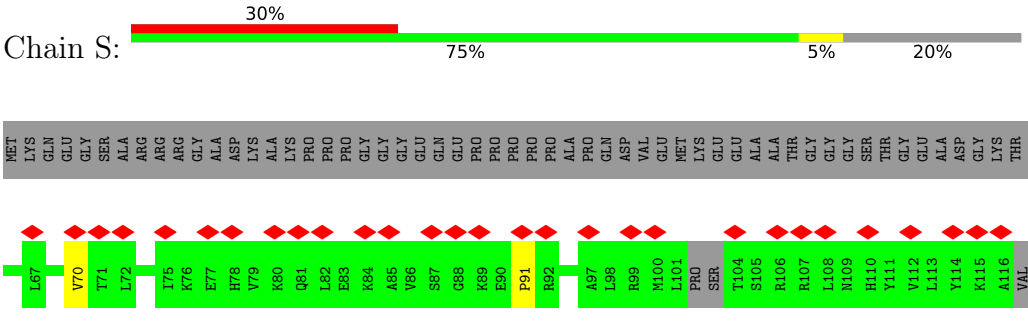
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

Chain 5:



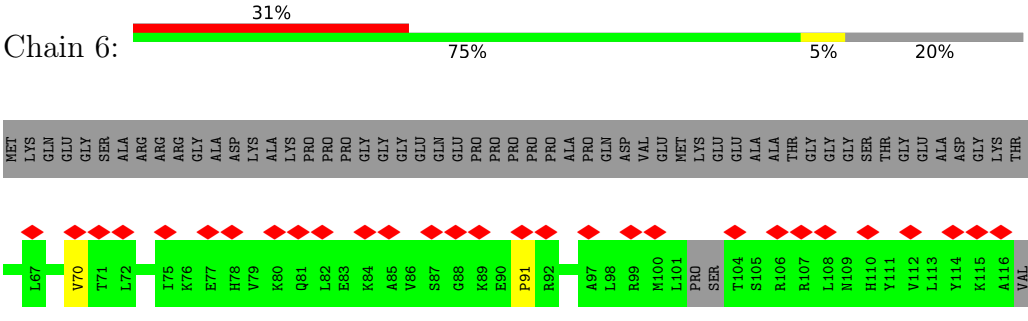
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 3

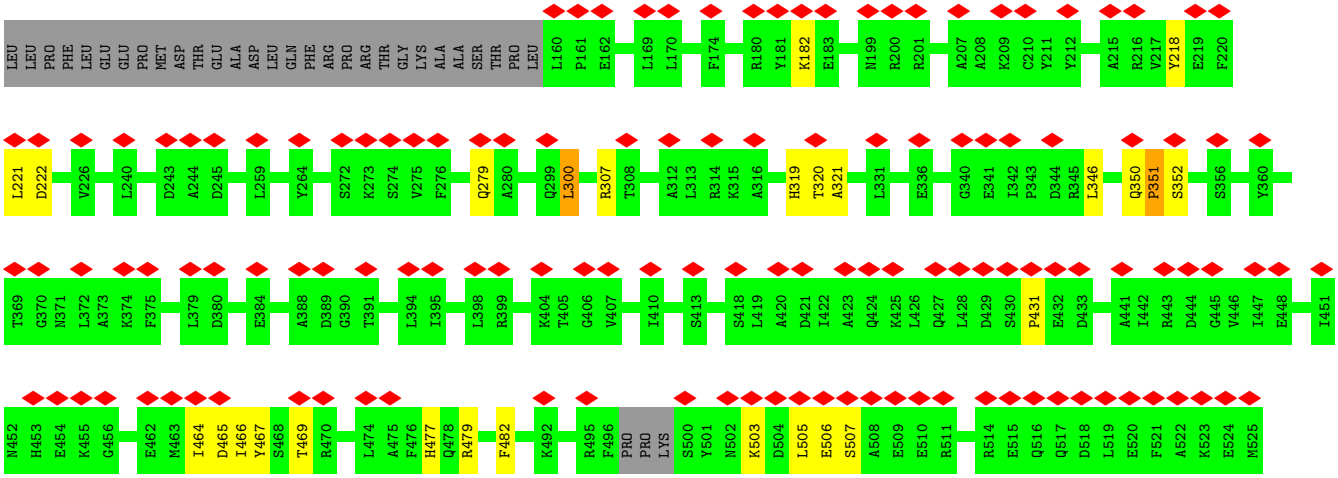
Chain S:



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

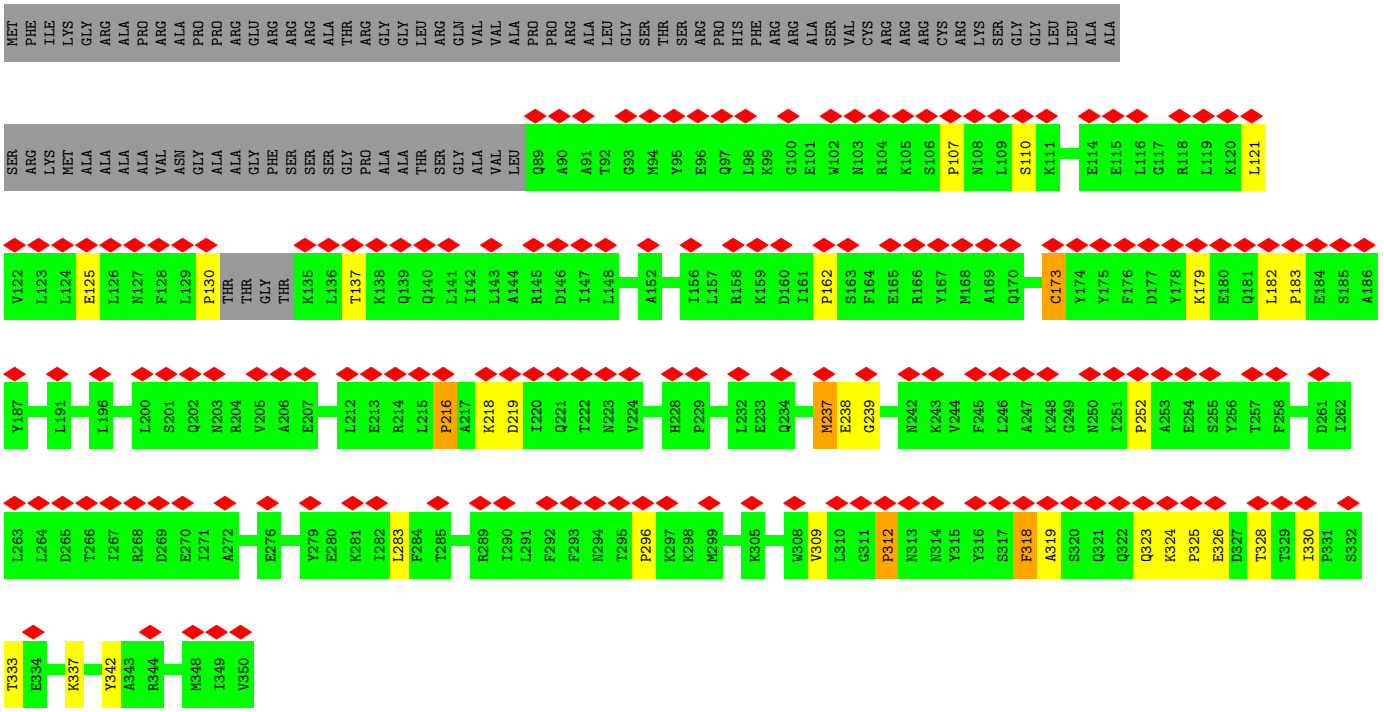
Chain 6:





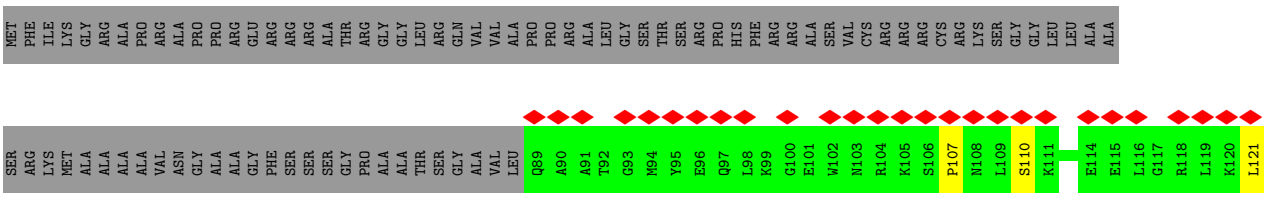
• Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

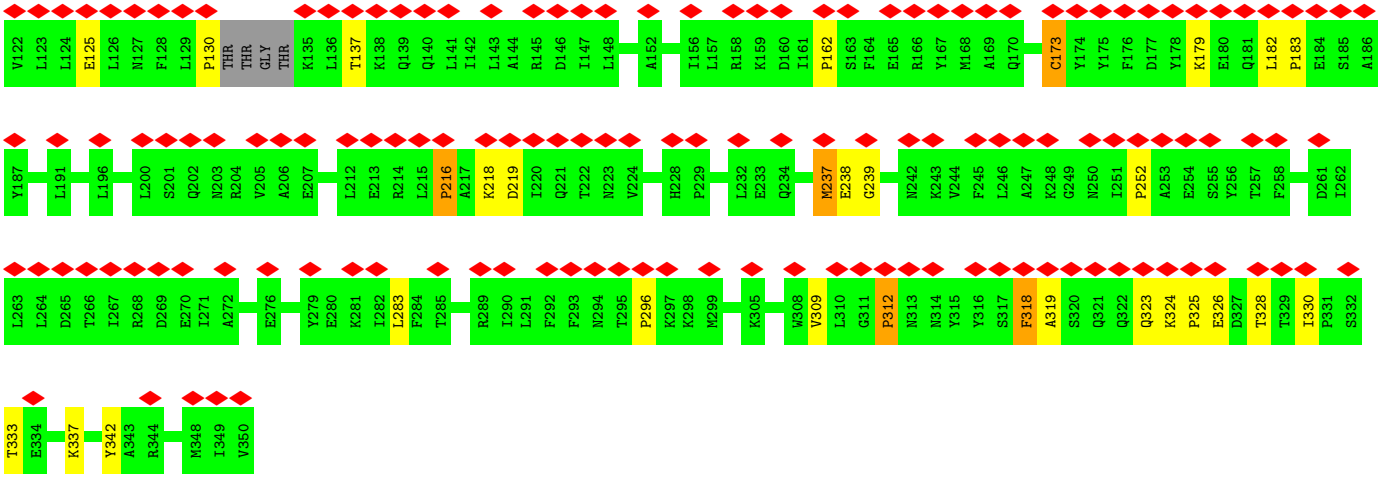
Chain T:



• Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

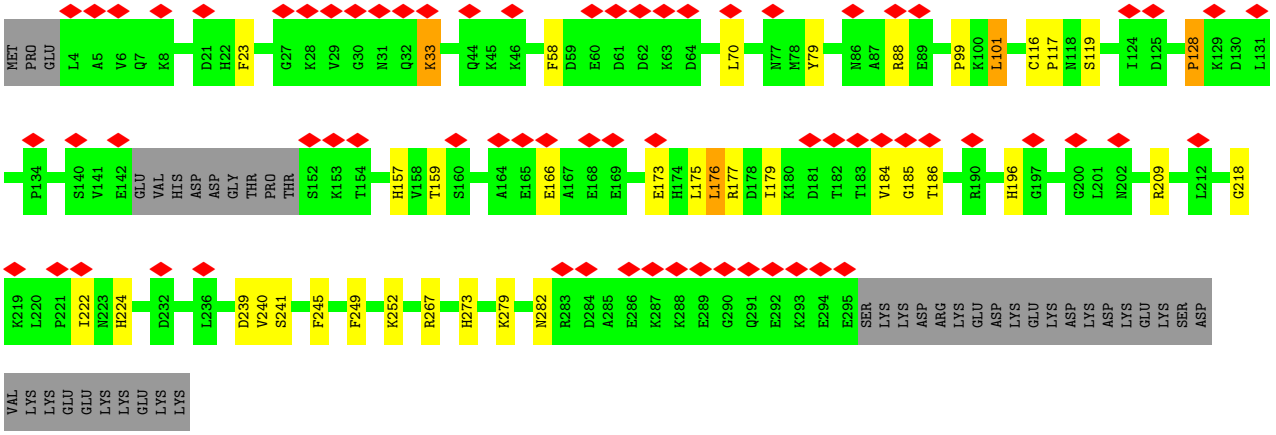
Chain 7:





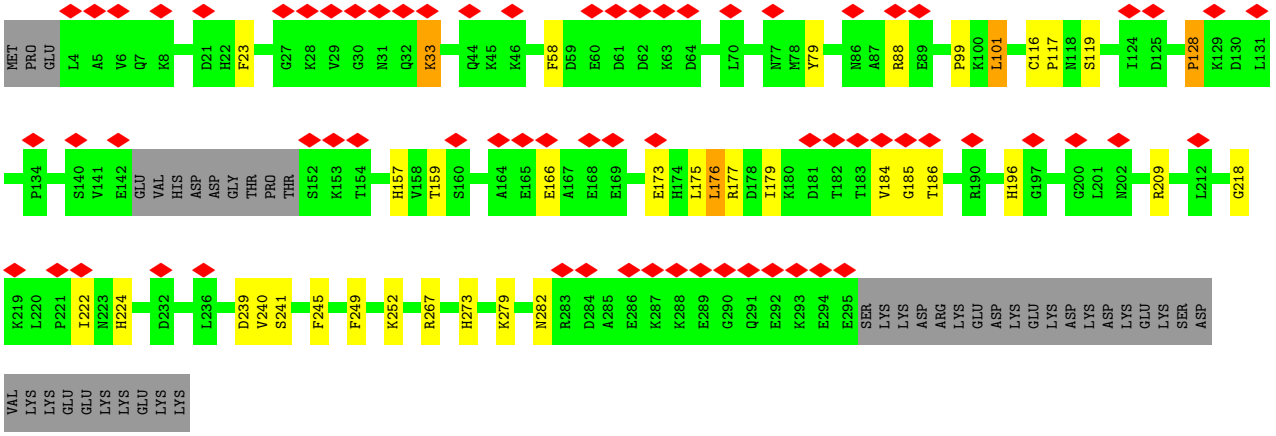
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 7

Chain U:



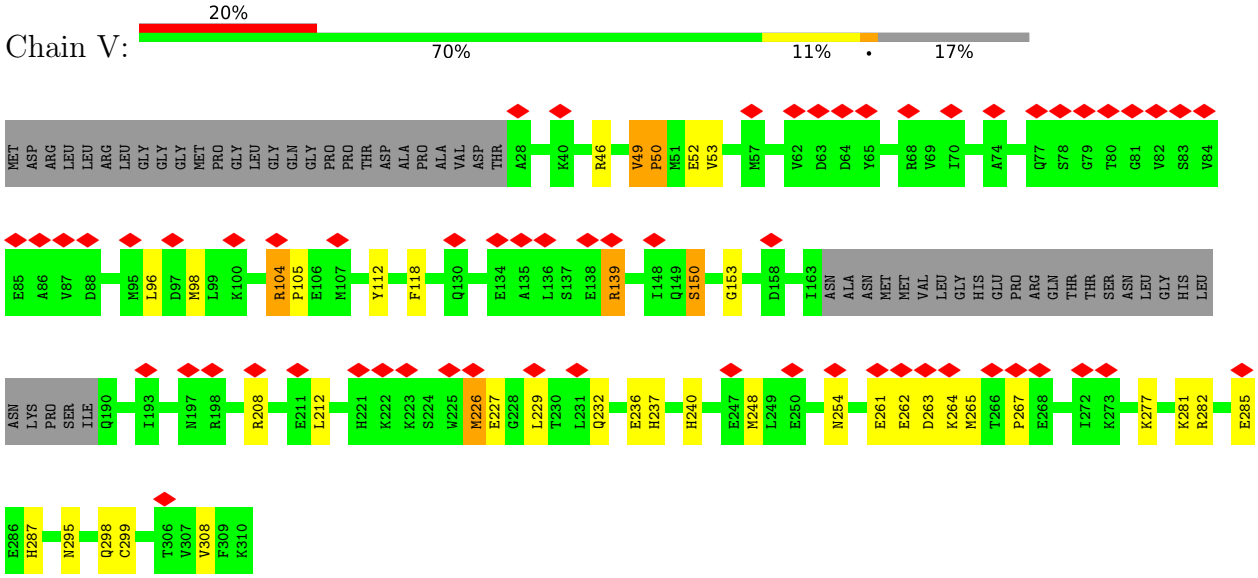
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 7

Chain 8:



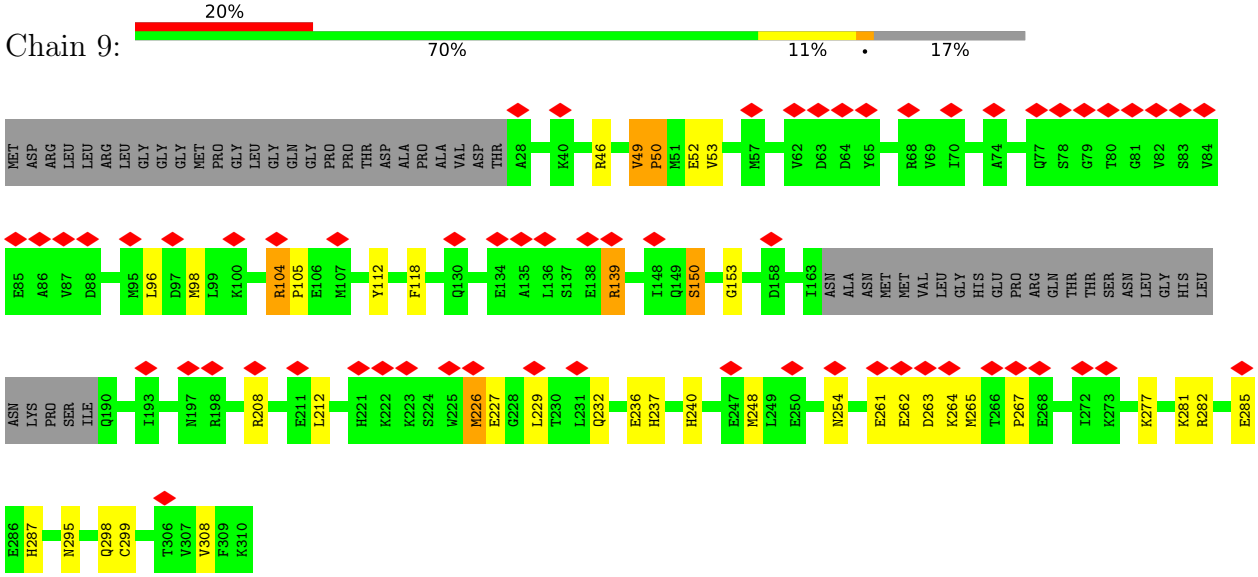
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

Chain V:



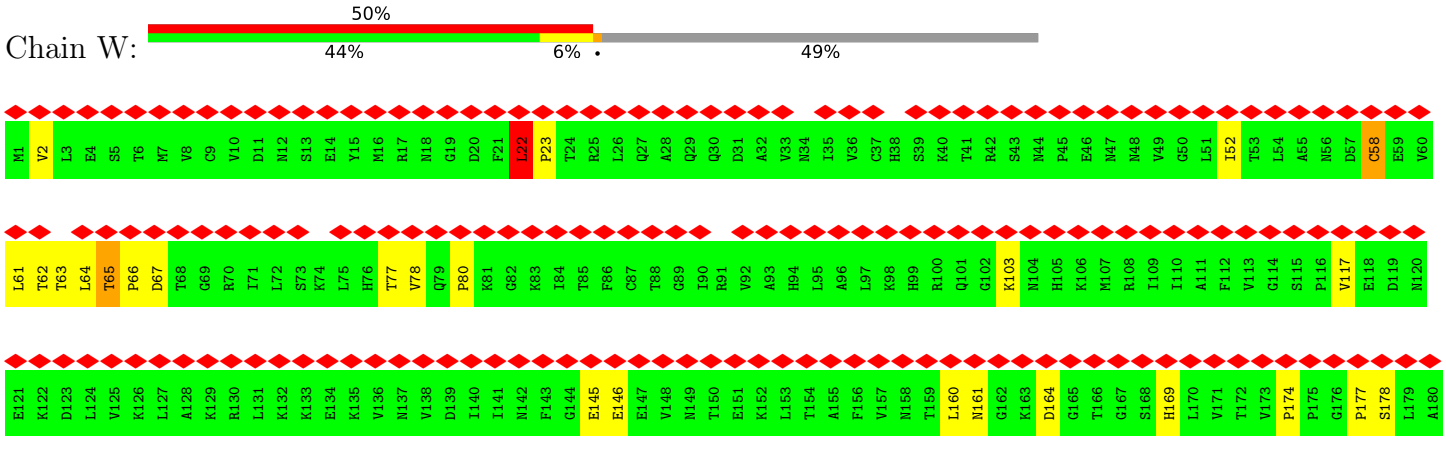
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

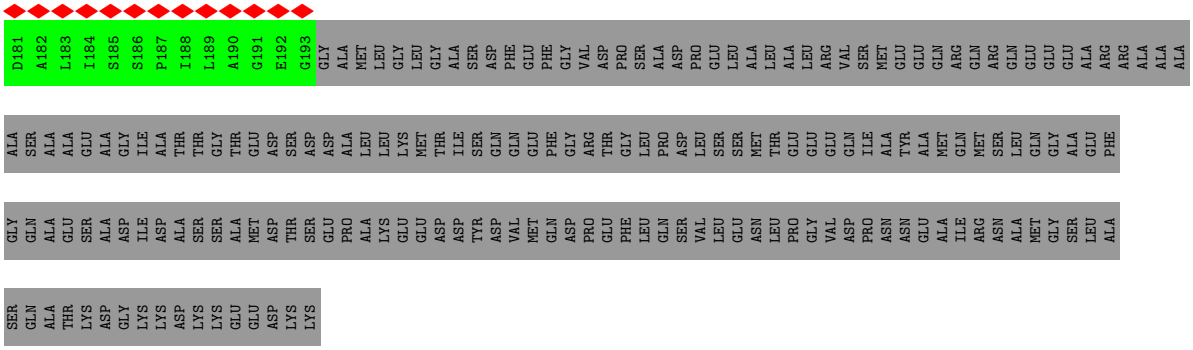
Chain 9:



• Molecule 16: 26S proteasome non-ATPase regulatory subunit 4

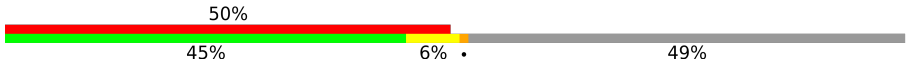
Chain W:

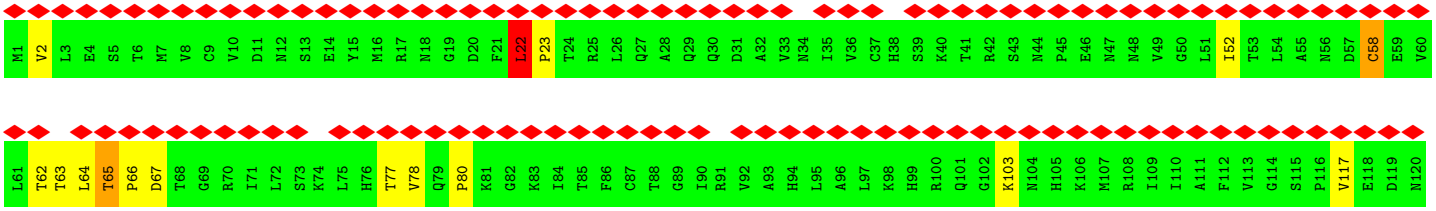


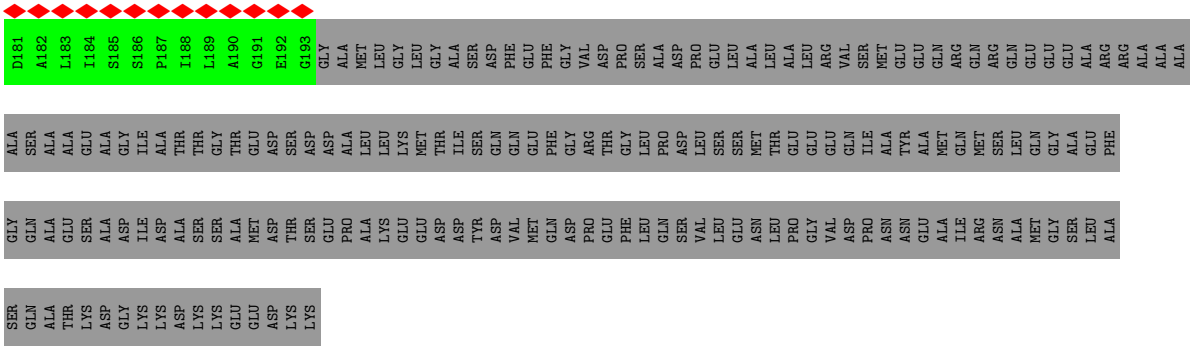


• Molecule 16: 26S proteasome non-ATPase regulatory subunit 4

Chain AA:

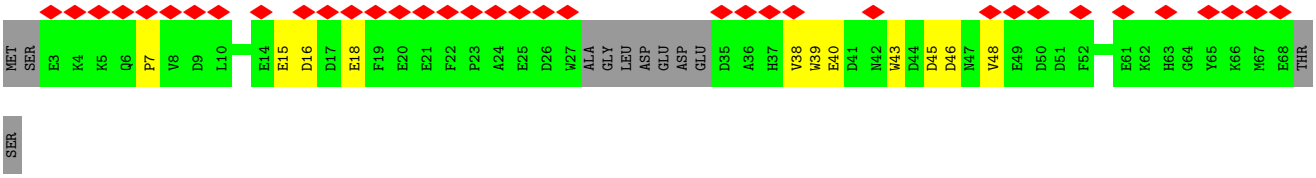






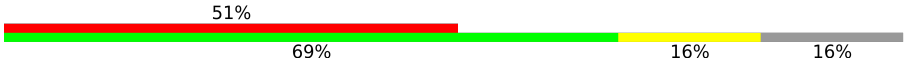
• Molecule 17: 26S proteasome complex subunit DSS1

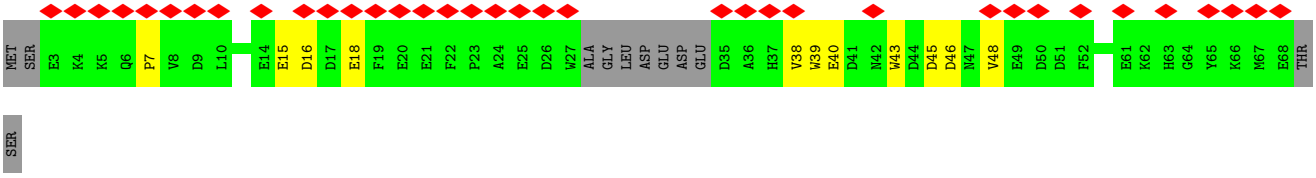
Chain Y:



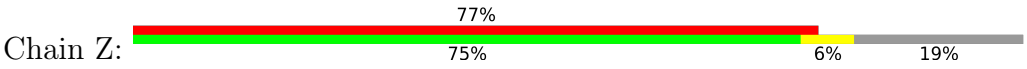
• Molecule 17: 26S proteasome complex subunit DSS1

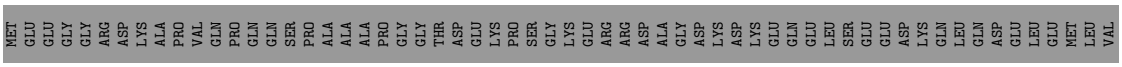
Chain AB:

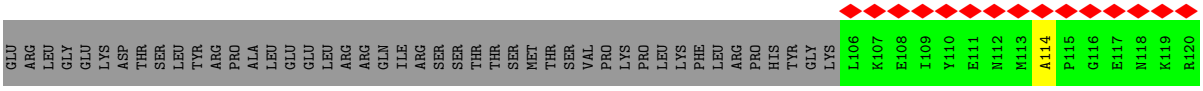


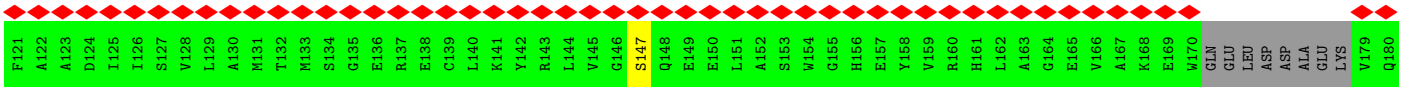


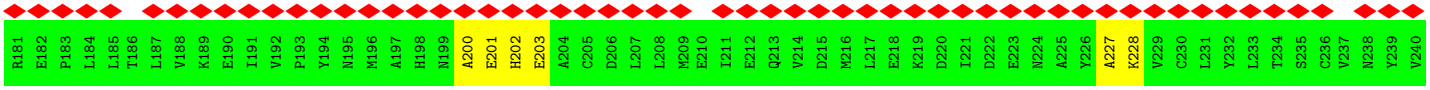
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

