



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:04 PM UTC

PDB ID : 5GJR / pdb_00005gjr
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

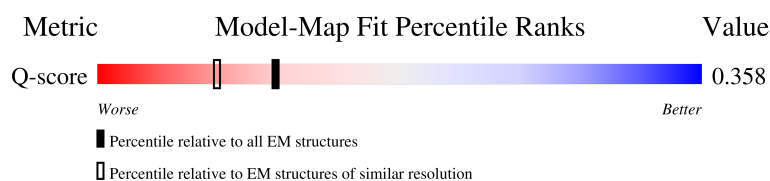
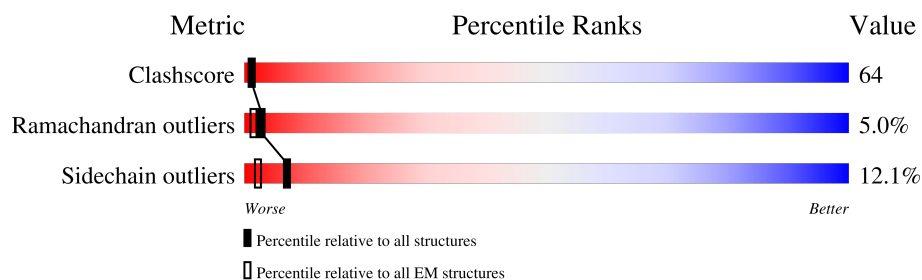
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	I	440	13% 13% 51% 14% • 18%
1	w	440	13% 13% 50% 15% • 18%
2	H	433	10% 17% 48% 20% • 12%
2	v	433	10% 16% 49% 19% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	389	
3	z	389	
4	0	439	
4	M	439	
5	J	406	
5	x	406	
6	K	418	
6	y	418	
7	1	953	
7	N	953	
8	2	376	
8	O	376	
9	3	456	
9	P	456	
10	4	422	
10	Q	422	
11	5	389	
11	R	389	
12	6	525	
12	S	525	
13	7	350	
13	T	350	
14	8	324	
14	U	324	
15	9	310	

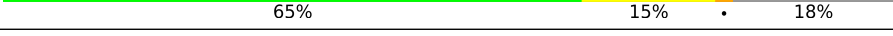
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	V	310	
16	AA	377	
16	W	377	
17	AB	70	
17	Y	70	
18	AC	908	
18	Z	908	
19	B	246	
19	h	246	
20	C	234	
20	i	234	
21	D	261	
21	j	261	
22	E	248	
22	k	248	
23	F	241	
23	l	241	
24	G	263	
24	m	263	
25	X	255	
25	n	255	
26	a	239	
26	o	239	
27	b	277	
27	p	277	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	c	205	
28	q	205	
29	d	201	
29	r	201	
30	e	263	
30	s	263	
31	f	241	
31	t	241	
32	g	264	
32	u	264	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	ADP	0	501	-	-	X	-
33	ADP	I	501	-	-	X	-
33	ADP	J	501	-	-	X	-
33	ADP	K	501	-	-	X	-
33	ADP	L	401	-	-	X	-
33	ADP	M	501	-	-	X	-
33	ADP	w	501	-	-	X	-
33	ADP	x	501	-	-	X	-
33	ADP	y	501	-	-	X	-
33	ADP	z	401	-	-	X	-

2 Entry composition

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

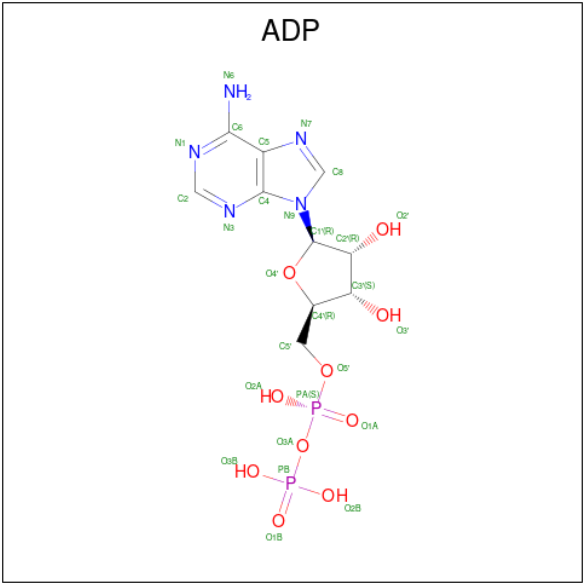
- Molecule 31 is a protein called Proteasome subunit beta type-1.

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
			Total	C	N	O	S		
32	g	216	1672	1055	286	319	12	0	0
32	u	217	1678	1058	290	318	12	0	0

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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	
33	x	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

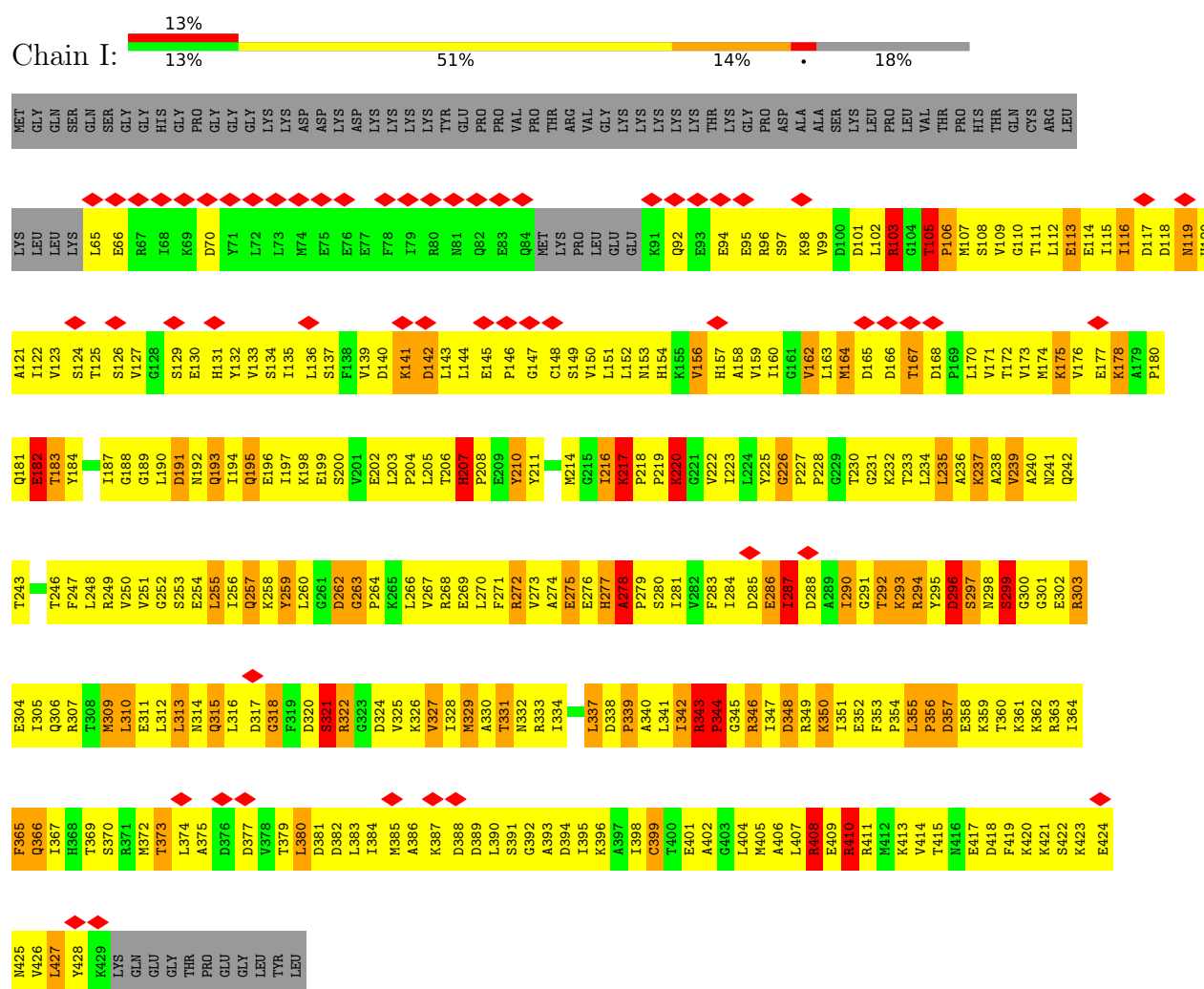
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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	

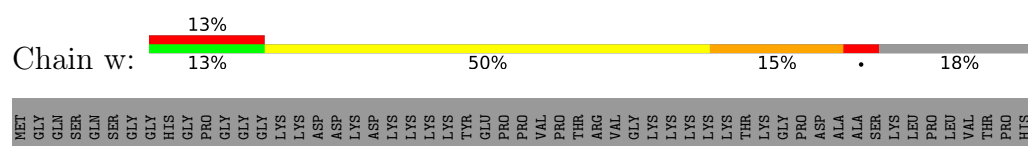
3 Residue-property plots

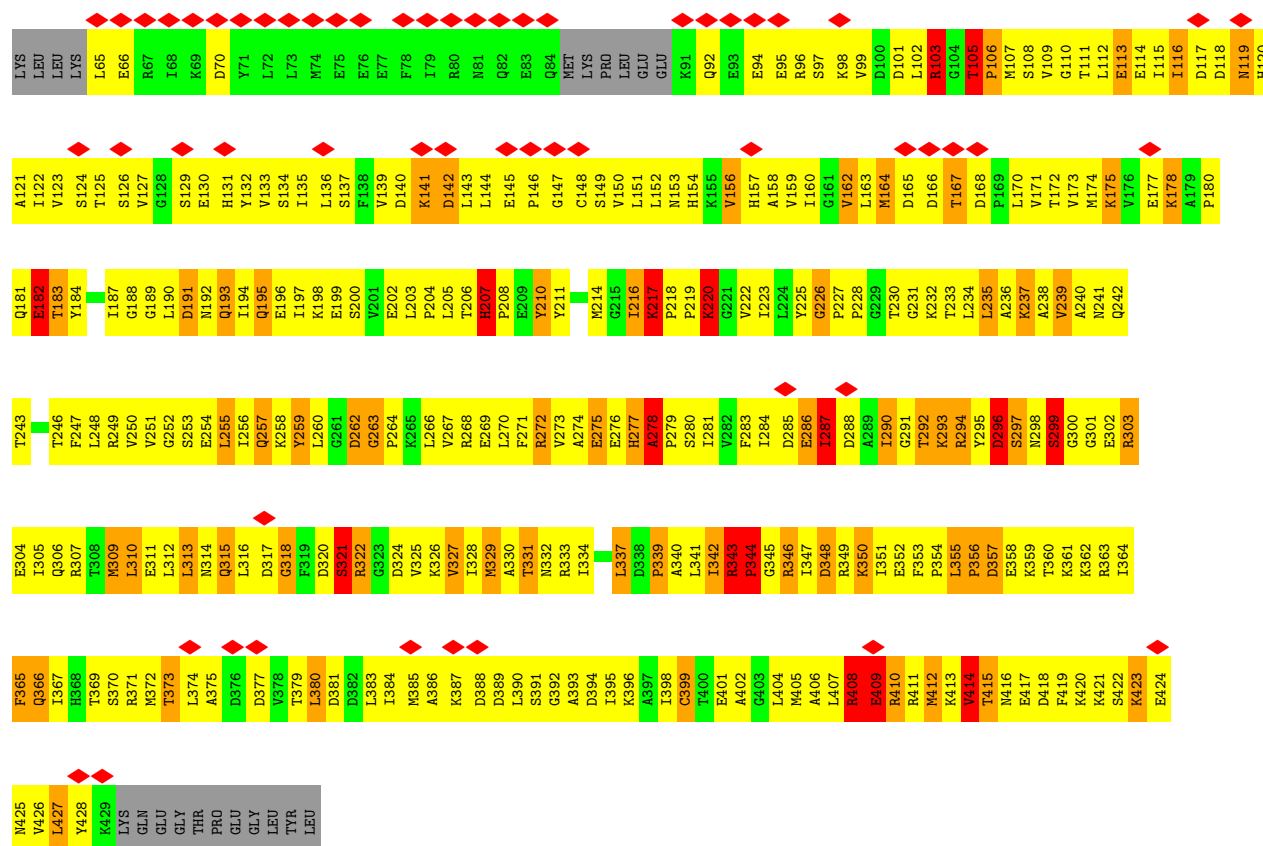
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

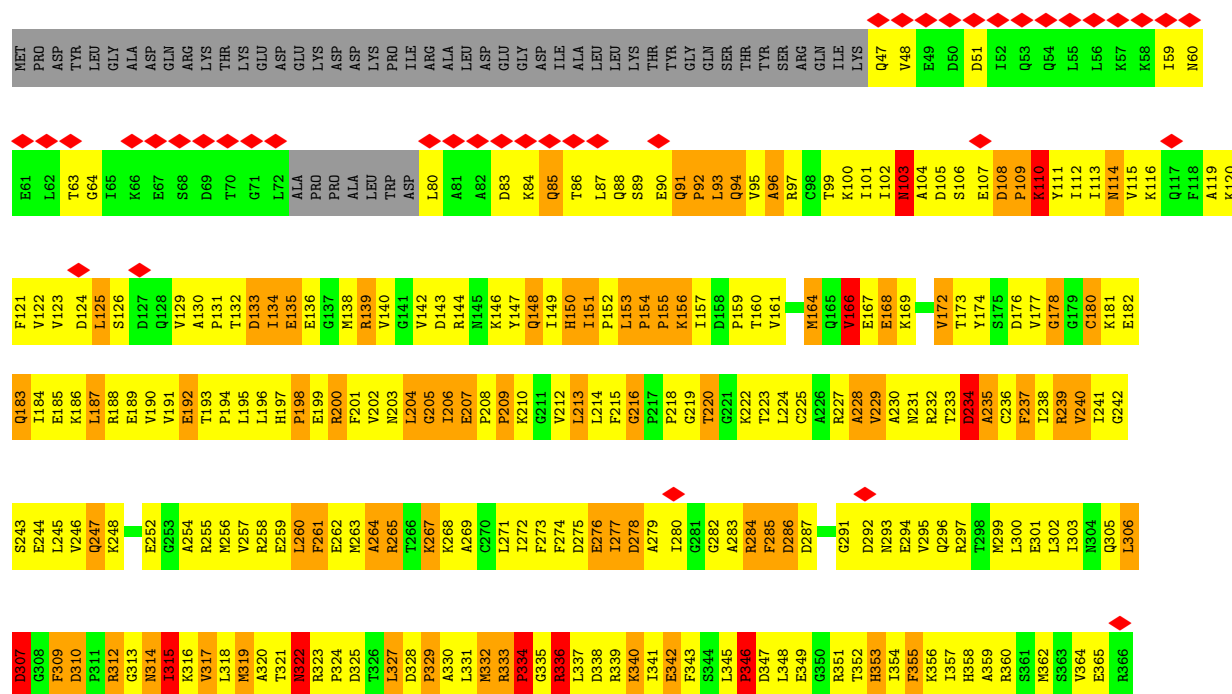
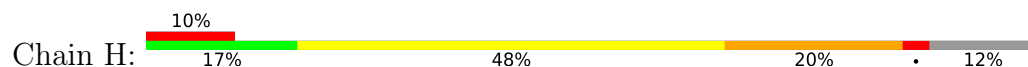


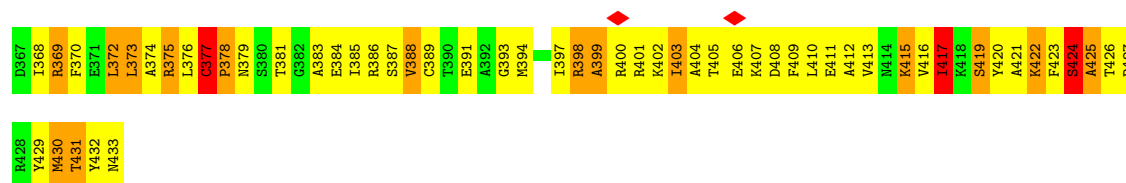
• Molecule 1: 26S protease regulatory subunit 4



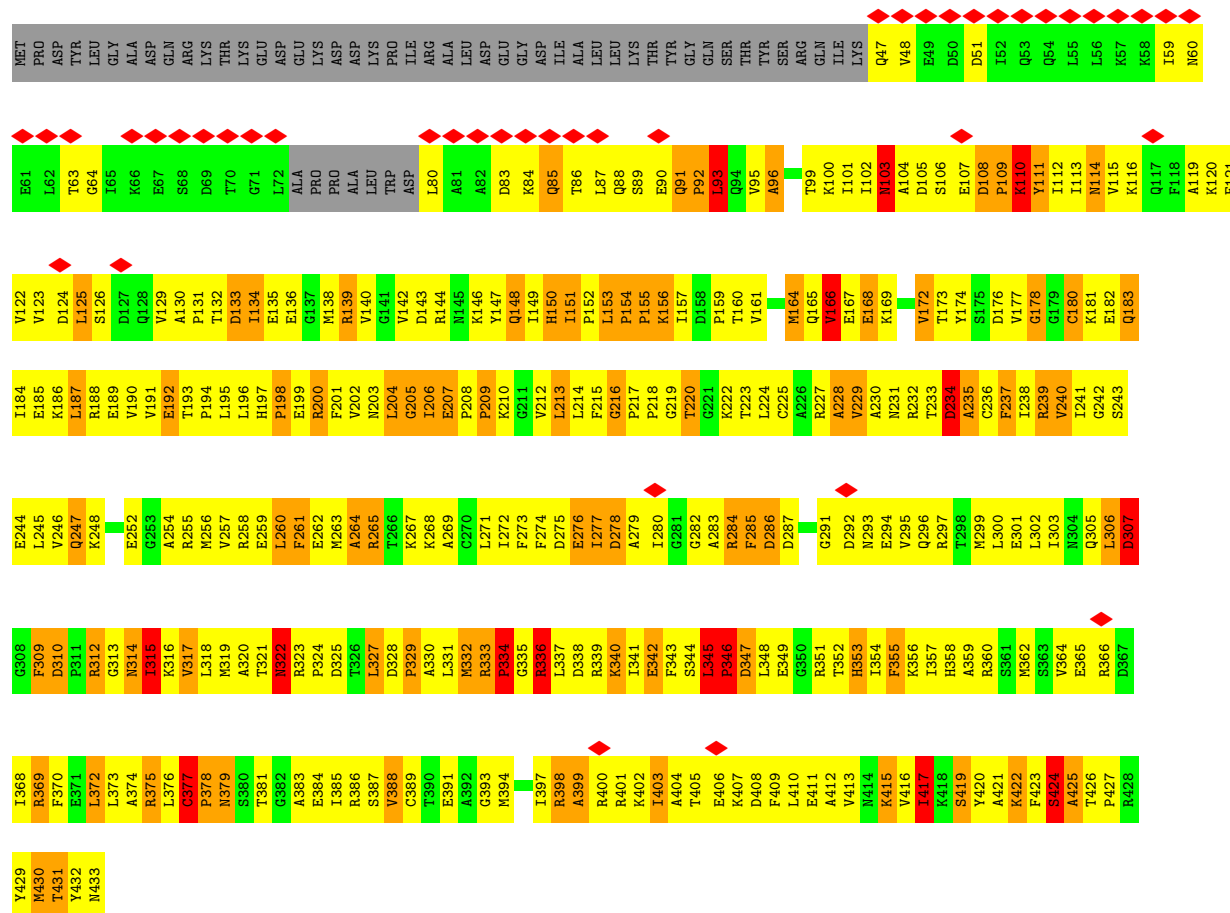
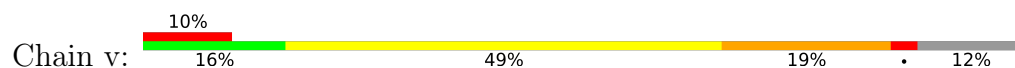


• Molecule 2: 26S protease regulatory subunit 7

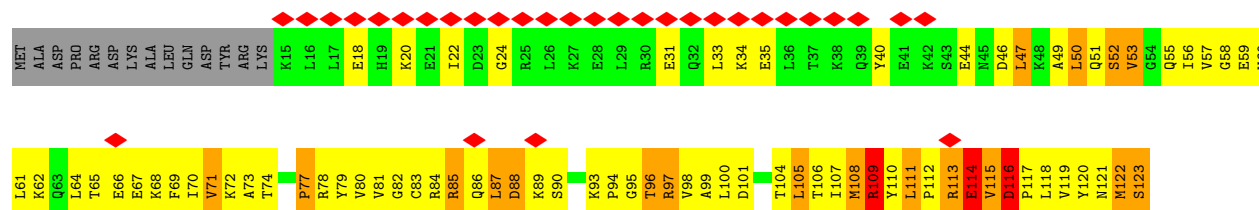
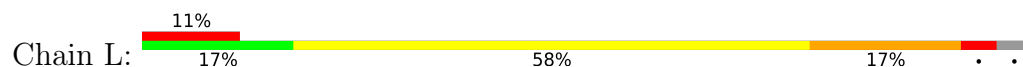


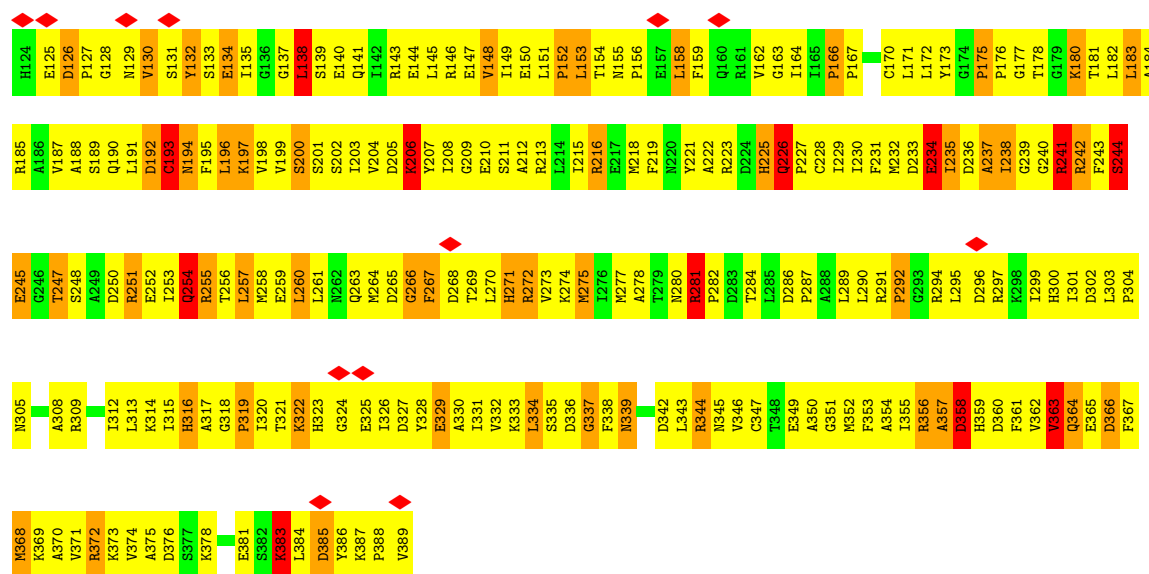


• Molecule 2: 26S protease regulatory subunit 7

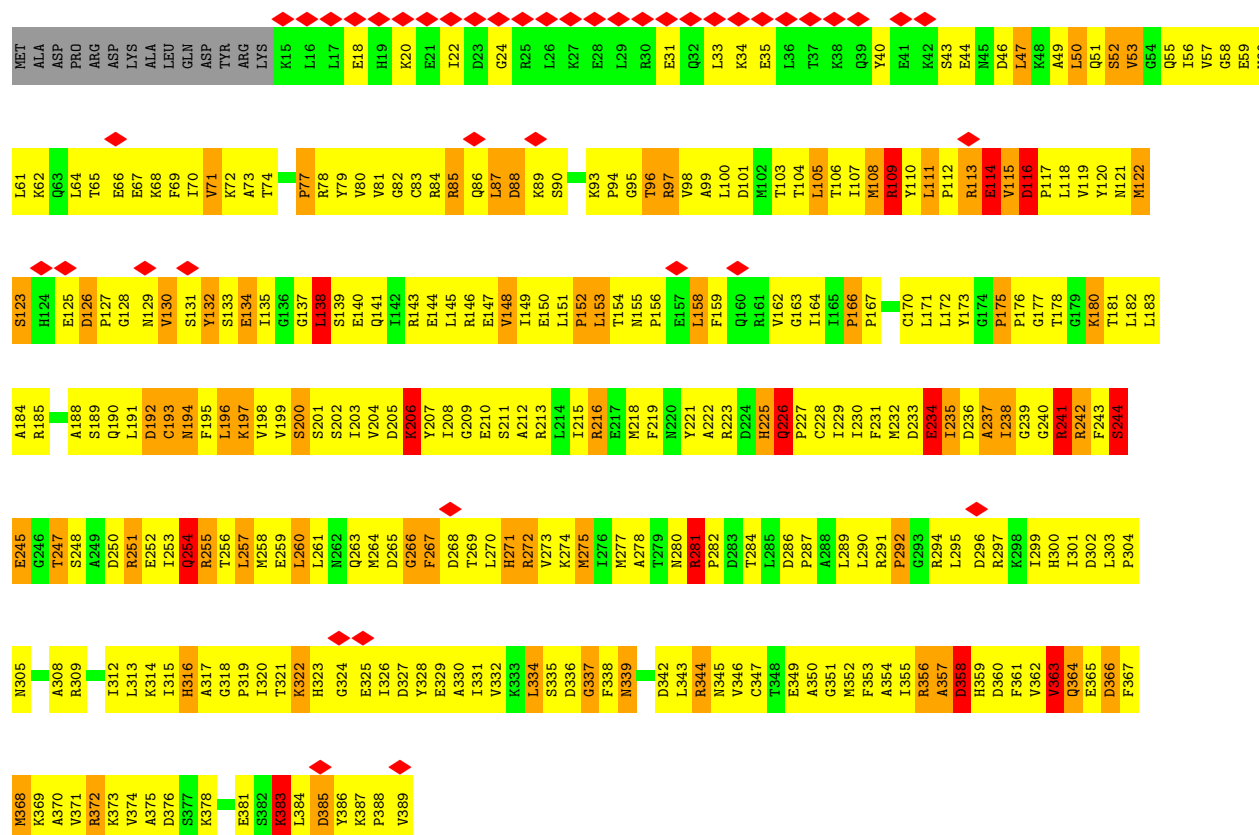
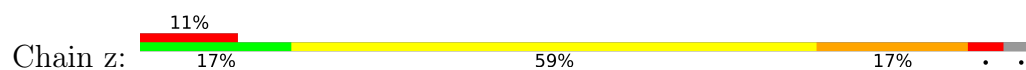


