



wwPDB EM Validation Summary Report ⓘ

Apr 28, 2025 – 05:48 PM EDT

PDB ID : 9NKI / pdb_00009nki
EMDB ID : EMD-49509
Title : Structure of substrate engaged MIDN-bound human 26S proteasome, EB
MIDN_UBL state (Composite map)
Authors : Peddada, N.; Beutler, B.
Deposited on : 2025-02-28
Resolution : 2.94 Å(reported)
Based on initial model : 6mse

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

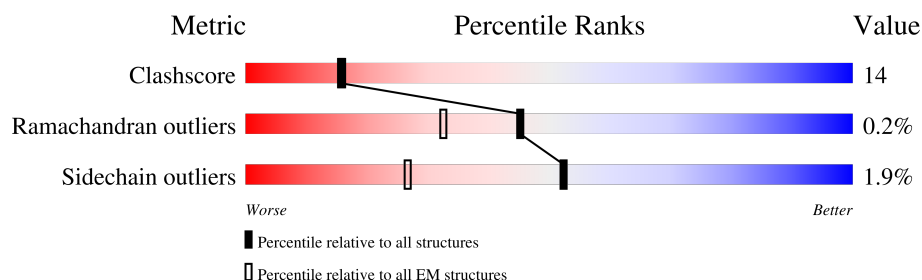
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	433	<div> <div>21%</div> <div>67%</div> <div>22%</div> <div>10%</div> </div>
2	B	440	<div> <div>32%</div> <div>54%</div> <div>33%</div> <div>11%</div> </div>
3	C	406	<div> <div>38%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
4	D	418	<div> <div>22%</div> <div>69%</div> <div>21%</div> <div>9%</div> </div>
5	E	403	<div> <div>25%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
6	F	439	<div> <div>27%</div> <div>72%</div> <div>21%</div> <div>5%</div> </div>
7	G	246	<div> <div>9%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
7	g	246	<div> <div>22%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	
18	r	263	
19	S	241	
19	s	241	
20	T	264	

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Mol	Chain	Length	Quality of chain
20	t	264	
21	V	534	
22	W	456	
23	X	422	
24	Y	389	
25	Z	324	
26	a	376	
27	b	377	
28	d	350	
29	e	70	
30	v	12	
31	z	468	
32	U	953	
33	c	310	
34	f	908	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 200583 atoms, of which 97961 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	390	Total	C	H	N	O	S	0	0
			6166	1928	3106	537	578	17		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	393	Total	C	H	N	O	S	0	0
			6129	1936	3053	524	601	15		

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	389	Total	C	H	N	O	S	0	0
			6264	1932	3193	550	571	18		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	380	Total	C	H	N	O	S	0	0
			6114	1923	3075	524	579	13		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	389	Total	C	H	N	O	S	0	0
			6248	1947	3150	552	582	17		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	415	Total	C	H	N	O	S	0	0
			6569	2038	3318	561	634	18		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	240	Total	C	H	N	O	S	0	0
			3394	1106	1656	304	316	12		
7	g	240	Total	C	H	N	O	S	0	0
			3445	1124	1687	306	316	12		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		
8	h	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	247	Total	C	H	N	O	S	0	0
			3543	1150	1741	322	320	10		
9	i	247	Total	C	H	N	O	S	0	0
			3503	1143	1717	320	313	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		
10	j	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	233	Total	C	H	N	O	S	0	0
			3264	1062	1597	287	307	11		
11	k	233	Total	C	H	N	O	S	0	0
			3249	1056	1589	287	306	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	9	TYR	ASP	conflict	UNP P28066

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Chain	Residue	Modelled	Actual	Comment	Reference
k	9	TYR	ASP	conflict	UNP P28066

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	233	Total	C	H	N	O	S	0	0
			3359	1090	1649	318	293	9		
12	l	233	Total	C	H	N	O	S	0	0
			3352	1089	1645	315	293	10		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	239	Total	C	H	N	O	S	0	0
			3440	1131	1680	308	311	10		
13	m	239	Total	C	H	N	O	S	0	0
			3444	1131	1683	308	312	10		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	202	Total	C	H	N	O	S	0	0
			2891	928	1422	257	272	12		
14	n	202	Total	C	H	N	O	S	0	0
			2881	926	1416	256	271	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	220	Total	C	H	N	O	S	0	0
			3139	1005	1559	272	294	9		
15	o	220	Total	C	H	N	O	S	0	0
			3131	1003	1555	272	292	9		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	204	Total	C	H	N	O	S	0	0
			3096	992	1550	262	273	19		
16	p	204	Total	C	H	N	O	S	0	0
			3081	989	1543	263	268	18		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	196	Total	C	H	N	O	S	0	0
			2986	974	1477	259	268	8		
17	q	196	Total	C	H	N	O	S	0	0
			2981	973	1475	259	266	8		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	200	Total	C	H	N	O	S	0	0
			2953	957	1449	271	267	9		
18	r	200	Total	C	H	N	O	S	0	0
			2938	954	1438	270	267	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	212	Total	C	H	N	O	S	0	0
			3163	1016	1579	279	279	10		
19	s	212	Total	C	H	N	O	S	0	0
			3168	1017	1581	279	281	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	212	Total	C	H	N	O	S	0	0
			3102	1003	1526	280	282	11		
20	t	212	Total	C	H	N	O	S	0	0
			3079	998	1511	279	280	11		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	442	Total	C	H	N	O	S	0	0
			7256	2293	3658	642	650	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	440	Total	C	N	O	S	0	0
			3588	2272	612	681	23		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	384	Total	C	H	N	O	S	0	0
			6174	1935	3134	513	580	12		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	380	Total	C	H	N	O	S	0	0
			6260	1995	3133	535	580	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	286	Total	C	H	N	O	S	0	0
			4593	1457	2312	392	427	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	373	Total	C	H	N	O	S	0	0
			6007	1911	3012	510	559	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	191	Total	C	H	N	O	S	0	0
			2963	910	1505	261	279	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	d	270	Total	C	H	N	O	S	0	0
			4414	1417	2221	360	407	9		

- Molecule 29 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	e	48	Total	C	H	N	O		0	0
			725	249	316	63	97			

- Molecule 30 is a protein called Unknown density-substrate density.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 31 is a protein called Midnolin.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	z	81	Total	C	H	N	O	S	0	0
			1257	383	645	111	116	2		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	U	818	Total	C	H	N	O	S	0	0
			12773	4046	6402	1085	1196	44		

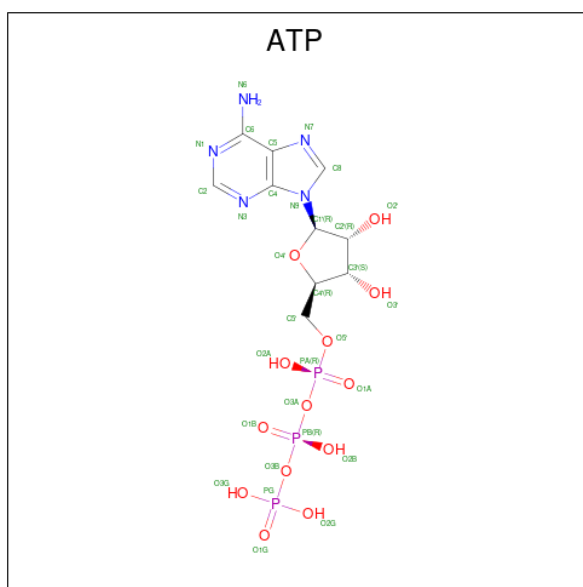
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	c	283	Total	C	H	N	O	S	0	0
			4473	1412	2241	385	418	17		

- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	f	836	Total	C	H	N	O	S	0	0
			12946	4084	6486	1097	1234	45		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	H	N	O	P
			43	10	12	5	13	3
35	B	1	Total	C	H	N	O	P
			43	10	12	5	13	3
35	D	1	Total	C	H	N	O	P
			43	10	12	5	13	3
35	F	1	Total	C	H	N	O	P
			43	10	12	5	13	3

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
37	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

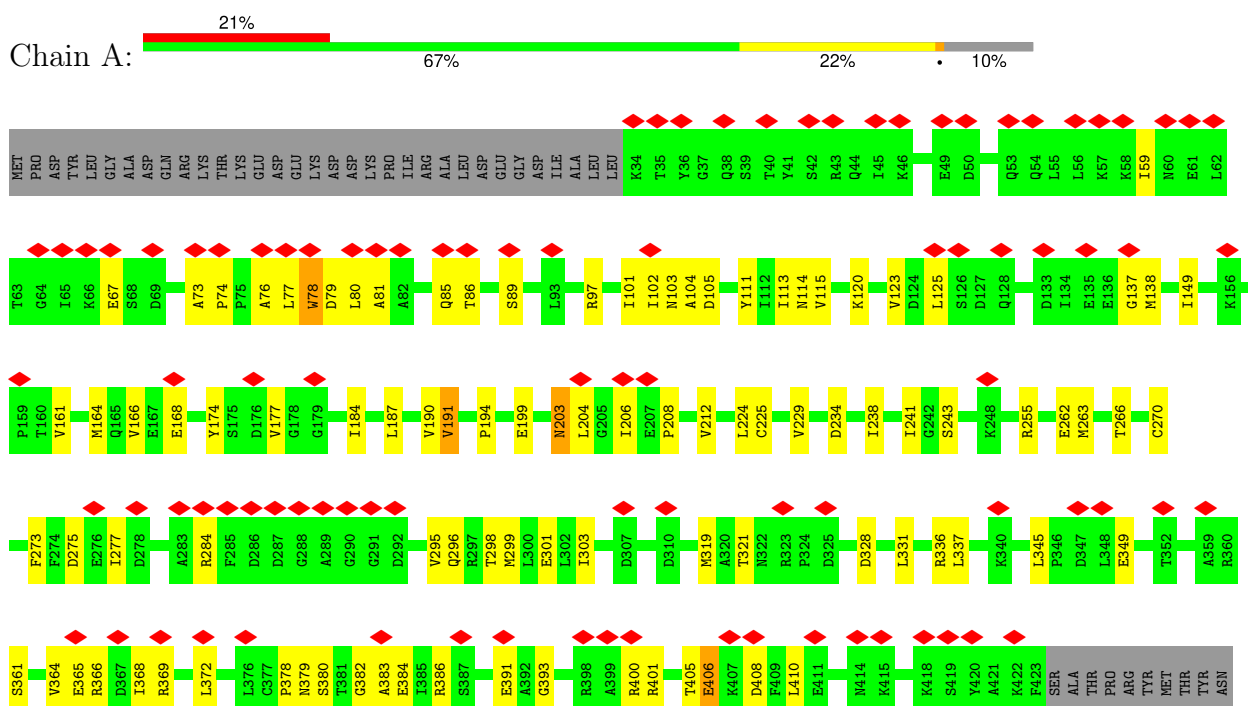
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

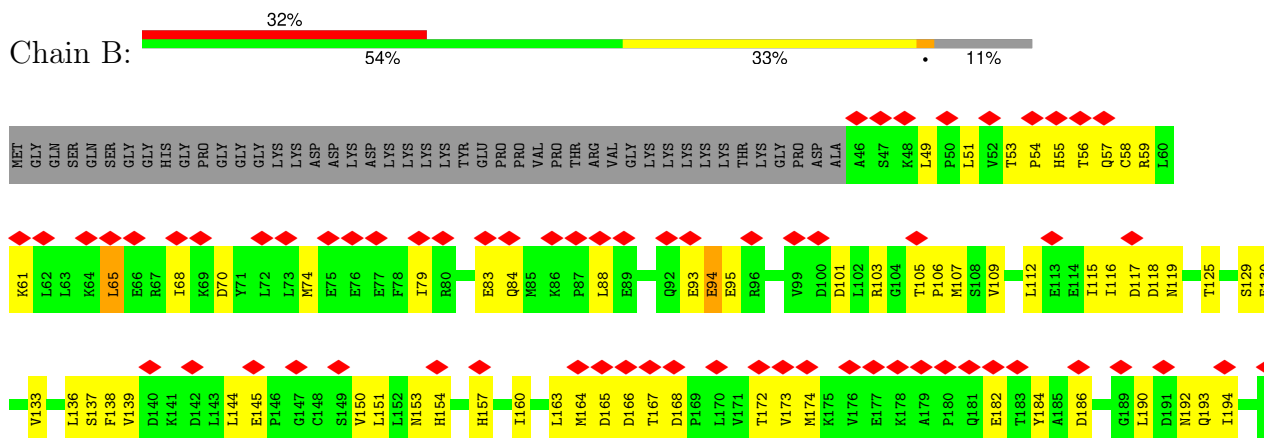
3 Residue-property plots

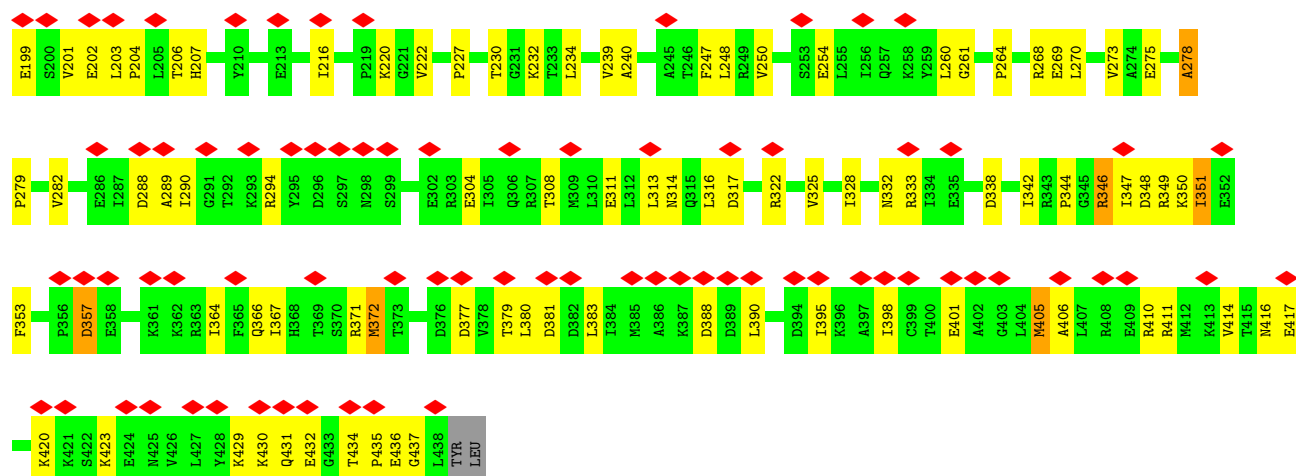
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 26S proteasome regulatory subunit 7

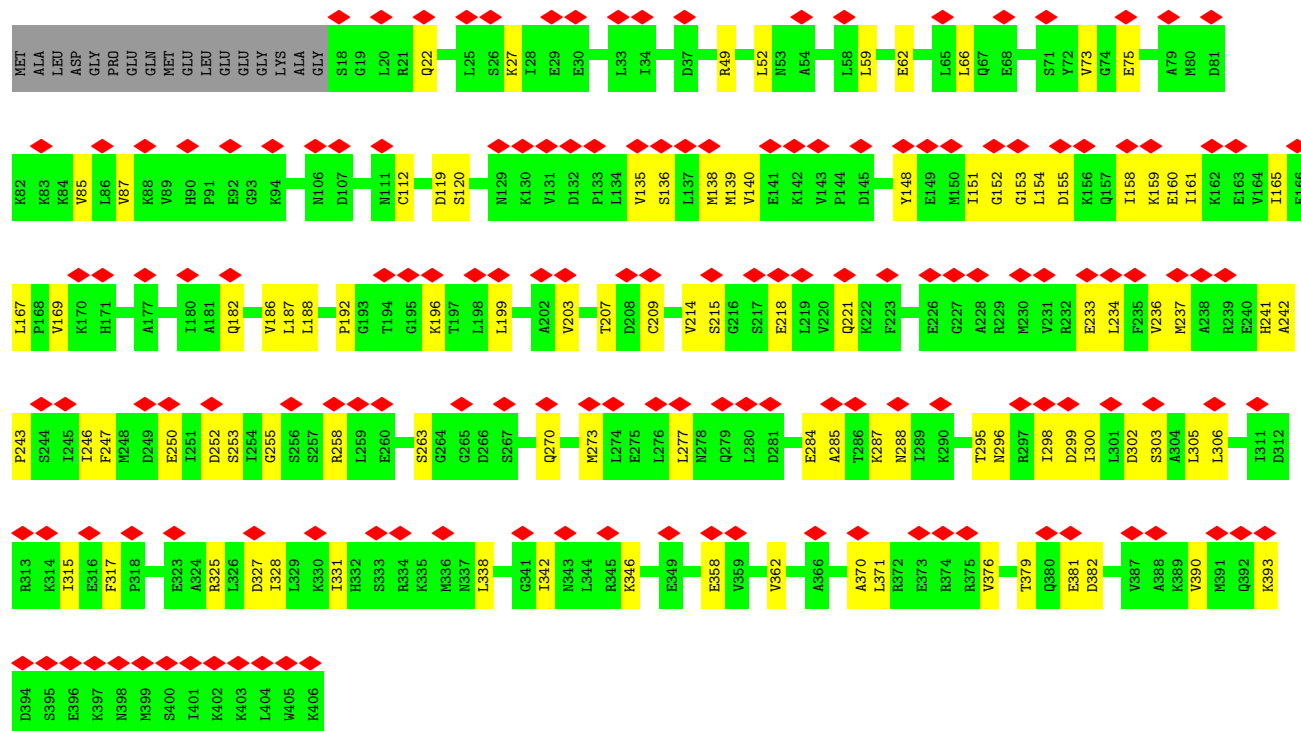
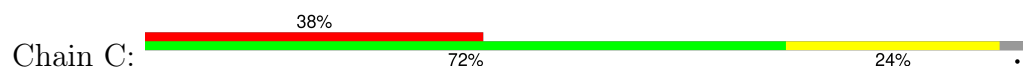