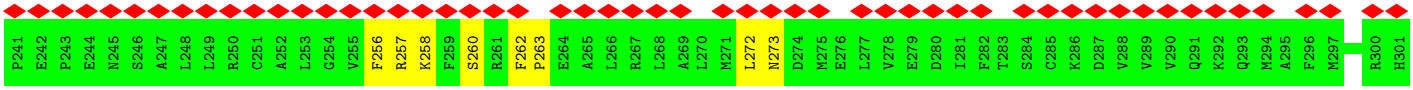


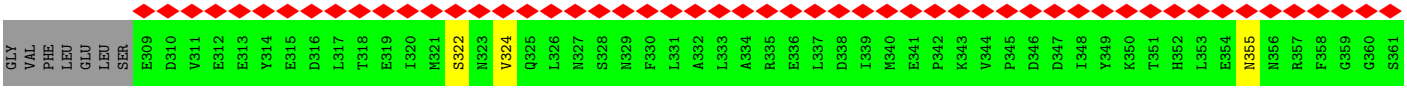


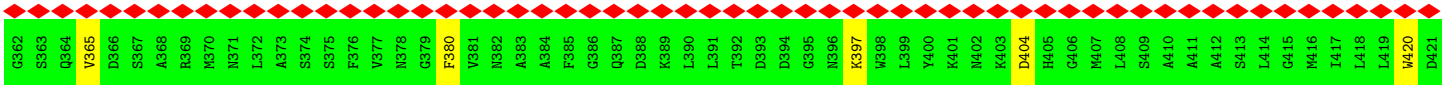


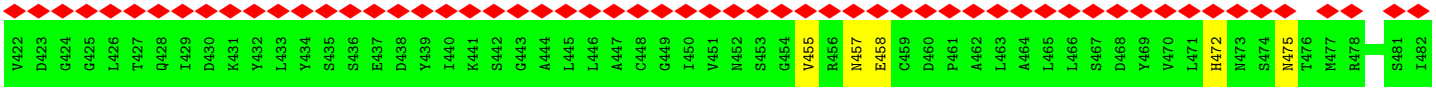


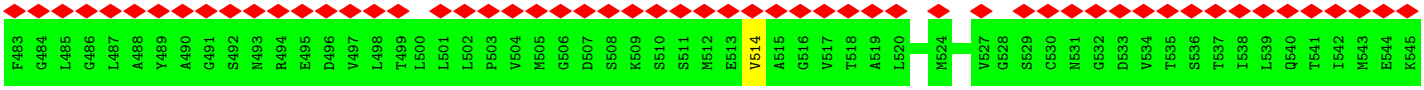


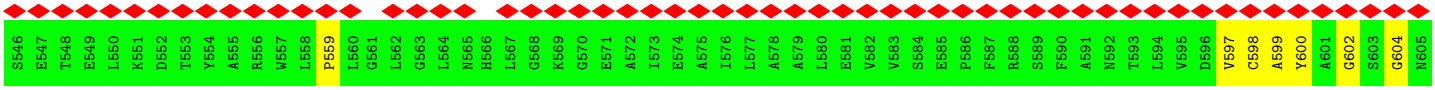


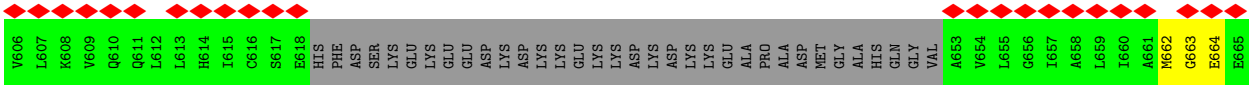


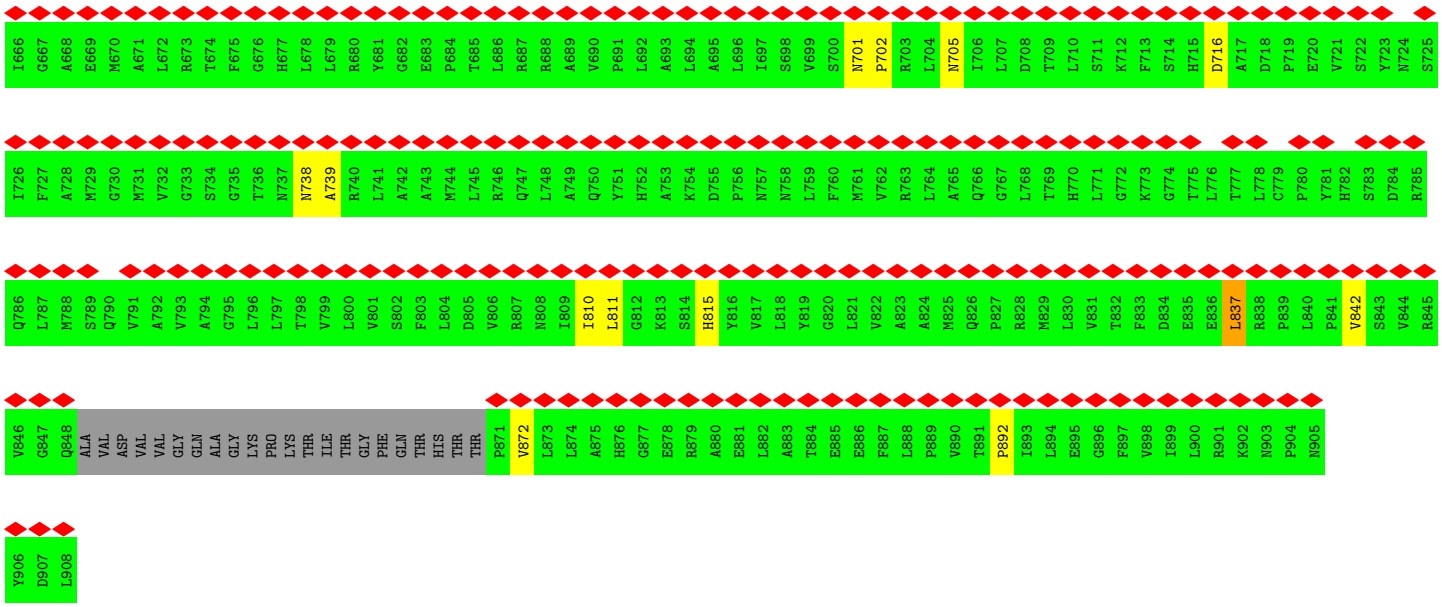






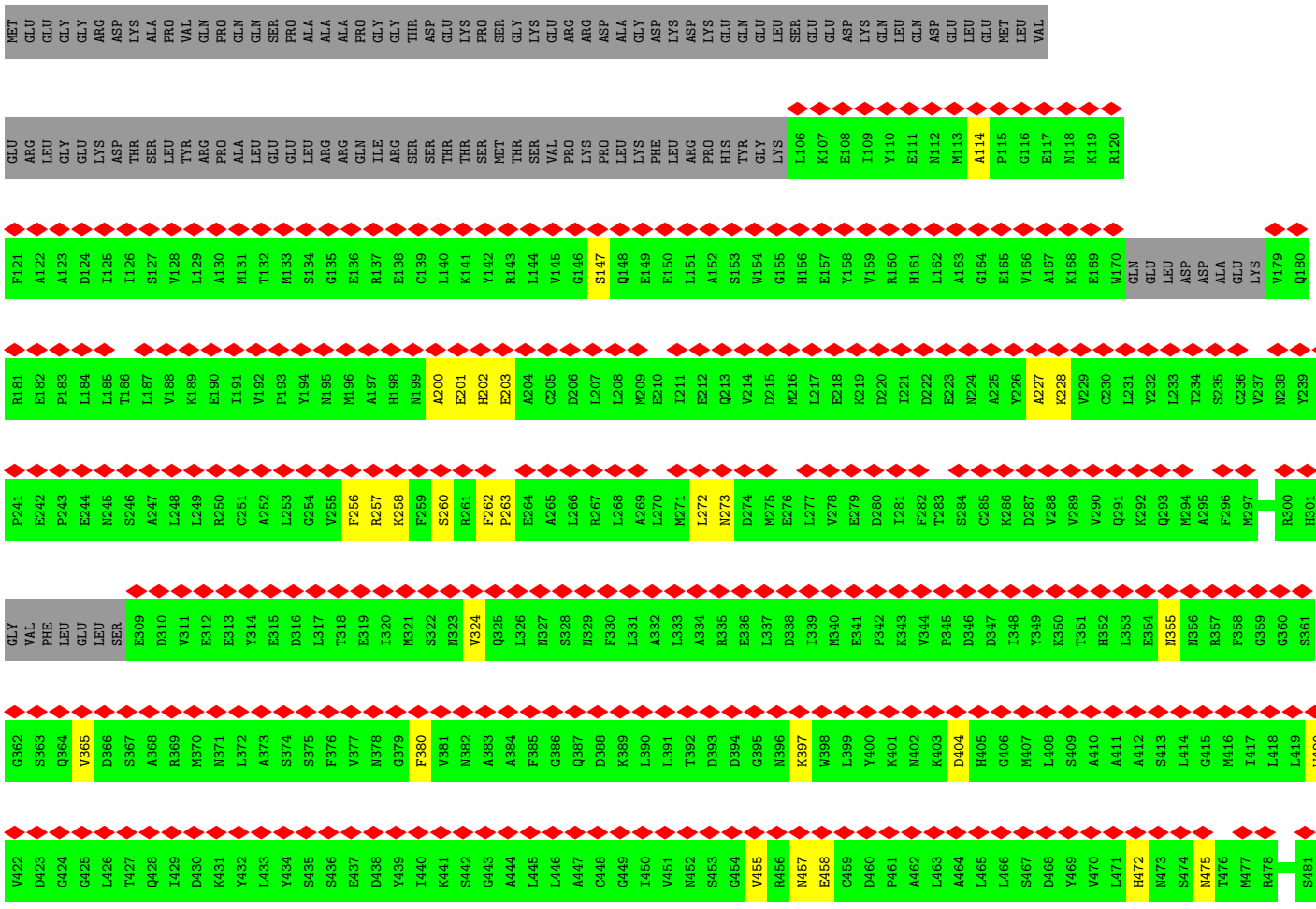


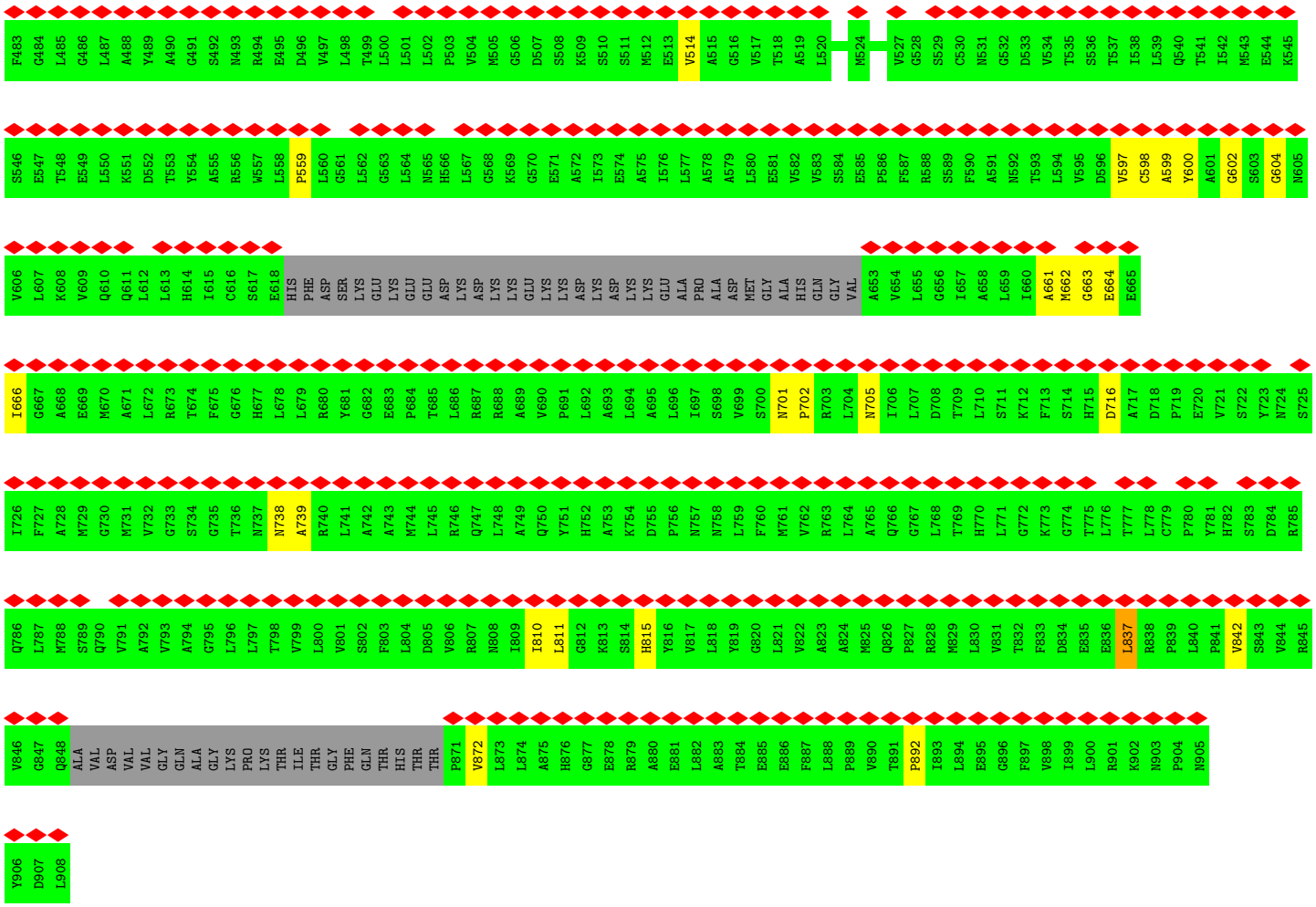




• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

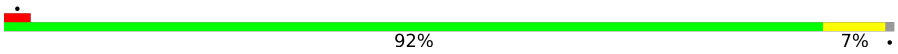
Chain AC:

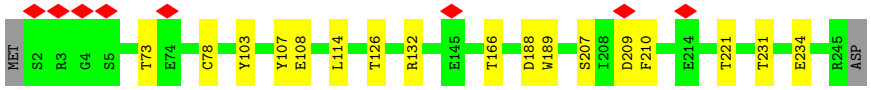




• Molecule 19: Proteasome subunit alpha type-6

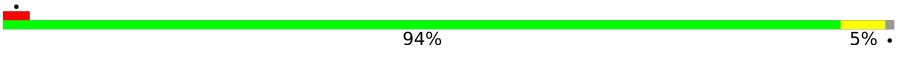
Chain B:





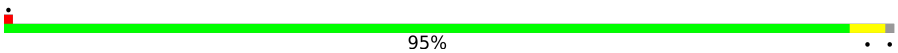
• Molecule 19: Proteasome subunit alpha type-6

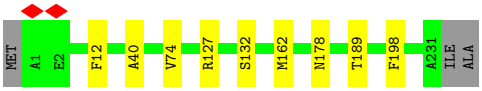
Chain h:



• Molecule 20: Proteasome subunit alpha type-2

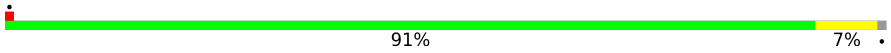
Chain C:





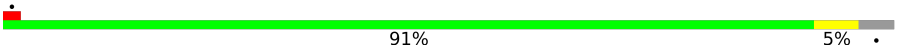
• Molecule 20: Proteasome subunit alpha type-2

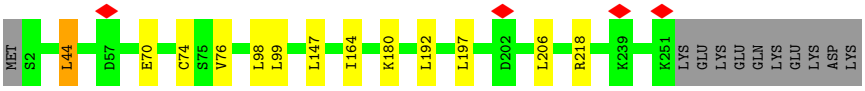
Chain i:



• Molecule 21: Proteasome subunit alpha type-4

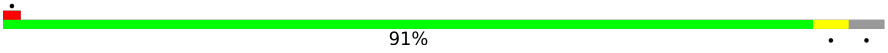
Chain D:

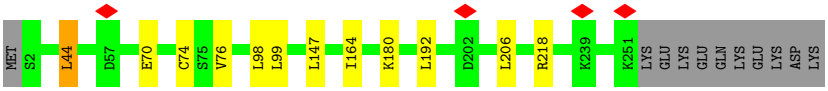




• Molecule 21: Proteasome subunit alpha type-4

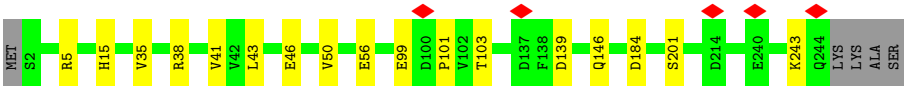
Chain j:





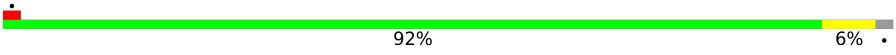
• Molecule 22: Proteasome subunit alpha type-7

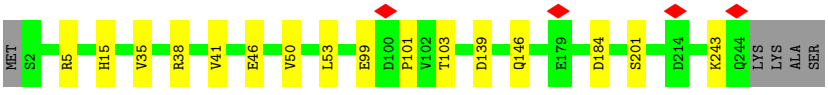
Chain E:



• Molecule 22: Proteasome subunit alpha type-7

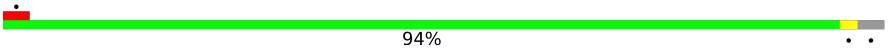
Chain k:

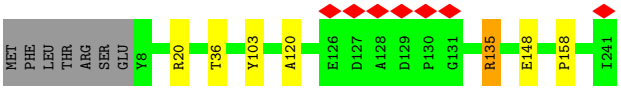




• Molecule 23: Proteasome subunit alpha type-5

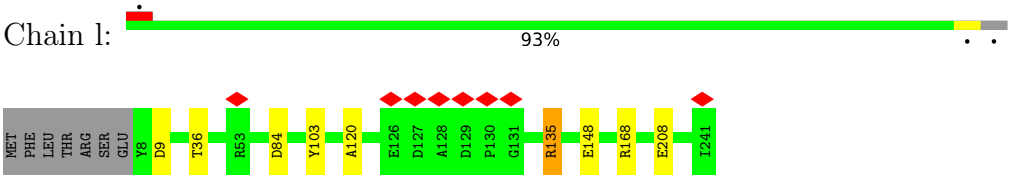
Chain F:





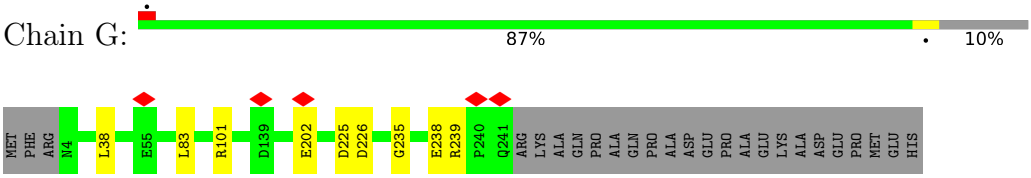
• Molecule 23: Proteasome subunit alpha type-5

Chain l:



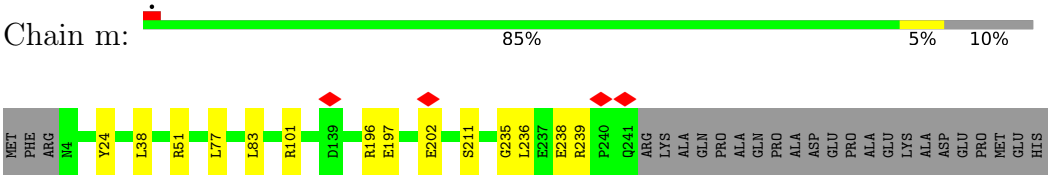
• Molecule 24: Proteasome subunit alpha type-1

Chain G:



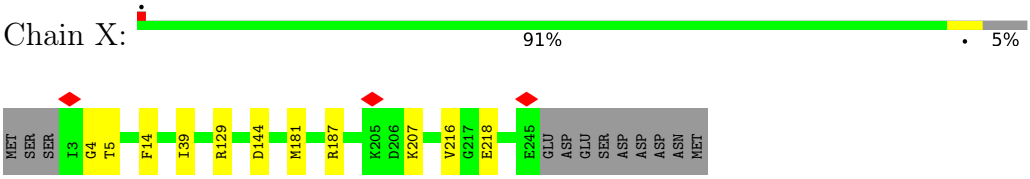
• Molecule 24: Proteasome subunit alpha type-1

Chain m:



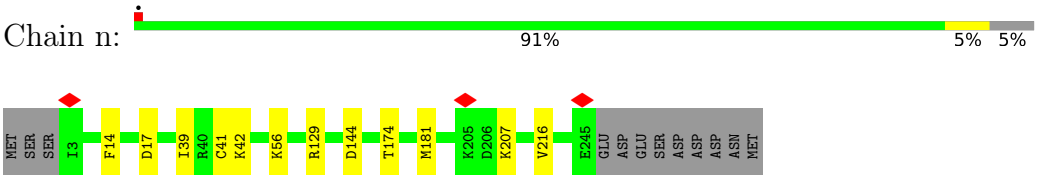
• Molecule 25: Proteasome subunit alpha type-3

Chain X:



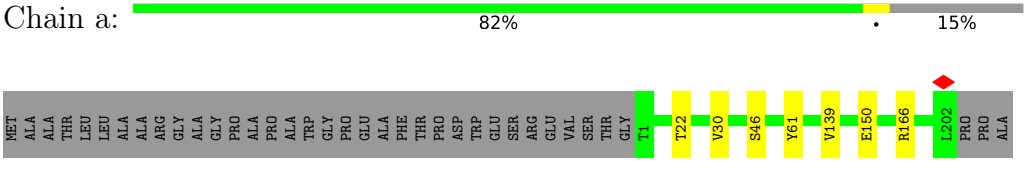
• Molecule 25: Proteasome subunit alpha type-3

Chain n:



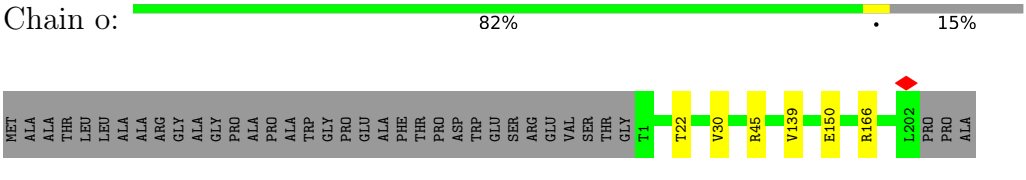
• Molecule 26: Proteasome subunit beta type-6

Chain a:



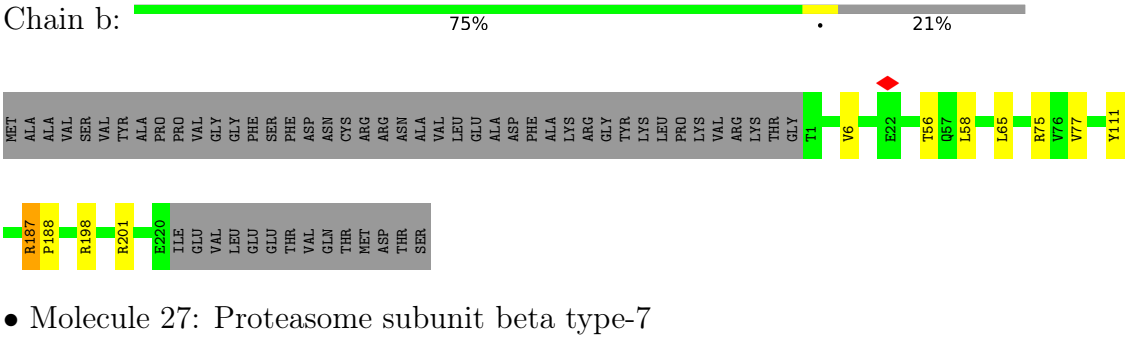
• Molecule 26: Proteasome subunit beta type-6

Chain o:



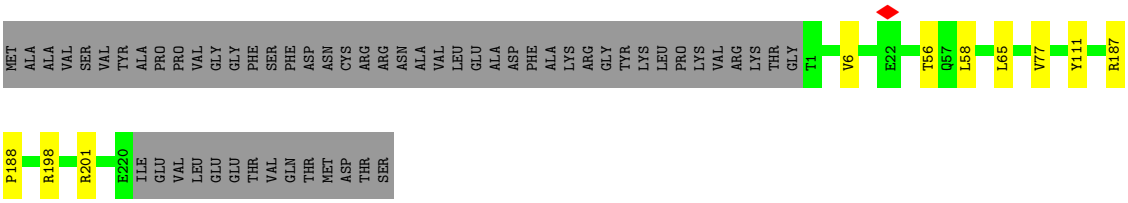
• Molecule 27: Proteasome subunit beta type-7

Chain b:



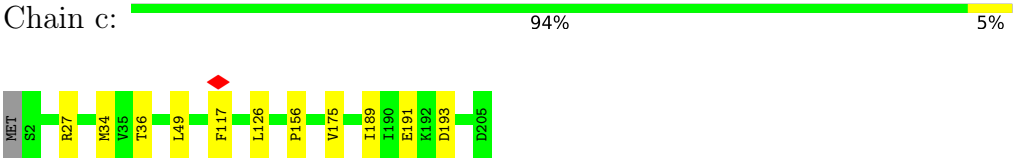
• Molecule 27: Proteasome subunit beta type-7

Chain p:



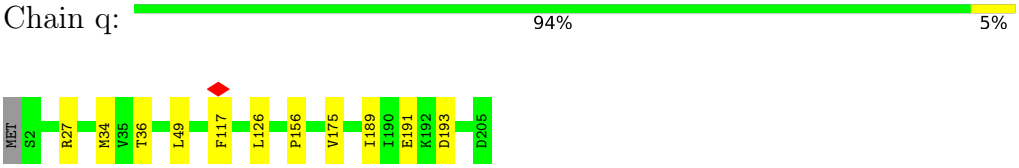
• Molecule 28: Proteasome subunit beta type-3

Chain c:



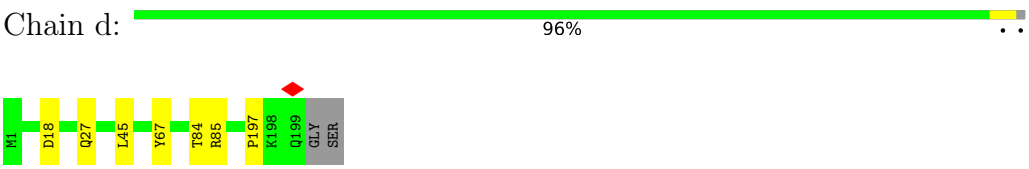
• Molecule 28: Proteasome subunit beta type-3

Chain q:



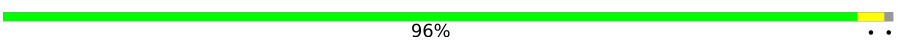
• Molecule 29: Proteasome subunit beta type-2

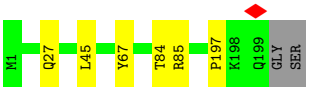
Chain d:



• Molecule 29: Proteasome subunit beta type-2

Chain r:



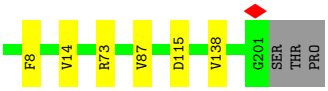


• Molecule 30: Proteasome subunit beta type-5

Chain e:

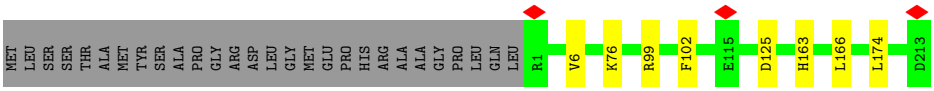
• Molecule 30: Proteasome subunit beta type-5

Chain s:



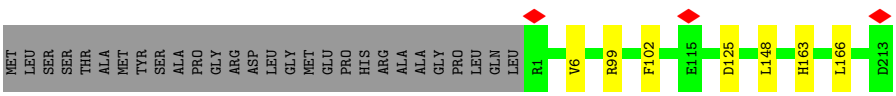
• Molecule 31: Proteasome subunit beta type-1

Chain f:



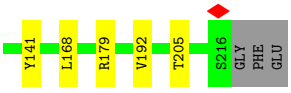
• Molecule 31: Proteasome subunit beta type-1

Chain t:



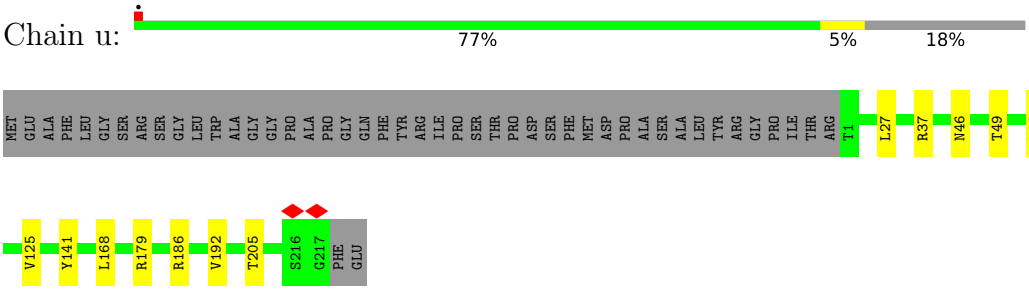
• Molecule 32: Proteasome subunit beta type-4

Chain g:



• Molecule 32: Proteasome subunit beta type-4

Chain u:


77%
5%
18%
MET GLU ALA PHE LEU GLY SER ARG SER GLY LEU TRP ALA GLY GLY PRO ALA PRO GLY GLN PHE TYR ARG ILE PRO SER THR PRO ASP SER PHE MET ASP PRO ALA SER ALA LEU TYR ARG GLY PRO ILE THR ARG T1 L27 R37 N46 T49 R86 R94 R99
V125 Y141 L168 R179 R186 V192 T205 S216 G217 PHE GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	165699	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	1.6	Depositor
Maximum defocus (nm)	2.6	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0336	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	I	0.66	2/2756 (0.1%)	1.09	7/3727 (0.2%)
1	w	0.66	2/2756 (0.1%)	1.09	7/3727 (0.2%)
2	H	0.76	3/2939 (0.1%)	0.96	9/3970 (0.2%)
2	v	0.76	2/2939 (0.1%)	0.97	11/3970 (0.3%)
3	L	0.66	0/2904	0.80	5/3924 (0.1%)
3	z	0.65	0/2904	0.79	4/3924 (0.1%)
4	0	0.65	0/2896	0.81	6/3912 (0.2%)
4	M	0.65	0/2896	0.81	6/3912 (0.2%)
5	J	0.59	0/2857	0.75	3/3844 (0.1%)
5	x	0.59	0/2857	0.75	3/3844 (0.1%)
6	K	0.61	0/3089	0.80	3/4168 (0.1%)
6	y	0.61	0/3089	0.80	3/4168 (0.1%)
7	1	0.41	0/5506	0.60	1/7425 (0.0%)
7	N	0.41	0/5506	0.60	1/7425 (0.0%)
8	2	0.43	0/2390	0.65	2/3215 (0.1%)
8	O	0.43	0/2383	0.65	2/3206 (0.1%)
9	3	0.45	0/2860	0.67	3/3860 (0.1%)
9	P	0.45	0/2861	0.67	3/3861 (0.1%)
10	4	0.49	2/2989 (0.1%)	0.63	6/4054 (0.1%)
10	Q	0.48	1/2989 (0.0%)	0.63	6/4054 (0.1%)
11	5	0.48	0/2820	0.65	3/3815 (0.1%)
11	R	0.48	0/2817	0.65	3/3812 (0.1%)
12	6	0.41	0/2754	0.59	3/3728 (0.1%)
12	S	0.41	0/2745	0.58	2/3717 (0.1%)
13	7	0.41	0/1713	0.63	4/2306 (0.2%)
13	T	0.41	0/1713	0.63	4/2306 (0.2%)
14	8	0.46	0/2167	0.60	0/2936
14	U	0.46	0/2167	0.60	0/2936
15	9	0.47	0/2045	0.73	2/2760 (0.1%)
15	V	0.47	0/2047	0.72	2/2763 (0.1%)
16	AA	0.44	0/1312	0.76	4/1769 (0.2%)
16	W	0.44	0/1312	0.76	4/1769 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AB	0.43	0/315	0.74	1/433 (0.2%)
17	Y	0.43	0/315	0.74	1/433 (0.2%)
18	AC	0.32	0/3603	0.55	1/5005 (0.0%)
18	Z	0.32	0/3603	0.55	1/5005 (0.0%)
19	B	0.75	0/1878	0.74	0/2549
19	h	0.81	0/1886	0.77	0/2557
20	C	0.85	1/1773 (0.1%)	0.78	1/2409 (0.0%)
20	i	0.86	1/1780 (0.1%)	0.79	1/2417 (0.0%)
21	D	1.13	4/1946 (0.2%)	0.85	6/2633 (0.2%)
21	j	1.39	3/1943 (0.2%)	0.83	6/2629 (0.2%)
22	E	0.77	0/1748	0.77	0/2386
22	k	0.78	0/1716	0.80	1/2347 (0.0%)
23	F	0.78	1/1794 (0.1%)	0.79	1/2430 (0.0%)
23	l	0.80	1/1753 (0.1%)	0.83	2/2346 (0.1%)
24	G	0.75	0/1885	0.77	0/2552
24	m	0.77	1/1885 (0.1%)	0.79	0/2552
25	X	0.83	2/1908 (0.1%)	0.76	0/2575
25	n	0.81	1/1908 (0.1%)	0.76	0/2575
26	a	0.88	5/1535 (0.3%)	0.86	4/2078 (0.2%)
26	o	0.86	3/1535 (0.2%)	0.87	4/2078 (0.2%)
27	b	0.79	1/1670 (0.1%)	0.84	3/2265 (0.1%)
27	p	0.80	1/1670 (0.1%)	0.82	2/2265 (0.1%)
28	c	0.87	0/1614	0.85	1/2177 (0.0%)
28	q	0.87	0/1614	0.85	1/2177 (0.0%)
29	d	0.87	1/1603 (0.1%)	0.83	0/2174
29	r	0.87	1/1603 (0.1%)	0.83	0/2174
30	e	0.92	0/1579	0.85	1/2134 (0.0%)
30	s	0.91	0/1582	0.84	1/2138 (0.0%)
31	f	0.85	0/1674	0.81	0/2257
31	t	0.85	0/1674	0.81	1/2257 (0.0%)
32	g	0.90	2/1705 (0.1%)	0.86	4/2312 (0.2%)
32	u	0.89	2/1711 (0.1%)	0.85	4/2319 (0.2%)
All	All	0.66	43/144386 (0.0%)	0.76	170/195445 (0.1%)

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	I	0	4
1	w	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
2	v	0	1
3	L	0	3
3	z	0	3
4	0	0	3
4	M	0	3
5	J	0	1
5	x	0	1
6	K	0	2
6	y	0	2
7	1	0	3
7	N	0	3
8	2	0	1
8	O	0	1
9	3	0	2
9	P	0	2
10	4	0	7
10	Q	0	7
11	5	0	9
11	R	0	9
13	7	0	2
13	T	0	2
14	8	0	1
14	U	0	1
15	9	0	3
15	V	0	3
16	AA	0	8
16	W	0	8
17	AB	0	2
17	Y	0	2
18	AC	0	7
18	Z	0	7
27	b	0	2
All	All	0	120

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	70	GLU	CD-OE1	44.40	1.74	1.25
21	D	70	GLU	CD-OE1	23.09	1.51	1.25
21	D	70	GLU	CD-OE2	22.37	1.50	1.25
21	j	70	GLU	CD-OE2	18.38	1.45	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	70	GLU	CG-CD	13.41	1.72	1.51

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	142	ASP	CB-CG-OD1	34.78	149.61	118.30
1	w	142	ASP	CB-CG-OD1	34.78	149.61	118.30
1	I	142	ASP	CB-CG-OD2	-25.59	95.27	118.30
1	w	142	ASP	CB-CG-OD2	-25.59	95.27	118.30
2	H	336	ARG	NE-CZ-NH1	-19.14	110.73	120.30

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	336	ARG	Sidechain
1	I	105	THR	Peptide
1	I	137	SER	Peptide
1	I	299	SER	Mainchain,Peptide
3	L	226	GLN	Mainchain

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	I	355/440 (81%)	255 (72%)	72 (20%)	28 (8%)	1 10
1	w	355/440 (81%)	255 (72%)	71 (20%)	29 (8%)	1 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	376/433 (87%)	248 (66%)	91 (24%)	37 (10%)	0 7
2	v	376/433 (87%)	249 (66%)	88 (23%)	39 (10%)	0 7
3	L	373/389 (96%)	264 (71%)	72 (19%)	37 (10%)	0 7
3	z	373/389 (96%)	263 (70%)	73 (20%)	37 (10%)	0 7
4	0	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0 5
4	M	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0 5
5	J	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	0 8
5	x	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	0 8
6	K	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0 6
6	y	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0 6
7	1	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	3 27
7	N	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	3 27
8	2	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	2 17
8	O	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	2 17
9	3	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	4 30
9	P	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	4 30
10	4	419/422 (99%)	331 (79%)	58 (14%)	30 (7%)	1 11
10	Q	419/422 (99%)	330 (79%)	58 (14%)	31 (7%)	1 11
11	5	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1 13
11	R	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1 13
12	6	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	3 23
12	S	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	3 23
13	7	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	1 14
13	T	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	1 14
14	8	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	2 17
14	U	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	2 17
15	9	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	2 20
15	V	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	2 20
16	AA	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	1 16
16	W	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	1 16
17	AB	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	Y	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0 3
18	AC	722/908 (80%)	557 (77%)	116 (16%)	49 (7%)	1 13
18	Z	722/908 (80%)	558 (77%)	116 (16%)	48 (7%)	1 13
19	B	242/246 (98%)	230 (95%)	8 (3%)	4 (2%)	9 42
19	h	242/246 (98%)	229 (95%)	13 (5%)	0	100 100
20	C	229/234 (98%)	204 (89%)	23 (10%)	2 (1%)	17 56
20	i	229/234 (98%)	206 (90%)	21 (9%)	2 (1%)	17 56
21	D	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	34 72
21	j	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	34 72
22	E	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	7 38
22	k	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	7 38
23	F	232/241 (96%)	217 (94%)	13 (6%)	2 (1%)	17 56
23	l	232/241 (96%)	214 (92%)	17 (7%)	1 (0%)	34 72
24	G	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	12 48
24	m	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	12 48
25	X	241/255 (94%)	234 (97%)	4 (2%)	3 (1%)	13 50
25	n	241/255 (94%)	235 (98%)	4 (2%)	2 (1%)	19 58
26	a	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29 68
26	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29 68
27	b	218/277 (79%)	209 (96%)	8 (4%)	1 (0%)	29 68
27	p	218/277 (79%)	208 (95%)	8 (4%)	2 (1%)	17 56
28	c	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15 54
28	q	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15 54
29	d	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	29 68
29	r	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	29 68
30	e	199/263 (76%)	195 (98%)	4 (2%)	0	100 100
30	s	199/263 (76%)	195 (98%)	4 (2%)	0	100 100
31	f	211/241 (88%)	203 (96%)	8 (4%)	0	100 100
31	t	211/241 (88%)	203 (96%)	8 (4%)	0	100 100
32	g	214/264 (81%)	203 (95%)	10 (5%)	1 (0%)	29 68
32	u	215/264 (81%)	206 (96%)	8 (4%)	1 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	19717/22846 (86%)	16137 (82%)	2604 (13%)	976 (5%)	4 19

