



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2023 – 06:59 pm GMT

PDB ID : 7QO5  
EMDB ID : EMD-14084  
Title : 26S proteasome Rpt1-RK -Ubp6-UbVS complex in the si state  
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsasser, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.  
Deposited on : 2021-12-23  
Resolution : 6.00 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](mailto: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>.

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

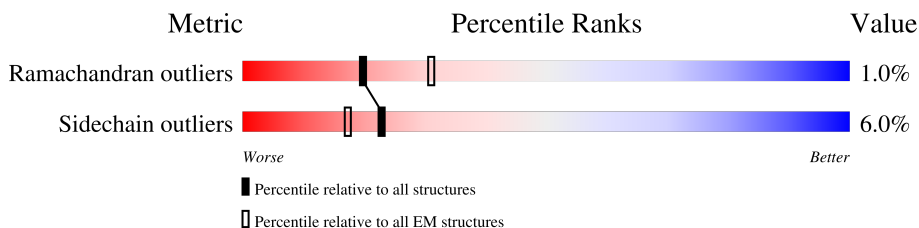
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 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 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	252	11% (upper red bar), 80% (green), 12% (yellow), 7% (orange), 2% (grey)
1	a	252	66% (upper red bar), 81% (green), 12% (yellow), 1% (orange), 2% (grey)
2	B	250	20% (upper red bar), 82% (green), 13% (yellow), 1% (orange), 4% (grey)
2	b	250	80% (green), 82% (green), 13% (yellow), 1% (orange), 5% (grey)
3	C	258	17% (upper red bar), 81% (green), 12% (yellow), 5% (orange), 5% (grey)
3	c	258	64% (upper red bar), 81% (green), 12% (yellow), 5% (orange), 5% (grey)
4	D	254	9% (upper red bar), 86% (green), 5% (yellow), 7% (orange), 1% (grey)
4	d	254	54% (upper red bar), 86% (green), 5% (yellow), 7% (orange), 1% (grey)
5	E	260	13% (upper red bar), 74% (green), 18% (yellow), 6% (orange), 1% (grey)

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Mol	Chain	Length	Quality of chain
5	e	260	62% 73% 17% .. 6%
6	F	234	11% 85% 12% ..
6	f	234	52% 85% 12% ..
7	G	288	12% 71% 11% . 16%
7	g	288	59% 70% 12% . 16%
8	1	215	14% 63% 18% 10% 9%
8	h	215	35% 63% 19% 9% 9%
9	2	261	17% 56% 16% 13% . 13%
9	i	261	54% 60% 16% 10% . 13%
10	3	205	24% 66% 17% 15% .
10	j	205	52% 72% 16% 12%
11	4	198	16% 57% 23% 18% ..
11	k	198	32% 58% 23% 18% ..
12	5	287	13% 48% 13% 12% . 26%
12	l	287	38% 49% 12% 12% . 26%
13	6	241	18% 61% 19% 11% . 8%
13	m	241	46% 57% 20% 14% . 8%
14	7	266	14% 81% 5% 14%
14	n	266	33% 82% . 14%
15	W	268	15% 69% .. 26%
16	V	306	16% 90% .. 6%
17	T	274	28% 93% ...
18	X	156	65% 77% .. 19%
19	Y	89	61% 93% 6% .
20	Z	993	48% 84% 5% . 9%

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Mol	Chain	Length	Quality of chain
21	N	945	15% 84% 12%
22	S	523	20% 84% 6% 9%
23	P	445	5% 95% ..
24	Q	434	15% 95% ..
25	R	429	15% 90% 5% 6%
26	U	338	14% 81% .. 14%
27	O	393	9% 96% ...
28	H	467	27% 75% 7% 16%
29	I	437	31% 79% 7% 12%
30	K	428	29% 85% 5% 8%
31	L	437	19% 80% 7% 11%
32	M	434	28% 87% 7% ..
33	J	405	32% 94% ..
34	8	499	46% 68% 5% 25%
35	9	76	66% 93% 5% .

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 112834 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		
5	E	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	289	2274	1425	389	446	14	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	266	2192	1405	349	432	6	0	0

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	127	1032	664	169	195	4	0	0

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Y	89	731	447	119	164	1	0	0

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Z	906	7005	4416	1150	1409	30	0	0

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	832	6418	4078	1077	1238	25	0	0

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	475	3894	2488	653	738	15	0	0

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	440	3608	2297	604	697	10	0	0

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	434	3499	2225	577	681	16	0	0

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	405	3258	2077	535	636	10	0	0

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	290	2306	1454	392	453	7	0	0

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	O	388	3186	2051	519	608	8	0	0

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	H	391	3064	1927	551	569	17	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ARG	SER	variant	UNP P33299
H	166	LYS	THR	variant	UNP P33299

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	I	384	3015	1895	507	596	17	0	0

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	K	394	3113	1951	548	604	10	0	0

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	L	388	3082	1942	548	580	12	0	0

- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	M	421	3285	2043	573	656	13	0	0

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	J	405	3171	1995	565	593	18	0	0

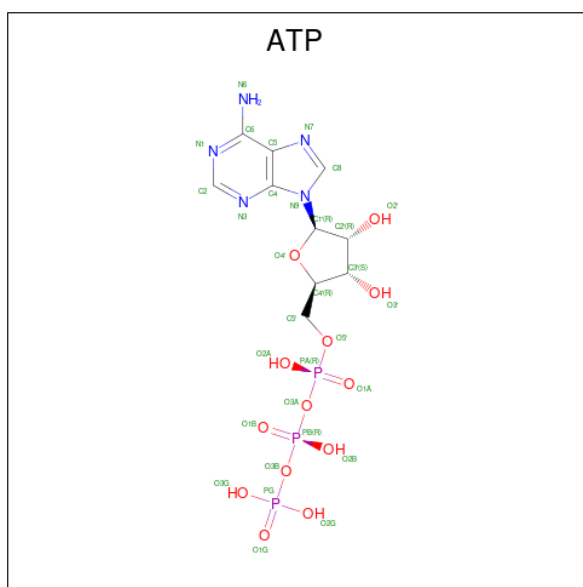
- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	8	372	3034	1918	521	583	12	0	0

- Molecule 35 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	9	76	601	378	105	117	1	0	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



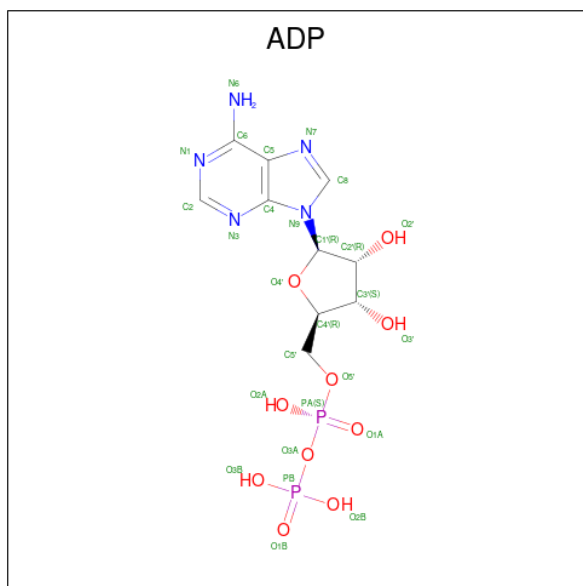
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	H	1	Total	Mg	0
			1	1	
37	I	1	Total	Mg	0
			1	1	
37	K	1	Total	Mg	0
			1	1	
37	L	1	Total	Mg	0
			1	1	
37	M	1	Total	Mg	0
			1	1	
37	J	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$ ).

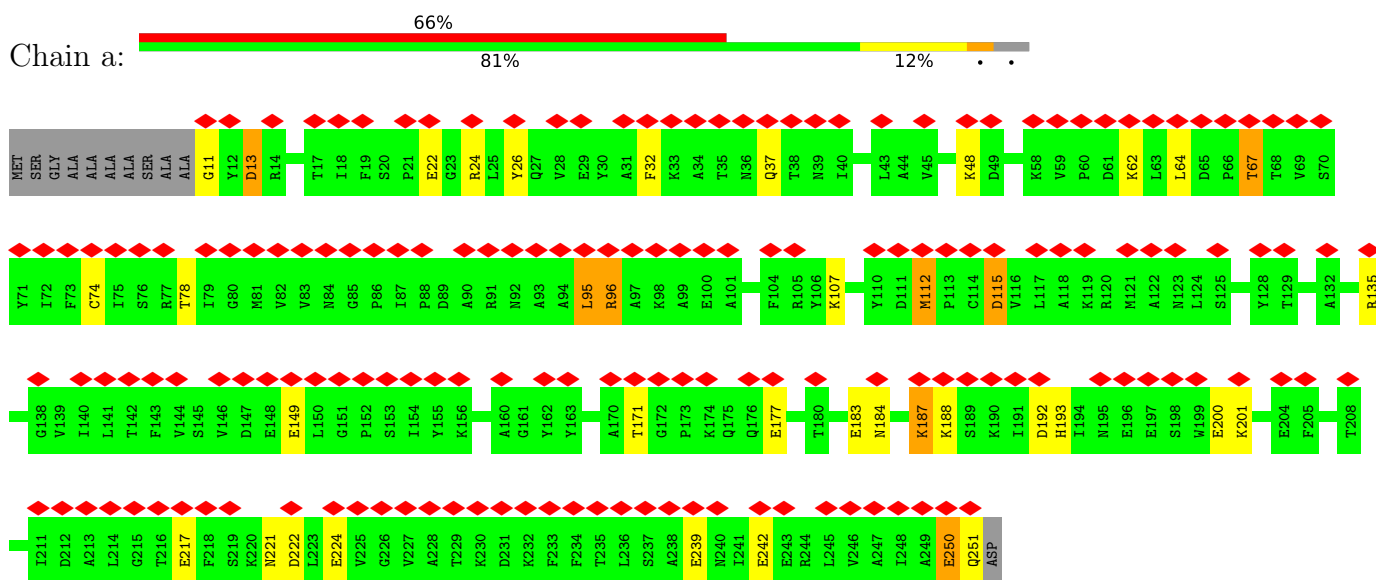


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
38	J	1	27	10	5	10	2	0

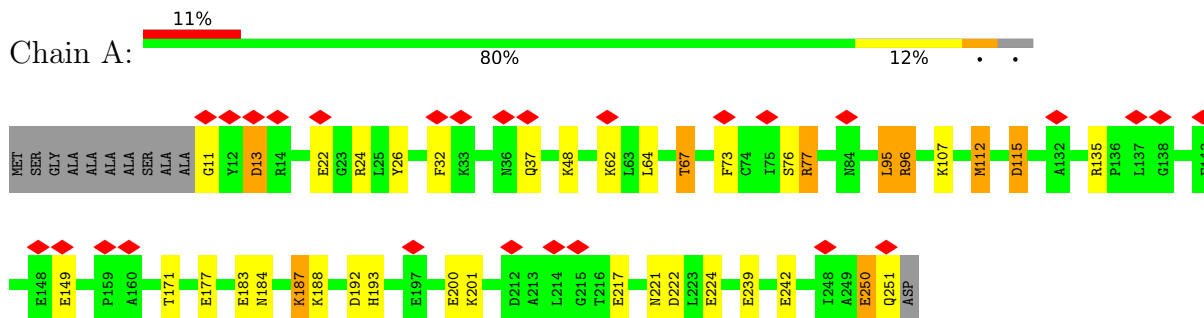
### 3 Residue-property plots [i](#)

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

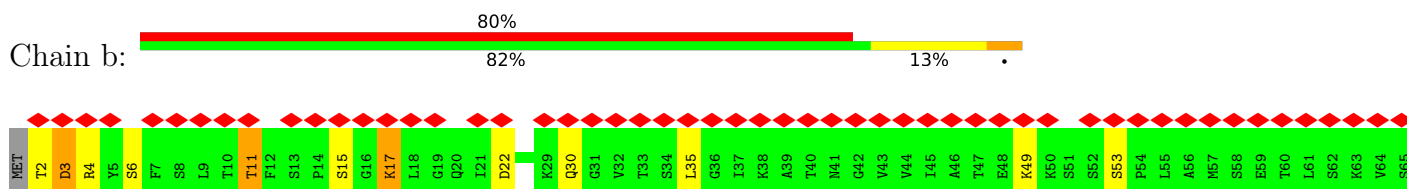
- Molecule 1: Proteasome subunit alpha type-1

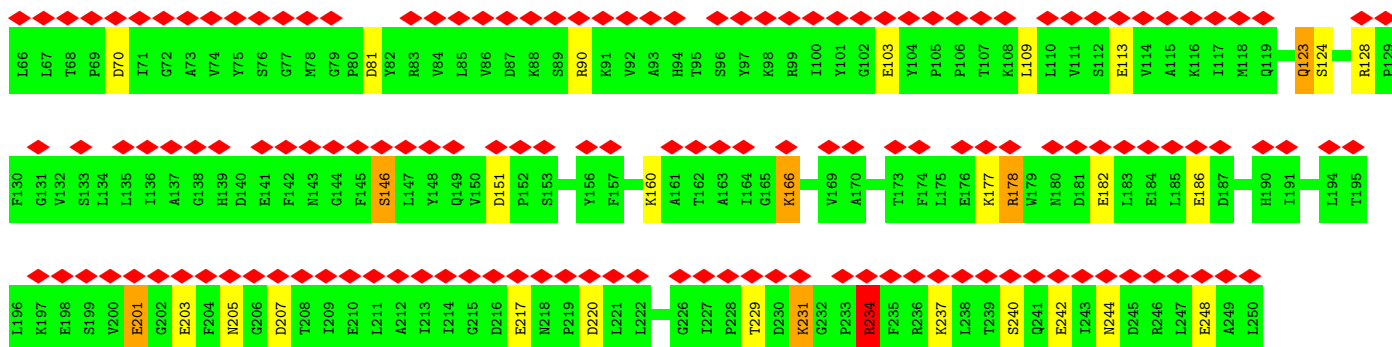


- Molecule 1: Proteasome subunit alpha type-1

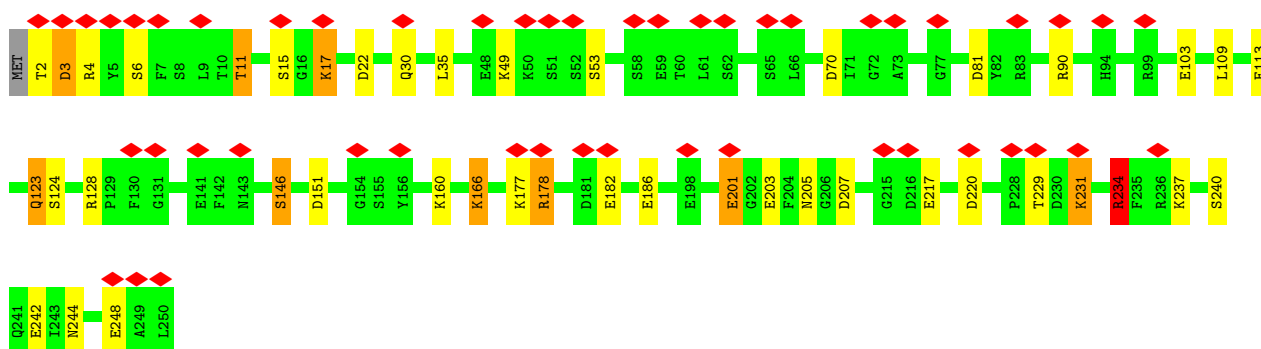
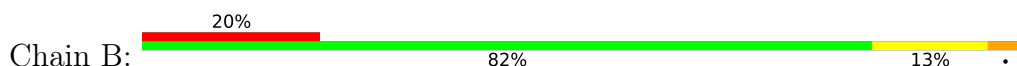


- Molecule 2: Proteasome subunit alpha type-2

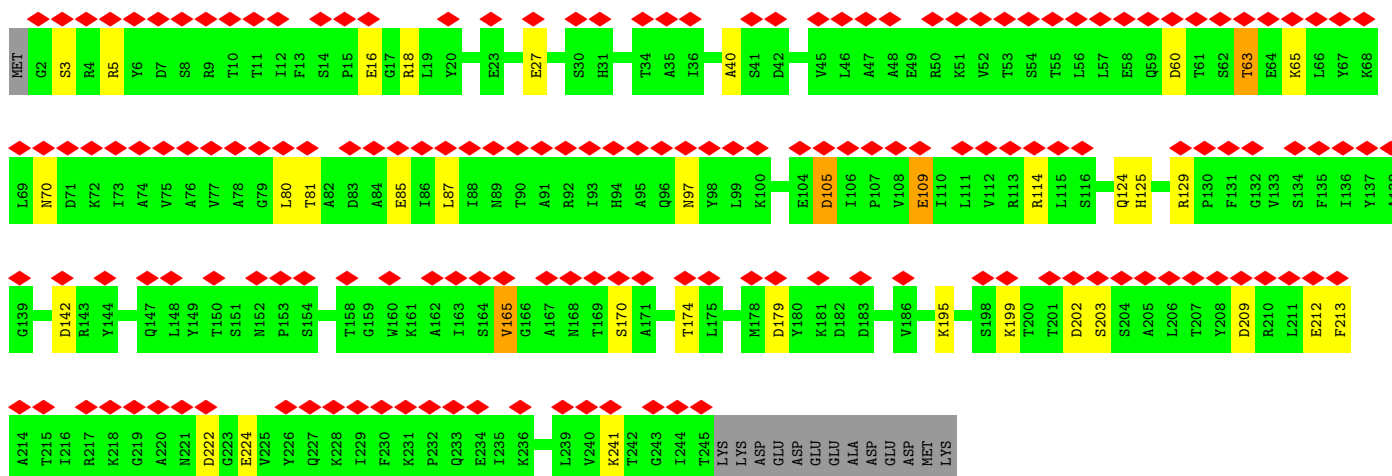
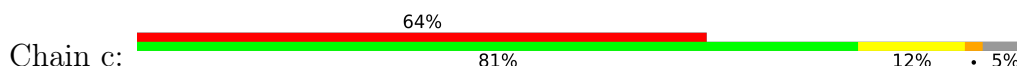




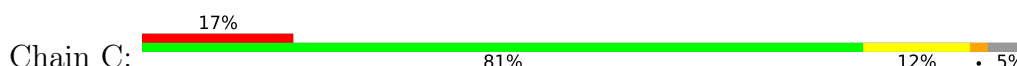
• Molecule 2: Proteasome subunit alpha type-2

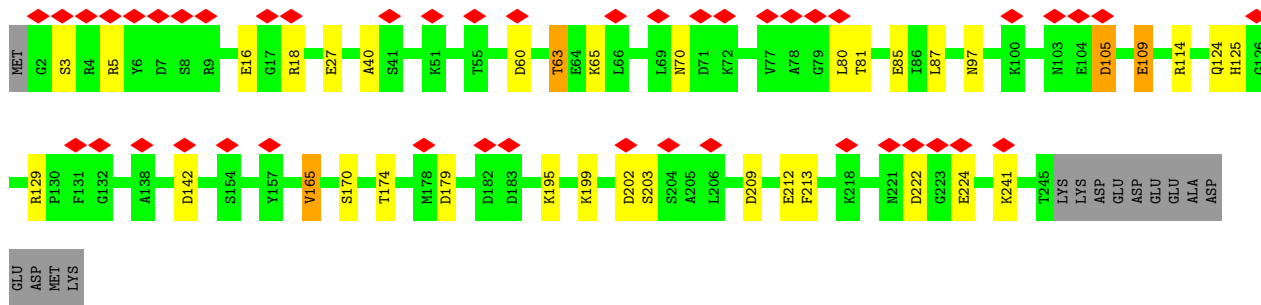


• Molecule 3: Proteasome subunit alpha type-3

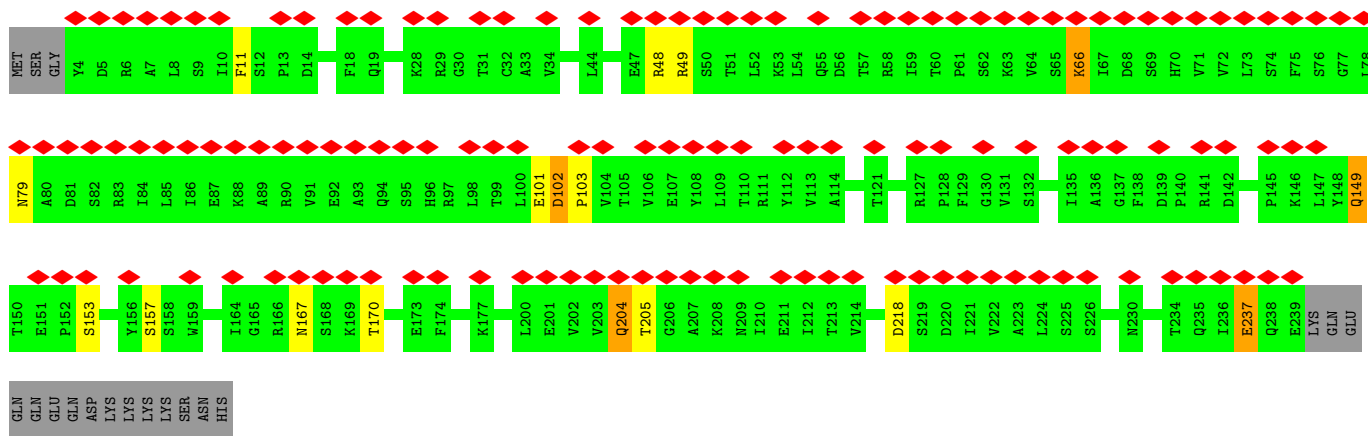
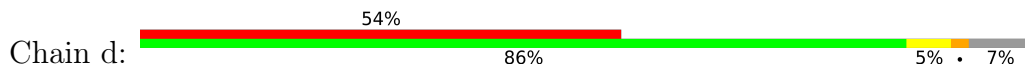


