



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:37 AM UTC

PDB ID : 7QO6 / pdb_00007qo6
EMDB ID : EMD-14085
Title : 26S proteasome Rpt1-RK -Ubp6-UbVS complex in the s2 state
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsassner, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on : 2021-12-23
Resolution : 6.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

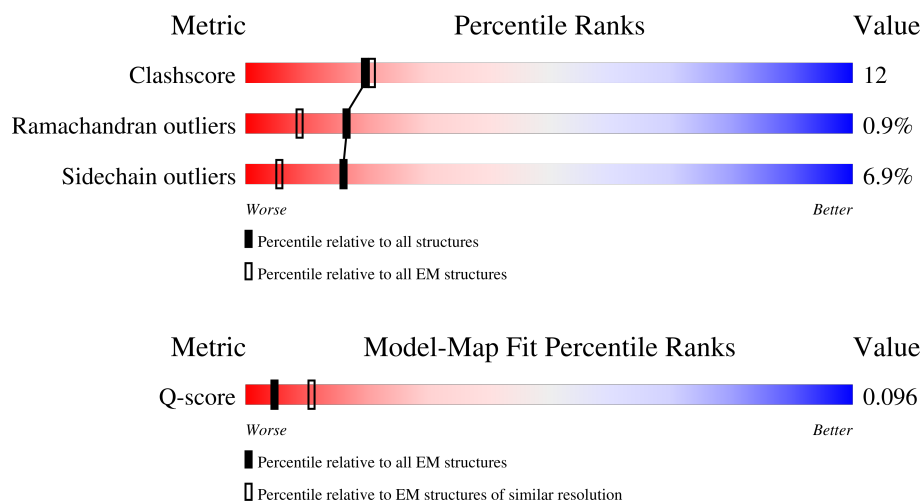
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 6.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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	252	15% 63% 23% 7% • •
1	a	252	80% 64% 22% 7% • •
2	B	250	23% 63% 27% 9%
2	b	250	90% 64% 26% 9%

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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	W	268	

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Mol	Chain	Length	Quality of chain
16	V	306	
17	T	274	
18	X	156	
19	Y	89	
20	Z	993	
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	
28	H	467	
29	I	437	
30	K	428	
31	L	437	
32	M	434	
33	J	405	
34	8	499	
35	9	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	GLZ	9	76	-	-	X	-
36	ATP	H	501	-	-	X	-
36	ATP	I	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	ATP	L	501	-	-	X	-
36	ATP	M	501	-	-	X	-
38	ADP	J	501	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 112930 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 BJ4_G0020160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	242	Total	C	N	O	S	0	0
			1912	1217	321	366	8		
1	A	242	Total	C	N	O	S	0	0
			1912	1217	321	366	8		

- Molecule 2 is a protein called HLJ1_G0039880.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
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 BJ4_G0021480.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
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 HLJ1_G0048980.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
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 EM14S01-3B_G0035190.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	249	Total	C	N	O	S	0	0
			1925	1204	324	390	7		
5	E	249	Total	C	N	O	S	0	0
			1925	1204	324	390	7		

- Molecule 6 is a protein called BJ4_G0043800.mRNA.1.CDS.1.

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 endopeptidase complex.

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 endopeptidase complex.

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.

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	l	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 HLJ1_G0013750.mRNA.1.CDS.1.

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 26S proteasome regulatory subunit RPN11.

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

- Molecule 17 is a protein called EM14S01-3B_G0050020.mRNA.1.CDS.1.

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

- Molecule 18 is a protein called HLJ1_G0030700.mRNA.1.CDS.1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ARG	SER	variant	UNP A0A6A5PV22
H	166	LYS	THR	variant	UNP A0A6A5PV22

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

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

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

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

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

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

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

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

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

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

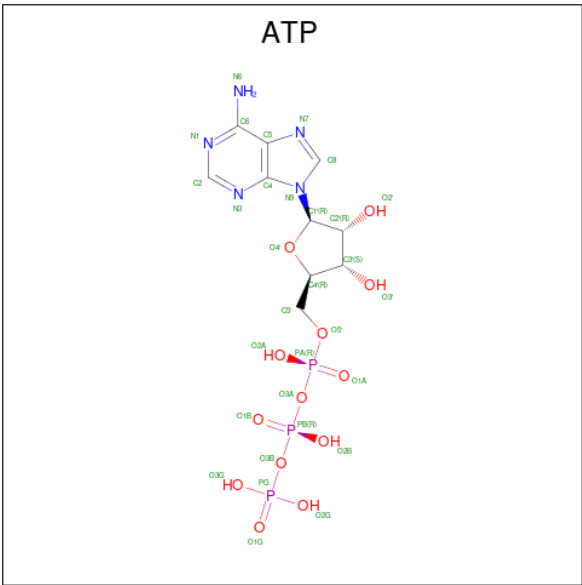
- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase.

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

- Molecule 35 is a protein called Polyubiquitin-B.

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

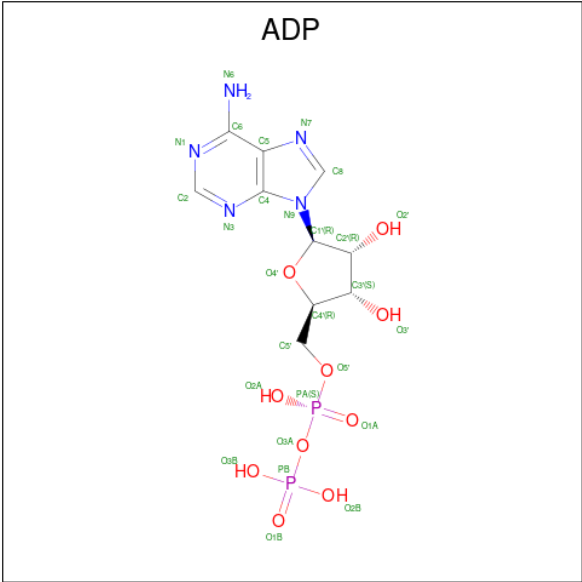


Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

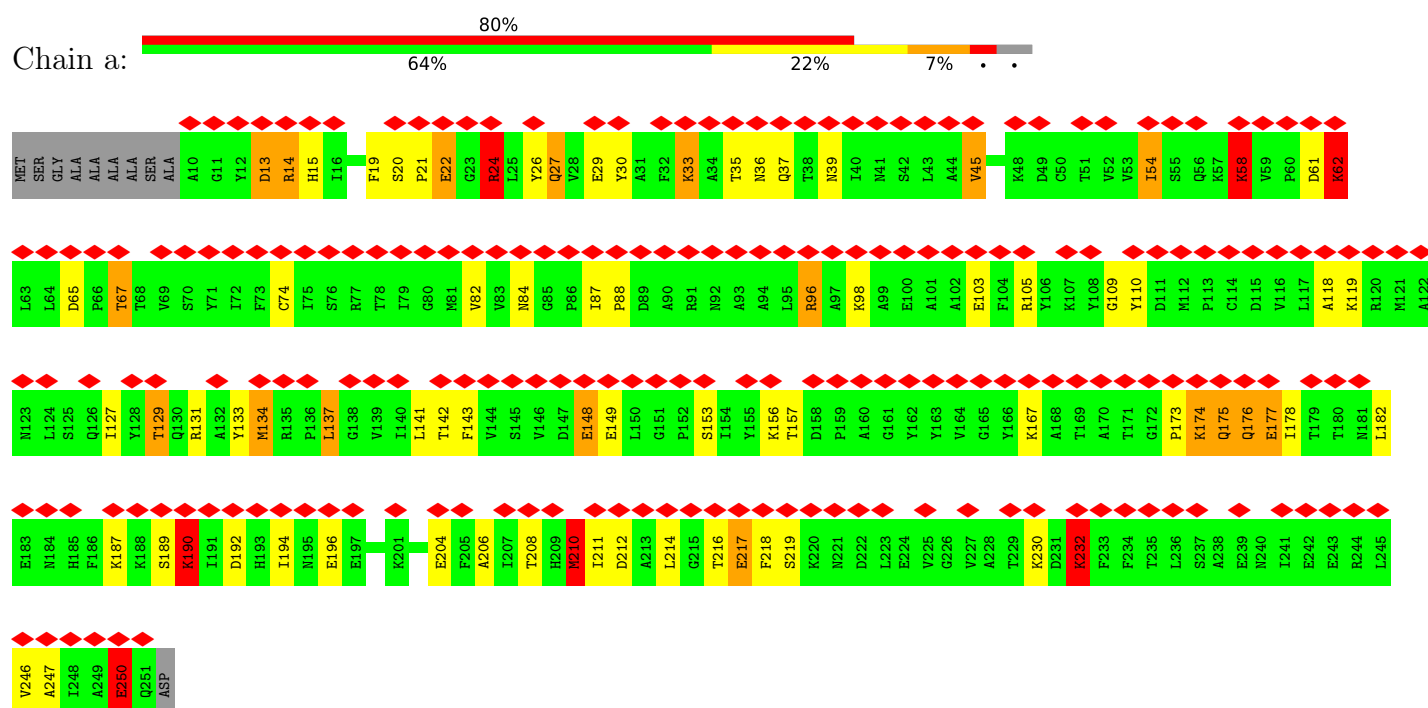


Mol	Chain	Residues	Atoms					AltConf
38	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

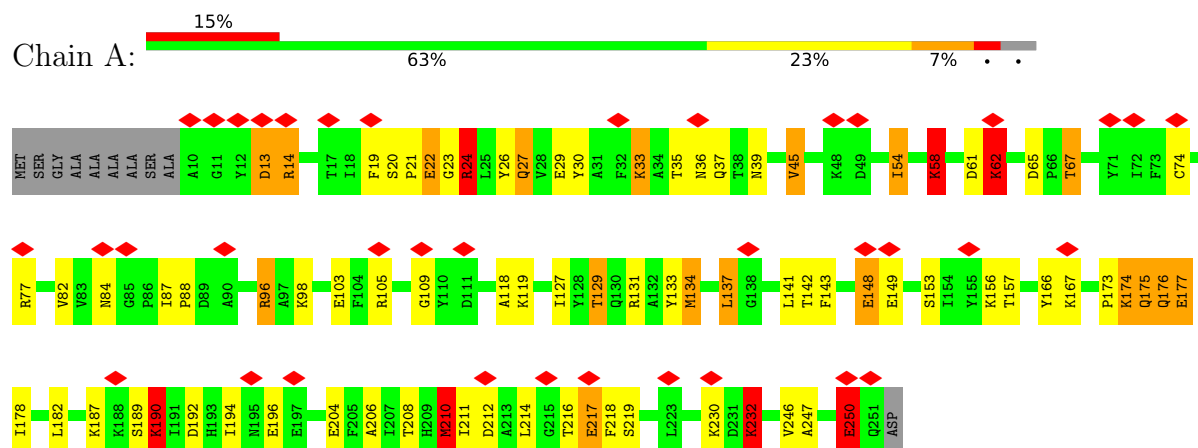
3 Residue-property plots

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

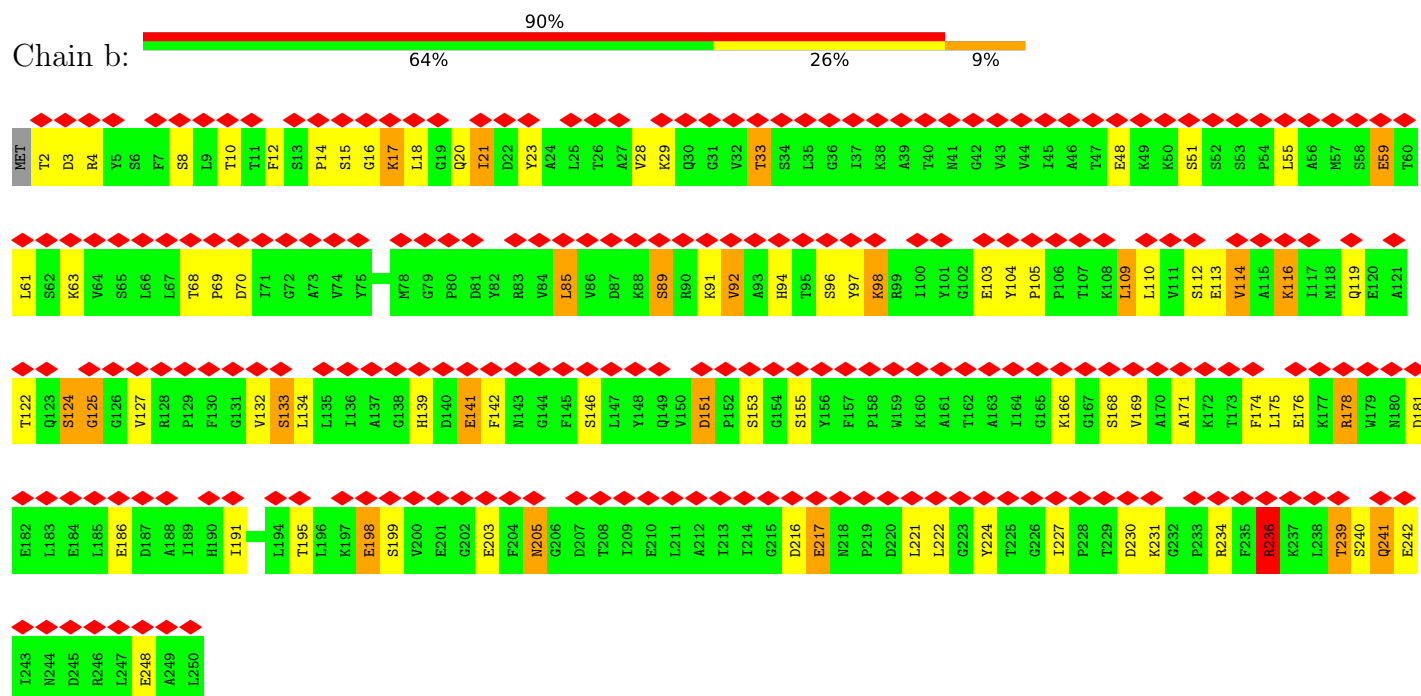
• Molecule 1: BJ4_G0020160.mRNA.1.CDS.1



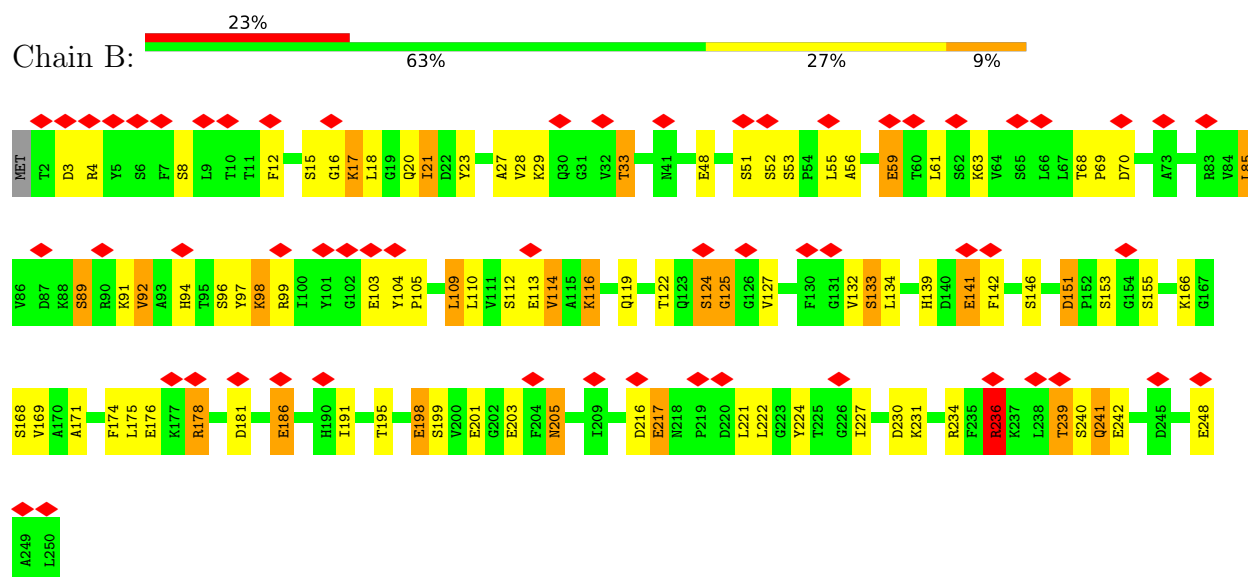
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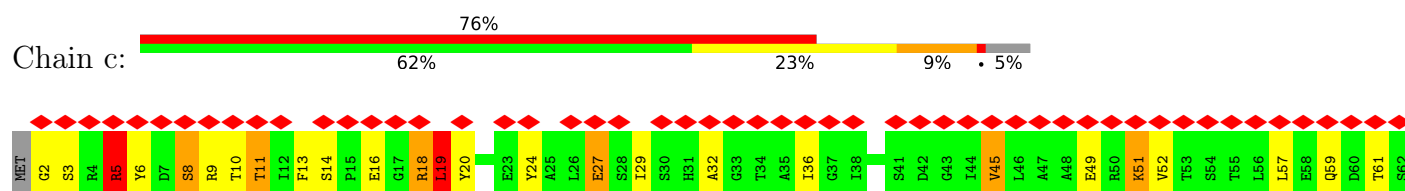
- Molecule 2: HLJ1_G0039880.mRNA.1.CDS.1

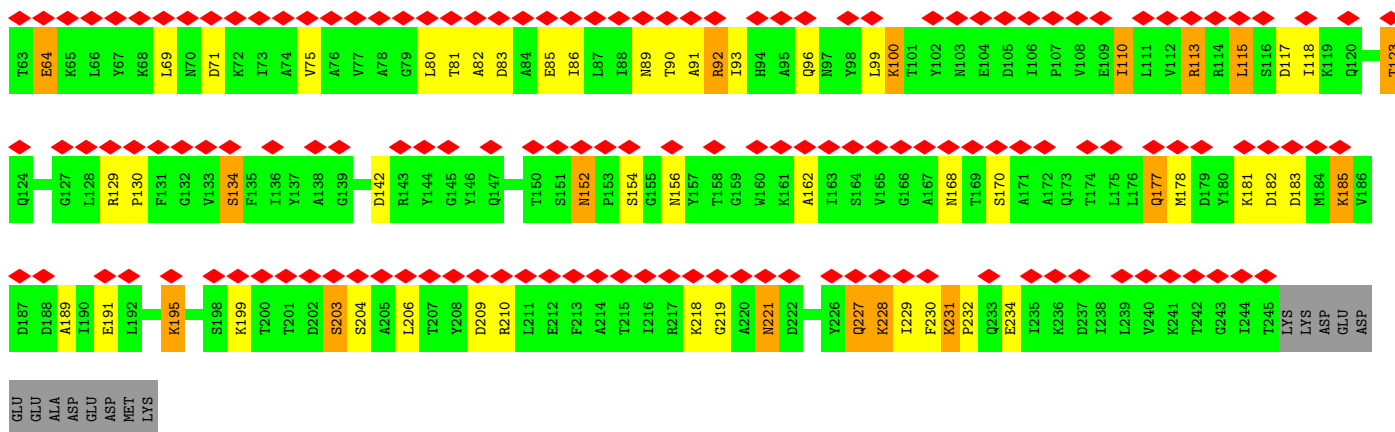


- Molecule 2: HLJ1_G0039880.mRNA.1.CDS.1

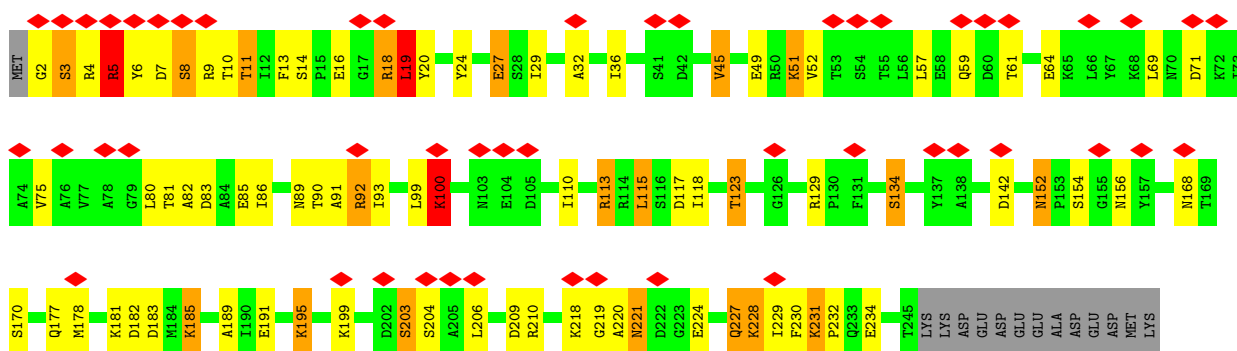


- Molecule 3: BJ4_G0021480.mRNA.1.CDS.1

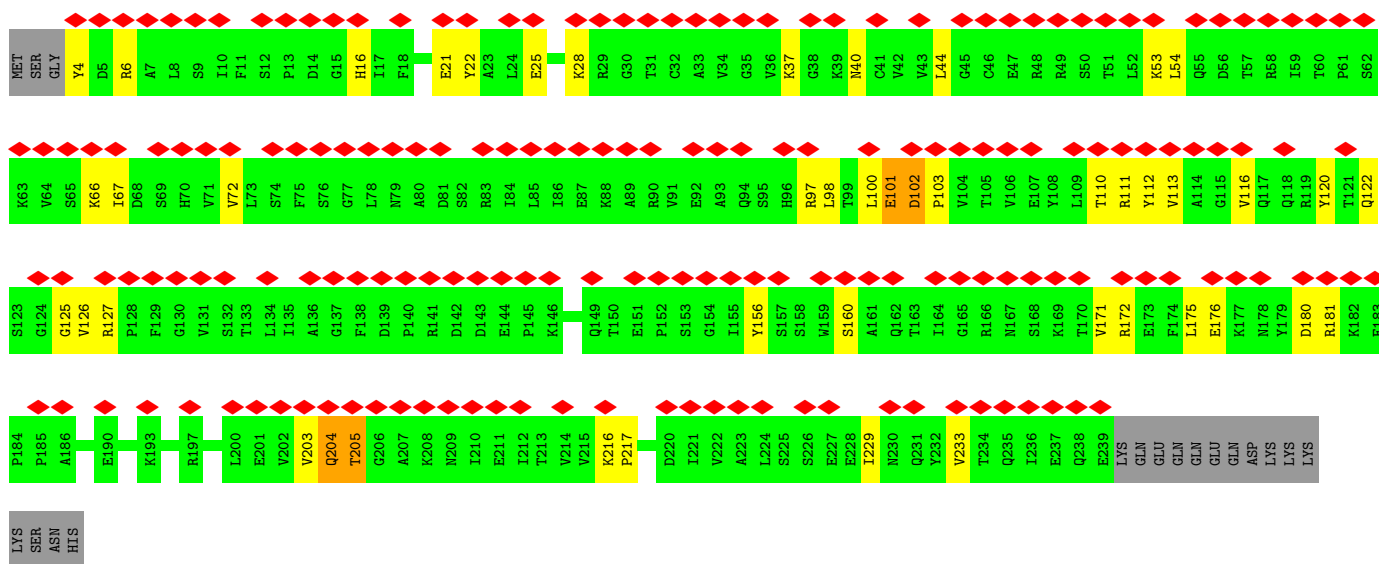
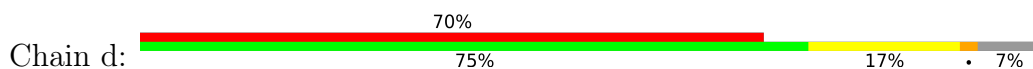