5 of 976 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	165	ASP
1	I	207	HIS
1	I	220	LYS
1	I	277	HIS
1	I	278	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	291/385 (76%)	229 (79%)	62 (21%)	1 5
1	w	291/385 (76%)	227 (78%)	64 (22%)	1 5
2	H	298/372 (80%)	232 (78%)	66 (22%)	1 5
2	v	297/372 (80%)	232 (78%)	65 (22%)	1 5
3	L	298/341 (87%)	233 (78%)	65 (22%)	1 5
3	z	298/341 (87%)	233 (78%)	65 (22%)	1 5
4	0	296/379 (78%)	240 (81%)	56 (19%)	1 8
4	M	296/379 (78%)	240 (81%)	56 (19%)	1 8
5	J	310/352 (88%)	244 (79%)	66 (21%)	1 5
5	x	310/352 (88%)	244 (79%)	66 (21%)	1 5
6	K	333/366 (91%)	272 (82%)	61 (18%)	1 8
6	y	333/366 (91%)	270 (81%)	63 (19%)	1 8
7	1	376/816 (46%)	344 (92%)	32 (8%)	10 39
7	N	376/816 (46%)	344 (92%)	32 (8%)	10 39
8	2	142/336 (42%)	124 (87%)	18 (13%)	4 22
8	O	141/336 (42%)	123 (87%)	18 (13%)	4 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	3	201/416 (48%)	181 (90%)	20 (10%)	7	32
9	P	202/416 (49%)	181 (90%)	21 (10%)	7	31
10	4	250/362 (69%)	210 (84%)	40 (16%)	2	14
10	Q	249/362 (69%)	209 (84%)	40 (16%)	2	14
11	5	229/344 (67%)	202 (88%)	27 (12%)	5	25
11	R	228/344 (66%)	202 (89%)	26 (11%)	5	26
12	6	164/452 (36%)	153 (93%)	11 (7%)	16	48
12	S	163/452 (36%)	152 (93%)	11 (7%)	16	48
13	7	108/294 (37%)	91 (84%)	17 (16%)	2	15
13	T	109/294 (37%)	92 (84%)	17 (16%)	2	16
14	8	211/295 (72%)	186 (88%)	25 (12%)	5	25
14	U	212/295 (72%)	186 (88%)	26 (12%)	4	23
15	9	218/268 (81%)	187 (86%)	31 (14%)	3	19
15	V	219/268 (82%)	188 (86%)	31 (14%)	3	19
16	AA	111/312 (36%)	104 (94%)	7 (6%)	18	51
16	W	111/312 (36%)	103 (93%)	8 (7%)	14	45
17	AB	6/63 (10%)	6 (100%)	0	100	100
17	Y	6/63 (10%)	6 (100%)	0	100	100
19	B	193/210 (92%)	180 (93%)	13 (7%)	16	48
19	h	195/210 (93%)	182 (93%)	13 (7%)	16	48
20	C	175/191 (92%)	170 (97%)	5 (3%)	42	71
20	i	177/191 (93%)	164 (93%)	13 (7%)	14	45
21	D	194/221 (88%)	186 (96%)	8 (4%)	30	63
21	j	193/221 (87%)	186 (96%)	7 (4%)	35	66
22	E	152/211 (72%)	140 (92%)	12 (8%)	12	41
22	k	142/211 (67%)	132 (93%)	10 (7%)	15	46
23	F	190/203 (94%)	186 (98%)	4 (2%)	53	79
23	l	191/203 (94%)	184 (96%)	7 (4%)	34	65
24	G	198/224 (88%)	192 (97%)	6 (3%)	41	71
24	m	198/224 (88%)	188 (95%)	10 (5%)	24	57
25	X	193/212 (91%)	187 (97%)	6 (3%)	40	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	n	193/212 (91%)	184 (95%)	9 (5%)	26 60
26	a	155/181 (86%)	151 (97%)	4 (3%)	46 74
26	o	155/181 (86%)	152 (98%)	3 (2%)	57 80
27	b	177/228 (78%)	171 (97%)	6 (3%)	37 68
27	p	177/228 (78%)	172 (97%)	5 (3%)	43 72
28	c	172/174 (99%)	164 (95%)	8 (5%)	26 60
28	q	172/174 (99%)	164 (95%)	8 (5%)	26 60
29	d	164/171 (96%)	159 (97%)	5 (3%)	41 71
29	r	164/171 (96%)	160 (98%)	4 (2%)	49 76
30	e	153/202 (76%)	149 (97%)	4 (3%)	46 74
30	s	154/202 (76%)	149 (97%)	5 (3%)	39 69
31	f	175/199 (88%)	167 (95%)	8 (5%)	27 61
31	t	175/199 (88%)	169 (97%)	6 (3%)	37 68
32	g	175/215 (81%)	167 (95%)	8 (5%)	27 61
32	u	175/215 (81%)	165 (94%)	10 (6%)	20 53
All	All	12610/17990 (70%)	11190 (89%)	1420 (11%)	9 27

5 of 1420 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	w	337	LEU
4	0	170	SER
5	x	69	GLN
1	w	333	ARG
6	y	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
32	g	81	HIS
5	x	171	HIS
16	AA	142	ASN
12	6	473	GLN
28	q	173	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
33	ADP	0	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	v	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
33	ADP	z	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
33	ADP	H	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
33	ADP	K	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
33	ADP	w	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.51	4 (13%)
33	ADP	x	501	-	24,29,29	0.90	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	I	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.51	4 (13%)
33	ADP	J	501	-	24,29,29	0.90	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	M	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	L	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
33	ADP	y	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)

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
33	ADP	0	501	-	-	3/12/32/32	0/3/3/3
33	ADP	v	501	-	-	1/12/32/32	0/3/3/3
33	ADP	z	401	-	-	1/12/32/32	0/3/3/3
33	ADP	H	501	-	-	1/12/32/32	0/3/3/3
33	ADP	K	501	-	-	5/12/32/32	0/3/3/3
33	ADP	w	501	-	-	3/12/32/32	0/3/3/3
33	ADP	x	501	-	-	4/12/32/32	0/3/3/3
33	ADP	I	501	-	-	3/12/32/32	0/3/3/3
33	ADP	J	501	-	-	4/12/32/32	0/3/3/3
33	ADP	M	501	-	-	3/12/32/32	0/3/3/3
33	ADP	L	401	-	-	1/12/32/32	0/3/3/3
33	ADP	y	501	-	-	5/12/32/32	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)
33	I	501	ADP	C5-C4	2.53	1.47	1.40
33	w	501	ADP	C5-C4	2.53	1.47	1.40
33	H	501	ADP	C5-C4	2.52	1.47	1.40
33	v	501	ADP	C5-C4	2.52	1.47	1.40
33	L	401	ADP	C5-C4	2.36	1.47	1.40

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	501	ADP	PA-O3A-PB	-4.55	117.22	132.83
33	x	501	ADP	PA-O3A-PB	-4.55	117.22	132.83
33	M	501	ADP	PA-O3A-PB	-4.47	117.47	132.83
33	0	501	ADP	PA-O3A-PB	-4.47	117.47	132.83
33	L	401	ADP	PA-O3A-PB	-3.60	120.46	132.83

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	M	501	ADP	C5'-O5'-PA-O1A
33	M	501	ADP	C5'-O5'-PA-O2A
33	J	501	ADP	C5'-O5'-PA-O3A

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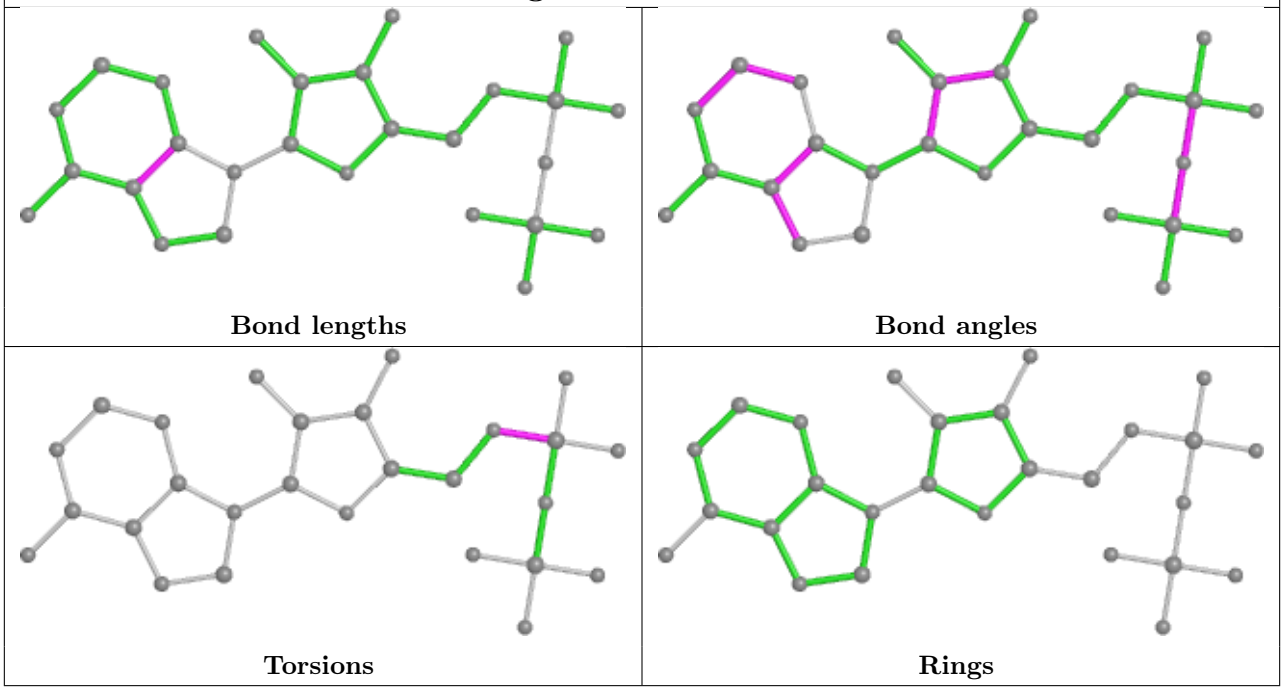
Mol	Chain	Res	Type	Atoms
33	K	501	ADP	C5'-O5'-PA-O1A
33	K	501	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

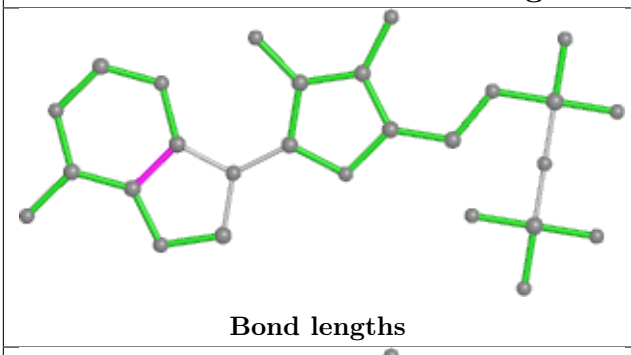
No monomer is involved in short contacts.

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.

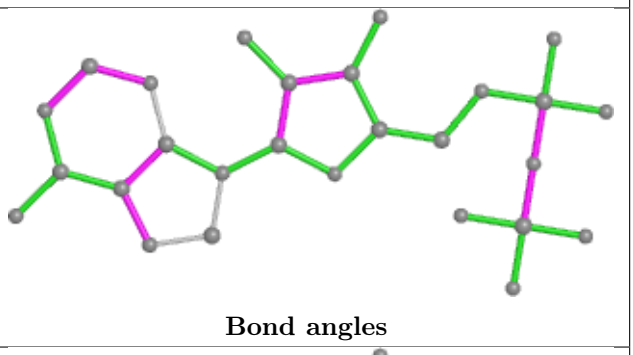
Ligand ADP 0 501



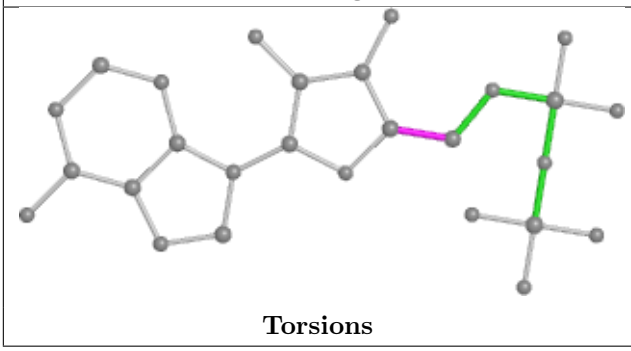
Ligand ADP v 501



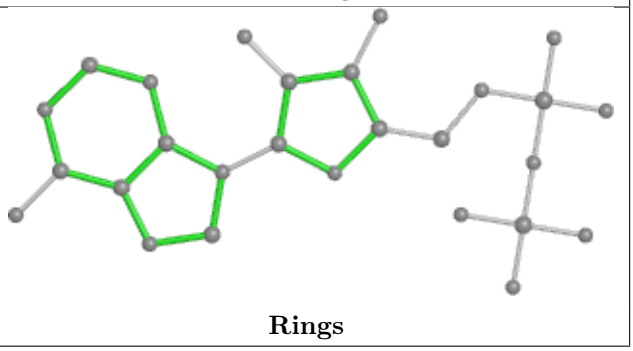
Bond lengths



Bond angles

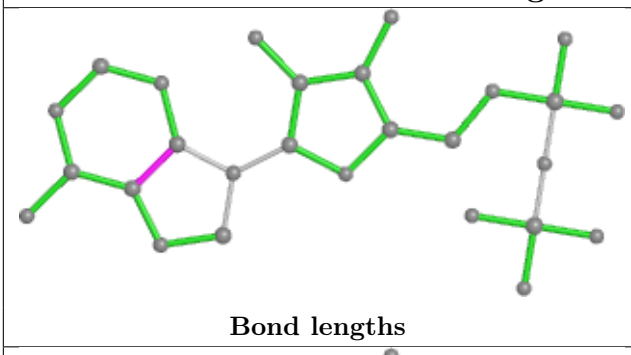


Torsions

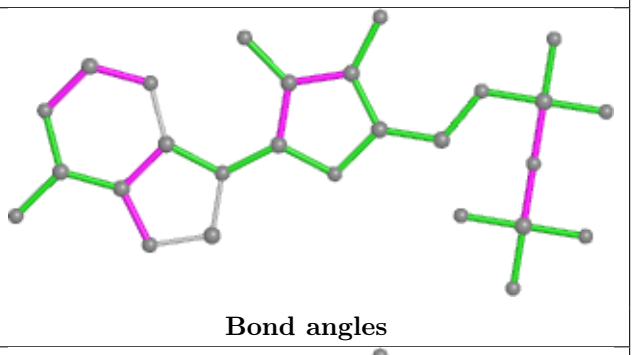


Rings

Ligand ADP z 401



Bond lengths



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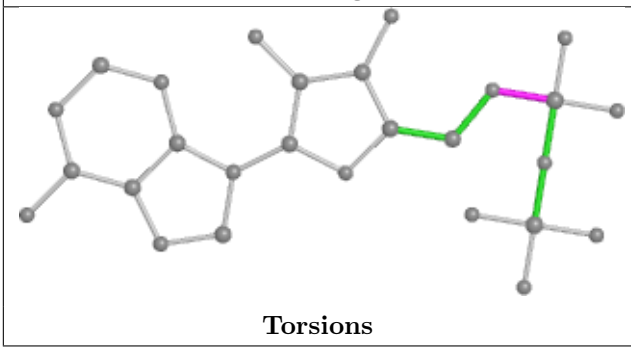
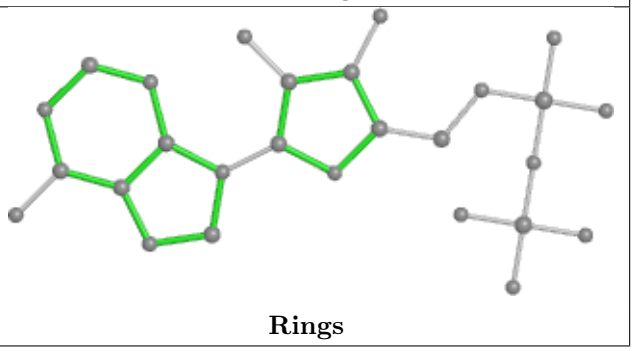
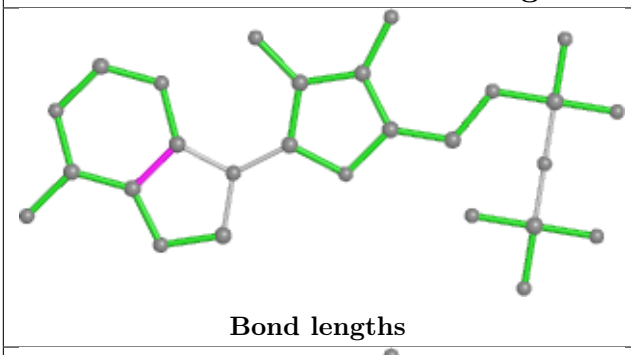