• Molecule 3: Proteasome subunit alpha type-3

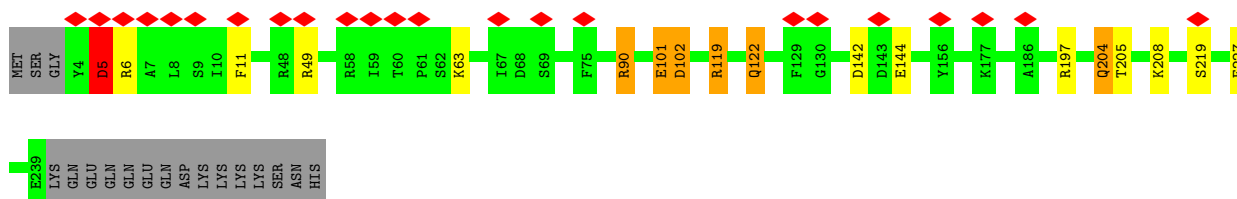
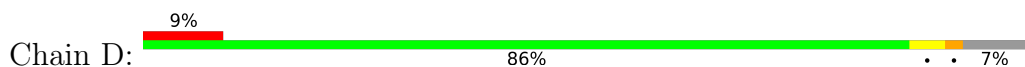




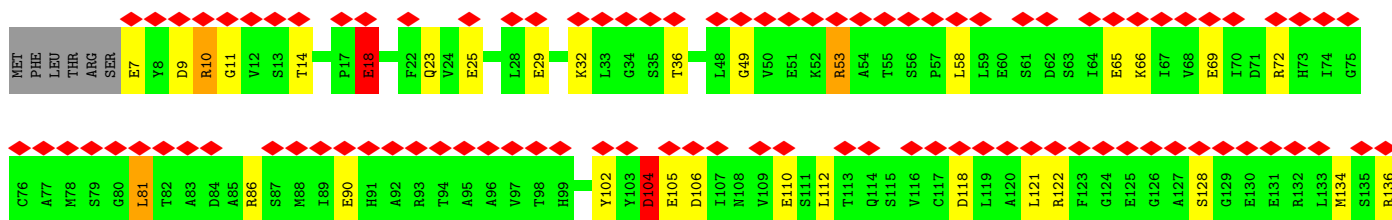
• Molecule 4: Proteasome subunit alpha type-4

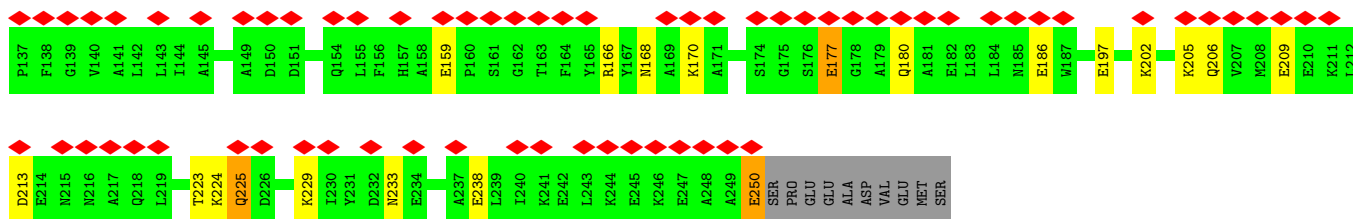


• Molecule 4: Proteasome subunit alpha type-4

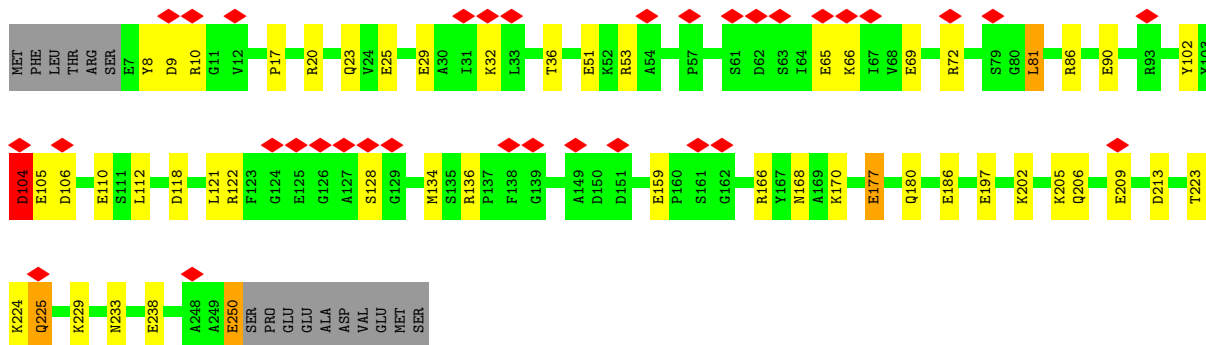
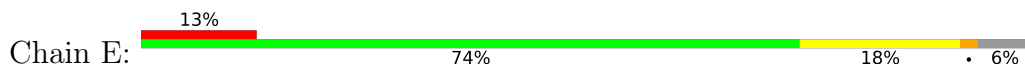


• Molecule 5: Proteasome subunit alpha type-5

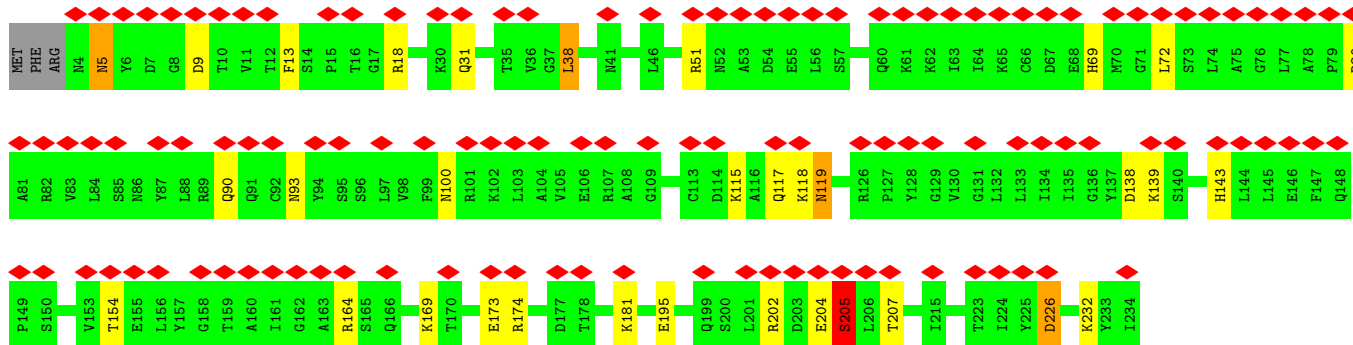
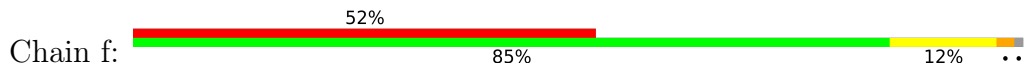




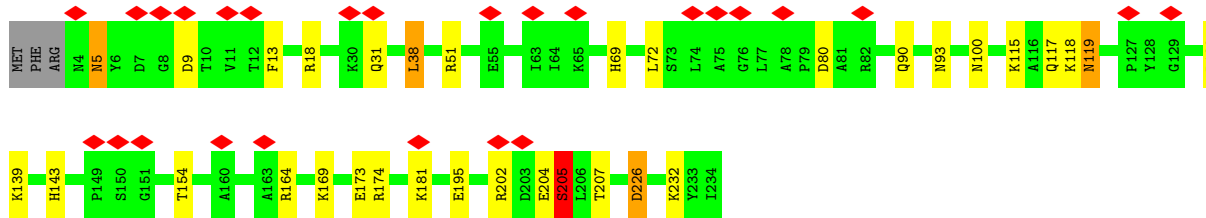
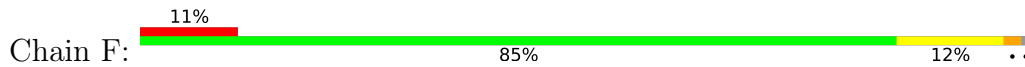
• Molecule 5: Proteasome subunit alpha type-5



• Molecule 6: Proteasome subunit alpha type-6



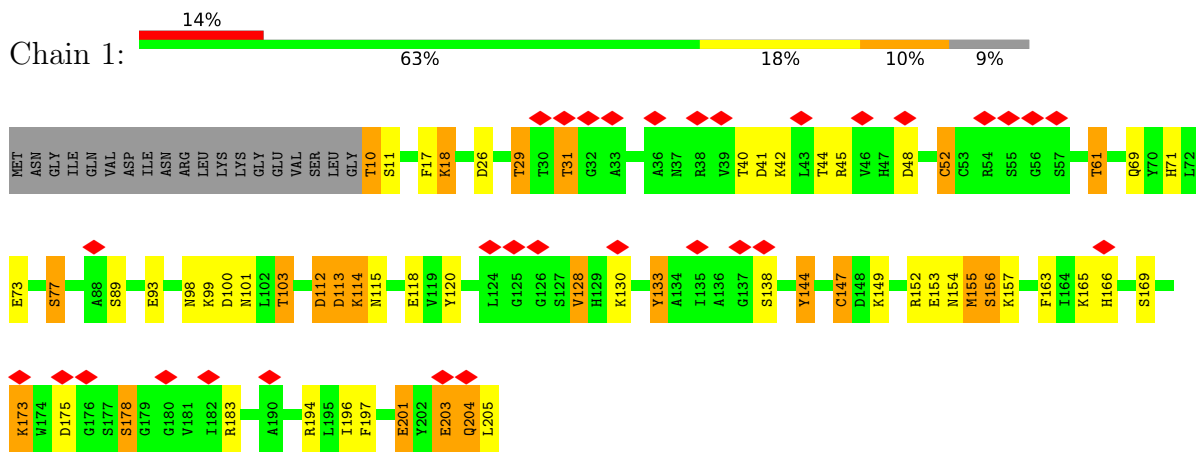
• Molecule 6: Proteasome subunit alpha type-6



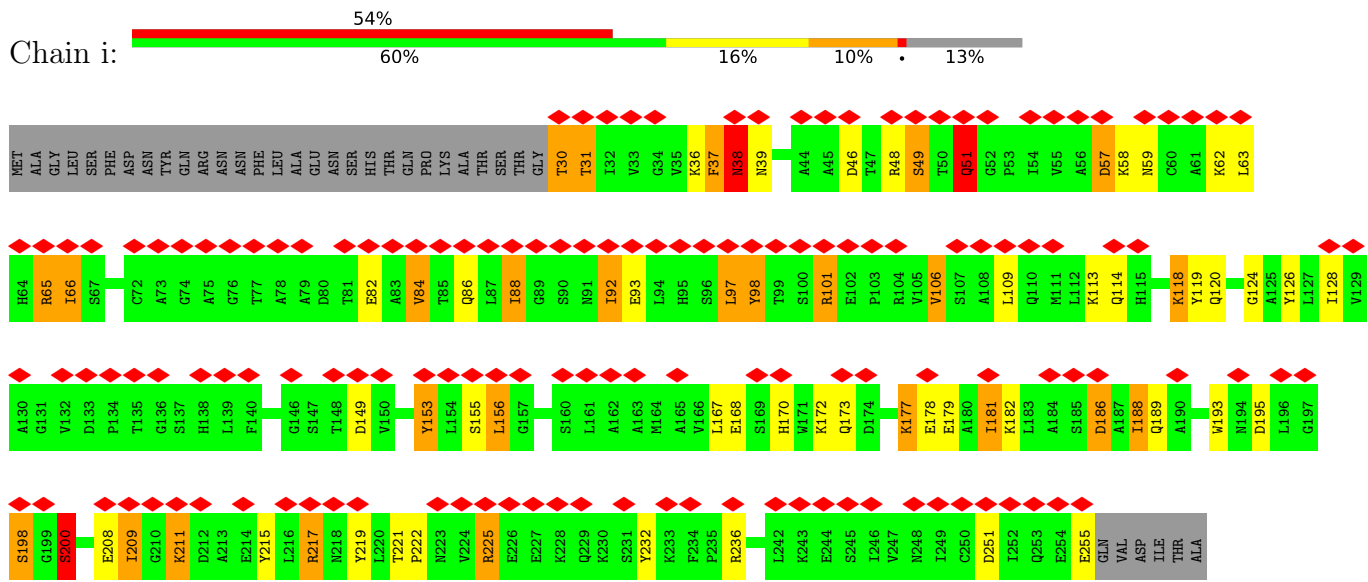
• Molecule 7: Probable proteasome subunit alpha type-7



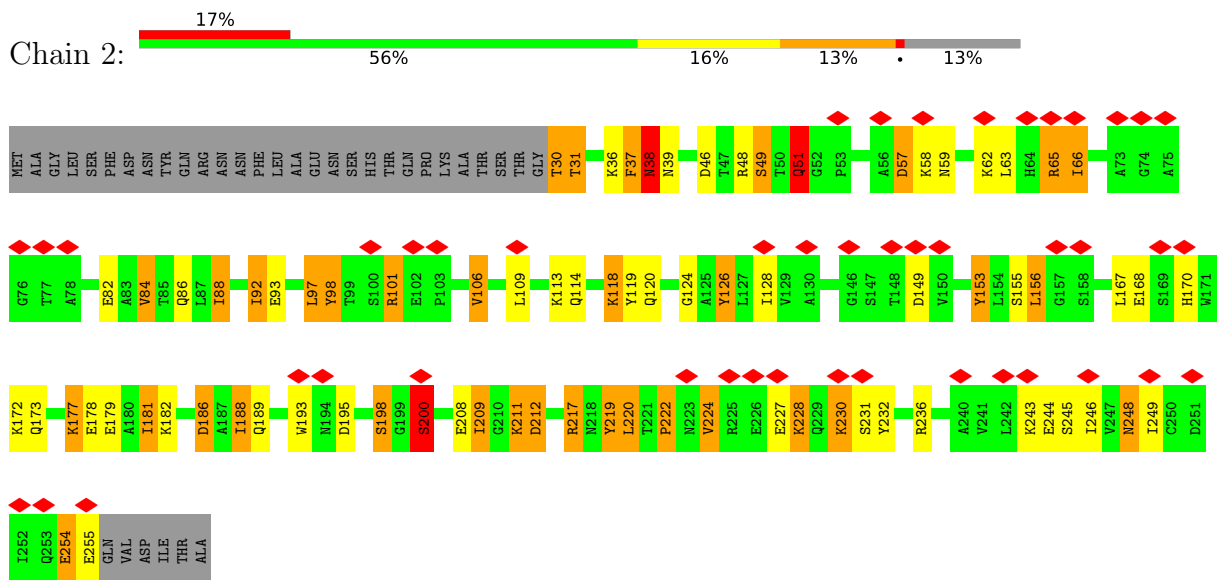




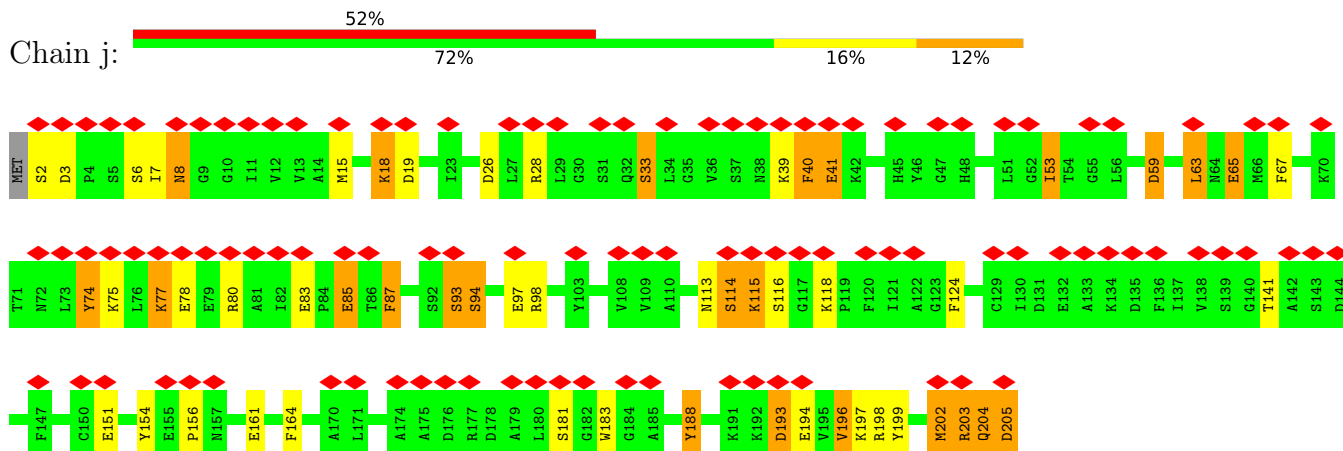
• Molecule 9: Proteasome subunit beta type-2



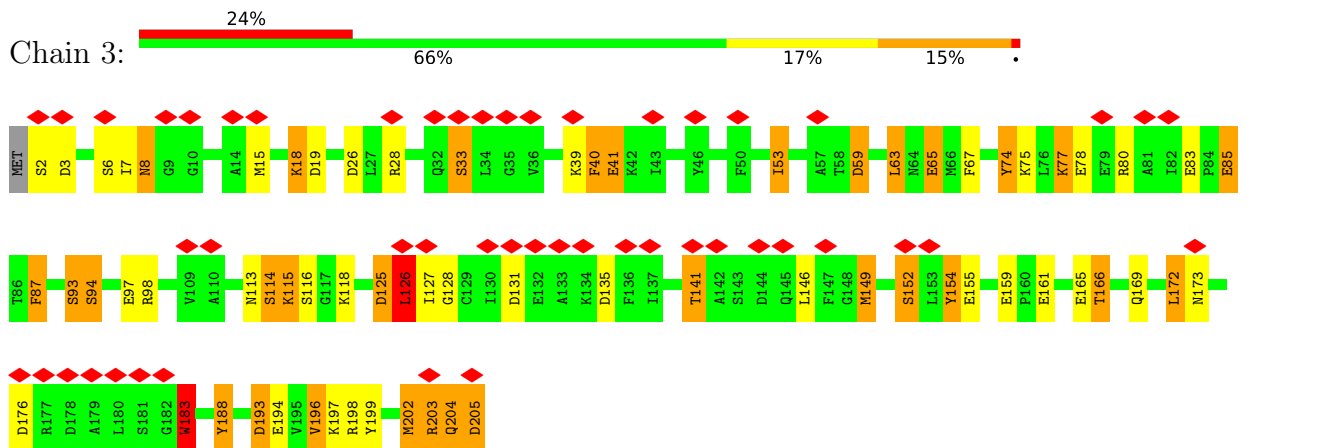
• Molecule 9: Proteasome subunit beta type-2



