



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 04:08 AM UTC

PDB ID : 2KU2 / pdb_00002ku2
Title : Dynamic Regulation of Archaeal Proteasome Gate Opening as Studied by TROSY-NMR
Authors : Religa, T.L.; Sprangers, R.; Kay, L.E.
Deposited on : 2010-02-11

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

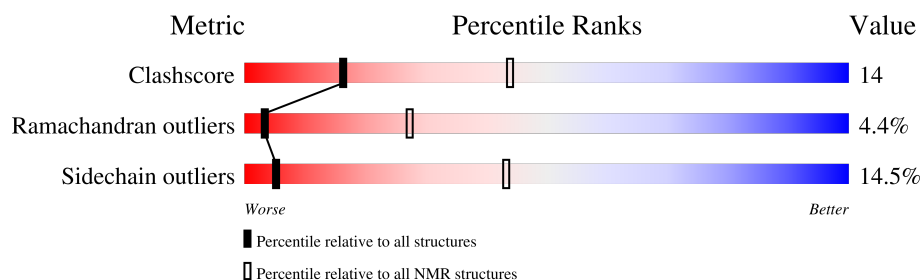
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	237	51% 35% 6% • 6%
1	B	237	57% 30% 7% 6%
1	C	237	57% 29% 8% 6%
1	D	237	57% 27% 9% 6%
1	E	237	51% 35% 7% 6%
1	F	237	55% 34% 5% 6%
1	G	237	54% 34% 5% 6%

2 Ensemble composition and analysis

This entry contains 50 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:233, B:12-B:233, C:12-C:233, D:12-D:233, E:12-E:233, F:12-F:233, G:12-G:233 (1554)	0.07	10

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 9 clusters and 1 single-model cluster was found.

Cluster number	Models
1	5, 6, 9, 10, 15, 16, 17, 19, 21, 26, 37, 39, 45, 47
2	2, 13, 29, 41, 42, 44, 48, 49, 50
3	14, 18, 32, 36, 38
4	7, 8, 25, 34, 43
5	11, 22, 23, 24, 40
6	27, 28, 31, 33
7	1, 3, 4
8	12, 20
9	35, 46
Single-model clusters	30

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25802 atoms, of which 13027 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	
1	B	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	
1	C	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	
1	D	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	
1	E	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	
1	F	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	
1	G	237	Total	C	H	N	O	S	0
			3686	1153	1861	312	354	6	

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P25156
A	-2	ALA	-	expression tag	UNP P25156
A	-1	MET	-	expression tag	UNP P25156
A	0	GLY	-	expression tag	UNP P25156
A	8	GLY	TYR	engineered mutation	UNP P25156
A	9	GLY	ASP	engineered mutation	UNP P25156
B	-3	GLY	-	expression tag	UNP P25156
B	-2	ALA	-	expression tag	UNP P25156
B	-1	MET	-	expression tag	UNP P25156
B	0	GLY	-	expression tag	UNP P25156
B	8	GLY	TYR	engineered mutation	UNP P25156
B	9	GLY	ASP	engineered mutation	UNP P25156
C	-3	GLY	-	expression tag	UNP P25156
C	-2	ALA	-	expression tag	UNP P25156
C	-1	MET	-	expression tag	UNP P25156
C	0	GLY	-	expression tag	UNP P25156
C	8	GLY	TYR	engineered mutation	UNP P25156
C	9	GLY	ASP	engineered mutation	UNP P25156
D	-3	GLY	-	expression tag	UNP P25156