• Molecule 3: BJ4_G0021480.mRNA.1.CDS.1

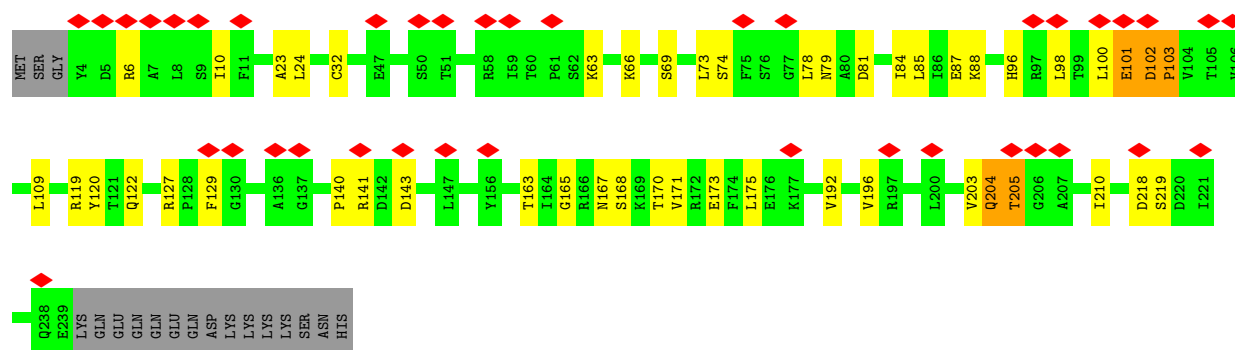


• Molecule 4: HLJ1_G0048980.mRNA.1.CDS.1



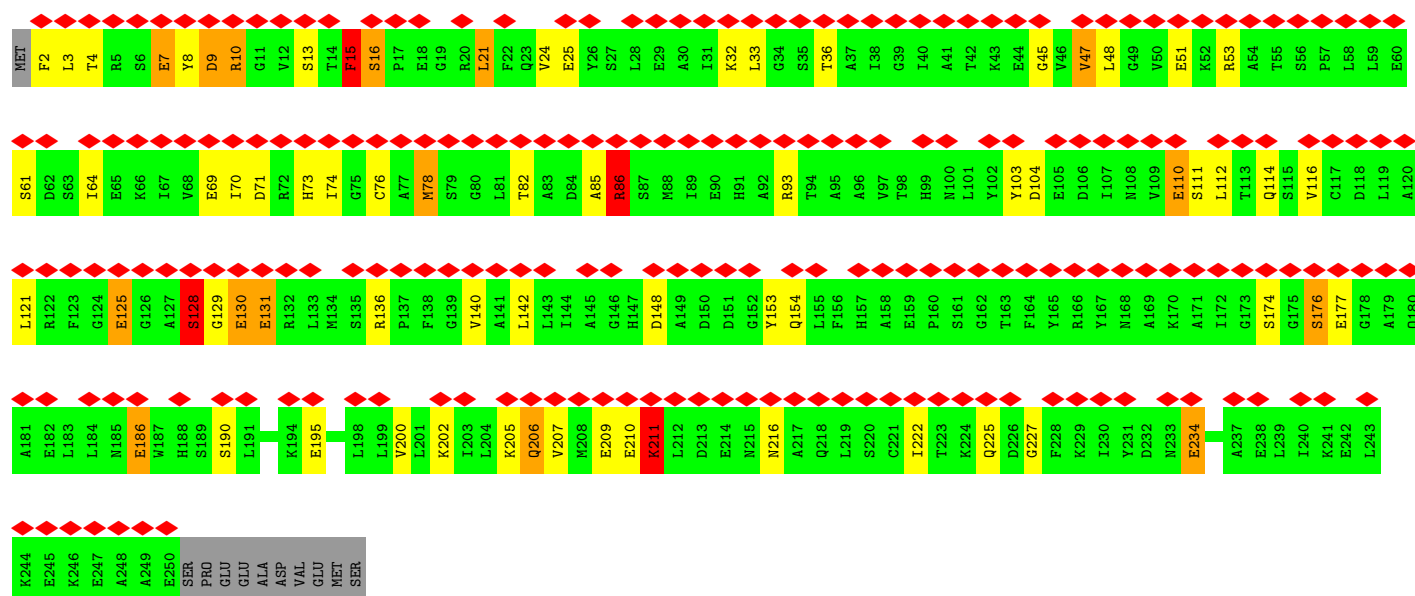
• Molecule 4: HLJ1_G0048980.mRNA.1.CDS.1

Chain D: 15% 74% 17% 7%



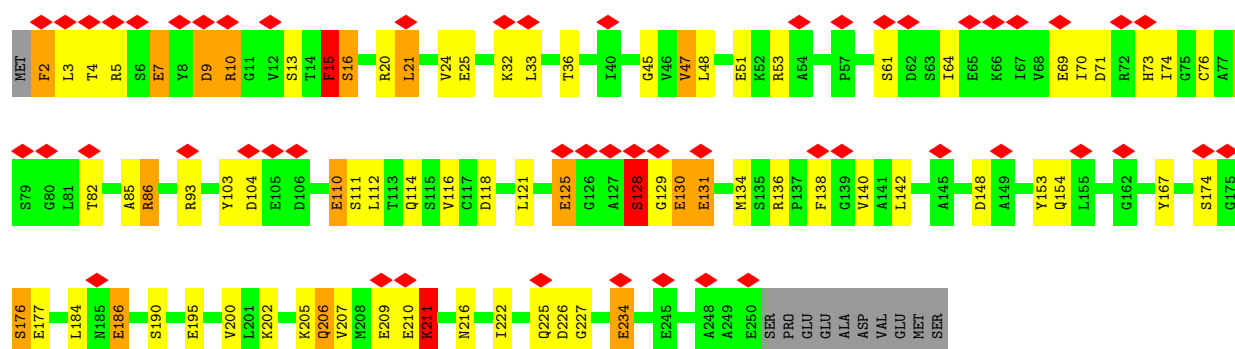
• Molecule 5: EM14S01-3B_G0035190.mRNA.1.CDS.1

Chain e: 83% 68% 20% 6%

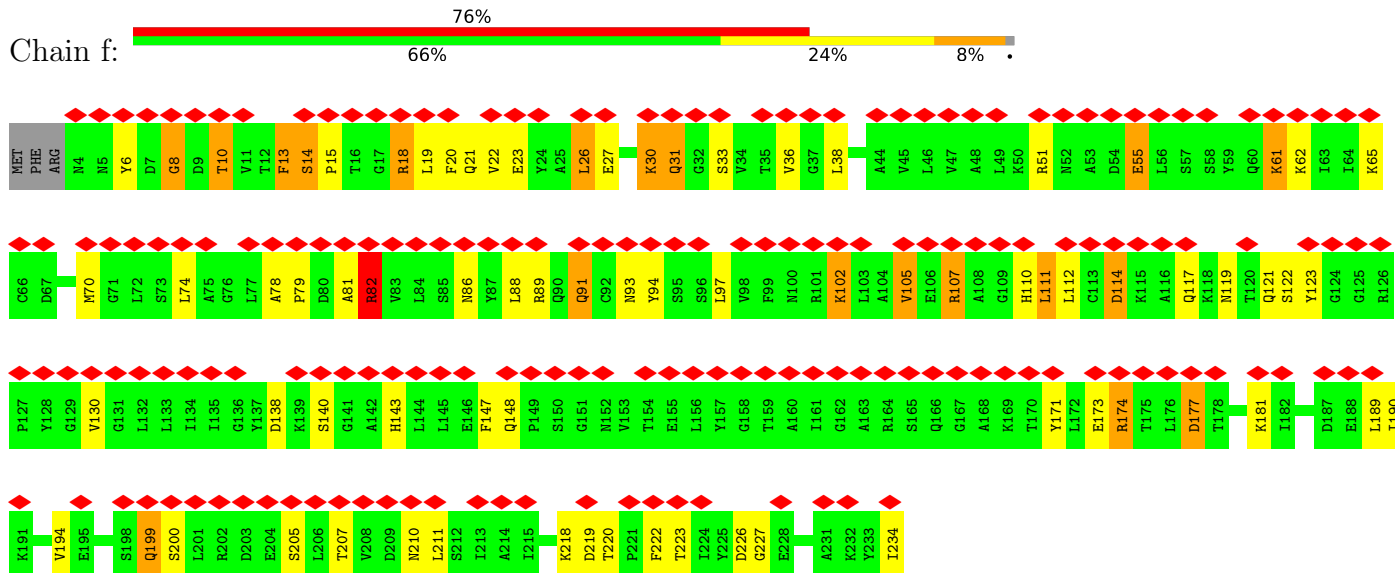


• Molecule 5: EM14S01-3B_G0035190.mRNA.1.CDS.1

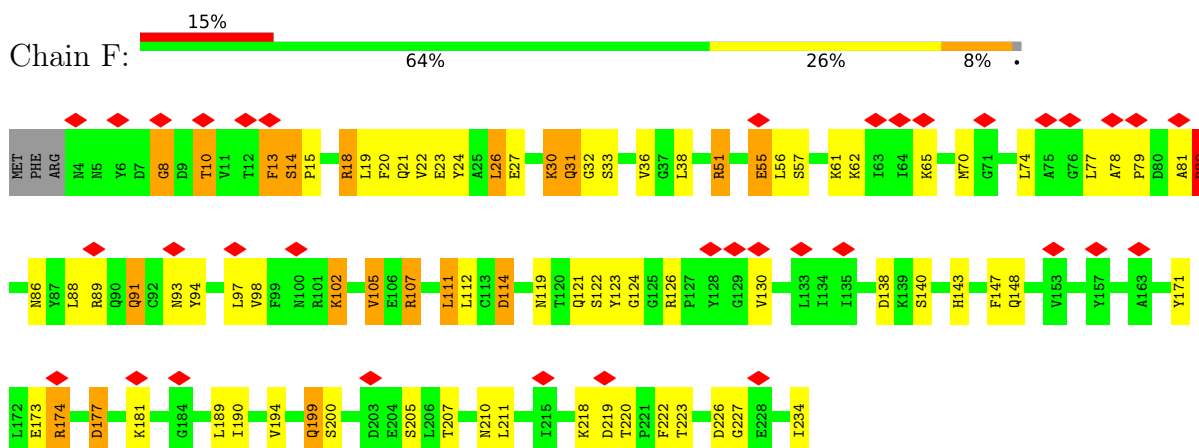
Chain E: 20% 65% 23% 7%



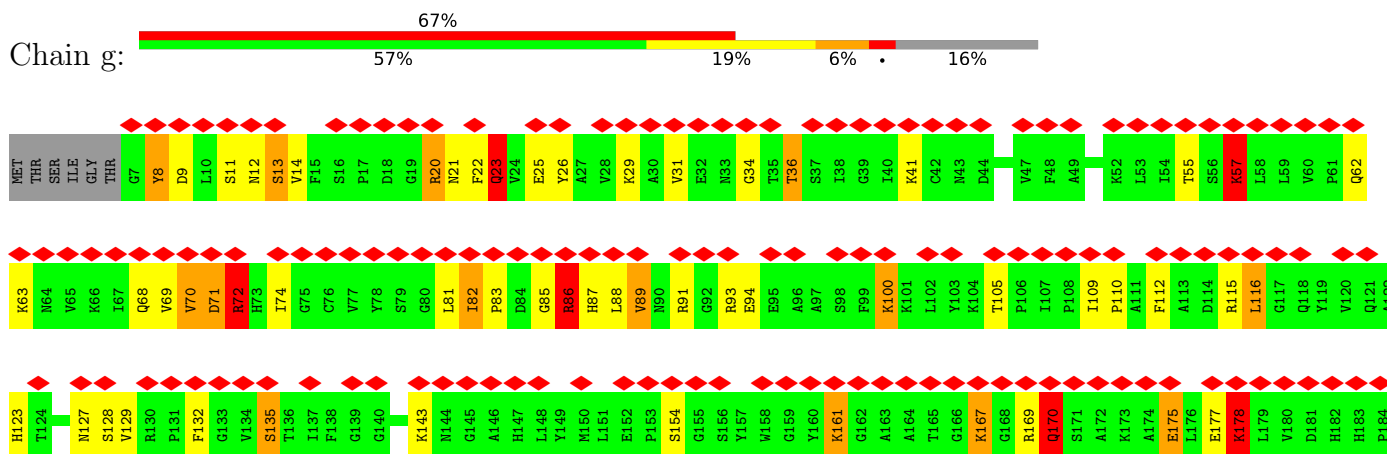
• Molecule 6: BJ4_G0043800.mRNA.1.CDS.1

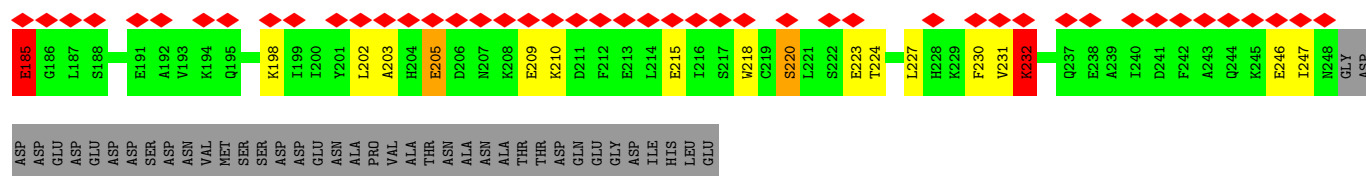


• Molecule 6: BJ4_G0043800.mRNA.1.CDS.1

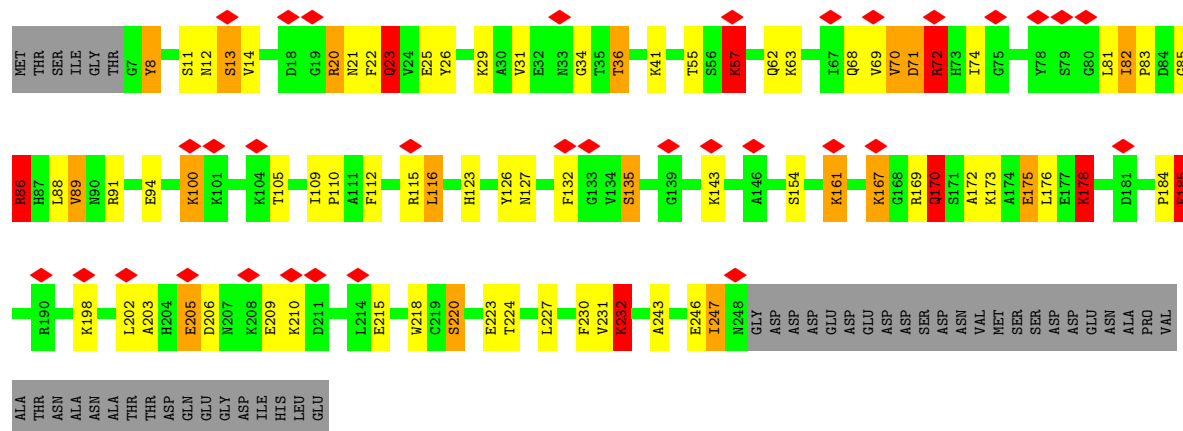


• Molecule 7: Probable proteasome subunit alpha type-7

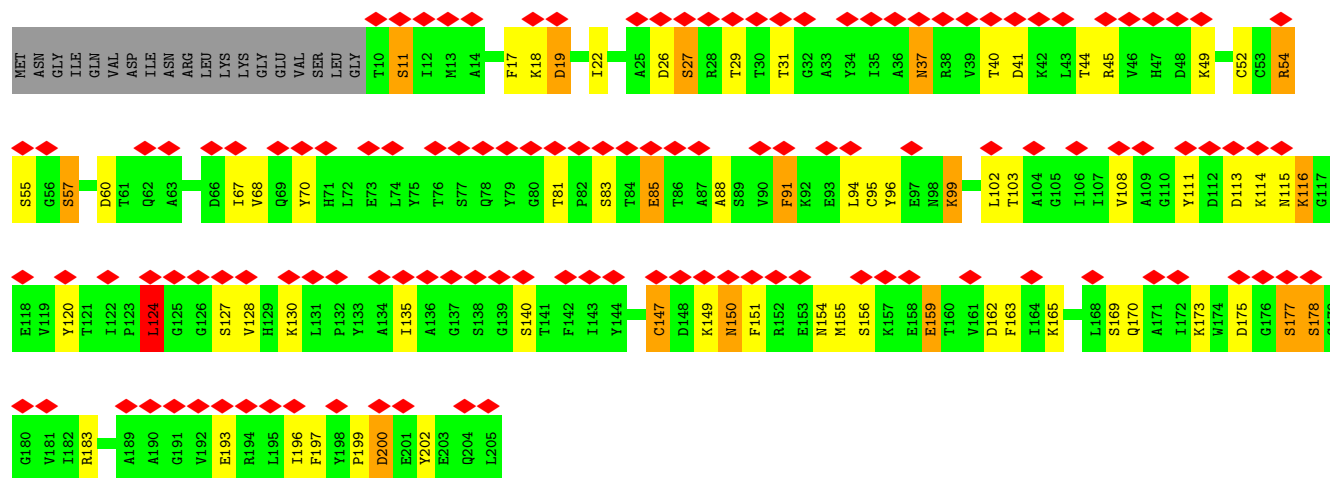




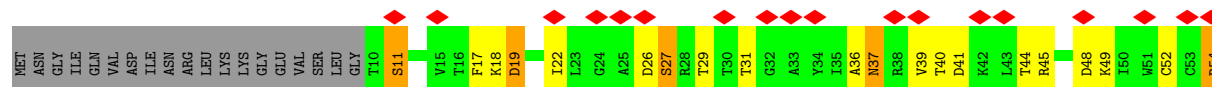
• Molecule 7: Probable proteasome subunit alpha type-7

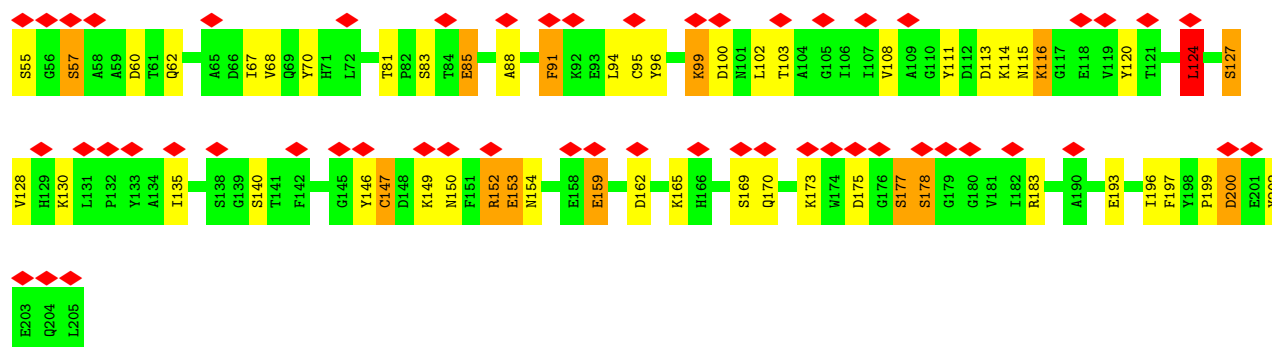


• Molecule 8: Proteasome subunit beta type-1

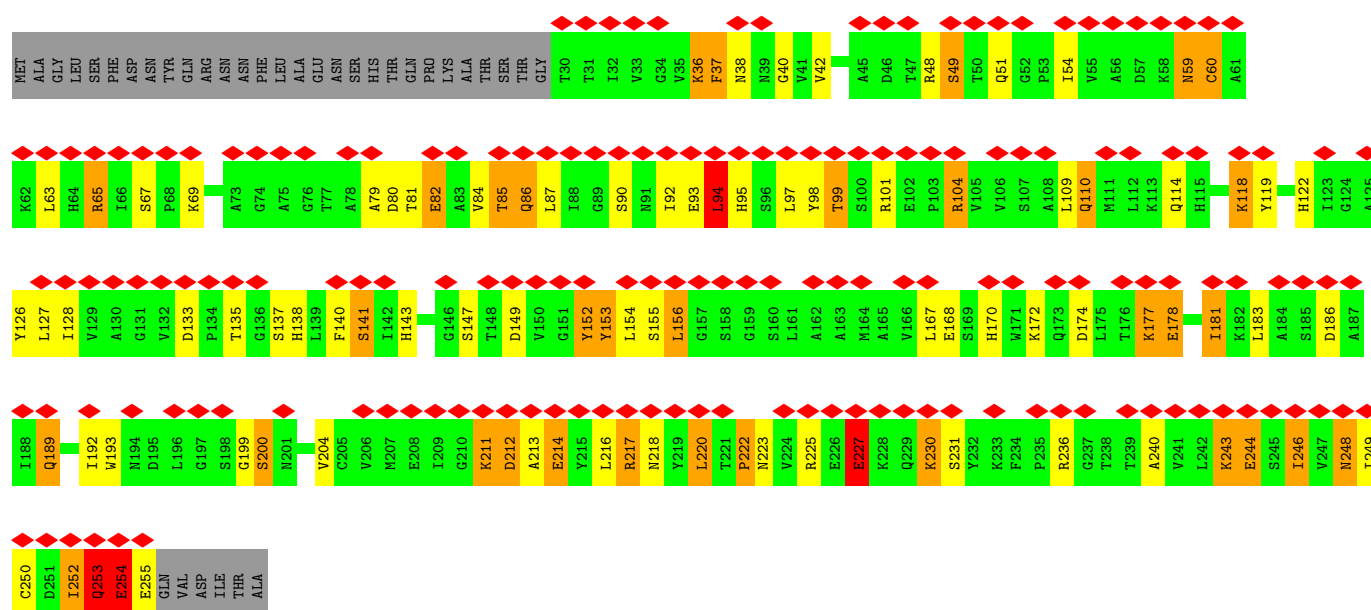


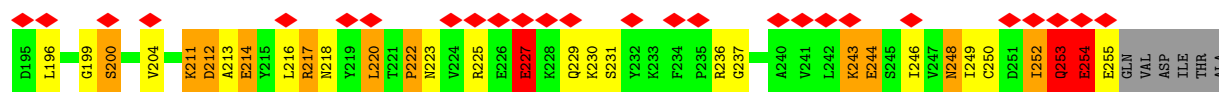
• Molecule 8: Proteasome subunit beta type-1