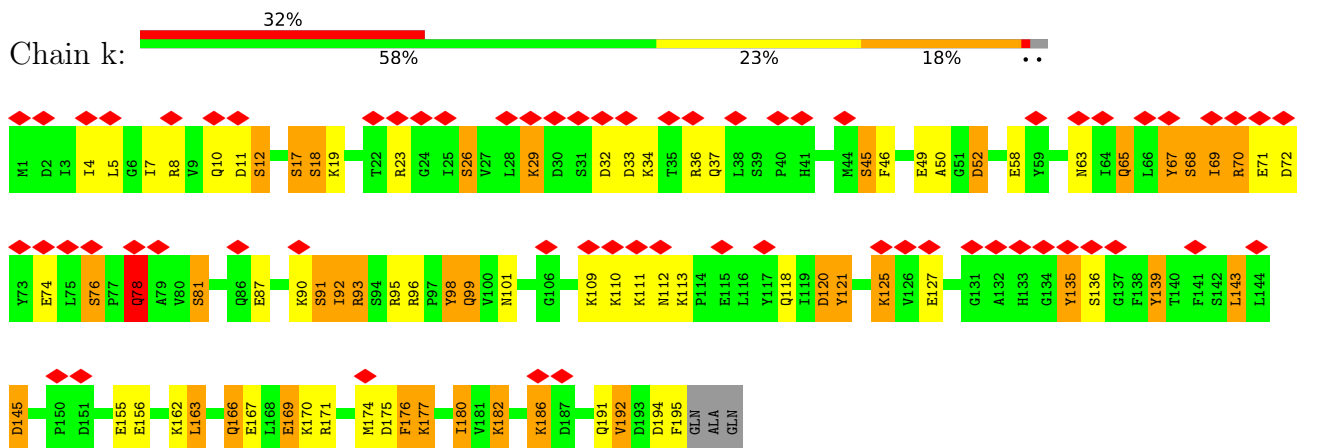
• Molecule 10: Proteasome subunit beta type-3



• Molecule 10: Proteasome subunit beta type-3

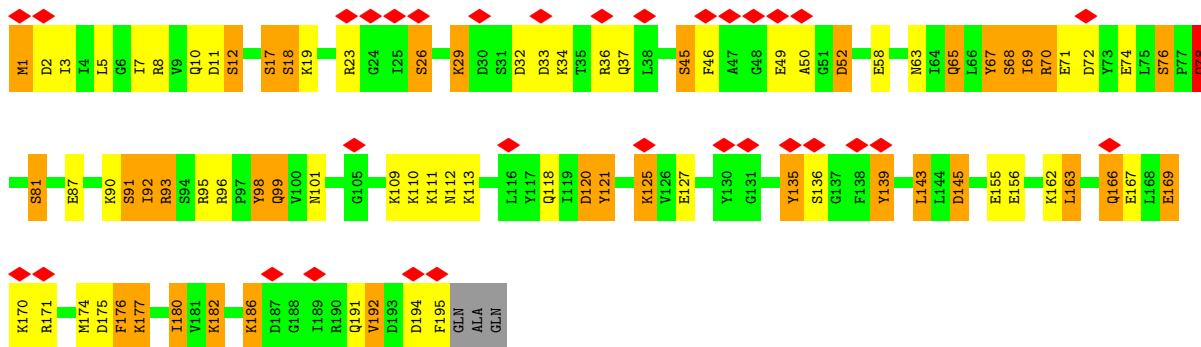


• Molecule 11: Proteasome subunit beta type-4

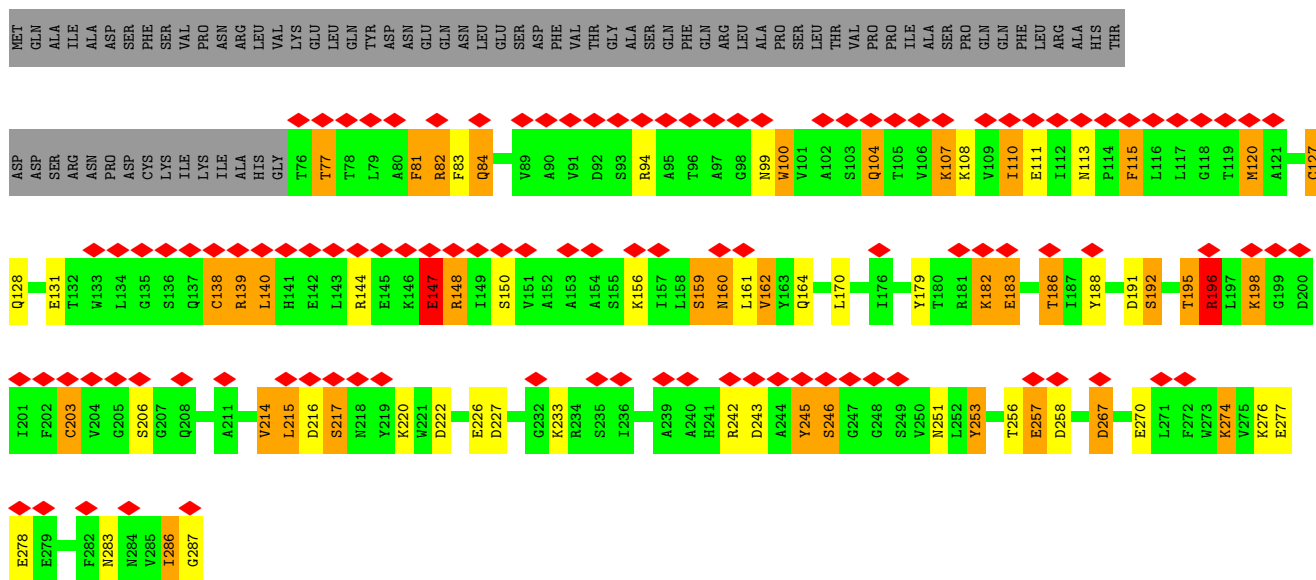


• Molecule 11: Proteasome subunit beta type-4

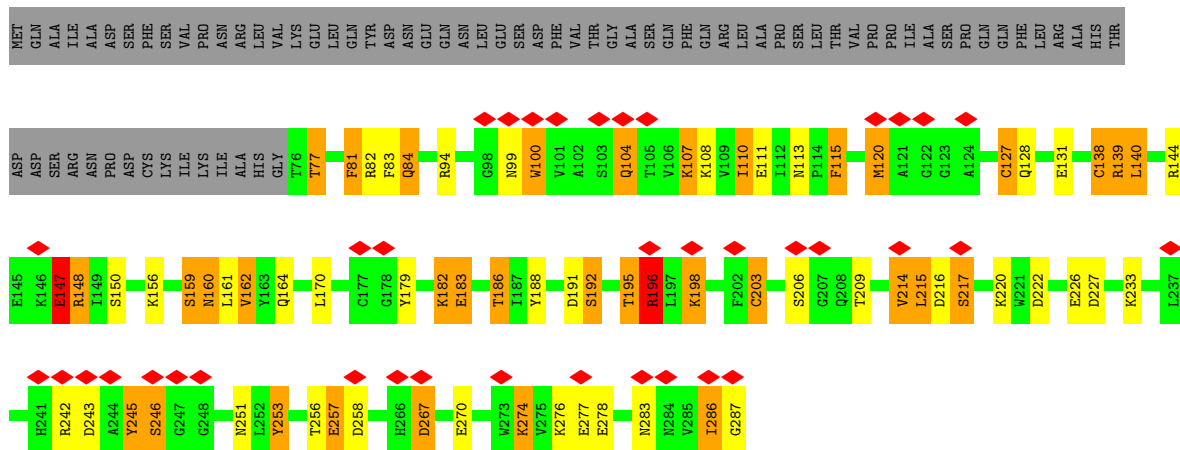




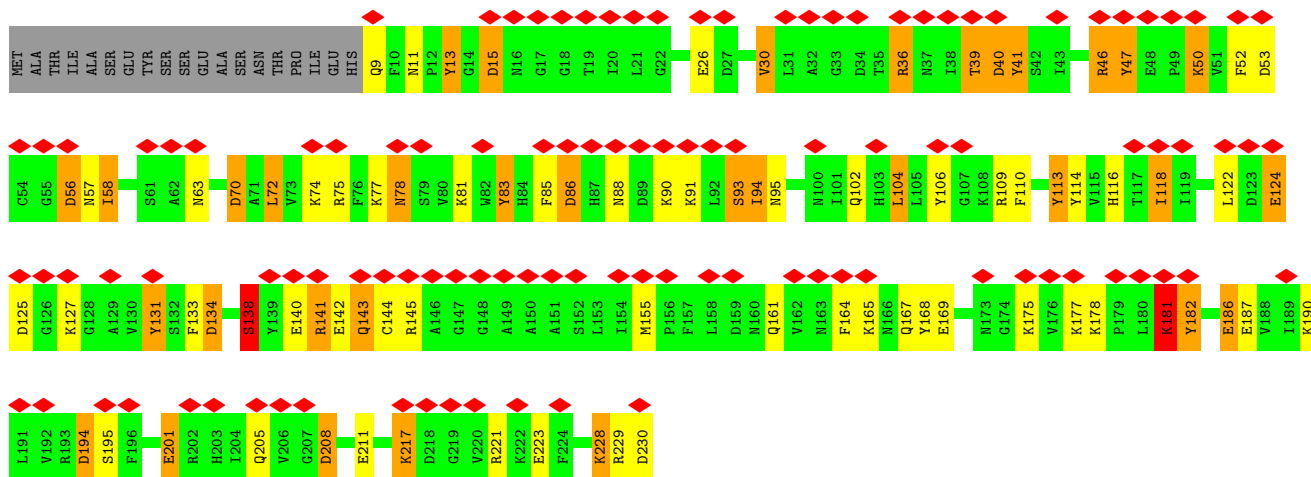
• Molecule 12: Proteasome subunit beta type-5



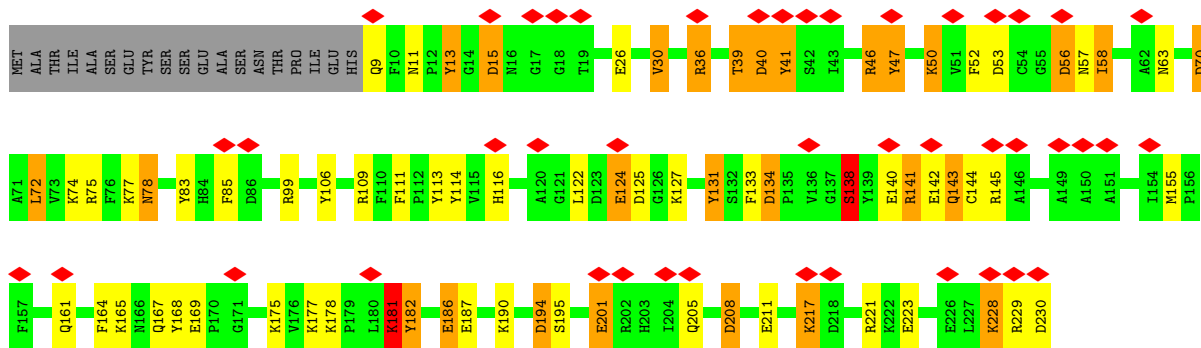
• Molecule 12: Proteasome subunit beta type-5



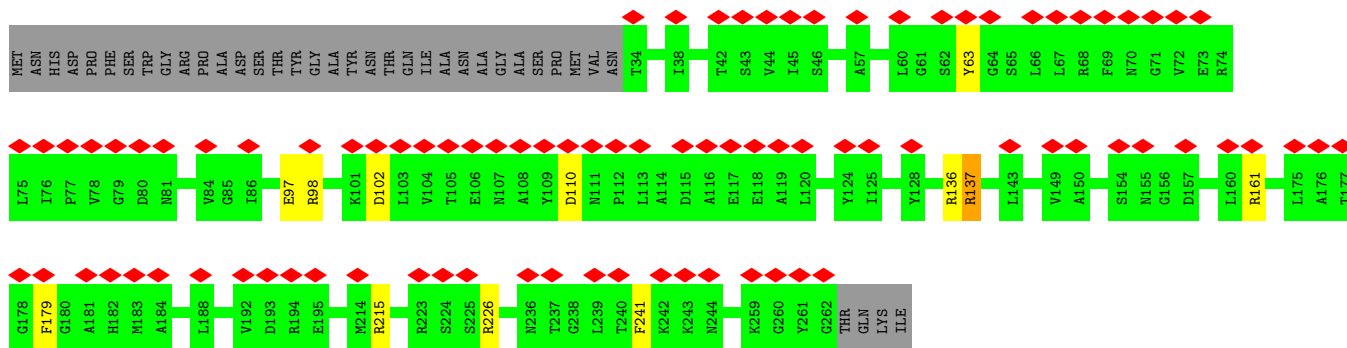
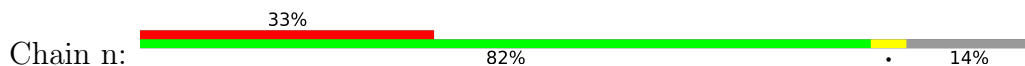
• Molecule 13: Proteasome subunit beta type-6



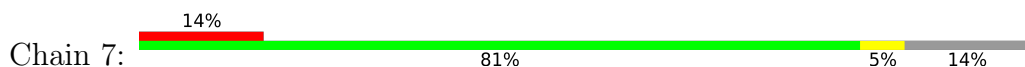
• Molecule 13: Proteasome subunit beta type-6

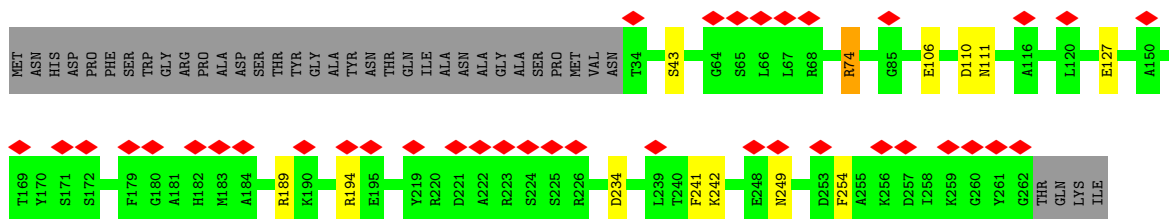


• Molecule 14: Proteasome subunit beta type-7

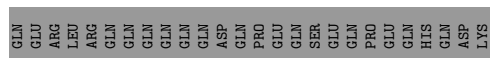
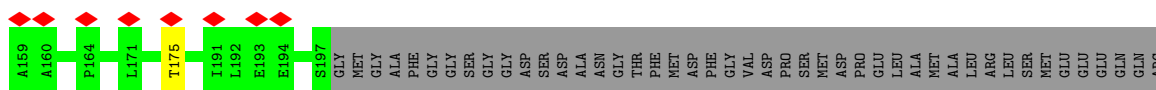
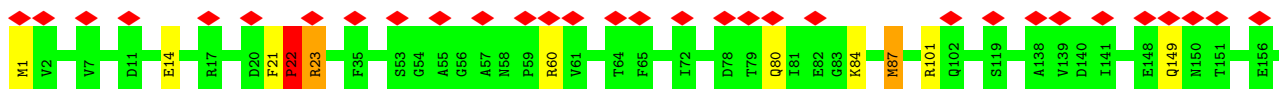


• Molecule 14: Proteasome subunit beta type-7

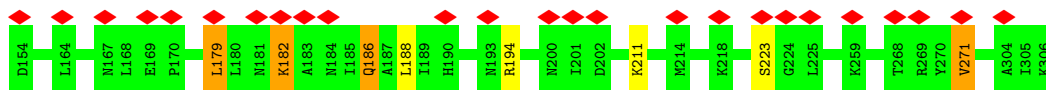
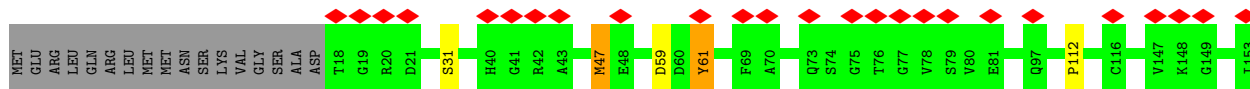
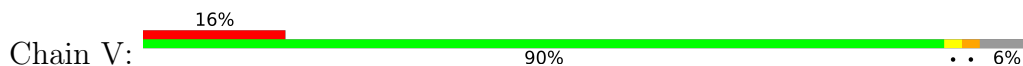




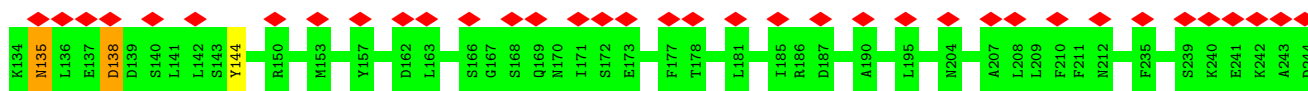
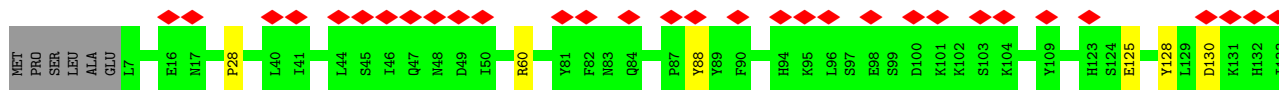
• Molecule 15: 26S proteasome regulatory subunit RPN10



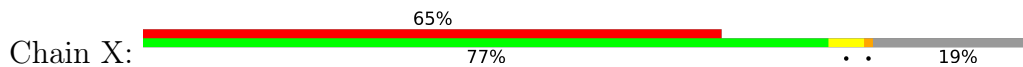
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

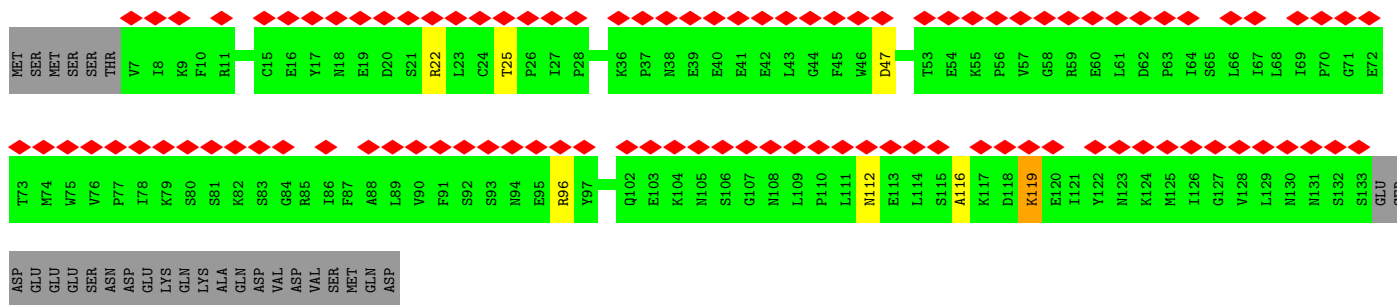


• Molecule 17: 26S proteasome regulatory subunit RPN12

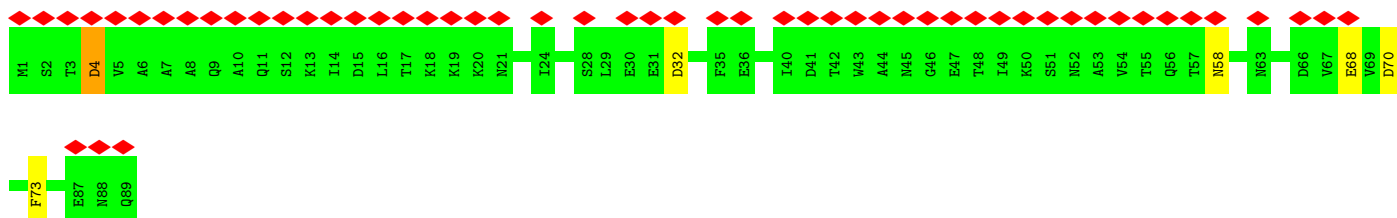
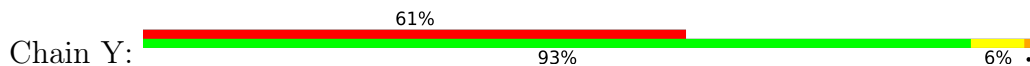