• Molecule 3: 26S protease regulatory subunit 10B

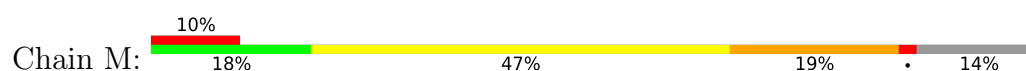


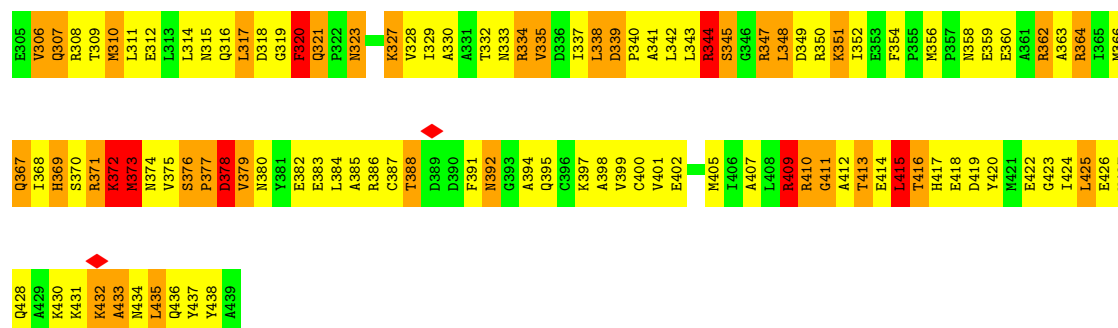


• Molecule 3: 26S protease regulatory subunit 10B

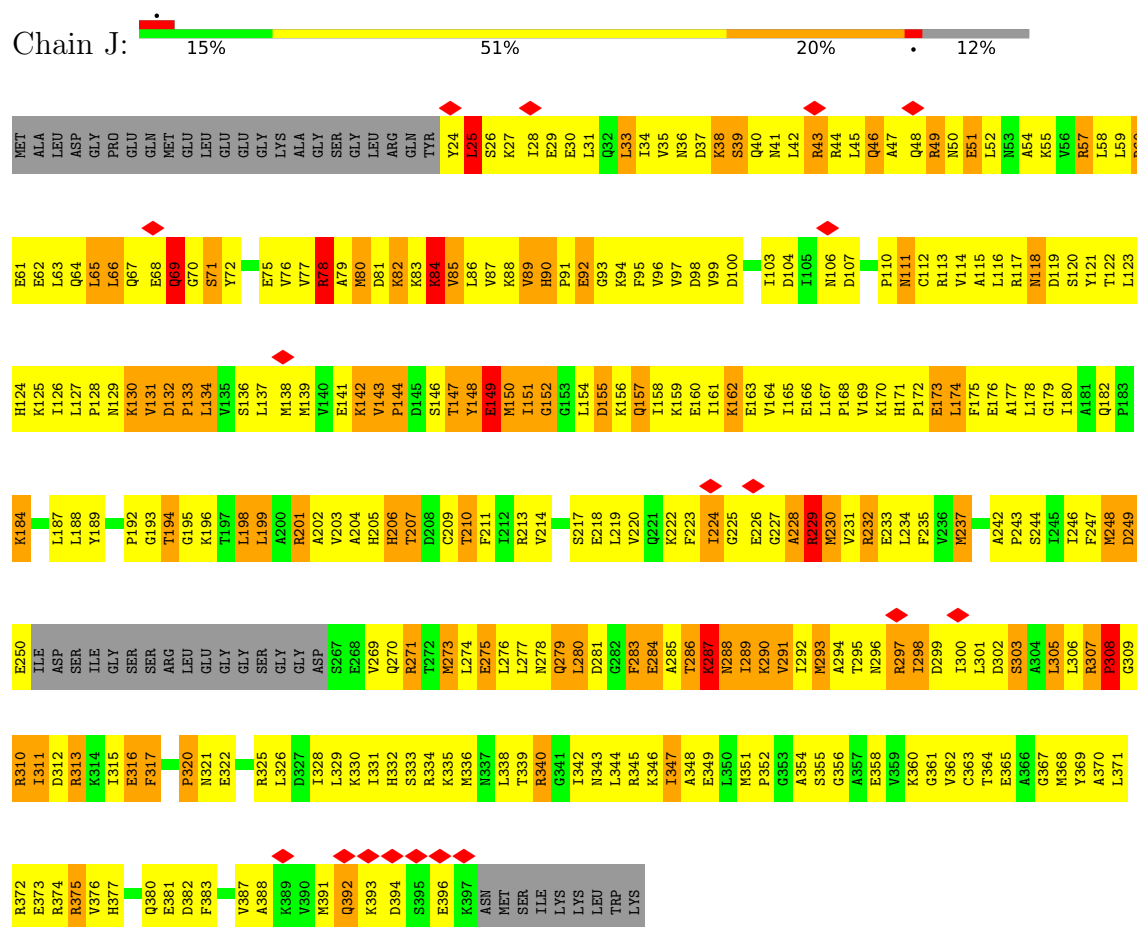


• Molecule 4: 26S protease regulatory subunit 6A

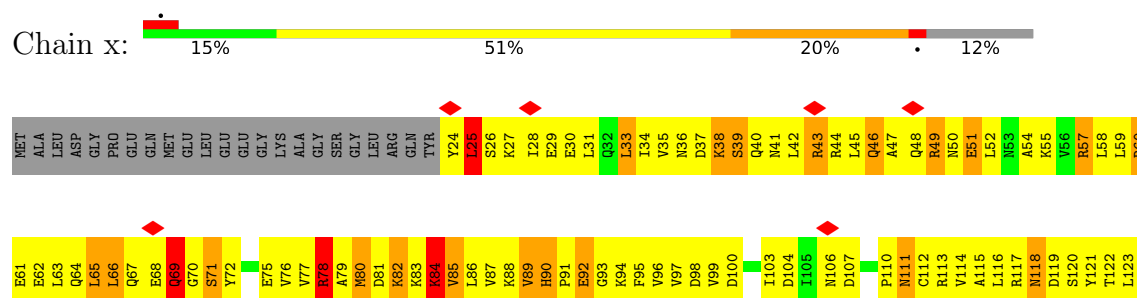


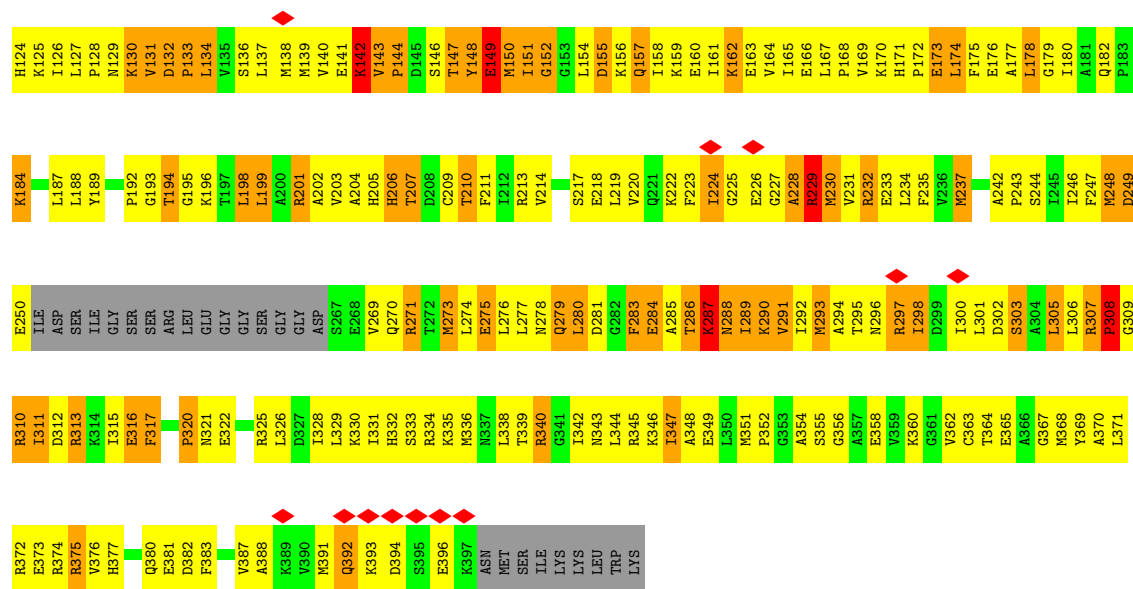


• Molecule 5: 26S protease regulatory subunit 8

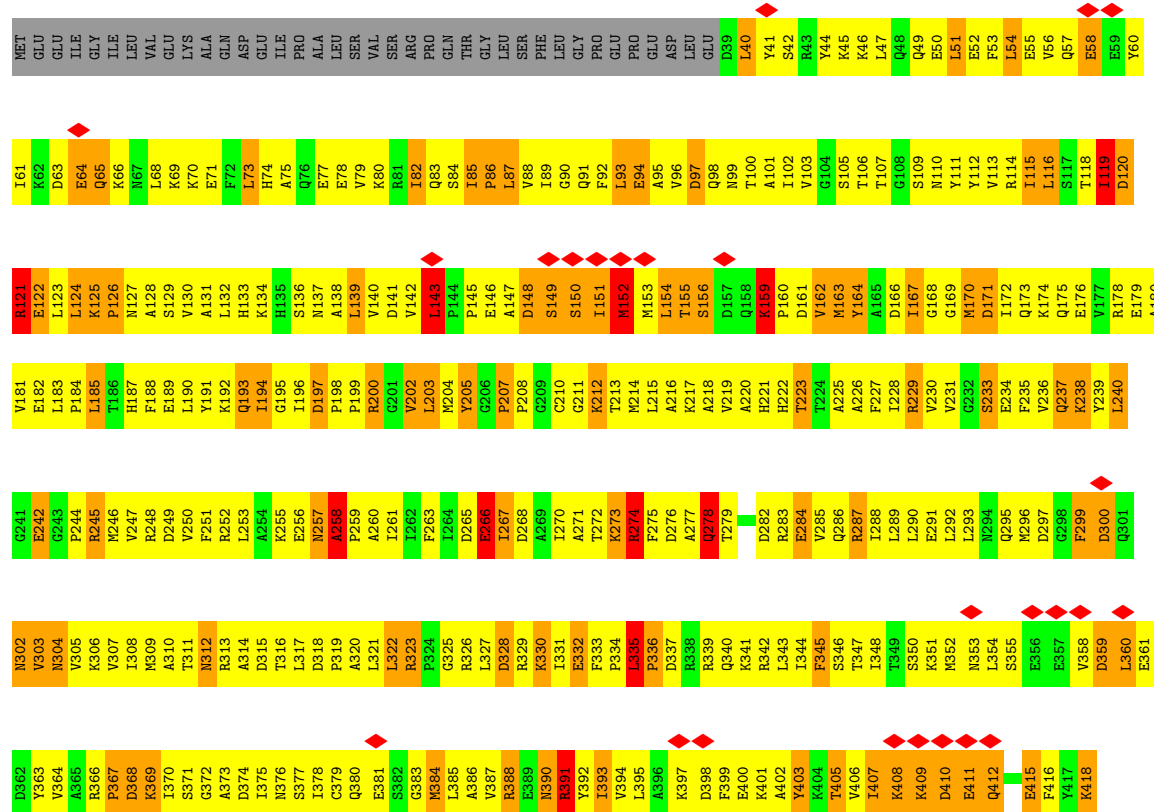
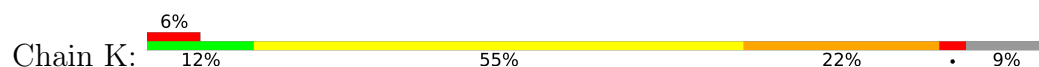


• Molecule 5: 26S protease regulatory subunit 8

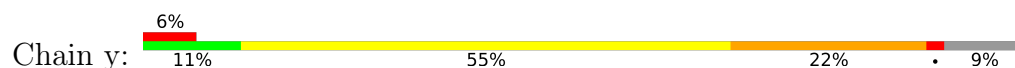




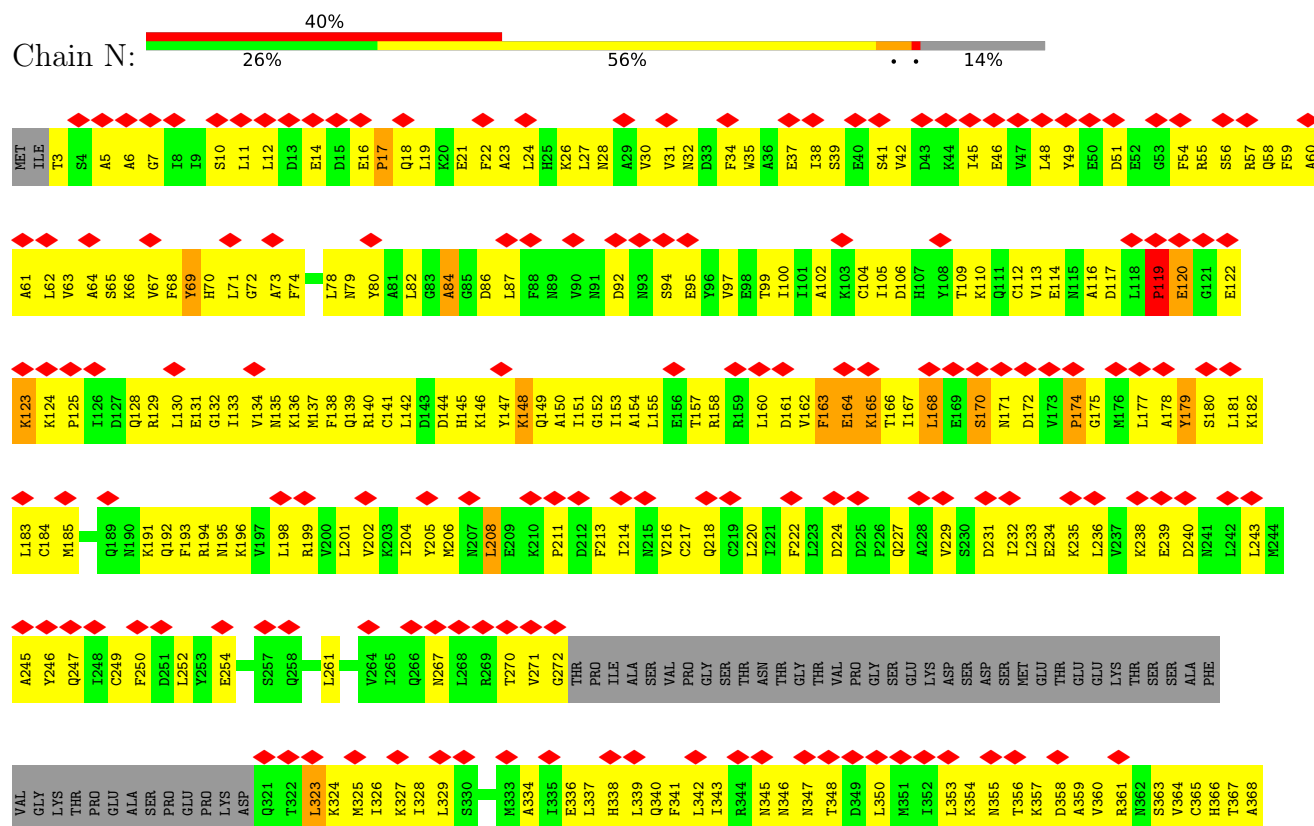
• Molecule 6: 26S protease regulatory subunit 6B

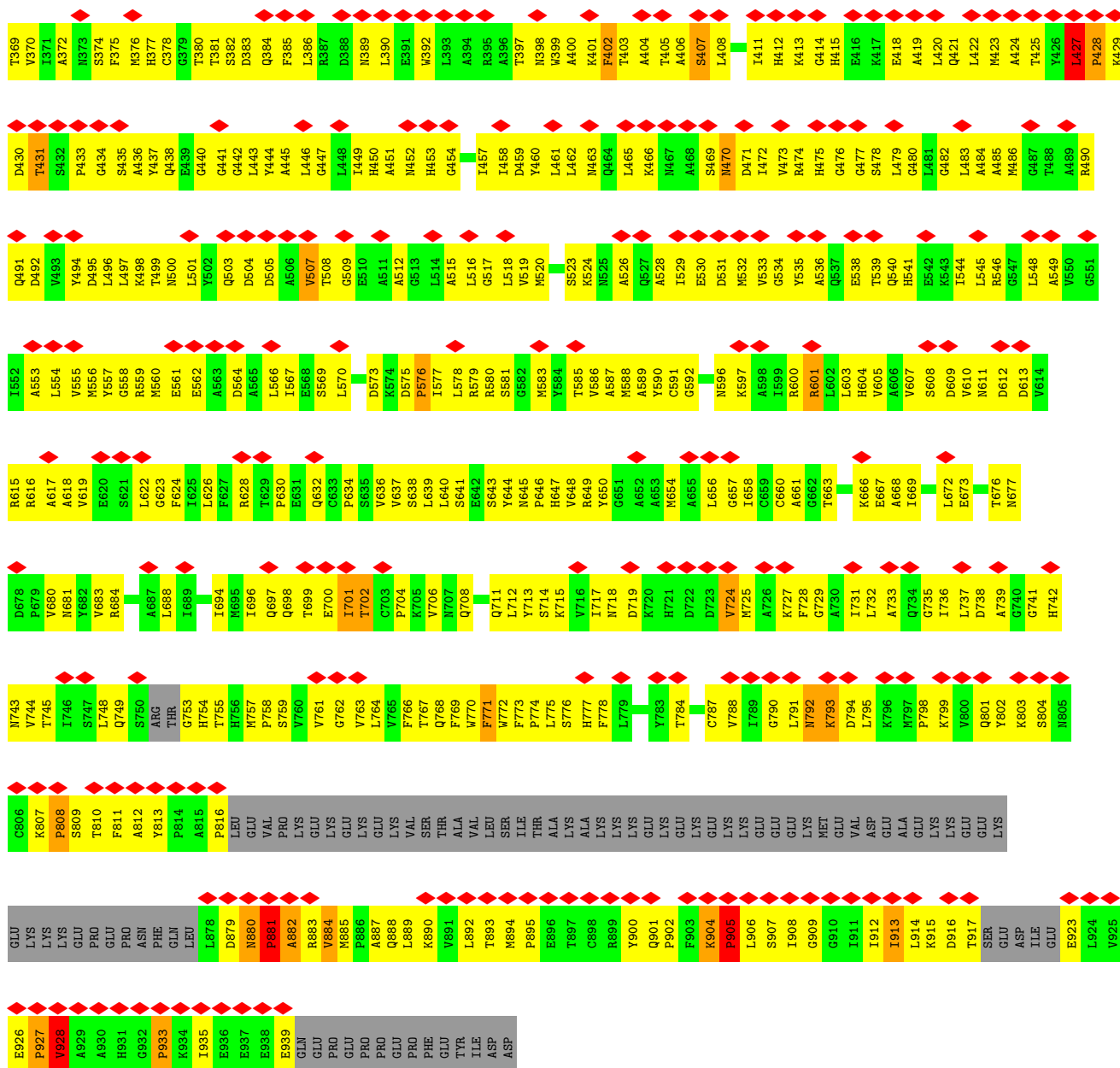


• Molecule 6: 26S protease regulatory subunit 6B

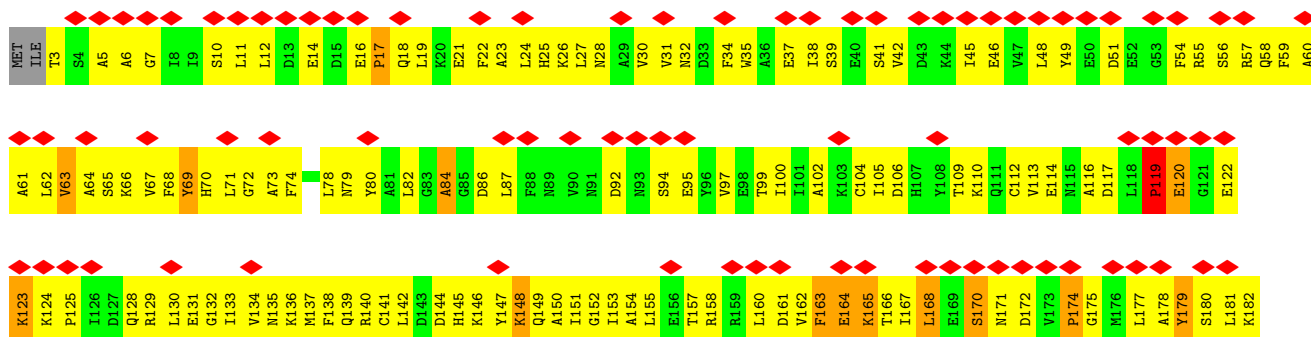


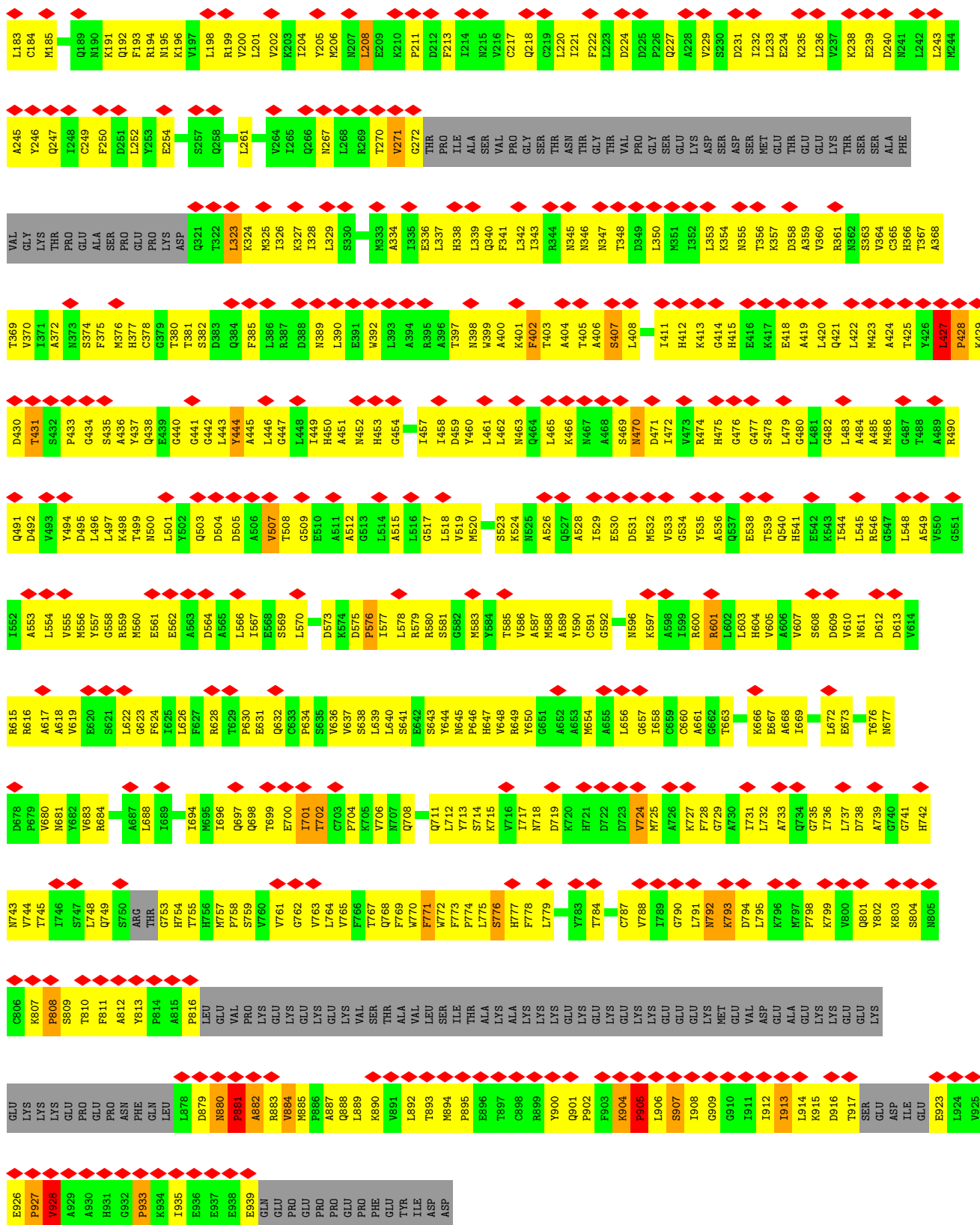
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 1