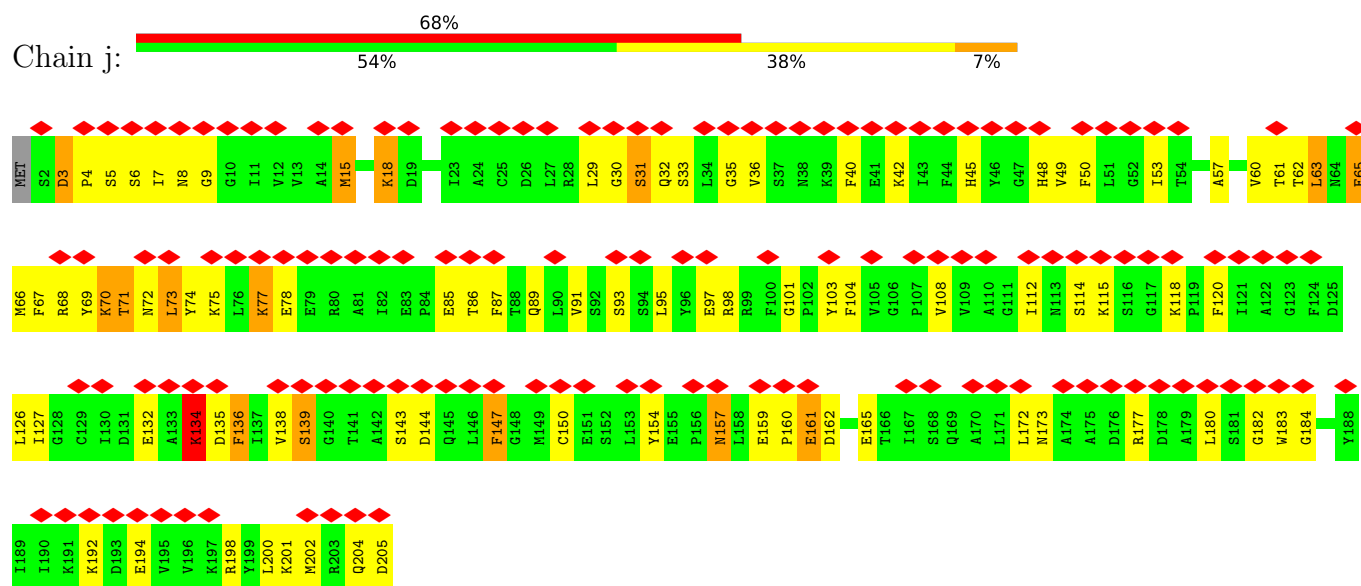


• Molecule 9: Proteasome endopeptidase complex

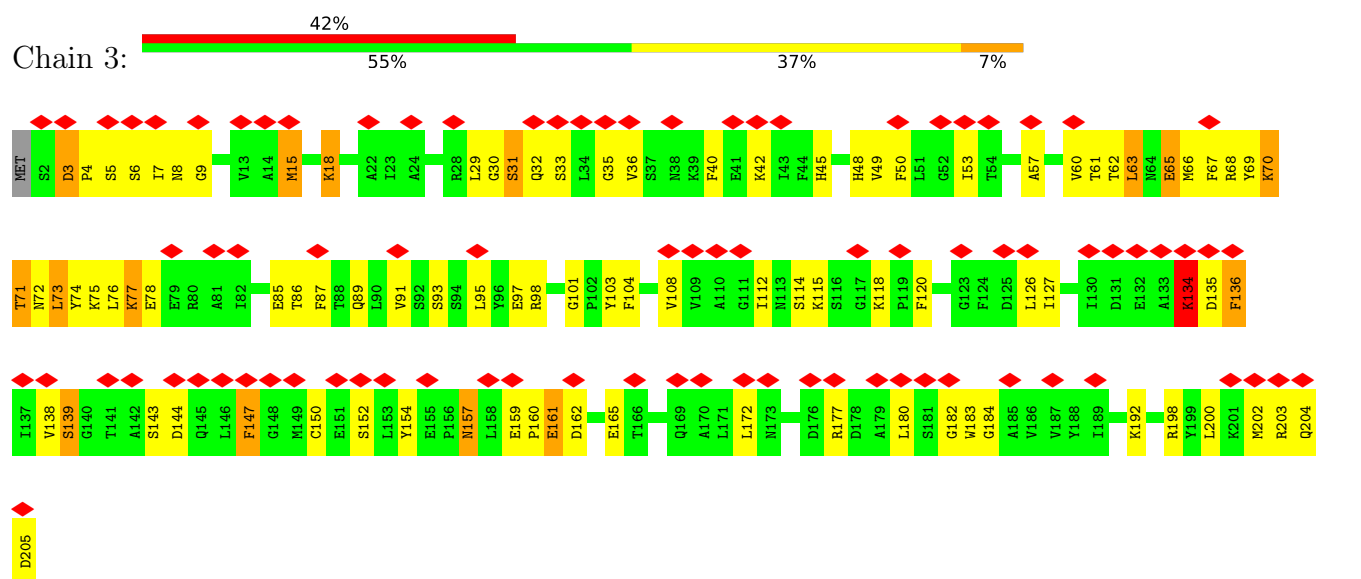




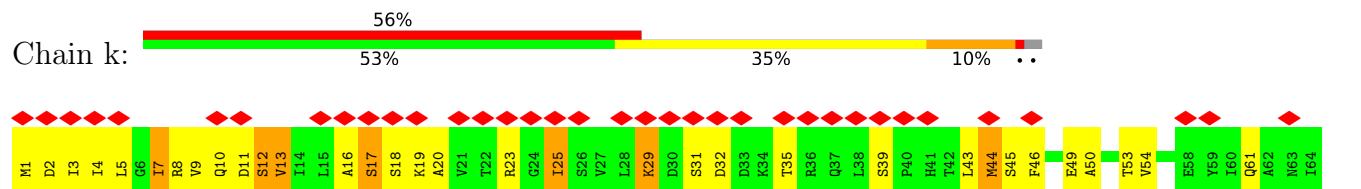
• Molecule 10: Proteasome endopeptidase complex

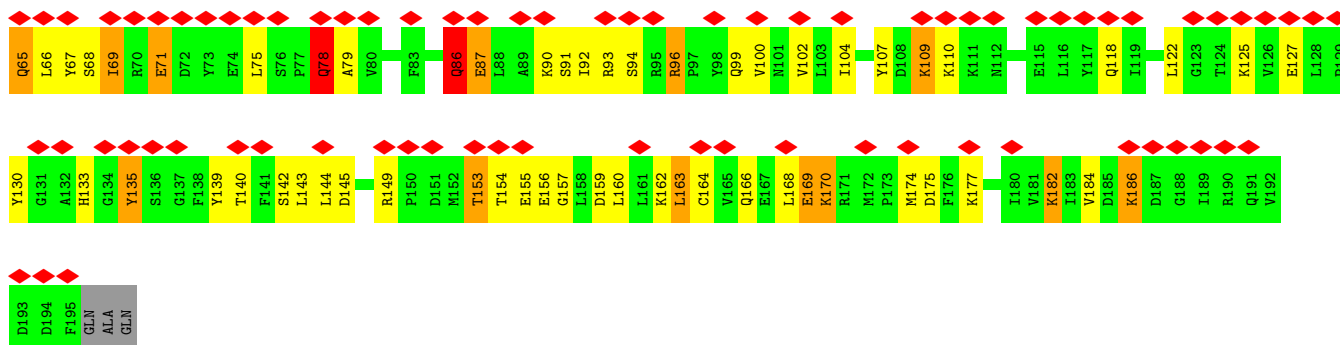


• Molecule 10: Proteasome endopeptidase complex

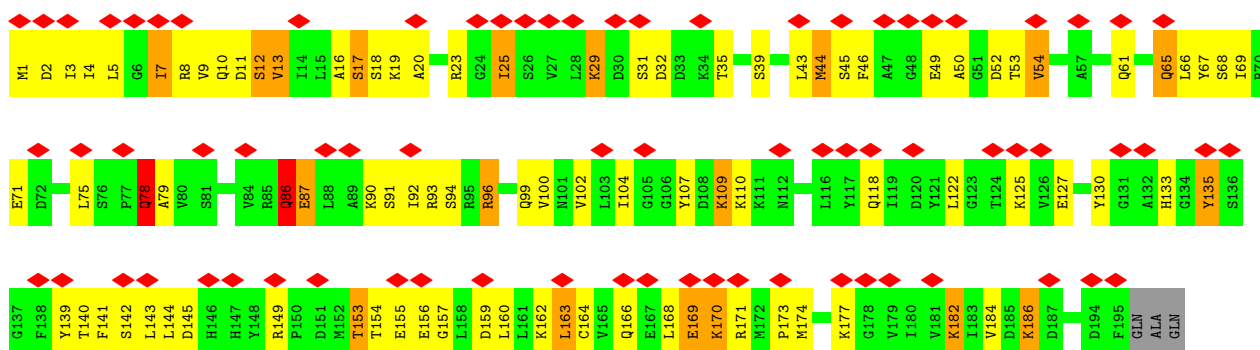


• Molecule 11: Proteasome subunit beta

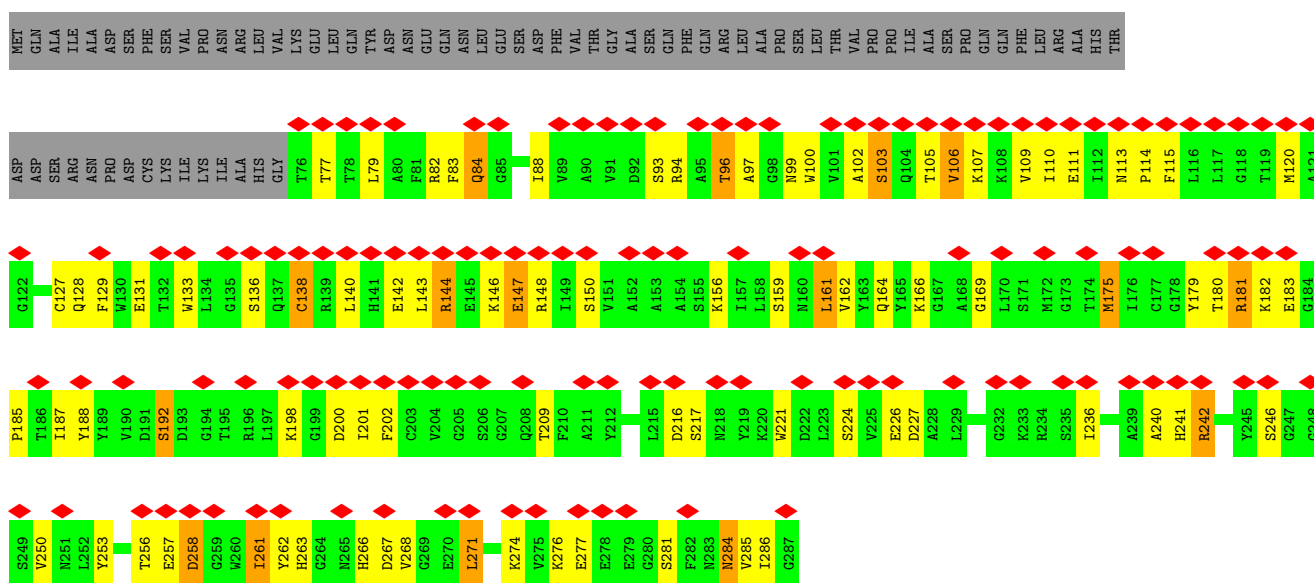




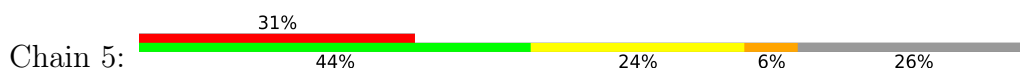
• Molecule 11: Proteasome subunit beta

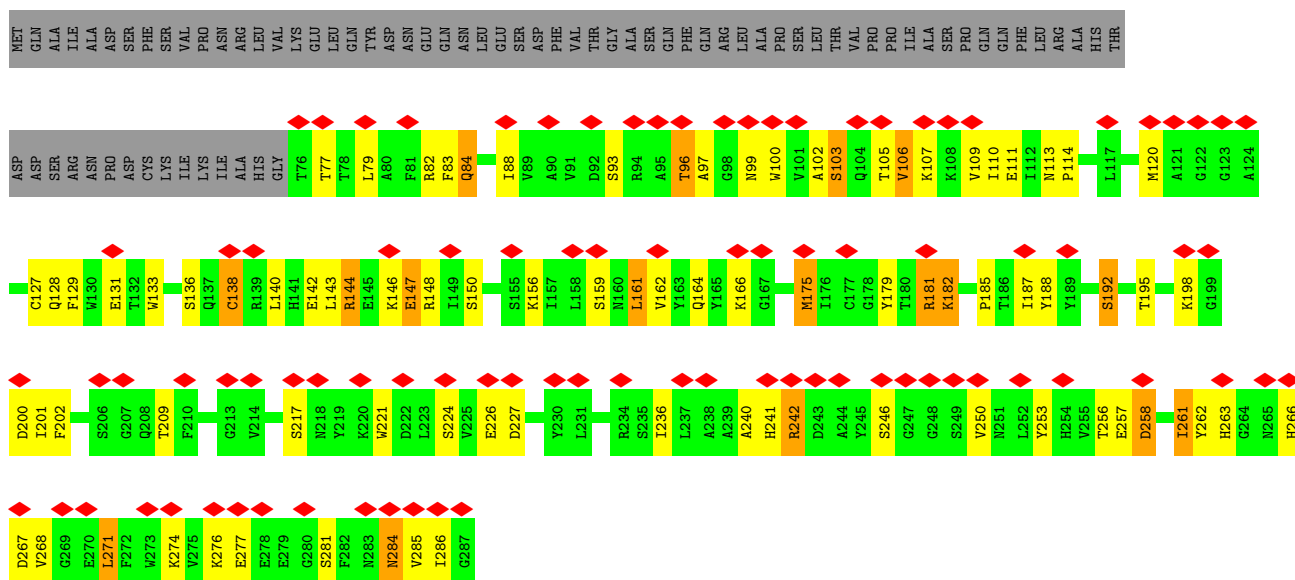


• Molecule 12: Proteasome subunit beta type-5

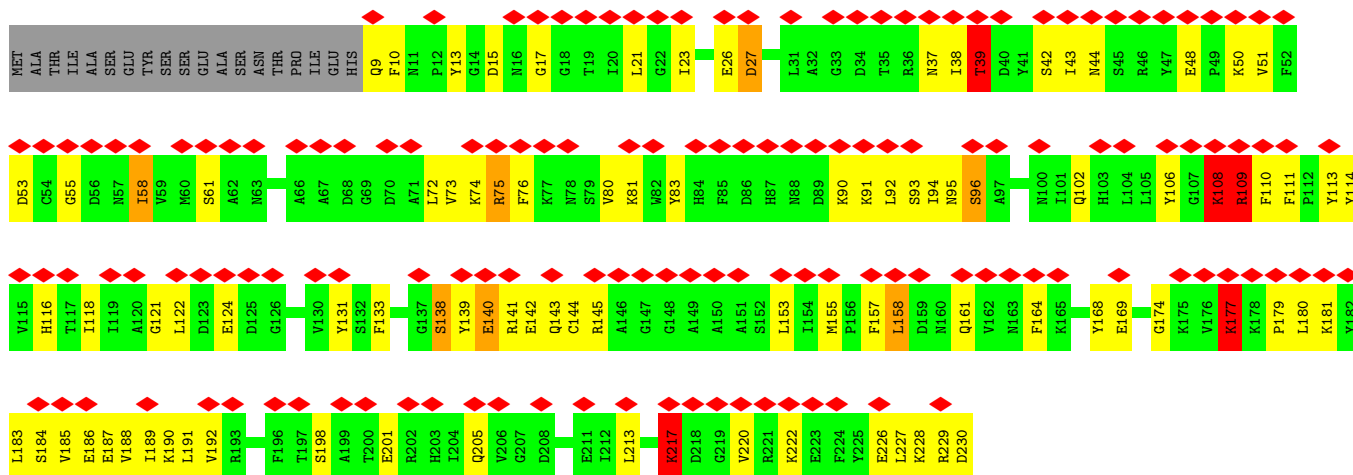


• Molecule 12: Proteasome subunit beta type-5

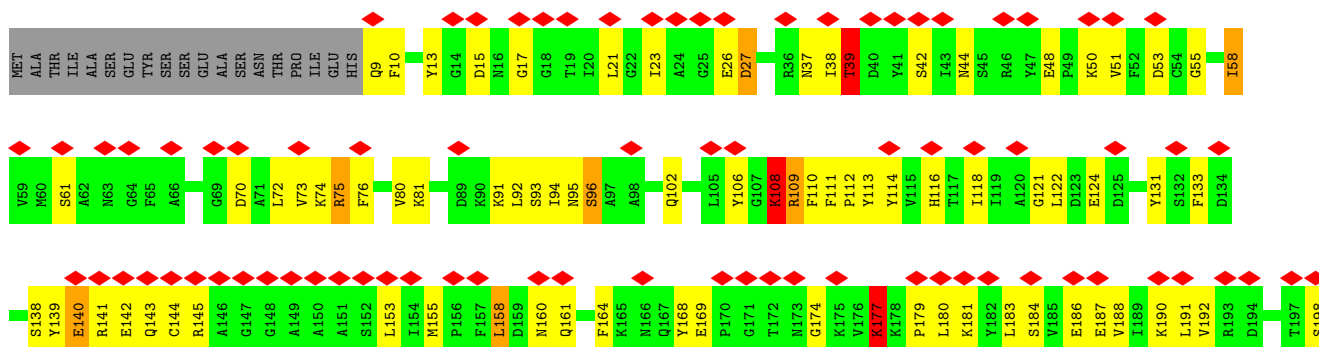
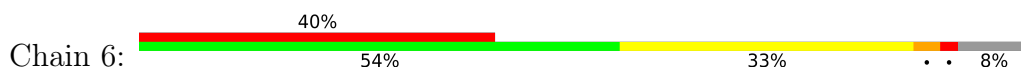


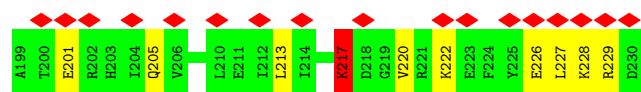


• Molecule 13: HLJ1_G0013750.mRNA.1.CDS.1

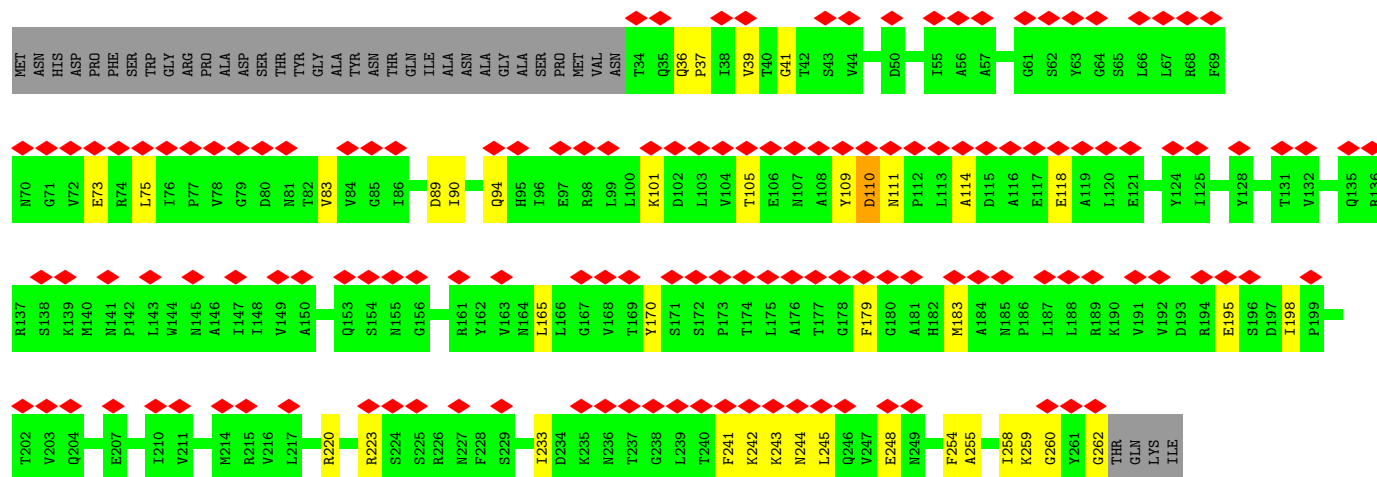
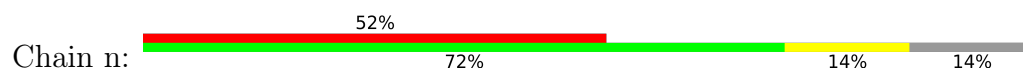


• Molecule 13: HLJ1_G0013750.mRNA.1.CDS.1

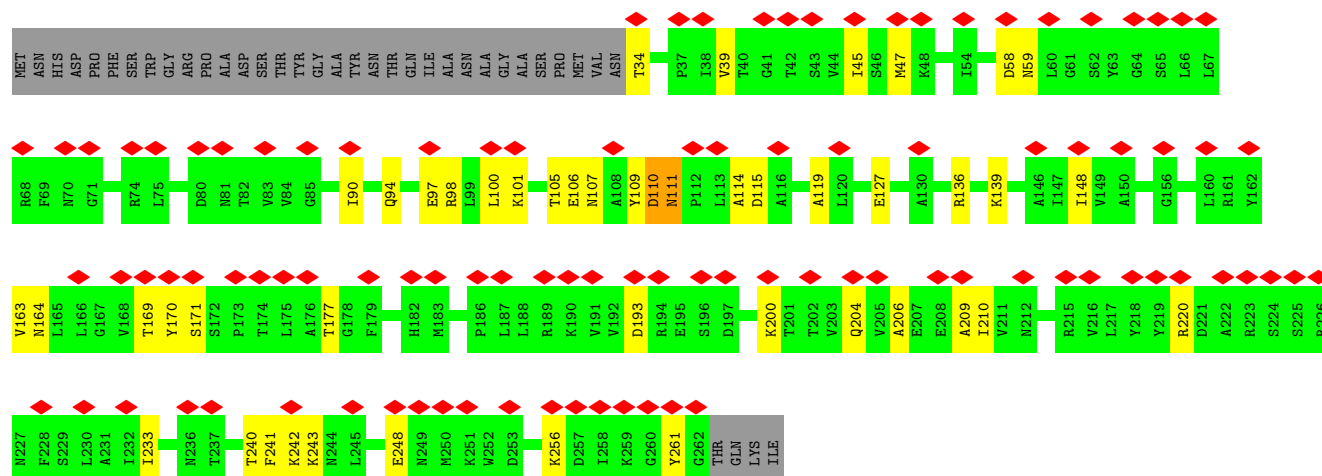




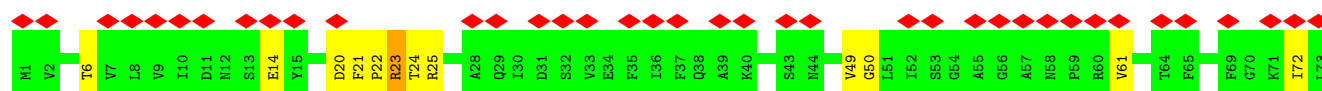
• Molecule 14: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-7