- Molecule 2: 26S proteasome regulatory subunit 4

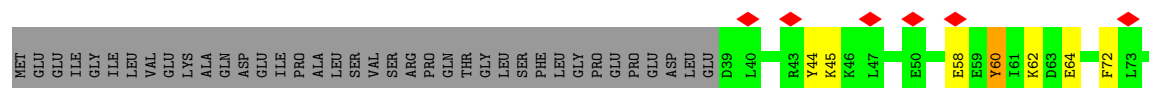


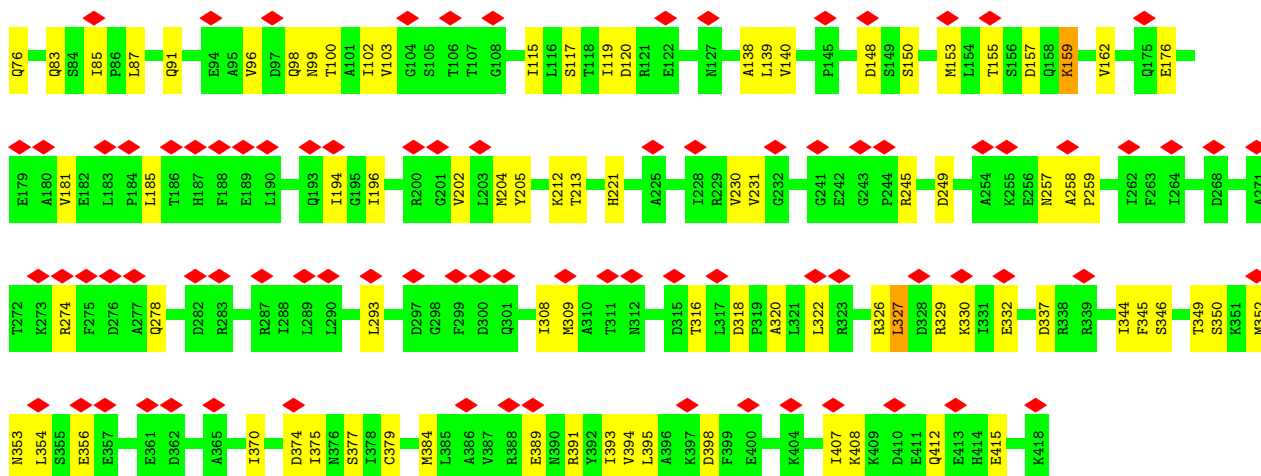


• Molecule 3: 26S protease regulatory subunit 8

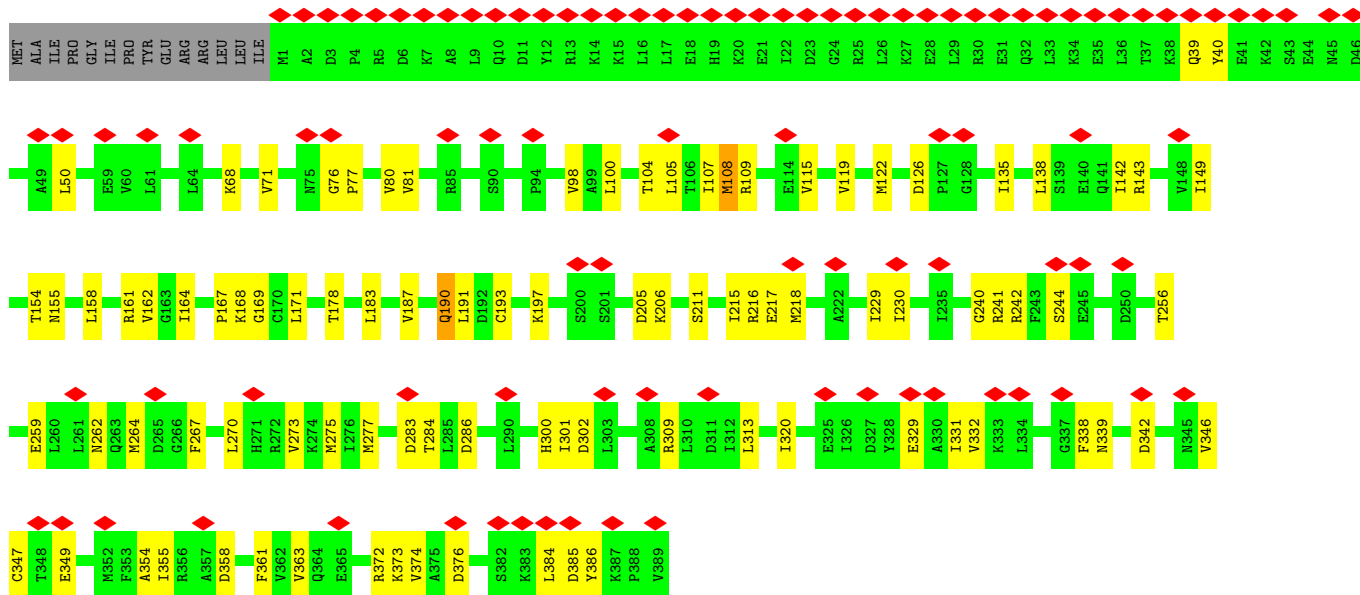


• Molecule 4: 26S proteasome regulatory subunit 6B

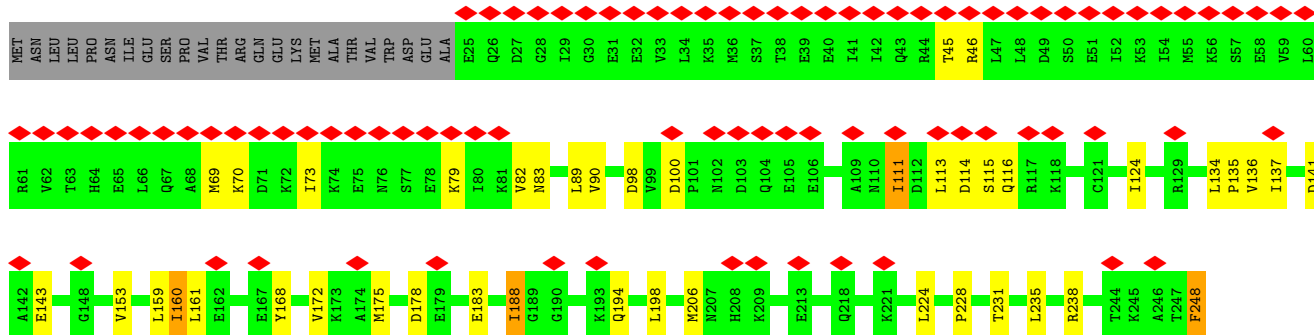


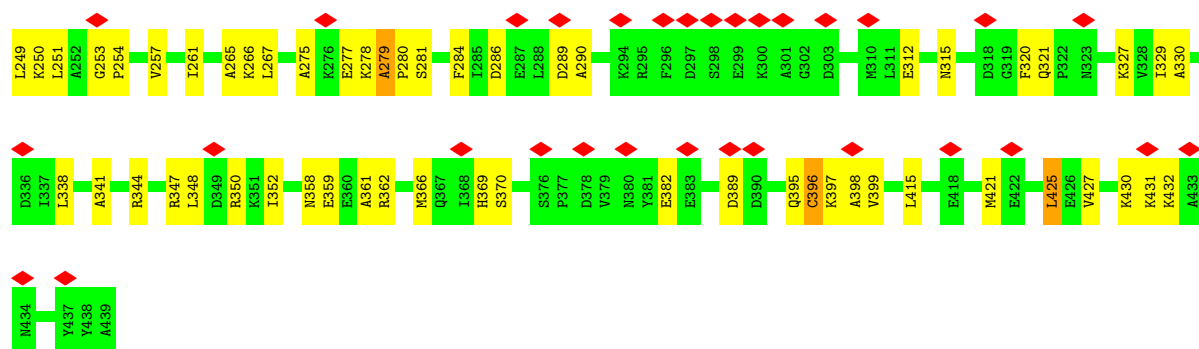


• Molecule 5: 26S proteasome regulatory subunit 10B



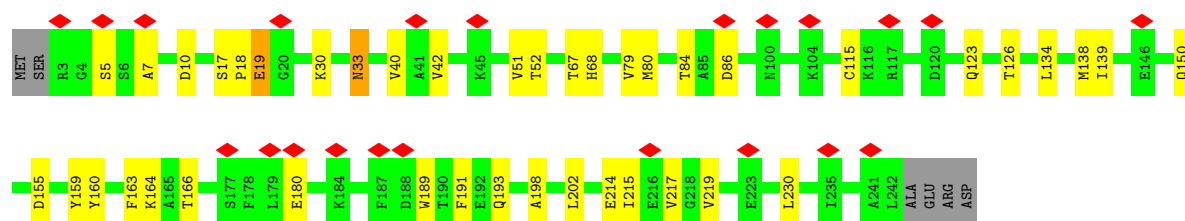
• Molecule 6: 26S proteasome regulatory subunit 6A





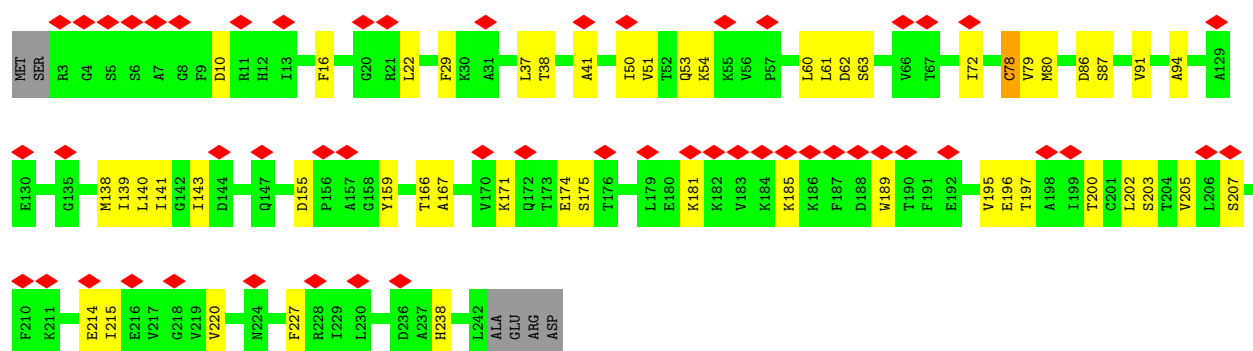
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 9% 80% 16% ..



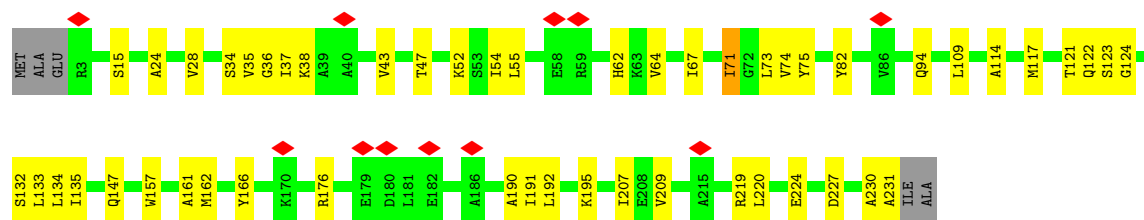
• Molecule 7: Proteasome subunit alpha type-6

Chain g: 22% 77% 20% .

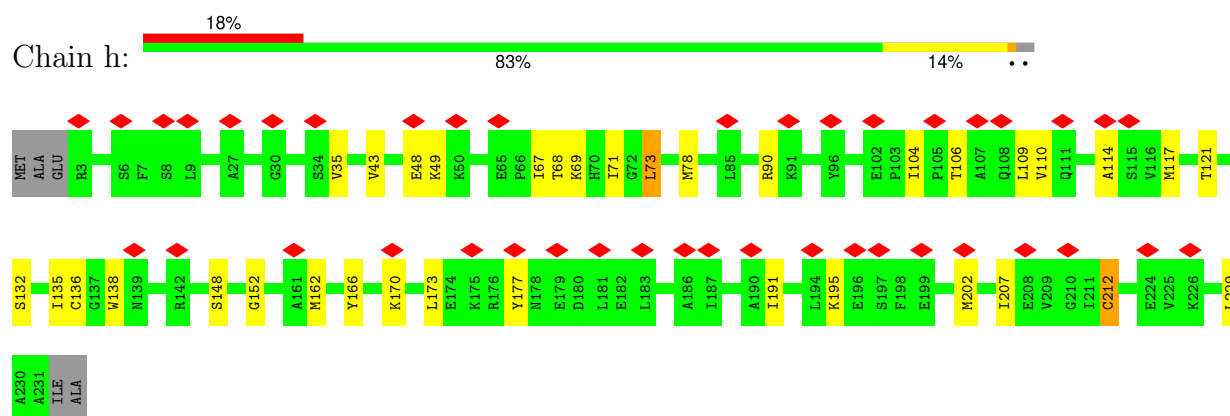


• Molecule 8: Proteasome subunit alpha type-2

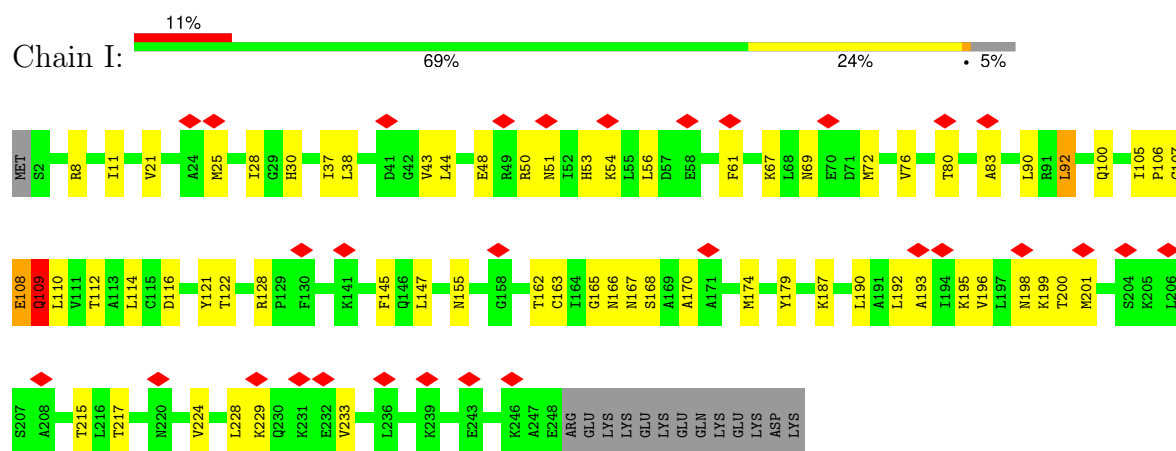
Chain H: 5% 76% 21% .



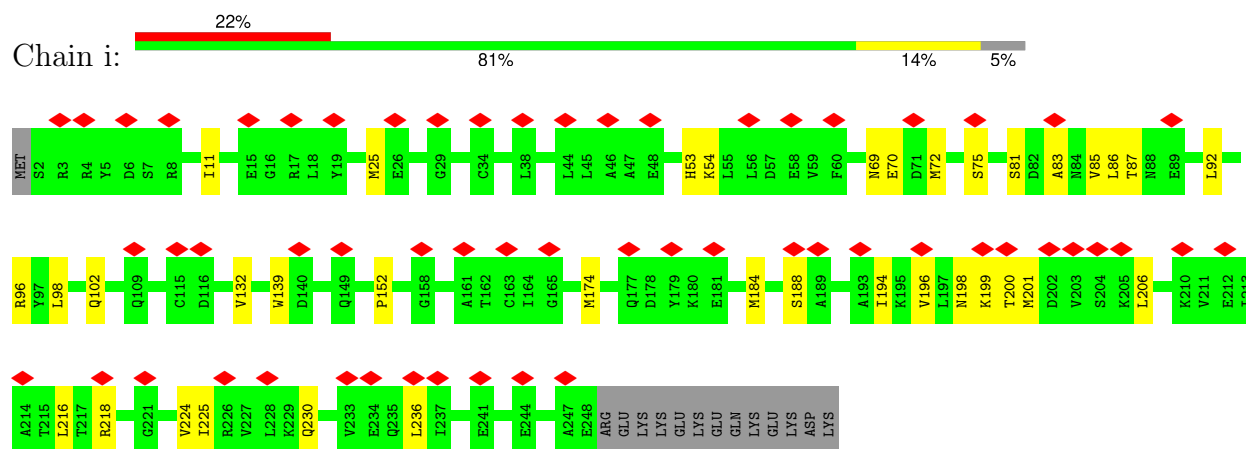
• Molecule 8: Proteasome subunit alpha type-2



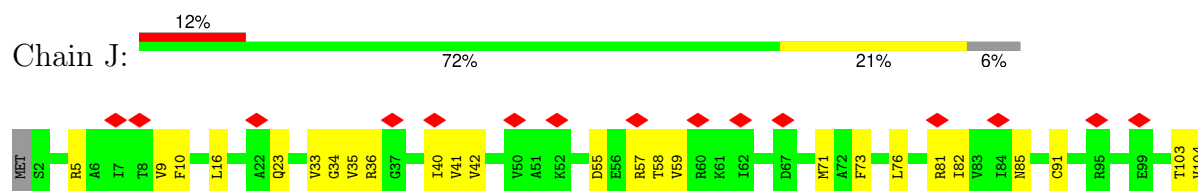
• Molecule 9: Proteasome subunit alpha type-4

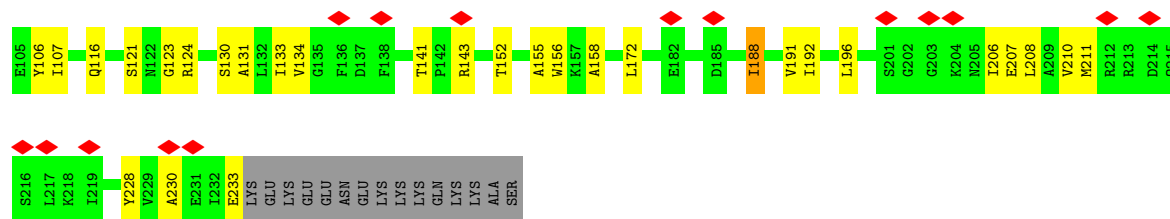


• Molecule 9: Proteasome subunit alpha type-4

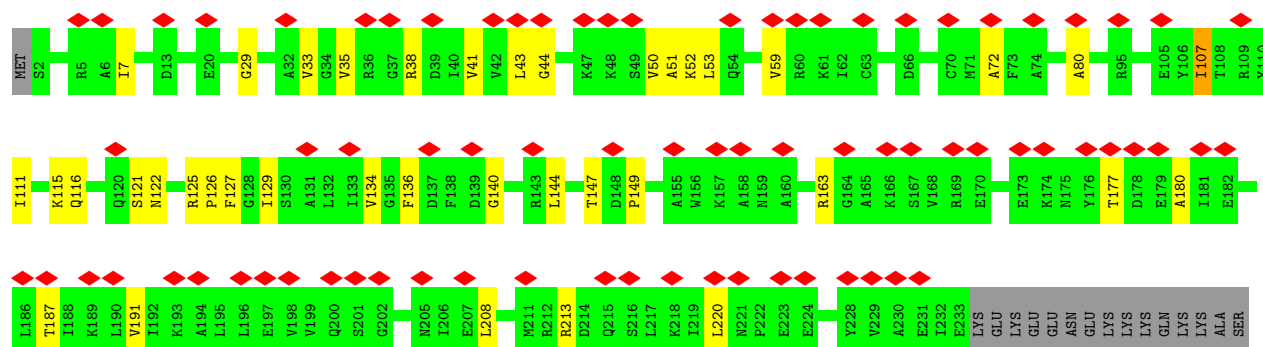
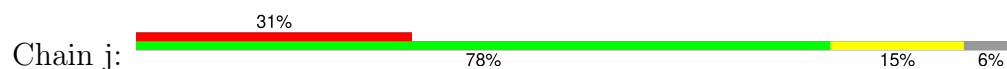


• Molecule 10: Proteasome subunit alpha type-7

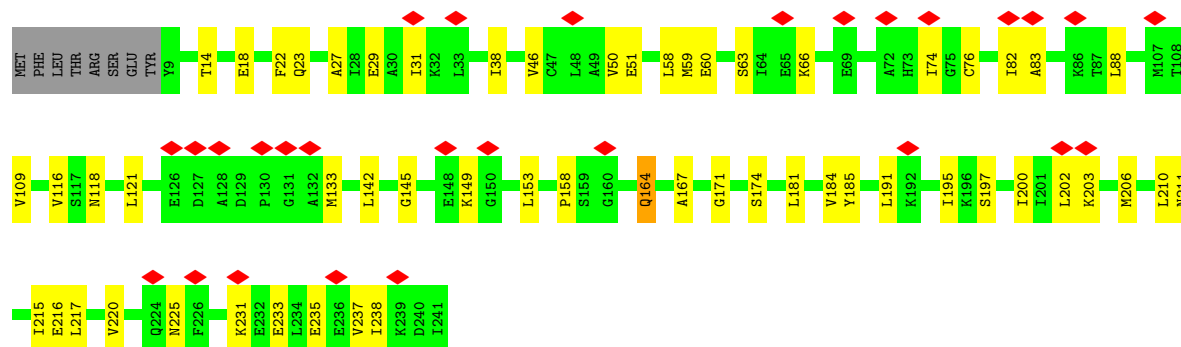
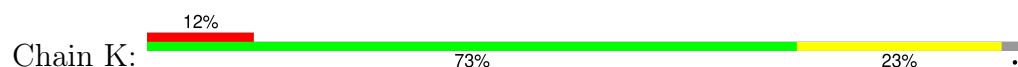