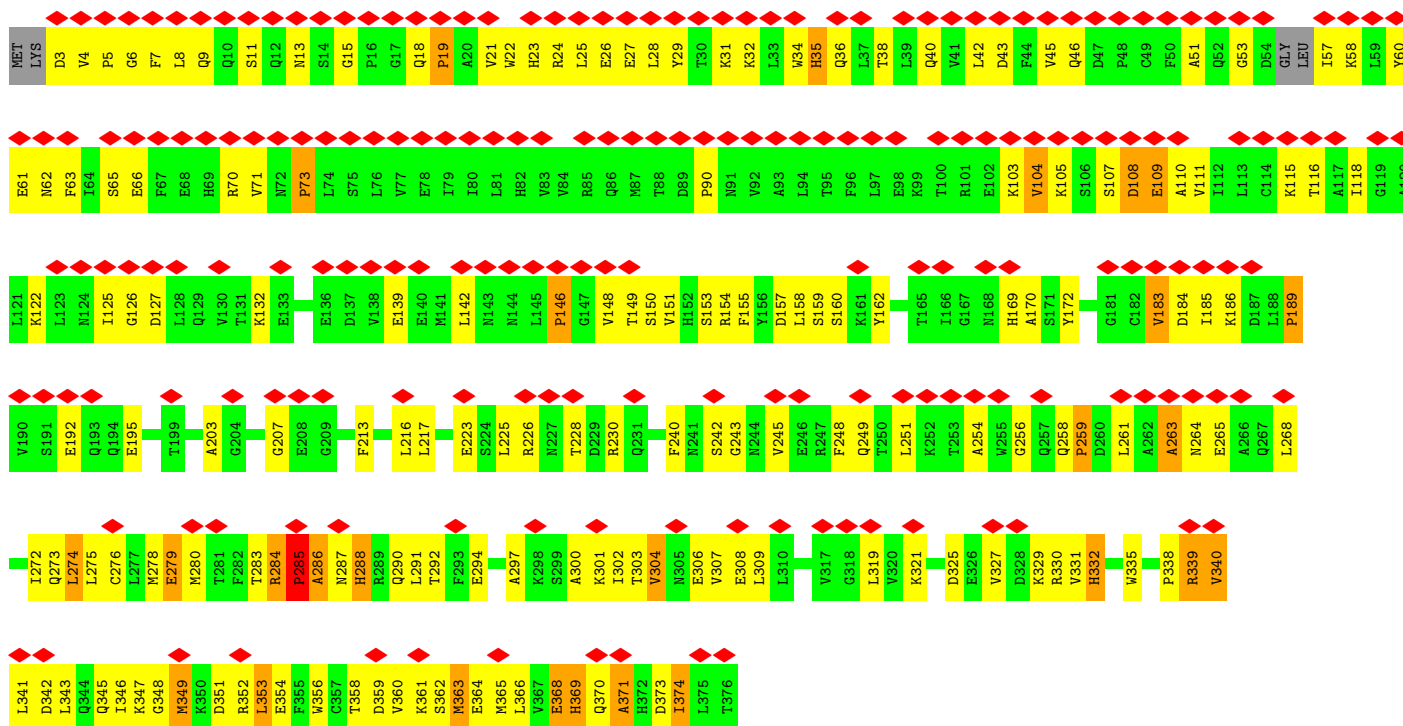
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1



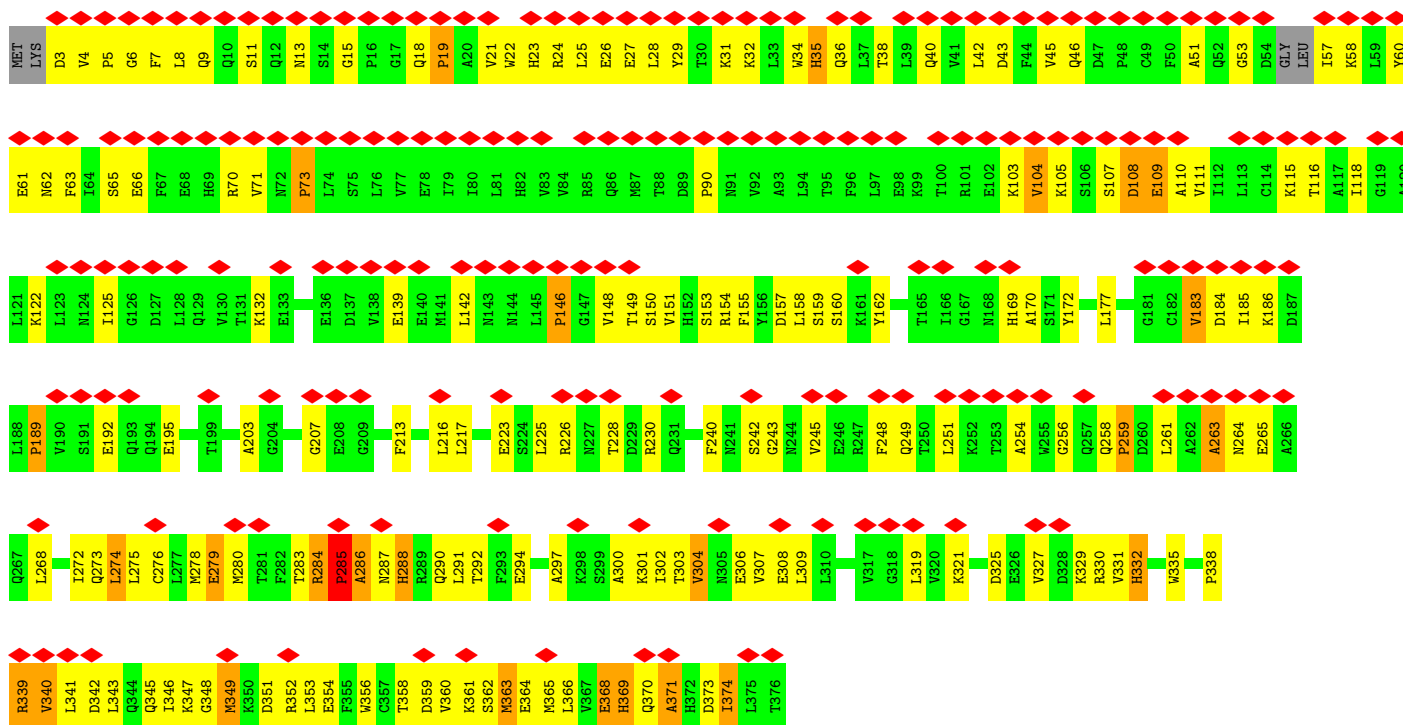


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13



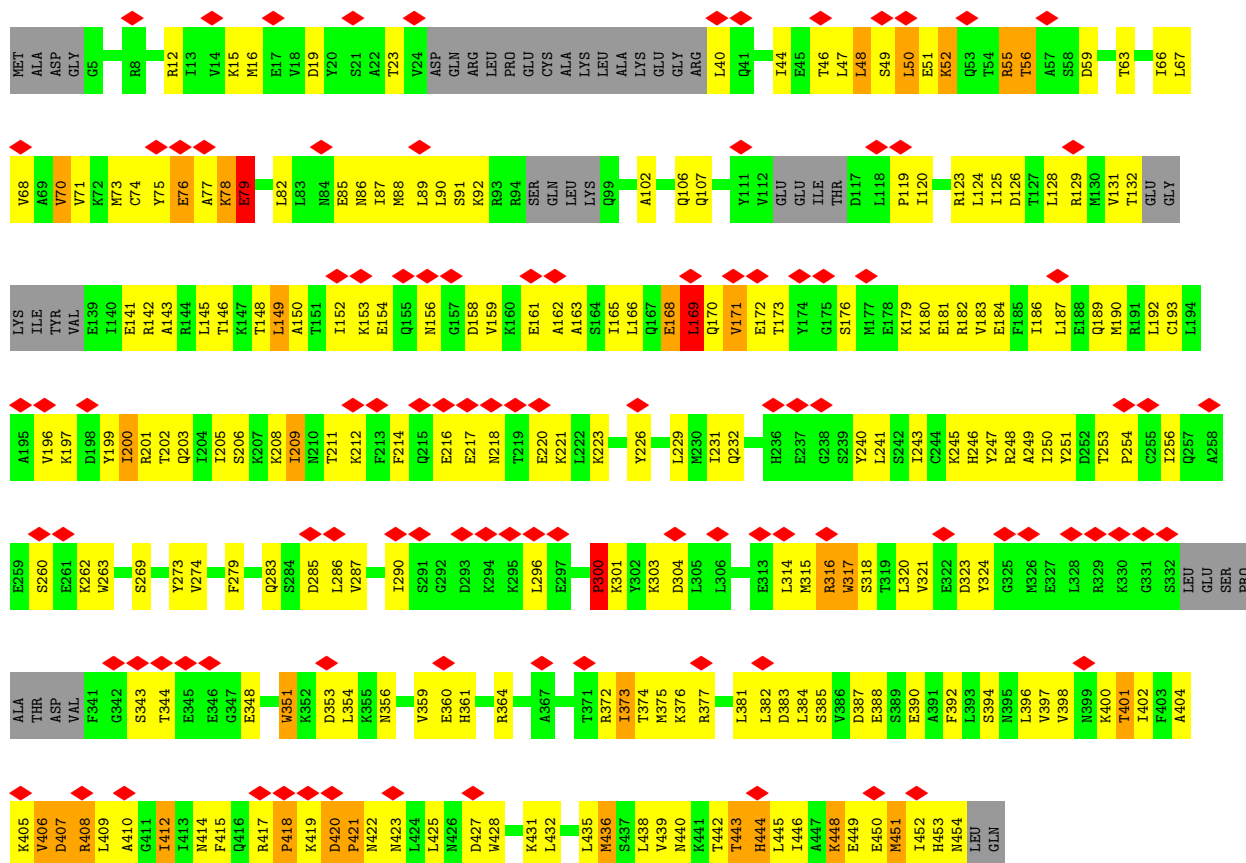


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

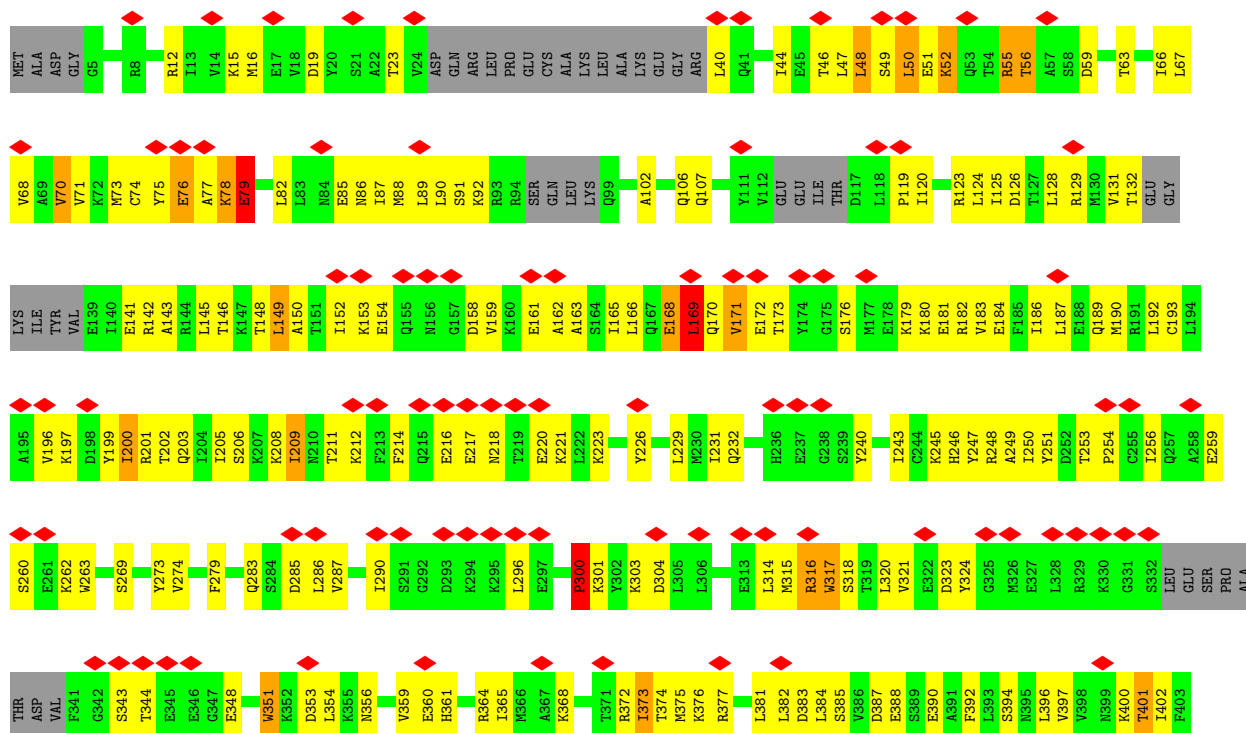


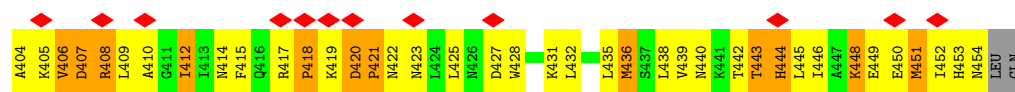
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



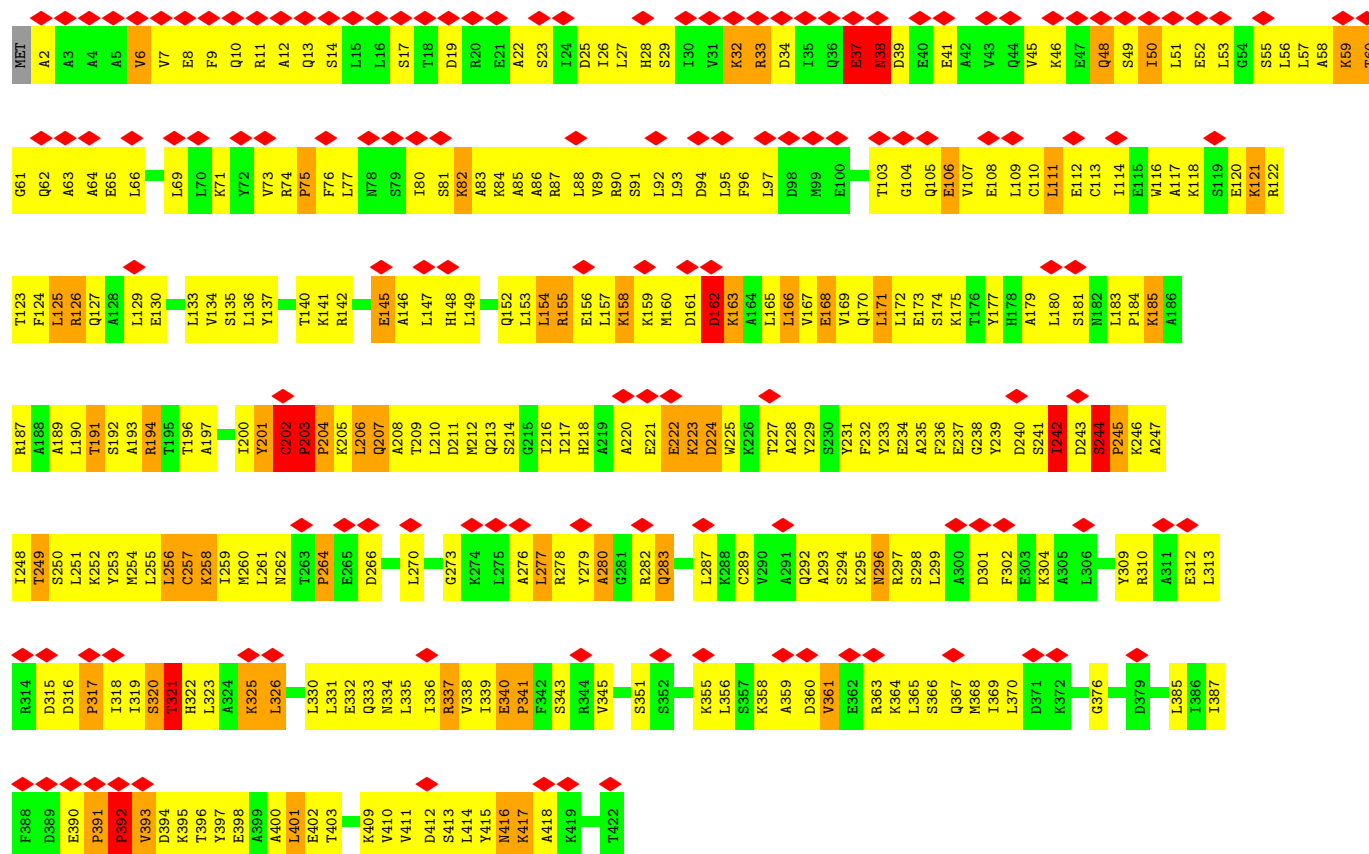


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

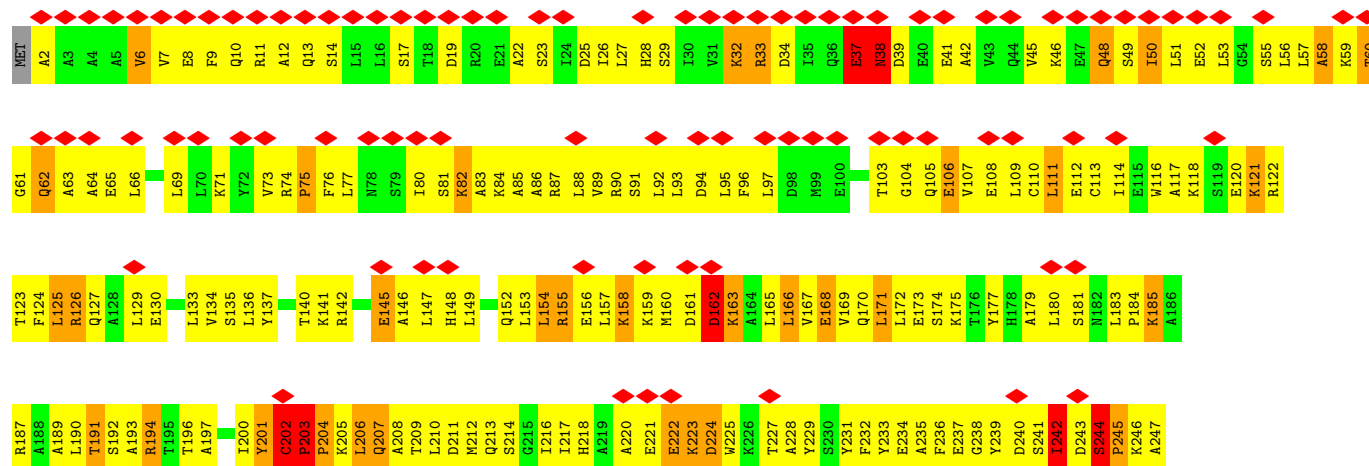




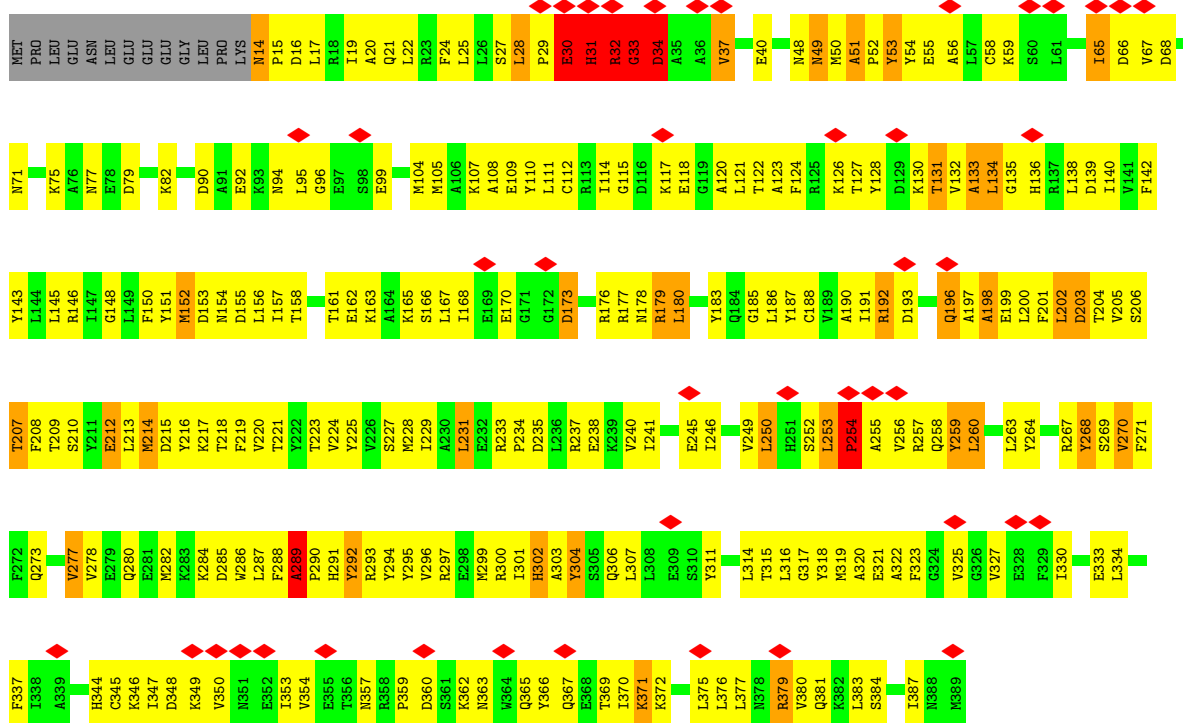
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



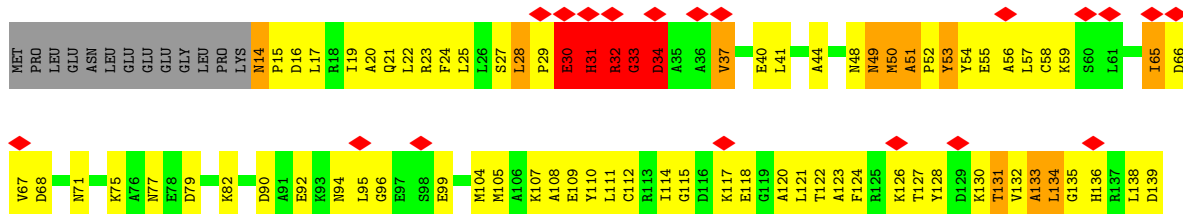
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



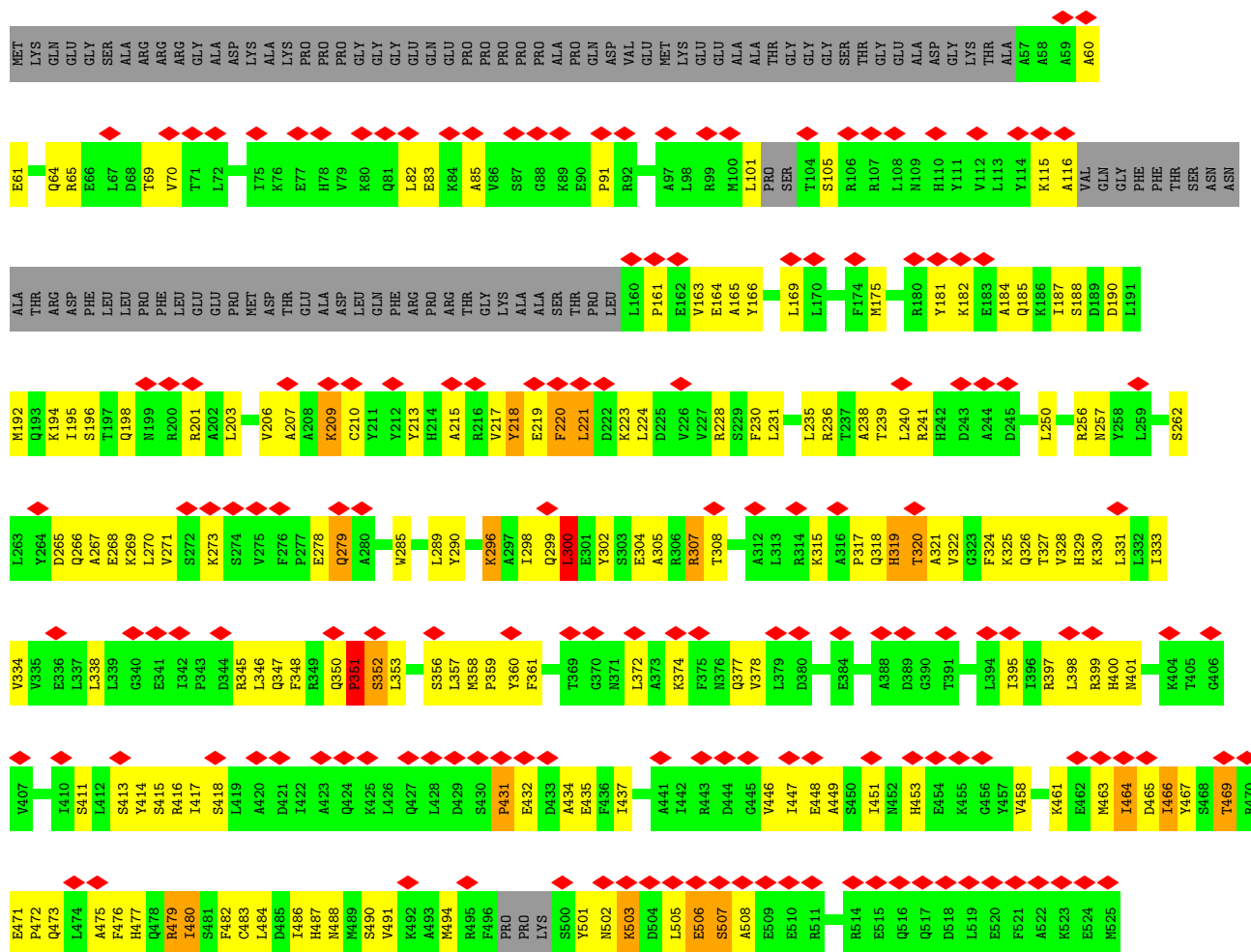
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6