• Molecule 18: 26S proteasome regulatory subunit RPN13

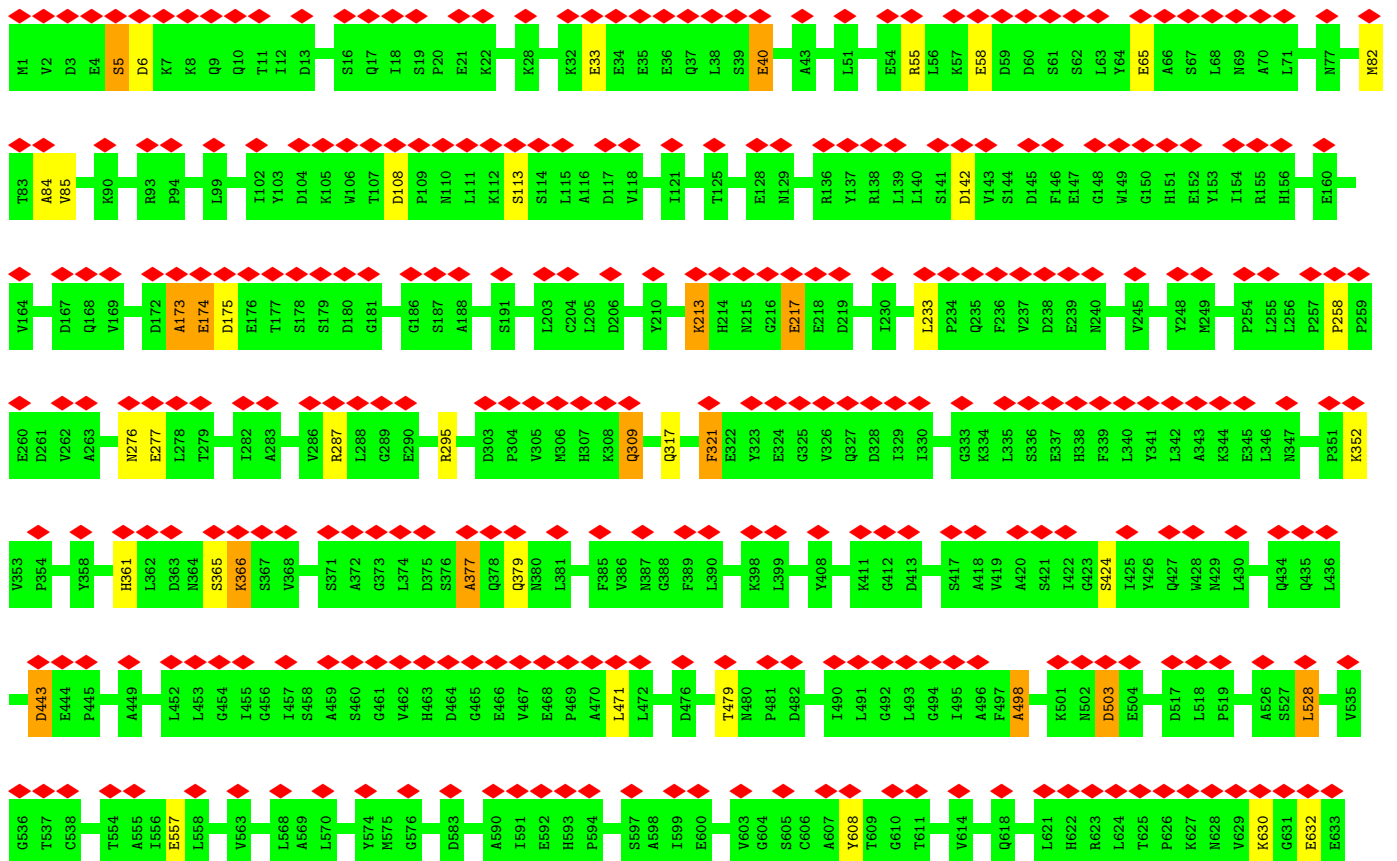
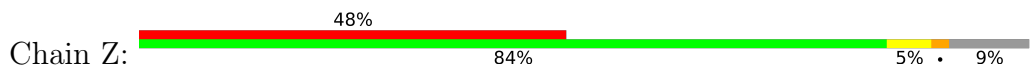


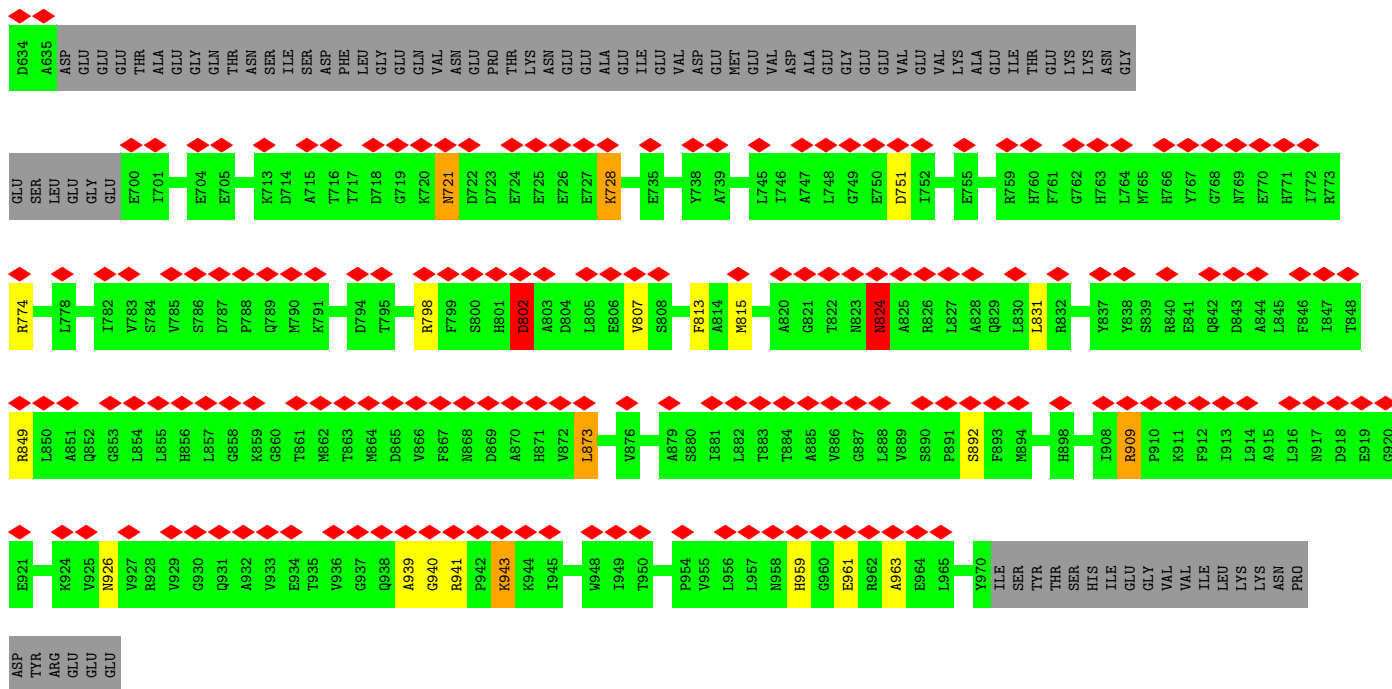


• Molecule 19: 26S proteasome complex subunit SEM1

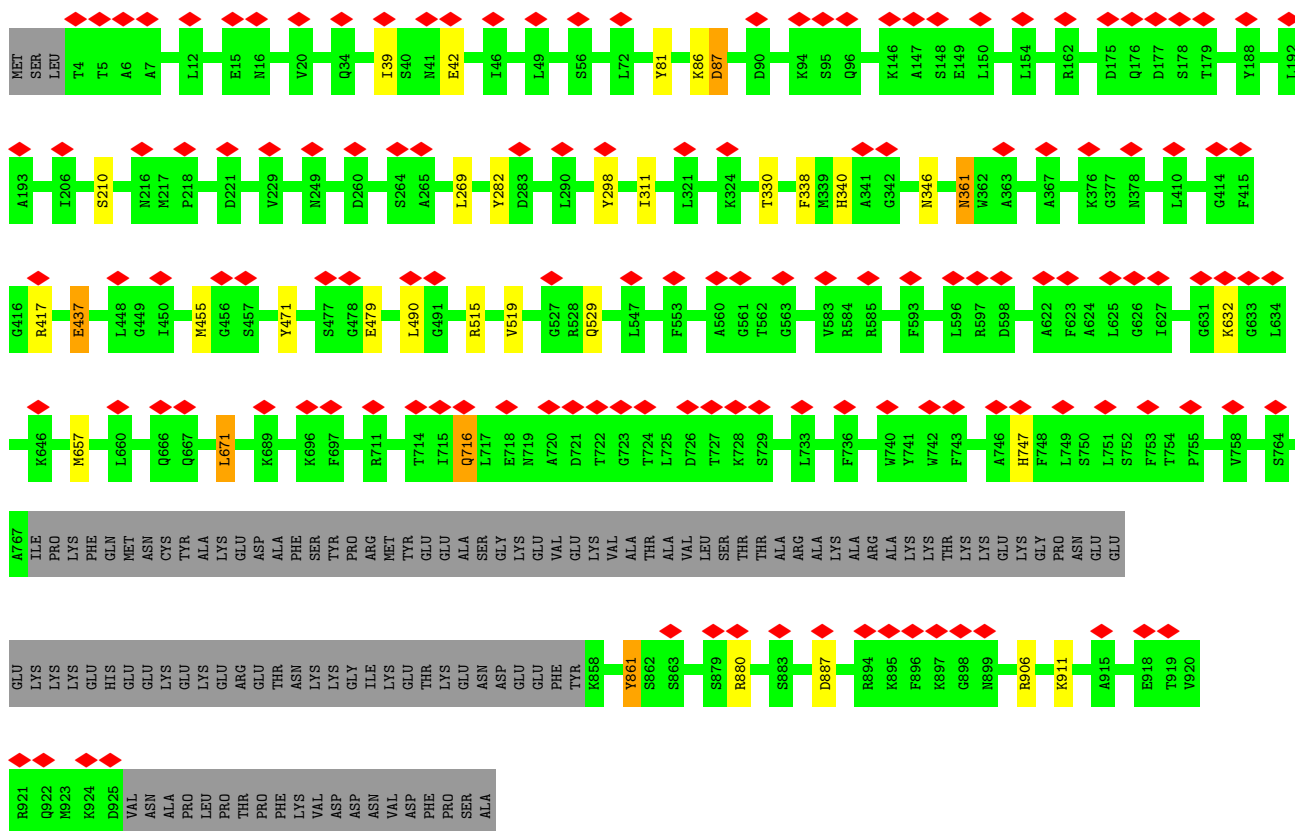
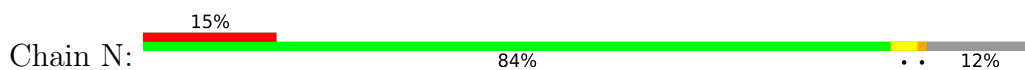


• Molecule 20: 26S proteasome regulatory subunit RPN1



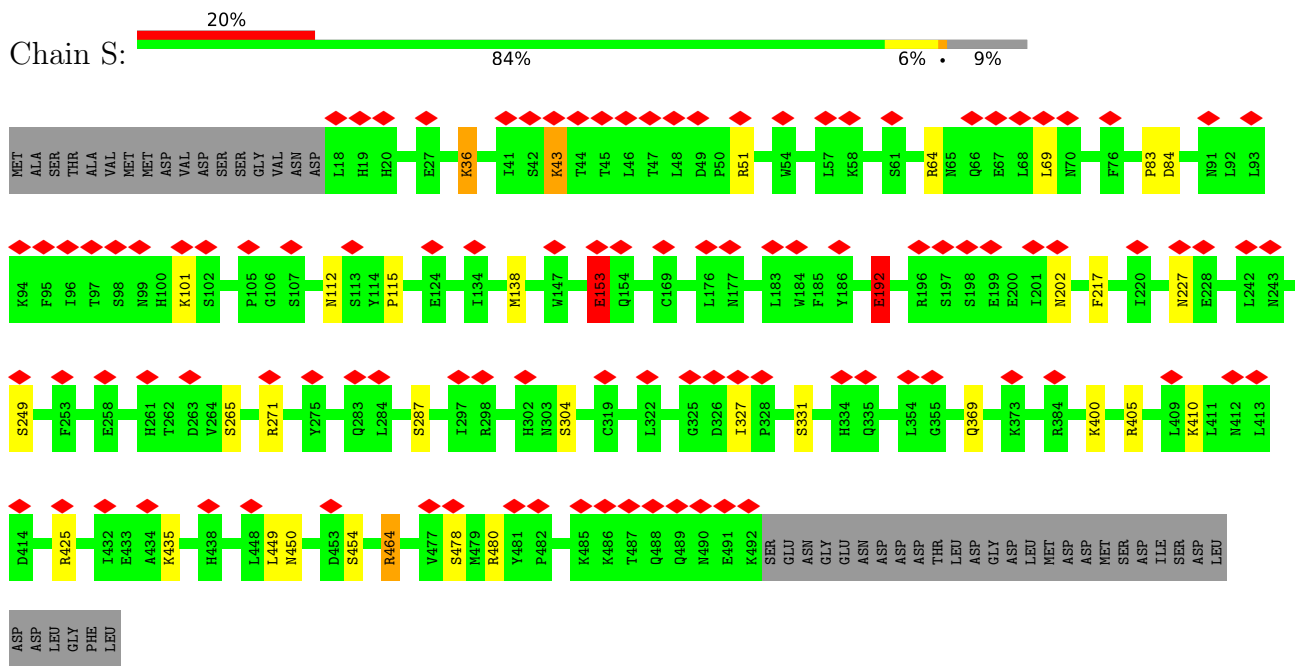


• Molecule 21: 26S proteasome regulatory subunit RPN2

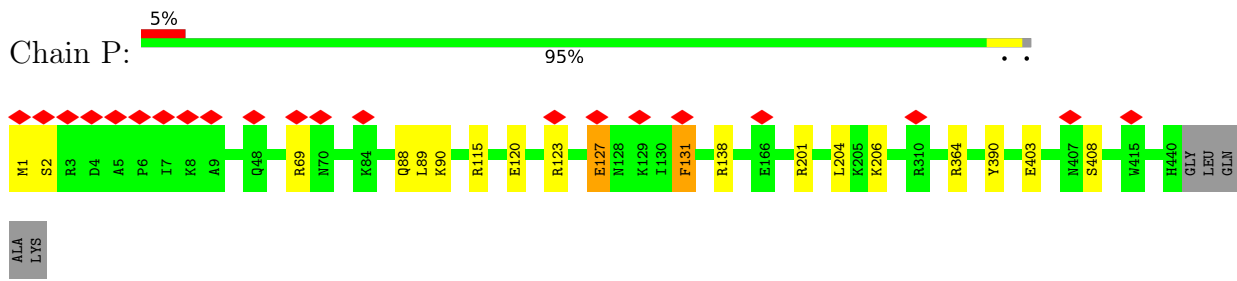


• Molecule 22: 26S proteasome regulatory subunit RPN3

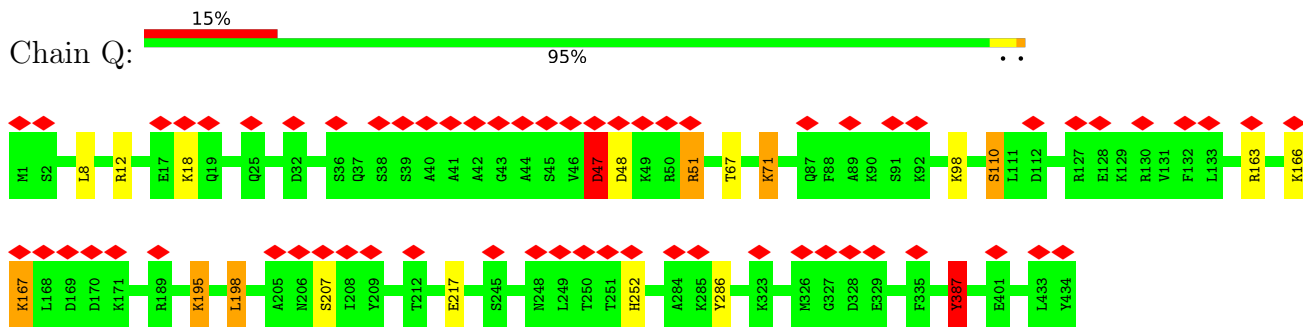




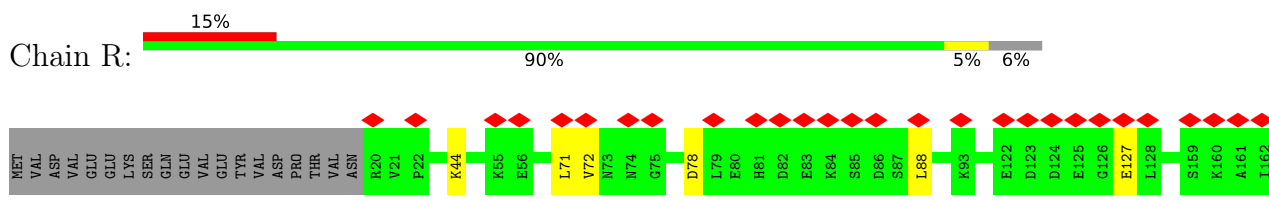
• Molecule 23: 26S proteasome regulatory subunit RPN5

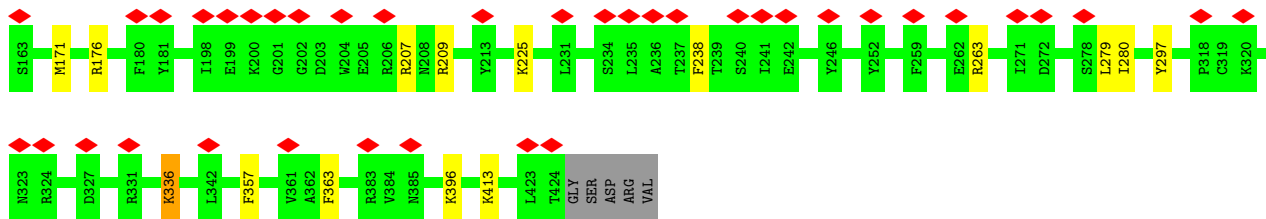


• Molecule 24: 26S proteasome regulatory subunit RPN6

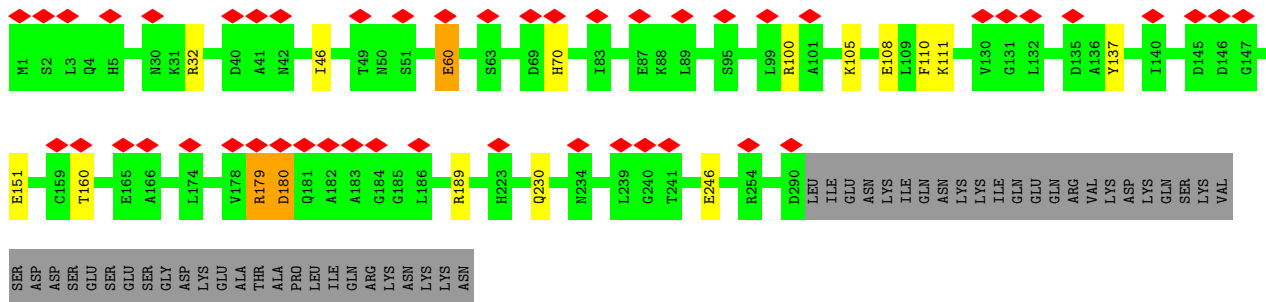
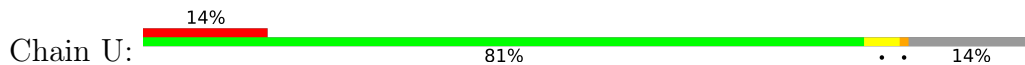


• Molecule 25: 26S proteasome regulatory subunit RPN7

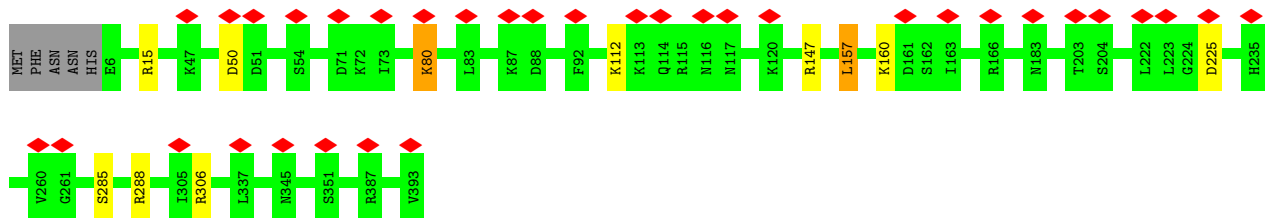




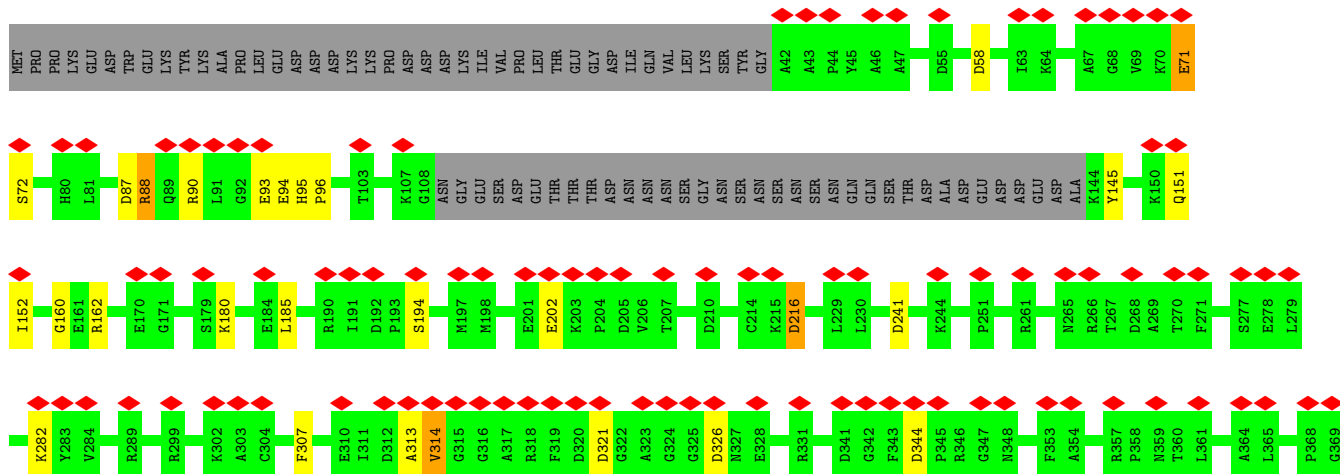
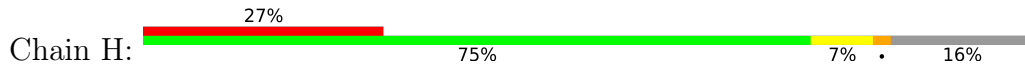
• Molecule 26: 26S proteasome regulatory subunit RPN8