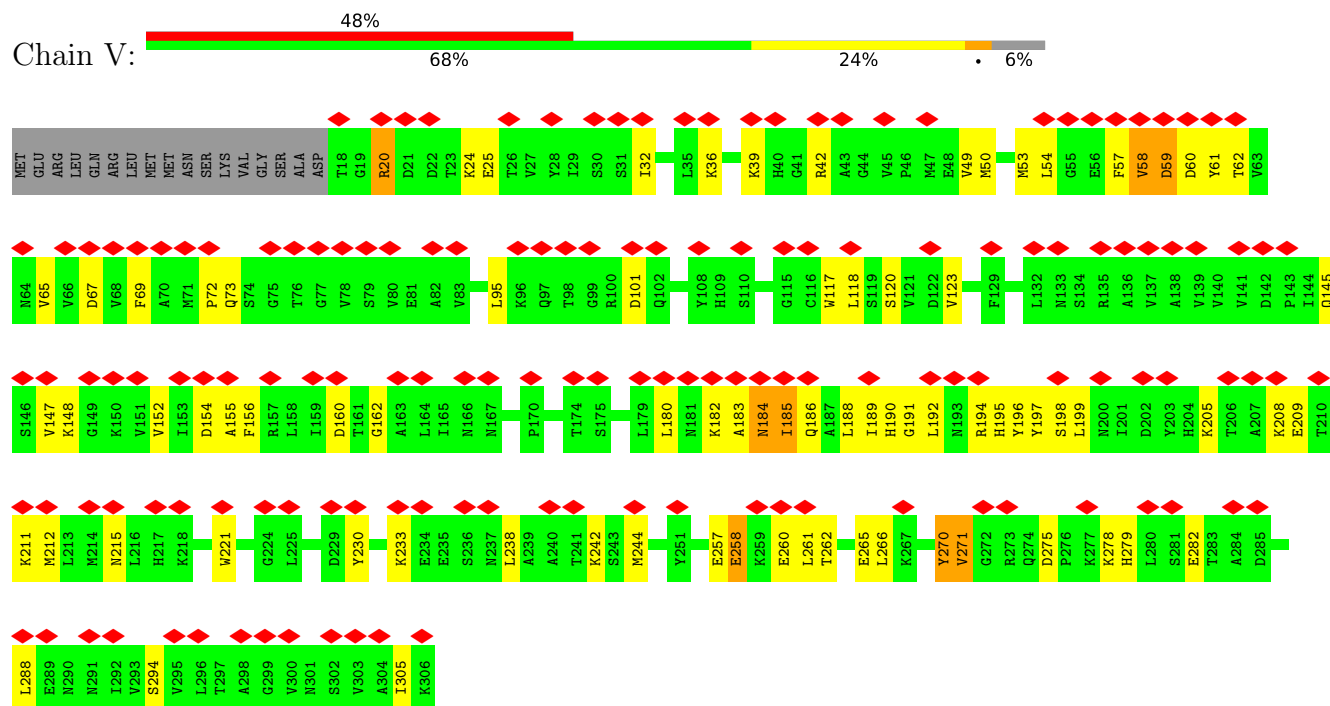


• Molecule 15: 26S proteasome regulatory subunit RPN10

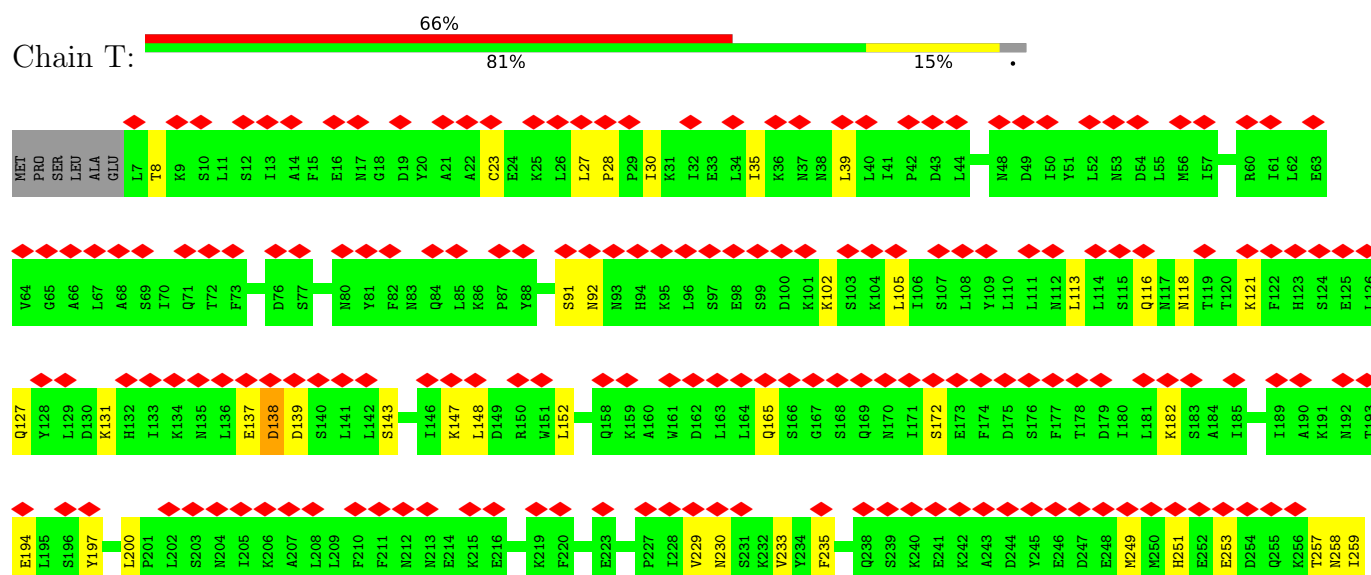


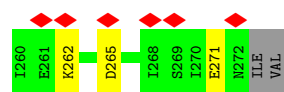


• Molecule 16: 26S proteasome regulatory subunit RPN11

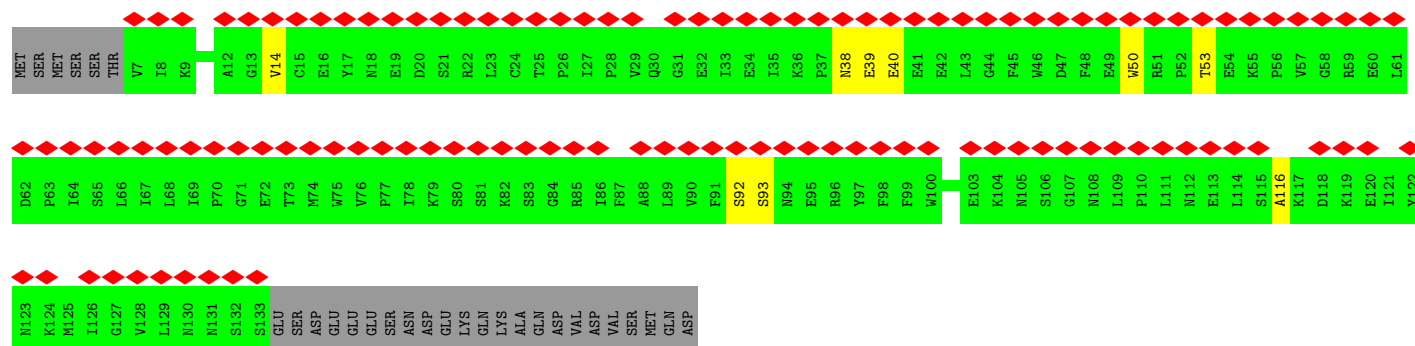
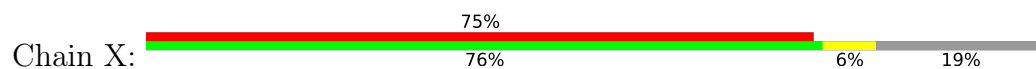


• Molecule 17: EM14S01-3B_G0050020.mRNA.1.CDS.1

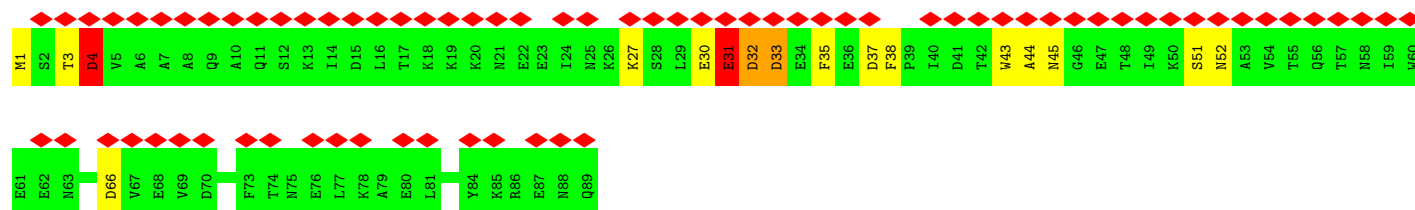
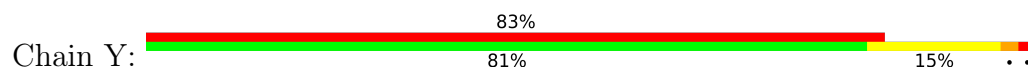




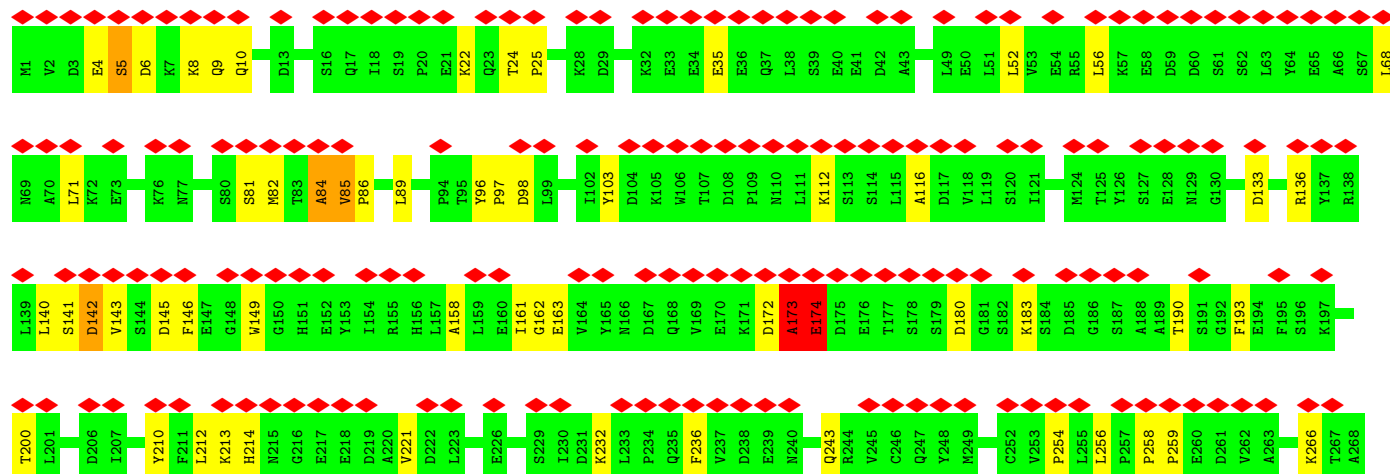
• Molecule 18: HLJ1_G0030700.mRNA.1.CDS.1

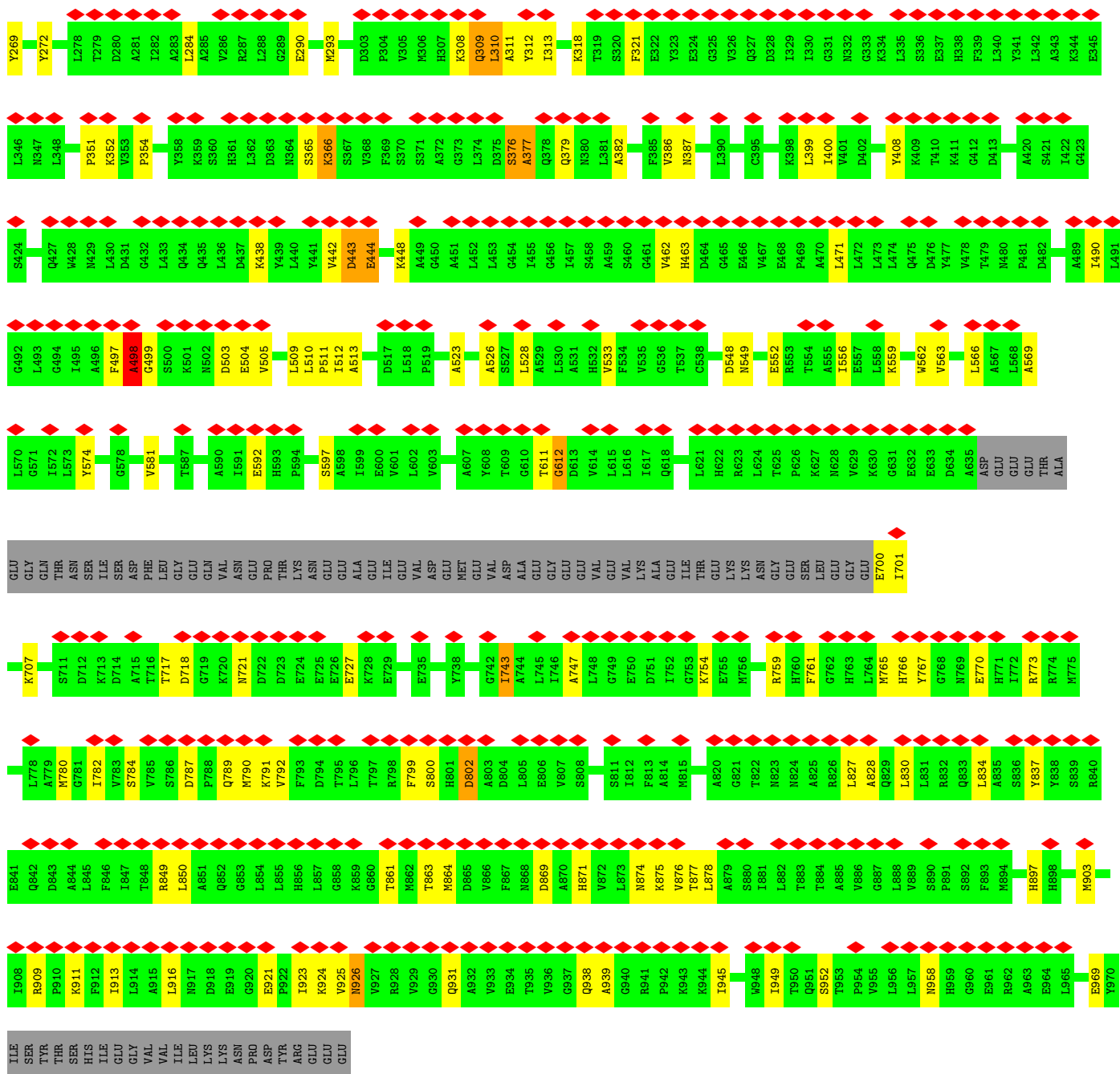


• Molecule 19: 26S proteasome complex subunit SEM1

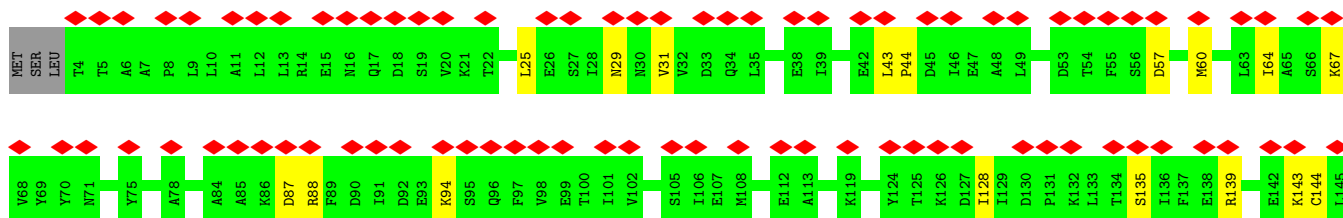
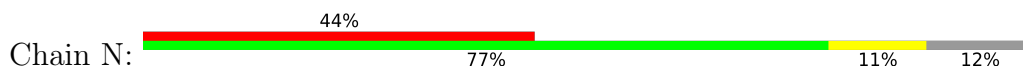


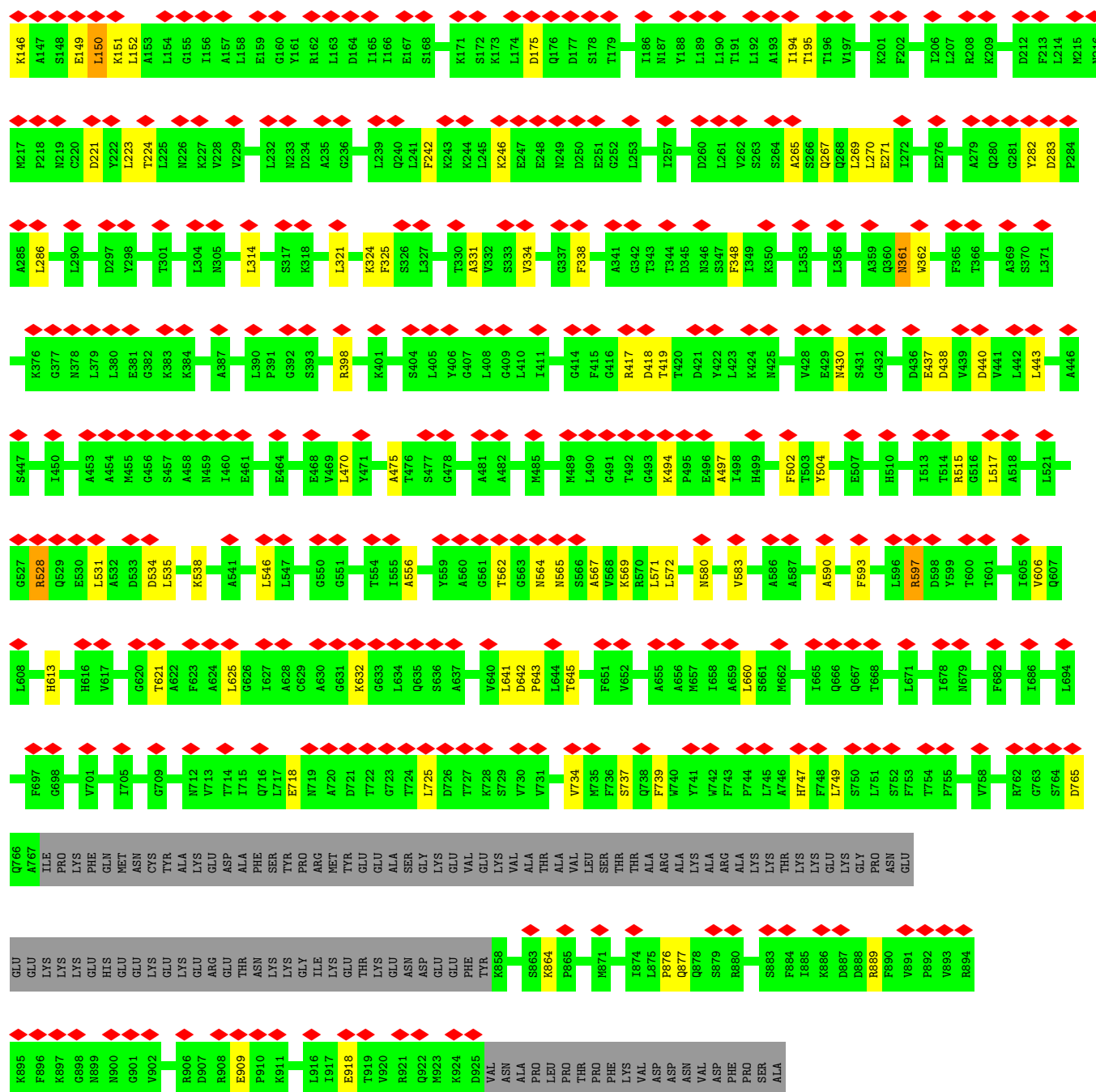
• Molecule 20: 26S proteasome regulatory subunit RPN1



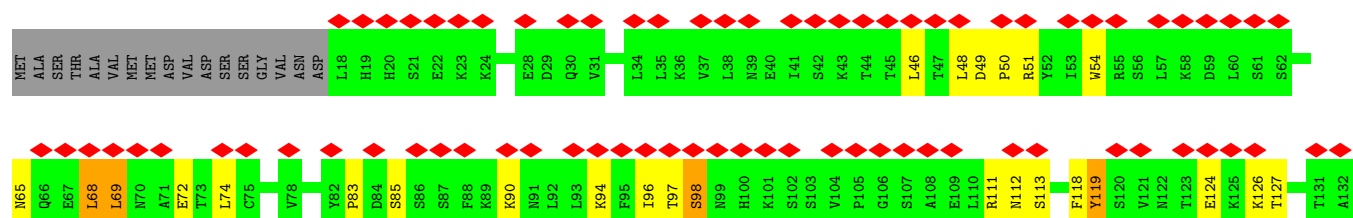
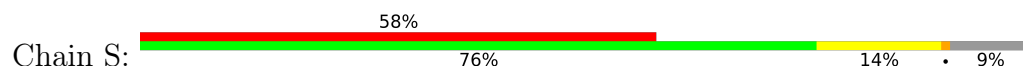


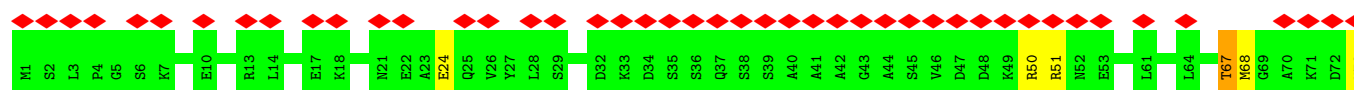
• Molecule 21: 26S proteasome regulatory subunit RPN2