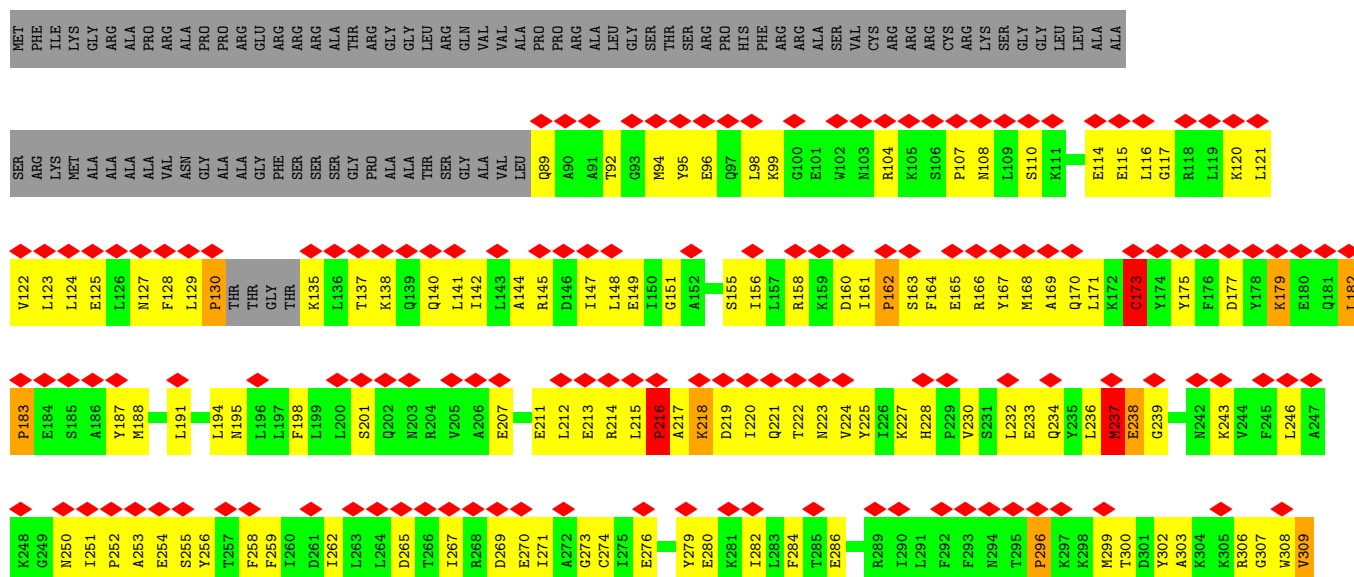
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6





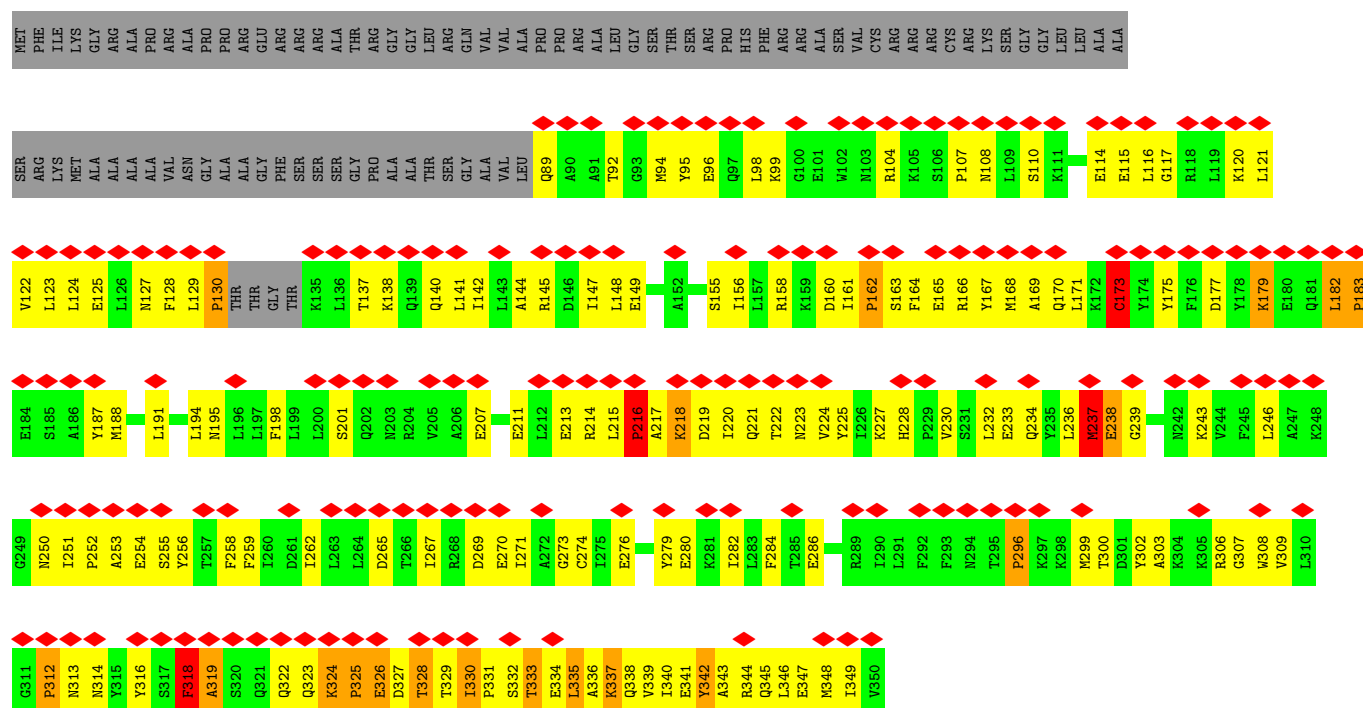


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

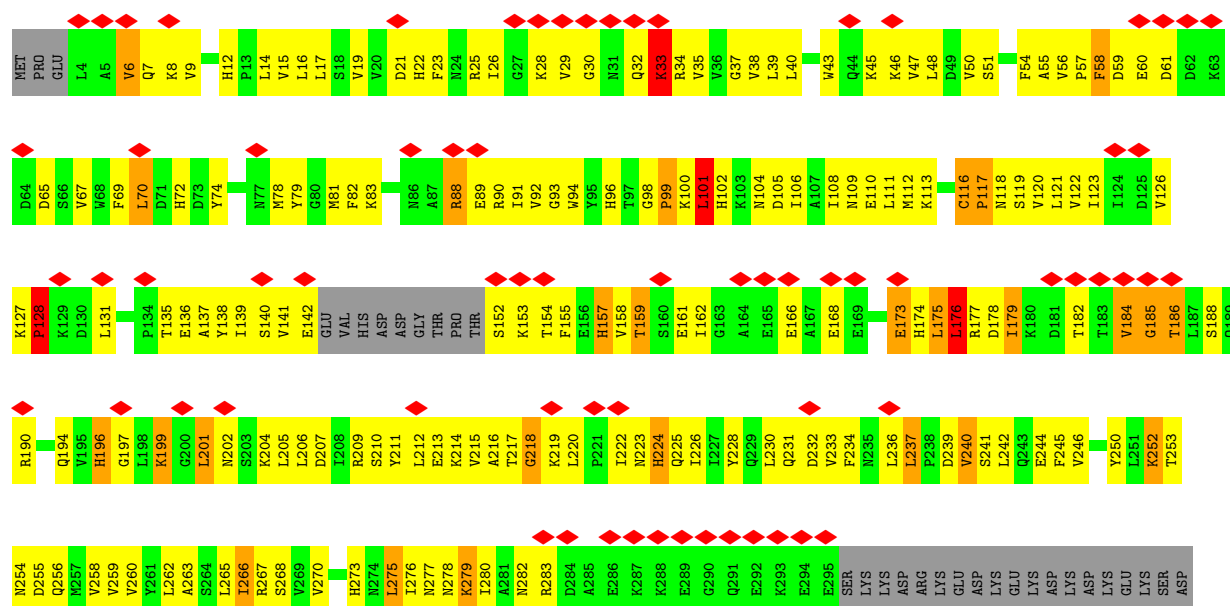


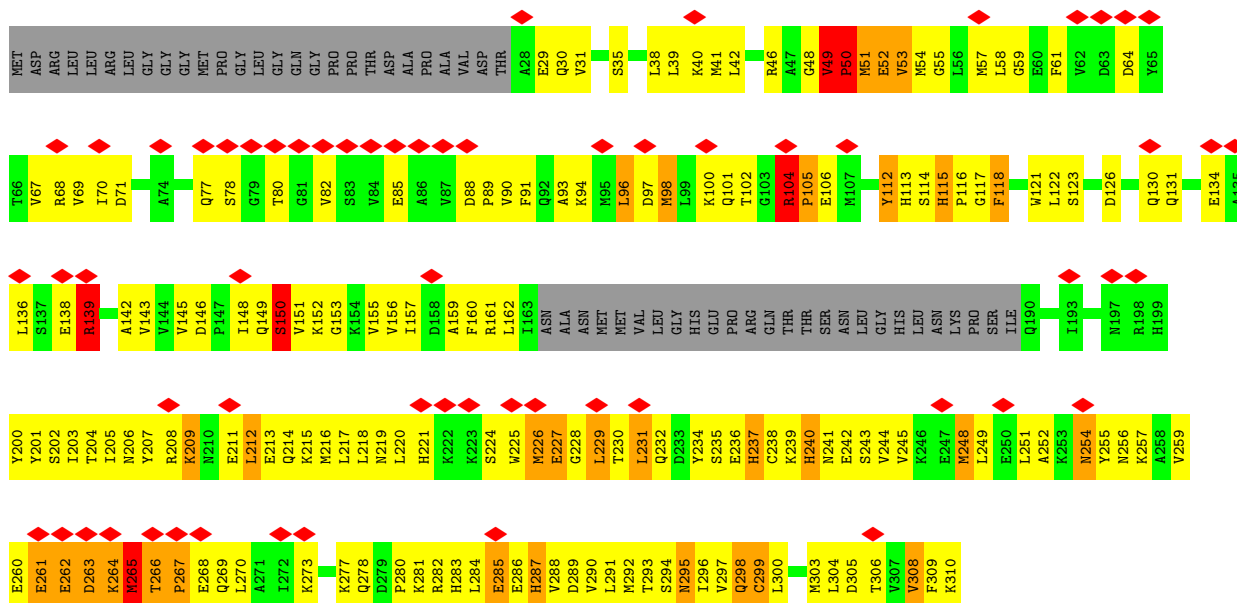


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

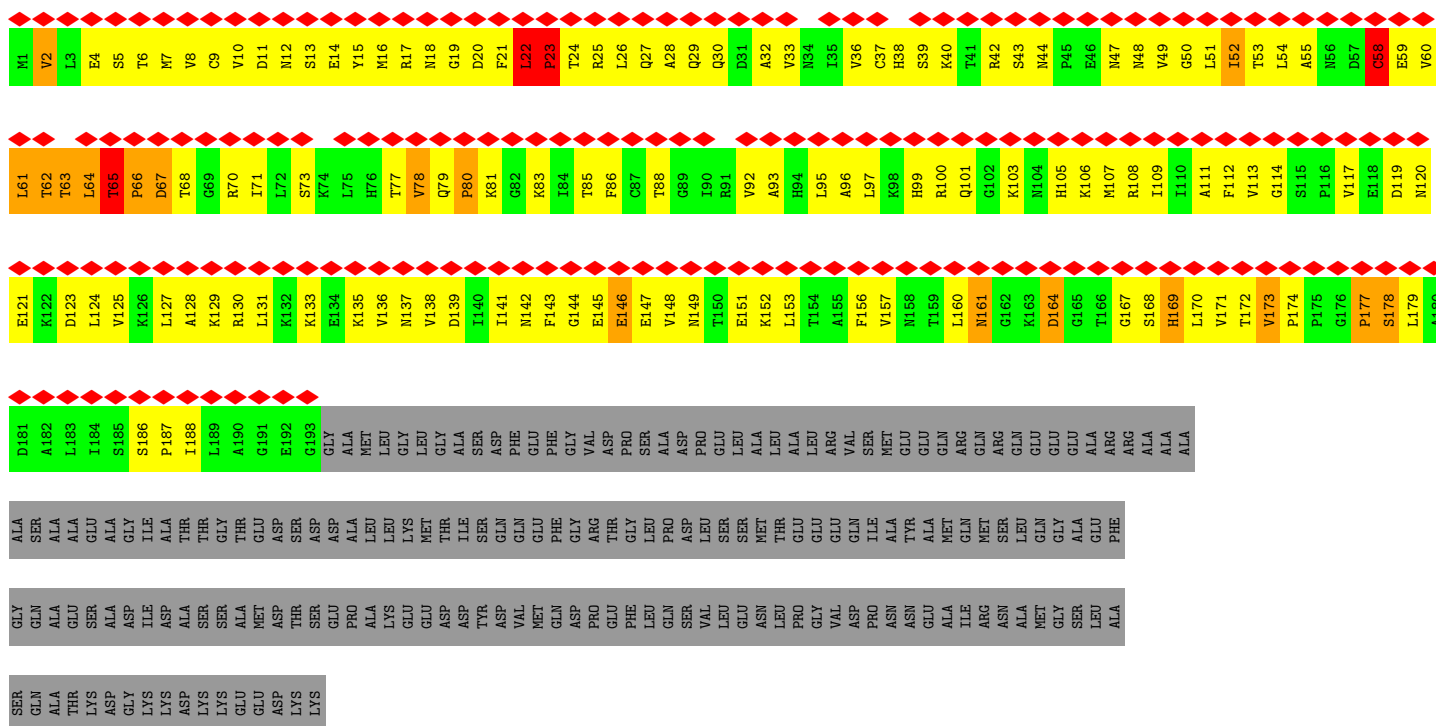


• Molecule 14: 26S proteasome non-ATPase regulatory subunit 7





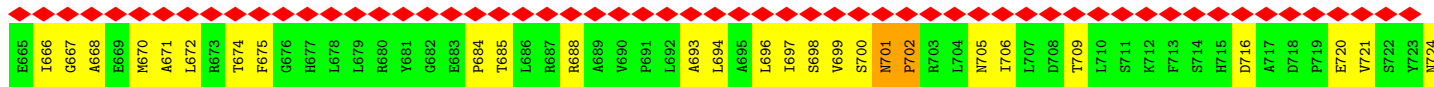
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 4



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



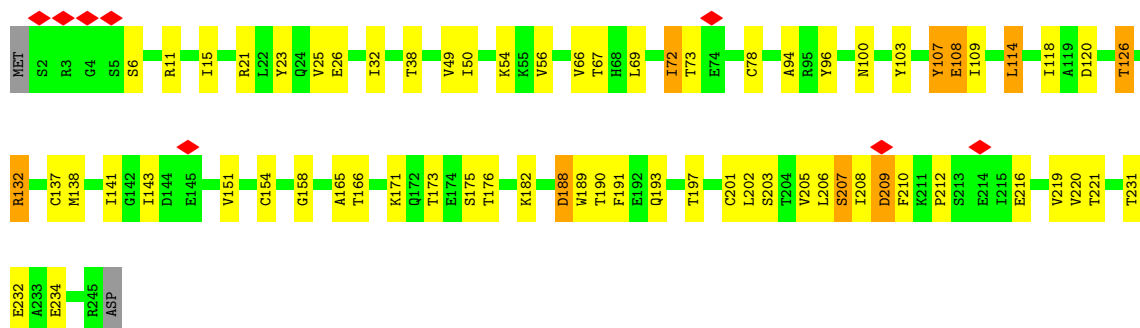
V844	D784	N724	E664	G604	E544	F483	V422	G362	GLY	P241	R181	F121	GLU
R845	R785	S725	E665	N605	K545	G484	D423	S363	VAL	E242	E182	A122	ARG
V846	Q786	T726	I666	V606	S846	L485	G424	Q364	PHE	P243	P183	A123	LEU
G847	L787	F727	G667	L607	E547	G486	G425	V365	LEU	E244	L184	D124	GLY
Q848	L788	A728	A668	K608	T548	L487	L426	D366	LEU	S246	L185	D125	GLU
ALA	M789	M729	E669	V609	E549	A488	T427	S367	SER	A247	T186	I126	ASP
VAL	Q790	G730	M670	Q610	L550	Y489	Q428	A368	E309	A248	L187	S127	THR
VAL	V791	M731	A671	D611	K551	A490	I429	R369	D310	L248	V188	V128	LEU
VAL	A792	V732	L672	L612	D552	G491	D430	M370	V311	L249	K189	V129	TYR
GLY	V793	G733	B673	L613	T553	S492	K431	N371	E312	R250	E190	A130	ARG
ALA	A794	S734	T674	H614	Y554	N493	Y432	N372	E313	L251	E191	L139	PRO
GLY	G795	G735	F675	L615	A555	R494	L433	A373	Y314	C251	I191	M131	ALA
LYS	L796	T736	G676	C616	R556	E495	Y434	S374	E315	A252	V192	T132	LEU
PRO	L797	M737	H677	S617	W557	D496	S435	S375	D316	L253	P193	M133	GLU
LYS	T798	M738	L678	E618	L558	V497	S436	F376	L317	G254	Y194	S134	LEU
THR	V799	A739	L679	HIS	P559	L498	E437	V377	T318	V255	N195	G135	ARG
THR	L800	R740	R680	PHE	L560	T499	D438	N378	I320	F256	M196	E136	ARG
GLY	R801	L741	Y681	ASP	G561	L500	Y439	G379	I321	K258	A197	R137	GLN
PHE	S802	A742	G682	SER	L562	L501	I440	F380	M321	F259	H198	E138	ILE
GLN	F803	A743	E683	LYS	G563	L502	K441	V381	S322	K260	A200	C139	ARG
THR	L804	M744	P684	LYS	L564	P503	S442	N382	V324	R261	A201	L140	THR
THR	D805	L745	T685	GLU	N565	V504	G443	A383	Q325	F262	H202	Y142	THR
V806	R806	R746	L686	ASP	H566	M505	A444	A384	Q326	P263	E203	R143	MET
R807	R807	Q747	L687	LYS	L567	G506	L445	F385	L327	E264	A204	L144	SER
N808	L748	L748	R688	LYS	G568	D507	L446	G386	N327	G266	C205	V145	VAL
I809	A749	Y750	A689	LYS	K569	S508	A447	Q387	S328	L266	D206	G146	PRO
I810	Q750	Y751	V690	LYS	G570	K509	C448	D388	N329	R267	L207	S147	LYS
L811	Y751	H752	P691	LYS	E571	S510	G449	K389	F330	L268	L208	Q148	PRO
G812	H752	A753	L692	ASP	A572	S511	I450	L390	A332	A269	M209	Q149	LEU
K813	A753	L754	A693	LYS	L573	M512	V451	L391	A333	L270	E210	E150	PHE
S814	K754	K754	L694	LYS	E574	E513	M452	T392	A334	M271	I211	L151	LEU
H815	D755	D755	A695	LYS	A575	V514	S453	D393	R335	L272	E212	A152	ARG
L696	P756	P756	L696	GLU	L576	A515	G454	D394	E336	D274	V214	W154	HIS
V817	M757	M757	L697	ALA	L577	G516	V455	G395	E336	D275	D215	G155	TYR
L818	M758	M758	S698	ALA	A578	V517	R456	N396	D338	E276	M216	G156	GLY
V819	L759	L759	V699	ALA	A579	T518	N457	K397	D338	L277	M217	H156	LYS
G820	F760	F760	S700	ASP	A579	A519	E458	W398	I339	V278	E157	E157	LEU
L821	M761	M761	N701	GLY	E581	L520	C459	L399	M340	E279	E158	E158	PHE
V822	V762	V762	F702	ALA	V582	A521	D460	Y400	E341	K219	V159	V159	LEU
R763	R763	R763	R703	HIS	G522	G523	P461	K401	P342	D280	K220	R160	ARG
A824	L764	L764	L704	GLN	G523	M524	A462	M402	K343	I281	I221	H161	TYR
M825	A765	A765	N705	VAL	E585	V527	L463	K403	V344	F282	D222	L162	GLY
Q826	Q766	Q766	T706	A653	F586	G528	A464	D404	P345	T283	E223	A163	LYS
P827	G767	G767	L707	V654	F587	S529	L465	H405	D345	S284	N224	G164	M113
R828	L768	L768	T708	L655	R588	S529	L466	G406	D347	C285	A225	E165	A114
M829	T769	T769	T709	G656	S589	C530	S467	M407	I348	K286	Y226	E166	P115
L830	H770	H770	L710	T657	F590	N531	D468	L408	Y349	D287	A227	V166	G116
V831	L771	L771	S711	A658	A591	G532	Y469	S409	K350	V288	K228	A167	E117
T832	G772	G772	K712	L659	N592	D533	V470	A410	T351	V289	V229	E168	K118
F833	K773	K773	F713	T660	T593	V534	L471	A411	H352	Q291	C230	K169	K119
D834	G774	G774	S714	A661	L594	T535	H472	A412	L353	Q292	L231	W170	R120
E835	T775	T775	H715	M662	V595	S536	H473	S413	E354	K293	L233	E169	
E836	L776	L776	D596	G663	V597	T537	N473	S414	N355	Q293	Y232	GLN	
L837	T777	T777	A717	V654	V597	L538	S474	L414	N356	M294	T234	LEU	
R838	L778	L778	D718	L655	C598	L539	N475	G415	R357	A295	ASP	GLU	
P839	G779	G779	F719	G656	A599	Q540	T476	M416	F358	F296	ALA	GLU	
L840	F780	F780	E720	T657	Y600	T541	R478	L418	G359	M297	LYS	GLU	
P841	H781	H781	W721	M662	A601	L542	R478	L419	G360	R300	N238	LYS	
V842	H782	H782	S722	G663	G602	M543	S481	W420	S361	H301	V179	Q180	
S843	S783	S783	Y723	G663	S603		L482	D421			V240		





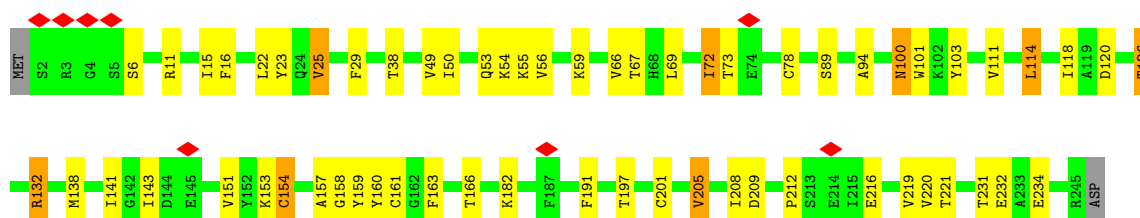
• Molecule 19: Proteasome subunit alpha type-6

Chain B: 72% 24%



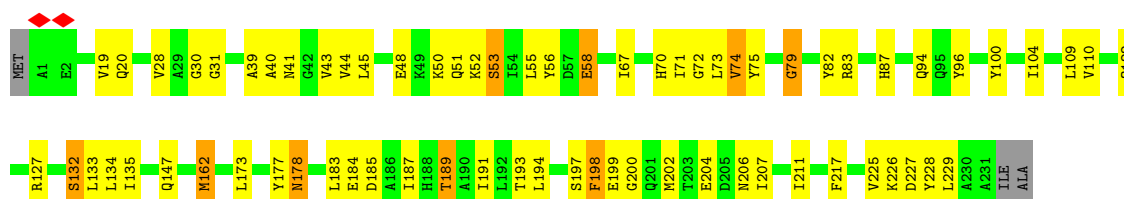
• Molecule 19: Proteasome subunit alpha type-6

Chain h: 74% 22%

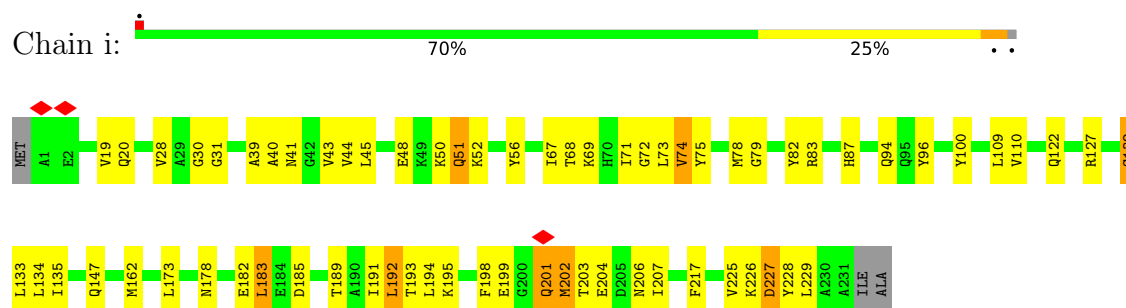


• Molecule 20: Proteasome subunit alpha type-2

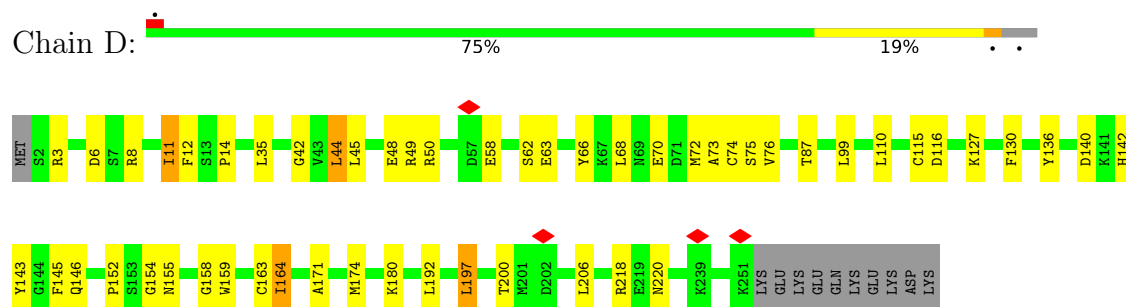
Chain C: 69% 26%



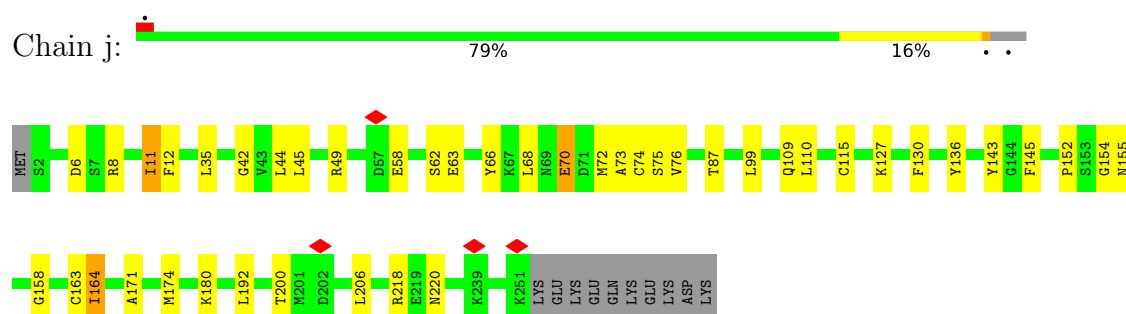
- Molecule 20: Proteasome subunit alpha type-2