Torsions

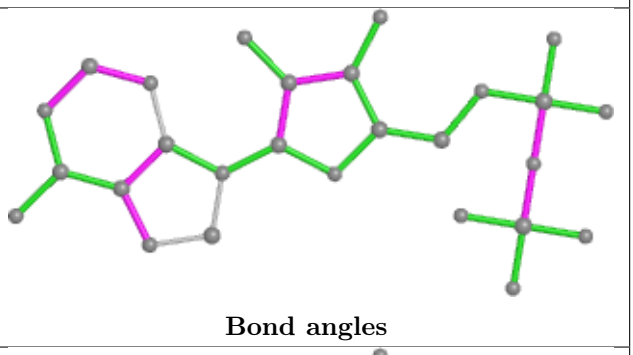


Rings

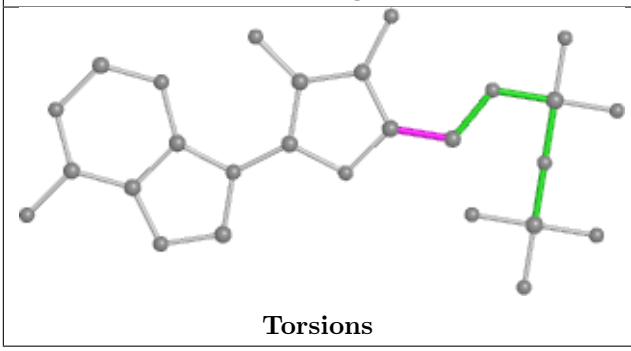
Ligand ADP H 501



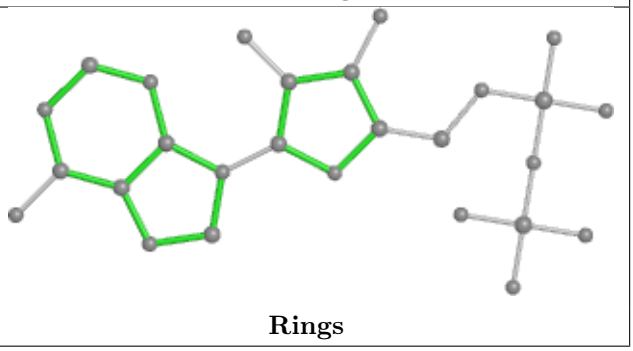
Bond lengths



Bond angles

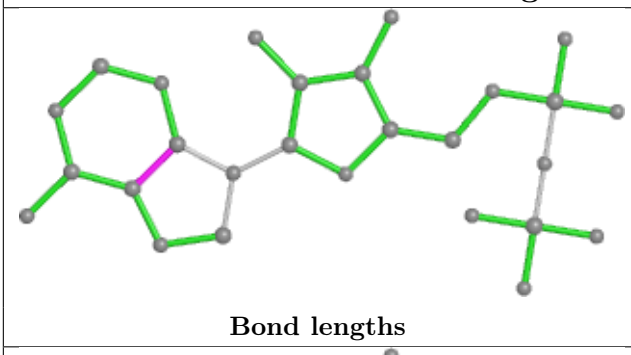


Torsions

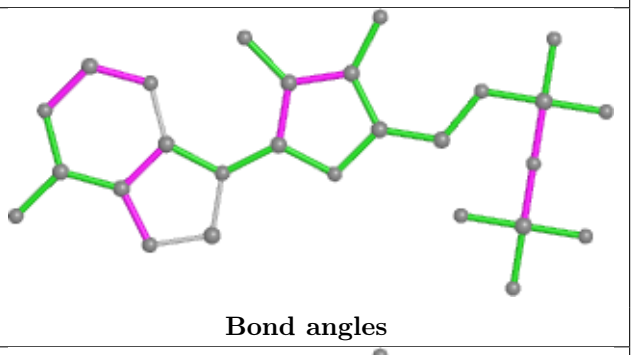


Rings

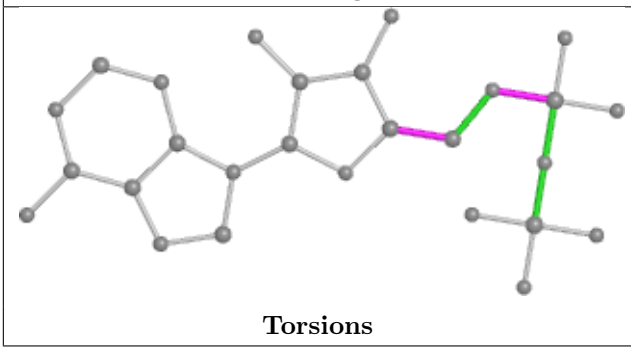
Ligand ADP K 501



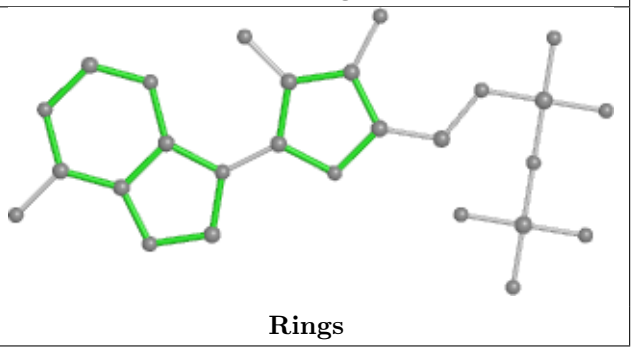
Bond lengths



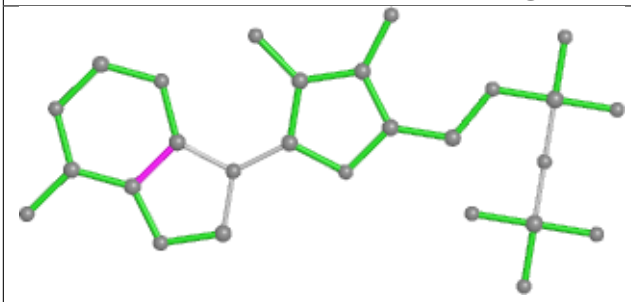
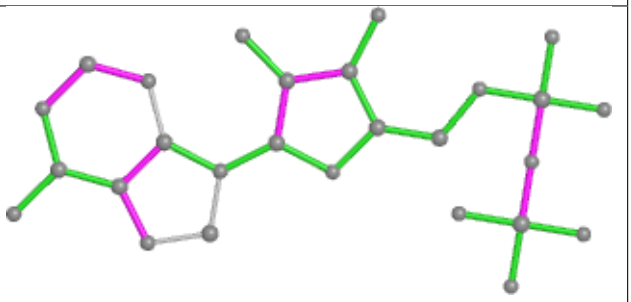
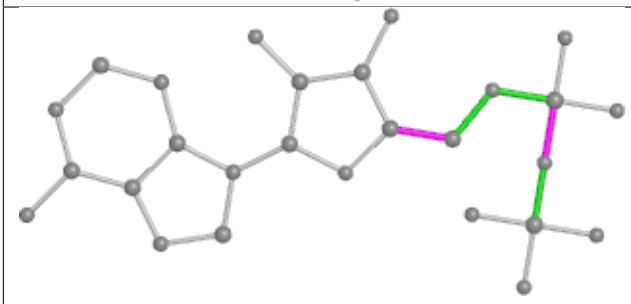
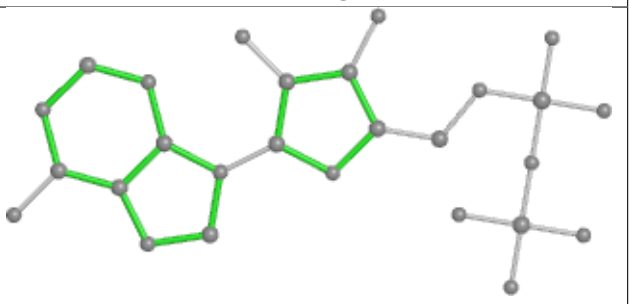
Bond angles

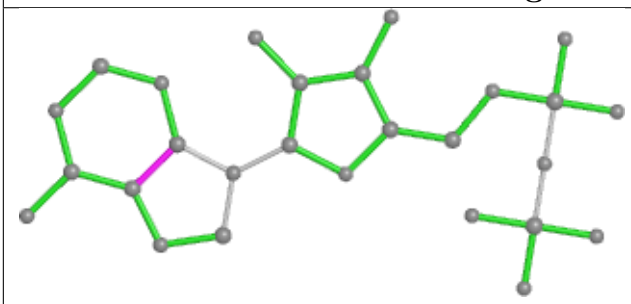
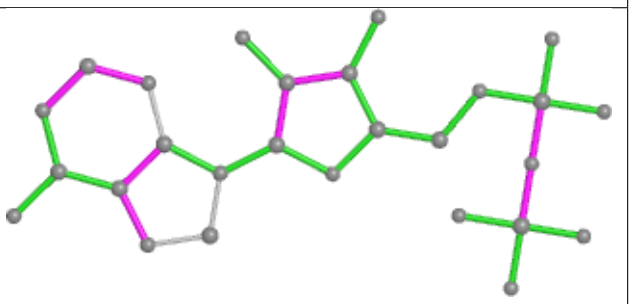
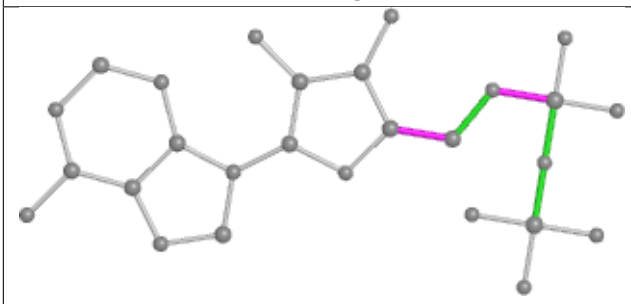
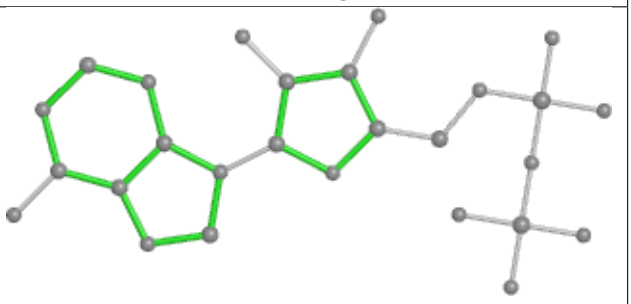


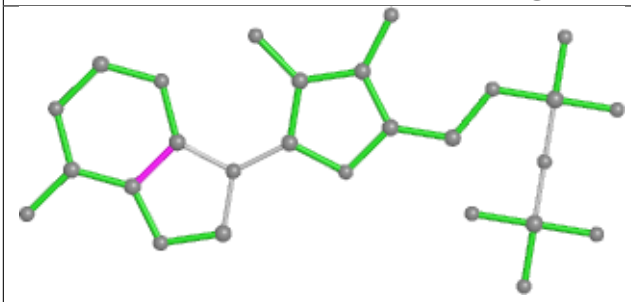
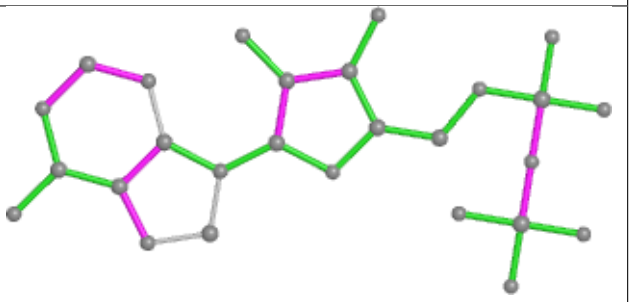
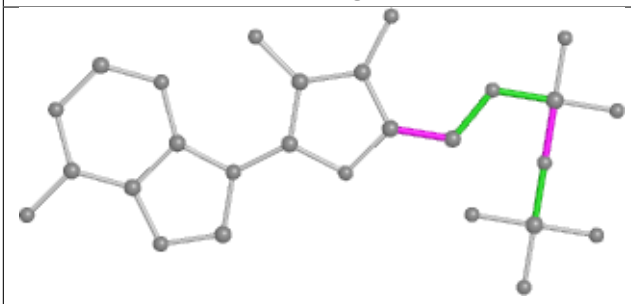
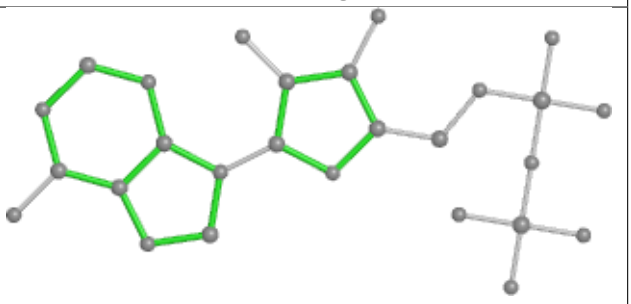
Torsions

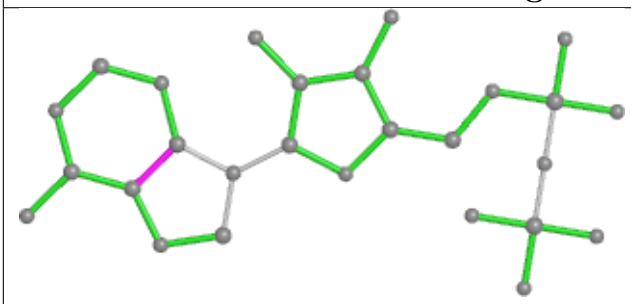
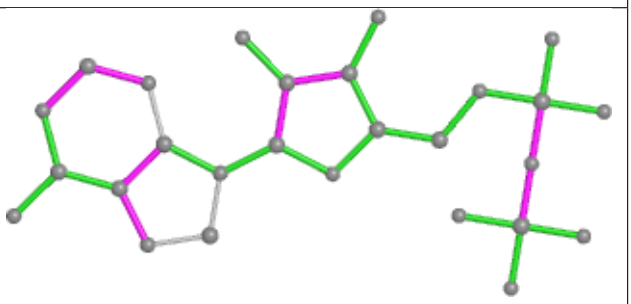
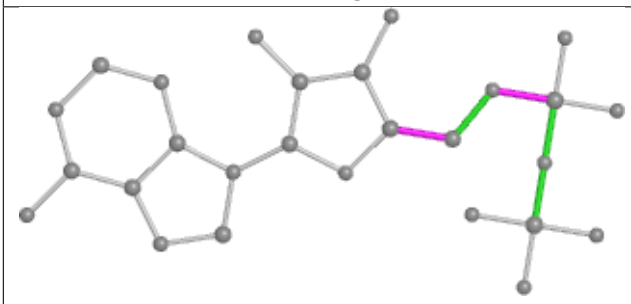
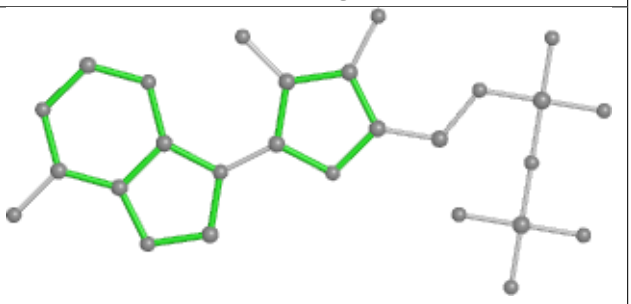


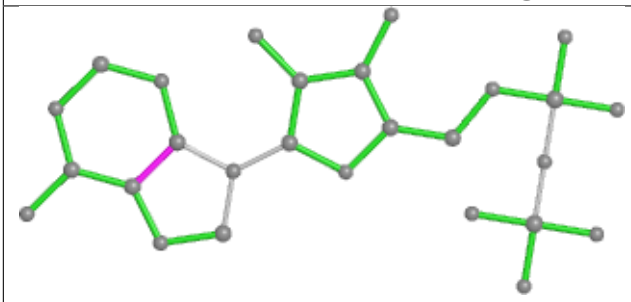
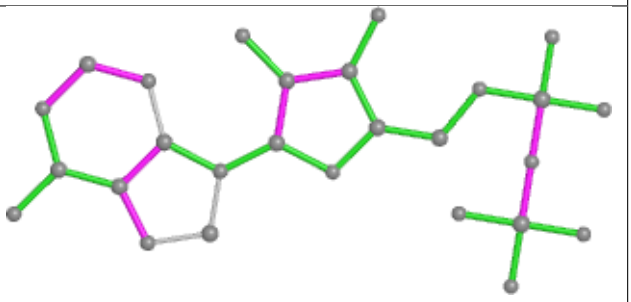
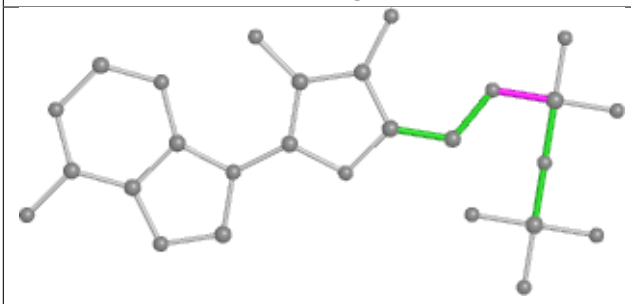
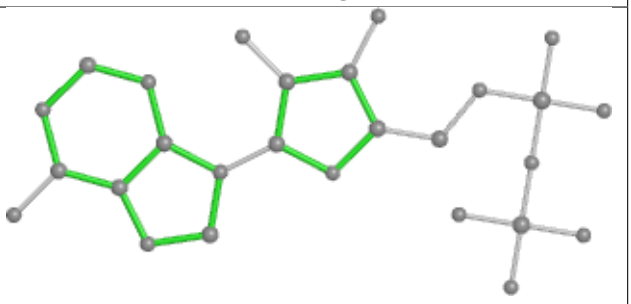
Rings