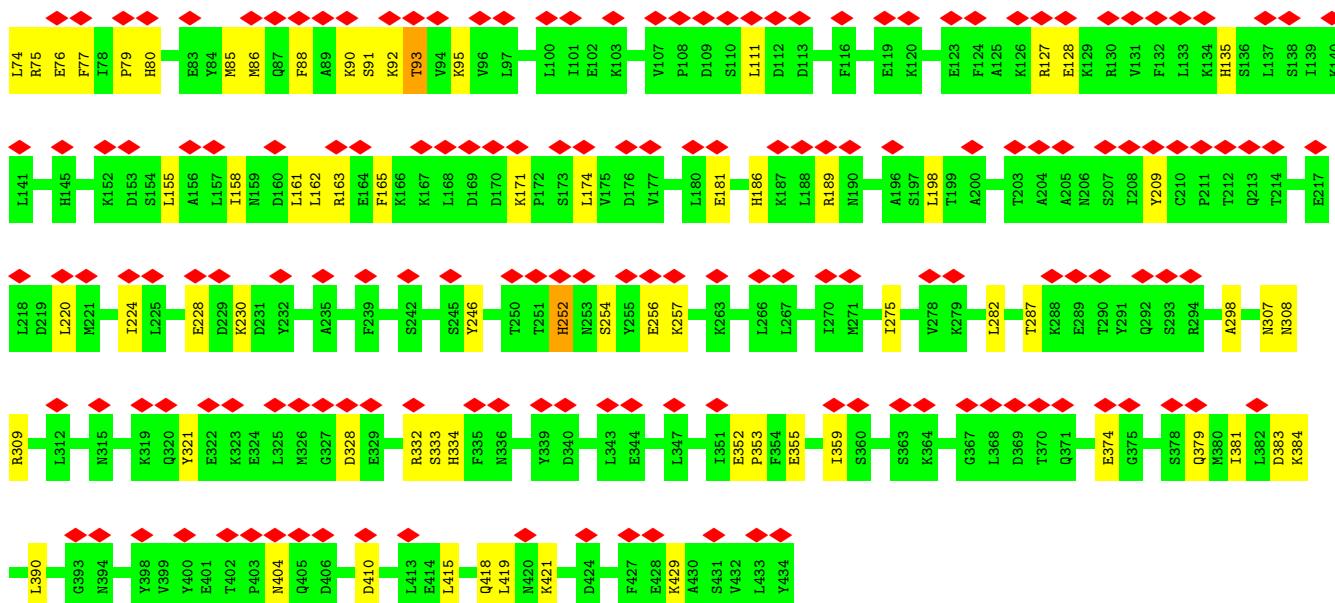




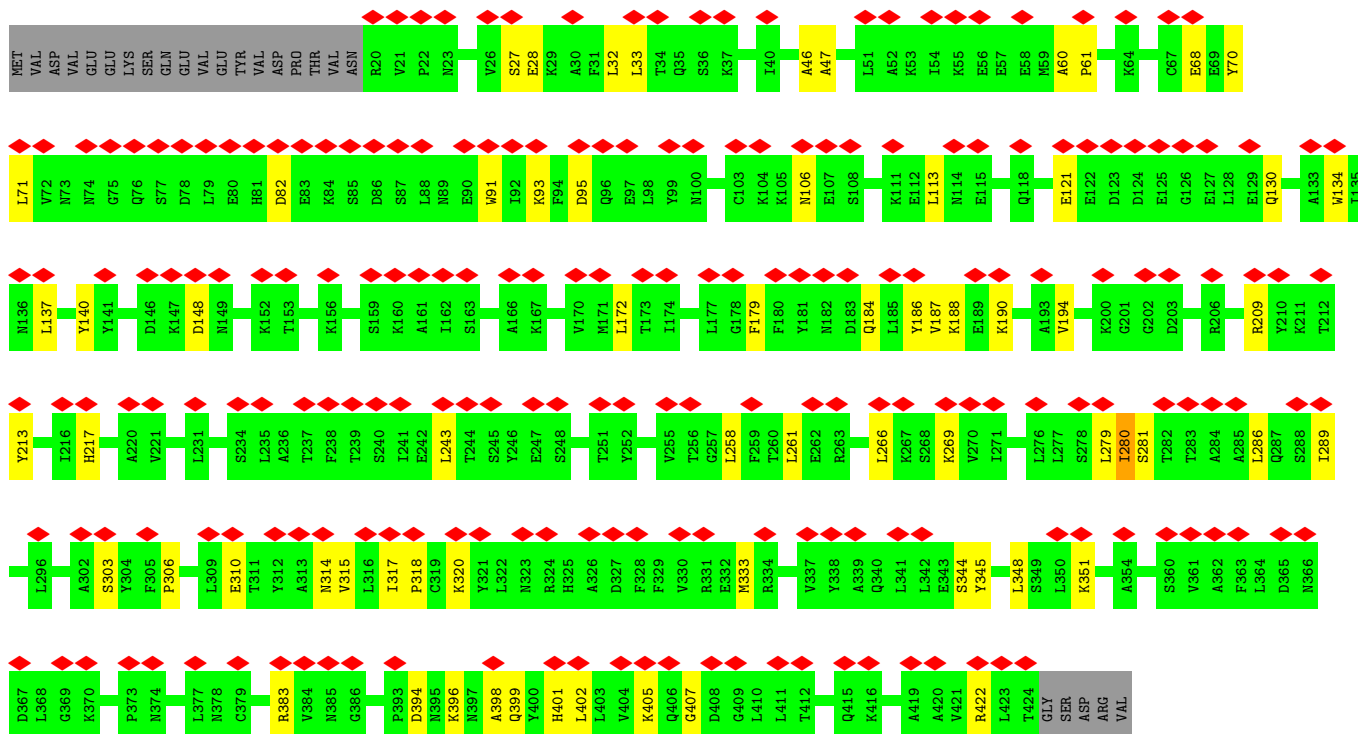
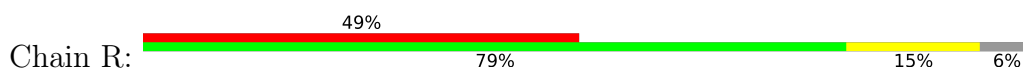
• Molecule 22: 26S proteasome regulatory subunit RPN3



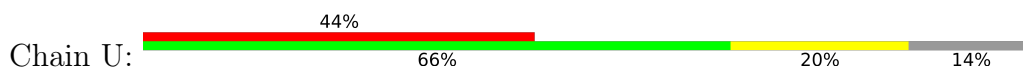


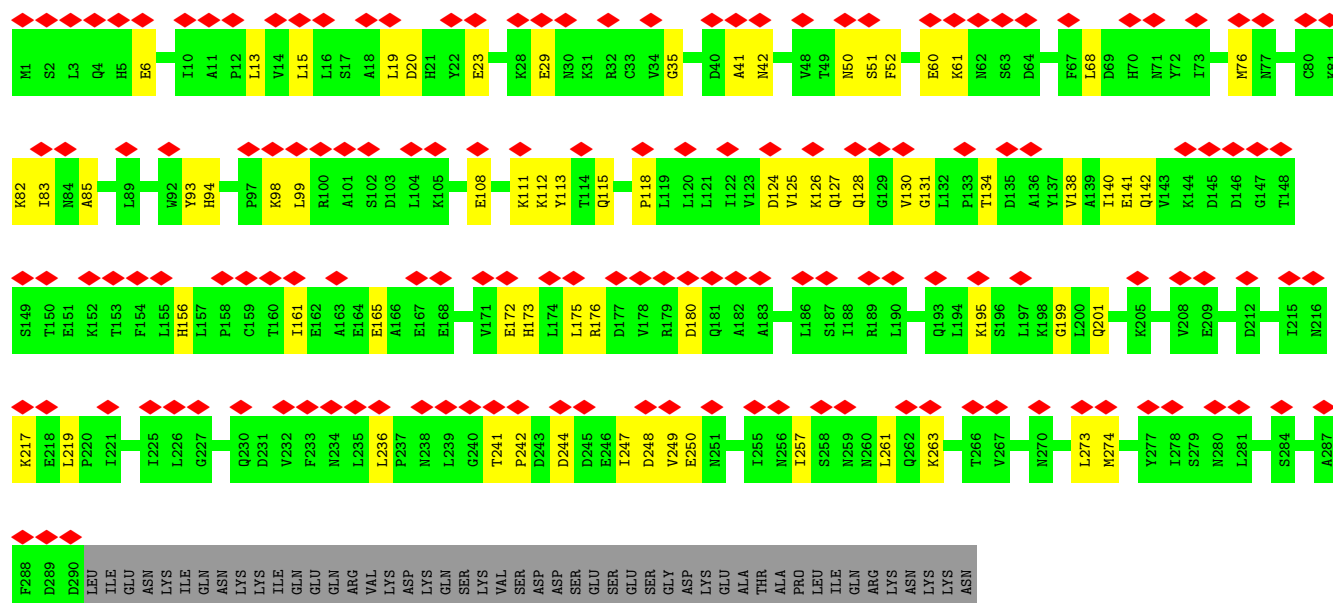


• Molecule 25: 26S proteasome regulatory subunit RPN7

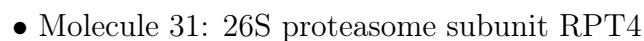


• Molecule 26: 26S proteasome regulatory subunit RPN8

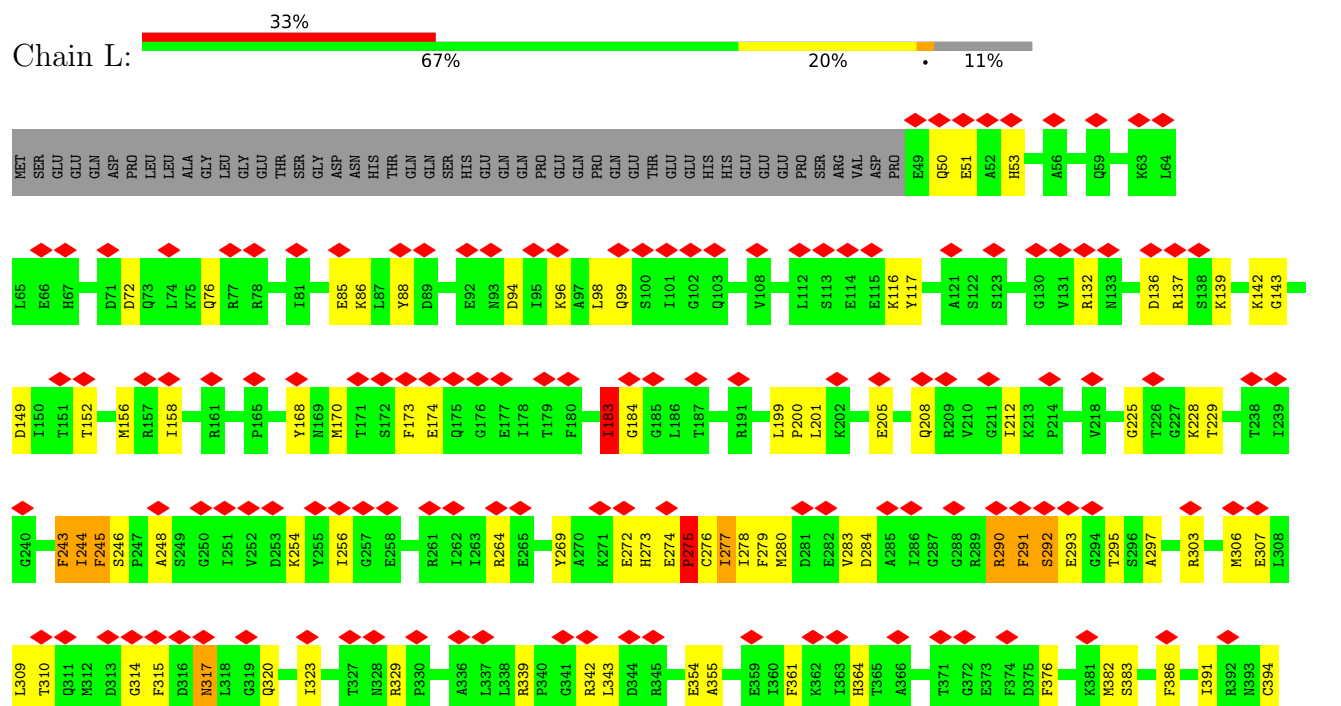


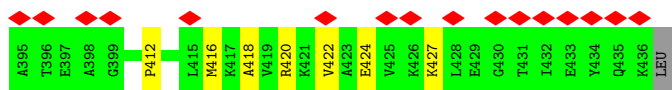


- Chain K:

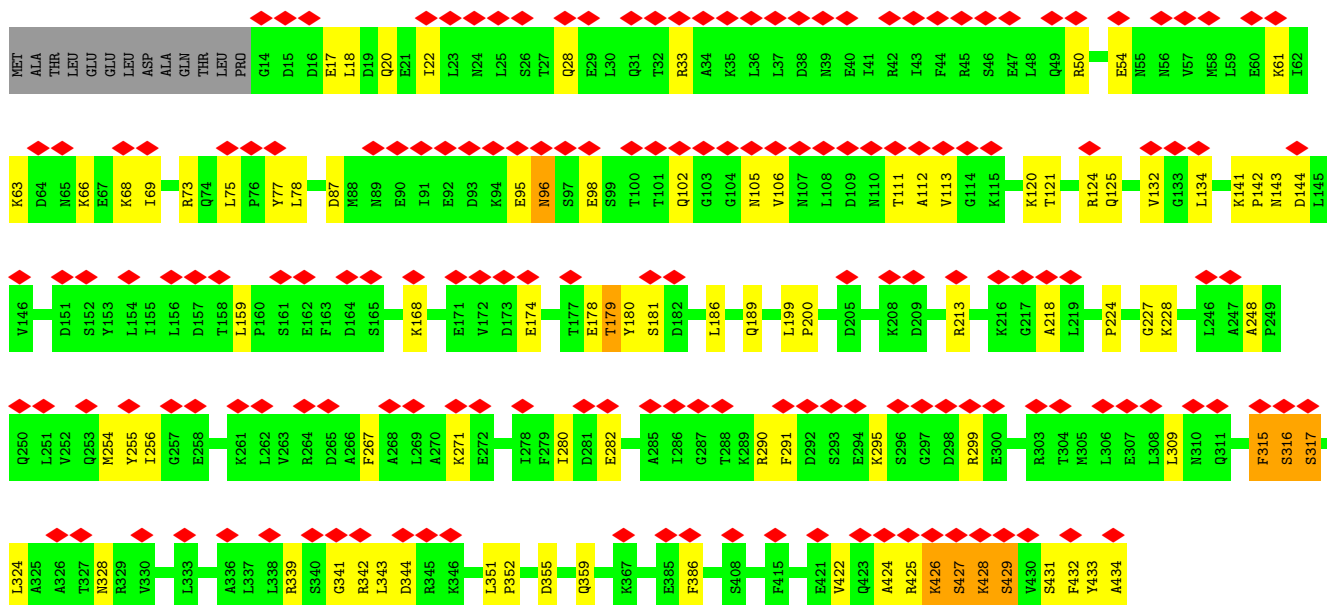
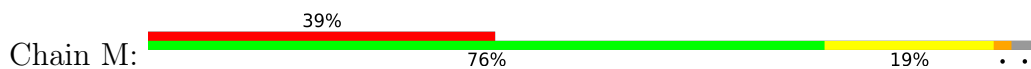


Chain L:

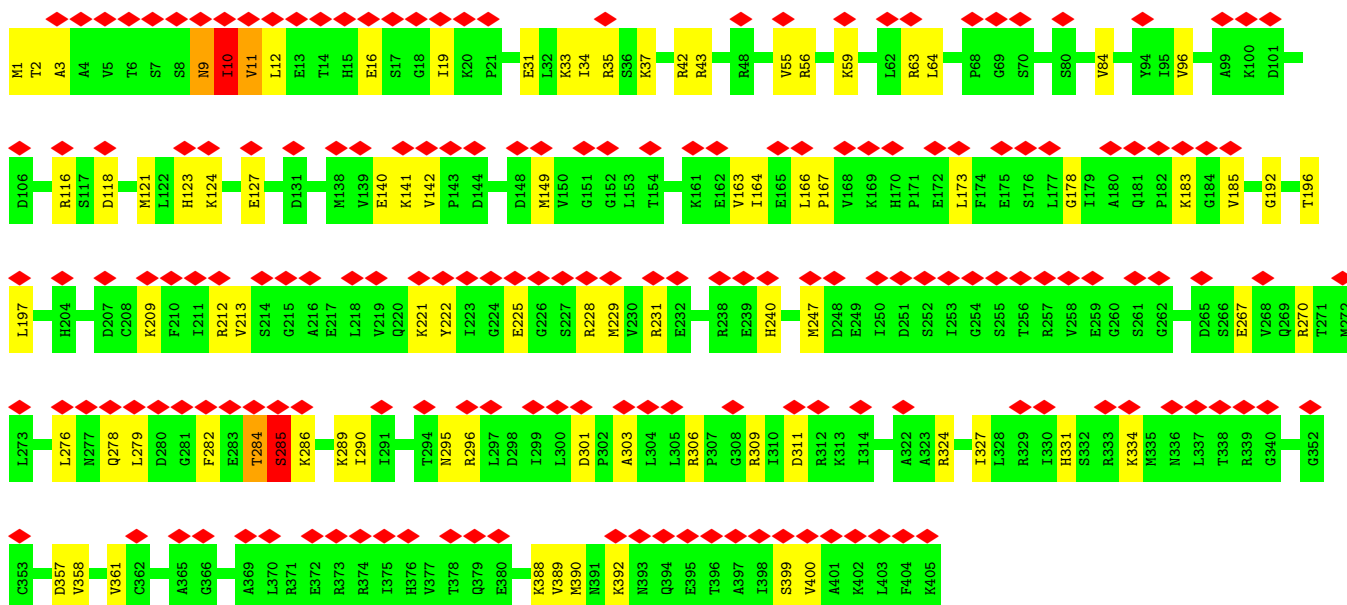
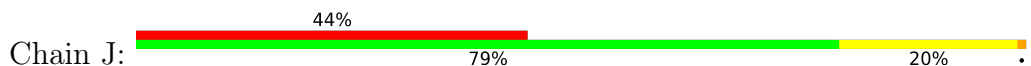




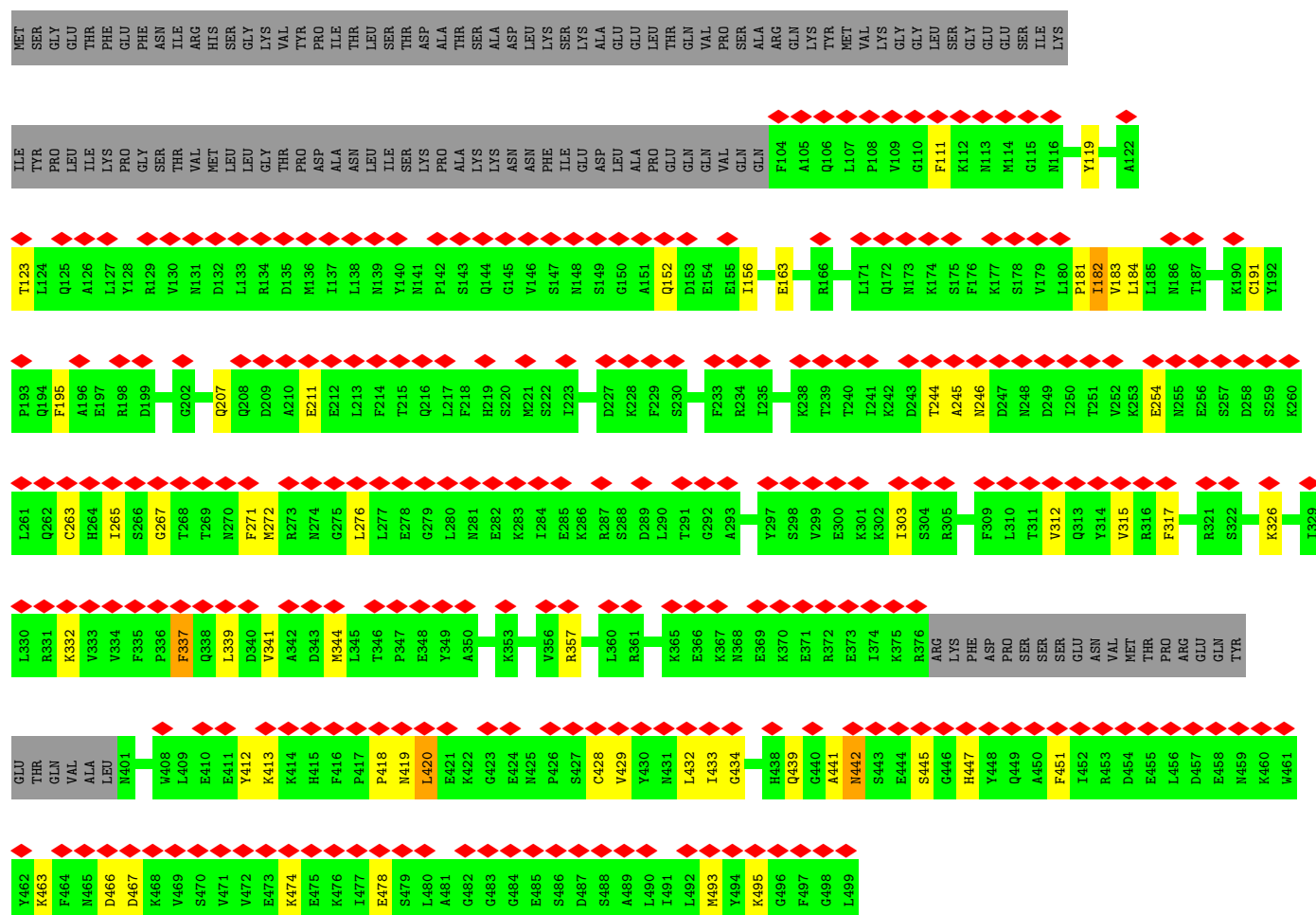
• Molecule 32: 26S proteasome regulatory subunit 6A



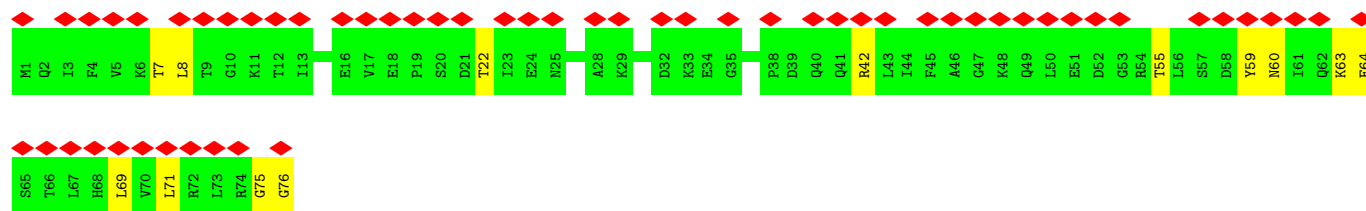
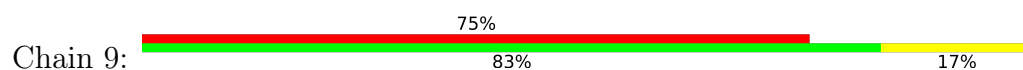
• Molecule 33: 26S proteasome regulatory subunit 8 homolog



• Molecule 34: Ubiquitin carboxyl-terminal hydrolase



• 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	74842	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	26.593	Depositor
Minimum map value	-21.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.913	Depositor
Recommended contour level	5.2	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 ⓘ