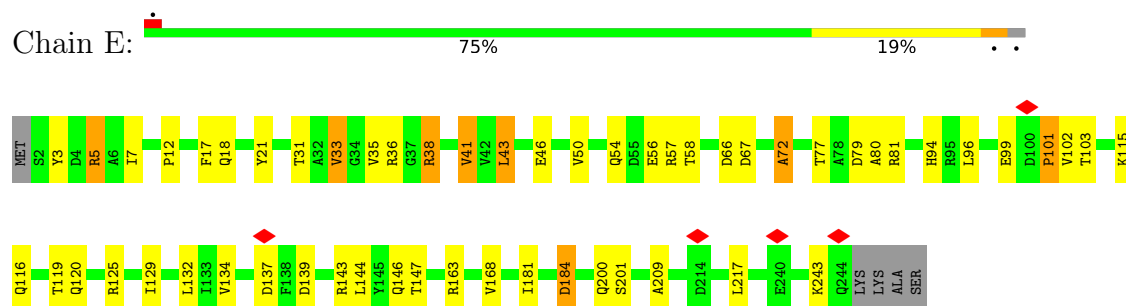
- Molecule 21: Proteasome subunit alpha type-4



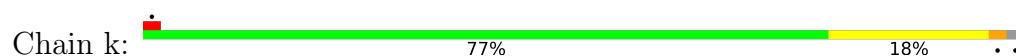
- Molecule 21: Proteasome subunit alpha type-4

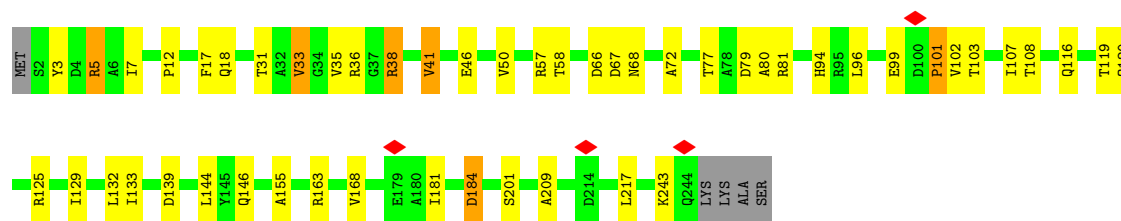


- Molecule 22: Proteasome subunit alpha type-7

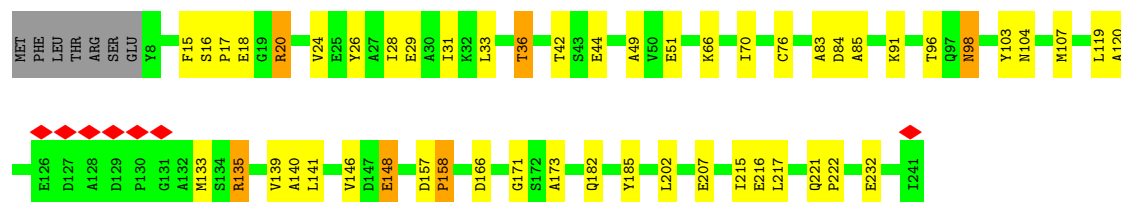
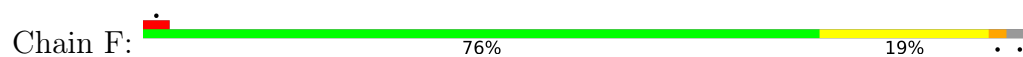


- Molecule 22: Proteasome subunit alpha type-7

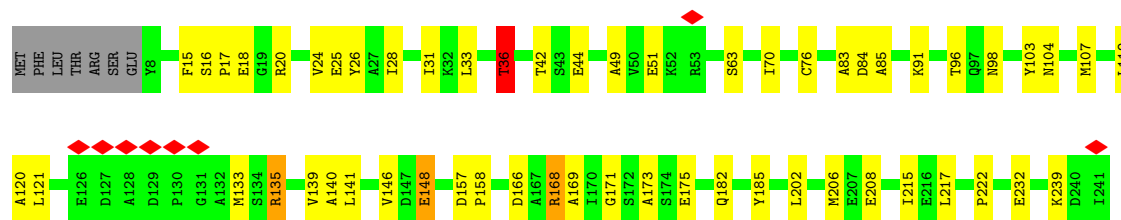




• Molecule 23: Proteasome subunit alpha type-5



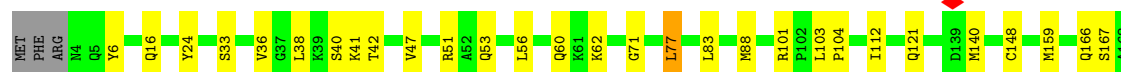
• Molecule 23: Proteasome subunit alpha type-5

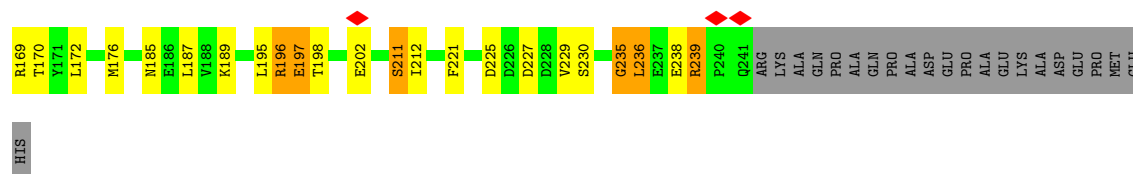


• Molecule 24: Proteasome subunit alpha type-1



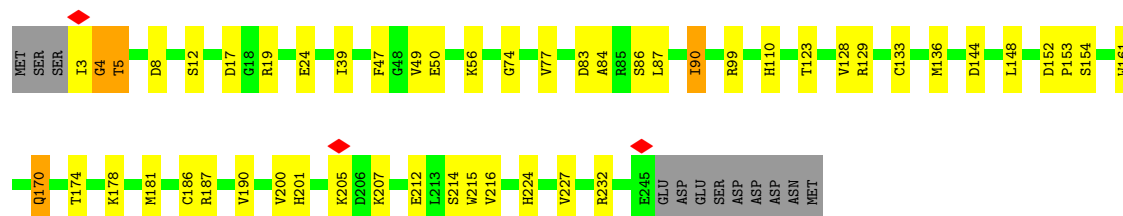
• Molecule 24: Proteasome subunit alpha type-1





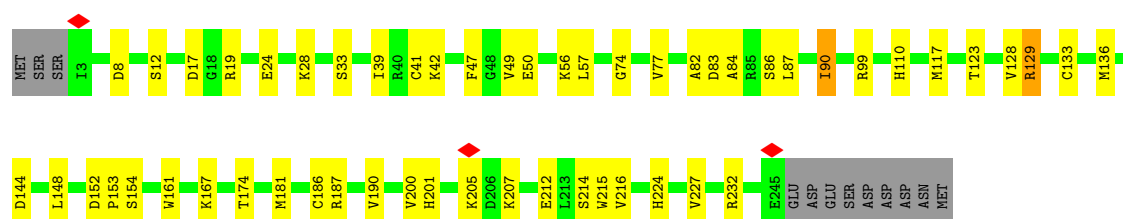
• Molecule 25: Proteasome subunit alpha type-3

Chain X: 75% 18% • 5%



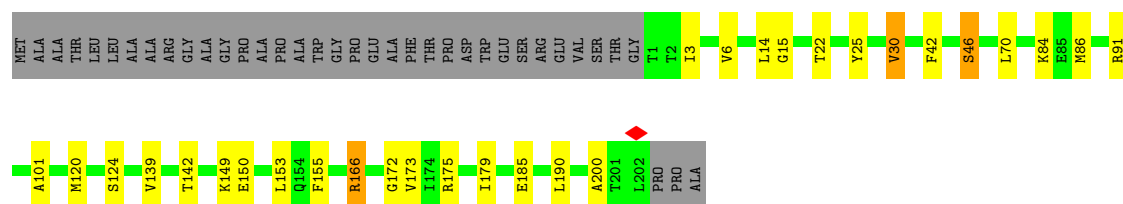
• Molecule 25: Proteasome subunit alpha type-3

Chain n: 74% 20% • 5%



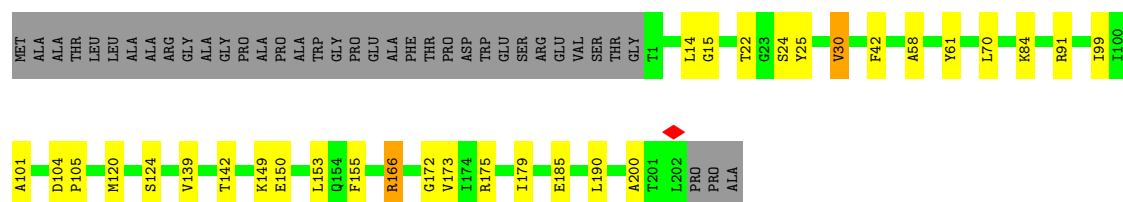
• Molecule 26: Proteasome subunit beta type-6

Chain a: 72% 11% • 15%

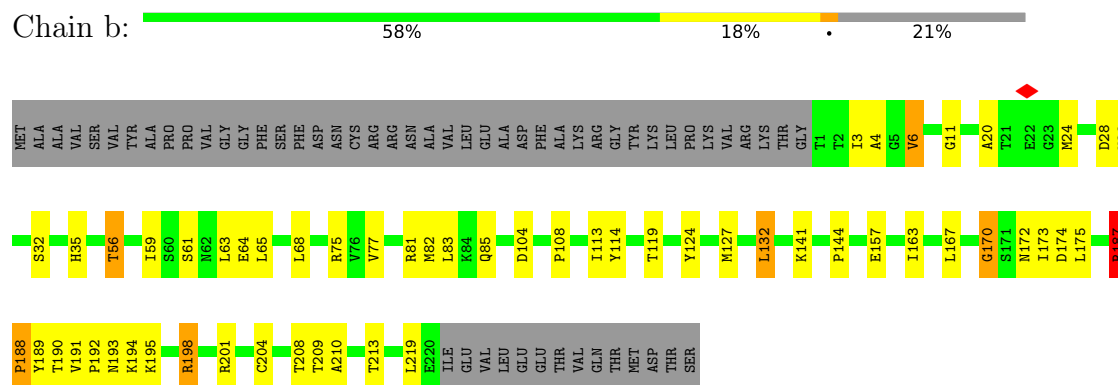


• Molecule 26: Proteasome subunit beta type-6

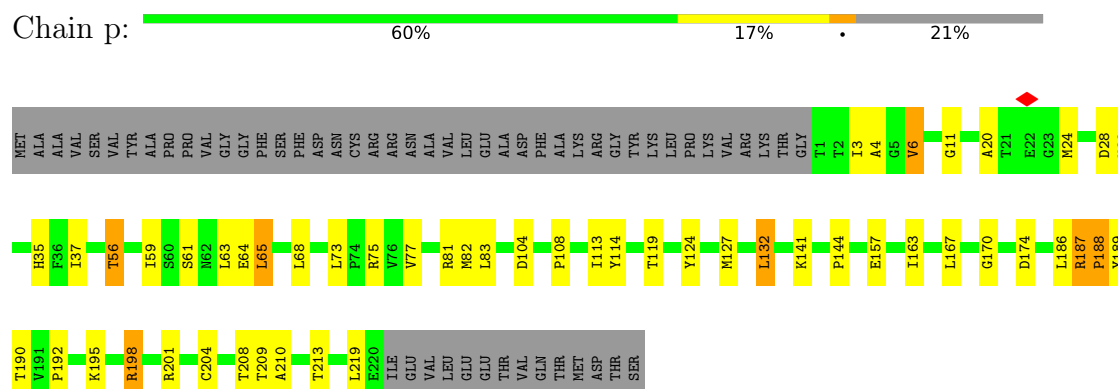
Chain o: 71% 13% • 15%



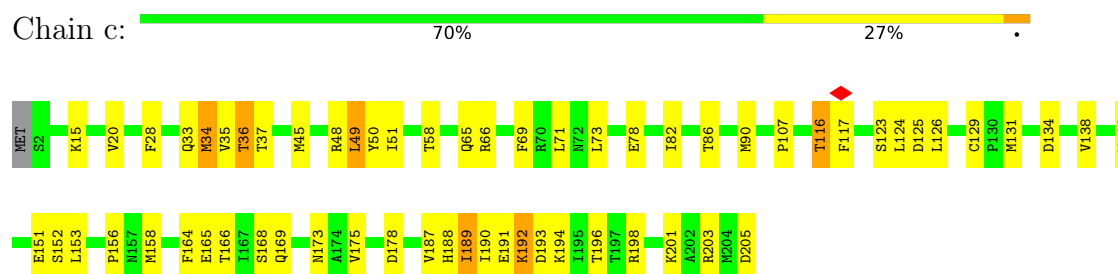
- Molecule 27: Proteasome subunit beta type-7



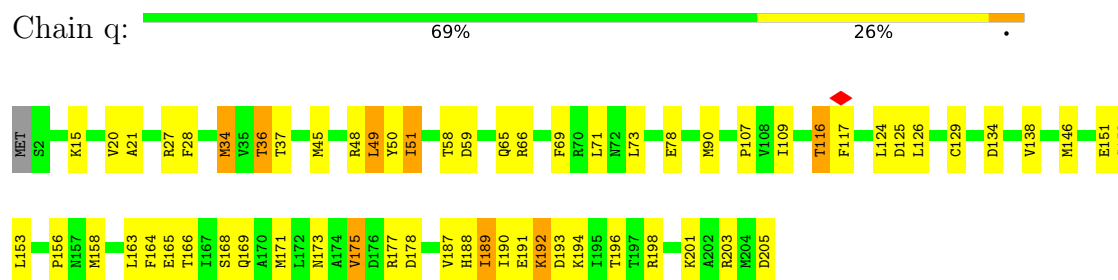
- Molecule 27: Proteasome subunit beta type-7



- Molecule 28: Proteasome subunit beta type-3

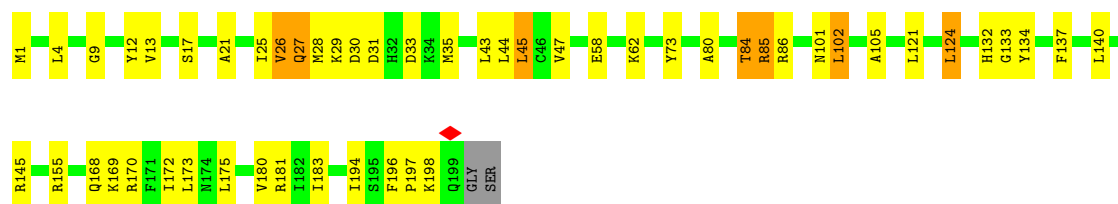


- Molecule 28: Proteasome subunit beta type-3



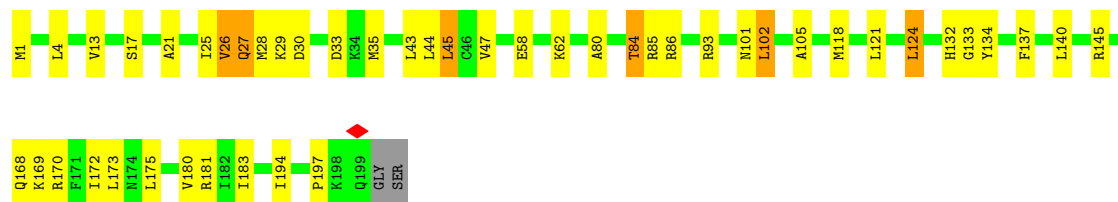
- Molecule 29: Proteasome subunit beta type-2

Chain d:  73% 22% . .



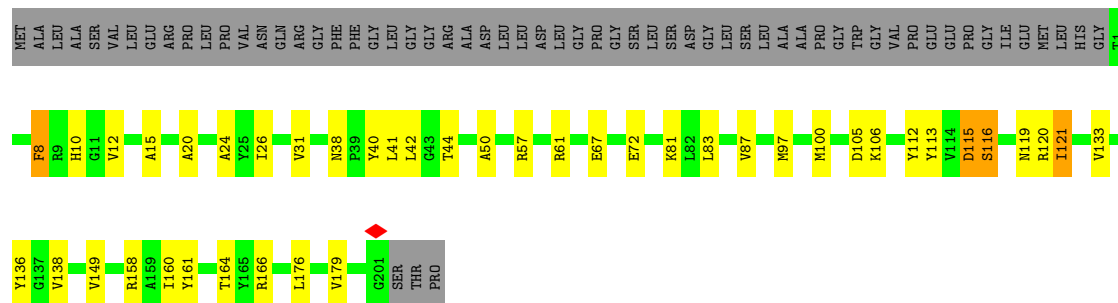
- Molecule 29: Proteasome subunit beta type-2

Chain r:  76% 20% . .



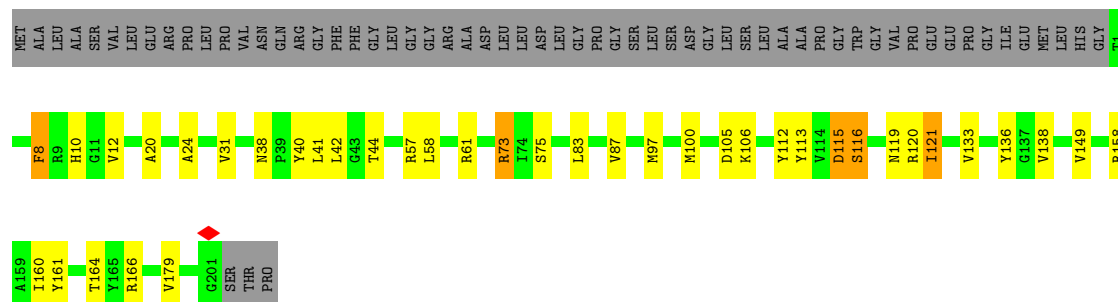
- Molecule 30: Proteasome subunit beta type-5

Chain e:  60% 15% . 24%



- Molecule 30: Proteasome subunit beta type-5

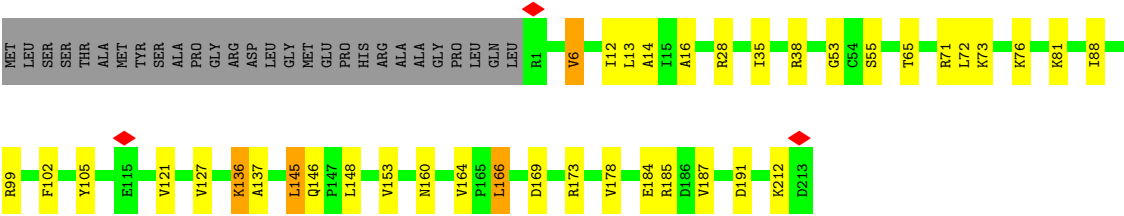
Chain s:  62% 13% . 24%



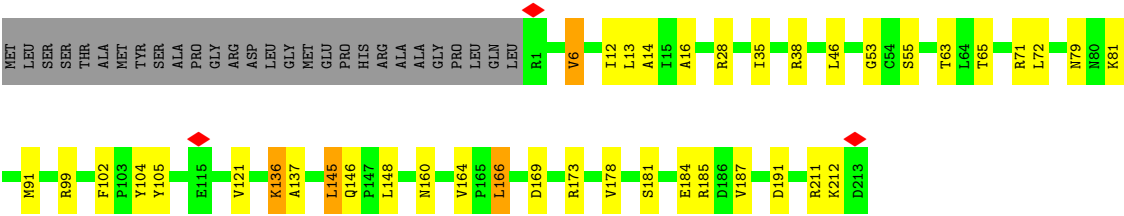
- Molecule 31: Proteasome subunit beta type-1

Chain f:  72% 15% . 12%

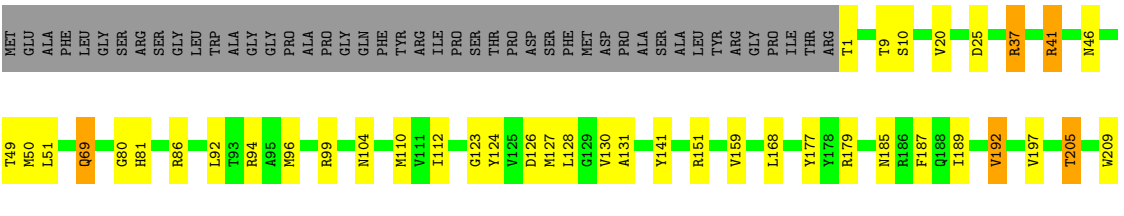




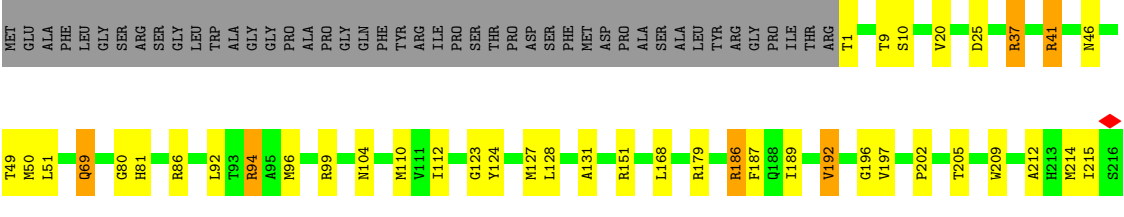
• Molecule 31: Proteasome subunit beta type-1



• Molecule 32: Proteasome subunit beta type-4



• Molecule 32: Proteasome subunit beta type-4



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.86	2/2756 (0.1%)	1.10	19/3727 (0.5%)
1	w	0.86	2/2756 (0.1%)	1.10	19/3727 (0.5%)
2	H	1.01	12/2939 (0.4%)	1.16	27/3970 (0.7%)
2	v	1.02	13/2939 (0.4%)	1.16	27/3970 (0.7%)
3	L	0.90	3/2904 (0.1%)	1.00	19/3924 (0.5%)
3	z	0.89	2/2904 (0.1%)	0.99	17/3924 (0.4%)
4	0	0.86	2/2896 (0.1%)	1.02	18/3912 (0.5%)
4	M	0.86	2/2896 (0.1%)	1.02	18/3912 (0.5%)
5	J	0.78	2/2857 (0.1%)	0.94	3/3844 (0.1%)
5	x	0.78	2/2857 (0.1%)	0.94	3/3844 (0.1%)
6	K	0.81	1/3089 (0.0%)	0.98	14/4168 (0.3%)
6	y	0.81	1/3089 (0.0%)	0.98	14/4168 (0.3%)
7	1	0.52	2/5506 (0.0%)	0.83	8/7425 (0.1%)
7	N	0.52	2/5506 (0.0%)	0.83	8/7425 (0.1%)
8	2	0.63	3/2390 (0.1%)	0.88	12/3215 (0.4%)
8	O	0.63	3/2383 (0.1%)	0.88	12/3206 (0.4%)
9	3	0.67	4/2860 (0.1%)	0.91	13/3860 (0.3%)
9	P	0.67	4/2861 (0.1%)	0.91	13/3861 (0.3%)
10	4	0.71	4/2989 (0.1%)	0.88	13/4054 (0.3%)
10	Q	0.68	4/2989 (0.1%)	0.88	11/4054 (0.3%)
11	5	0.65	3/2820 (0.1%)	0.85	9/3815 (0.2%)
11	R	0.65	3/2817 (0.1%)	0.85	9/3812 (0.2%)
12	6	0.58	1/2754 (0.0%)	0.83	5/3728 (0.1%)
12	S	0.58	1/2745 (0.0%)	0.83	5/3717 (0.1%)
13	7	0.55	0/1713	0.80	2/2306 (0.1%)
13	T	0.55	0/1713	0.80	2/2306 (0.1%)
14	8	0.58	0/2167	0.76	2/2936 (0.1%)
14	U	0.58	0/2167	0.76	2/2936 (0.1%)
15	9	0.60	0/2045	0.81	5/2760 (0.2%)
15	V	0.60	0/2047	0.81	5/2763 (0.2%)
16	AA	0.57	0/1312	1.00	7/1769 (0.4%)
16	W	0.57	0/1312	1.00	7/1769 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AB	0.64	0/315	1.33	4/433 (0.9%)
17	Y	0.64	0/315	1.33	4/433 (0.9%)
18	AC	0.54	1/3603 (0.0%)	0.89	8/5005 (0.2%)
18	Z	0.55	2/3603 (0.1%)	0.90	7/5005 (0.1%)
19	B	0.96	1/1878 (0.1%)	0.99	5/2549 (0.2%)
19	h	1.01	3/1886 (0.2%)	0.99	5/2557 (0.2%)
20	C	1.06	1/1773 (0.1%)	0.99	2/2409 (0.1%)
20	i	1.07	1/1780 (0.1%)	0.99	0/2417
21	D	1.11	5/1946 (0.3%)	0.98	2/2633 (0.1%)
21	j	1.21	6/1943 (0.3%)	0.98	3/2629 (0.1%)
22	E	0.97	1/1748 (0.1%)	0.97	1/2386 (0.0%)
22	k	0.98	2/1716 (0.1%)	1.00	1/2347 (0.0%)
23	F	1.00	2/1794 (0.1%)	1.01	3/2430 (0.1%)
23	l	1.03	2/1753 (0.1%)	1.04	3/2346 (0.1%)
24	G	0.97	0/1885	0.97	2/2552 (0.1%)
24	m	0.97	0/1885	0.97	2/2552 (0.1%)
25	X	1.00	0/1908	0.96	2/2575 (0.1%)
25	n	0.99	1/1908 (0.1%)	0.96	1/2575 (0.0%)
26	a	1.09	4/1535 (0.3%)	0.99	1/2078 (0.0%)
26	o	1.09	5/1535 (0.3%)	0.99	2/2078 (0.1%)
27	b	1.01	1/1670 (0.1%)	1.06	4/2265 (0.2%)
27	p	1.02	1/1670 (0.1%)	1.02	0/2265
28	c	1.19	3/1614 (0.2%)	1.05	1/2177 (0.0%)
28	q	1.19	4/1614 (0.2%)	1.04	1/2177 (0.0%)
29	d	1.06	3/1603 (0.2%)	0.97	2/2174 (0.1%)
29	r	1.07	3/1603 (0.2%)	0.97	2/2174 (0.1%)
30	e	1.16	4/1579 (0.3%)	0.97	0/2134
30	s	1.15	4/1582 (0.3%)	0.97	0/2138
31	f	1.13	3/1674 (0.2%)	0.99	1/2257 (0.0%)
31	t	1.13	3/1674 (0.2%)	0.98	1/2257 (0.0%)
32	g	1.12	5/1705 (0.3%)	1.00	1/2312 (0.0%)
32	u	1.11	6/1711 (0.4%)	0.99	0/2319
All	All	0.85	155/144386 (0.1%)	0.95	419/195445 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	4
1	w	0	4

Continued on next page...