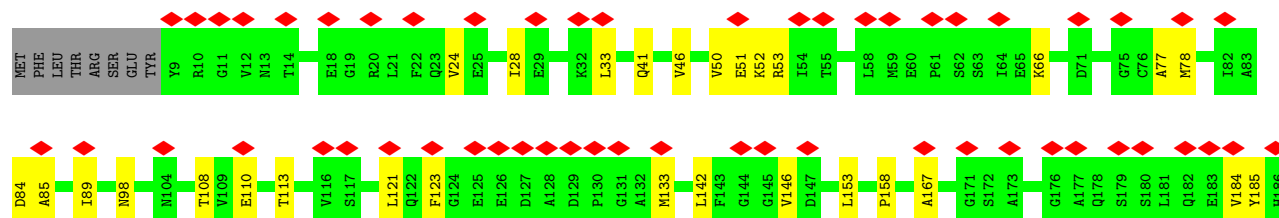
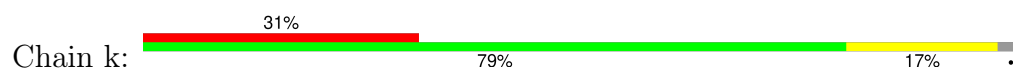
• Molecule 10: Proteasome subunit alpha type-7

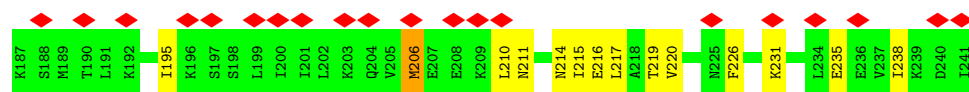


• Molecule 11: Proteasome subunit alpha type-5

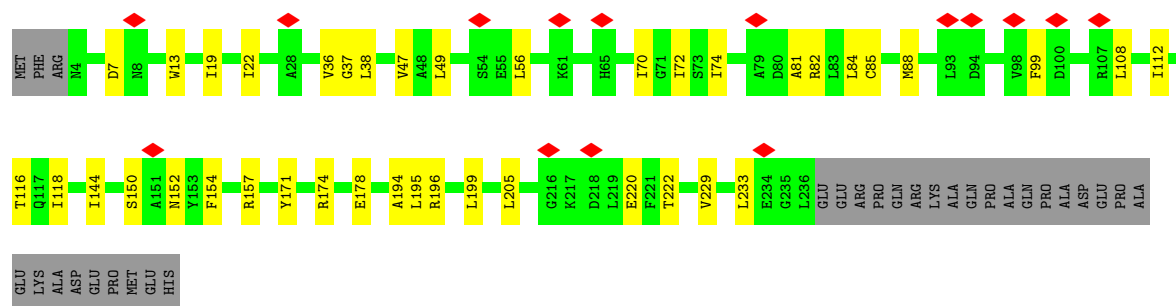
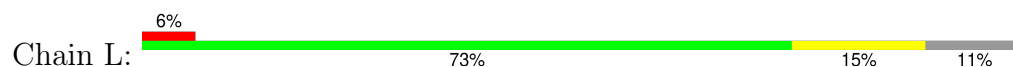


• Molecule 11: Proteasome subunit alpha type-5

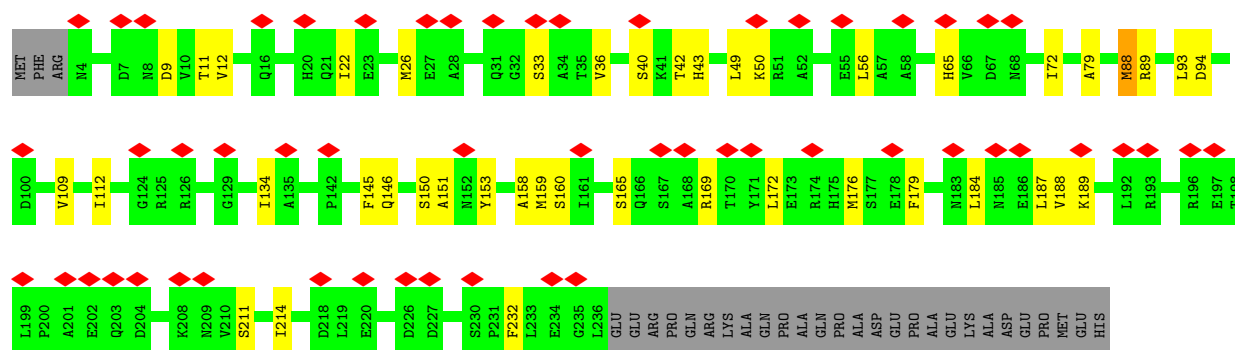




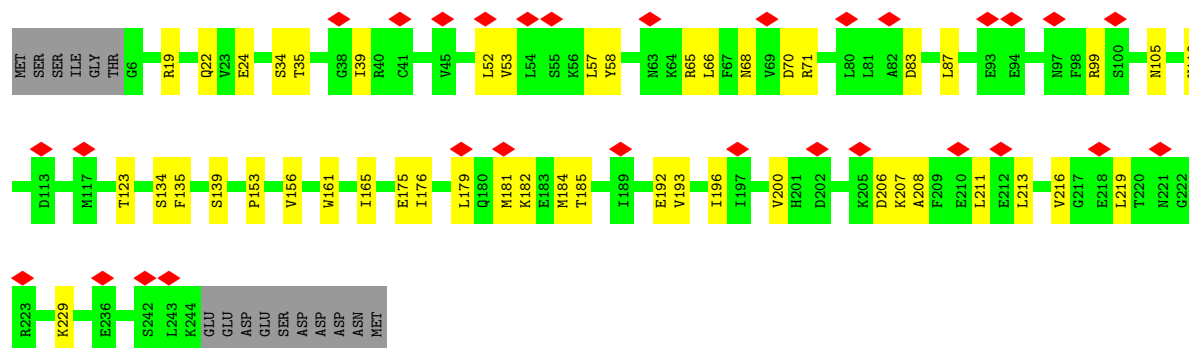
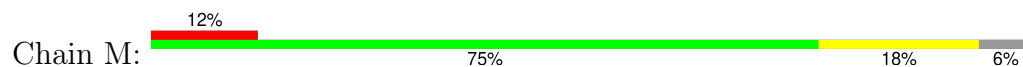
• Molecule 12: Proteasome subunit alpha type-1



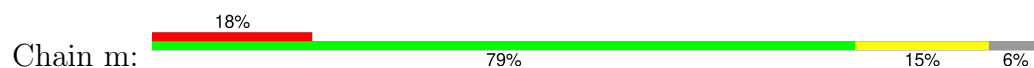
• Molecule 12: Proteasome subunit alpha type-1

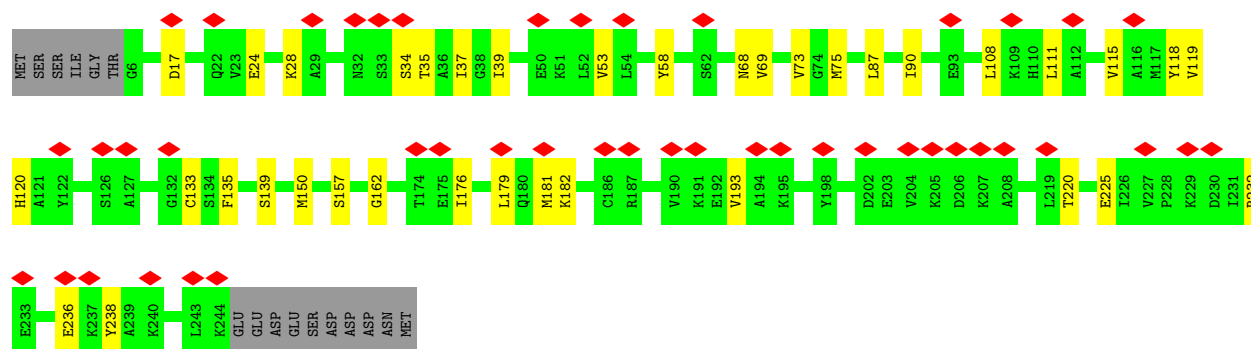


• Molecule 13: Proteasome subunit alpha type-3

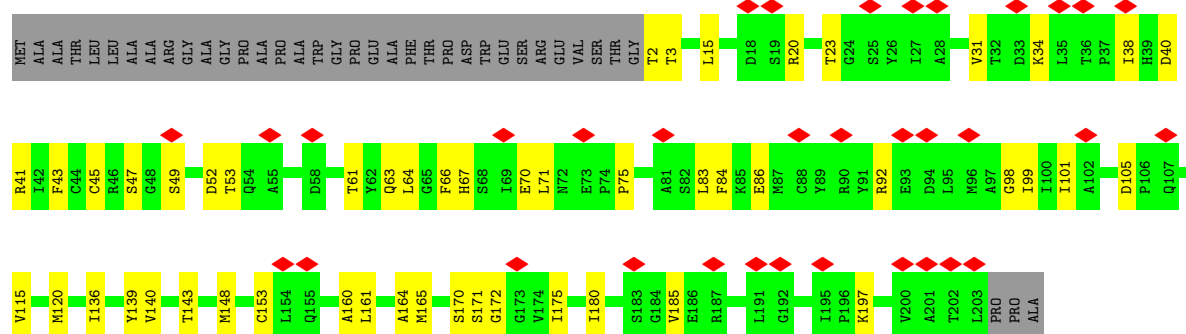


• Molecule 13: Proteasome subunit alpha type-3

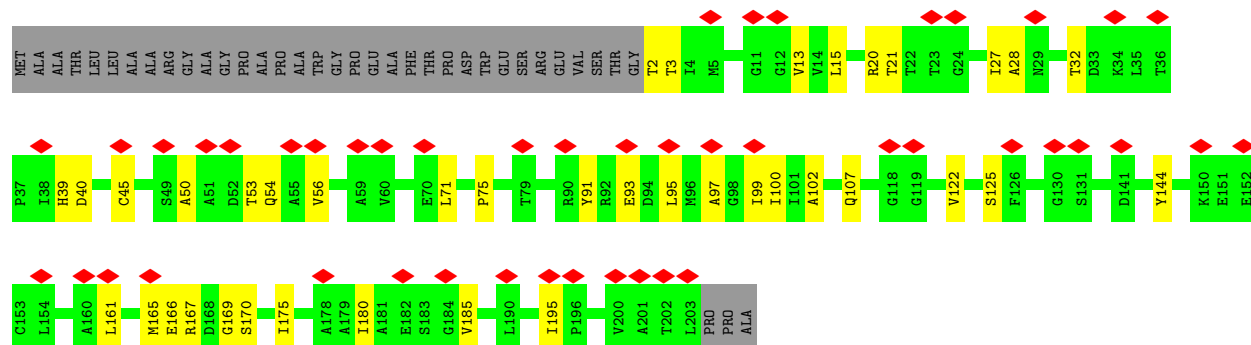




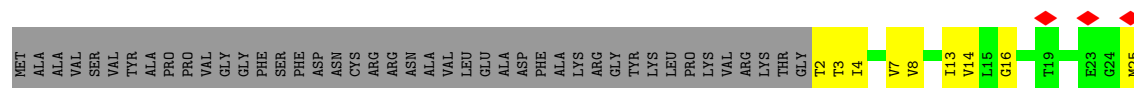
• Molecule 14: Proteasome subunit beta type-6

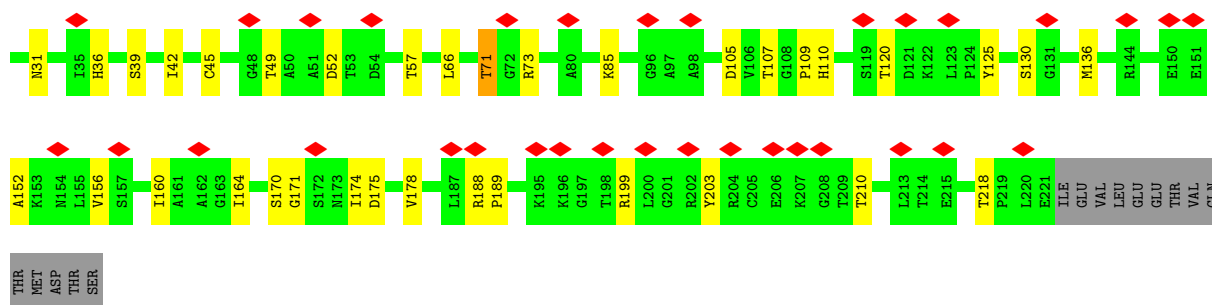


• Molecule 14: Proteasome subunit beta type-6

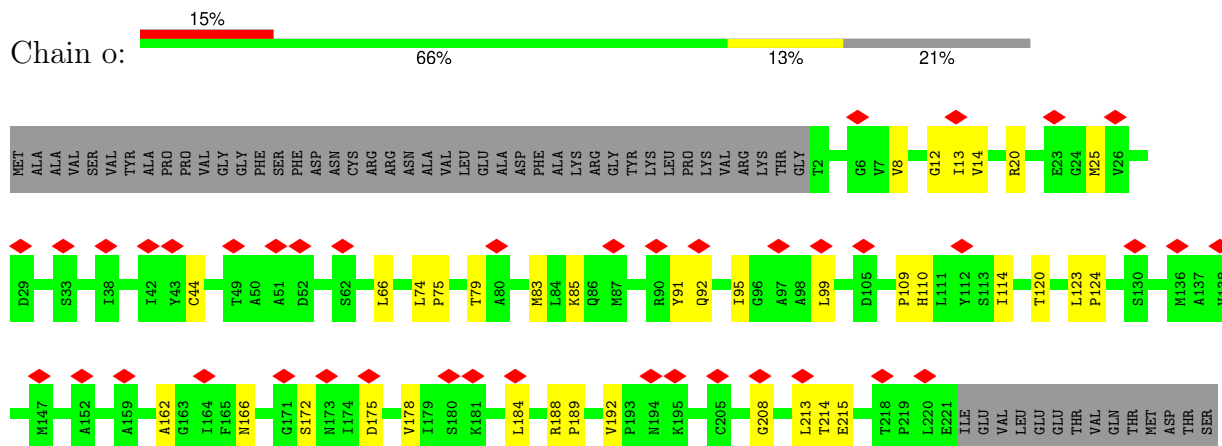


• Molecule 15: Proteasome subunit beta type-7

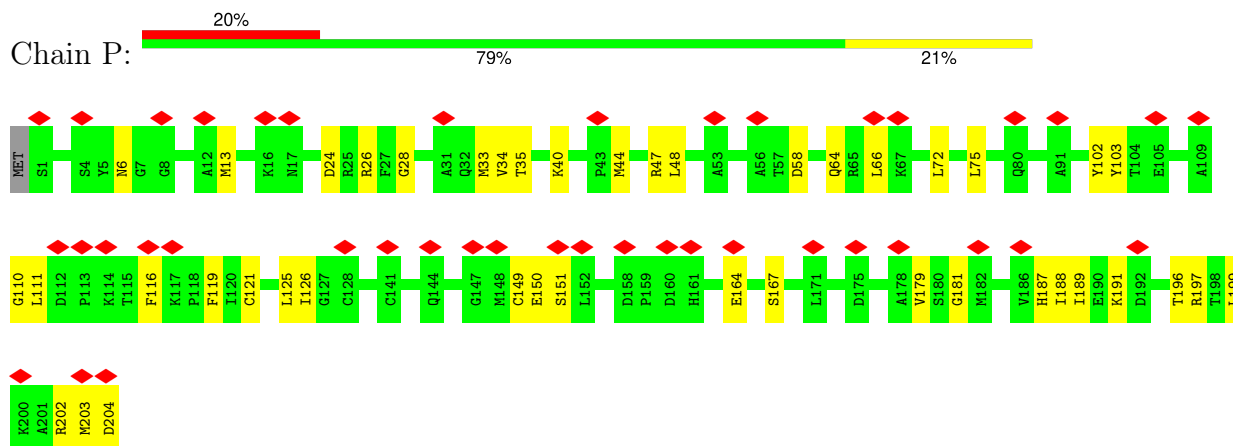




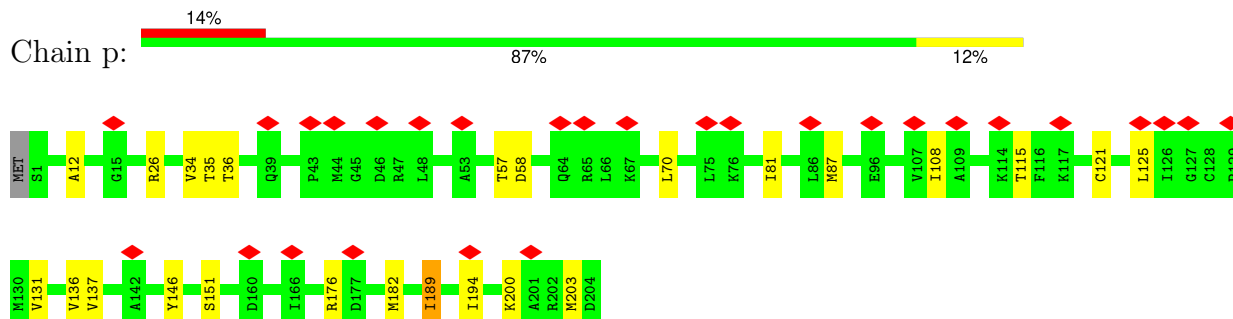
• Molecule 15: Proteasome subunit beta type-7



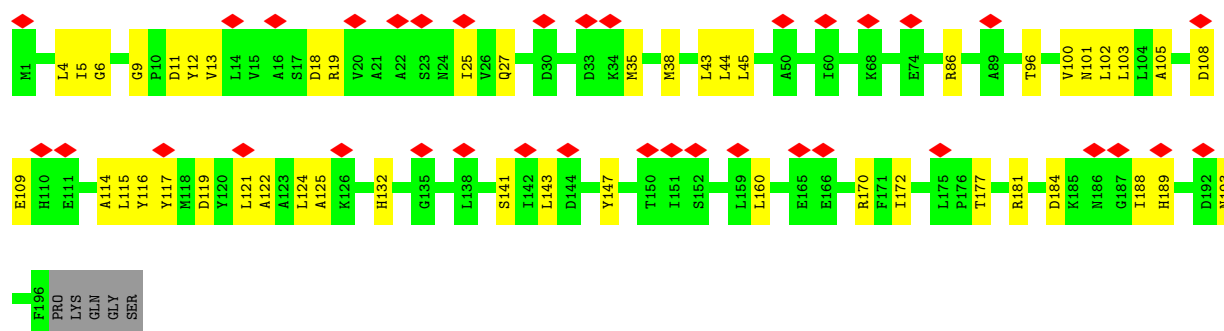
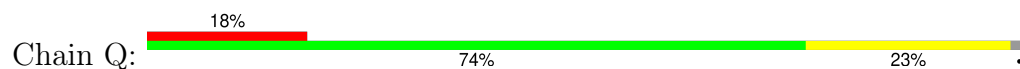
• Molecule 16: Proteasome subunit beta type-3



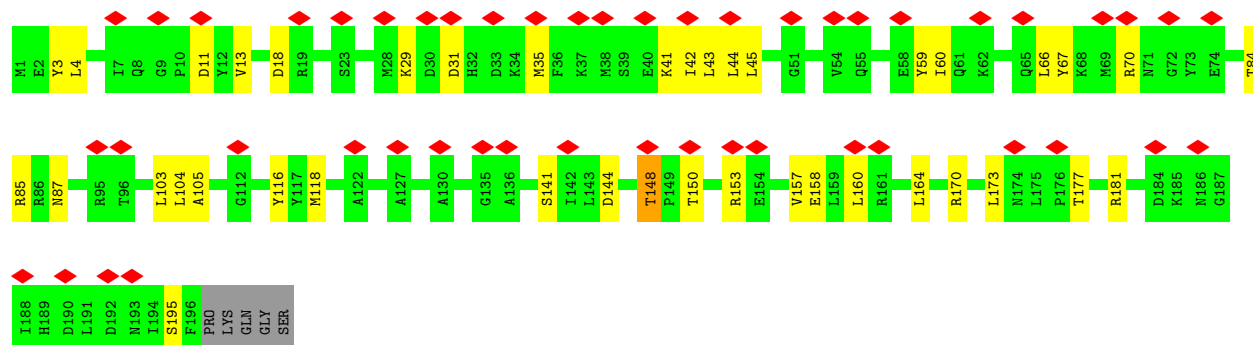
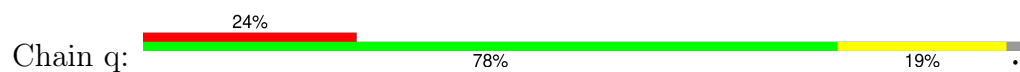
• Molecule 16: Proteasome subunit beta type-3