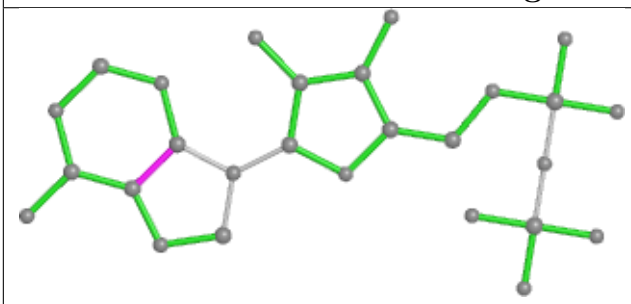
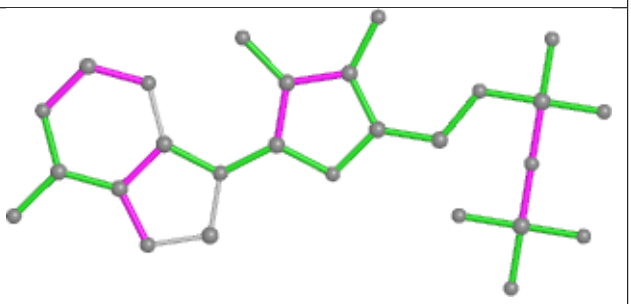
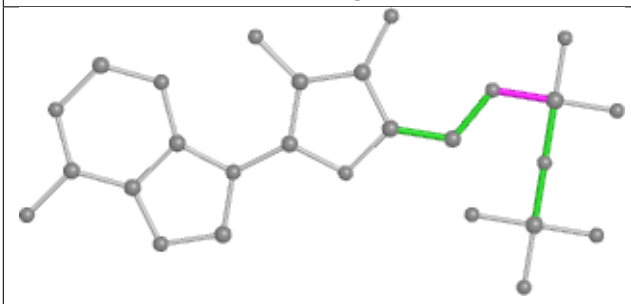
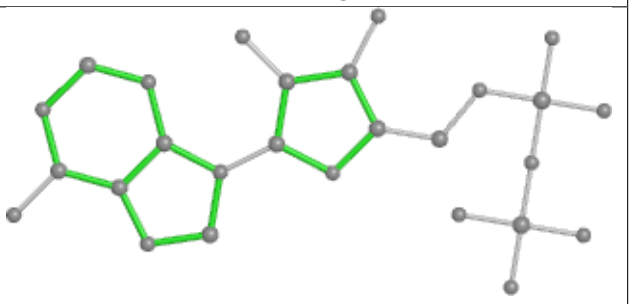
Ligand ADP w 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP x 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

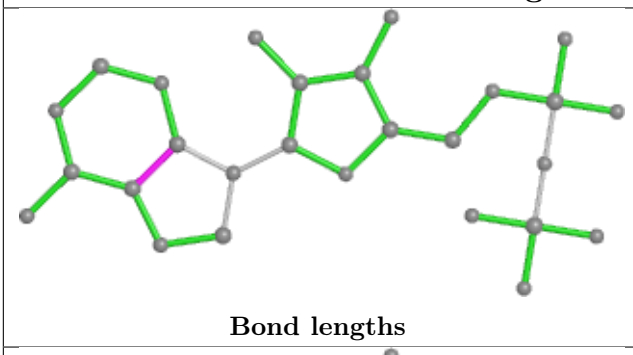
Ligand ADP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

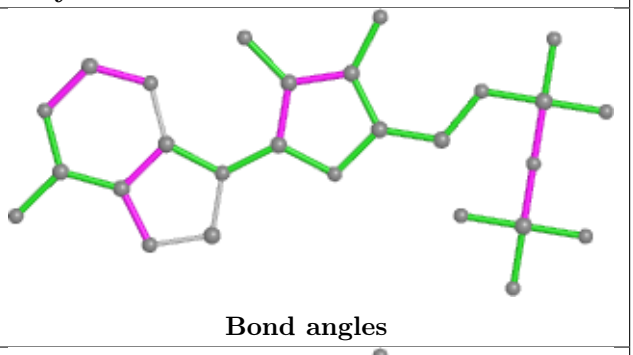
Ligand ADP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP L 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

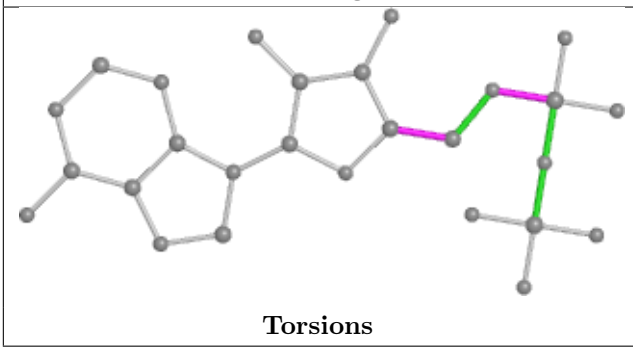
Ligand ADP y 501



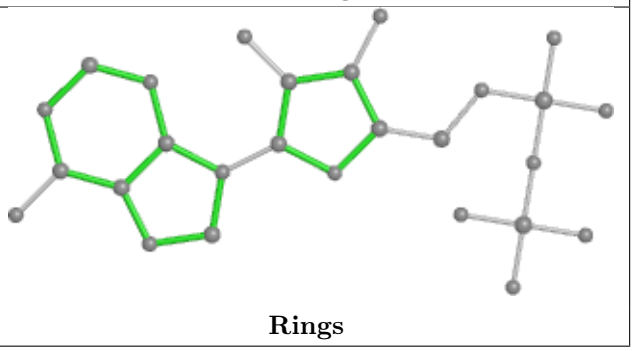
Bond lengths



Bond angles



Torsions



Rings

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.

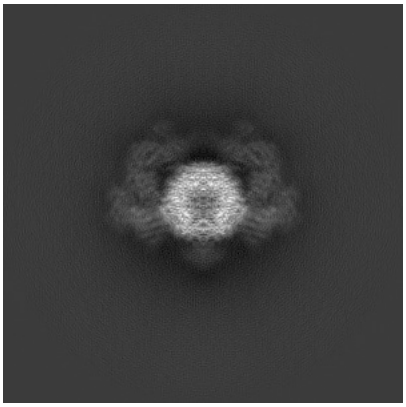
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9512. These allow visual inspection of the internal detail of the map and identification of artifacts.

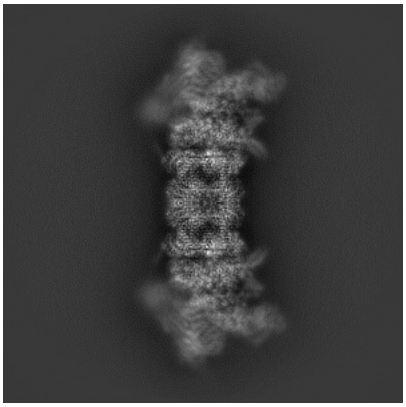
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

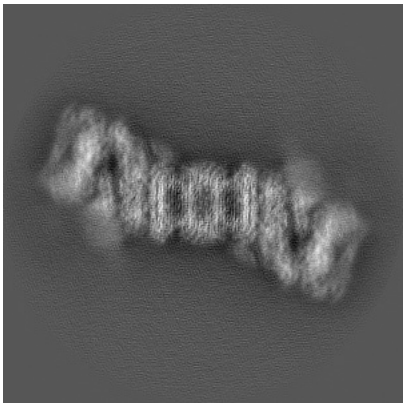
6.1.1 Primary map



X



Y

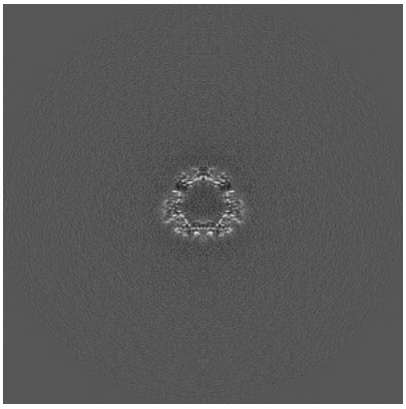


Z

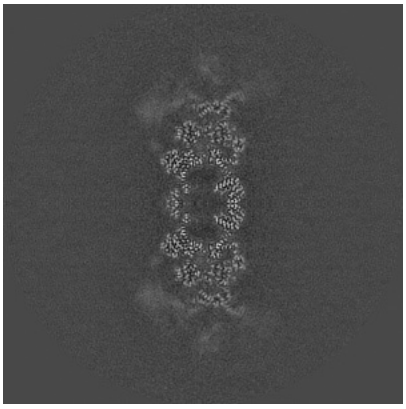
The images above show the map projected in three orthogonal directions.

6.2 Central slices

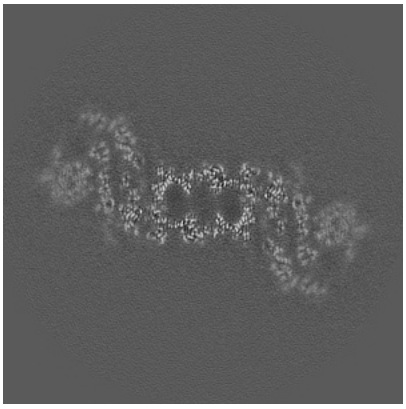
6.2.1 Primary map



X Index: 256



Y Index: 256

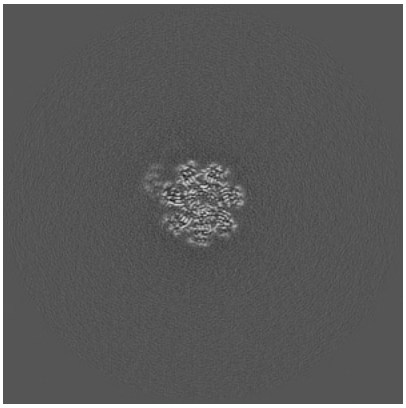


Z Index: 256

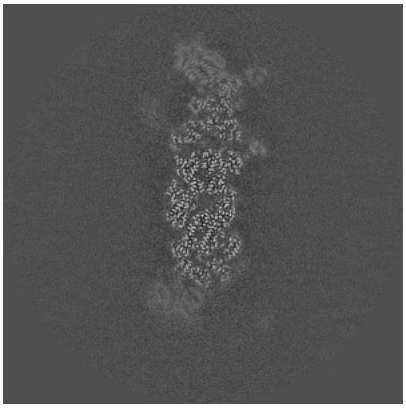
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

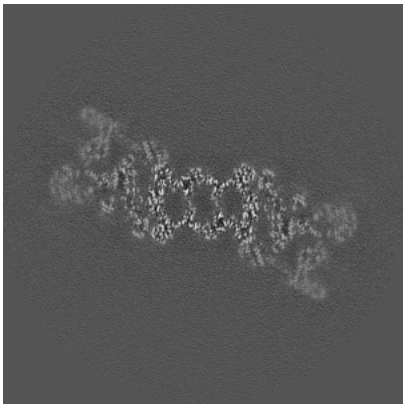
6.3.1 Primary map



X Index: 309



Y Index: 233



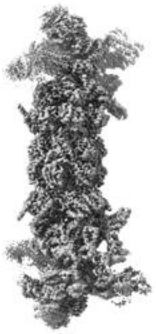
Z Index: 270

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

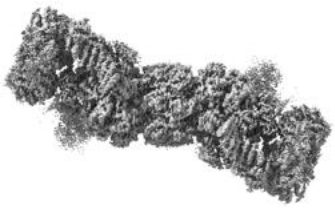
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

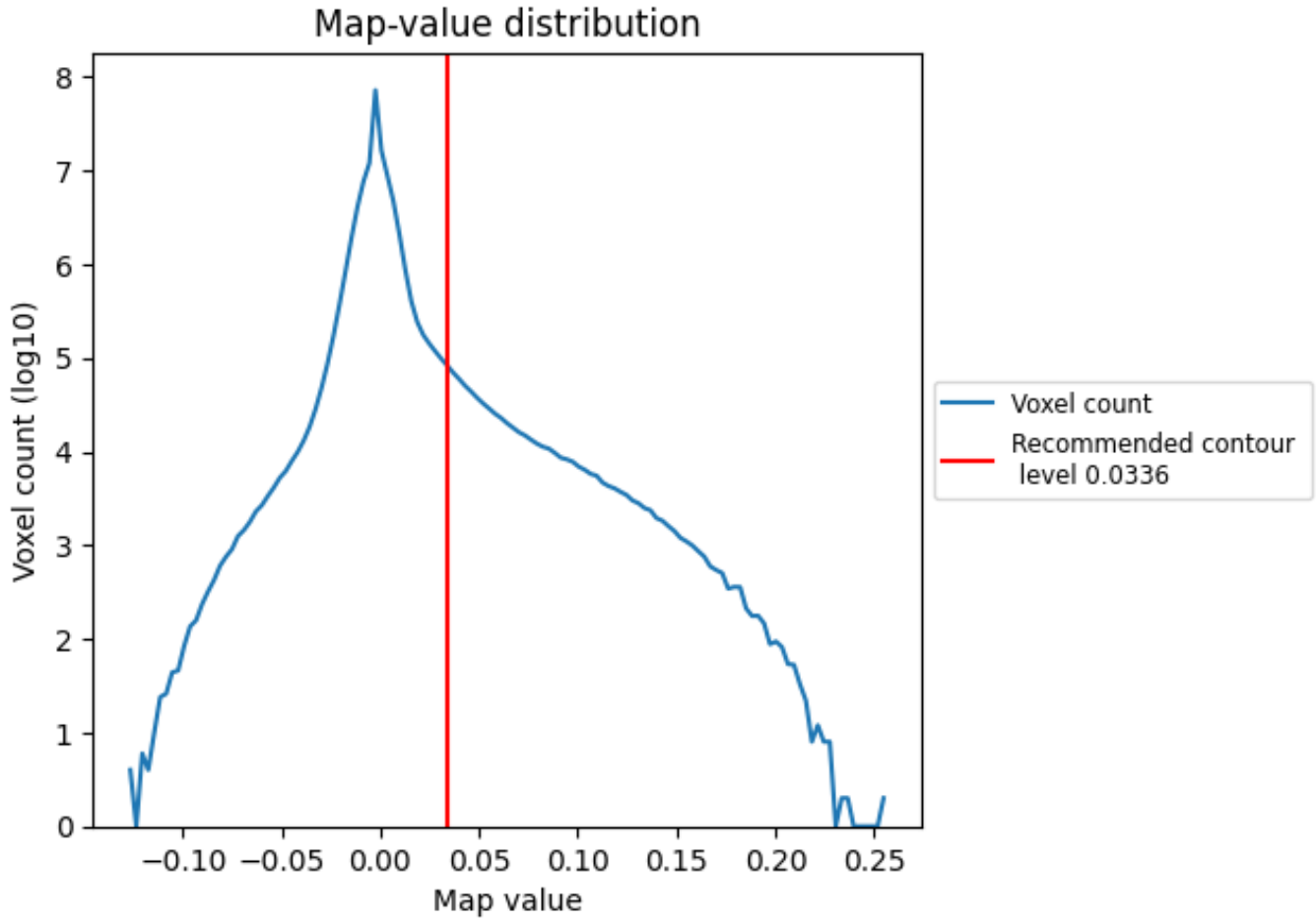
6.5 Mask visualisation (i)

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

7 Map analysis

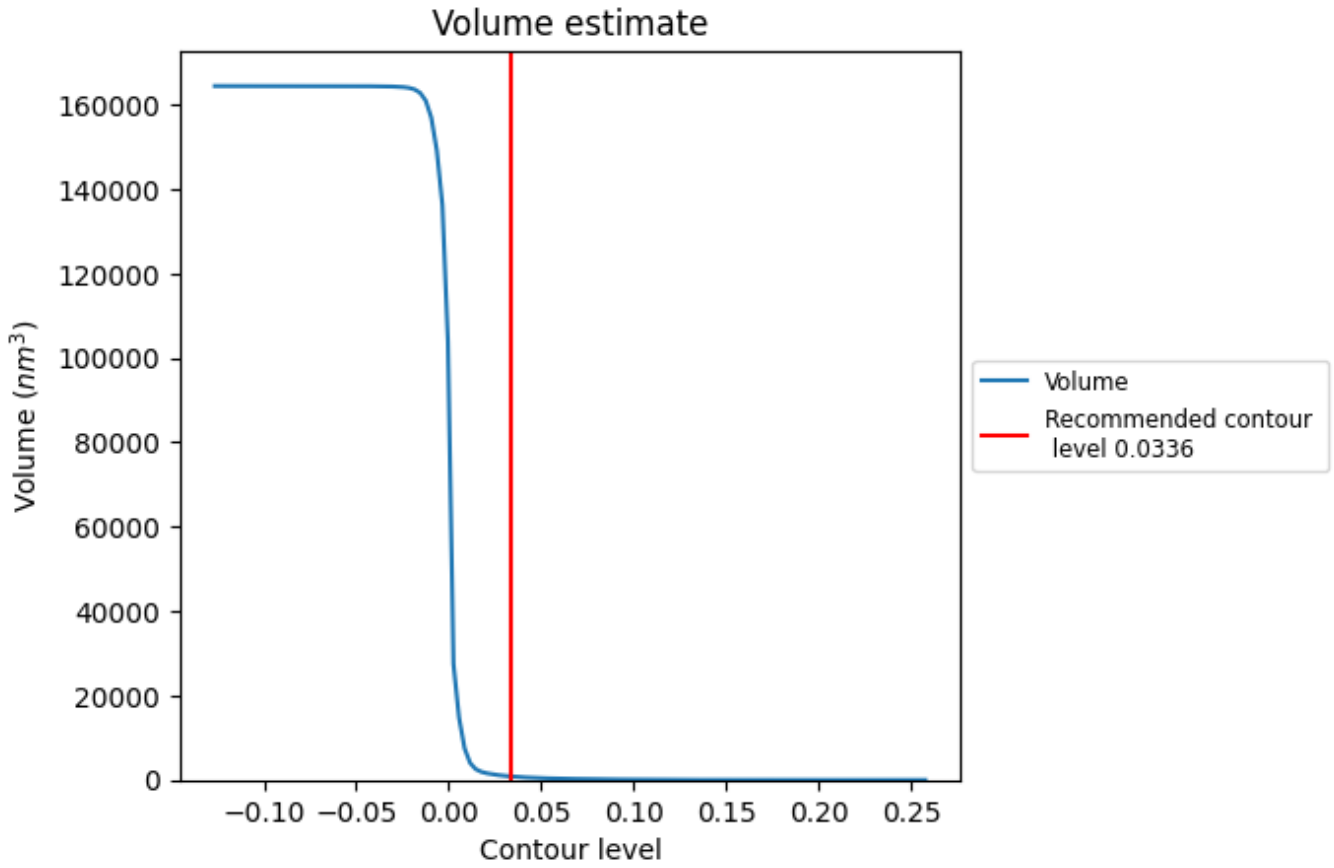
This section contains the results of statistical analysis of the map.