Continued from previous page...

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 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	70	GLU	CD-OE1	25.86	1.74	1.25
21	D	70	GLU	CD-OE1	13.53	1.51	1.25
21	D	70	GLU	CD-OE2	13.11	1.50	1.25
10	4	48	GLN	C-N	12.92	1.51	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	168	GLU	CA-C	-12.36	1.46	1.52

The worst 5 of 419 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	168	GLU	CA-C-O	14.27	127.90	119.77
9	3	168	GLU	CA-C-O	14.27	127.90	119.77
4	M	169	ASP	N-CA-C	13.72	130.95	110.64
4	0	169	ASP	N-CA-C	13.72	130.95	110.64
1	I	142	ASP	CB-CG-OD1	13.57	149.61	118.40

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	Peptide,Mainchain
3	L	226	GLN	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2720	0	2686	913	0
1	w	2720	0	2686	909	0
2	H	2893	0	2843	750	0
2	v	2893	0	2843	735	0
3	L	2860	0	2826	818	0
3	z	2860	0	2826	829	0
4	0	2858	0	2853	744	0
4	M	2858	0	2853	729	0
5	J	2820	0	2927	776	0
5	x	2820	0	2927	781	0
6	K	3039	0	3076	972	0
6	y	3039	0	3076	974	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	5449	0	4576	670	0
7	N	5449	0	4576	671	0
8	2	2375	0	1869	225	0
8	O	2369	0	1862	215	0
9	3	2831	0	2386	367	0
9	P	2832	0	2388	362	0
10	4	2956	0	2669	586	0
10	Q	2956	0	2669	575	0
11	5	2770	0	2480	497	0
11	R	2767	0	2473	502	0
12	6	2732	0	2215	289	0
12	S	2723	0	2202	288	0
13	7	1699	0	1364	228	0
13	T	1699	0	1364	234	0
14	8	2131	0	2039	414	0
14	U	2131	0	2039	398	0
15	9	2009	0	1973	303	0
15	V	2011	0	1980	302	0
16	AA	1300	0	1134	206	0
16	W	1300	0	1134	218	0
17	AB	316	0	160	24	0
17	Y	316	0	160	25	0
18	AC	3608	0	1688	202	0
18	Z	3608	0	1688	212	0
19	B	1845	0	1805	64	0
19	h	1853	0	1827	52	0
20	C	1737	0	1673	77	0
20	i	1744	0	1693	71	0
21	D	1916	0	1857	38	0
21	j	1913	0	1848	30	0
22	E	1724	0	1525	47	0
22	k	1691	0	1468	40	0
23	F	1766	0	1714	49	0
23	l	1726	0	1722	68	0
24	G	1850	0	1822	57	0
24	m	1850	0	1822	63	0
25	X	1873	0	1832	49	0
25	n	1873	0	1832	31	0
26	a	1509	0	1473	23	0
26	o	1509	0	1473	24	0
27	b	1643	0	1644	56	0
27	p	1643	0	1644	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	1585	0	1598	36	0
28	q	1585	0	1598	38	0
29	d	1570	0	1547	42	0
29	r	1570	0	1547	40	0
30	e	1548	0	1499	36	0
30	s	1551	0	1508	30	0
31	f	1644	0	1627	32	0
31	t	1644	0	1627	32	0
32	g	1672	0	1630	38	0
32	u	1678	0	1640	37	0
33	O	27	0	12	11	0
33	H	27	0	12	6	0
33	I	27	0	12	23	0
33	J	27	0	12	21	0
33	K	27	0	12	23	0
33	L	27	0	12	15	0
33	M	27	0	12	12	0
33	v	27	0	12	6	0
33	w	27	0	12	22	0
33	x	27	0	12	19	0
33	y	27	0	12	22	0
33	z	27	0	12	16	0
All	All	142753	0	130149	17440	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

The worst 5 of 17440 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:y:207:PRO:HG2	6:y:335:LEU:CD2	1.23	1.66
14:8:70:LEU:HD21	14:8:111:LEU:CD2	1.28	1.64
3:L:238:ILE:HD11	3:L:257:LEU:CA	1.17	1.63
1:I:339:PRO:HB3	2:H:425:ALA:CB	1.28	1.61
18:Z:667:GLY:HA2	18:Z:671:ALA:CB	1.19	1.61

There are no symmetry-related clashes.

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	I	355/440 (81%)	255 (72%)	72 (20%)	28 (8%)	1	8
1	w	355/440 (81%)	255 (72%)	71 (20%)	29 (8%)	0	8
2	H	376/433 (87%)	248 (66%)	91 (24%)	37 (10%)	0	6
2	v	376/433 (87%)	249 (66%)	88 (23%)	39 (10%)	0	5
3	L	373/389 (96%)	264 (71%)	72 (19%)	37 (10%)	0	6
3	z	373/389 (96%)	263 (70%)	73 (20%)	37 (10%)	0	6
4	0	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0	4
4	M	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0	4
5	J	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	0	6
5	x	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	0	6
6	K	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0	5
6	y	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0	5
7	1	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	3	23
7	N	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	3	23
8	2	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	1	14
8	O	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	1	14
9	3	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	3	25
9	P	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	3	25
10	4	419/422 (99%)	331 (79%)	58 (14%)	30 (7%)	1	9
10	Q	419/422 (99%)	330 (79%)	58 (14%)	31 (7%)	1	9
11	5	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1	11
11	R	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1	11
12	6	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	2	19
12	S	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	2	19
13	7	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	T	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	1	12
14	8	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	1	14
14	U	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	1	14
15	9	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	2	17
15	V	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	2	17
16	AA	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	1	13
16	W	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	1	13
17	AB	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0	3
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	10
18	Z	722/908 (80%)	558 (77%)	116 (16%)	48 (7%)	1	11
19	B	242/246 (98%)	230 (95%)	8 (3%)	4 (2%)	7	35
19	h	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
20	C	229/234 (98%)	204 (89%)	23 (10%)	2 (1%)	14	47
20	i	229/234 (98%)	206 (90%)	21 (9%)	2 (1%)	14	47
21	D	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	30	62
21	j	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	30	62
22	E	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	5	31
22	k	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	5	31
23	F	232/241 (96%)	217 (94%)	13 (6%)	2 (1%)	14	47
23	l	232/241 (96%)	214 (92%)	17 (7%)	1 (0%)	30	62
24	G	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	9	39
24	m	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	9	39
25	X	241/255 (94%)	234 (97%)	4 (2%)	3 (1%)	10	41
25	n	241/255 (94%)	235 (98%)	4 (2%)	2 (1%)	16	49
26	a	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	24	57
26	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	24	57
27	b	218/277 (79%)	209 (96%)	8 (4%)	1 (0%)	24	57
27	p	218/277 (79%)	208 (95%)	8 (4%)	2 (1%)	14	47
28	c	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	12	44
28	q	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	12	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	24	57
29	r	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	24	57
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%)	24	57
32	u	215/264 (81%)	206 (96%)	8 (4%)	1 (0%)	24	57
All	All	19717/22846 (86%)	16137 (82%)	2604 (13%)	976 (5%)	3	15

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 ⓘ

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%)	224 (77%)	67 (23%)	1	5
1	w	291/385 (76%)	219 (75%)	72 (25%)	1	4
2	H	298/372 (80%)	230 (77%)	68 (23%)	1	5
2	v	297/372 (80%)	228 (77%)	69 (23%)	1	5
3	L	298/341 (87%)	234 (78%)	64 (22%)	1	6
3	z	298/341 (87%)	234 (78%)	64 (22%)	1	6
4	0	296/379 (78%)	231 (78%)	65 (22%)	1	5
4	M	296/379 (78%)	231 (78%)	65 (22%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	310/352 (88%)	235 (76%)	75 (24%)	1	4
5	x	310/352 (88%)	235 (76%)	75 (24%)	1	4
6	K	333/366 (91%)	261 (78%)	72 (22%)	1	6
6	y	333/366 (91%)	260 (78%)	73 (22%)	1	5
7	1	376/816 (46%)	343 (91%)	33 (9%)	9	32
7	N	376/816 (46%)	344 (92%)	32 (8%)	10	34
8	2	142/336 (42%)	122 (86%)	20 (14%)	3	18
8	O	141/336 (42%)	121 (86%)	20 (14%)	3	18
9	3	201/416 (48%)	178 (89%)	23 (11%)	5	24
9	P	202/416 (49%)	178 (88%)	24 (12%)	5	23
10	4	250/362 (69%)	207 (83%)	43 (17%)	2	12
10	Q	249/362 (69%)	206 (83%)	43 (17%)	2	11
11	5	229/344 (67%)	205 (90%)	24 (10%)	6	27
11	R	228/344 (66%)	205 (90%)	23 (10%)	7	28
12	6	164/452 (36%)	154 (94%)	10 (6%)	17	43
12	S	163/452 (36%)	153 (94%)	10 (6%)	17	43
13	7	108/294 (37%)	89 (82%)	19 (18%)	2	11
13	T	109/294 (37%)	90 (83%)	19 (17%)	2	11
14	8	211/295 (72%)	188 (89%)	23 (11%)	6	26
14	U	212/295 (72%)	188 (89%)	24 (11%)	5	25
15	9	218/268 (81%)	184 (84%)	34 (16%)	2	15
15	V	219/268 (82%)	185 (84%)	34 (16%)	2	15
16	AA	111/312 (36%)	104 (94%)	7 (6%)	16	42
16	W	111/312 (36%)	103 (93%)	8 (7%)	13	38
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%)	182 (94%)	11 (6%)	18	45
19	h	195/210 (93%)	183 (94%)	12 (6%)	16	43
20	C	175/191 (92%)	166 (95%)	9 (5%)	21	48
20	i	177/191 (93%)	164 (93%)	13 (7%)	13	38
21	D	194/221 (88%)	183 (94%)	11 (6%)	18	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	j	193/221 (87%)	183 (95%)	10 (5%)	21	47
22	E	152/211 (72%)	140 (92%)	12 (8%)	11	36
22	k	142/211 (67%)	132 (93%)	10 (7%)	14	39
23	F	190/203 (94%)	185 (97%)	5 (3%)	40	62
23	l	191/203 (94%)	186 (97%)	5 (3%)	40	62
24	G	198/224 (88%)	191 (96%)	7 (4%)	32	57
24	m	198/224 (88%)	186 (94%)	12 (6%)	17	43
25	X	193/212 (91%)	186 (96%)	7 (4%)	31	57
25	n	193/212 (91%)	183 (95%)	10 (5%)	21	47
26	a	155/181 (86%)	150 (97%)	5 (3%)	34	59
26	o	155/181 (86%)	151 (97%)	4 (3%)	40	62
27	b	177/228 (78%)	168 (95%)	9 (5%)	21	48
27	p	177/228 (78%)	169 (96%)	8 (4%)	24	50
28	c	172/174 (99%)	161 (94%)	11 (6%)	16	42
28	q	172/174 (99%)	162 (94%)	10 (6%)	18	44
29	d	164/171 (96%)	158 (96%)	6 (4%)	30	56
29	r	164/171 (96%)	159 (97%)	5 (3%)	36	60
30	e	153/202 (76%)	149 (97%)	4 (3%)	40	62
30	s	154/202 (76%)	149 (97%)	5 (3%)	34	59
31	f	175/199 (88%)	169 (97%)	6 (3%)	32	57
31	t	175/199 (88%)	170 (97%)	5 (3%)	37	60
32	g	175/215 (81%)	166 (95%)	9 (5%)	21	48
32	u	175/215 (81%)	166 (95%)	9 (5%)	21	48
All	All	12610/17990 (70%)	11078 (88%)	1532 (12%)	7	22

5 of 1532 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	v	345	LEU
6	y	312	ASN
1	w	141	LYS
2	v	342	GLU
5	x	118	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 263 such sidechains are listed below:

Mol	Chain	Res	Type
10	4	207	GLN
11	5	363	ASN
16	AA	101	GLN
15	V	221	HIS
14	U	278	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 oligosaccharides 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	w	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	9 (20%)
33	ADP	0	501	-	28,29,29	1.34	5 (17%)	43,45,45	1.84	10 (23%)
33	ADP	M	501	-	28,29,29	1.34	5 (17%)	43,45,45	1.84	10 (23%)
33	ADP	H	501	-	28,29,29	1.43	4 (14%)	43,45,45	1.86	9 (20%)
33	ADP	L	401	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	7 (16%)
33	ADP	y	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ADP	I	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	9 (20%)
33	ADP	K	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	11 (25%)
33	ADP	x	501	-	28,29,29	1.33	5 (17%)	43,45,45	1.82	10 (23%)
33	ADP	J	501	-	28,29,29	1.33	5 (17%)	43,45,45	1.82	10 (23%)
33	ADP	z	401	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	7 (16%)
33	ADP	v	501	-	28,29,29	1.43	4 (14%)	43,45,45	1.86	9 (20%)

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	w	501	-	-	3/16/32/32	0/3/3/3
33	ADP	0	501	-	-	3/16/32/32	0/3/3/3
33	ADP	M	501	-	-	3/16/32/32	0/3/3/3
33	ADP	H	501	-	-	1/16/32/32	0/3/3/3
33	ADP	L	401	-	-	0/16/32/32	0/3/3/3
33	ADP	y	501	-	-	6/16/32/32	0/3/3/3
33	ADP	I	501	-	-	3/16/32/32	0/3/3/3
33	ADP	K	501	-	-	6/16/32/32	0/3/3/3
33	ADP	x	501	-	-	4/16/32/32	0/3/3/3
33	ADP	J	501	-	-	4/16/32/32	0/3/3/3
33	ADP	z	401	-	-	0/16/32/32	0/3/3/3
33	ADP	v	501	-	-	1/16/32/32	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	I	501	ADP	C5-C4	4.79	1.47	1.39
33	w	501	ADP	C5-C4	4.79	1.47	1.39
33	H	501	ADP	C5-C4	4.76	1.47	1.39
33	v	501	ADP	C5-C4	4.76	1.47	1.39
33	L	401	ADP	C5-C4	4.54	1.47	1.39

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	L	401	ADP	C5-C4-N3	-5.97	118.49	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	z	401	ADP	C5-C4-N3	-5.97	118.49	126.72
33	I	501	ADP	C5-C4-N3	-5.90	118.60	126.72
33	w	501	ADP	C5-C4-N3	-5.90	118.60	126.72
33	H	501	ADP	C5-C4-N3	-5.87	118.64	126.72

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	M	501	ADP	C5'-O5'-PA-O3A
33	J	501	ADP	C5'-O5'-PA-O3A
33	K	501	ADP	C5'-O5'-PA-O1A

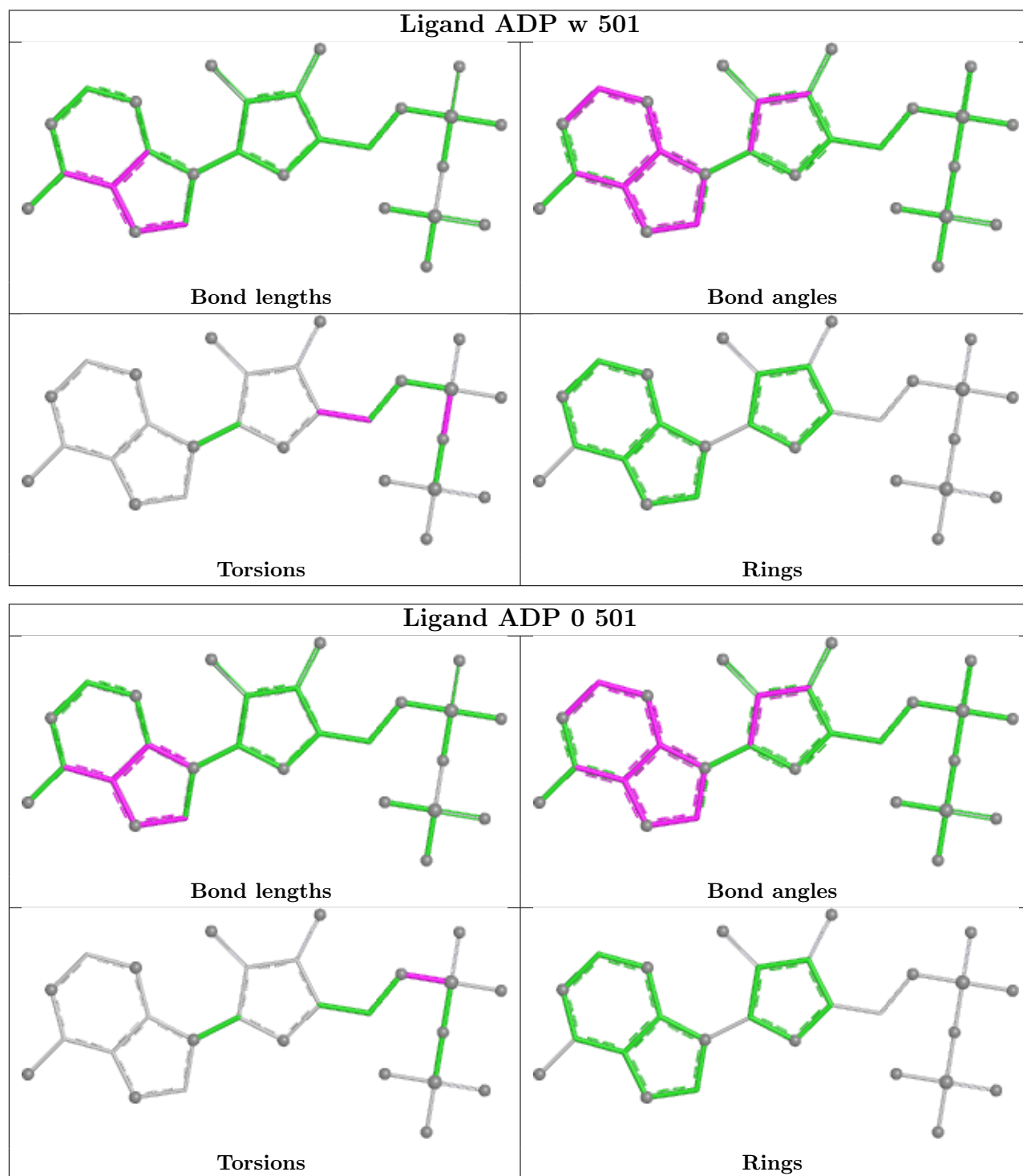
There are no ring outliers.

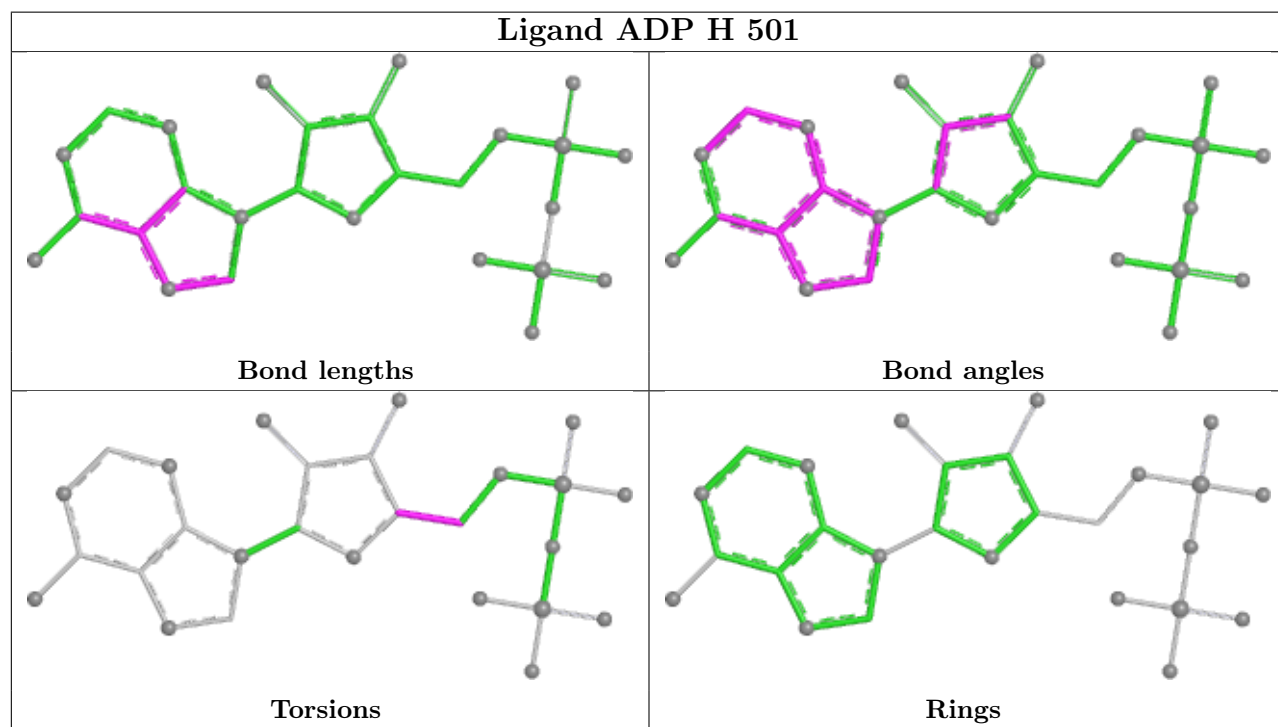
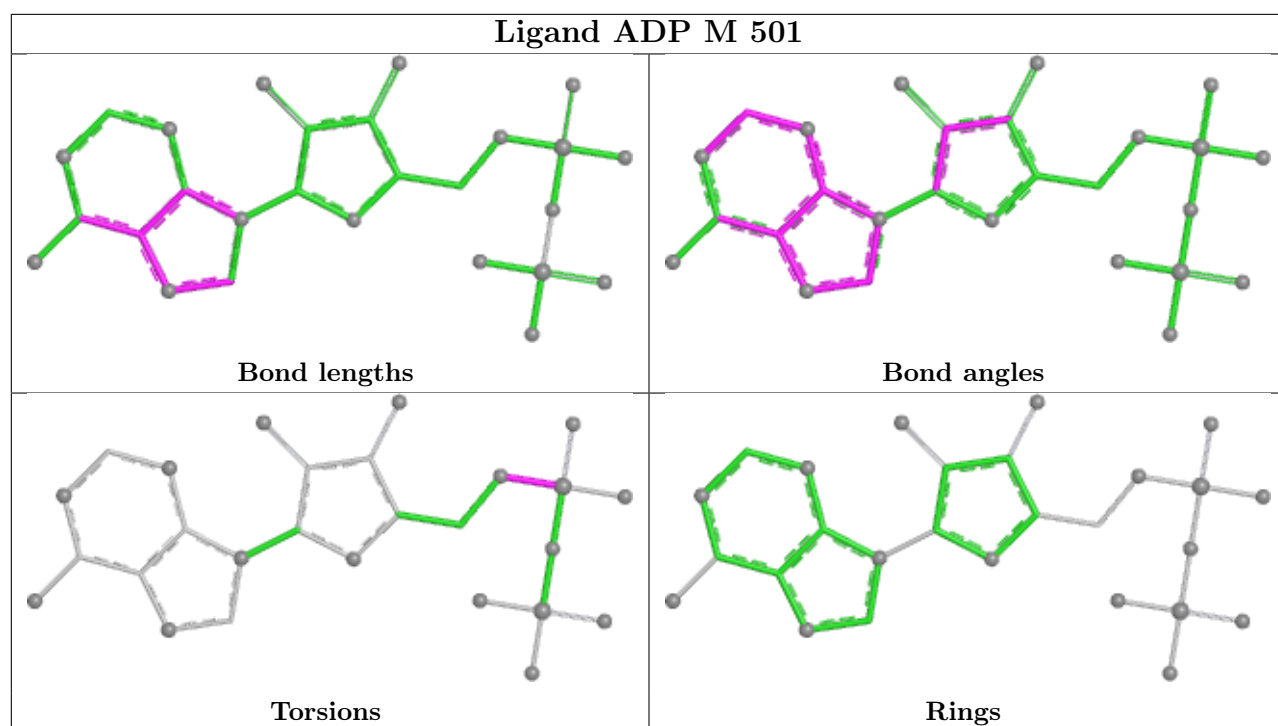
12 monomers are involved in 196 short contacts:

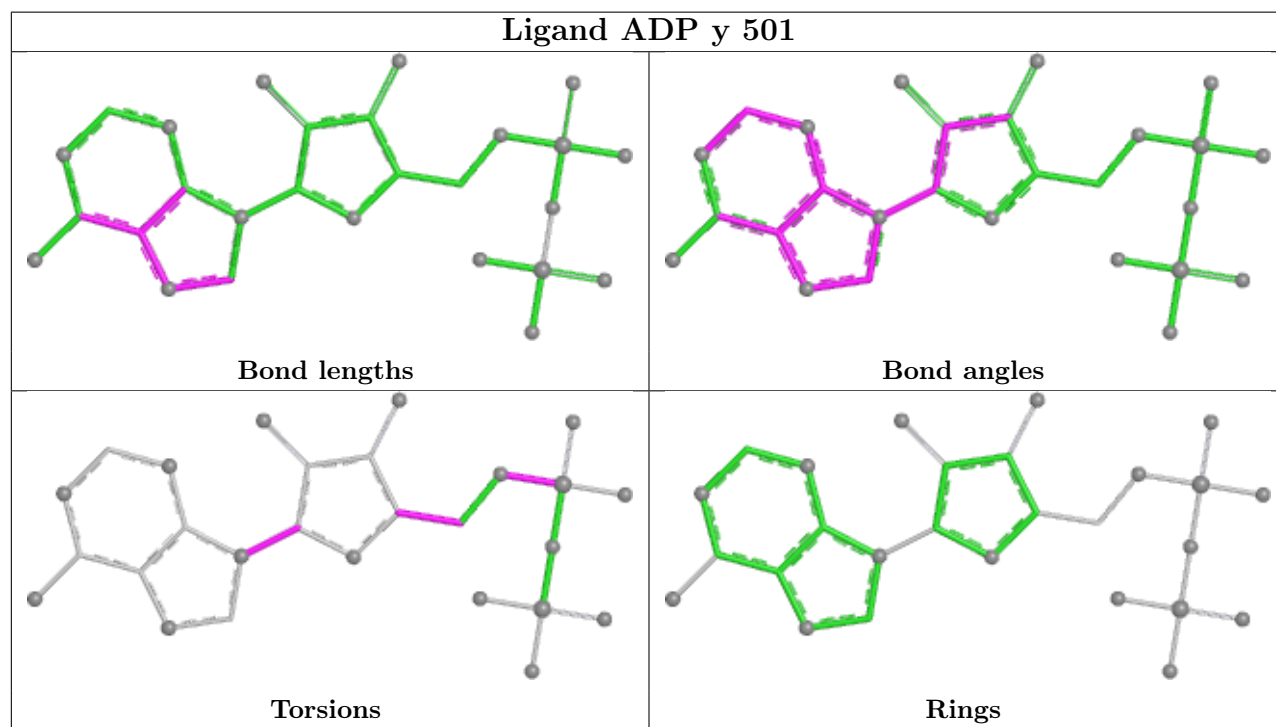
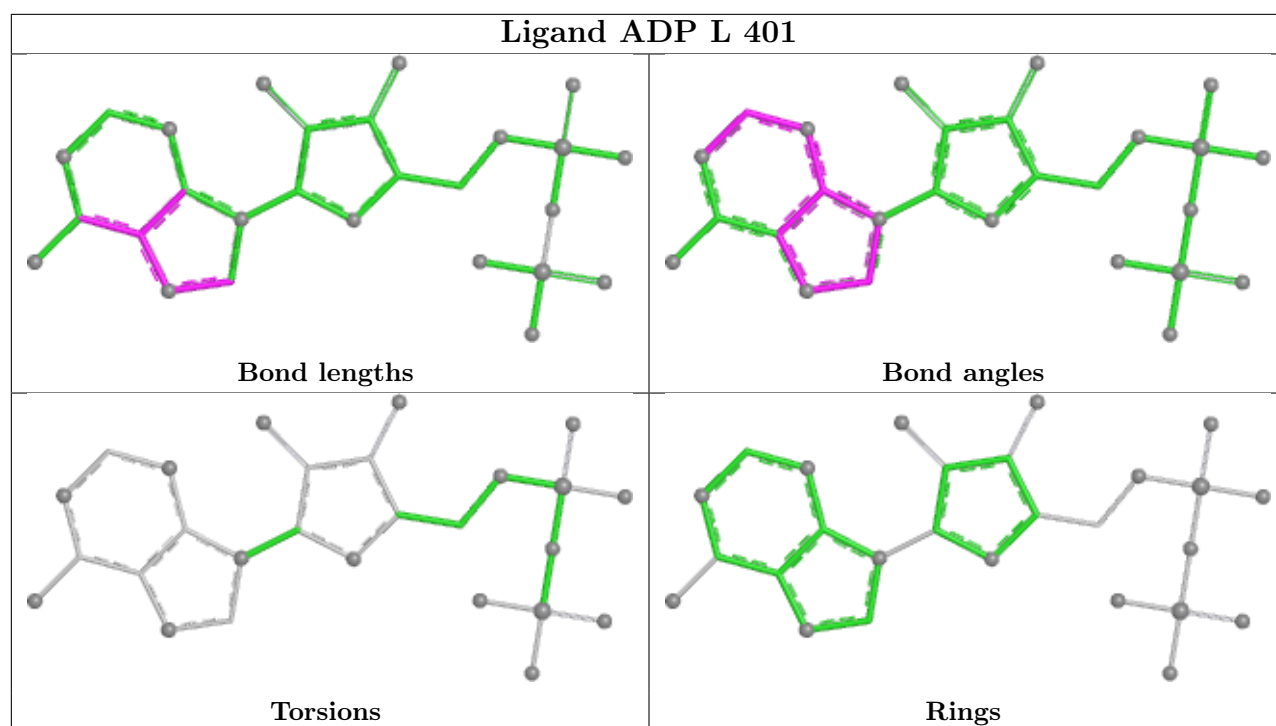
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	w	501	ADP	22	0
33	0	501	ADP	11	0
33	M	501	ADP	12	0
33	H	501	ADP	6	0
33	L	401	ADP	15	0
33	y	501	ADP	22	0
33	I	501	ADP	23	0
33	K	501	ADP	23	0
33	x	501	ADP	19	0
33	J	501	ADP	21	0
33	z	401	ADP	16	0
33	v	501	ADP	6	0

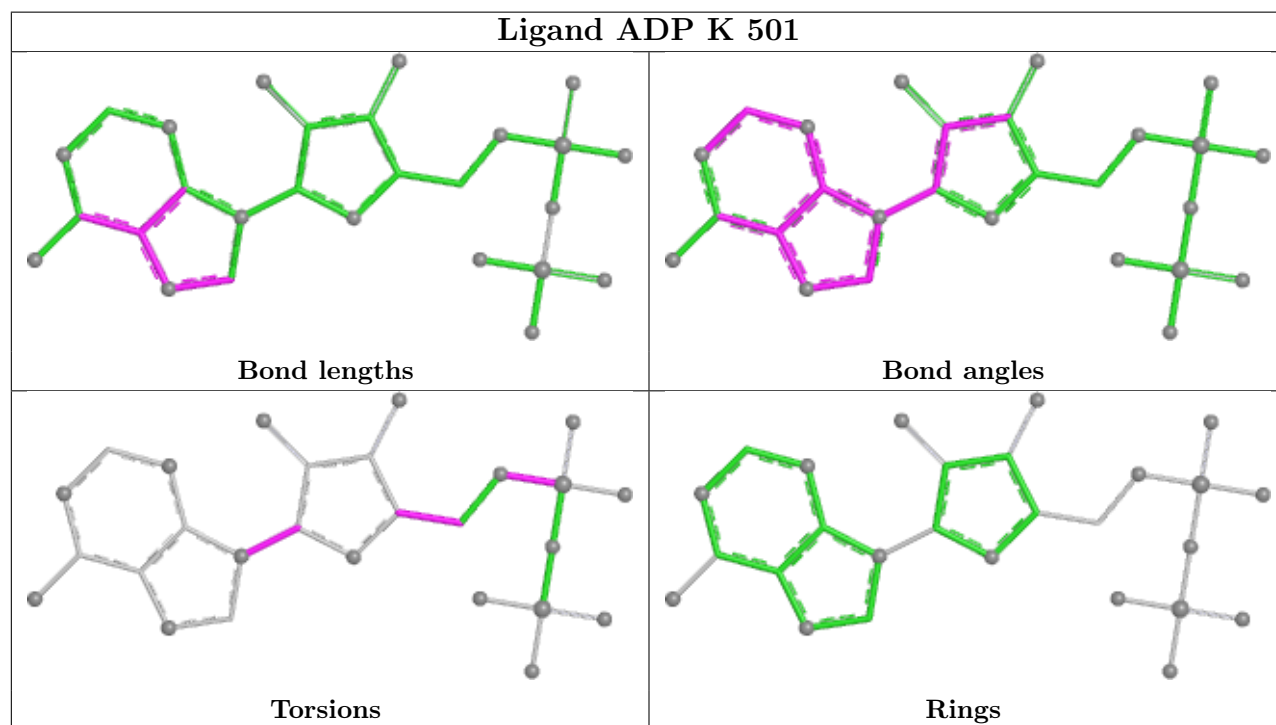
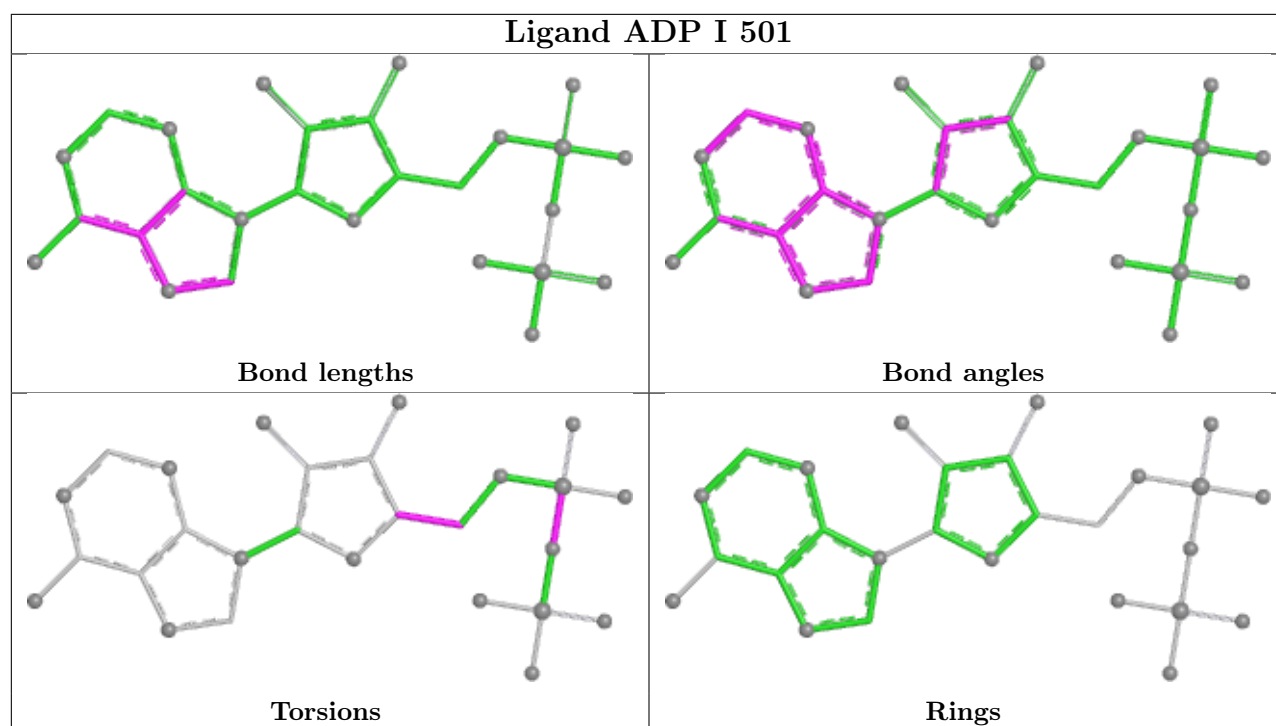
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

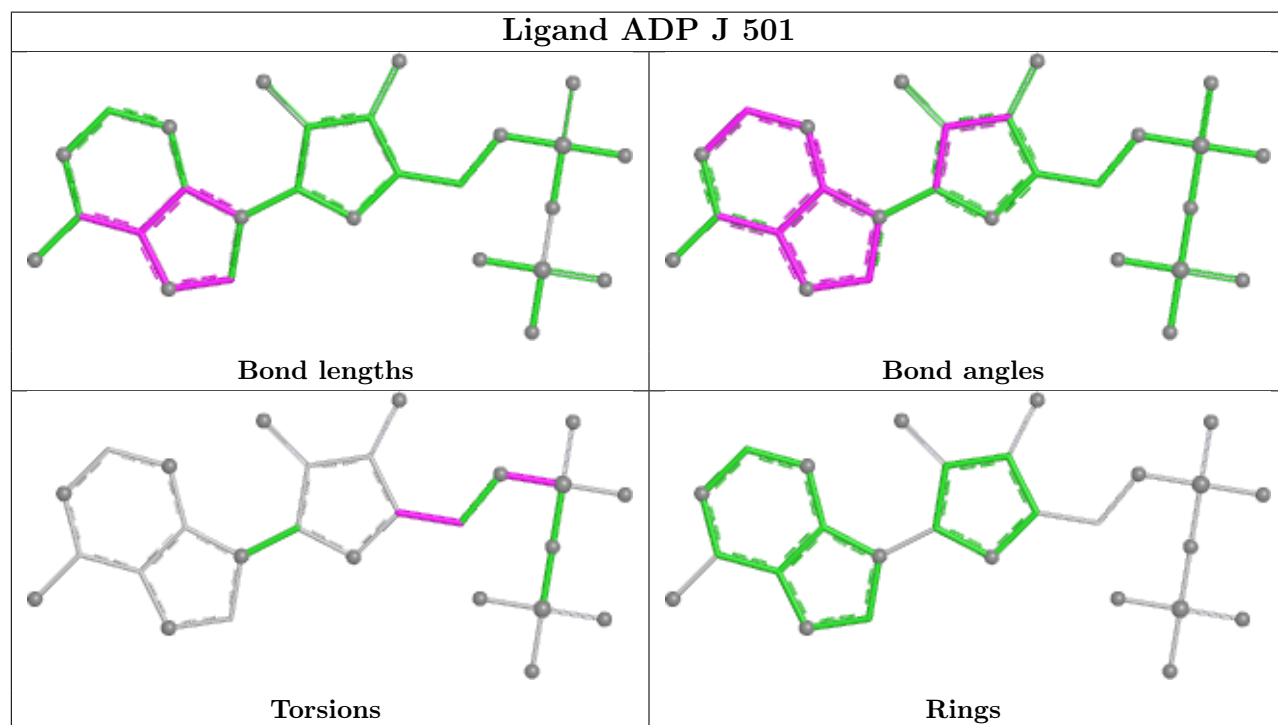
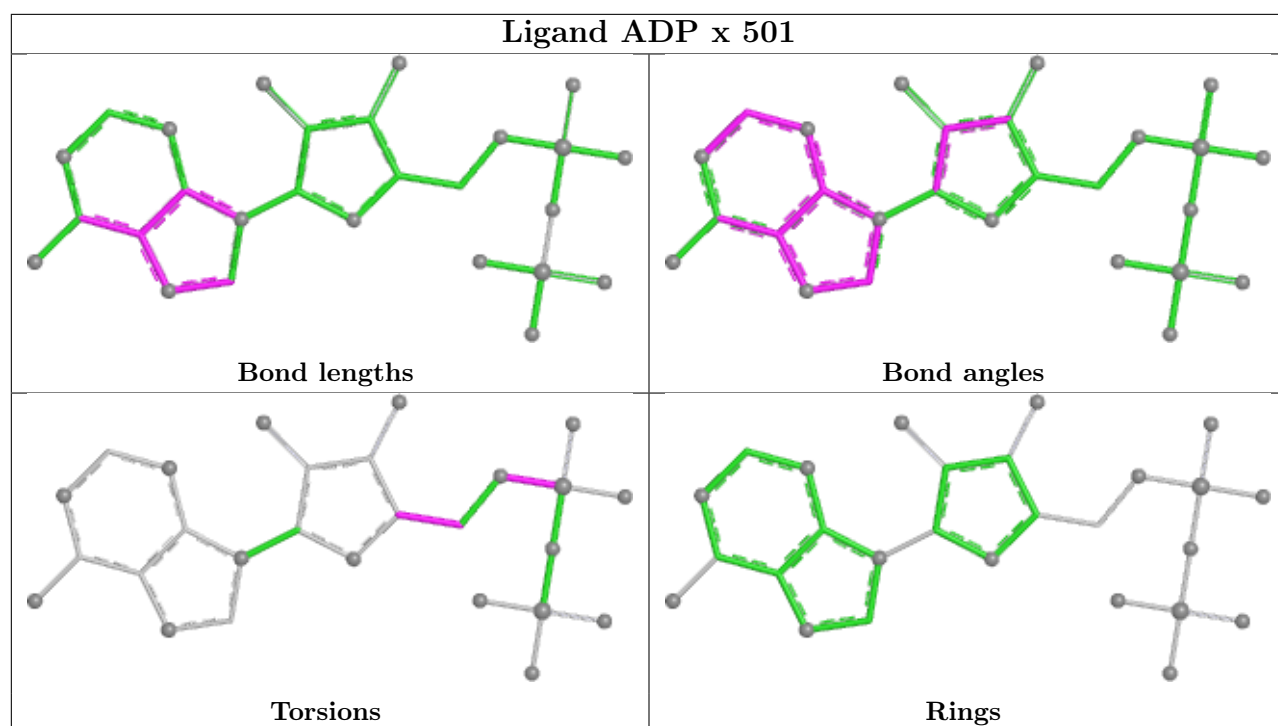
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

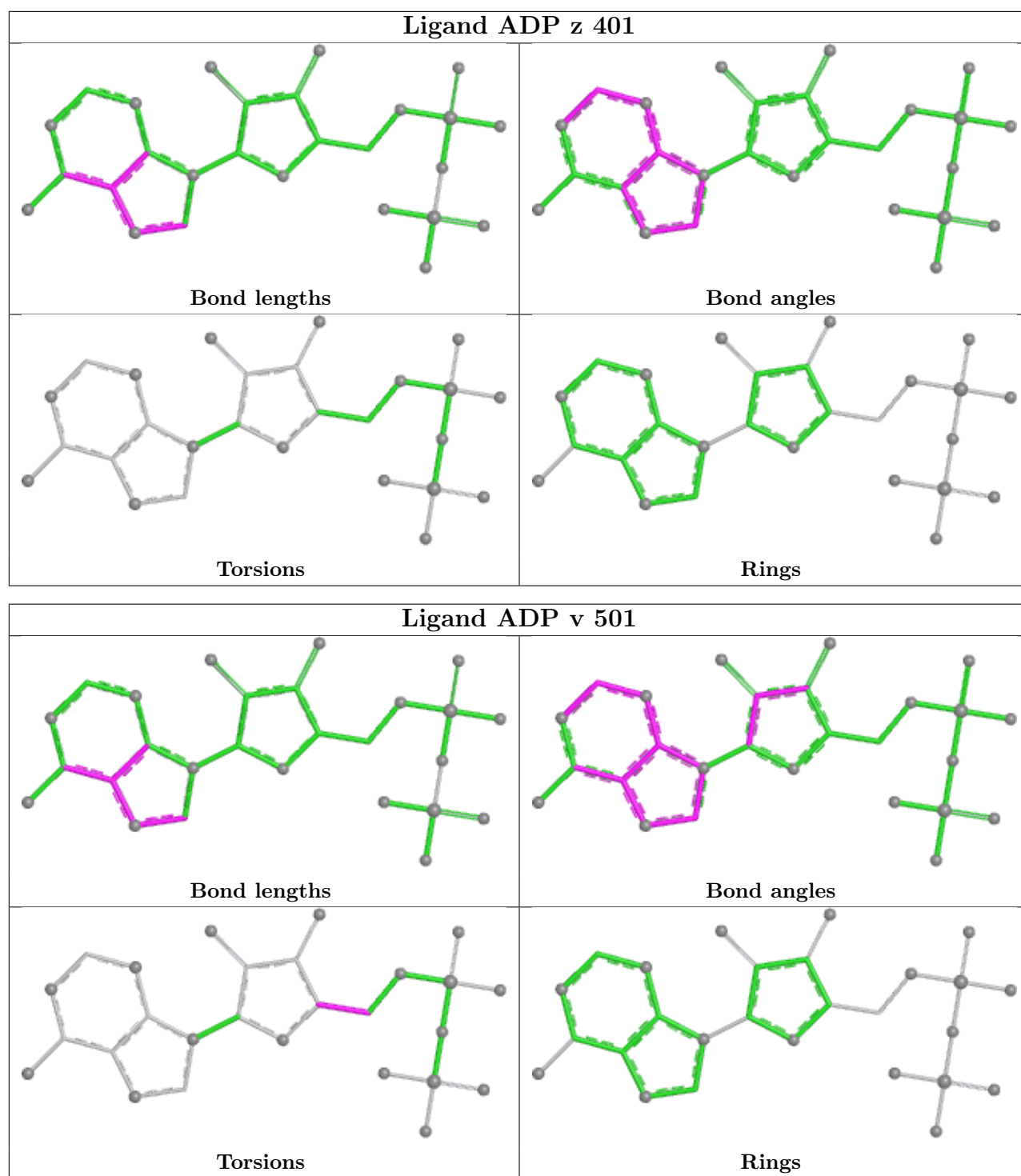












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

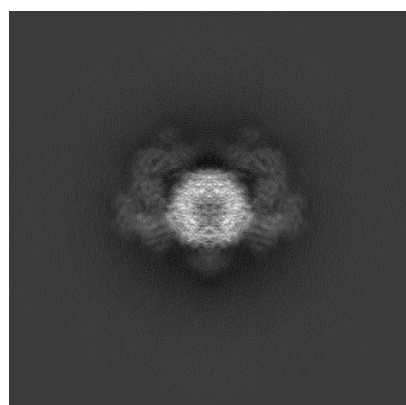
6 Map visualisation [i](#)

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.

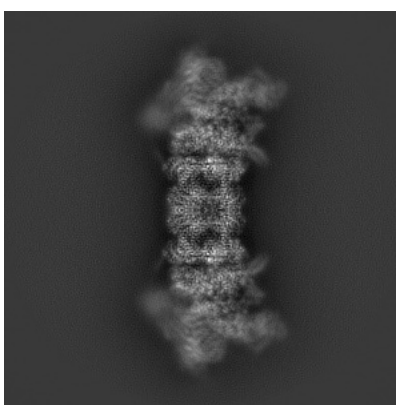
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

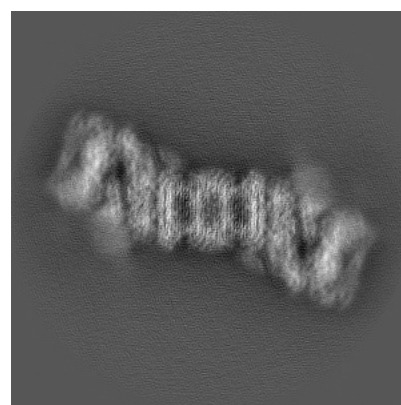
6.1.1 Primary map



X



Y

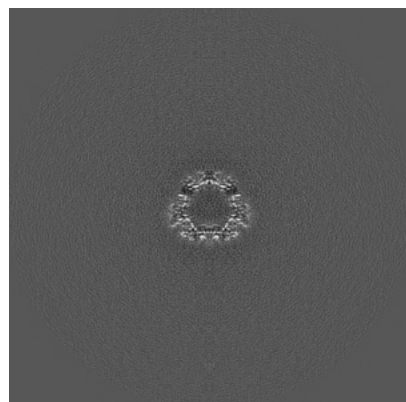


Z

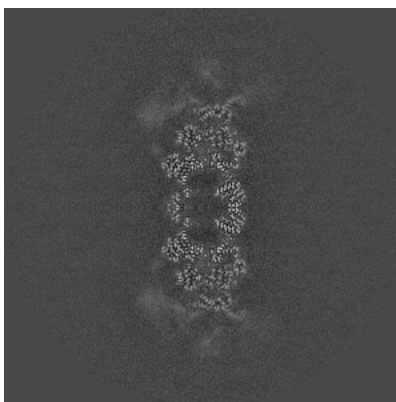
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

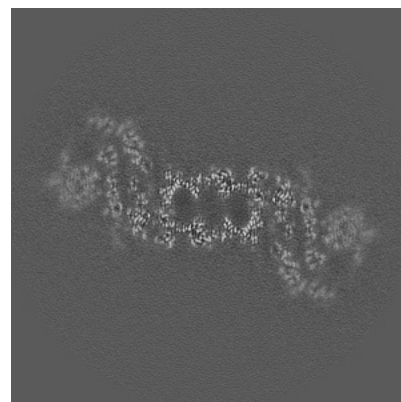
6.2.1 Primary map



X Index: 256



Y Index: 256

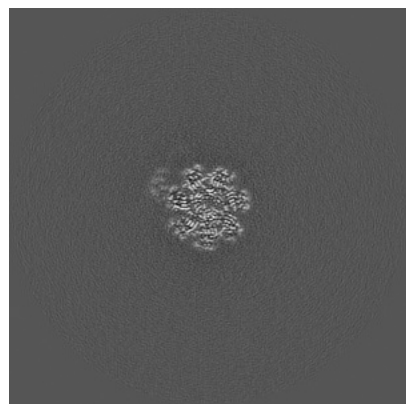


Z Index: 256

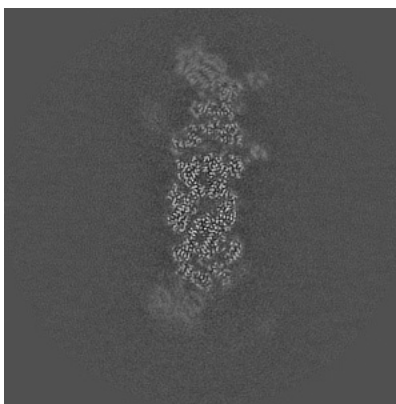
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

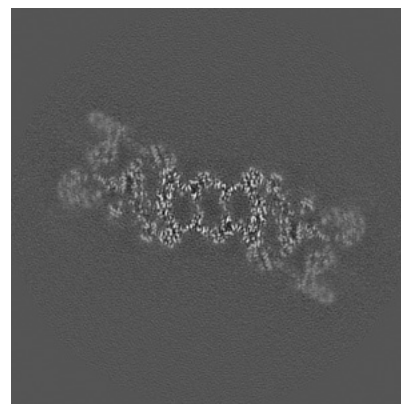
6.3.1 Primary map



X Index: 309



Y Index: 233

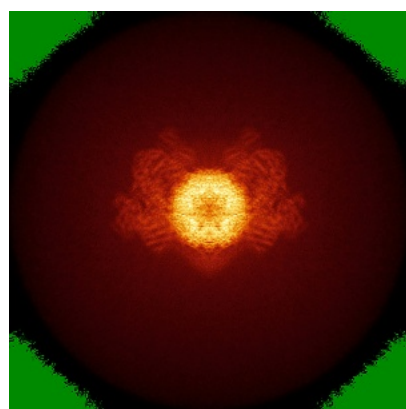


Z Index: 270

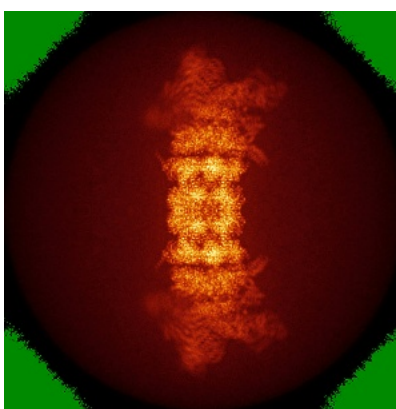
The images above show the largest variance slices of the map in three orthogonal directions.