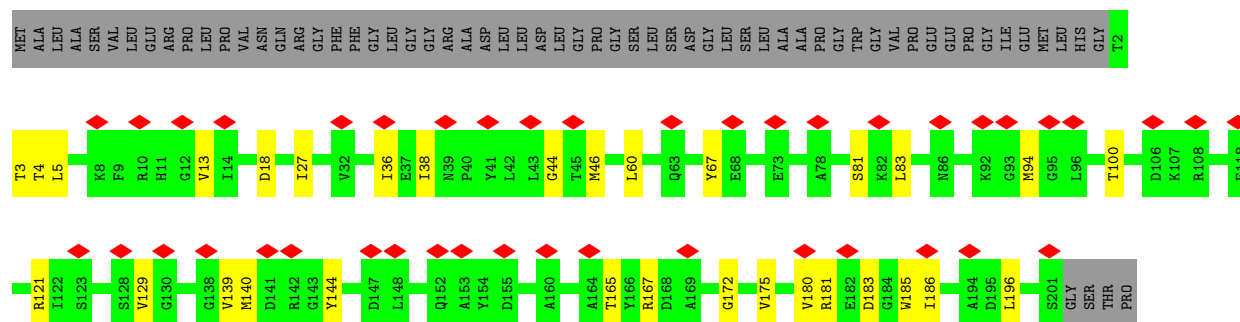
- Molecule 17: Proteasome subunit beta type-2



- Molecule 17: Proteasome subunit beta type-2

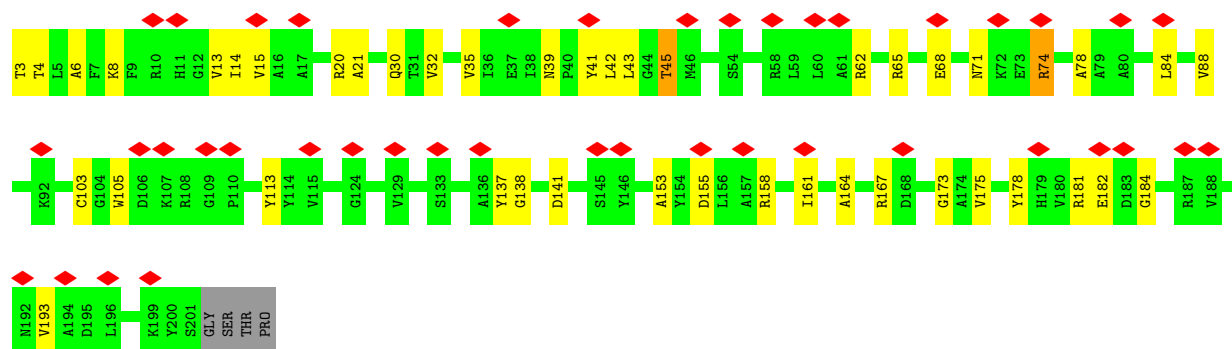


- Molecule 18: Proteasome subunit beta type-5

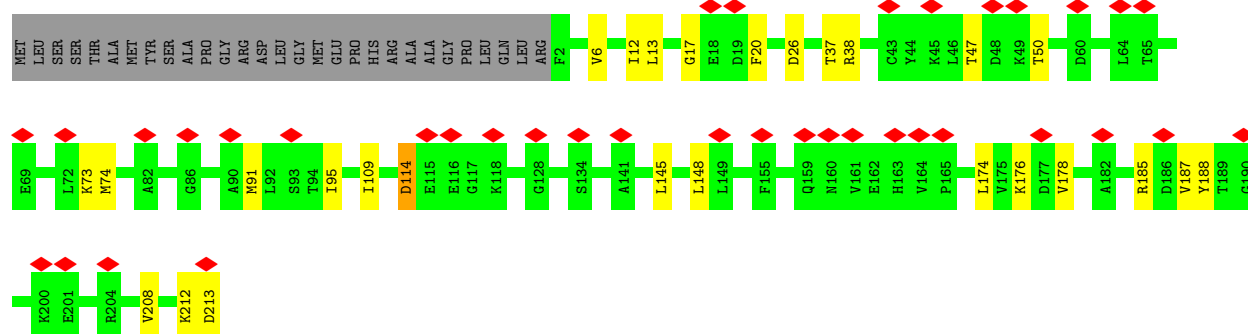


- Molecule 18: Proteasome subunit beta type-5

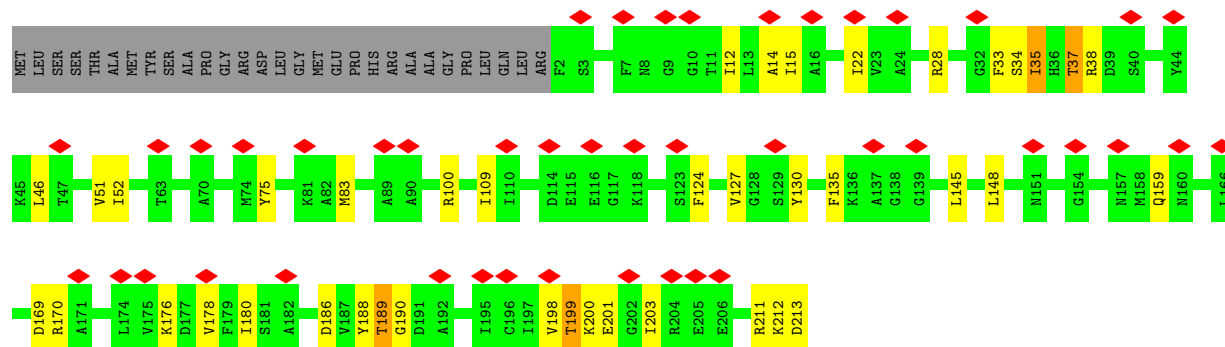




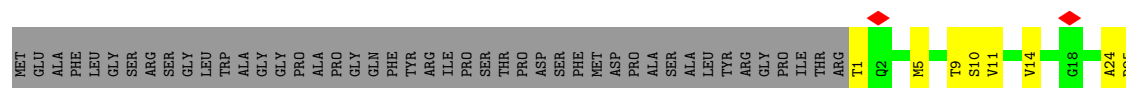
- Molecule 19: Proteasome subunit beta type-1

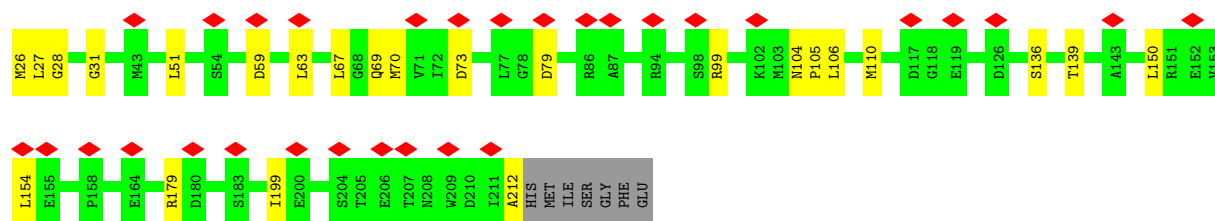


- Molecule 19: Proteasome subunit beta type-1

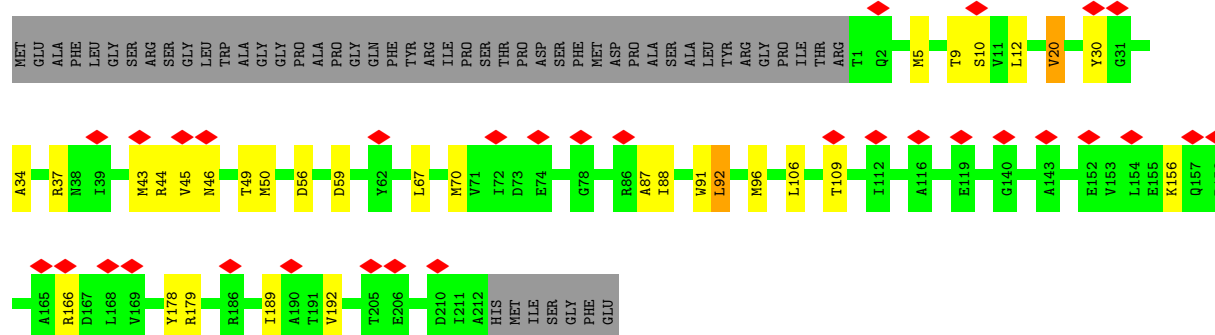


- Molecule 20: Proteasome subunit beta type-4

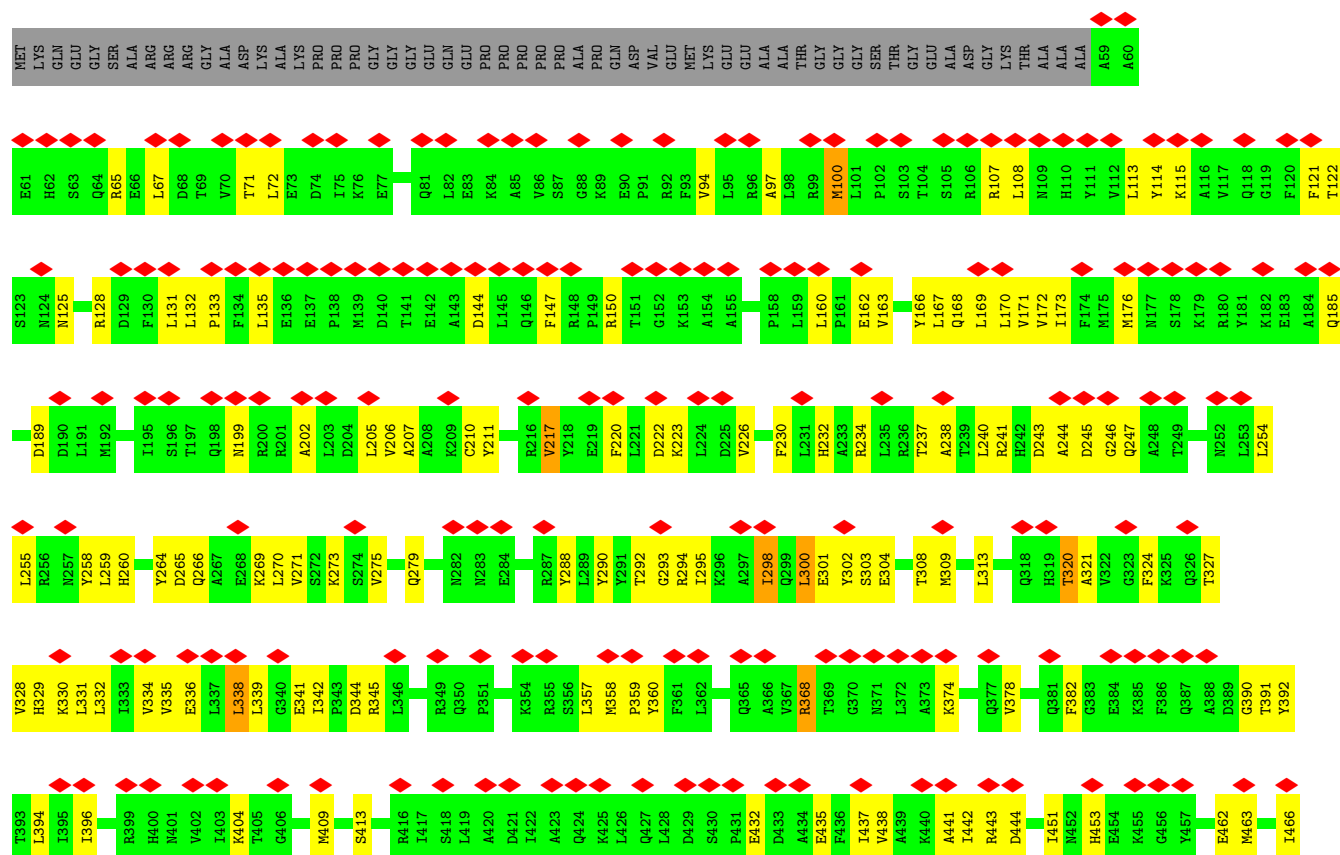


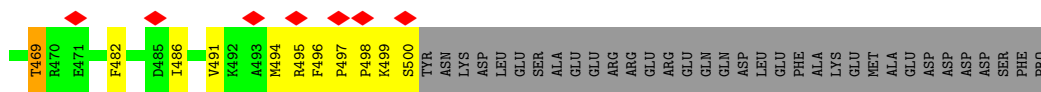


• Molecule 20: Proteasome subunit beta type-4

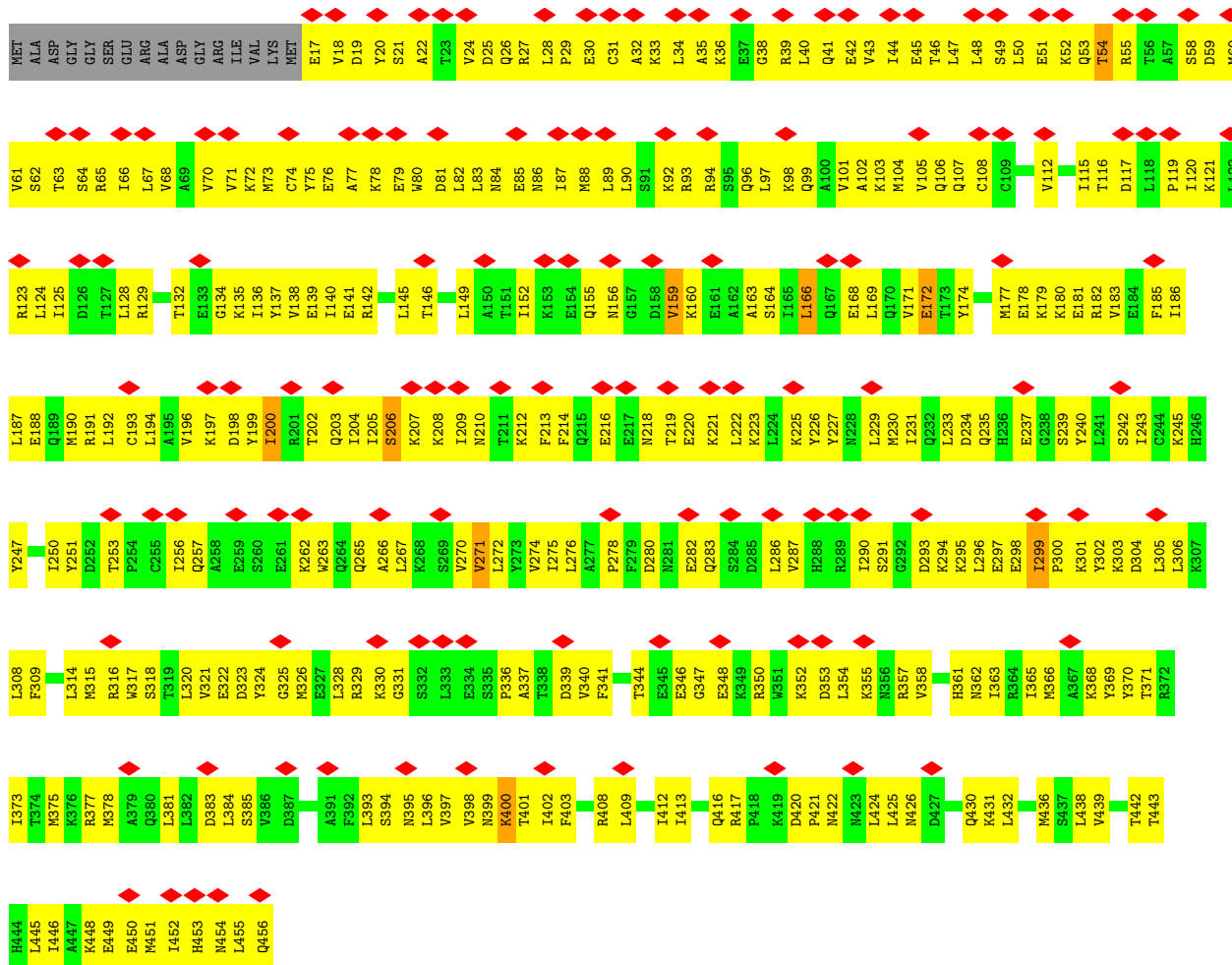
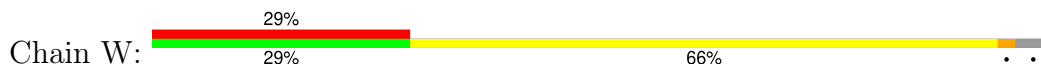


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 3

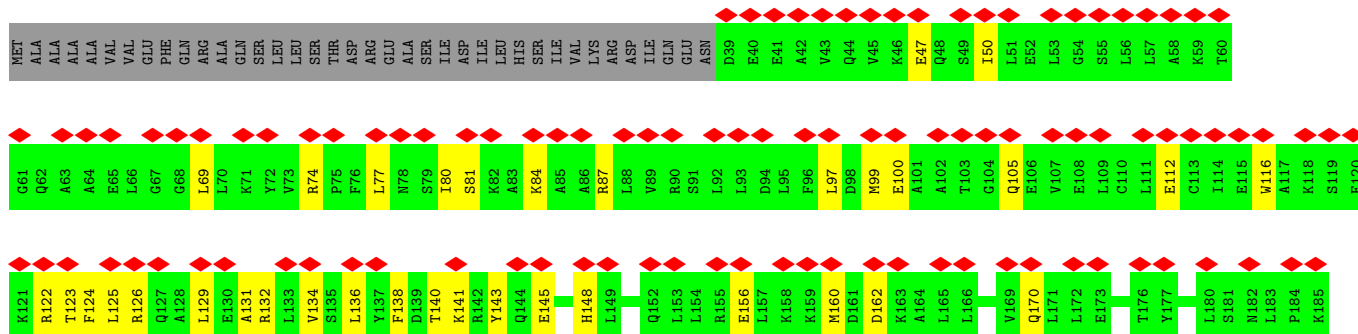




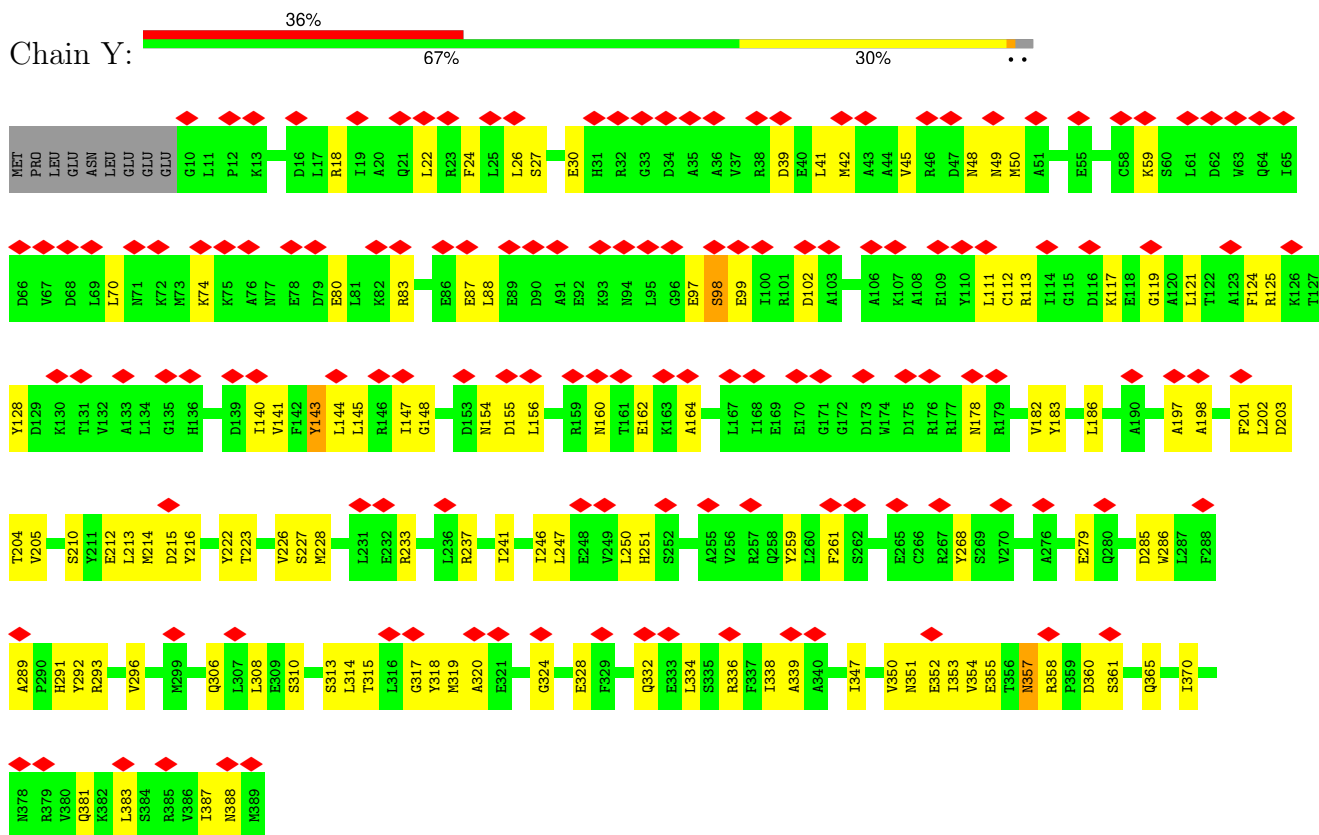
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12