5.1 Standard geometry ⓘ

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	0.40	0/1950	0.94	14/2641 (0.5%)
1	a	0.40	0/1950	0.94	14/2641 (0.5%)
2	B	0.39	0/1944	0.71	4/2632 (0.2%)
2	b	0.39	0/1944	0.71	4/2632 (0.2%)
3	C	0.43	0/1934	0.92	10/2618 (0.4%)
3	c	0.43	0/1934	0.92	10/2618 (0.4%)
4	D	0.45	0/1879	0.63	0/2546
4	d	0.25	0/1879	0.62	0/2546
5	E	0.39	0/1952	0.77	5/2630 (0.2%)
5	e	0.39	0/1952	0.77	5/2630 (0.2%)
6	F	0.41	0/1800	0.82	3/2433 (0.1%)
6	f	0.41	0/1800	0.82	3/2433 (0.1%)
7	G	0.56	1/1925 (0.1%)	0.91	14/2599 (0.5%)
7	g	0.56	1/1925 (0.1%)	0.91	14/2599 (0.5%)
8	1	0.42	0/1541	0.81	2/2087 (0.1%)
8	h	0.58	0/1541	0.94	7/2087 (0.3%)
9	2	0.64	2/1750 (0.1%)	1.00	13/2373 (0.5%)
9	i	0.47	0/1750	0.92	7/2373 (0.3%)
10	3	0.45	0/1611	0.86	4/2174 (0.2%)
10	j	0.45	0/1611	0.86	4/2174 (0.2%)
11	4	0.52	0/1589	0.92	6/2142 (0.3%)
11	k	0.52	0/1589	0.92	6/2142 (0.3%)
12	5	0.47	0/1681	1.02	6/2274 (0.3%)
12	l	0.47	0/1681	1.02	6/2274 (0.3%)
13	6	0.41	0/1795	0.86	9/2420 (0.4%)
13	m	0.41	0/1795	0.86	9/2420 (0.4%)
14	7	0.40	0/1821	0.61	0/2470
14	n	0.28	0/1821	0.57	0/2470
15	W	0.57	5/1557 (0.3%)	0.75	5/2111 (0.2%)
16	V	0.36	0/2309	0.65	4/3115 (0.1%)
17	T	0.24	0/2235	0.56	0/3017
18	X	0.19	0/1058	0.63	2/1432 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.24	0/741	0.74	2/1000 (0.2%)
20	Z	0.31	2/7122 (0.0%)	0.68	7/9645 (0.1%)
21	N	0.31	0/6521	0.51	2/8824 (0.0%)
22	S	0.29	0/3966	0.57	0/5355
23	P	0.31	0/3663	0.51	0/4940
24	Q	0.28	0/3556	0.57	1/4787 (0.0%)
25	R	0.29	0/3313	0.53	0/4469
26	U	0.48	1/2340 (0.0%)	0.66	5/3168 (0.2%)
27	O	0.28	0/3247	0.53	0/4380
28	H	0.37	0/3113	0.64	2/4187 (0.0%)
29	I	0.56	4/3054 (0.1%)	0.82	10/4111 (0.2%)
30	K	0.44	2/3156 (0.1%)	0.75	10/4261 (0.2%)
31	L	0.62	3/3128 (0.1%)	0.88	17/4204 (0.4%)
32	M	0.38	0/3323	0.65	1/4478 (0.0%)
33	J	0.39	1/3212 (0.0%)	0.66	3/4316 (0.1%)
34	8	0.44	5/3089 (0.2%)	0.68	7/4144 (0.2%)
35	9	0.26	0/603	0.57	0/811
All	All	0.41	27/114650 (0.0%)	0.74	257/154833 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
5	E	0	1
5	e	0	1
6	F	0	3
6	f	0	3
7	G	0	1
7	g	0	1
8	h	0	1
9	2	0	7
9	i	0	6
10	3	0	1
10	j	0	1
11	4	0	1
11	k	0	1
13	6	0	1
13	m	0	1
16	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	T	0	3
19	Y	0	1
20	Z	0	2
21	N	0	1
22	S	0	3
24	Q	0	2
25	R	0	1
27	O	0	1
28	H	0	8
29	I	0	6
30	K	0	2
31	L	0	6
32	M	0	4
33	J	0	4
34	8	0	2
All	All	0	78

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	82	ILE	CA-CB	-10.87	1.48	1.54
7	G	82	ILE	CA-CB	-10.83	1.48	1.54
9	2	114	GLN	C-N	-10.08	1.21	1.33
15	W	25	ARG	CA-C	-7.83	1.42	1.52
29	I	86	GLU	C-N	-6.98	1.24	1.34

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	19	LEU	CB-CG-CD1	19.12	168.05	110.70
3	C	19	LEU	CB-CG-CD1	19.12	168.05	110.70
12	5	144	ARG	CG-CD-NE	-17.21	74.14	112.00
12	l	144	ARG	CG-CD-NE	-17.20	74.16	112.00
12	l	161	LEU	CB-CG-CD1	14.89	155.36	110.70

There are no chirality outliers.

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	d	16	HIS	Peptide
5	e	15	PHE	Peptide

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Mol	Chain	Res	Type	Group
6	f	13	PHE	Peptide
6	f	18	ARG	Peptide
6	f	8	GLY	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	1912	0	1906	74	0
1	a	1912	0	1906	66	0
2	B	1907	0	1917	67	0
2	b	1907	0	1917	68	0
3	C	1904	0	1901	72	0
3	c	1904	0	1901	65	0
4	D	1850	0	1862	59	0
4	d	1850	0	1862	42	0
5	E	1925	0	1896	63	0
5	e	1925	0	1896	54	0
6	F	1773	0	1775	62	0
6	f	1773	0	1775	62	0
7	G	1885	0	1876	80	0
7	g	1885	0	1876	89	0
8	1	1512	0	1478	63	0
8	h	1512	0	1478	61	0
9	2	1719	0	1716	96	0
9	i	1719	0	1716	85	0
10	3	1581	0	1571	83	0
10	j	1581	0	1571	80	0
11	4	1561	0	1569	67	0
11	k	1561	0	1569	67	0
12	5	1644	0	1592	66	0
12	l	1644	0	1592	80	0
13	6	1757	0	1708	69	0
13	m	1757	0	1708	74	0
14	7	1790	0	1790	41	0
14	n	1790	0	1790	47	0
15	W	1534	0	1542	16	0
16	V	2274	0	2273	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	T	2192	0	2161	25	0
18	X	1032	0	1017	3	0
19	Y	731	0	675	16	0
20	Z	7005	0	6932	161	0
21	N	6418	0	6487	90	0
22	S	3894	0	3938	67	0
23	P	3608	0	3694	39	0
24	Q	3499	0	3524	52	0
25	R	3258	0	3263	56	0
26	U	2306	0	2331	58	0
27	O	3186	0	3213	43	0
28	H	3064	0	3141	112	0
29	I	3015	0	3084	132	0
30	K	3113	0	3168	83	0
31	L	3082	0	3157	80	0
32	M	3285	0	3320	102	0
33	J	3171	0	3311	88	0
34	8	3034	0	3005	48	0
35	9	601	0	629	12	0
36	H	31	0	12	32	0
36	I	31	0	11	20	0
36	K	31	0	12	7	0
36	L	31	0	12	10	0
36	M	31	0	11	15	0
37	H	1	0	0	0	0
37	I	1	0	0	0	0
37	J	1	0	0	0	0
37	K	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
38	J	27	0	11	14	0
All	All	112930	0	113048	2815	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 12.

The worst 5 of 2815 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)
20:Z:916:LEU:HD12	29:I:54:ARG:O	1.29	1.28
29:I:393:GLN:HE22	36:I:501:ATP:C4'	1.49	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:916:LEU:CD1	29:I:54:ARG:O	1.84	1.24
20:Z:916:LEU:HD11	29:I:54:ARG:N	1.57	1.19
1:A:14:ARG:NE	7:G:8:TYR:OH	1.76	1.19

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	240/252 (95%)	236 (98%)	4 (2%)	0	100	100
1	a	240/252 (95%)	236 (98%)	4 (2%)	0	100	100
2	B	247/250 (99%)	238 (96%)	7 (3%)	2 (1%)	16	54
2	b	247/250 (99%)	238 (96%)	7 (3%)	2 (1%)	16	54
3	C	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
3	c	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
4	D	234/254 (92%)	224 (96%)	5 (2%)	5 (2%)	5	29
4	d	234/254 (92%)	224 (96%)	5 (2%)	5 (2%)	5	29
5	E	247/260 (95%)	238 (96%)	6 (2%)	3 (1%)	10	43
5	e	247/260 (95%)	238 (96%)	6 (2%)	3 (1%)	10	43
6	F	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	67
6	f	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	67
7	G	240/288 (83%)	235 (98%)	4 (2%)	1 (0%)	30	67
7	g	240/288 (83%)	235 (98%)	4 (2%)	1 (0%)	30	67
8	1	194/215 (90%)	187 (96%)	6 (3%)	1 (0%)	24	63
8	h	194/215 (90%)	187 (96%)	5 (3%)	2 (1%)	12	48
9	2	224/261 (86%)	210 (94%)	10 (4%)	4 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	224/261 (86%)	211 (94%)	10 (4%)	3 (1%)	9	42
10	3	202/205 (98%)	183 (91%)	18 (9%)	1 (0%)	24	63
10	j	202/205 (98%)	183 (91%)	18 (9%)	1 (0%)	24	63
11	4	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	63
11	k	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	63
12	5	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
12	l	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
13	6	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	24	63
13	m	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	24	63
14	7	227/266 (85%)	215 (95%)	10 (4%)	2 (1%)	14	50
14	n	227/266 (85%)	214 (94%)	11 (5%)	2 (1%)	14	50
15	W	195/268 (73%)	182 (93%)	12 (6%)	1 (0%)	24	63
16	V	287/306 (94%)	264 (92%)	19 (7%)	4 (1%)	9	40
17	T	264/274 (96%)	247 (94%)	13 (5%)	4 (2%)	8	39
18	X	125/156 (80%)	116 (93%)	8 (6%)	1 (1%)	16	54
19	Y	87/89 (98%)	73 (84%)	9 (10%)	5 (6%)	1	13
20	Z	902/993 (91%)	822 (91%)	65 (7%)	15 (2%)	7	36
21	N	828/945 (88%)	800 (97%)	26 (3%)	2 (0%)	43	77
22	S	473/523 (90%)	439 (93%)	27 (6%)	7 (2%)	8	39
23	P	438/445 (98%)	419 (96%)	17 (4%)	2 (0%)	24	63
24	Q	432/434 (100%)	404 (94%)	27 (6%)	1 (0%)	43	77
25	R	403/429 (94%)	384 (95%)	18 (4%)	1 (0%)	43	77
26	U	288/338 (85%)	280 (97%)	8 (3%)	0	100	100
27	O	386/393 (98%)	373 (97%)	13 (3%)	0	100	100
28	H	387/467 (83%)	353 (91%)	27 (7%)	7 (2%)	6	34
29	I	382/437 (87%)	342 (90%)	29 (8%)	11 (3%)	3	23
30	K	392/428 (92%)	371 (95%)	18 (5%)	3 (1%)	16	54
31	L	386/437 (88%)	358 (93%)	25 (6%)	3 (1%)	16	54
32	M	419/434 (96%)	387 (92%)	22 (5%)	10 (2%)	4	27
33	J	403/405 (100%)	368 (91%)	31 (8%)	4 (1%)	12	48
34	8	368/499 (74%)	345 (94%)	20 (5%)	3 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	9	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	14217/15714 (90%)	13424 (94%)	665 (5%)	128 (1%)	16	50

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	125	GLY
4	d	101	GLU
4	d	204	GLN
8	h	116	LYS
9	i	200	SER

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	206/210 (98%)	168 (82%)	38 (18%)	1	8
1	a	206/210 (98%)	168 (82%)	38 (18%)	1	8
2	B	208/209 (100%)	167 (80%)	41 (20%)	1	7
2	b	208/209 (100%)	167 (80%)	41 (20%)	1	7
3	C	203/216 (94%)	160 (79%)	43 (21%)	1	6
3	c	203/216 (94%)	160 (79%)	43 (21%)	1	6
4	D	209/226 (92%)	209 (100%)	0	100	100
4	d	209/226 (92%)	209 (100%)	0	100	100
5	E	205/215 (95%)	169 (82%)	36 (18%)	2	9
5	e	205/215 (95%)	169 (82%)	36 (18%)	2	9
6	F	190/193 (98%)	158 (83%)	32 (17%)	2	10
6	f	190/193 (98%)	158 (83%)	32 (17%)	2	10
7	G	200/239 (84%)	167 (84%)	33 (16%)	2	10
7	g	200/239 (84%)	167 (84%)	33 (16%)	2	10
8	1	162/178 (91%)	132 (82%)	30 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	162/178 (91%)	134 (83%)	28 (17%)	2	9
9	2	185/214 (86%)	137 (74%)	48 (26%)	0	3
9	i	185/214 (86%)	136 (74%)	49 (26%)	0	3
10	3	172/173 (99%)	146 (85%)	26 (15%)	3	12
10	j	172/173 (99%)	146 (85%)	26 (15%)	3	12
11	4	173/175 (99%)	139 (80%)	34 (20%)	1	7
11	k	173/175 (99%)	139 (80%)	34 (20%)	1	7
12	5	169/235 (72%)	135 (80%)	34 (20%)	1	7
12	l	169/235 (72%)	135 (80%)	34 (20%)	1	7
13	6	185/201 (92%)	158 (85%)	27 (15%)	3	13
13	m	185/201 (92%)	158 (85%)	27 (15%)	3	13
14	7	195/224 (87%)	195 (100%)	0	100	100
14	n	195/224 (87%)	195 (100%)	0	100	100
15	W	171/230 (74%)	170 (99%)	1 (1%)	78	83
16	V	253/268 (94%)	253 (100%)	0	100	100
17	T	249/256 (97%)	249 (100%)	0	100	100
18	X	116/144 (81%)	116 (100%)	0	100	100
19	Y	81/81 (100%)	81 (100%)	0	100	100
20	Z	773/850 (91%)	772 (100%)	1 (0%)	88	89
21	N	698/797 (88%)	698 (100%)	0	100	100
22	S	447/489 (91%)	447 (100%)	0	100	100
23	P	412/415 (99%)	412 (100%)	0	100	100
24	Q	391/391 (100%)	389 (100%)	2 (0%)	81	83
25	R	356/379 (94%)	356 (100%)	0	100	100
26	U	263/308 (85%)	263 (100%)	0	100	100
27	O	363/368 (99%)	363 (100%)	0	100	100
28	H	330/399 (83%)	328 (99%)	2 (1%)	78	83
29	I	341/385 (89%)	339 (99%)	2 (1%)	78	83
30	K	346/374 (92%)	345 (100%)	1 (0%)	86	85
31	L	332/377 (88%)	330 (99%)	2 (1%)	78	83
32	M	364/375 (97%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	J	352/352 (100%)	352 (100%)	0	100	100
34	8	337/449 (75%)	337 (100%)	0	100	100
35	9	68/68 (100%)	68 (100%)	0	100	100
All	All	12367/13571 (91%)	11513 (93%)	854 (7%)	16	36

5 of 854 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	THR
5	E	202	LYS
12	5	182	LYS
2	B	124	SER
2	B	21	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 241 such sidechains are listed below:

Mol	Chain	Res	Type
16	V	290	ASN
32	M	107	ASN
20	Z	926	ASN
31	L	317	ASN
34	8	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.54	0	1,2,2	0.06	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	9	76	GLZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	32,33,33	1.57	4 (12%)	48,52,52	2.52	21 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ATP	M	501	37	32,33,33	1.40	5 (15%)	48,52,52	2.38	15 (31%)
36	ATP	K	501	37	32,33,33	2.55	5 (15%)	48,52,52	2.46	16 (33%)
36	ATP	H	501	37	32,33,33	1.83	7 (21%)	48,52,52	2.29	21 (43%)
38	ADP	J	501	37	28,29,29	1.86	6 (21%)	43,45,45	2.95	20 (46%)
36	ATP	L	501	37	32,33,33	2.17	8 (25%)	48,52,52	1.51	4 (8%)

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	-	4/22/38/38	0/3/3/3
36	ATP	M	501	37	-	5/22/38/38	0/3/3/3
36	ATP	K	501	37	-	5/22/38/38	0/3/3/3
36	ATP	H	501	37	-	6/22/38/38	0/3/3/3
38	ADP	J	501	37	-	3/16/32/32	0/3/3/3
36	ATP	L	501	37	-	4/22/38/38	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	501	ATP	PA-O3A	8.14	1.68	1.59
36	K	501	ATP	PB-O3A	7.90	1.68	1.59
38	J	501	ADP	PA-O3A	6.25	1.66	1.59
36	L	501	ATP	PA-O3A	6.17	1.66	1.59
36	L	501	ATP	PB-O3A	5.97	1.65	1.59

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	J	501	ADP	C4-N9-C8	8.82	115.00	105.74
36	M	501	ATP	C4-N9-C8	8.58	114.75	105.74
36	K	501	ATP	C5-C4-N3	-7.87	115.88	126.72
36	L	501	ATP	O2B-PB-O3A	6.13	123.83	107.27
36	I	501	ATP	C5-C4-N3	-5.96	118.52	126.72

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

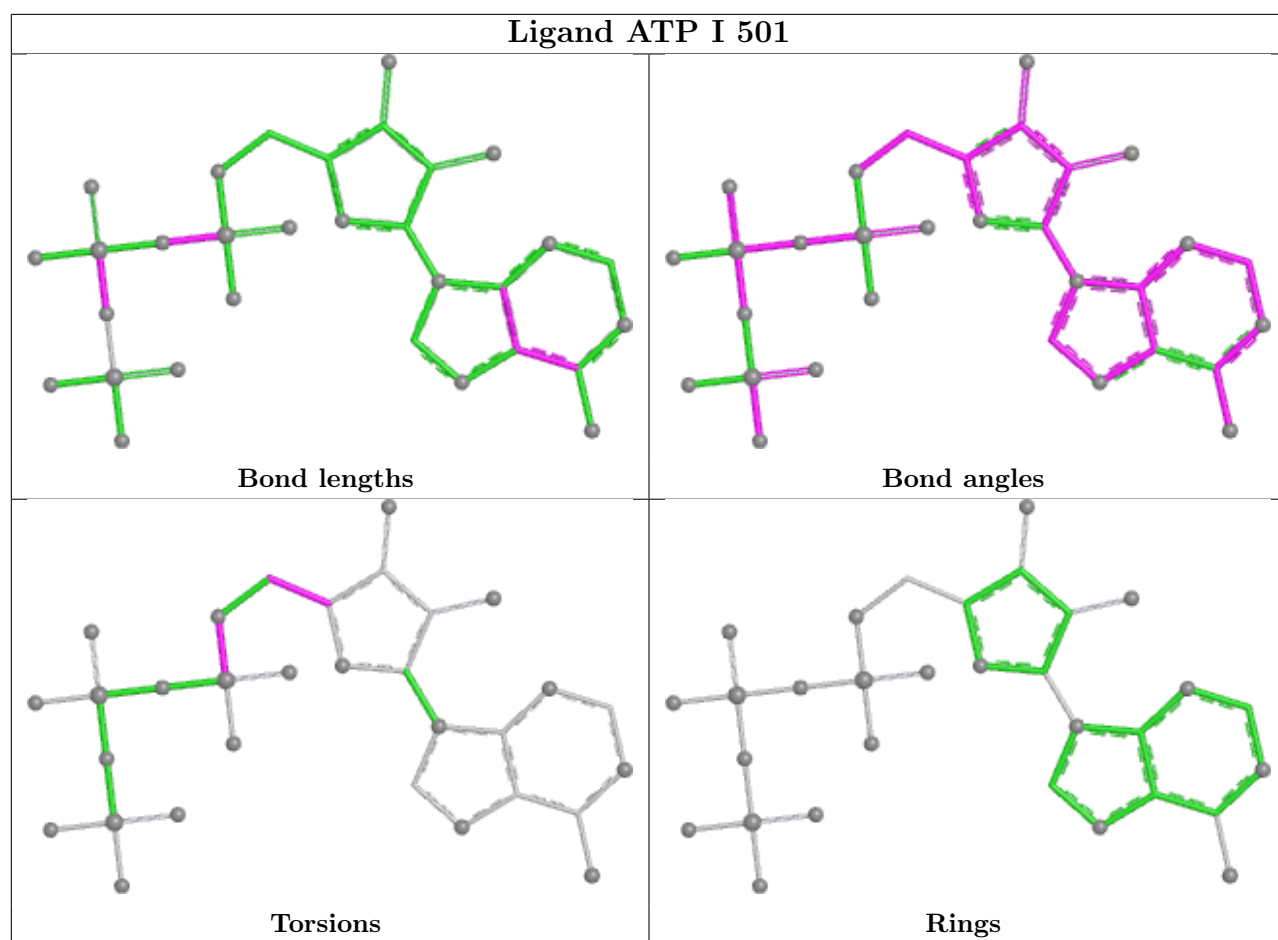
Mol	Chain	Res	Type	Atoms
36	H	501	ATP	PB-O3B-PG-O3G
36	H	501	ATP	C5'-O5'-PA-O2A
36	H	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	C5'-O5'-PA-O1A
36	I	501	ATP	C5'-O5'-PA-O2A

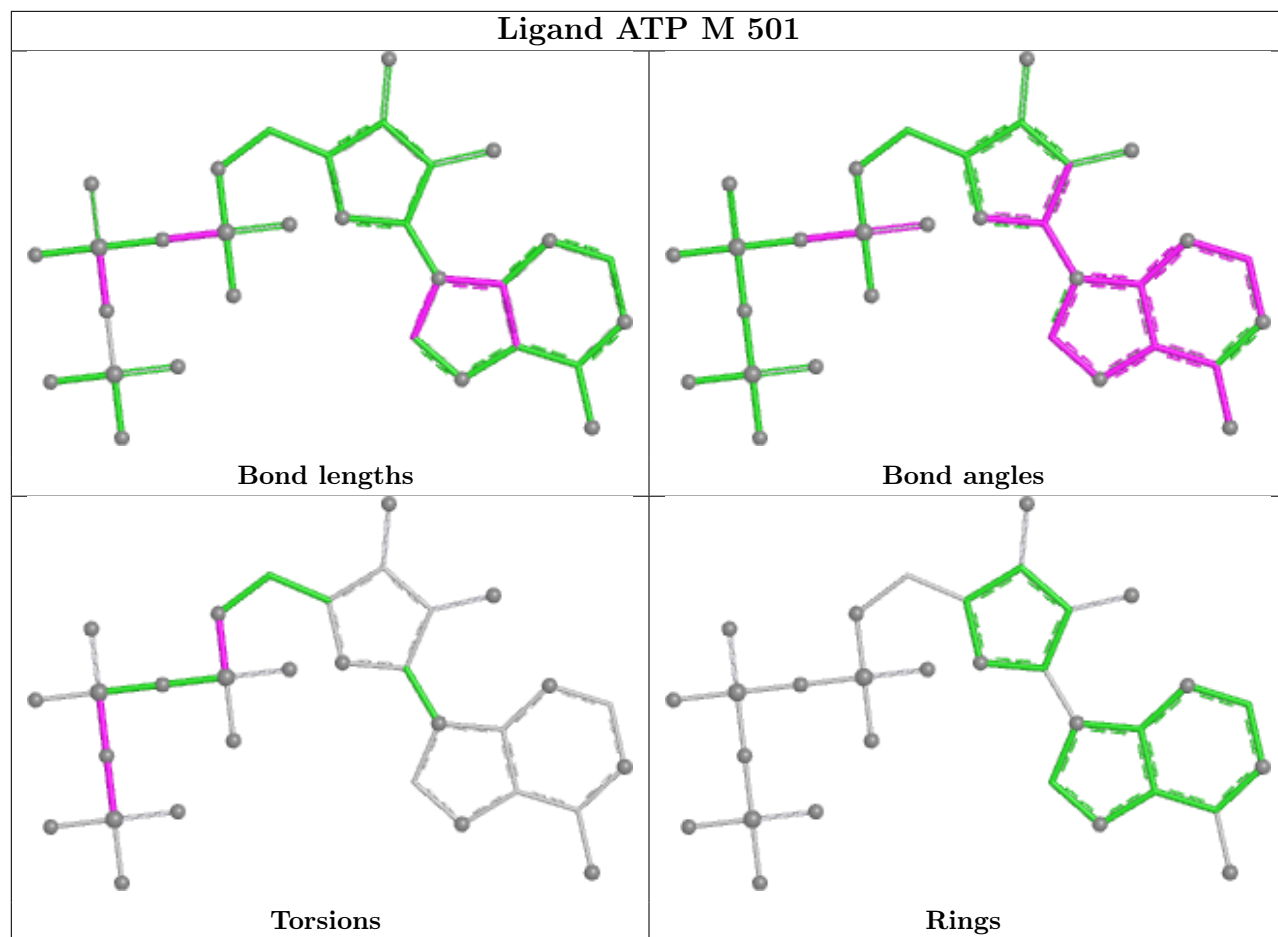
There are no ring outliers.