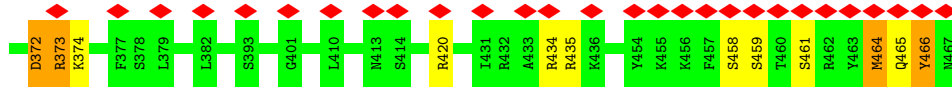


• Molecule 27: 26S proteasome regulatory subunit RPN9

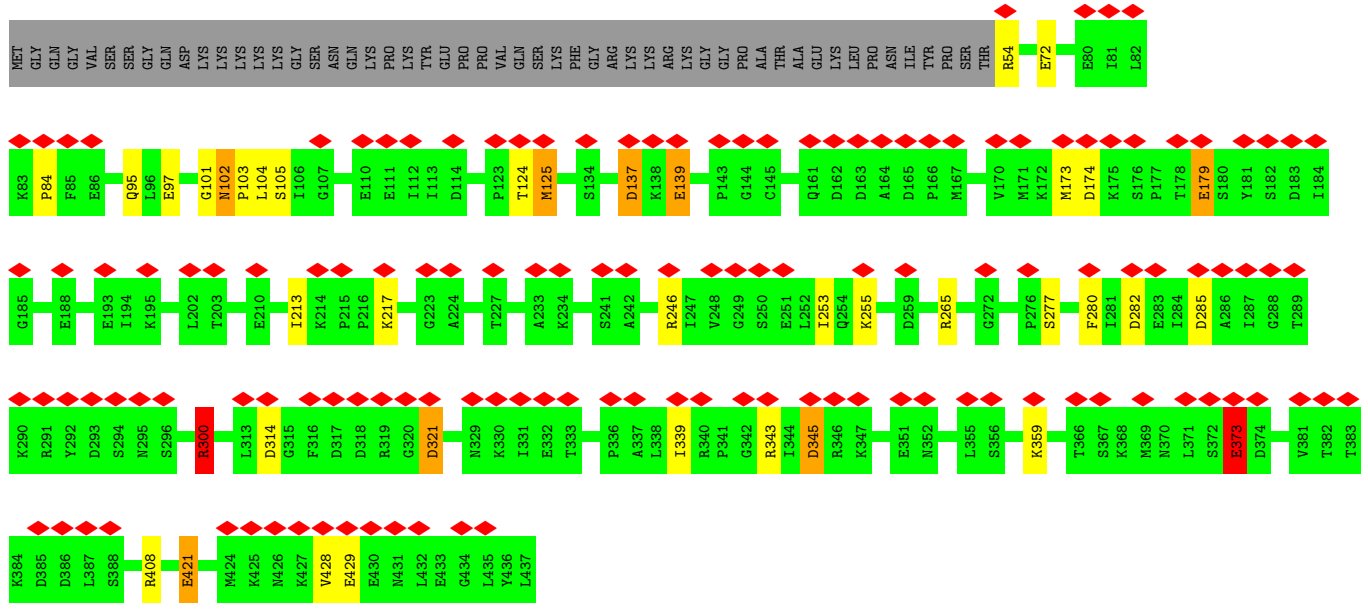
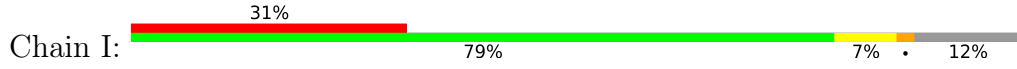


• Molecule 28: 26S proteasome regulatory subunit 7 homolog

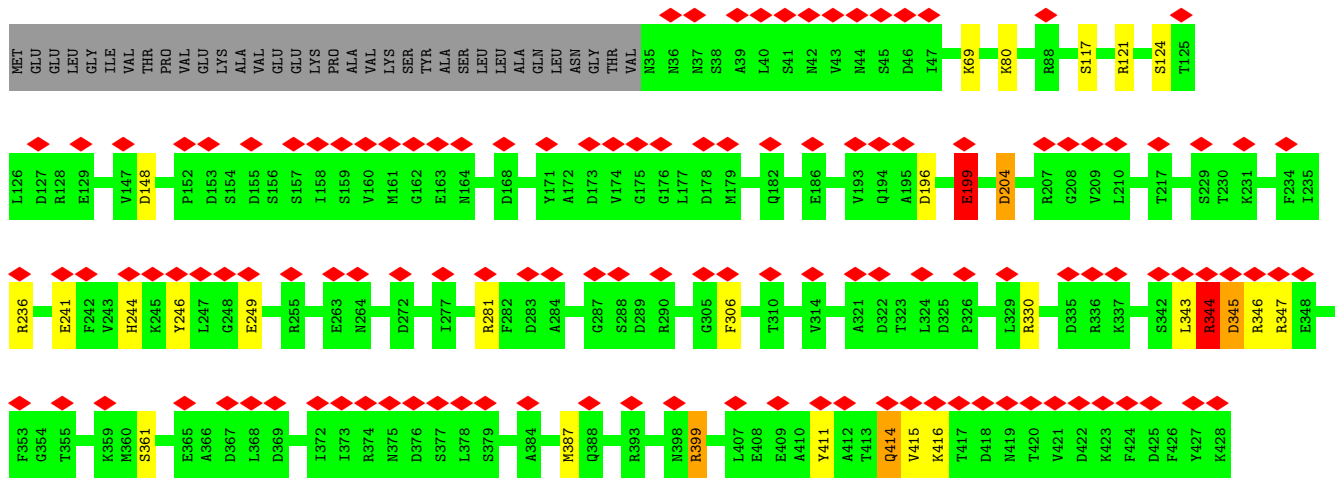
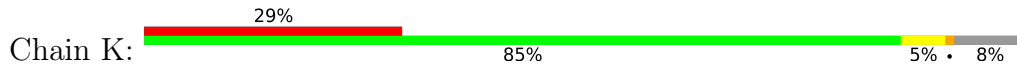




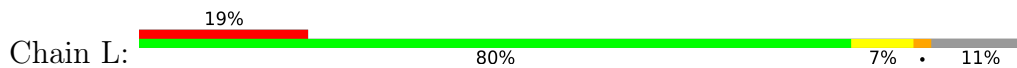
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

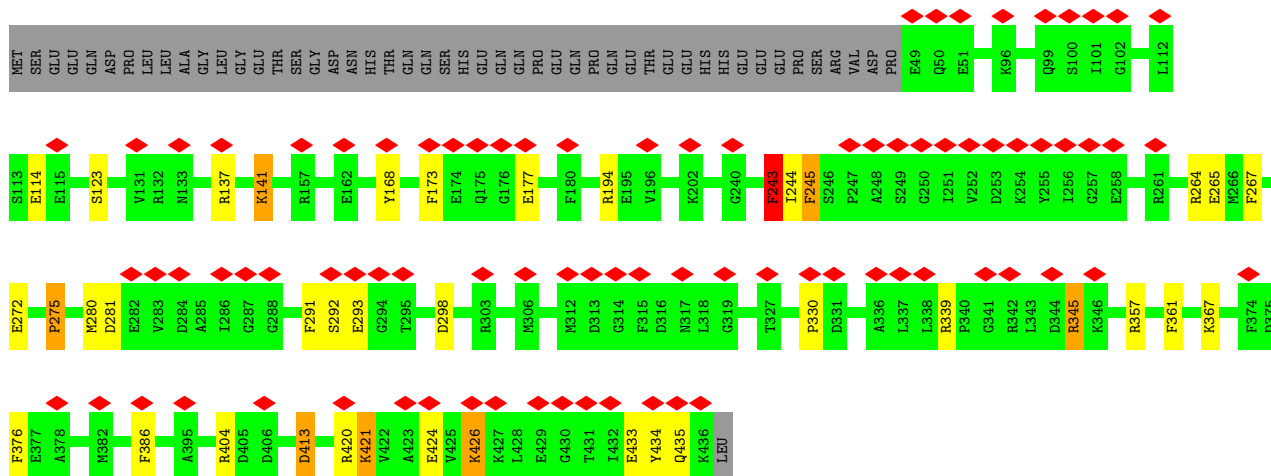


• Molecule 30: 26S proteasome regulatory subunit 6B homolog

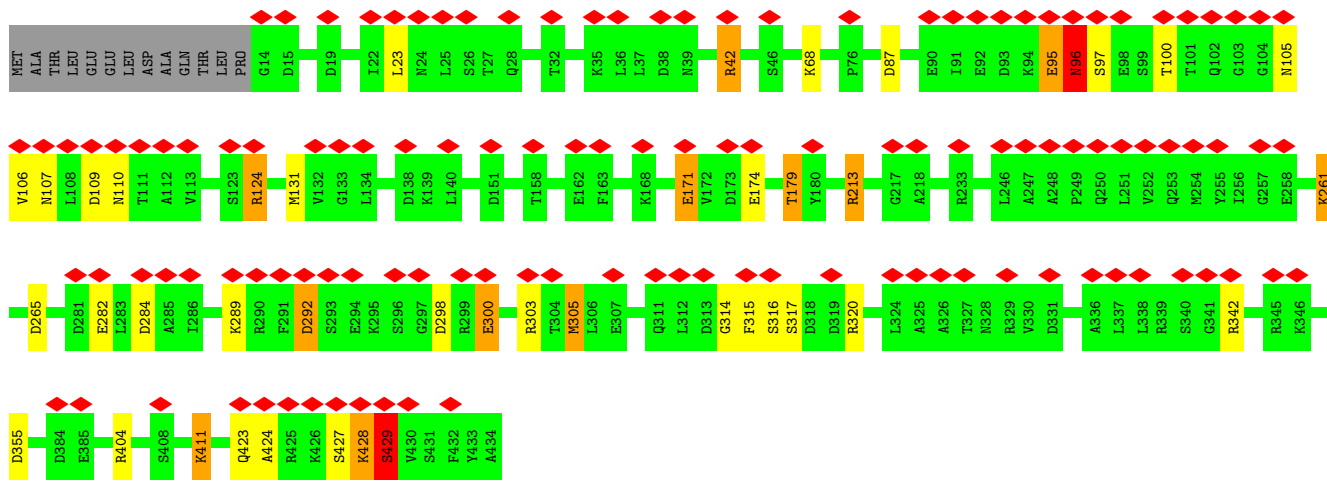
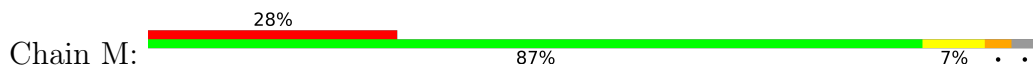


• Molecule 31: 26S proteasome subunit RPT4

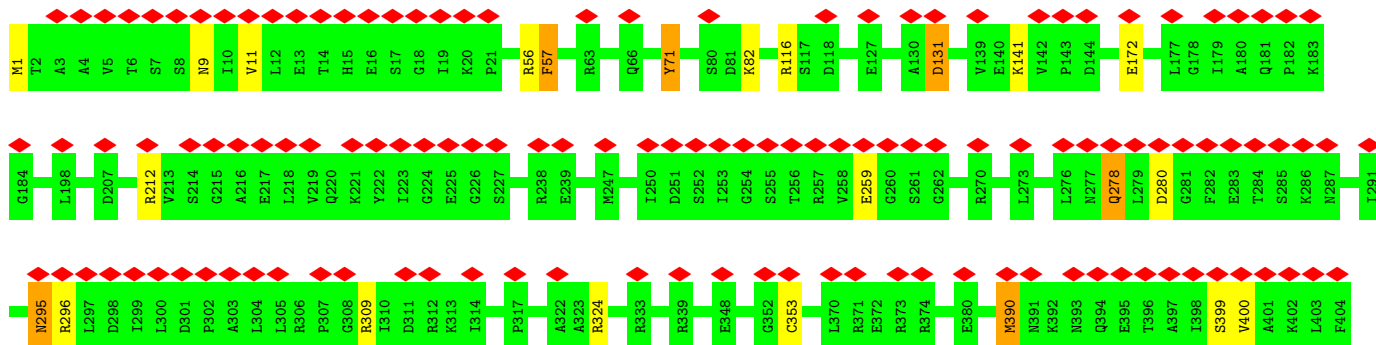




• Molecule 32: 26S proteasome regulatory subunit 6A

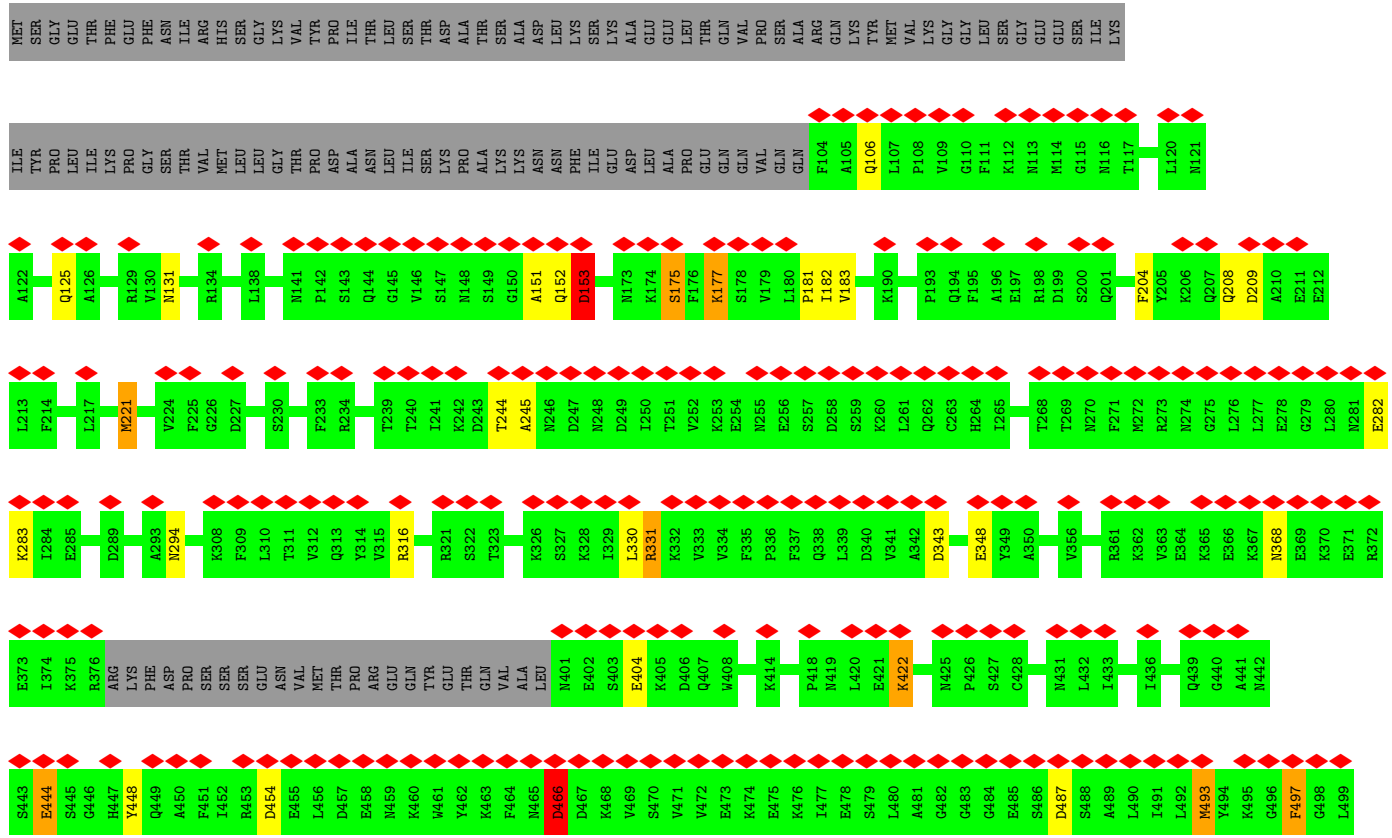


• Molecule 33: 26S proteasome regulatory subunit 8 homolog

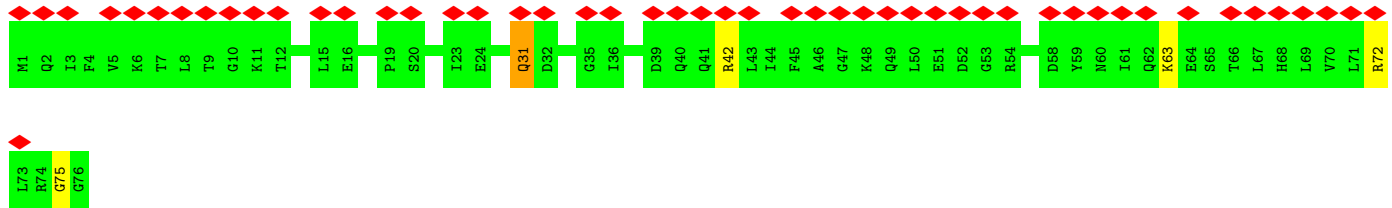
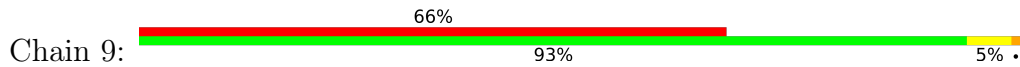


K405

• Molecule 34: Ubiquitin carboxyl-terminal hydrolase 6



• Molecule 35: Polyubiquitin-B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64766	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 ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.895	Depositor
Minimum map value	-17.249	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.920	Depositor
Recommended contour level	4.8	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GLZ, MG, 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	A	1.61	51/1945 (2.6%)	1.60	41/2634 (1.6%)
1	a	1.60	52/1945 (2.7%)	1.57	36/2634 (1.4%)
2	B	1.57	40/1944 (2.1%)	1.55	38/2632 (1.4%)
2	b	1.57	40/1944 (2.1%)	1.55	38/2632 (1.4%)
3	C	1.45	35/1934 (1.8%)	1.59	42/2618 (1.6%)
3	c	1.45	34/1934 (1.8%)	1.59	42/2618 (1.6%)
4	D	0.63	1/1879 (0.1%)	1.07	10/2546 (0.4%)
4	d	0.65	1/1879 (0.1%)	1.01	4/2546 (0.2%)
5	E	1.67	50/1908 (2.6%)	1.76	51/2571 (2.0%)
5	e	1.79	57/1908 (3.0%)	1.68	57/2571 (2.2%)
6	F	1.16	18/1800 (1.0%)	1.23	24/2433 (1.0%)
6	f	1.16	18/1800 (1.0%)	1.23	24/2433 (1.0%)
7	G	1.35	14/1925 (0.7%)	1.48	31/2599 (1.2%)
7	g	1.50	34/1925 (1.8%)	1.40	34/2599 (1.3%)
8	1	2.97	92/1541 (6.0%)	2.44	80/2087 (3.8%)
8	h	2.84	78/1541 (5.1%)	2.42	82/2087 (3.9%)
9	2	3.77	132/1750 (7.5%)	3.04	125/2373 (5.3%)
9	i	3.28	101/1750 (5.8%)	2.83	100/2373 (4.2%)
10	3	3.58	113/1611 (7.0%)	2.51	113/2174 (5.2%)
10	j	3.12	86/1611 (5.3%)	2.44	93/2174 (4.3%)
11	4	4.18	154/1589 (9.7%)	2.88	121/2142 (5.6%)
11	k	4.18	153/1589 (9.6%)	2.88	121/2142 (5.6%)
12	5	3.47	108/1681 (6.4%)	2.48	106/2274 (4.7%)
12	l	3.47	109/1681 (6.5%)	2.48	106/2274 (4.7%)
13	6	3.87	140/1795 (7.8%)	2.80	139/2420 (5.7%)
13	m	4.15	164/1795 (9.1%)	2.83	150/2420 (6.2%)
14	7	0.58	0/1821	1.03	6/2470 (0.2%)
14	n	0.67	2/1821 (0.1%)	1.08	11/2470 (0.4%)
15	W	0.68	0/1557	1.21	12/2111 (0.6%)
16	V	0.60	0/2309	1.09	12/3115 (0.4%)
17	T	0.64	2/2235 (0.1%)	1.08	6/3017 (0.2%)
18	X	0.61	0/1058	1.10	4/1432 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	Y	0.58	0/741	1.00	2/1000 (0.2%)
20	Z	0.62	7/7122 (0.1%)	1.10	44/9645 (0.5%)
21	N	0.61	2/6521 (0.0%)	0.96	22/8824 (0.2%)
22	S	0.59	1/3966 (0.0%)	1.09	20/5355 (0.4%)
23	P	0.59	0/3663	0.95	12/4940 (0.2%)
24	Q	0.59	0/3556	1.08	15/4787 (0.3%)
25	R	0.64	1/3313 (0.0%)	1.10	20/4469 (0.4%)
26	U	0.64	1/2340 (0.0%)	1.08	14/3168 (0.4%)
27	O	0.57	0/3247	0.97	12/4380 (0.3%)
28	H	0.64	1/3113 (0.0%)	1.12	18/4187 (0.4%)
29	I	0.69	3/3054 (0.1%)	1.34	27/4111 (0.7%)
30	K	0.66	2/3156 (0.1%)	1.16	24/4261 (0.6%)
31	L	0.68	3/3128 (0.1%)	1.33	33/4204 (0.8%)
32	M	0.70	3/3323 (0.1%)	1.35	28/4478 (0.6%)
33	J	0.61	0/3212	1.08	13/4316 (0.3%)
34	8	0.69	0/3089	1.16	21/4144 (0.5%)
35	9	0.55	0/603	1.12	5/811 (0.6%)
All	All	1.72	1903/114552 (1.7%)	1.58	2189/154701 (1.4%)