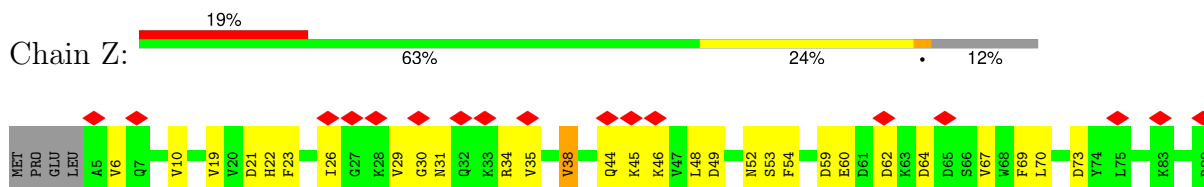
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11



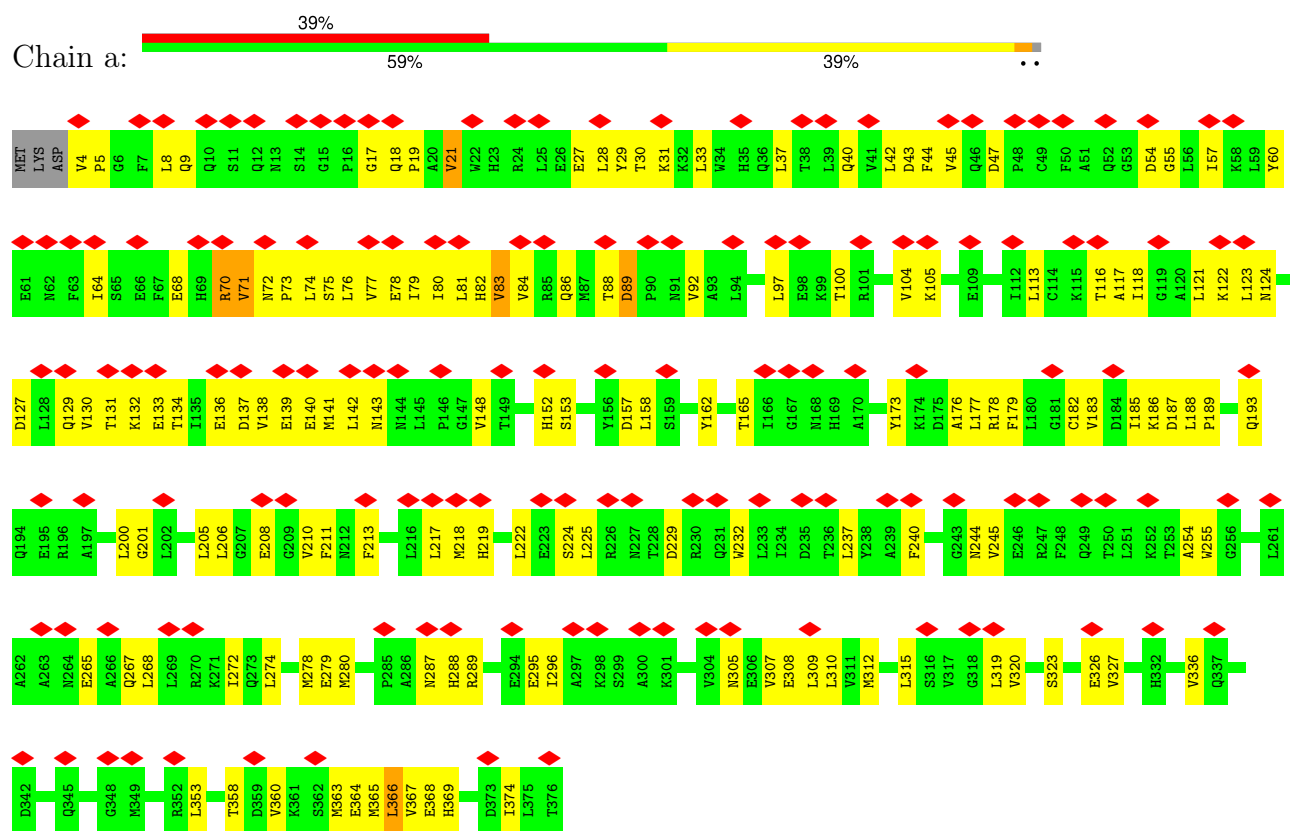
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 6



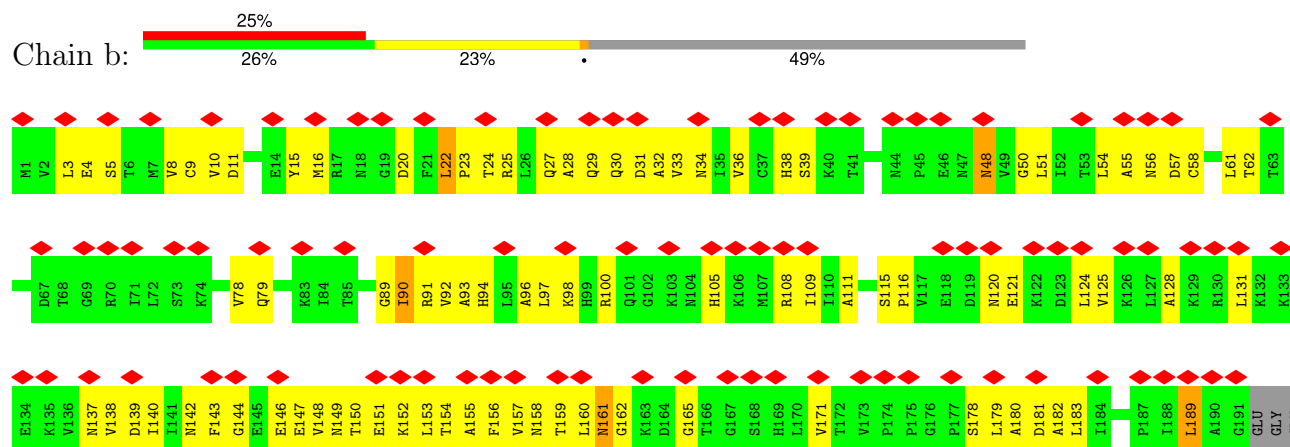
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 7



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



- Molecule 27: 26S proteasome non-ATPase regulatory subunit 4



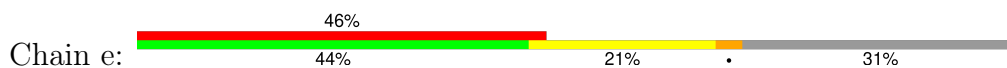
ASP LYS LYS	ASP THR SER GLU ALA LYS GLU ASP ASP THR SER VAL GLN MET GLN THR GLU ASN ASN GLU ALA ILE ARG ASN MET GLY SER LEU ALA GLU THR LYS ASP GLU LYS LYS LYS GLU	ASP THR SER GLU ALA LYS GLU ASP ASP THR SER VAL GLN MET GLN THR GLU ASN ASN GLU ALA ILE ARG ASN MET GLY SER LEU ALA GLU THR LYS ASP GLU LYS LYS LYS GLU	ASP SER ASP ALA LEU LEU LYS MET THR ILE SER GLN GLN PHE GLY THR ARG GLY LEU PRO SER ASP LEU SER GLU ASN LEU VAL GLY VAL PRO ASN ASN GLU ALA ILE ARG TYR ALA MET GLN MET SER LEU GLN GLY ALA SER LEU GLU GLU ILE GLN TYR ALA MET GLN MET SER LEU GLN GLY SER LEU GLU LYS ASP GLY LYS LYS LYS GLU	ALA MET GLY LEU GLY SER ALA ALA ALA ALA SER ALA ARG ARG GLU GLU GLN ARG GLN ARG GLN MET GLU GLN ILE ALA ARG GLN GLY MET GLU THR THR MET SER LEU SER THR THR THR THR THR THR MET
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- Molecule 28: 26S proteasome non-ATPase regulatory subunit 8



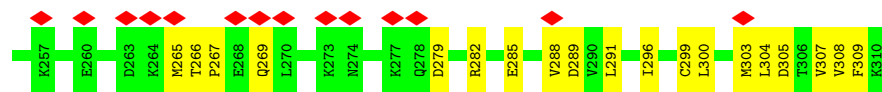
P312	A247	S186	L121	SER	THR	ARG	ALA
N313	K248	A186	V122	ARG	GLY	GLY	ALA
N314	G249	Y187	L123	LYS	LEU	LEU	ALA
Y315	N250	M188	L124	MET	ARG	ARG	ALA
Y316	I251	H189	E125	ALA	ALA	ALA	ALA
S317	F252	Q190	L126	ALA	ALA	ALA	ALA
F318	A253	L191	M127	ALA	ALA	ALA	ALA
A319	E254	L192	F128	ASN	ASN	ASN	ALA
S320	S255	G193	L129	VAL	GLY	GLY	ALA
Q321	Y256	L194	F130	ALA	ALA	ALA	ALA
Q322	T257	M195	T131	ALA	ALA	ALA	ALA
Q323		L196	G133	GLY	GLY	GLY	ALA
K324	D261	L197	T134	PHE	ARG	ARG	ALA
P325	I262	F198	K135	SER	SER	ARG	ALA
E326	L263	L200	L136	SER	GLY	GLY	ALA
D327	L264	S201	T137	PRO	PRO	PRO	ALA
	D265	Q202	K138	A81	A81	A81	
I330	T266	N203	Q139	A82	A82	A82	
P331	I267	R204	Q140	T83	T83	T83	
S332	R268	R205	L141	S84	S84	S84	
T333	D269	V206	I142	G85	G85	G85	
E334	E270	A206	L143	A86	A86	A86	
L335	I271	F208	A144	V87	V87	V87	
		H209	R145	L88	L88	L88	
V339	G274	T210	D146	Q89	Q89	Q89	
I340	I275	E211	I147	A90	A90	A90	
E341	E276	L212		A91	A91	A91	
L346	K277	E213	I150	T92	T92	T92	
	A278			S93	S93	S93	
V350	Y279	A217	Q153	M94	M94	M94	
	E280	K218	W154				
	K281	D219	S155	Y95	Y95	Y95	
	I282	I220	I156	E96	E96	E96	
	L283	Q221	L157	Q97	Q97	Q97	
	F284	T222	R158	L98	L98	L98	
	T285	N223	K159	K99	K99	K99	
	E286	V224	D160	G100	G100	G100	
		Y225	I161	E101	E101	E101	
		T226	P162	W102	W102	W102	
	R289	K227	S163	M103	M103	M103	
	I290	H228	F164	R104	R104	R104	
	F292	P229		K105	K105	K105	
	F293	V230	Y167	S106	S106	S106	
	N294	S231	M168	P107	P107	P107	
	T295	L232	A169	M108	M108	M108	
	P296	E233	Q170	N109	N109	N109	
	K297	Q234	L171	S110	S110	S110	
		Y235	K172	K111	K111	K111	
	R298	L236	Y175	C112	C112	C112	
	M299	M237	D176	G113	G113	G113	
		E238	F177	E114	E114	E114	
	Y302	G239	Y178	E115	E115	E115	
A303	K304	S240	K179	L116	L116	L116	
K306	K305	Y241	E180	G117	G117	G117	
R307	G306	N242	Q181	R118	R118	R118	
G307	L307	K243	L182	L119	L119	L119	
W308		V244	P183	K120	K120	K120	
		F245	E184				
		L246					

- Molecule 29: 26S proteasome complex subunit SEM1

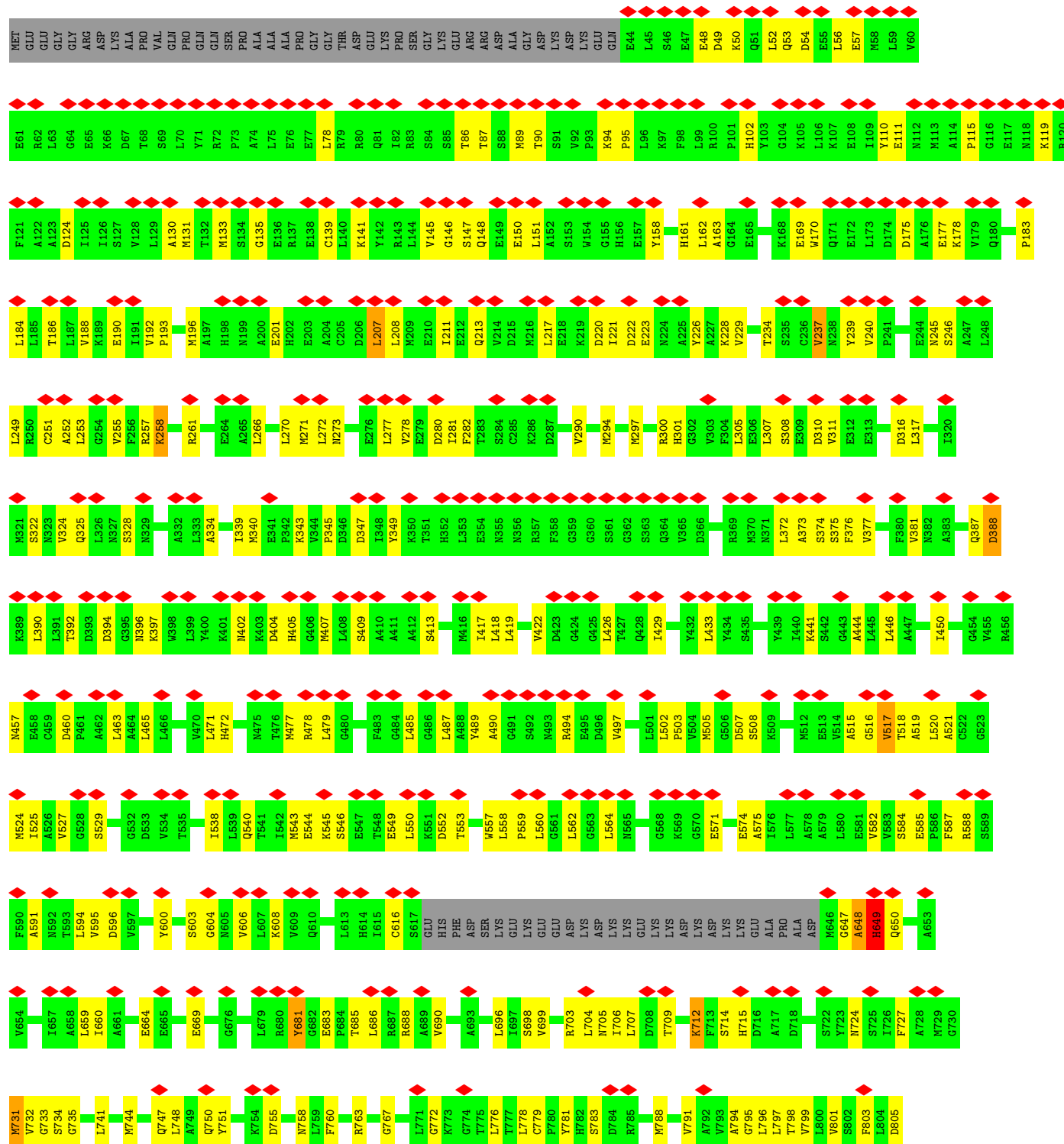
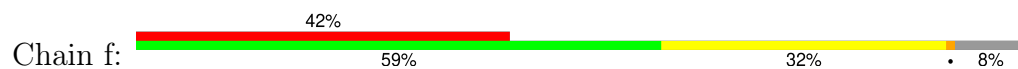
[illegible]

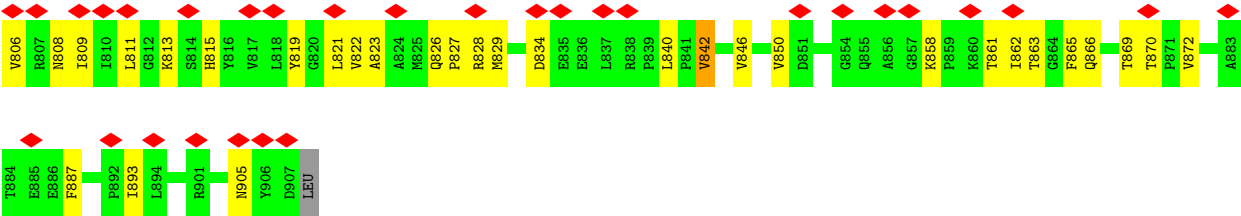
- Molecule 30: Unknown density-substrate density





• Molecule 34: 26S proteasome non-ATPase regulatory subunit 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.227	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	518.322, 518.322, 518.322	wwPDB
Map dimensions	602, 602, 602	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86100006, 0.86100006, 0.86100006	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, MG, ZN, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/3110	0.48	1/4196 (0.0%)
2	B	0.31	0/3120	0.48	0/4210
3	C	0.27	0/3112	0.42	0/4182
4	D	0.34	0/3089	0.48	0/4168
5	E	0.34	0/3146	0.43	0/4233
6	F	0.34	0/3292	0.47	2/4435 (0.0%)
7	G	0.34	0/1767	0.43	0/2398
7	g	0.31	0/1790	0.44	0/2429
8	H	0.33	0/1701	0.44	0/2318
8	h	0.29	0/1701	0.39	0/2318
9	I	0.43	1/1831 (0.1%)	0.71	5/2487 (0.2%)
9	i	0.29	0/1815	0.38	0/2466
10	J	0.29	0/1657	0.45	0/2261
10	j	0.28	0/1657	0.44	0/2261
11	K	0.31	0/1694	0.47	0/2301
11	k	0.29	0/1686	0.42	0/2290
12	L	0.34	0/1744	0.44	0/2371
12	l	0.30	0/1741	0.41	0/2367
13	M	0.33	0/1795	0.43	0/2434
13	m	0.29	0/1796	0.41	0/2435
14	N	0.31	0/1495	0.43	0/2026
14	n	0.30	0/1491	0.42	0/2021
15	O	0.30	0/1607	0.43	0/2185
15	o	0.31	0/1603	0.45	0/2180
16	P	0.31	0/1575	0.44	0/2128
16	p	0.32	0/1567	0.44	0/2118
17	Q	0.31	0/1541	0.44	0/2092
17	q	0.33	0/1538	0.44	0/2088
18	R	0.31	0/1535	0.43	0/2080
18	r	0.35	0/1531	0.45	0/2076
19	S	0.30	0/1614	0.41	0/2178
19	s	0.30	0/1617	0.44	0/2182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.32	0/1606	0.46	0/2179
20	t	0.32	0/1598	0.47	0/2170
21	V	0.26	0/3668	0.47	2/4953 (0.0%)
22	W	0.26	0/3636	0.41	0/4891
23	X	0.24	0/3084	0.42	0/4157
24	Y	0.29	0/3185	0.45	0/4290
25	Z	0.35	0/2324	0.50	0/3150
26	a	0.30	0/3053	0.50	0/4133
27	b	0.24	0/1478	0.49	0/2001
28	d	0.22	0/2239	0.43	0/3025
29	e	0.19	0/420	0.37	0/572
31	z	0.27	0/620	0.42	0/836
32	U	0.31	0/6486	0.46	0/8777
33	c	0.34	0/2274	0.47	0/3072
34	f	0.32	1/6569 (0.0%)	0.55	6/8893 (0.1%)
All	All	0.31	2/104198 (0.0%)	0.46	16/141013 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
7	g	0	1
9	I	0	1
20	t	0	1
34	f	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	649	HIS	CG-CD2	6.31	1.42	1.35
9	I	109	GLN	N-CA	6.12	1.53	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	649	HIS	N-CA-CB	12.69	129.09	110.06
9	I	109	GLN	CB-CG-CD	-10.44	94.86	112.60
9	I	108	GLU	CA-C-N	-10.38	106.52	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	108	GLU	C-N-CA	-10.38	106.52	120.54
34	f	648	ALA	CA-C-N	-10.15	106.47	120.38