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

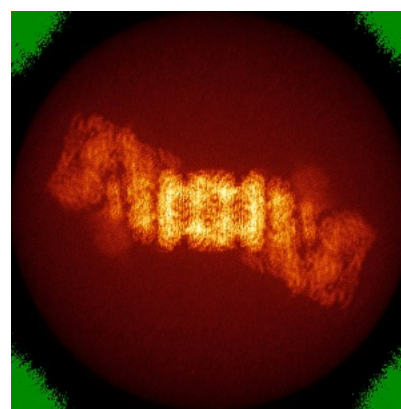
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

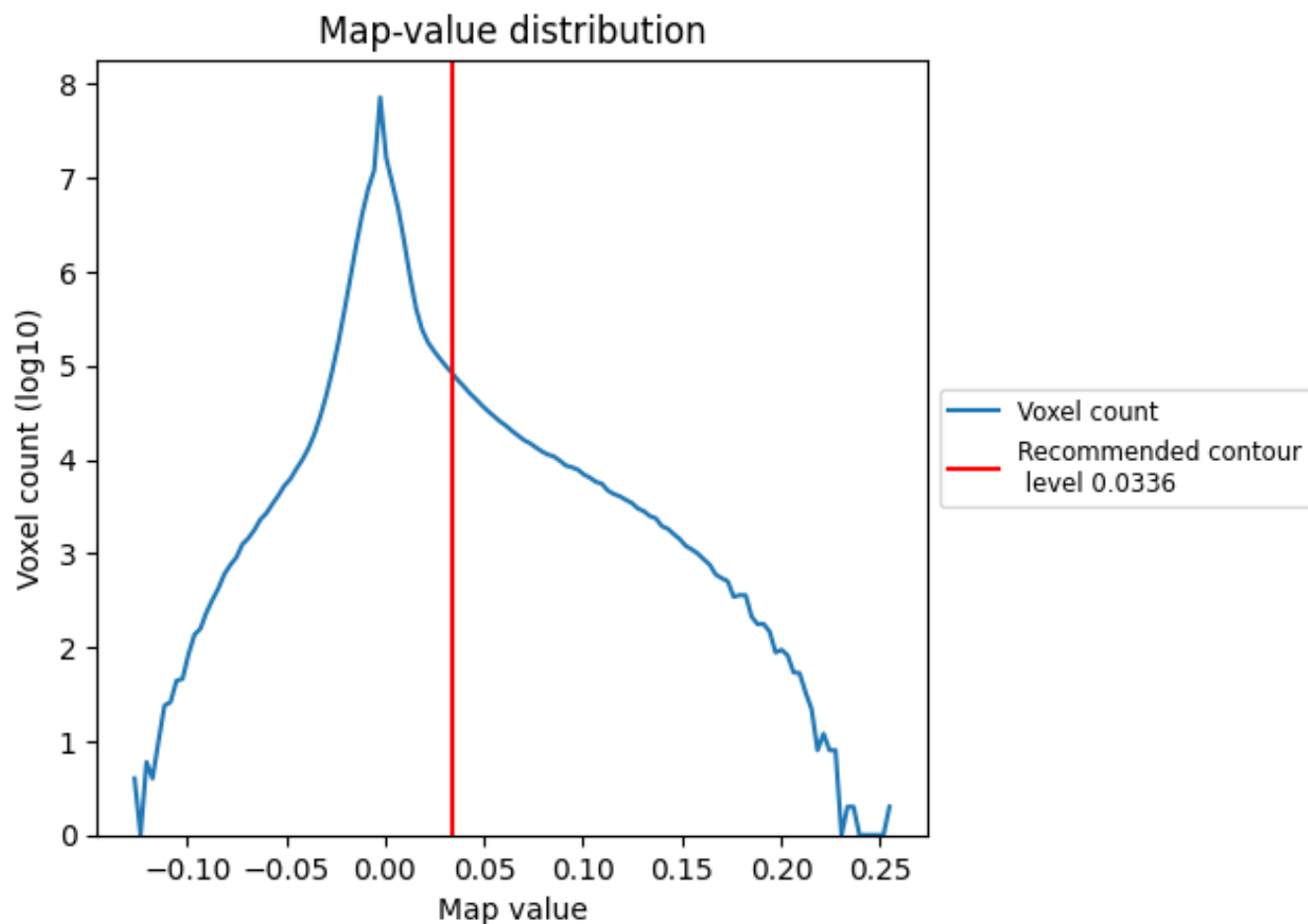
6.6 Mask visualisation

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

7 Map analysis [i](#)

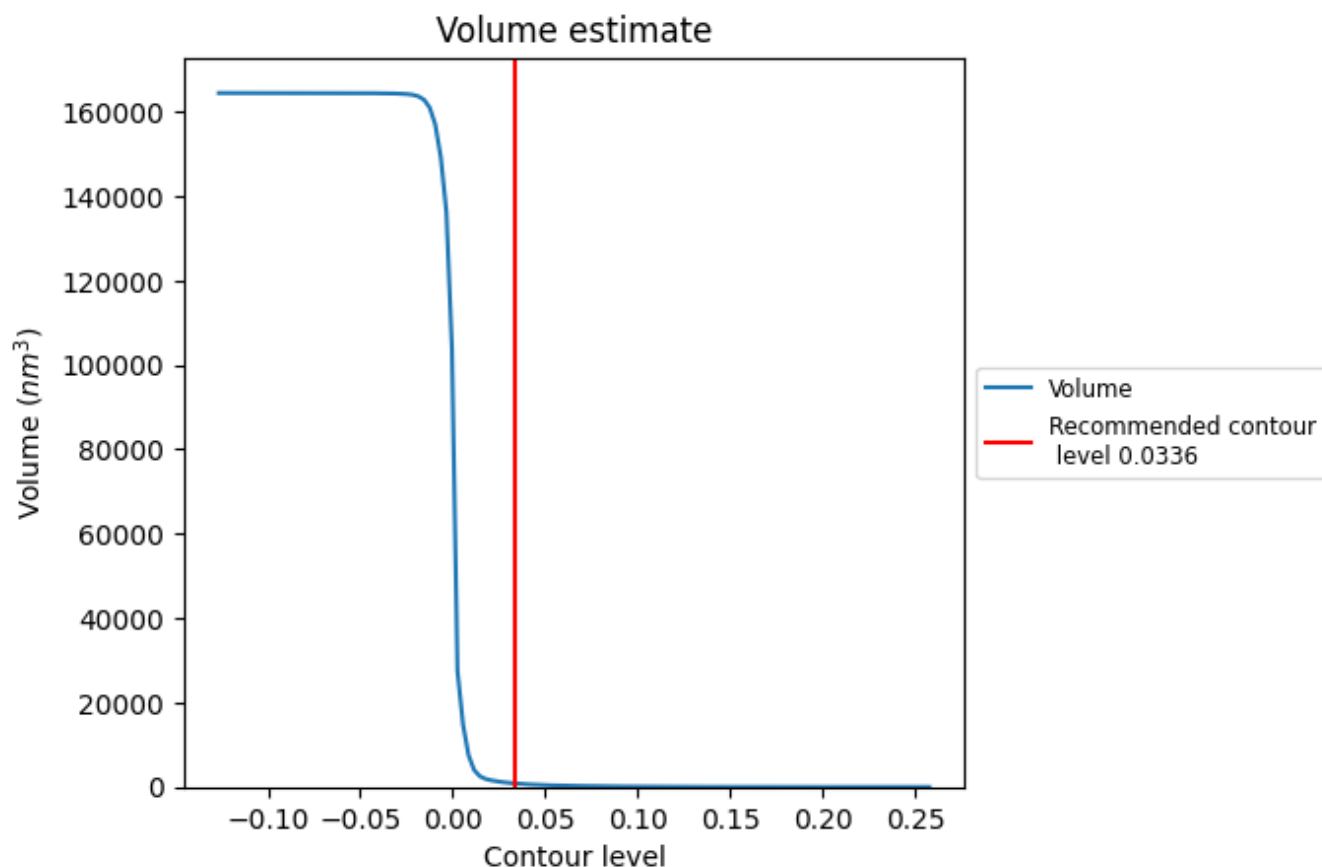
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

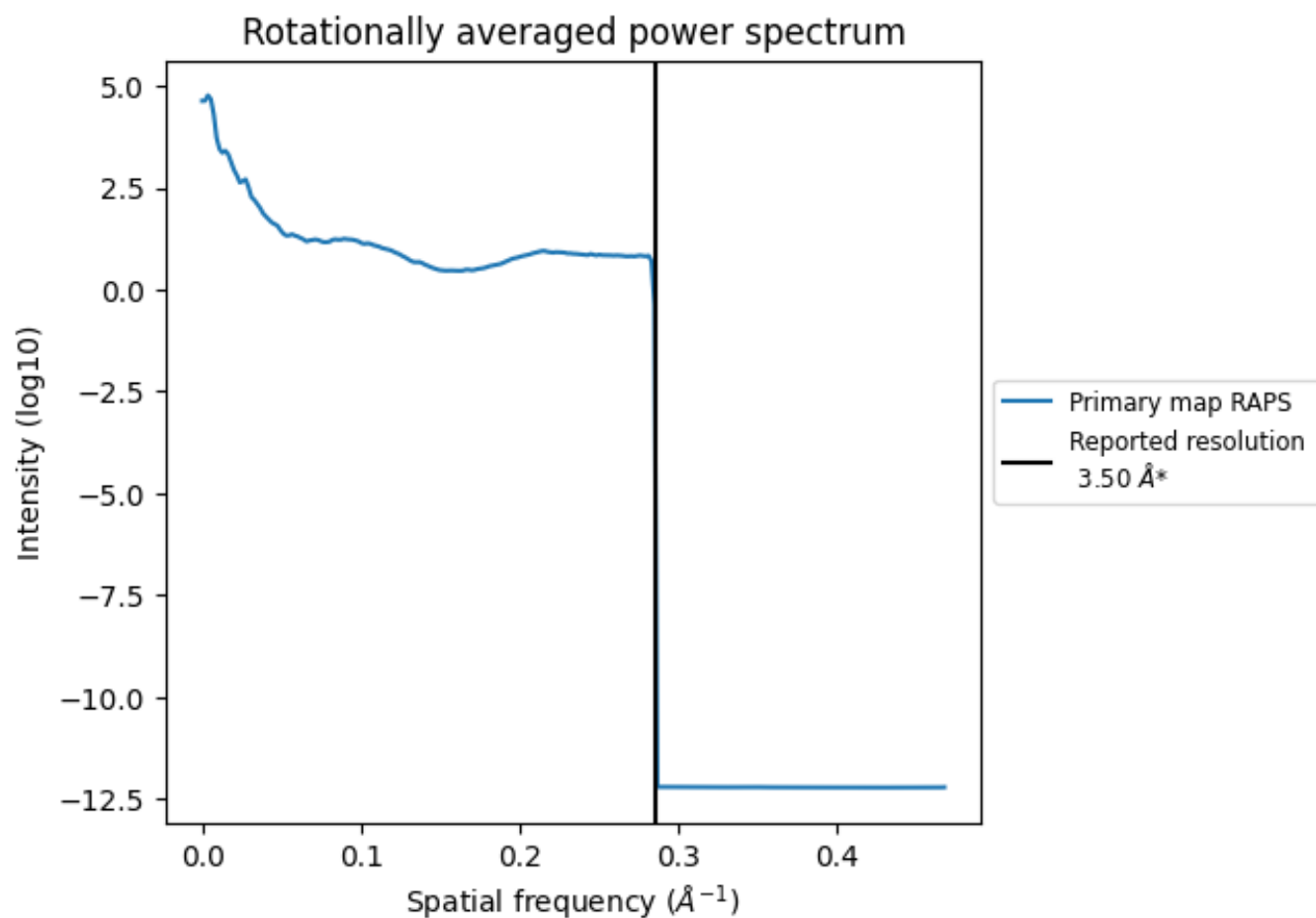
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 841 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

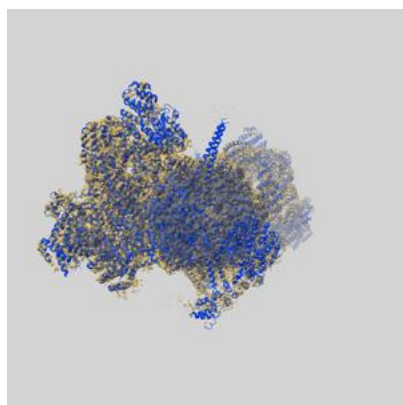
8 Fourier-Shell correlation

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

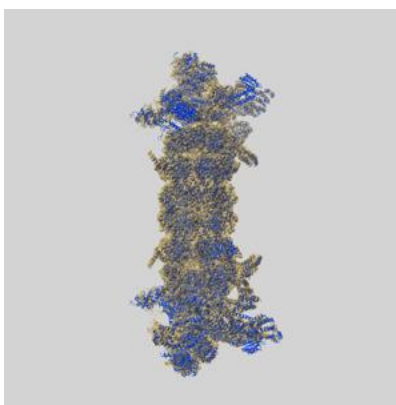
9 Map-model fit [i](#)

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](#).

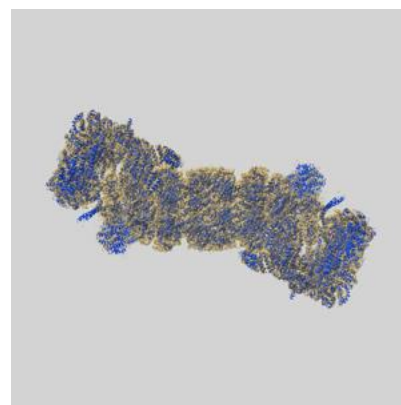
9.1 Map-model overlay [i](#)



X



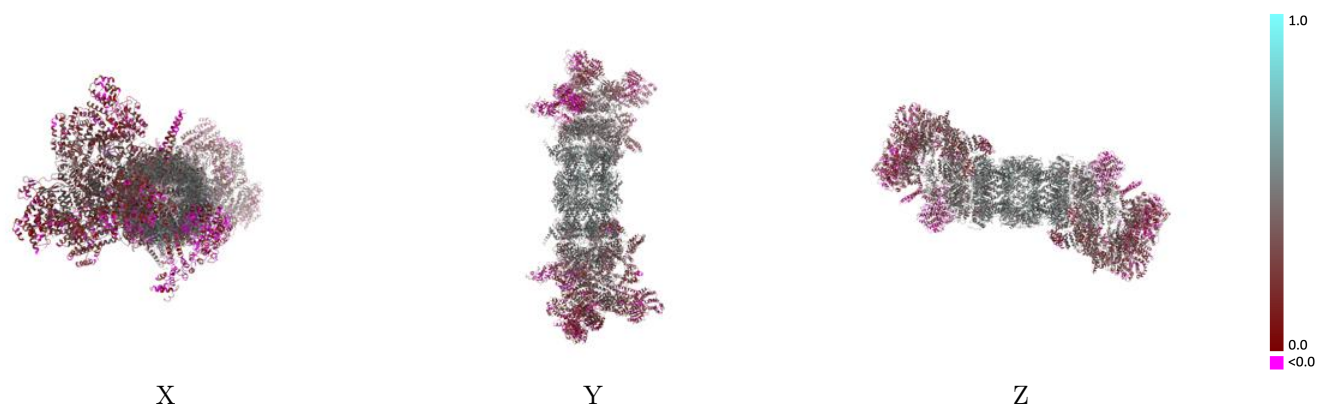
Y



Z

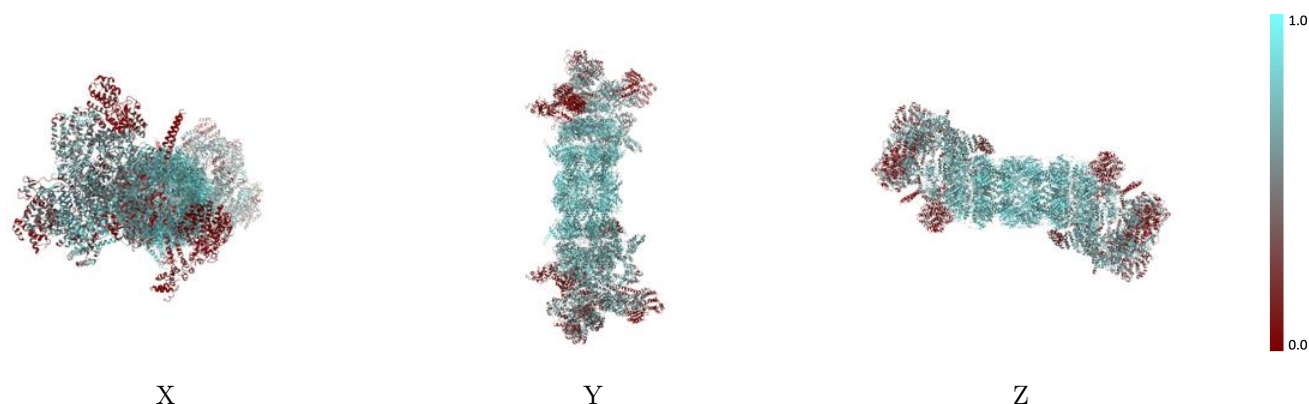
The images above show the 3D surface view of the map at the recommended contour level 0.0336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



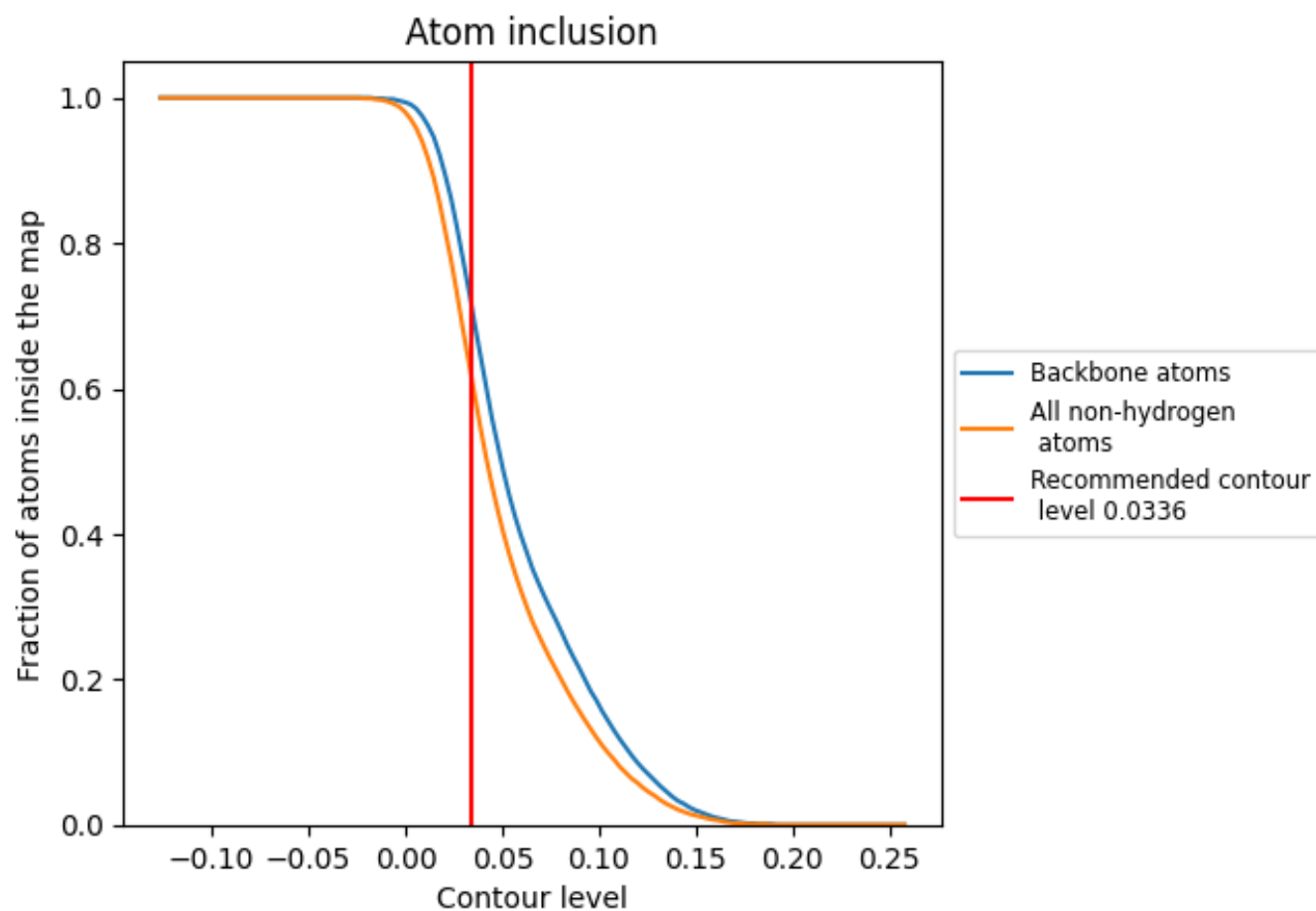
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0336).

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	 0.6230	 0.3580
0	 0.7070	 0.4190
1	 0.4270	 0.1720
2	 0.4060	 0.2280
3	 0.5740	 0.2790
4	 0.5240	 0.3320
5	 0.6560	 0.3430
6	 0.5060	 0.2500
7	 0.3210	 0.1730
8	 0.5410	 0.3120
9	 0.5620	 0.3400
AA	 0.0840	 0.1490
AB	 0.3510	 0.2790
AC	 0.0760	 0.0730
B	 0.8100	 0.4750
C	 0.8200	 0.4900
D	 0.7970	 0.4650
E	 0.8200	 0.4670
F	 0.7900	 0.4770
G	 0.8110	 0.4780
H	 0.7030	 0.4060
I	 0.6540	 0.3830
J	 0.6920	 0.3980
K	 0.6740	 0.3960
L	 0.6910	 0.3930
M	 0.7070	 0.4190
N	 0.4280	 0.1710
O	 0.4070	 0.2280
P	 0.5740	 0.2800
Q	 0.5240	 0.3330
R	 0.6560	 0.3420
S	 0.5070	 0.2500
T	 0.3210	 0.1720
U	 0.5420	 0.3150
V	 0.5610	 0.3400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
W	 0.0840	 0.1470
X	 0.8020	 0.4730
Y	 0.3510	 0.2760
Z	 0.0760	 0.0720
a	 0.8350	 0.4930
b	 0.8270	 0.4920
c	 0.8380	 0.4950
d	 0.8390	 0.4920
e	 0.8540	 0.4970
f	 0.8360	 0.4880
g	 0.8450	 0.4940
h	 0.8060	 0.4770
i	 0.8220	 0.4870
j	 0.7980	 0.4650
k	 0.8360	 0.4740
l	 0.7940	 0.4800
m	 0.8160	 0.4790
n	 0.7990	 0.4740
o	 0.8360	 0.4930
p	 0.8270	 0.4930
q	 0.8380	 0.4970
r	 0.8400	 0.4920
s	 0.8550	 0.4950
t	 0.8340	 0.4880
u	 0.8440	 0.4940
v	 0.7050	 0.4080
w	 0.6530	 0.3820
x	 0.6920	 0.3990
y	 0.6750	 0.3960
z	 0.6910	 0.3930