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	A	0	3
1	a	0	2
2	B	0	1
2	b	0	1
3	C	0	3
3	c	0	3
4	D	0	4
4	d	0	4
5	E	0	4
5	e	0	4
6	F	0	3
6	f	0	3
7	G	0	6
7	g	0	4
8	1	0	1
8	h	0	1
9	2	0	6

*Continued on next page...*



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Mol	Chain	#Chirality outliers	#Planarity outliers
9	i	0	7
10	3	0	2
10	j	0	1
11	4	0	1
11	k	0	1
12	5	0	3
12	l	0	3
13	6	0	5
13	m	0	8
14	7	0	2
15	W	0	4
16	V	0	1
17	T	0	3
19	Y	0	3
20	Z	0	22
21	N	0	5
22	S	0	5
23	P	0	2
24	Q	0	6
25	R	0	2
26	U	0	5
27	O	0	2
28	H	0	9
29	I	0	15
30	K	0	7
31	L	0	10
32	M	0	20
33	J	0	7
34	8	0	15
35	9	0	1
All	All	0	230

The worst 5 of 1903 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	153	TYR	CD1-CE1	-33.59	0.89	1.39
9	i	153	TYR	CD1-CE1	-33.55	0.89	1.39
11	k	67	TYR	CE1-CZ	-31.35	0.97	1.38
9	2	232	TYR	CE2-CZ	-31.34	0.97	1.38
11	4	67	TYR	CE1-CZ	-31.33	0.97	1.38

The worst 5 of 2189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	65	ARG	NE-CZ-NH1	-46.33	97.13	120.30
9	2	65	ARG	NE-CZ-NH1	-46.27	97.17	120.30
9	i	65	ARG	NE-CZ-NH2	43.31	141.96	120.30
9	2	65	ARG	NE-CZ-NH2	43.26	141.93	120.30
11	4	70	ARG	NE-CZ-NH1	38.29	139.45	120.30

There are no chirality outliers.

5 of 230 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	115	ASP	Sidechain
1	a	250	GLU	Sidechain
2	b	234	ARG	Sidechain
3	c	105	ASP	Sidechain
3	c	63	THR	Mainchain

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
1	a	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
2	B	247/250 (99%)	237 (96%)	8 (3%)	2 (1%)	19	60
2	b	247/250 (99%)	237 (96%)	8 (3%)	2 (1%)	19	60
3	C	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	72
3	c	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	72
4	D	234/254 (92%)	219 (94%)	10 (4%)	5 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	234/254 (92%)	218 (93%)	11 (5%)	5 (2%)	7	36
5	E	242/260 (93%)	227 (94%)	14 (6%)	1 (0%)	34	72
5	e	242/260 (93%)	224 (93%)	15 (6%)	3 (1%)	13	50
6	F	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	34	72
6	f	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	34	72
7	G	240/288 (83%)	225 (94%)	14 (6%)	1 (0%)	34	72
7	g	240/288 (83%)	227 (95%)	12 (5%)	1 (0%)	34	72
8	l	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
8	h	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
9	2	224/261 (86%)	213 (95%)	9 (4%)	2 (1%)	17	56
9	i	224/261 (86%)	209 (93%)	12 (5%)	3 (1%)	12	48
10	3	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	54
10	j	202/205 (98%)	193 (96%)	7 (4%)	2 (1%)	15	54
11	4	193/198 (98%)	183 (95%)	9 (5%)	1 (0%)	29	69
11	k	193/198 (98%)	183 (95%)	8 (4%)	2 (1%)	15	54
12	5	210/287 (73%)	199 (95%)	10 (5%)	1 (0%)	29	69
12	l	210/287 (73%)	198 (94%)	11 (5%)	1 (0%)	29	69
13	6	220/241 (91%)	206 (94%)	12 (6%)	2 (1%)	17	56
13	m	220/241 (91%)	206 (94%)	12 (6%)	2 (1%)	17	56
14	7	227/266 (85%)	206 (91%)	18 (8%)	3 (1%)	12	48
14	n	227/266 (85%)	210 (92%)	17 (8%)	0	100	100
15	W	195/268 (73%)	177 (91%)	17 (9%)	1 (0%)	29	69
16	V	287/306 (94%)	261 (91%)	22 (8%)	4 (1%)	11	46
17	T	264/274 (96%)	239 (90%)	24 (9%)	1 (0%)	34	72
18	X	125/156 (80%)	107 (86%)	17 (14%)	1 (1%)	19	60
19	Y	87/89 (98%)	77 (88%)	7 (8%)	3 (3%)	3	26
20	Z	902/993 (91%)	822 (91%)	63 (7%)	17 (2%)	8	38
21	N	828/945 (88%)	796 (96%)	28 (3%)	4 (0%)	29	69
22	S	473/523 (90%)	437 (92%)	27 (6%)	9 (2%)	8	38
23	P	438/445 (98%)	418 (95%)	17 (4%)	3 (1%)	22	62
24	Q	432/434 (100%)	397 (92%)	30 (7%)	5 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	R	403/429 (94%)	377 (94%)	23 (6%)	3 (1%)	22	62
26	U	288/338 (85%)	276 (96%)	11 (4%)	1 (0%)	41	76
27	O	386/393 (98%)	372 (96%)	14 (4%)	0	100	100
28	H	387/467 (83%)	355 (92%)	25 (6%)	7 (2%)	8	40
29	I	382/437 (87%)	331 (87%)	42 (11%)	9 (2%)	6	33
30	K	392/428 (92%)	360 (92%)	30 (8%)	2 (0%)	29	69
31	L	386/437 (88%)	349 (90%)	33 (8%)	4 (1%)	15	54
32	M	419/434 (96%)	374 (89%)	35 (8%)	10 (2%)	6	33
33	J	403/405 (100%)	356 (88%)	42 (10%)	5 (1%)	13	50
34	8	368/499 (74%)	329 (89%)	30 (8%)	9 (2%)	6	33
35	9	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
All	All	14205/15714 (90%)	13230 (93%)	832 (6%)	143 (1%)	20	54

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	3	ASP
4	d	204	GLN
5	e	128	SER
9	i	200	SER
9	i	222	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	198 (96%)	8 (4%)	32	56
1	a	206/210 (98%)	197 (96%)	9 (4%)	28	53
2	B	208/209 (100%)	192 (92%)	16 (8%)	13	37
2	b	208/209 (100%)	192 (92%)	16 (8%)	13	37
3	C	203/216 (94%)	197 (97%)	6 (3%)	41	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	203/216 (94%)	197 (97%)	6 (3%)	41	63
4	D	209/226 (92%)	199 (95%)	10 (5%)	25	51
4	d	209/226 (92%)	200 (96%)	9 (4%)	29	54
5	E	200/215 (93%)	189 (94%)	11 (6%)	21	47
5	e	200/215 (93%)	187 (94%)	13 (6%)	17	42
6	F	190/193 (98%)	178 (94%)	12 (6%)	18	43
6	f	190/193 (98%)	178 (94%)	12 (6%)	18	43
7	G	200/239 (84%)	189 (94%)	11 (6%)	21	47
7	g	200/239 (84%)	188 (94%)	12 (6%)	19	44
8	1	162/178 (91%)	134 (83%)	28 (17%)	2	11
8	h	162/178 (91%)	136 (84%)	26 (16%)	2	13
9	2	185/214 (86%)	144 (78%)	41 (22%)	1	6
9	i	185/214 (86%)	155 (84%)	30 (16%)	2	13
10	3	172/173 (99%)	137 (80%)	35 (20%)	1	7
10	j	172/173 (99%)	145 (84%)	27 (16%)	2	14
11	4	173/175 (99%)	131 (76%)	42 (24%)	0	4
11	k	173/175 (99%)	133 (77%)	40 (23%)	1	5
12	5	169/235 (72%)	130 (77%)	39 (23%)	1	5
12	l	169/235 (72%)	130 (77%)	39 (23%)	1	5
13	6	185/201 (92%)	160 (86%)	25 (14%)	4	17
13	m	185/201 (92%)	154 (83%)	31 (17%)	2	12
14	7	195/224 (87%)	190 (97%)	5 (3%)	46	67
14	n	195/224 (87%)	192 (98%)	3 (2%)	65	80
15	W	171/230 (74%)	166 (97%)	5 (3%)	42	64
16	V	253/268 (94%)	247 (98%)	6 (2%)	49	69
17	T	249/256 (97%)	245 (98%)	4 (2%)	62	79
18	X	116/144 (81%)	112 (97%)	4 (3%)	37	60
19	Y	81/81 (100%)	81 (100%)	0	100	100
20	Z	773/850 (91%)	749 (97%)	24 (3%)	40	62
21	N	698/797 (88%)	684 (98%)	14 (2%)	55	74
22	S	447/489 (91%)	429 (96%)	18 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	P	412/415 (99%)	407 (99%)	5 (1%)	71	84
24	Q	391/391 (100%)	379 (97%)	12 (3%)	40	62
25	R	356/379 (94%)	354 (99%)	2 (1%)	86	92
26	U	263/308 (85%)	261 (99%)	2 (1%)	81	89
27	O	363/368 (99%)	359 (99%)	4 (1%)	73	84
28	H	330/399 (83%)	313 (95%)	17 (5%)	23	48
29	I	341/385 (89%)	333 (98%)	8 (2%)	50	71
30	K	346/374 (92%)	333 (96%)	13 (4%)	33	57
31	L	332/377 (88%)	320 (96%)	12 (4%)	35	59
32	M	364/375 (97%)	349 (96%)	15 (4%)	30	55
33	J	352/352 (100%)	345 (98%)	7 (2%)	55	74
34	8	337/449 (75%)	327 (97%)	10 (3%)	41	63
35	9	68/68 (100%)	66 (97%)	2 (3%)	42	64
All	All	12357/13571 (91%)	11611 (94%)	746 (6%)	23	44

5 of 746 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	4	69	ILE
17	T	28	PRO
11	4	125	LYS
11	4	68	SER
12	5	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
12	5	251	ASN
21	N	360	GLN
13	6	87	HIS
17	T	17	ASN
24	Q	252	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
35	GLZ	9	76	35	3,3,3	0.17	0	0,2,2	-	-

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
35	GLZ	9	76	35	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
36	ATP	I	501	37	26,33,33	1.30	2 (7%)	31,52,52	1.15	3 (9%)
36	ATP	M	501	-	26,33,33	2.09	4 (15%)	31,52,52	1.76	6 (19%)
38	ADP	J	501	-	24,29,29	1.82	6 (25%)	29,45,45	1.34	5 (17%)
36	ATP	K	501	37	26,33,33	1.41	3 (11%)	31,52,52	1.59	7 (22%)
36	ATP	H	501	37	26,33,33	1.25	2 (7%)	31,52,52	1.72	7 (22%)
36	ATP	L	501	37	26,33,33	1.48	5 (19%)	31,52,52	1.55	6 (19%)

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
36	ATP	I	501	37	-	8/18/38/38	0/3/3/3
36	ATP	M	501	-	-	3/18/38/38	0/3/3/3
38	ADP	J	501	-	-	2/12/32/32	0/3/3/3
36	ATP	K	501	37	-	6/18/38/38	0/3/3/3
36	ATP	H	501	37	-	5/18/38/38	0/3/3/3
36	ATP	L	501	37	-	3/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	501	ATP	O4'-C1'	6.74	1.50	1.41
36	M	501	ATP	C4-N3	-4.97	1.28	1.35
36	M	501	ATP	C8-N7	-4.81	1.26	1.34
36	K	501	ATP	C8-N7	-4.60	1.26	1.34
38	J	501	ADP	C2-N3	4.18	1.38	1.32

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	501	ATP	PA-O3A-PB	5.13	150.41	132.83
36	M	501	ATP	C5-C6-N6	4.30	126.88	120.35
36	K	501	ATP	N6-C6-N1	3.99	126.86	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	M	501	ATP	PA-O3A-PB	3.88	146.16	132.83
38	J	501	ADP	C5-C6-N6	3.74	126.04	120.35

There are no chirality outliers.

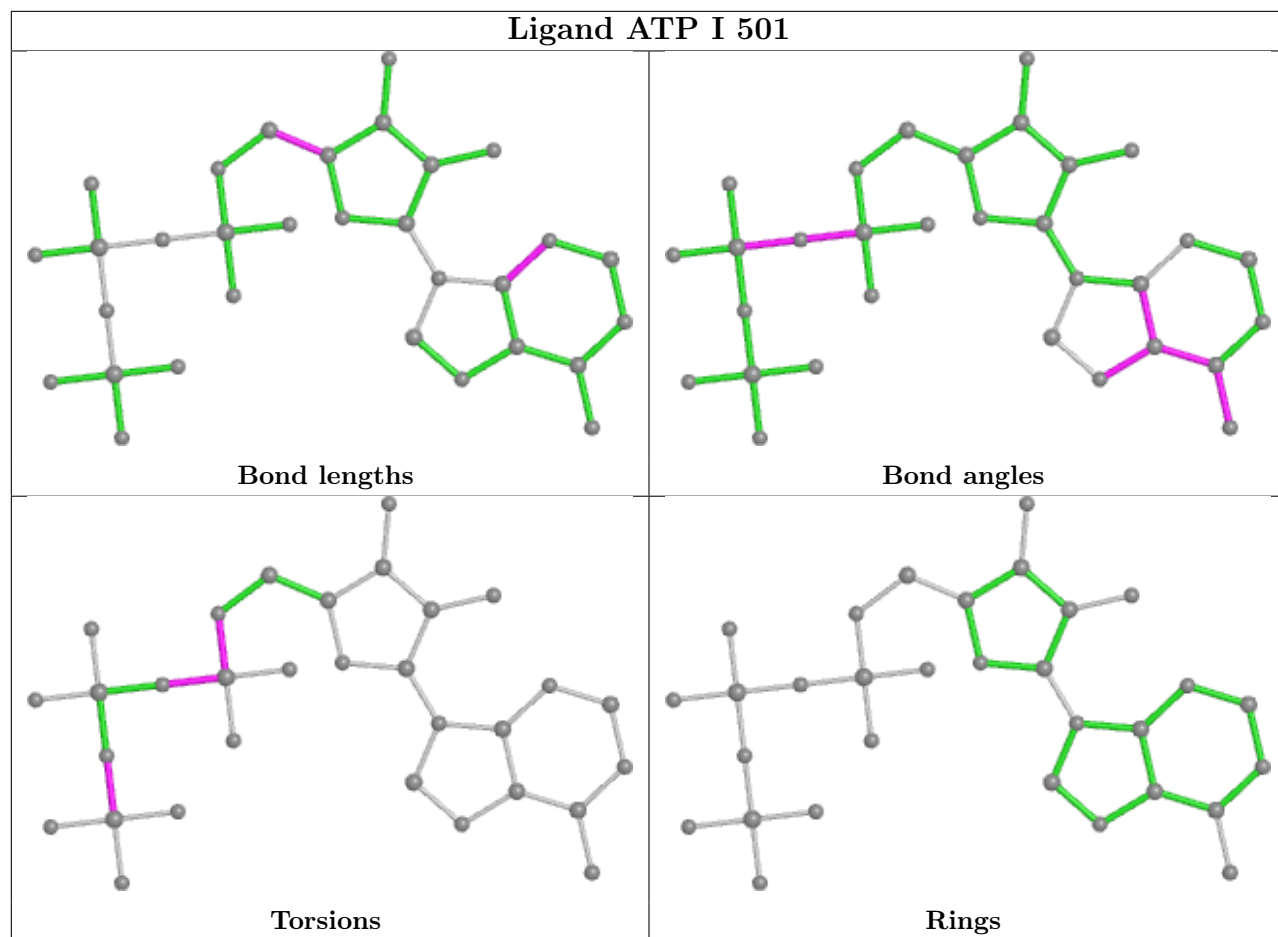
5 of 27 torsion outliers are listed below:

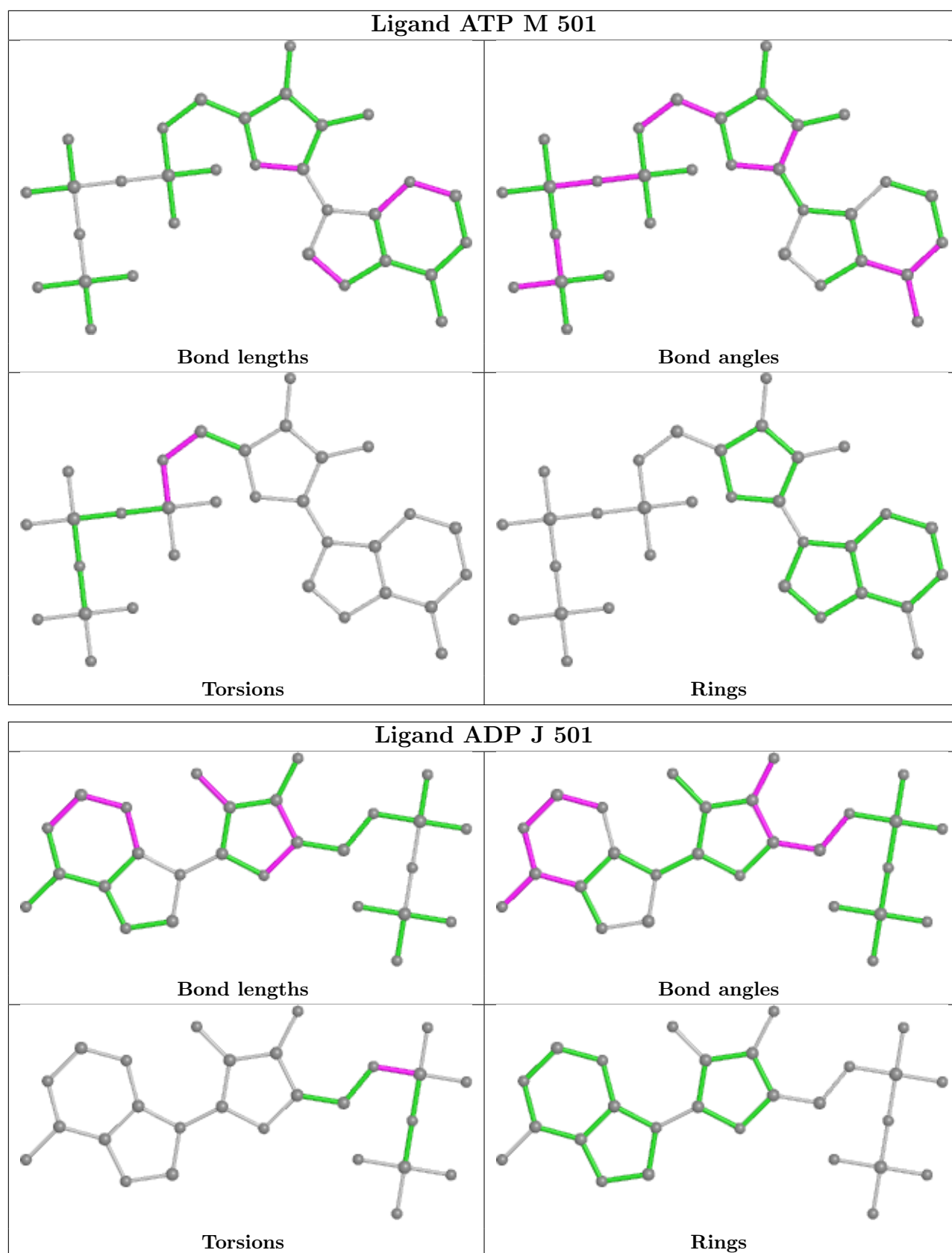
Mol	Chain	Res	Type	Atoms
36	H	501	ATP	PB-O3B-PG-O2G
36	H	501	ATP	C5'-O5'-PA-O2A
36	H	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3B-PG-O2G
36	I	501	ATP	C5'-O5'-PA-O1A