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	395	GLN	Peptide
9	I	109	GLN	Sidechain
34	f	647	GLY	Peptide
7	g	78	CYS	Peptide
20	t	109	THR	Peptide

5.2 Too-close contacts [i](#)

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	A	3060	3106	3107	93	0
2	B	3076	3053	3129	151	0
3	C	3071	3193	3193	73	0
4	D	3039	3075	3076	77	0
5	E	3098	3150	3174	79	0
6	F	3251	3318	3316	83	0
7	G	1738	1656	1656	26	0
7	g	1758	1687	1687	33	0
8	H	1662	1590	1590	45	0
8	h	1662	1590	1590	24	0
9	I	1802	1741	1741	51	0
9	i	1786	1717	1717	29	0
10	J	1633	1518	1518	42	0
10	j	1633	1518	1518	28	0
11	K	1667	1597	1596	49	0
11	k	1660	1589	1589	31	0
12	L	1710	1649	1649	29	0
12	l	1707	1645	1645	31	0
13	M	1760	1680	1680	37	0
13	m	1761	1683	1683	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1469	1422	1422	37	0
14	n	1465	1416	1416	24	0
15	O	1580	1559	1559	40	0
15	o	1576	1555	1555	31	0
16	P	1546	1550	1552	29	0
16	p	1538	1543	1545	19	0
17	Q	1509	1477	1477	37	0
17	q	1506	1475	1475	26	0
18	R	1504	1449	1449	20	0
18	r	1500	1438	1438	38	0
19	S	1584	1579	1579	18	0
19	s	1587	1581	1581	32	0
20	T	1576	1526	1528	21	0
20	t	1568	1511	1513	22	0
21	V	3598	3658	3658	116	0
22	W	3588	0	3704	483	0
23	X	3040	3134	3134	82	0
24	Y	3127	3133	3133	89	0
25	Z	2281	2312	2312	76	0
26	a	2995	3012	3012	159	0
27	b	1458	1505	1505	75	0
28	d	2193	2221	2221	80	0
29	e	409	316	316	17	0
30	v	60	0	14	0	0
31	z	612	645	645	17	0
32	U	6371	6402	6407	222	0
33	c	2232	2241	2242	73	0
34	f	6460	6486	6487	224	0
35	A	31	12	12	1	0
35	B	31	12	12	3	0
35	D	31	12	12	0	0
35	F	31	12	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	E	27	12	12	1	0
38	c	1	0	0	0	0
All	All	102622	97961	101793	2925	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 14.

The worst 5 of 2925 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)
22:W:205:ILE:HA	22:W:208:LYS:HD2	1.24	1.13
22:W:205:ILE:HD12	22:W:208:LYS:HD3	1.23	1.13
32:U:446:LEU:HD21	32:U:457:ILE:HD12	1.36	1.07
22:W:79:GLU:HB3	22:W:82:LEU:HB2	1.34	1.04
25:Z:186:THR:OG1	25:Z:190:ARG:NH2	1.93	1.01

There are no symmetry-related clashes.

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	A	388/433 (90%)	354 (91%)	34 (9%)	0	100	100
2	B	391/440 (89%)	341 (87%)	48 (12%)	2 (0%)	25	50
3	C	387/406 (95%)	349 (90%)	38 (10%)	0	100	100
4	D	378/418 (90%)	352 (93%)	25 (7%)	1 (0%)	37	60
5	E	387/403 (96%)	362 (94%)	25 (6%)	0	100	100
6	F	413/439 (94%)	382 (92%)	30 (7%)	1 (0%)	44	66
7	G	238/246 (97%)	222 (93%)	15 (6%)	1 (0%)	30	55
7	g	238/246 (97%)	233 (98%)	5 (2%)	0	100	100
8	H	227/234 (97%)	217 (96%)	10 (4%)	0	100	100
8	h	227/234 (97%)	218 (96%)	9 (4%)	0	100	100
9	I	245/261 (94%)	228 (93%)	17 (7%)	0	100	100
9	i	245/261 (94%)	237 (97%)	8 (3%)	0	100	100
10	J	230/248 (93%)	216 (94%)	14 (6%)	0	100	100
10	j	230/248 (93%)	222 (96%)	7 (3%)	1 (0%)	30	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
11	k	231/241 (96%)	223 (96%)	8 (4%)	0	100	100
12	L	231/263 (88%)	222 (96%)	9 (4%)	0	100	100
12	l	231/263 (88%)	221 (96%)	10 (4%)	0	100	100
13	M	237/255 (93%)	230 (97%)	7 (3%)	0	100	100
13	m	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
15	o	218/277 (79%)	210 (96%)	7 (3%)	1 (0%)	25	50
16	P	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	25	50
17	q	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
18	R	198/263 (75%)	191 (96%)	7 (4%)	0	100	100
18	r	198/263 (75%)	186 (94%)	12 (6%)	0	100	100
19	S	210/241 (87%)	202 (96%)	8 (4%)	0	100	100
19	s	210/241 (87%)	203 (97%)	7 (3%)	0	100	100
20	T	210/264 (80%)	199 (95%)	10 (5%)	1 (0%)	25	50
20	t	210/264 (80%)	195 (93%)	15 (7%)	0	100	100
21	V	440/534 (82%)	413 (94%)	25 (6%)	2 (0%)	25	50
22	W	438/456 (96%)	411 (94%)	27 (6%)	0	100	100
23	X	382/422 (90%)	364 (95%)	18 (5%)	0	100	100
24	Y	378/389 (97%)	356 (94%)	21 (6%)	1 (0%)	37	60
25	Z	284/324 (88%)	258 (91%)	23 (8%)	3 (1%)	12	30
26	a	371/376 (99%)	325 (88%)	44 (12%)	2 (0%)	25	50
27	b	189/377 (50%)	151 (80%)	37 (20%)	1 (0%)	25	50
28	d	268/350 (77%)	246 (92%)	20 (8%)	2 (1%)	19	41
29	e	46/70 (66%)	37 (80%)	8 (17%)	1 (2%)	5	16
31	z	79/468 (17%)	78 (99%)	1 (1%)	0	100	100
32	U	812/953 (85%)	762 (94%)	49 (6%)	1 (0%)	48	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	c	279/310 (90%)	257 (92%)	21 (8%)	1 (0%)	30	55
34	f	832/908 (92%)	779 (94%)	53 (6%)	0	100	100
All	All	13284/15352 (86%)	12454 (94%)	807 (6%)	23 (0%)	45	66

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	65	LEU
25	Z	149	THR
2	B	278	ALA
24	Y	98	SER
25	Z	194	GLN

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	A	333/372 (90%)	329 (99%)	4 (1%)	67	81
2	B	344/385 (89%)	332 (96%)	12 (4%)	31	55
3	C	340/352 (97%)	337 (99%)	3 (1%)	75	85
4	D	333/366 (91%)	330 (99%)	3 (1%)	75	85
5	E	341/353 (97%)	336 (98%)	5 (2%)	60	78
6	F	357/379 (94%)	351 (98%)	6 (2%)	56	76
7	G	164/210 (78%)	157 (96%)	7 (4%)	25	49
7	g	168/210 (80%)	166 (99%)	2 (1%)	67	81
8	H	150/191 (78%)	146 (97%)	4 (3%)	40	64
8	h	150/191 (78%)	146 (97%)	4 (3%)	40	64
9	I	166/221 (75%)	158 (95%)	8 (5%)	21	44
9	i	160/221 (72%)	159 (99%)	1 (1%)	84	90
10	J	136/211 (64%)	133 (98%)	3 (2%)	47	70
10	j	136/211 (64%)	135 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	159/203 (78%)	158 (99%)	1 (1%)	84	90
11	k	158/203 (78%)	156 (99%)	2 (1%)	65	80
12	L	161/224 (72%)	161 (100%)	0	100	100
12	l	161/224 (72%)	159 (99%)	2 (1%)	67	81
13	M	162/212 (76%)	159 (98%)	3 (2%)	52	73
13	m	163/212 (77%)	161 (99%)	2 (1%)	67	81
14	N	141/181 (78%)	139 (99%)	2 (1%)	62	79
14	n	140/181 (77%)	138 (99%)	2 (1%)	62	79
15	O	158/228 (69%)	156 (99%)	2 (1%)	65	80
15	o	157/228 (69%)	157 (100%)	0	100	100
16	P	159/174 (91%)	157 (99%)	2 (1%)	65	80
16	p	156/174 (90%)	153 (98%)	3 (2%)	52	73
17	Q	149/171 (87%)	147 (99%)	2 (1%)	65	80
17	q	148/171 (86%)	146 (99%)	2 (1%)	62	79
18	R	139/202 (69%)	136 (98%)	3 (2%)	47	70
18	r	138/202 (68%)	136 (99%)	2 (1%)	62	79
19	S	158/199 (79%)	154 (98%)	4 (2%)	42	66
19	s	159/199 (80%)	155 (98%)	4 (2%)	42	66
20	T	151/215 (70%)	150 (99%)	1 (1%)	81	89
20	t	149/215 (69%)	147 (99%)	2 (1%)	65	80
21	V	389/460 (85%)	379 (97%)	10 (3%)	41	65
22	W	405/416 (97%)	393 (97%)	12 (3%)	36	60
23	X	330/362 (91%)	326 (99%)	4 (1%)	67	81
24	Y	335/344 (97%)	327 (98%)	8 (2%)	44	68
25	Z	257/295 (87%)	250 (97%)	7 (3%)	40	64
26	a	333/336 (99%)	324 (97%)	9 (3%)	40	64
27	b	167/312 (54%)	161 (96%)	6 (4%)	30	54
28	d	237/294 (81%)	233 (98%)	4 (2%)	56	76
29	e	43/63 (68%)	42 (98%)	1 (2%)	45	69
31	z	68/377 (18%)	67 (98%)	1 (2%)	60	78
32	U	695/816 (85%)	680 (98%)	15 (2%)	47	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	c	249/268 (93%)	242 (97%)	7 (3%)	38	63
34	f	704/763 (92%)	690 (98%)	14 (2%)	50	72
All	All	10556/12997 (81%)	10354 (98%)	202 (2%)	52	73

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Z	214	LYS
10	j	107	ILE
34	f	744	MET
26	a	105	LYS
27	b	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
9	i	100	GLN
19	s	151	ASN
9	i	198	ASN
15	o	31	ASN
32	U	801	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
37	ADP	E	401	-	24,29,29	0.87	0	29,45,45	1.17	1 (3%)
35	ATP	A	501	36	28,33,33	0.85	0	34,52,52	1.09	6 (17%)
35	ATP	F	501	36	28,33,33	1.20	2 (7%)	34,52,52	1.27	6 (17%)
35	ATP	B	501	36	28,33,33	0.85	1 (3%)	34,52,52	1.26	5 (14%)
35	ATP	D	502	36	28,33,33	0.84	0	34,52,52	1.17	4 (11%)

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
37	ADP	E	401	-	-	4/12/32/32	0/3/3/3
35	ATP	A	501	36	-	3/18/38/38	0/3/3/3
35	ATP	F	501	36	-	4/18/38/38	0/3/3/3
35	ATP	B	501	36	-	3/18/38/38	0/3/3/3
35	ATP	D	502	36	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	501	ATP	PA-O3A	-3.70	1.55	1.59
35	F	501	ATP	PB-O3B	-3.38	1.55	1.59
35	B	501	ATP	PA-O3A	-2.24	1.57	1.59

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	501	ATP	C4'-O4'-C1'	-4.35	105.94	109.92
35	F	501	ATP	C4'-O4'-C1'	-4.27	106.01	109.92
37	E	401	ADP	N3-C2-N1	-4.05	123.18	128.67
35	D	502	ATP	C4'-O4'-C1'	-3.91	106.35	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	501	ATP	C5-C6-N6	2.41	123.98	120.31

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

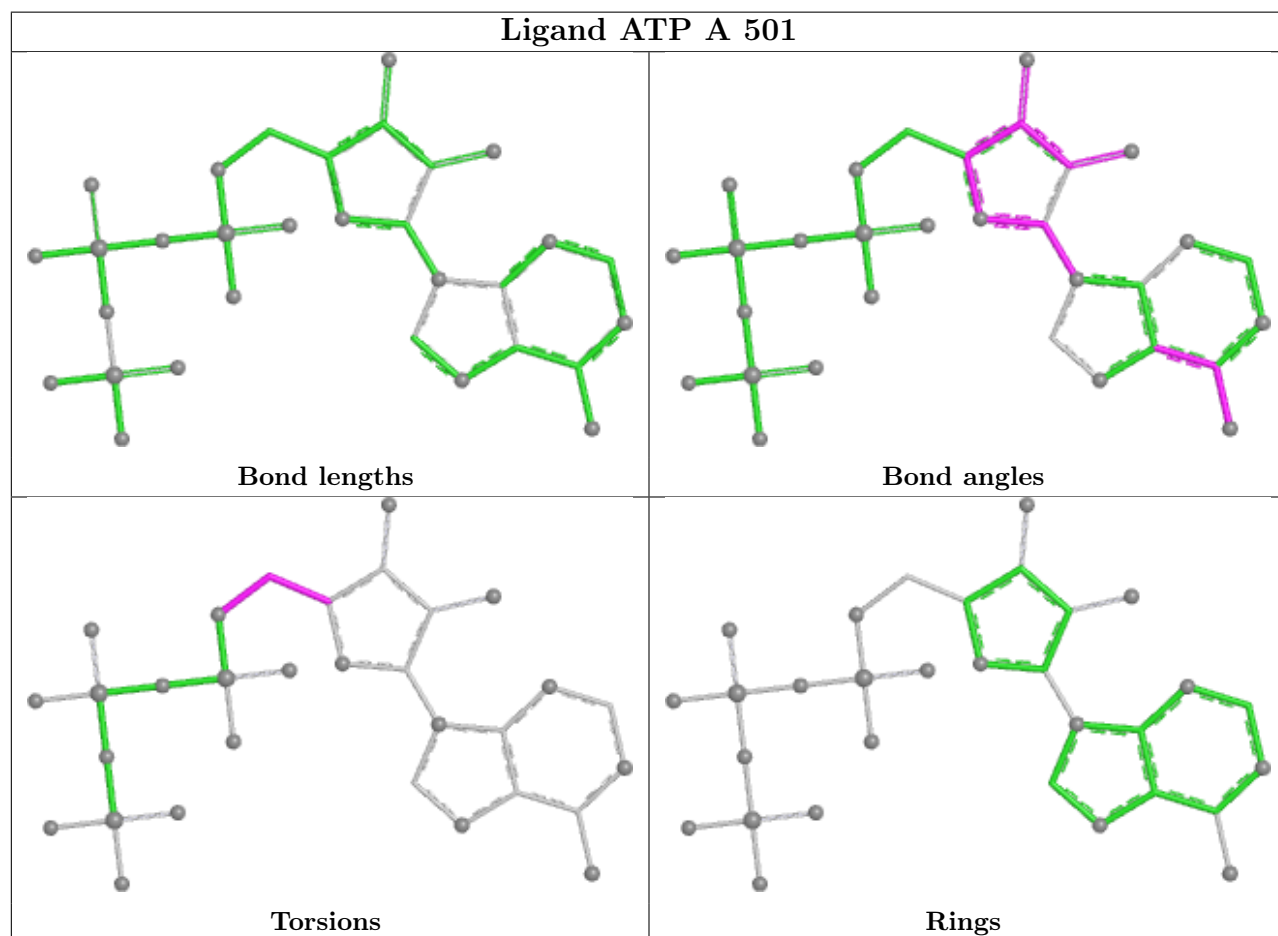
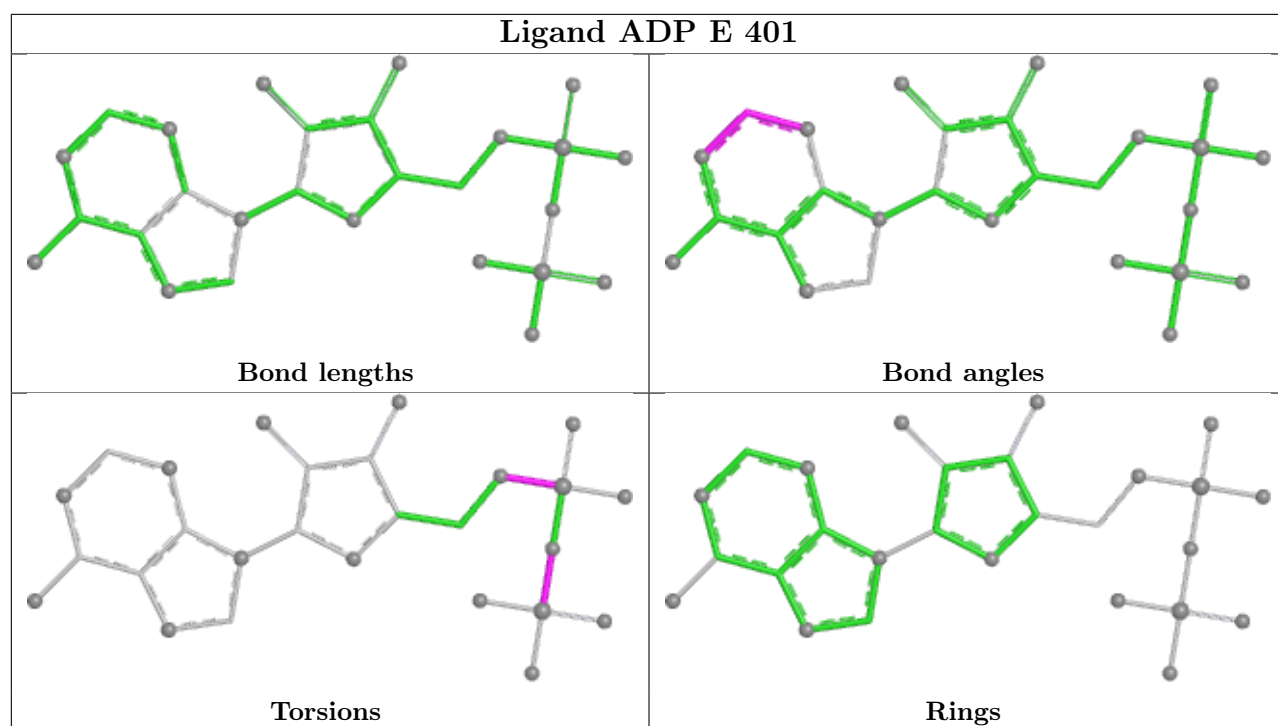
Mol	Chain	Res	Type	Atoms
35	D	502	ATP	C5'-O5'-PA-O1A
35	D	502	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	C5'-O5'-PA-O3A
37	E	401	ADP	PA-O3A-PB-O2B

There are no ring outliers.