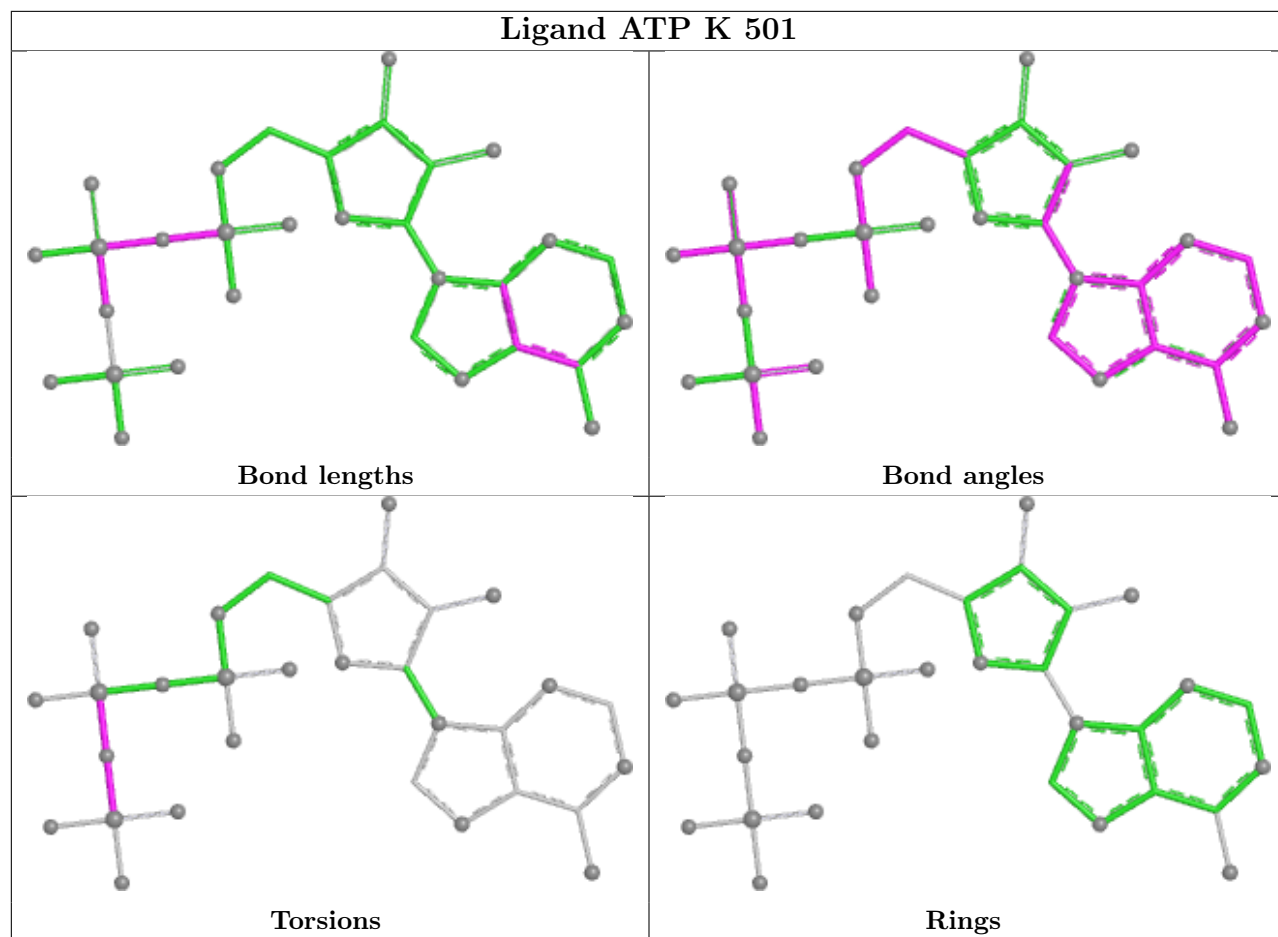
6 monomers are involved in 98 short contacts:

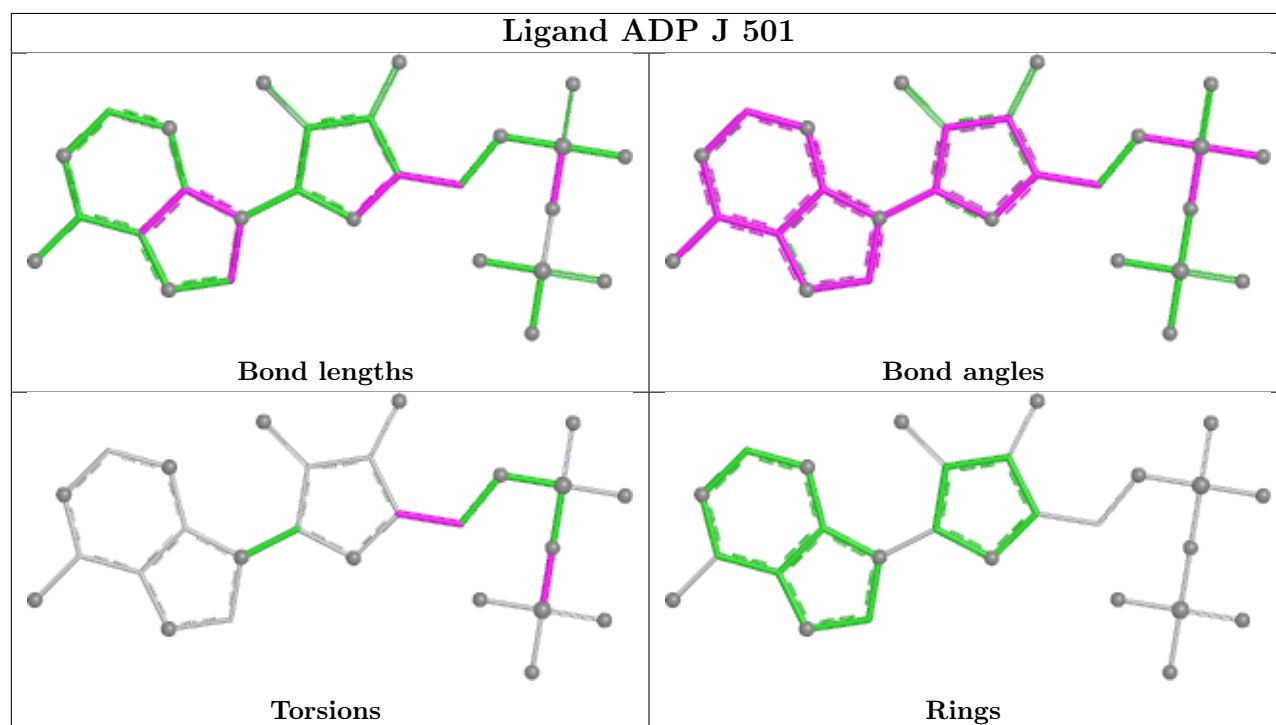
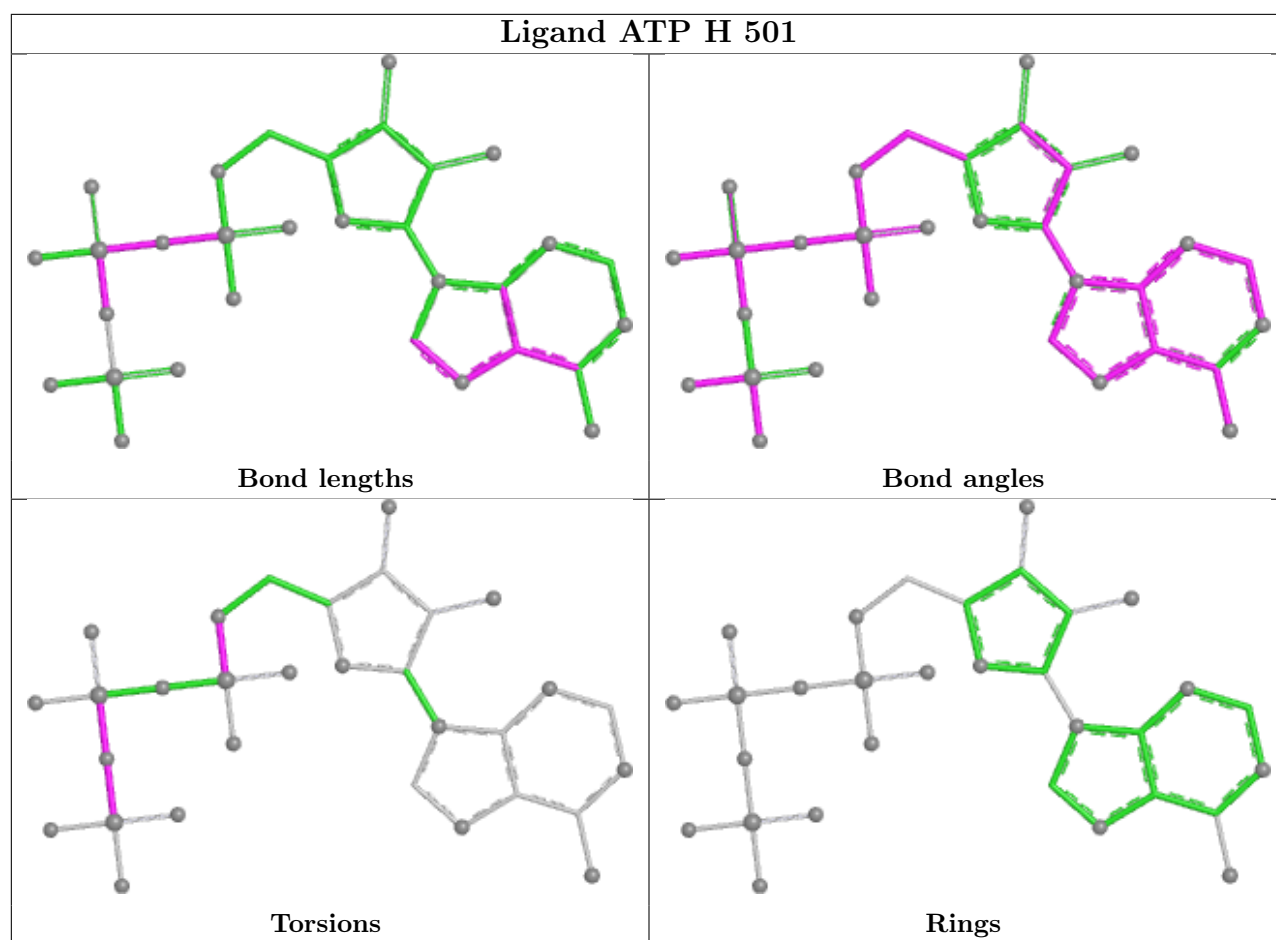
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	I	501	ATP	20	0
36	M	501	ATP	15	0
36	K	501	ATP	7	0
36	H	501	ATP	32	0
38	J	501	ADP	14	0
36	L	501	ATP	10	0

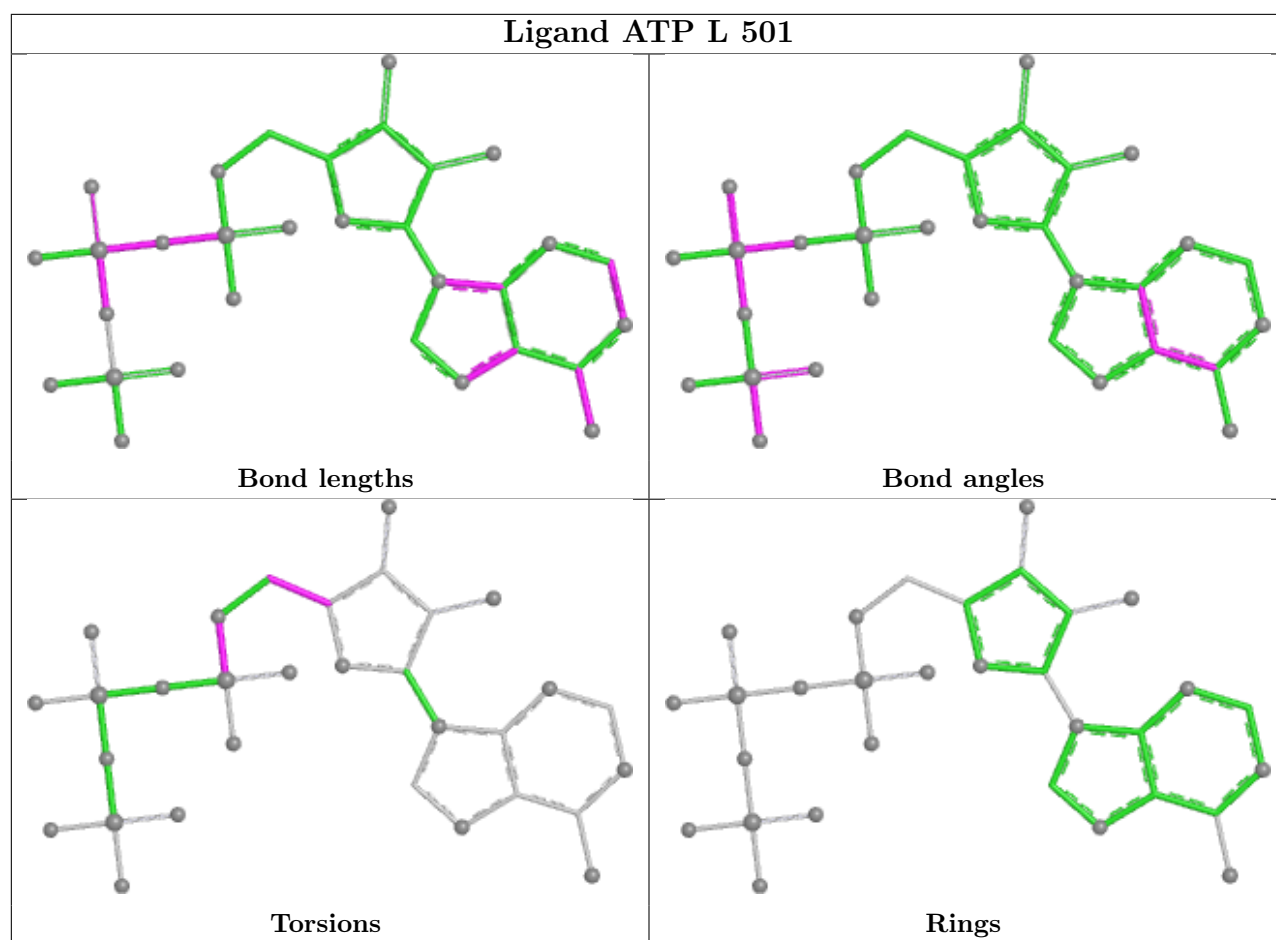
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

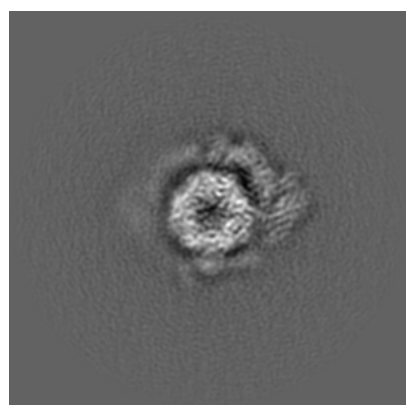
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14085. These allow visual inspection of the internal detail of the map and identification of artifacts.

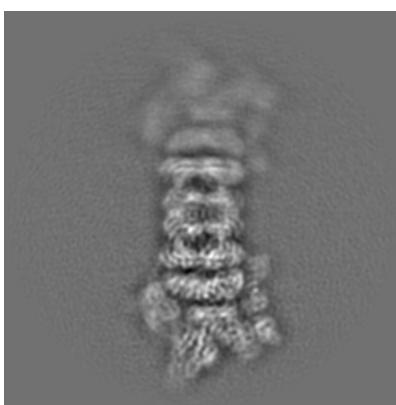
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

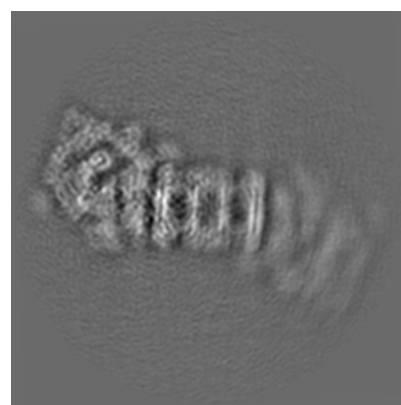
6.1.1 Primary map



X



Y

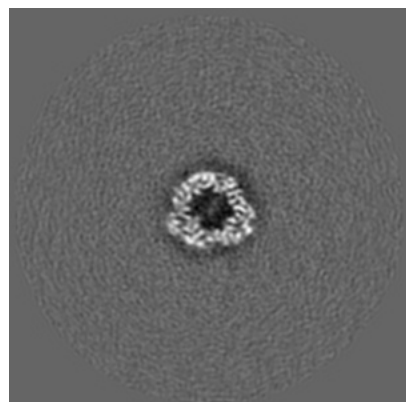


Z

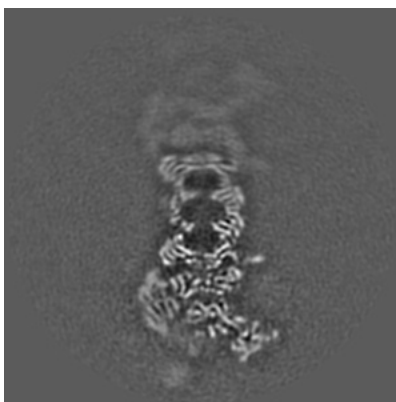
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

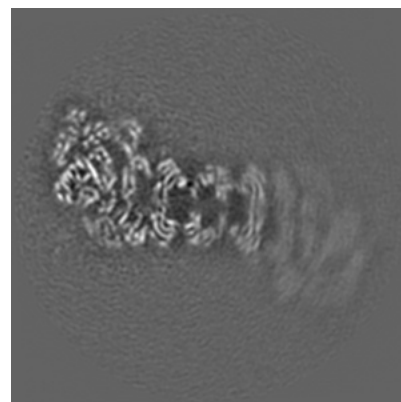
6.2.1 Primary map



X Index: 192



Y Index: 192

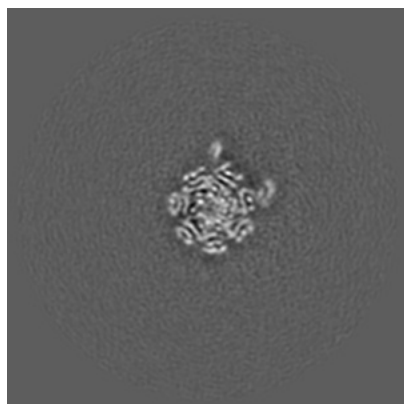


Z Index: 192

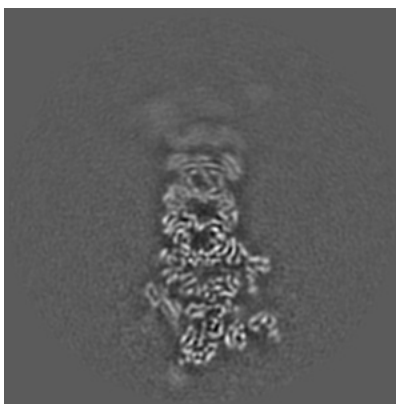
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

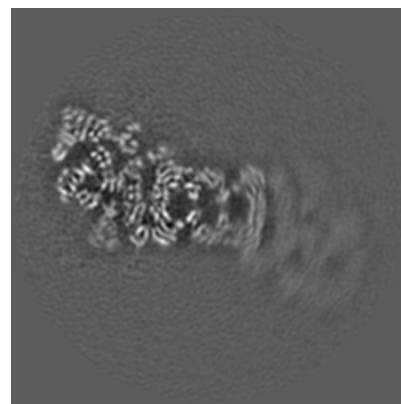
6.3.1 Primary map



X Index: 148



Y Index: 208

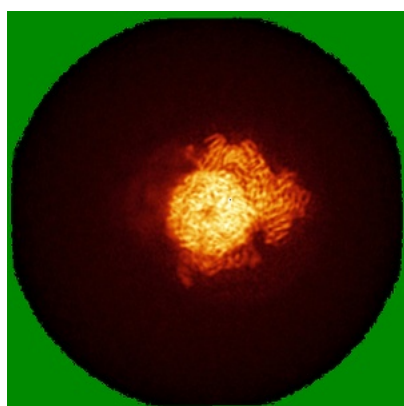


Z Index: 197

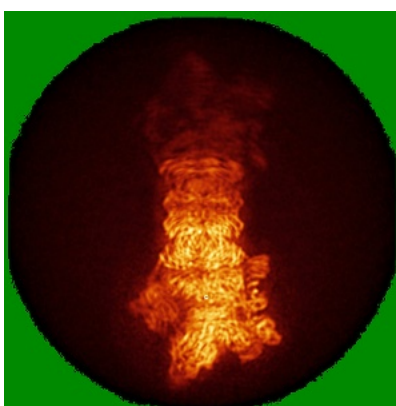
The images above show the largest variance slices of the map in three orthogonal directions.