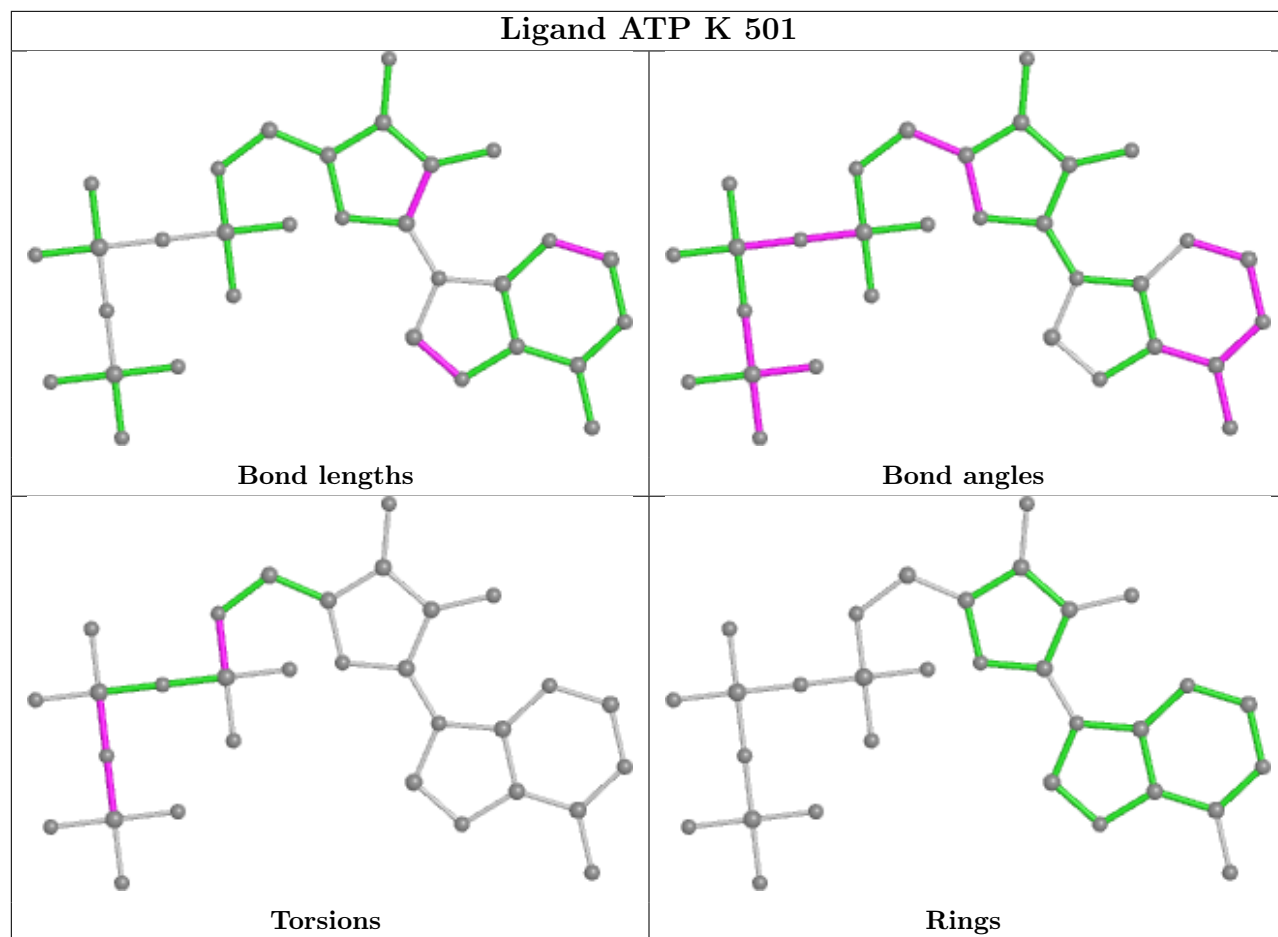
There are no ring outliers.

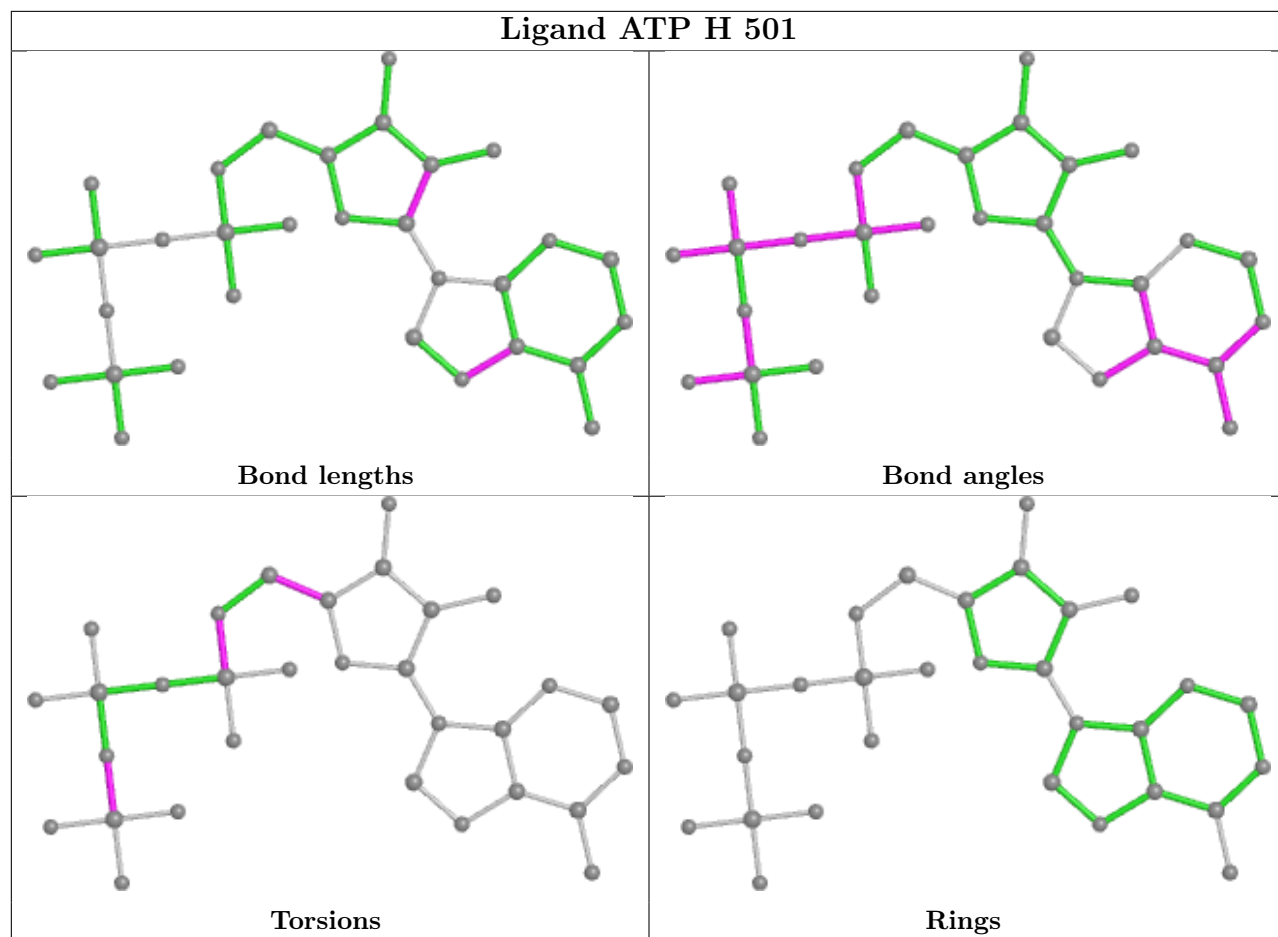
No monomer is involved in short contacts.

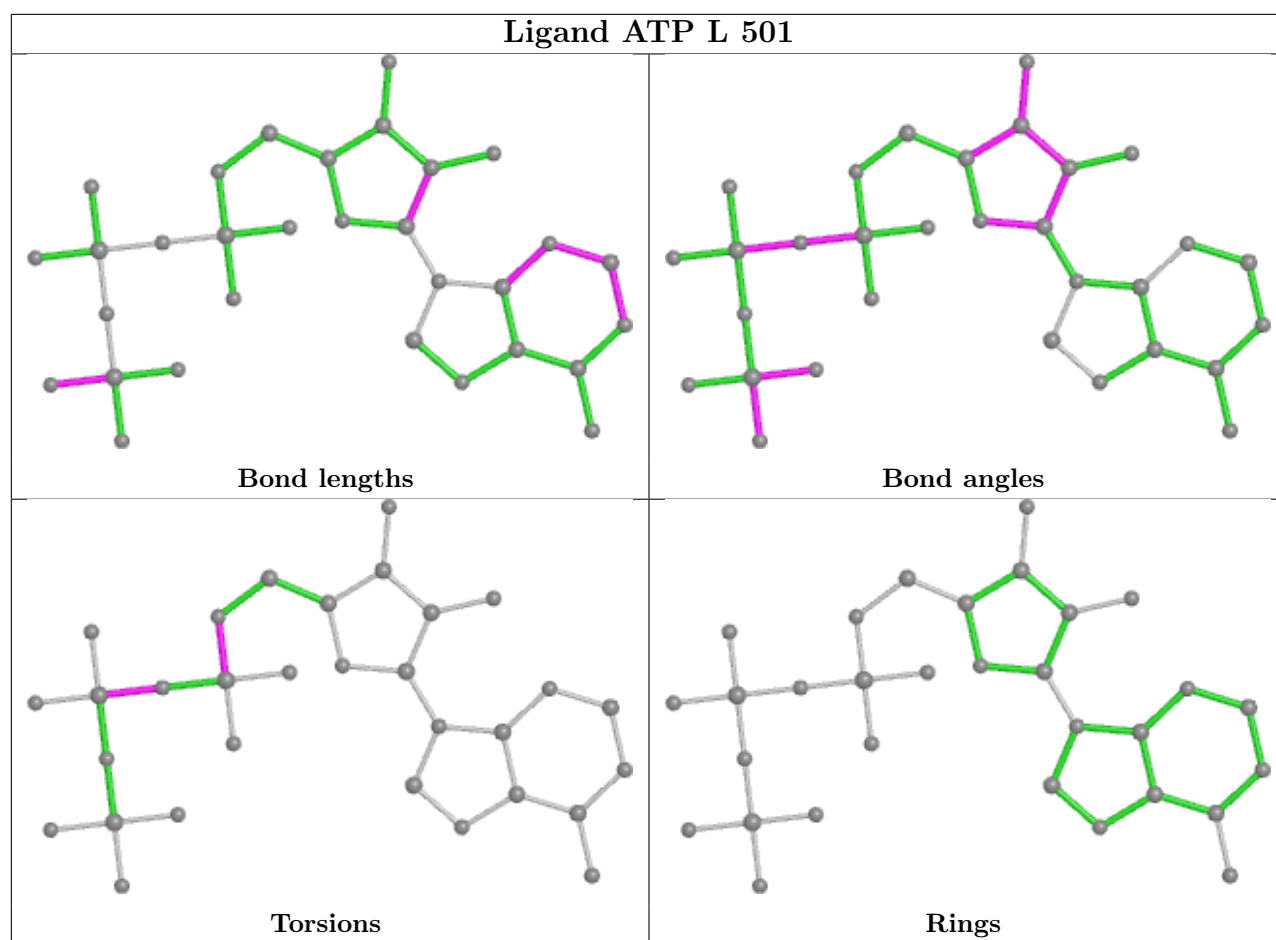
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

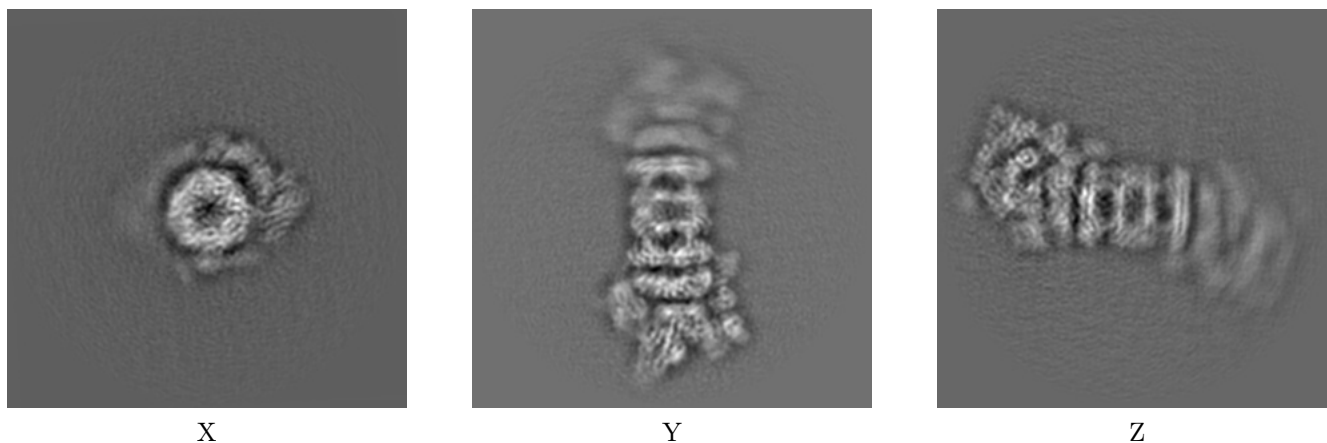
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14084. 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](#)

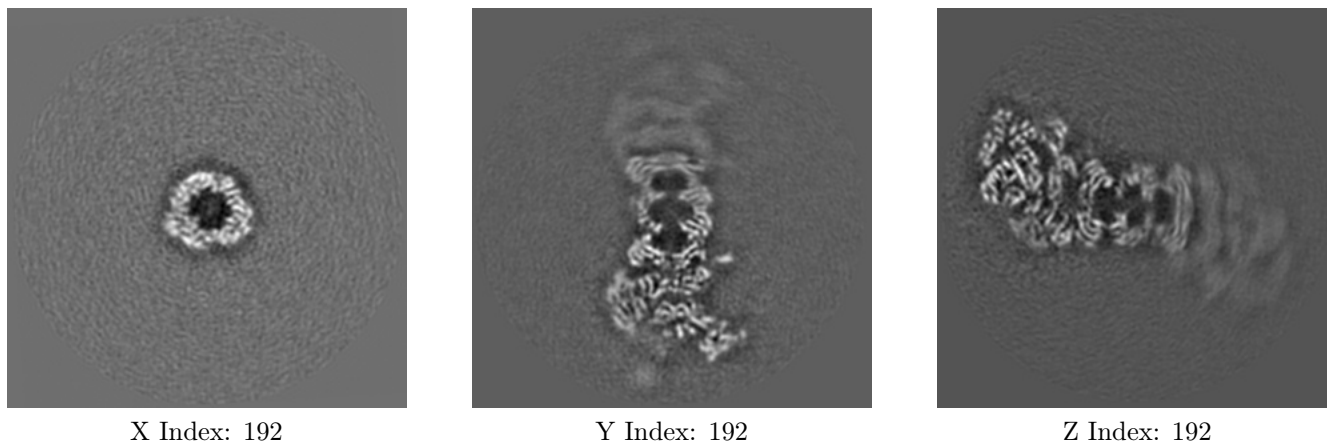
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

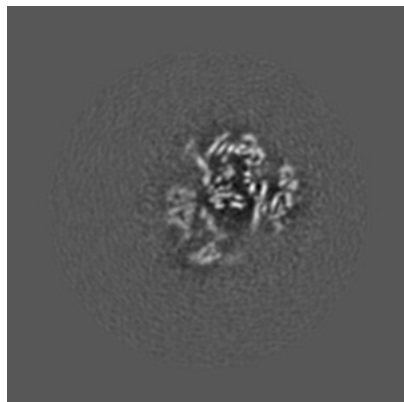
#### 6.2.1 Primary map



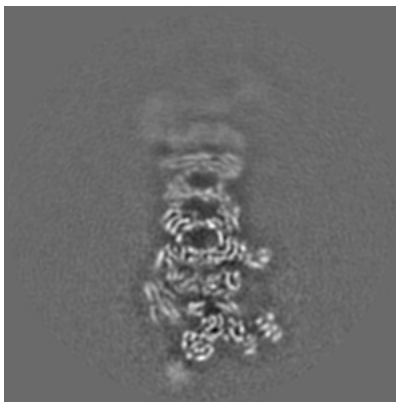
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

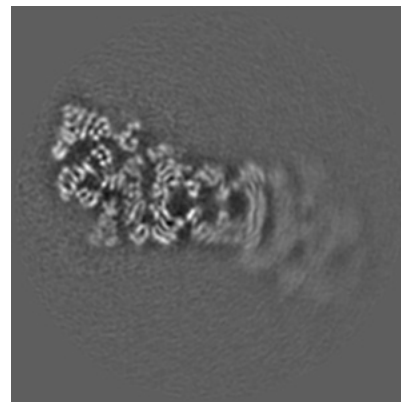
### 6.3.1 Primary map



X Index: 82



Y Index: 204

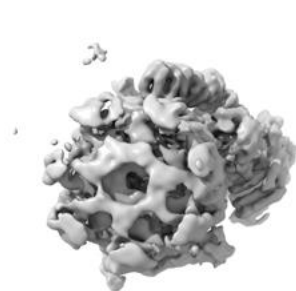


Z Index: 197

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

## 6.4 Orthogonal surface views [i](#)

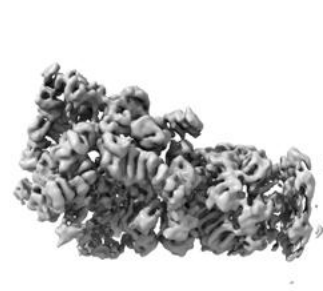
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