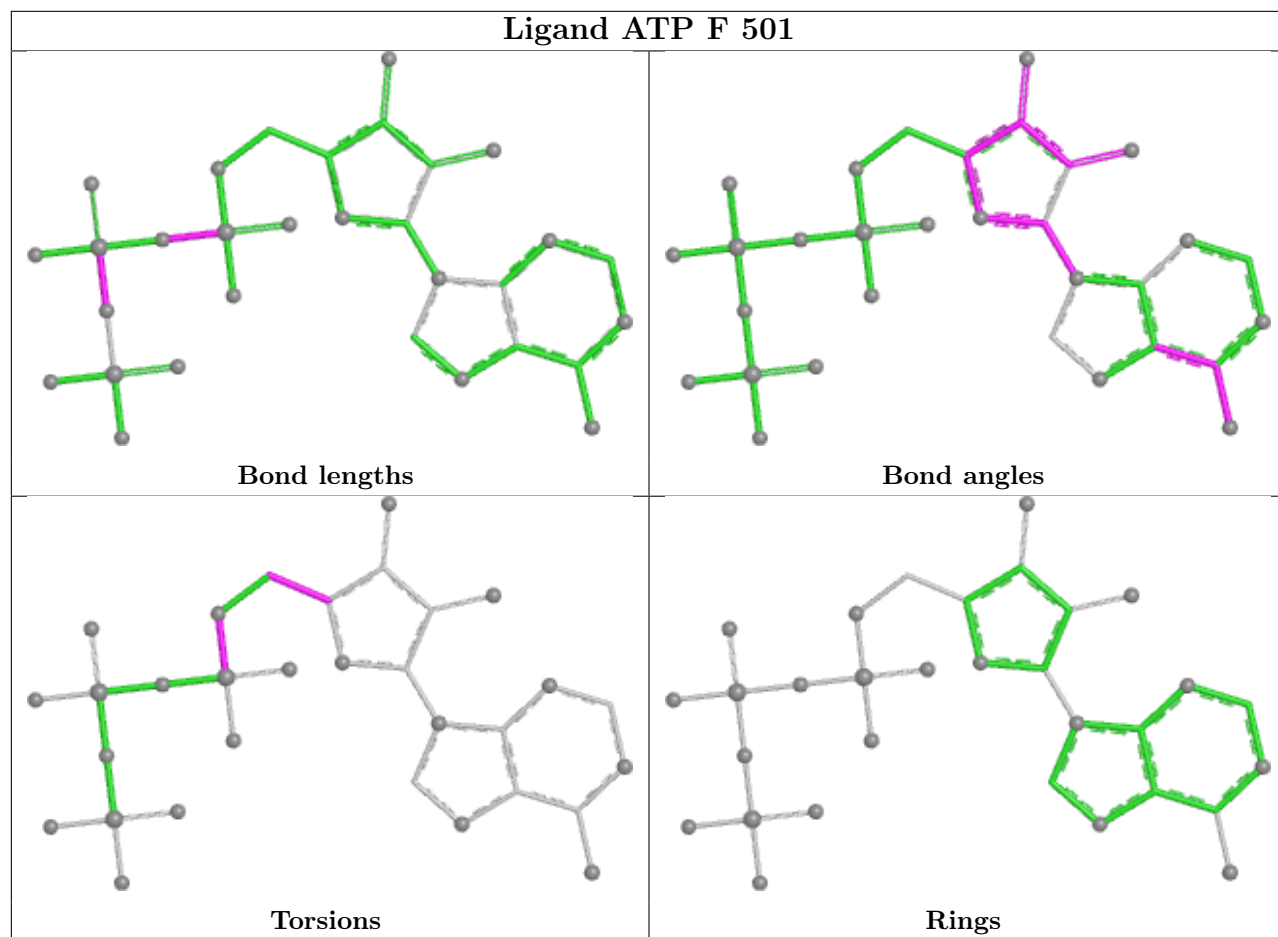
4 monomers are involved in 6 short contacts:

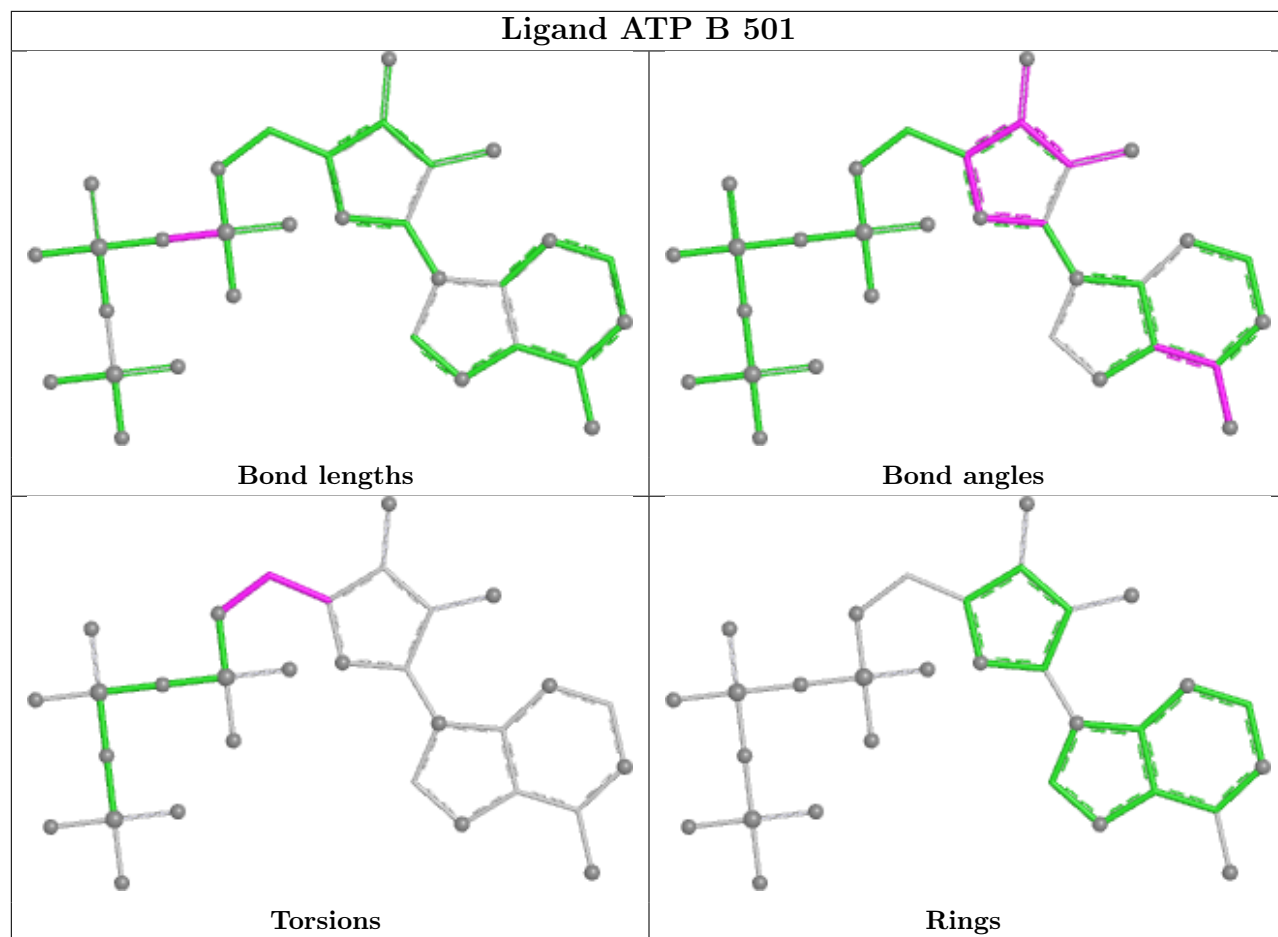
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	401	ADP	1	0
35	A	501	ATP	1	0
35	F	501	ATP	1	0
35	B	501	ATP	3	0

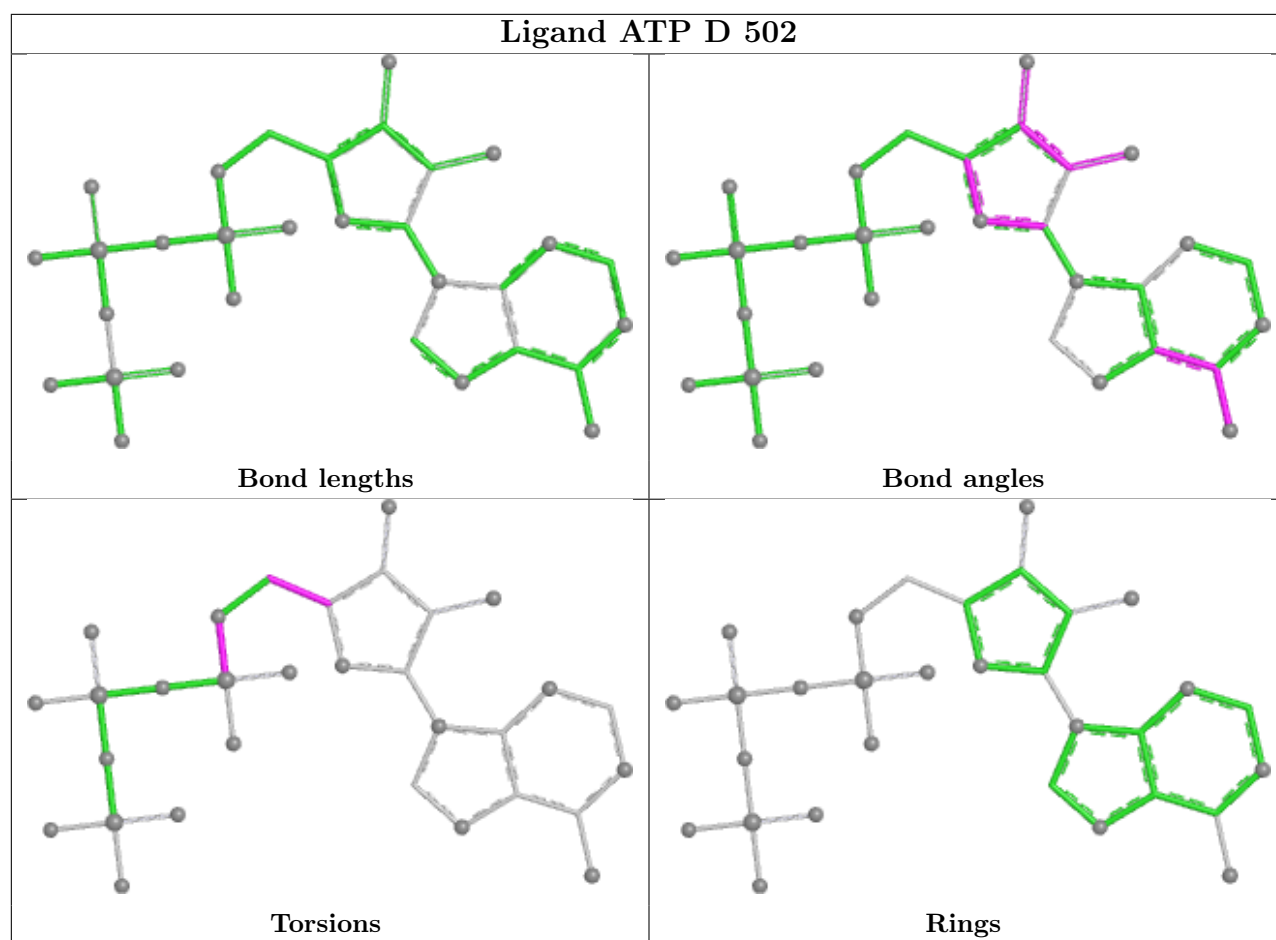
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand ATP F 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

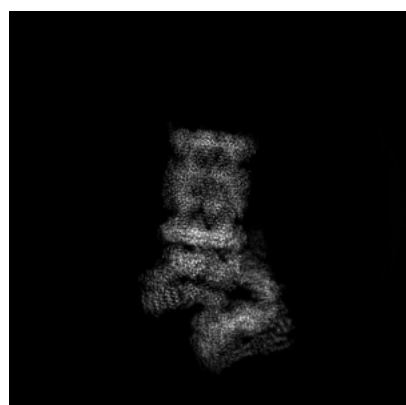
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49509. These allow visual inspection of the internal detail of the map and identification of artifacts.

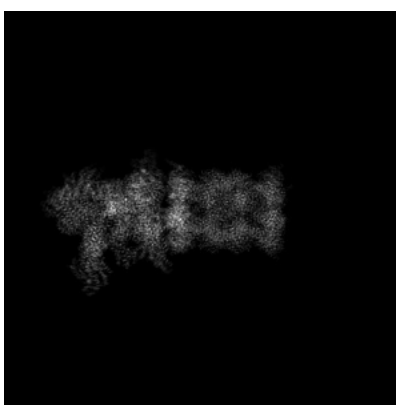
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

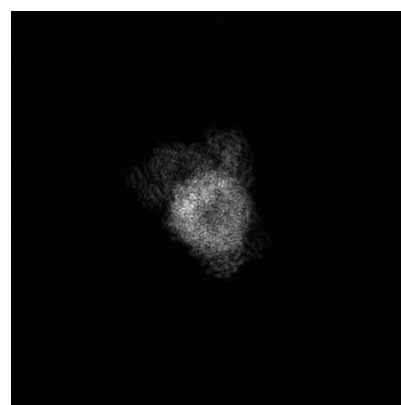
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

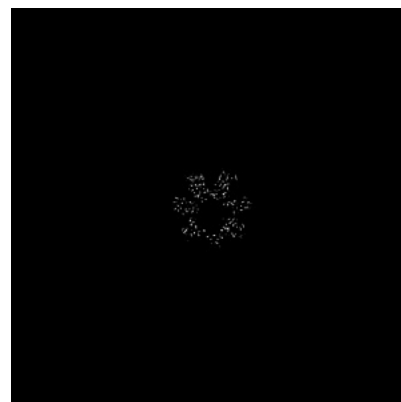
6.2.1 Primary map



X Index: 301



Y Index: 301

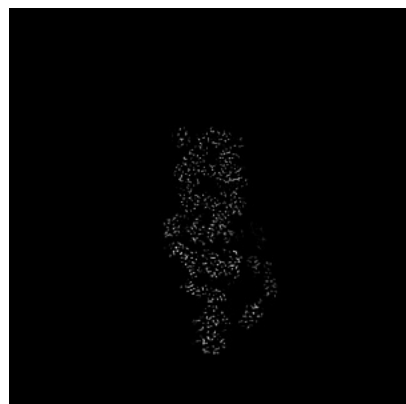


Z Index: 301

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: 273



Y Index: 319

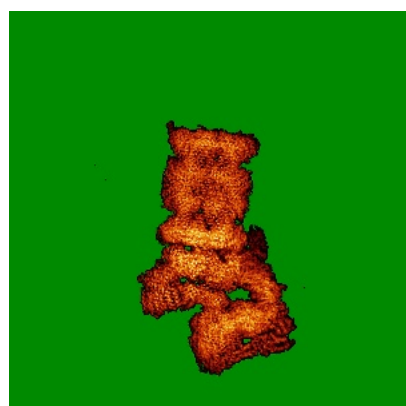


Z Index: 265

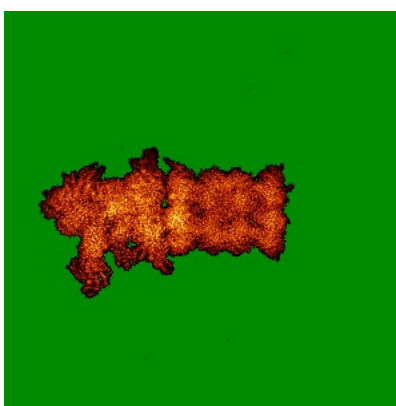
The images above show the largest variance slices of the map in three orthogonal directions.

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

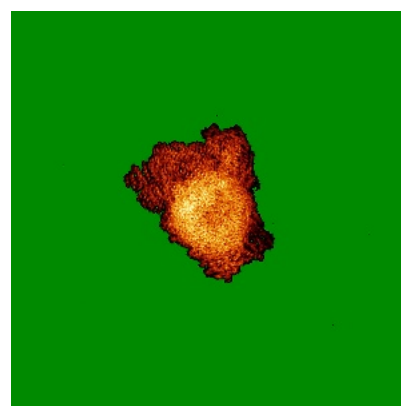
6.4.1 Primary map



X



Y

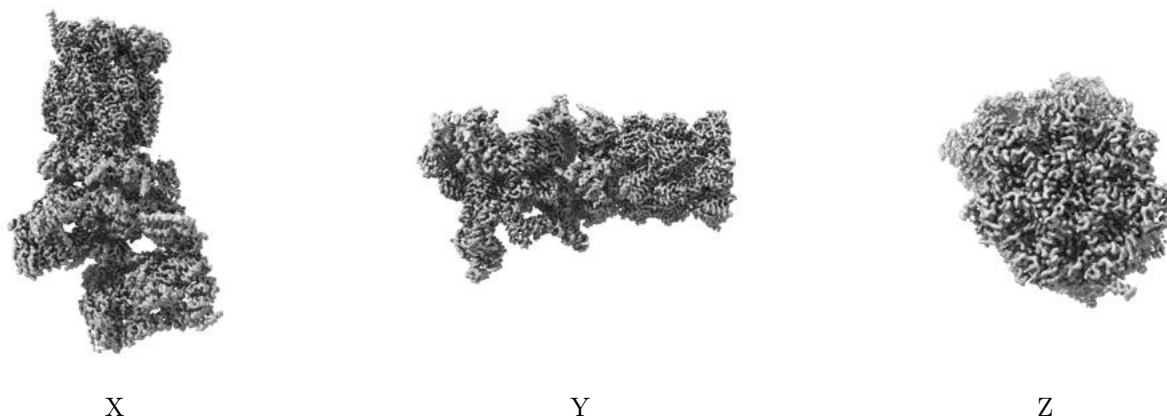


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

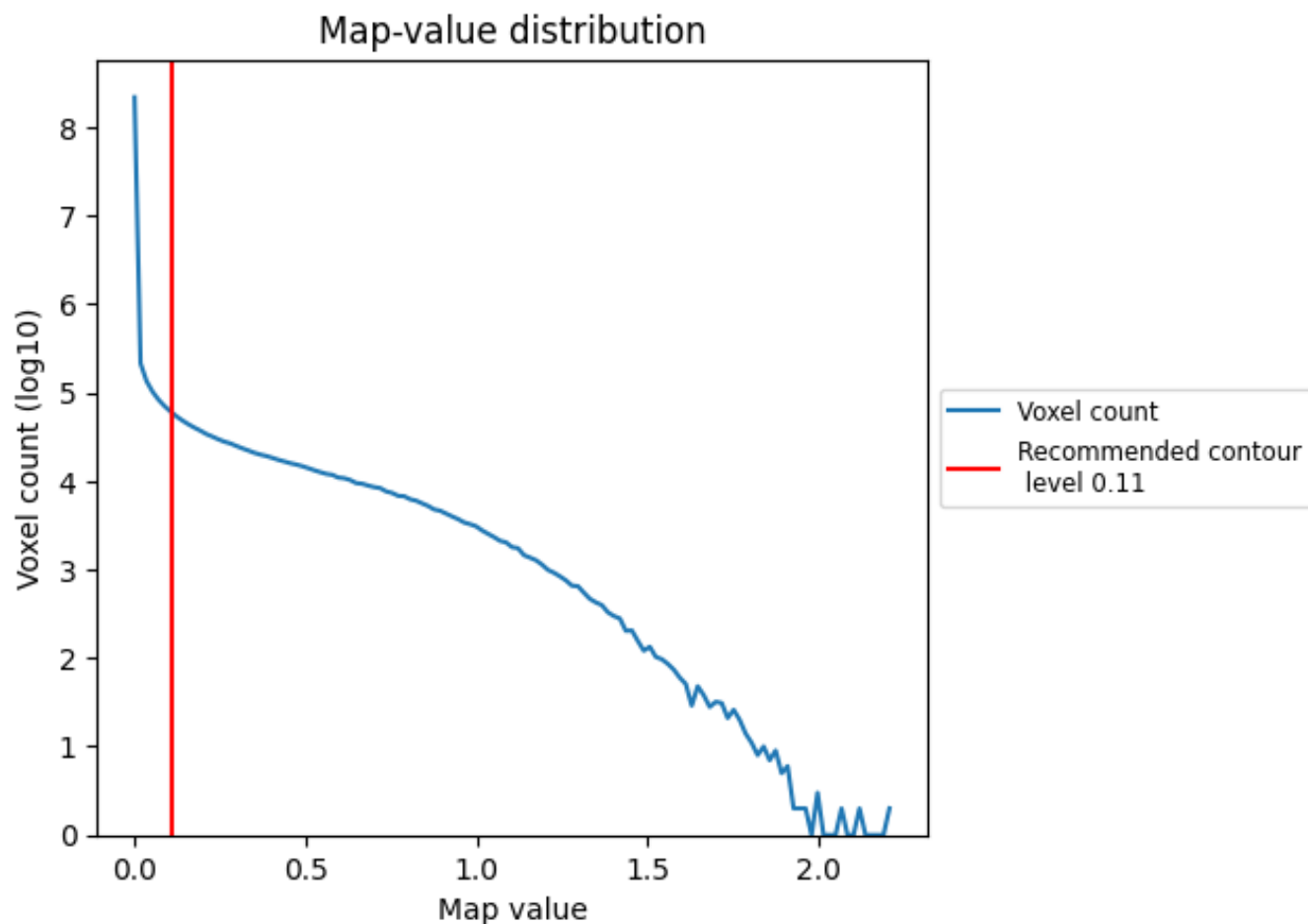
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