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

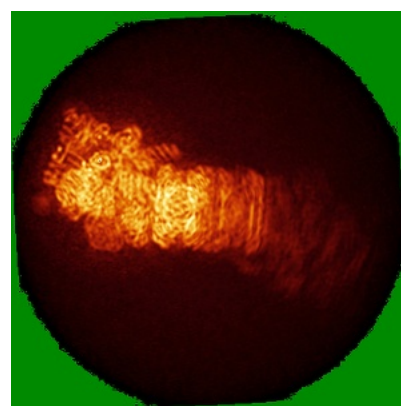
6.4.1 Primary map



X



Y

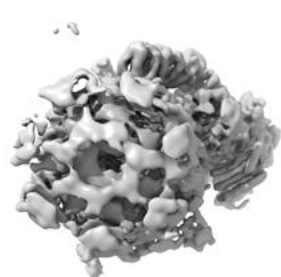


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

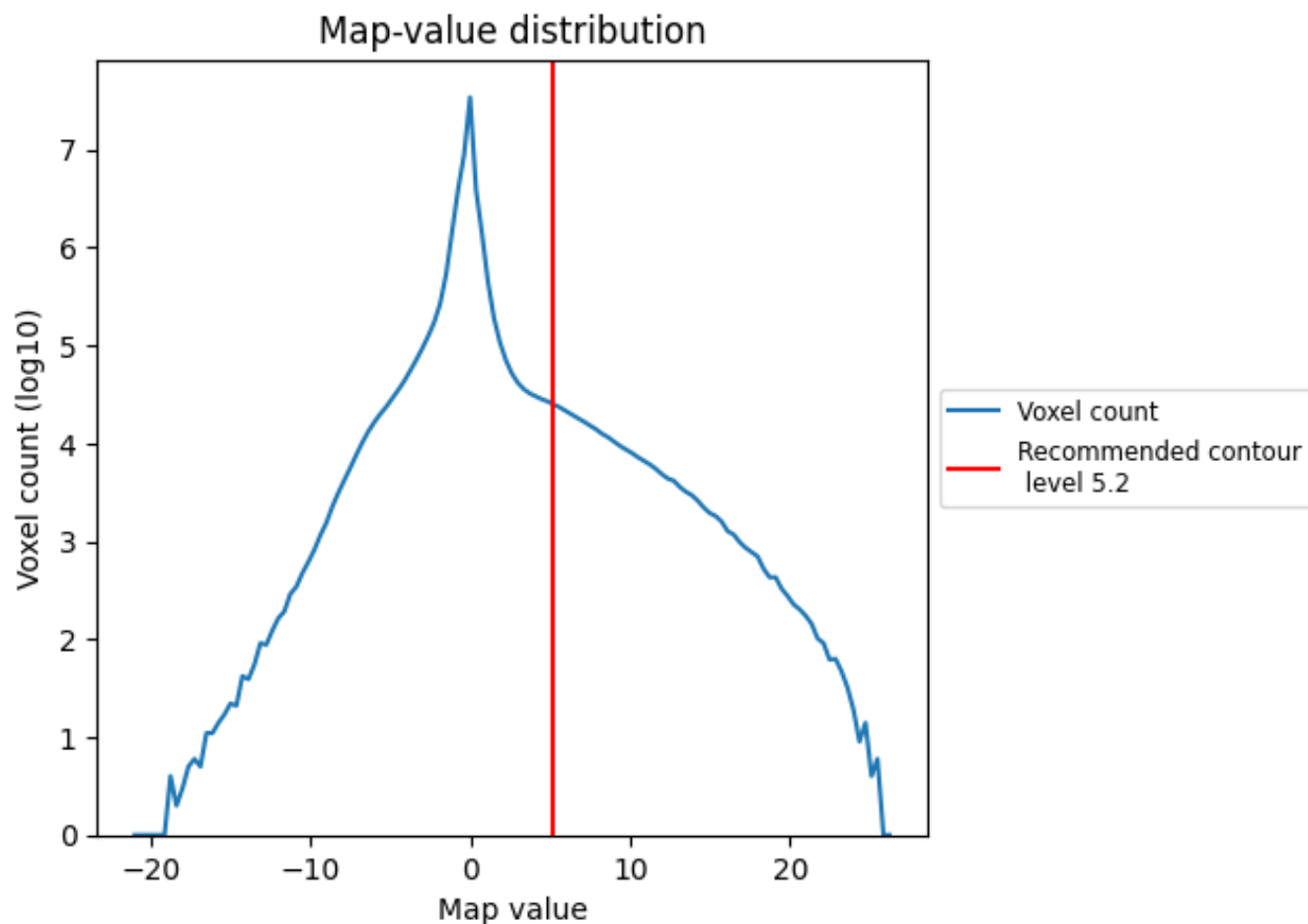
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

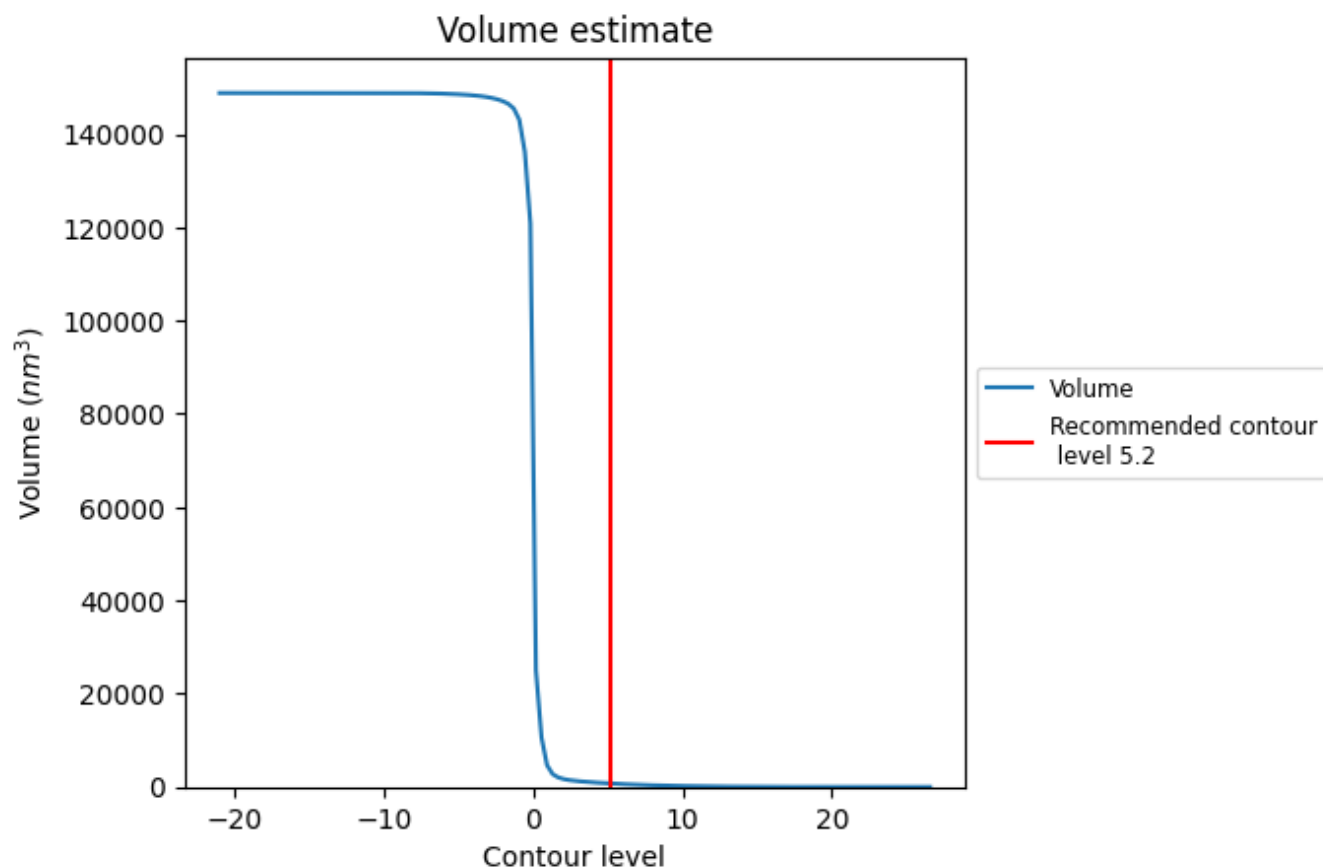
This section contains the results of statistical analysis of the map.

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.

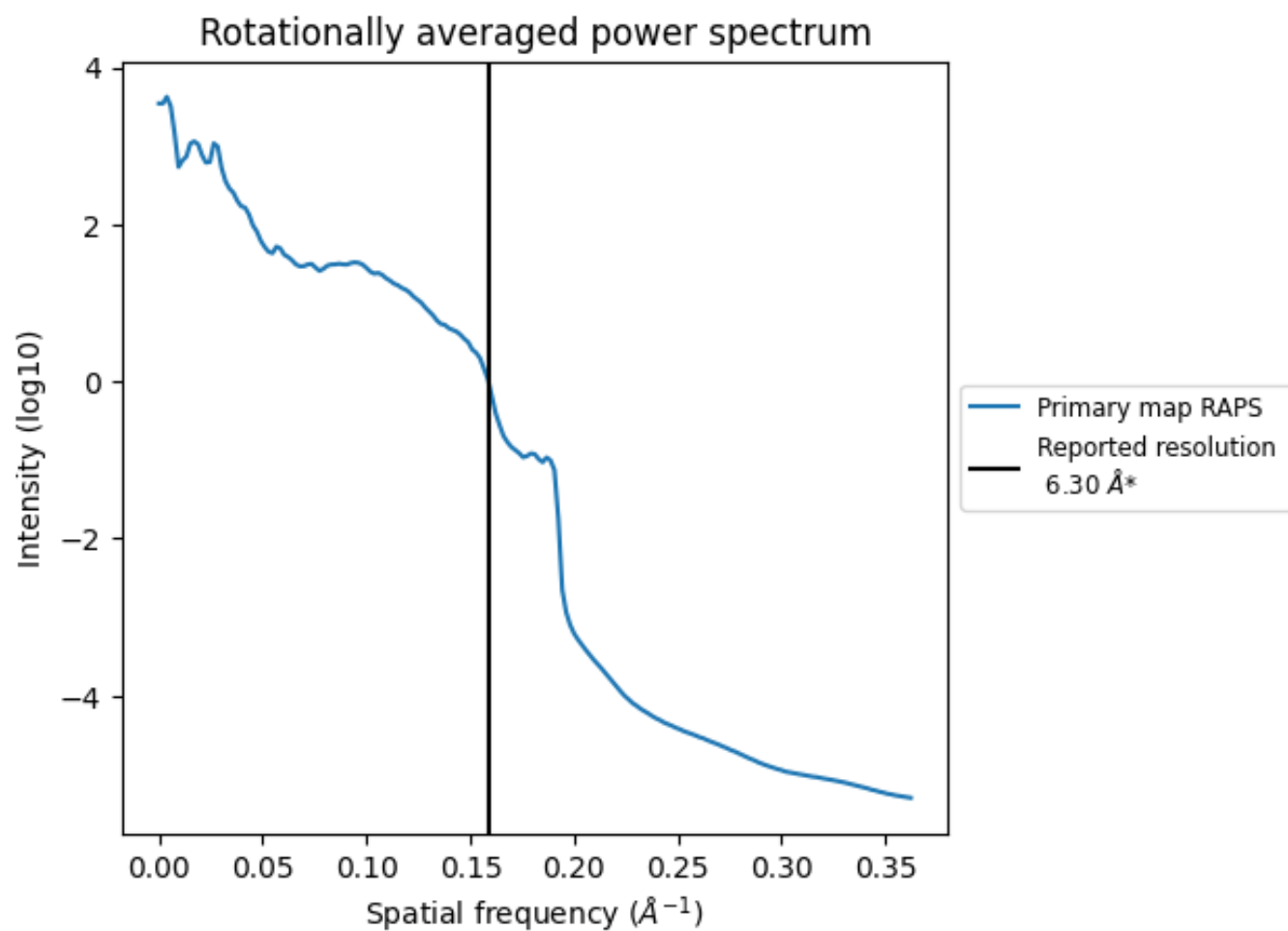
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 745 nm^3 ; this corresponds to an approximate mass of 673 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 0.159 Å⁻¹

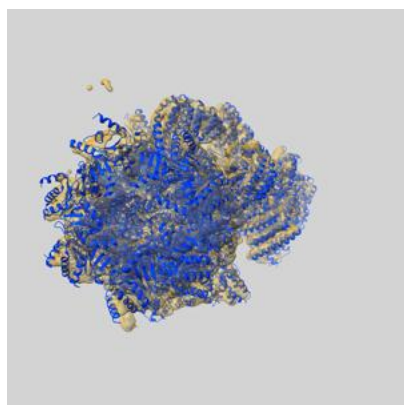
8 Fourier-Shell correlation

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

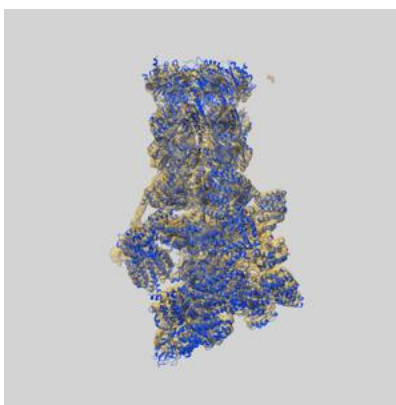
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14085 and PDB model 7QO6. Per-residue inclusion information can be found in section 3 on page 14.

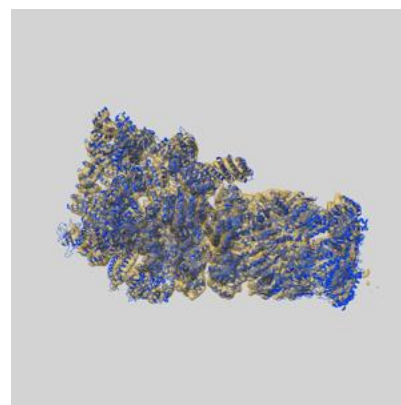
9.1 Map-model overlay [i](#)



X



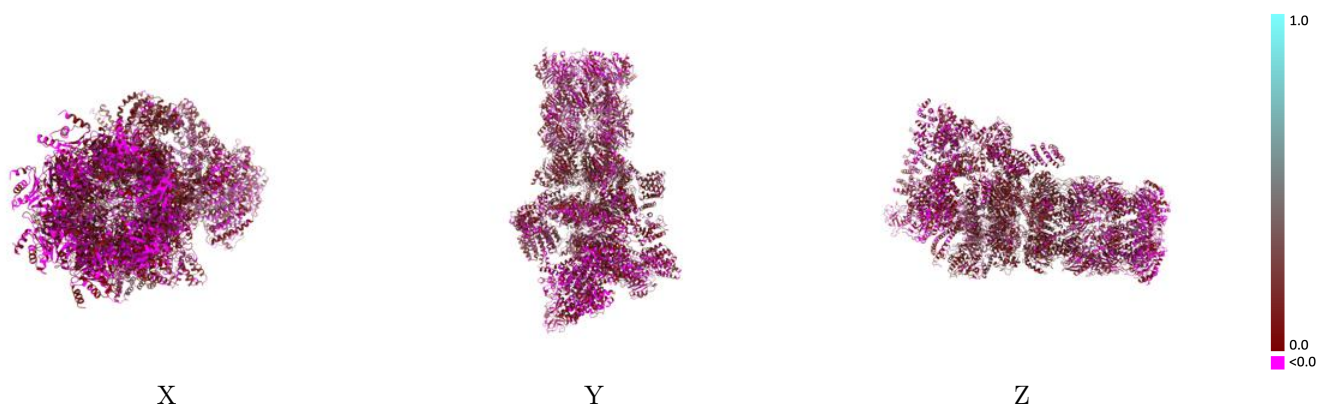
Y



Z

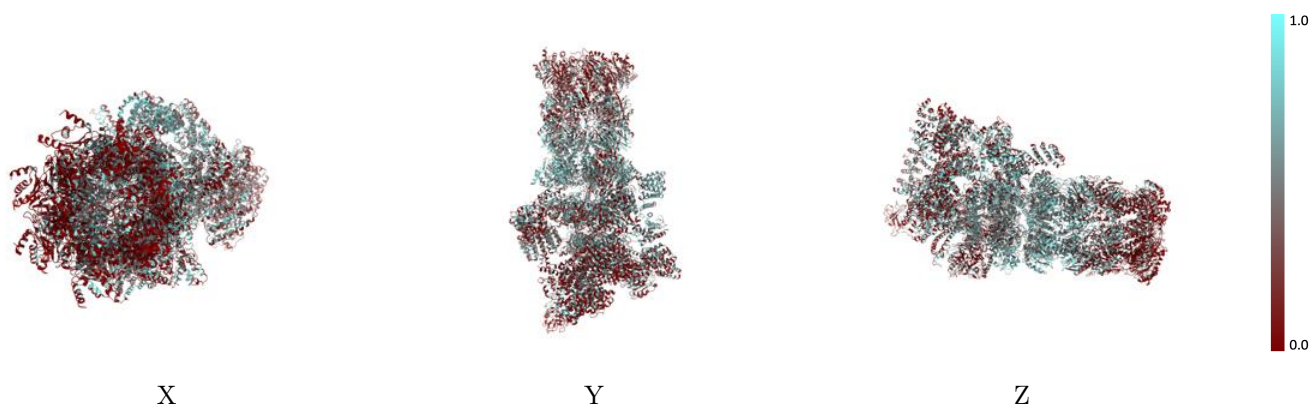
The images above show the 3D surface view of the map at the recommended contour level 5.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



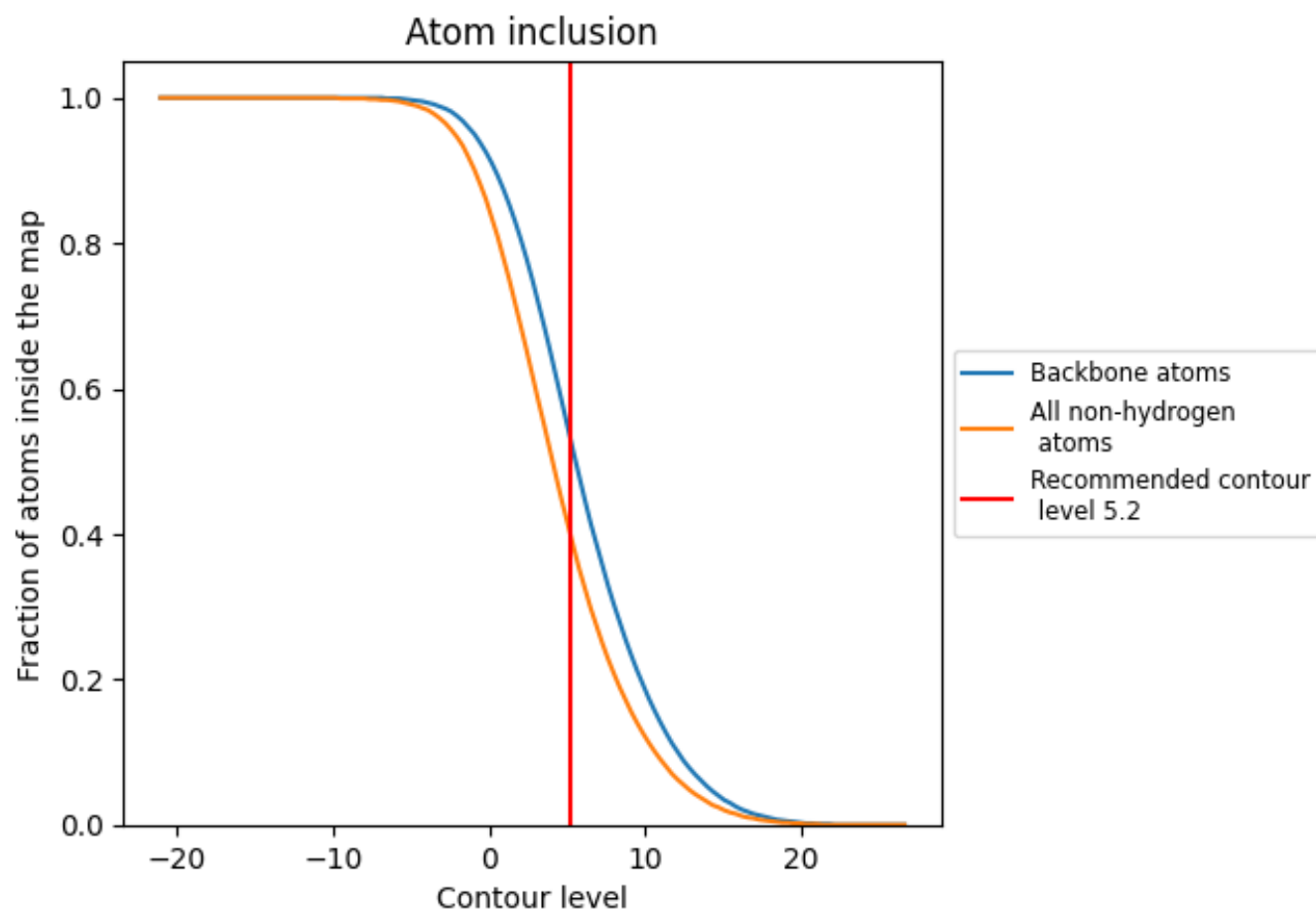
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 40% 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 (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3990	 0.0960
1	 0.5360	 0.1020
2	 0.4980	 0.1120
3	 0.4630	 0.0920
4	 0.5220	 0.0970
5	 0.5080	 0.1010
6	 0.4690	 0.0980
7	 0.4990	 0.1070
8	 0.2550	 0.1370
9	 0.2330	 0.1490
A	 0.5950	 0.1630
B	 0.5470	 0.1640
C	 0.5670	 0.1530
D	 0.6000	 0.1650
E	 0.5780	 0.1510
F	 0.6050	 0.1570
G	 0.6020	 0.1720
H	 0.4720	 0.1510
I	 0.4490	 0.1450
J	 0.4540	 0.1260
K	 0.4430	 0.1300
L	 0.4870	 0.1330
M	 0.4700	 0.1380
N	 0.4360	 0.0810
O	 0.4130	 0.0770
P	 0.5720	 0.1220
Q	 0.4490	 0.0970
R	 0.4240	 0.0760
S	 0.3240	 0.0270
T	 0.2800	 0.0620
U	 0.4290	 0.0920
V	 0.4310	 0.0920
W	 0.3920	 0.0590
X	 0.0920	 0.0550
Y	 0.1870	 0.0620



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Chain	Atom inclusion	Q-score
Z	 0.3130	 0.0990
a	 0.1620	 0.0110
b	 0.0930	 0.0010
c	 0.1800	 0.0020
d	 0.2110	 0.0180
e	 0.1510	 0.0110
f	 0.2080	 0.0090
g	 0.1770	 0.0150
h	 0.3560	 0.0760
i	 0.2460	 0.0720
j	 0.2860	 0.0880
k	 0.3790	 0.0880
l	 0.3350	 0.0850
m	 0.2930	 0.0750
n	 0.3460	 0.0880