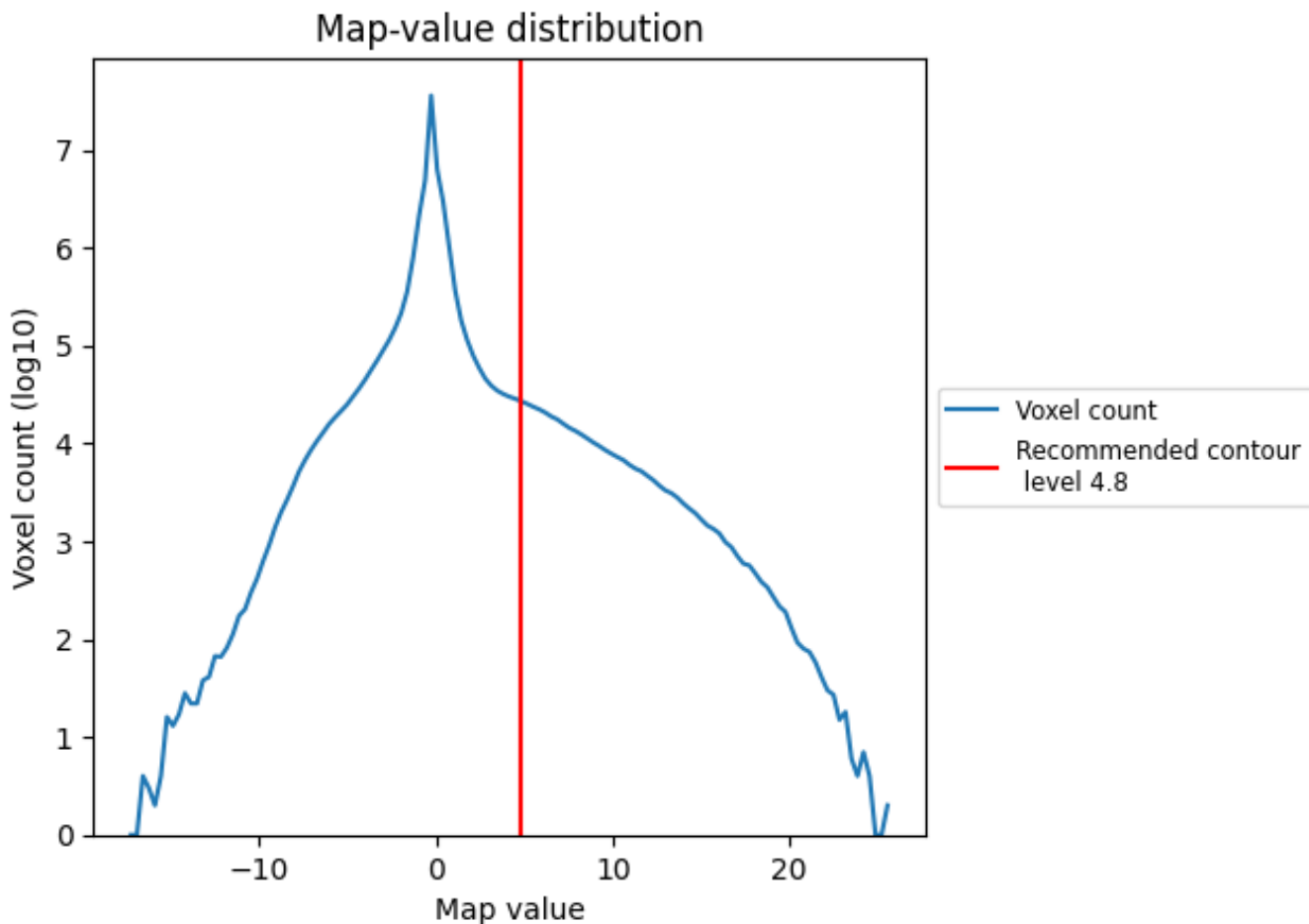
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

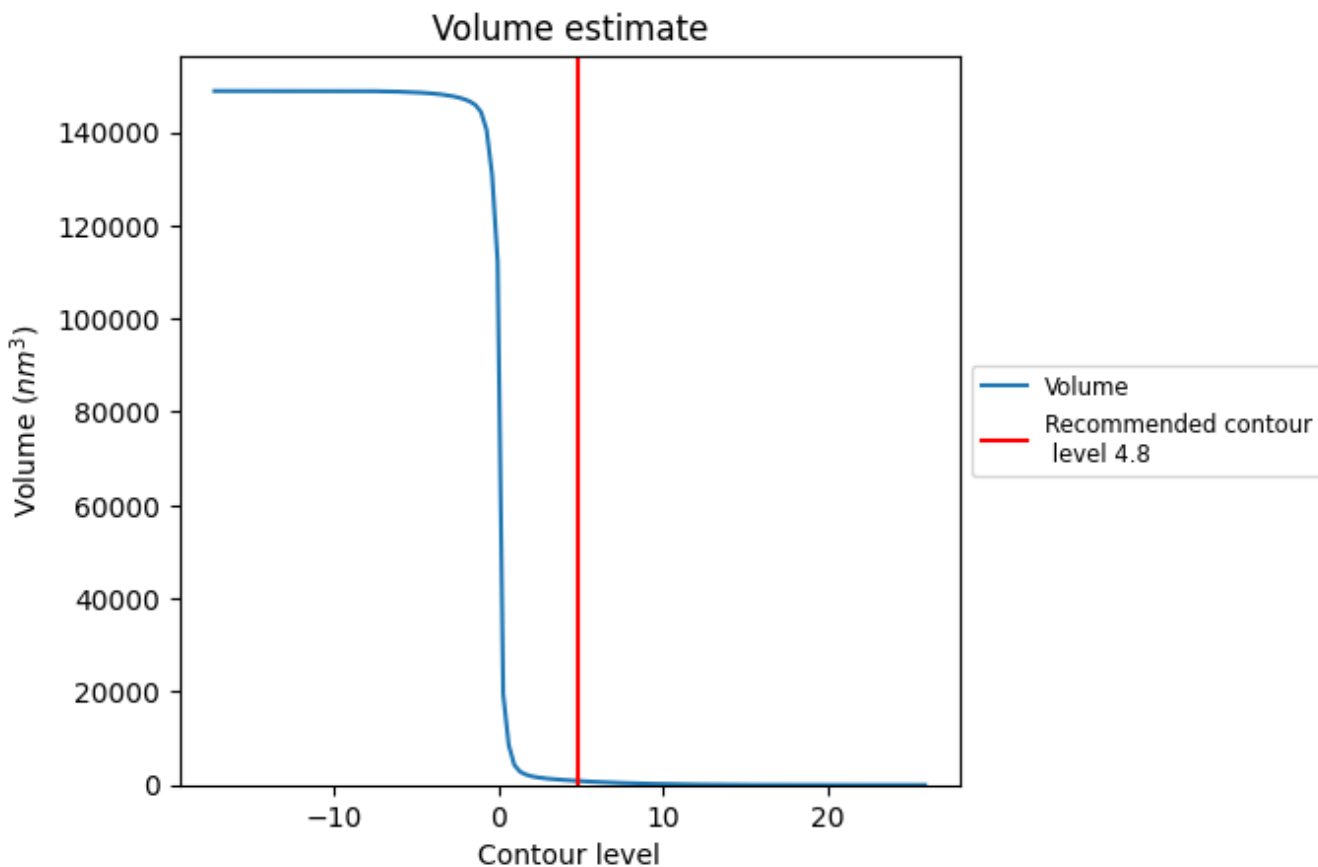
This section contains the results of statistical analysis of the map.

### 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.

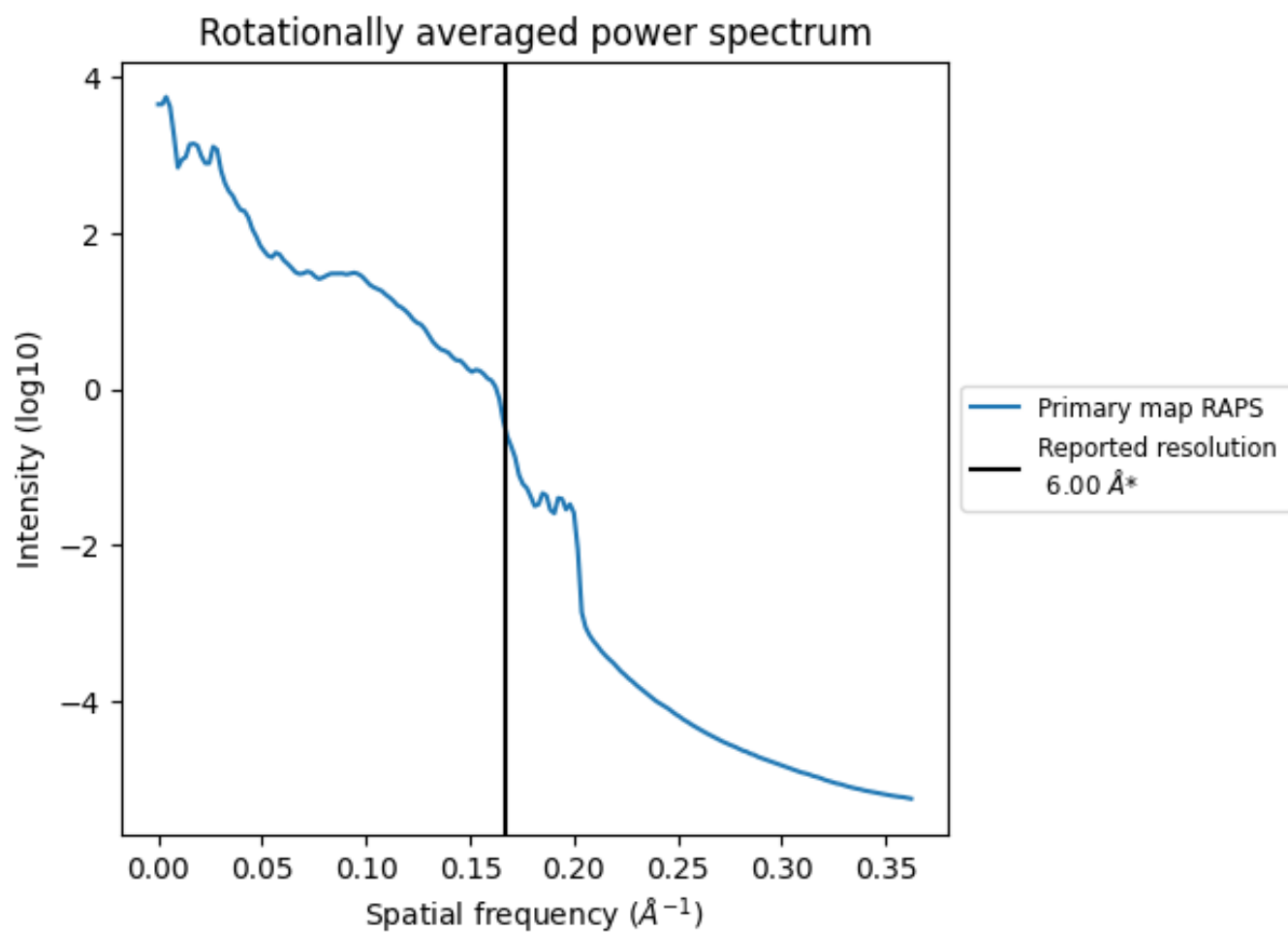
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 874  $\text{nm}^3$ ; this corresponds to an approximate mass of 789 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.167 \text{\AA}^{-1}$

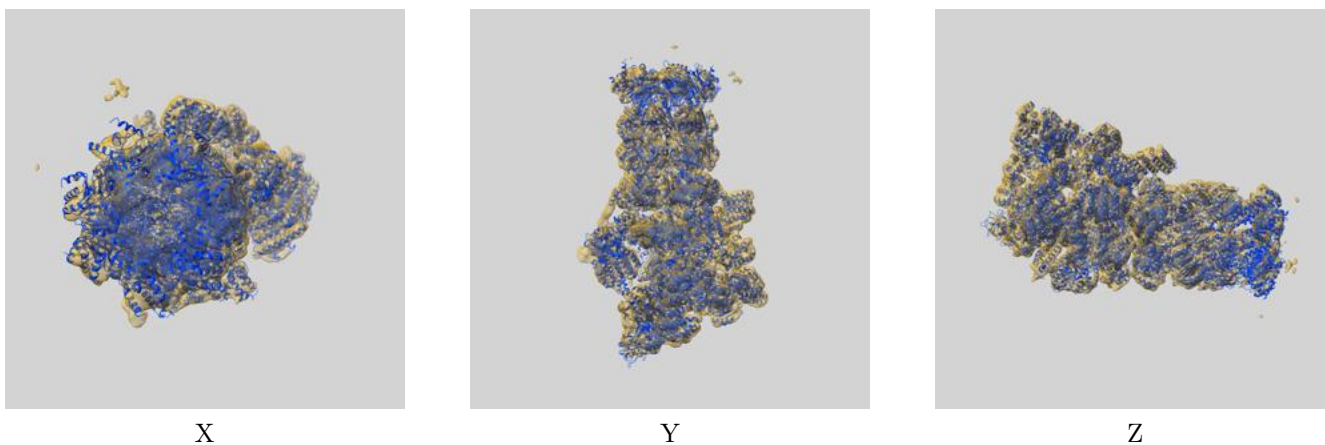
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

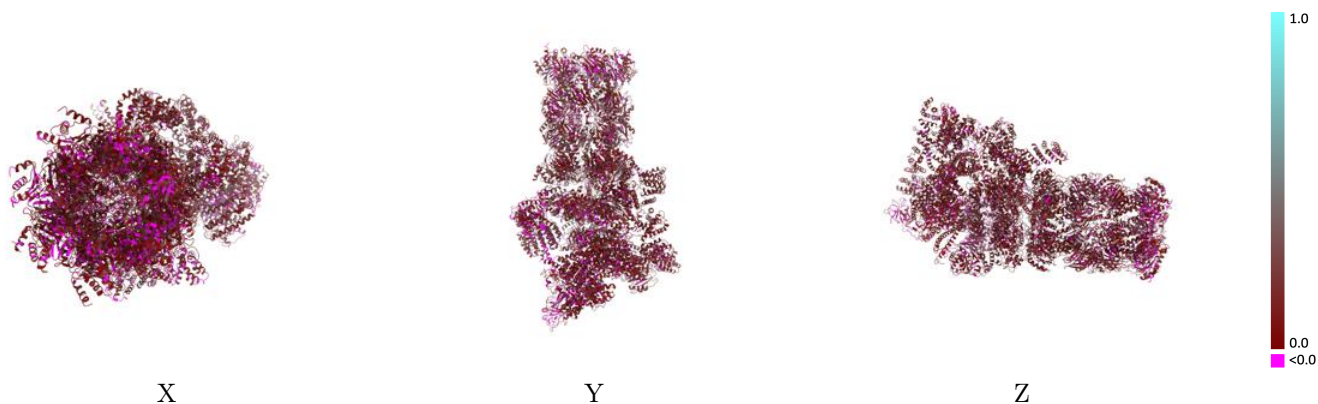
This section contains information regarding the fit between EMDB map EMD-14084 and PDB model 7QO5. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



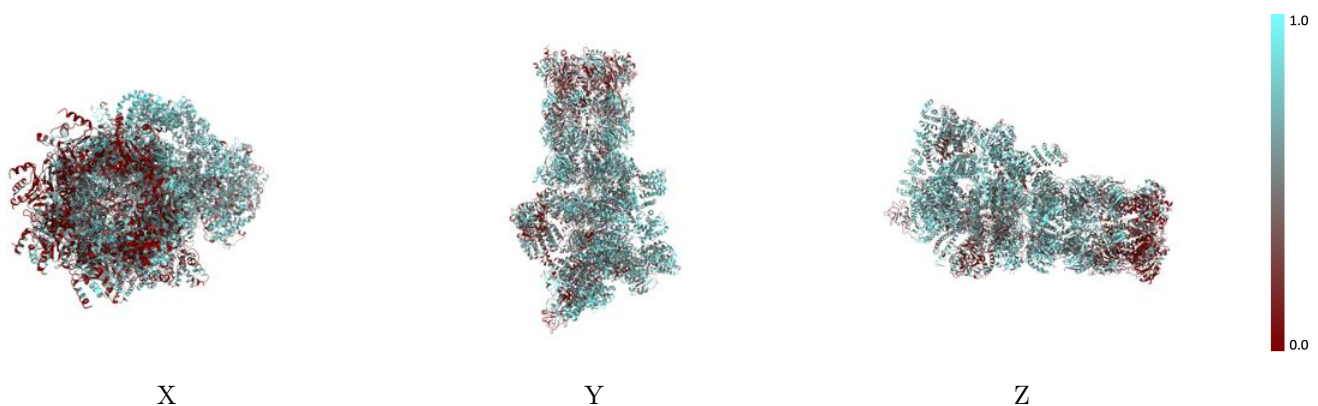
The images above show the 3D surface view of the map at the recommended contour level 4.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



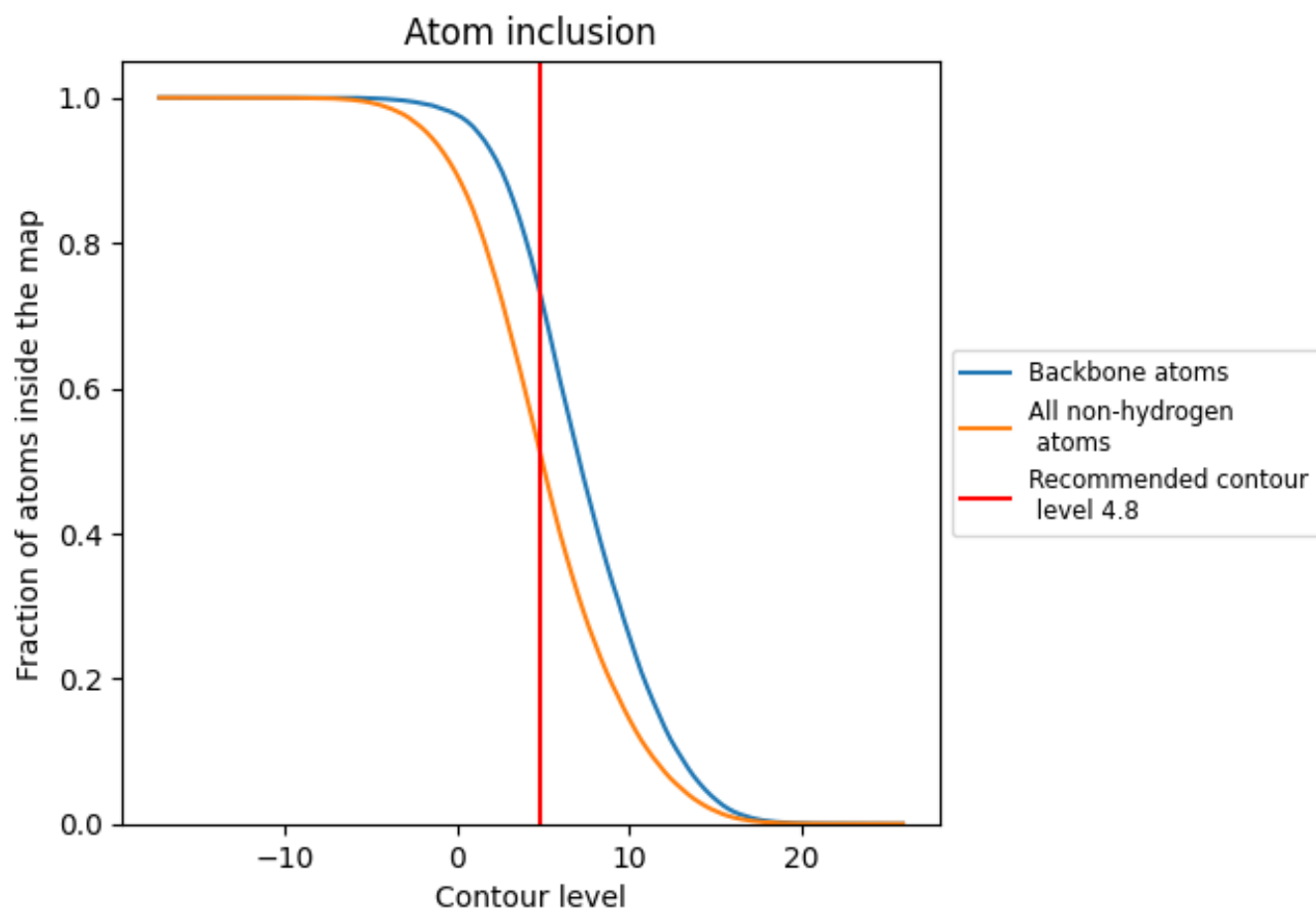
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.8).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 74% of all backbone atoms, 52% 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 (4.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5152	 0.1330
1	 0.6408	 0.1550
2	 0.6092	 0.1530
3	 0.5649	 0.1330
4	 0.6211	 0.1550
5	 0.6128	 0.1530
6	 0.5859	 0.1500
7	 0.5990	 0.1490
8	 0.3036	 0.1120
9	 0.3024	 0.1250
A	 0.6291	 0.1590
B	 0.5583	 0.1500
C	 0.5996	 0.1460
D	 0.6322	 0.1530
E	 0.6201	 0.1490
F	 0.6452	 0.1570
G	 0.6286	 0.1600
H	 0.5028	 0.1450
I	 0.4682	 0.1390
J	 0.5021	 0.1300
K	 0.4928	 0.1420
L	 0.5573	 0.1430
M	 0.5362	 0.1370
N	 0.6427	 0.1440
O	 0.6655	 0.1500
P	 0.7176	 0.1500
Q	 0.6425	 0.1430
R	 0.6200	 0.1310
S	 0.5585	 0.1340
T	 0.5424	 0.1320
U	 0.5840	 0.1430
V	 0.5944	 0.1540
W	 0.6177	 0.1360
X	 0.1945	 0.0320
Y	 0.3333	 0.0640



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Chain	Atom inclusion	Q-score
Z	 0.3947	 0.0860
a	 0.2822	 0.1120
b	 0.1854	 0.0940
c	 0.3017	 0.1030
d	 0.3606	 0.1140
e	 0.2930	 0.1050
f	 0.3807	 0.1130
g	 0.2863	 0.1080
h	 0.4919	 0.1430
i	 0.3483	 0.1300
j	 0.3779	 0.1250
k	 0.5124	 0.1370
l	 0.4375	 0.1230
m	 0.4309	 0.1250
n	 0.4889	 0.1440