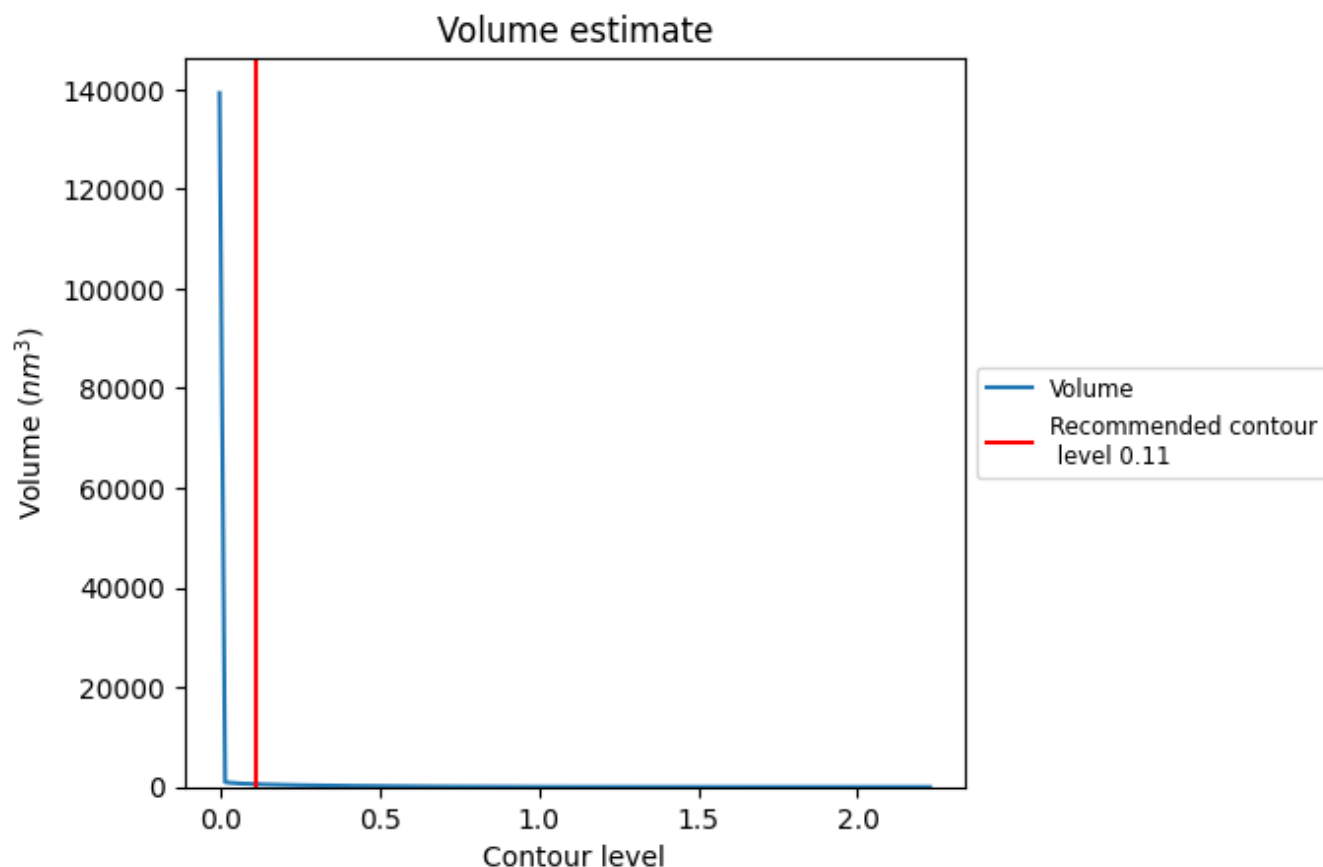
This section contains the results of statistical analysis of the map.

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.

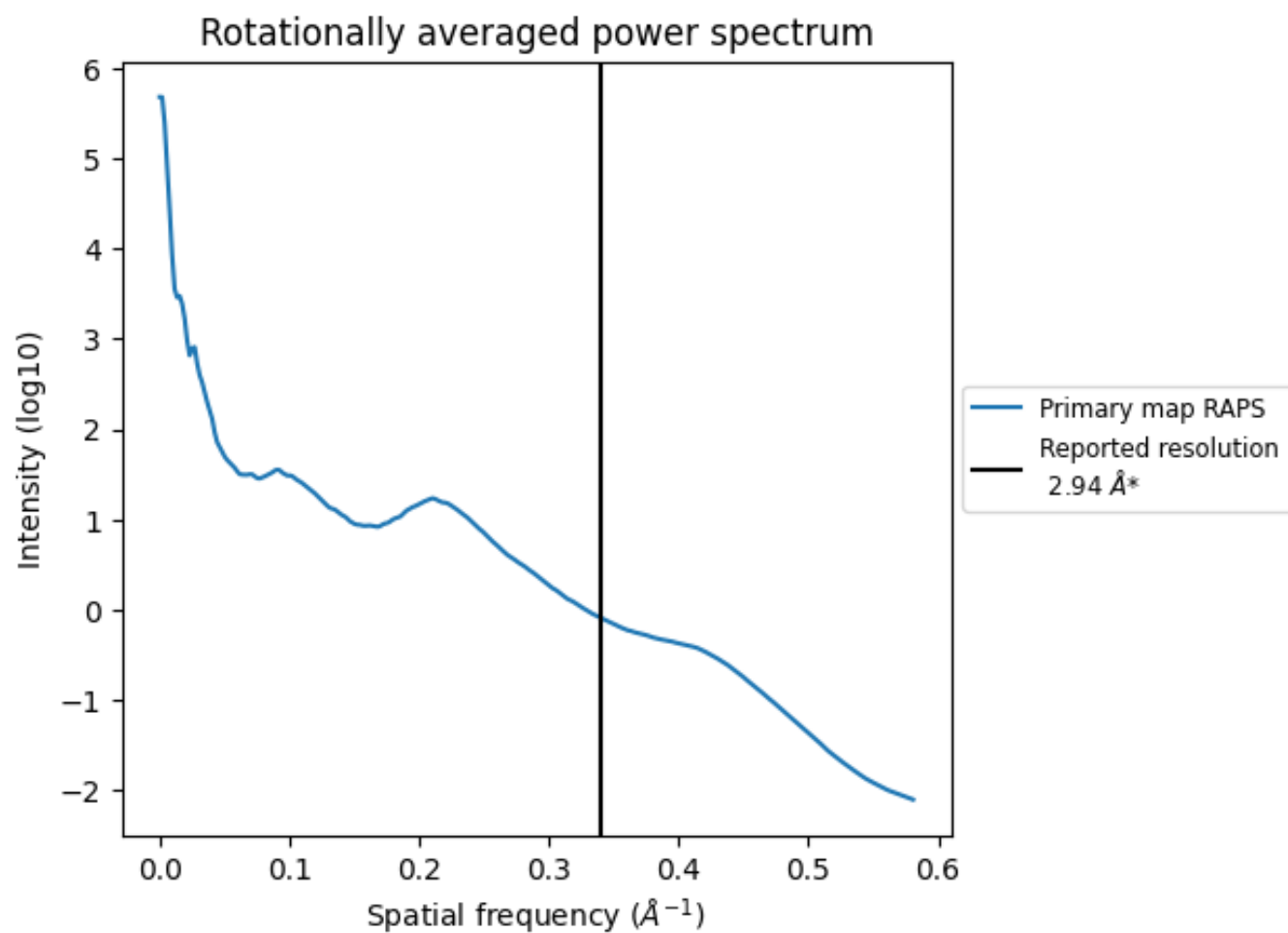
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 569 nm^3 ; this corresponds to an approximate mass of 514 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 0.340 Å⁻¹

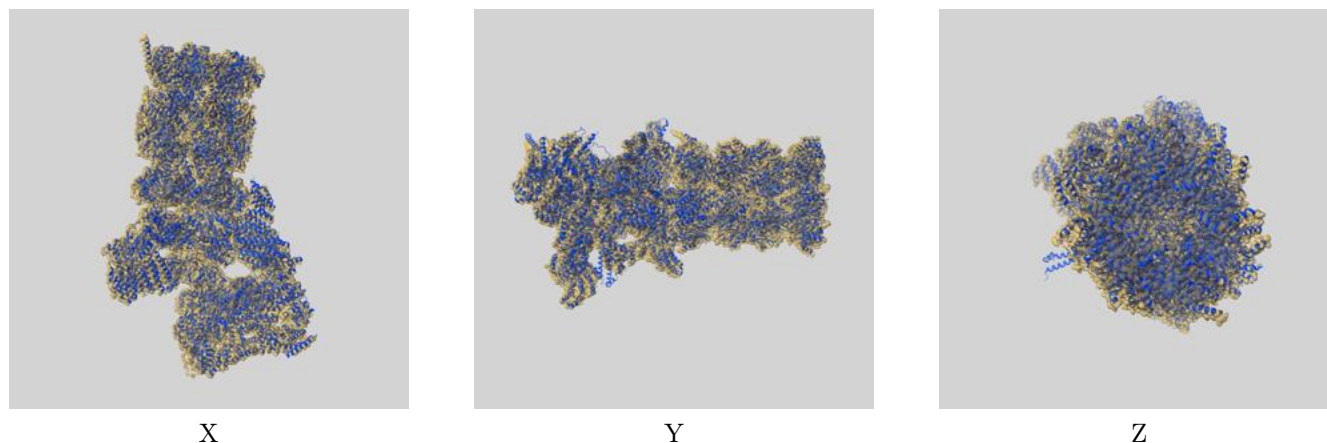
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

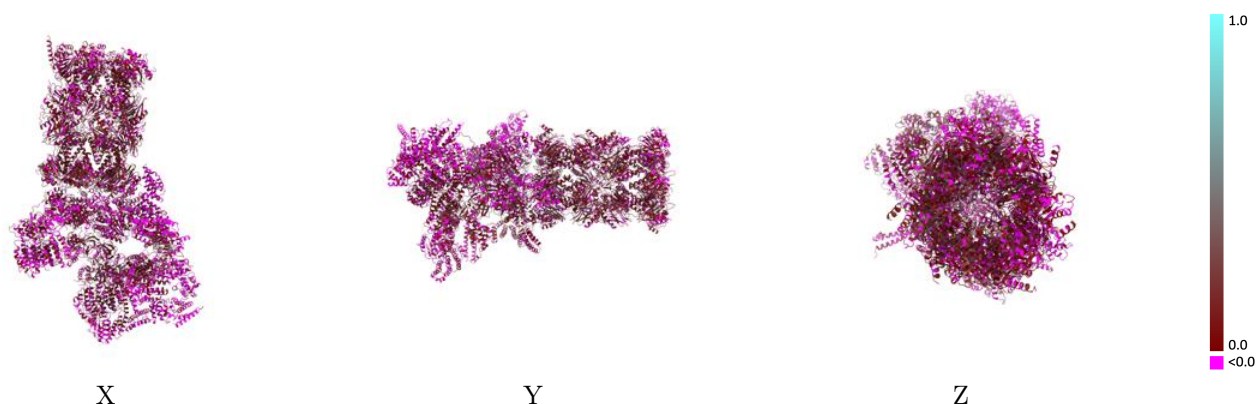
This section contains information regarding the fit between EMDB map EMD-49509 and PDB model 9NKI. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



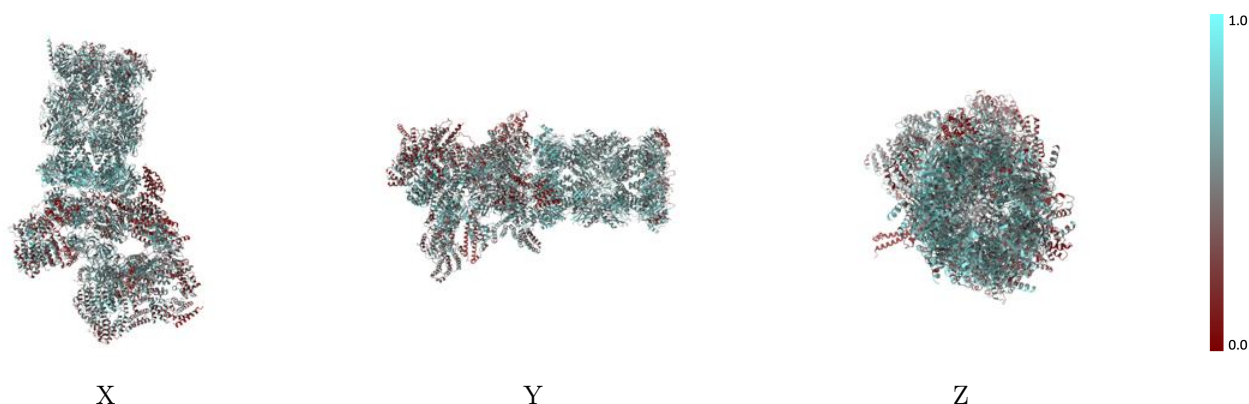
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



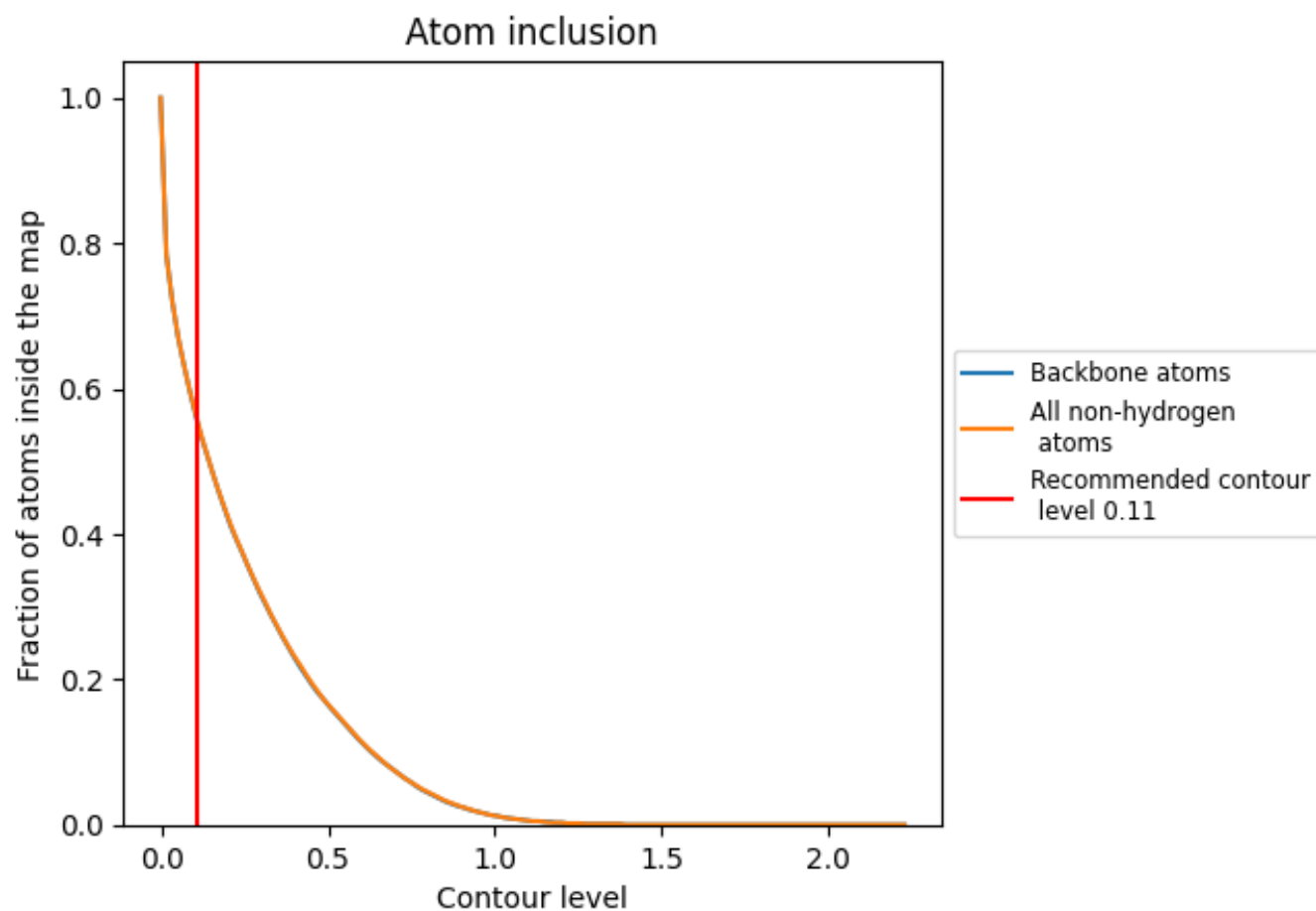
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.1090
A	 0.5720	 0.1290
B	 0.5120	 0.0770
C	 0.4780	 0.0660
D	 0.5940	 0.1290
E	 0.5650	 0.1400
F	 0.5130	 0.1220
G	 0.7030	 0.1770
H	 0.7340	 0.1890
I	 0.6730	 0.1470
J	 0.6880	 0.1260
K	 0.6650	 0.1480
L	 0.7190	 0.1760
M	 0.6970	 0.1680
N	 0.6120	 0.1600
O	 0.6280	 0.1440
P	 0.5850	 0.1260
Q	 0.6000	 0.1180
R	 0.6000	 0.1110
S	 0.5920	 0.1620
T	 0.6210	 0.1430
U	 0.5350	 0.0880
V	 0.4600	 0.0390
W	 0.5510	 0.1450
X	 0.3610	 0.0240
Y	 0.5110	 0.0730
Z	 0.5910	 0.1270
a	 0.5020	 0.0680
b	 0.4300	 0.0320
c	 0.6090	 0.1450
d	 0.3720	 0.0070
e	 0.2950	 0.0400
f	 0.4580	 0.0460
g	 0.5780	 0.1480
h	 0.6190	 0.1490



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Chain	Atom inclusion	Q-score
i	 0.5650	 0.1080
j	 0.5520	 0.0850
k	 0.5120	 0.0800
l	 0.5760	 0.1200
m	 0.6010	 0.1490
n	 0.5970	 0.1310
o	 0.5960	 0.1520
p	 0.6030	 0.1280
q	 0.5900	 0.1070
r	 0.5880	 0.1280
s	 0.5970	 0.1390
t	 0.6210	 0.1730
v	 0.7000	 0.2410
z	 0.4910	 0.0950