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.

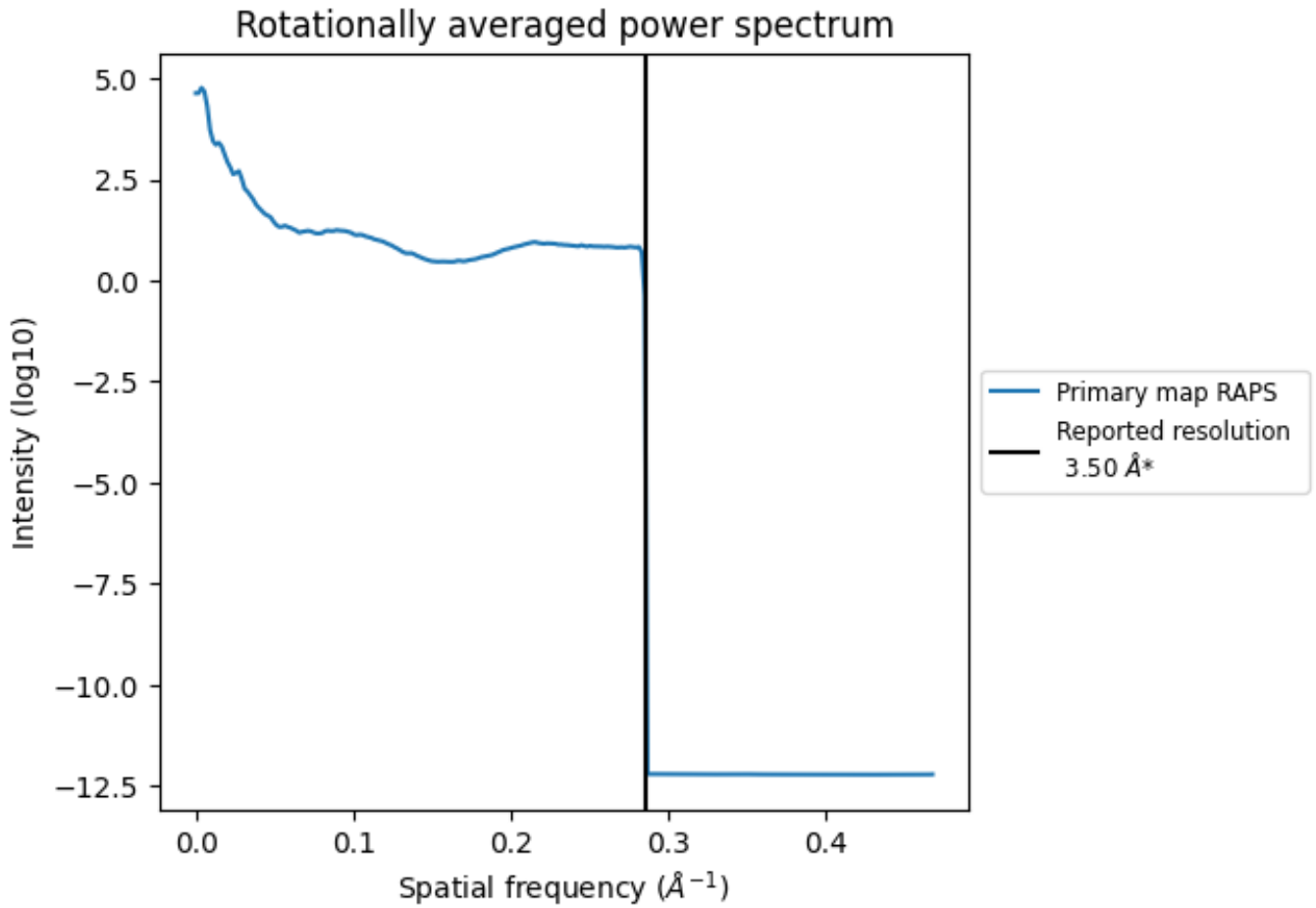
7.2 Volume estimate (i)



The volume at the recommended contour level is 841 nm^3; this corresponds to an approximate mass of 760 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 0.286 $Å^{-1}$

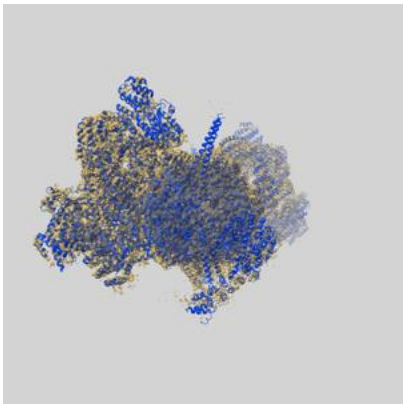
8 Fourier-Shell correlation

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

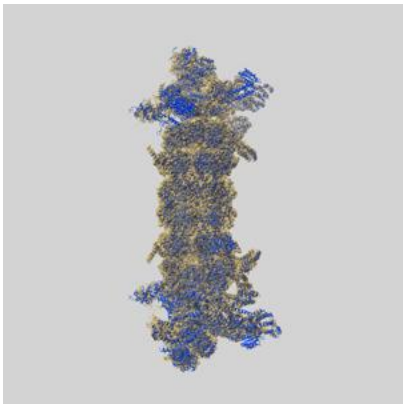
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9512 and PDB model 5GJR. Per-residue inclusion information can be found in section 3 on page 14.

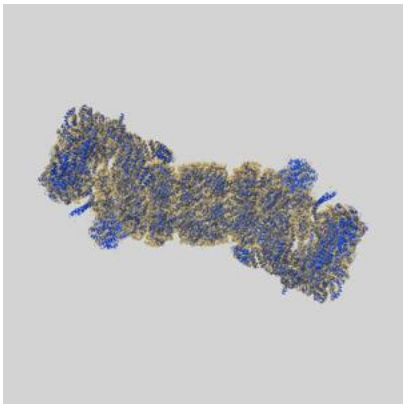
9.1 Map-model overlay



X



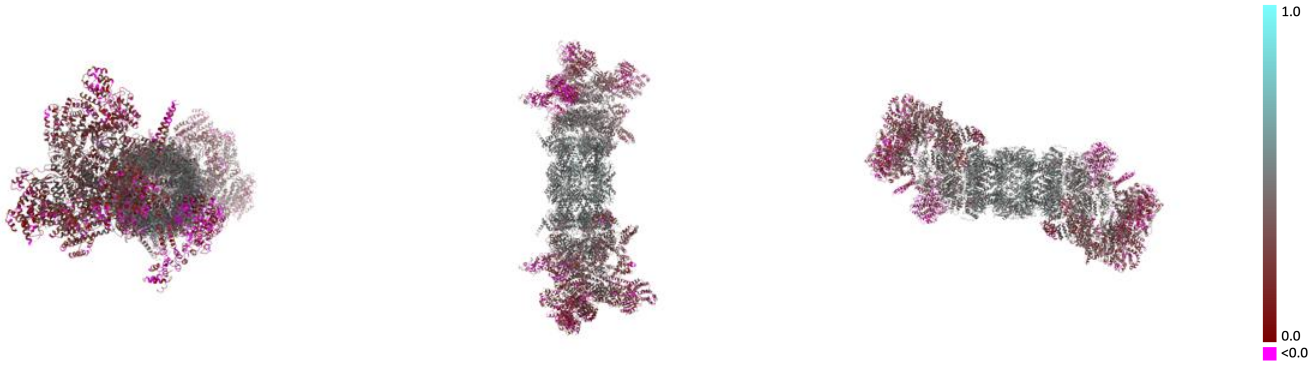
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0336 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.

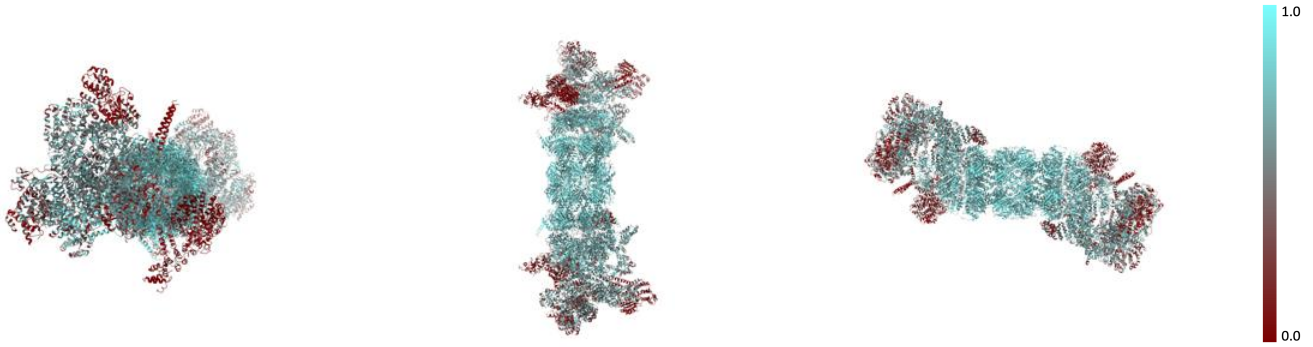
9.2 Q-score mapped to coordinate model



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.

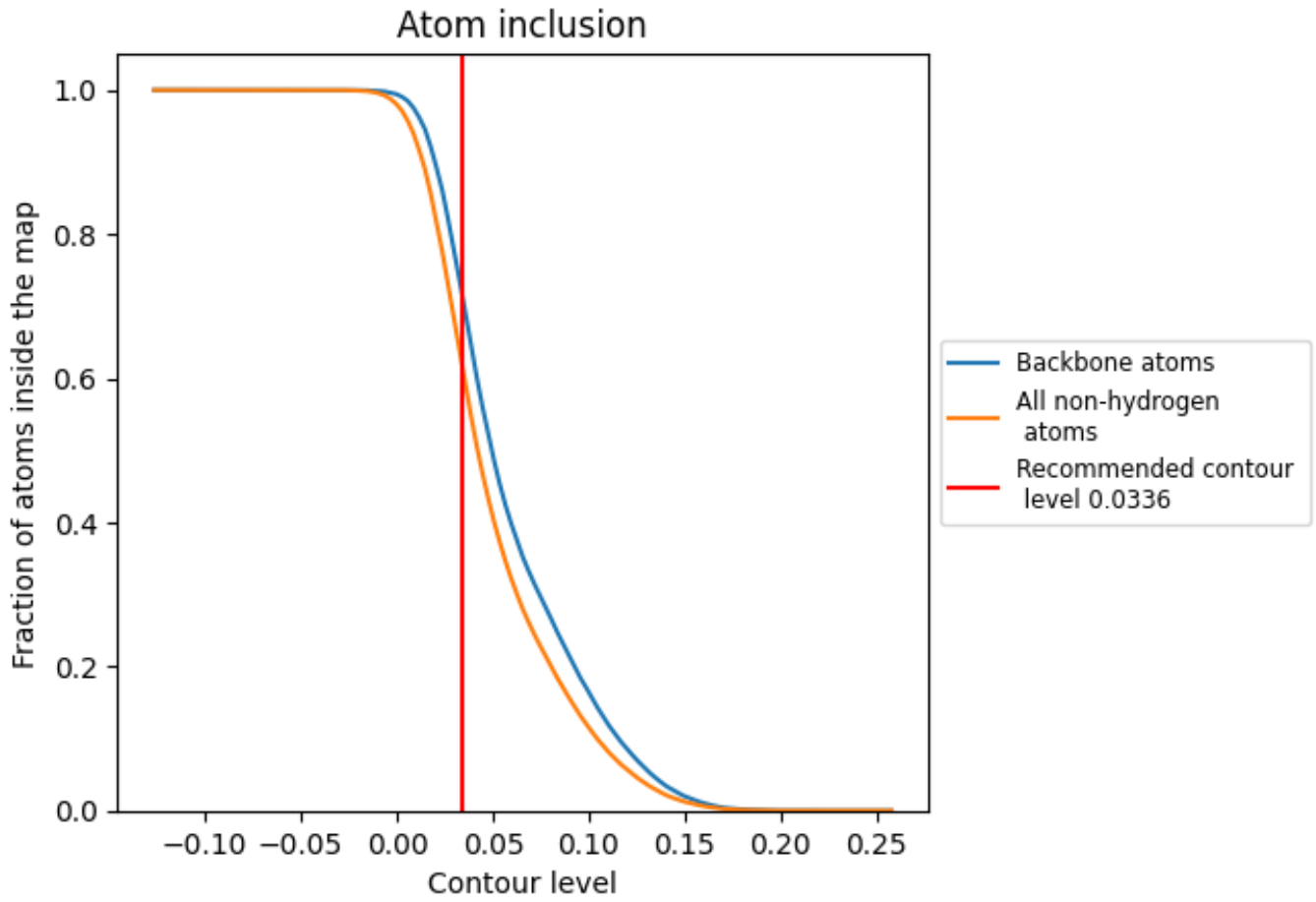
9.3 Atom inclusion mapped to coordinate model



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 (0.0336).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.0336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6228	0.3580
0	0.7066	0.4190
1	0.4272	0.1720
2	0.4059	0.2280
3	0.5741	0.2790
4	0.5242	0.3320
5	0.6562	0.3430
6	0.5056	0.2500
7	0.3209	0.1730
8	0.5413	0.3120
9	0.5616	0.3400
AA	0.0837	0.1490
AB	0.3513	0.2790
AC	0.0757	0.0730
B	0.8099	0.4750
C	0.8198	0.4900
D	0.7971	0.4650
E	0.8203	0.4670
F	0.7902	0.4770
G	0.8107	0.4780
H	0.7034	0.4060
I	0.6543	0.3830
J	0.6919	0.3980
K	0.6744	0.3960
L	0.6907	0.3930
M	0.7066	0.4190
N	0.4278	0.1710
O	0.4070	0.2280
P	0.5739	0.2800
Q	0.5238	0.3330
R	0.6562	0.3420
S	0.5069	0.2500
T	0.3209	0.1720
U	0.5418	0.3150
V	0.5615	0.3400

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
W	0.0837	0.1470
X	0.8021	0.4730
Y	0.3513	0.2760
Z	0.0757	0.0720
a	0.8348	0.4930
b	0.8271	0.4920
c	0.8376	0.4950
d	0.8391	0.4920
e	0.8538	0.4970
f	0.8358	0.4880
g	0.8452	0.4940
h	0.8058	0.4770
i	0.8223	0.4870
j	0.7979	0.4650
k	0.8355	0.4740
l	0.7942	0.4800
m	0.8163	0.4790
n	0.7993	0.4740
o	0.8362	0.4930
p	0.8271	0.4930
q	0.8376	0.4970
r	0.8404	0.4920
s	0.8548	0.4950
t	0.8340	0.4880
u	0.8444	0.4940
v	0.7051	0.4080
w	0.6532	0.3820
x	0.6922	0.3990
y	0.6748	0.3960
z	0.6907	0.3930