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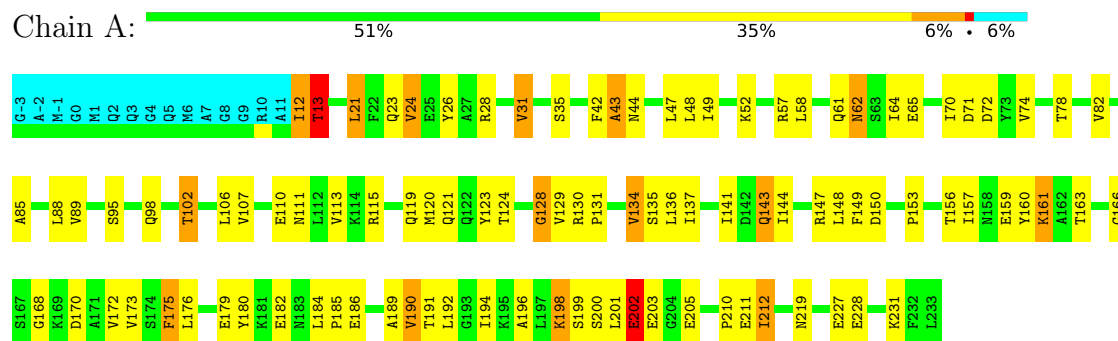
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	-	expression tag	UNP P25156
D	-1	MET	-	expression tag	UNP P25156
D	0	GLY	-	expression tag	UNP P25156
D	8	GLY	TYR	engineered mutation	UNP P25156
D	9	GLY	ASP	engineered mutation	UNP P25156
E	-3	GLY	-	expression tag	UNP P25156
E	-2	ALA	-	expression tag	UNP P25156
E	-1	MET	-	expression tag	UNP P25156
E	0	GLY	-	expression tag	UNP P25156
E	8	GLY	TYR	engineered mutation	UNP P25156
E	9	GLY	ASP	engineered mutation	UNP P25156
F	-3	GLY	-	expression tag	UNP P25156
F	-2	ALA	-	expression tag	UNP P25156
F	-1	MET	-	expression tag	UNP P25156
F	0	GLY	-	expression tag	UNP P25156
F	8	GLY	TYR	engineered mutation	UNP P25156
F	9	GLY	ASP	engineered mutation	UNP P25156
G	-3	GLY	-	expression tag	UNP P25156
G	-2	ALA	-	expression tag	UNP P25156
G	-1	MET	-	expression tag	UNP P25156
G	0	GLY	-	expression tag	UNP P25156
G	8	GLY	TYR	engineered mutation	UNP P25156
G	9	GLY	ASP	engineered mutation	UNP P25156

4 Residue-property plots

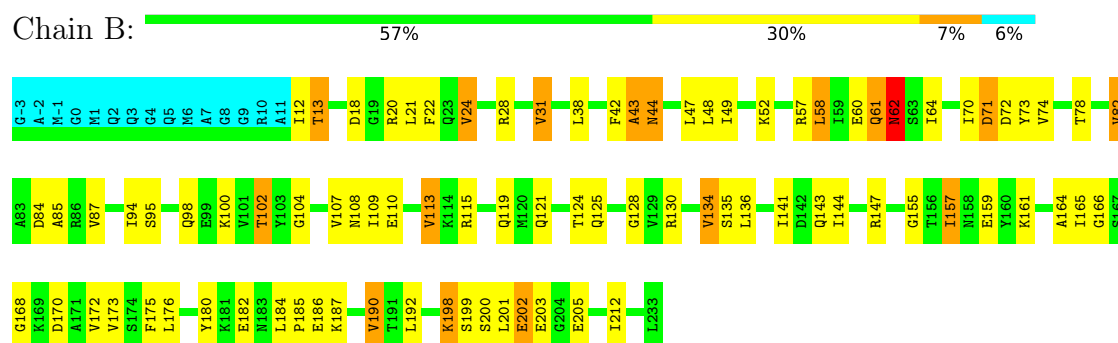
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

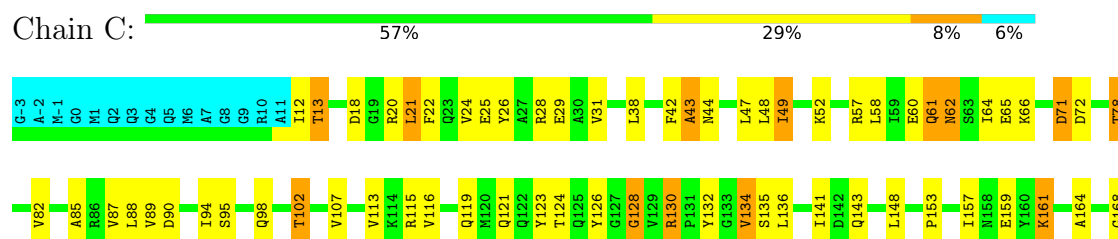
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha





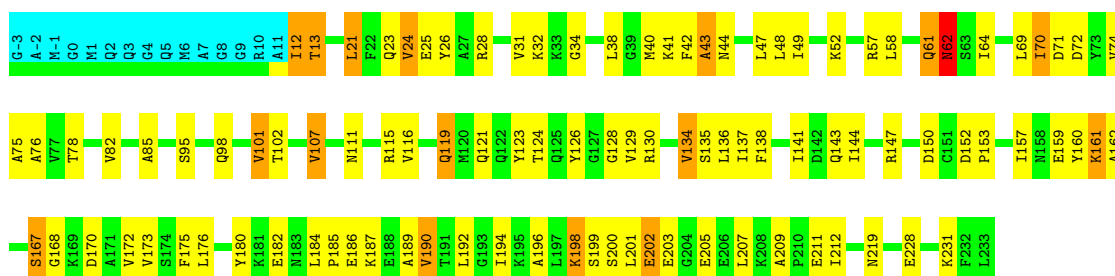
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



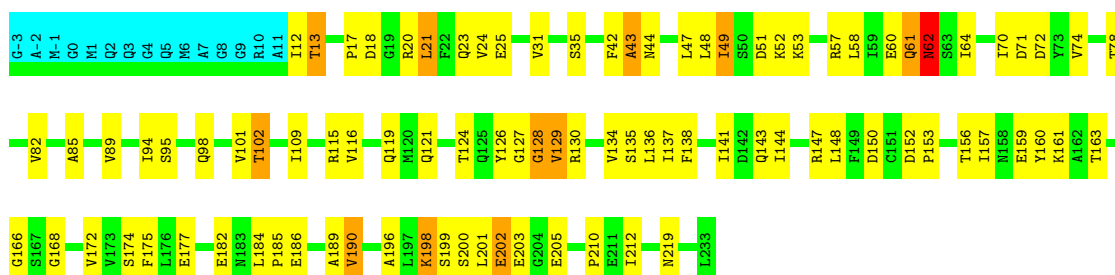
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



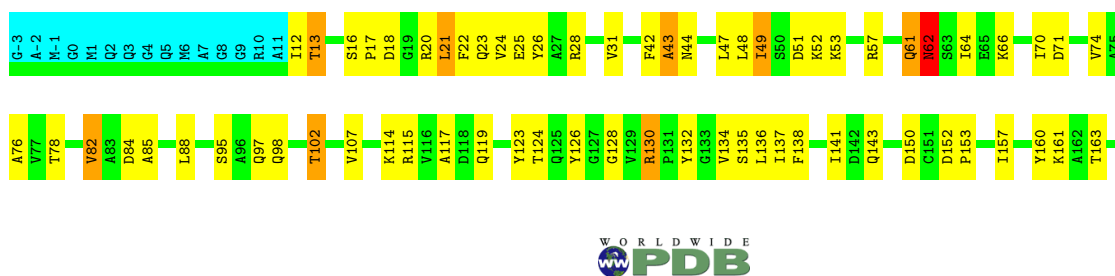
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 34% 5% 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 54% 34% 5% 6%



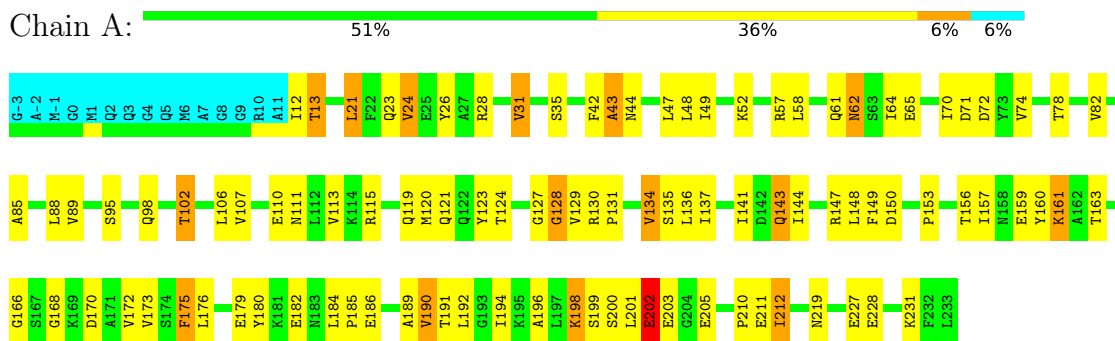


4.2 Scores per residue for each member of the ensemble

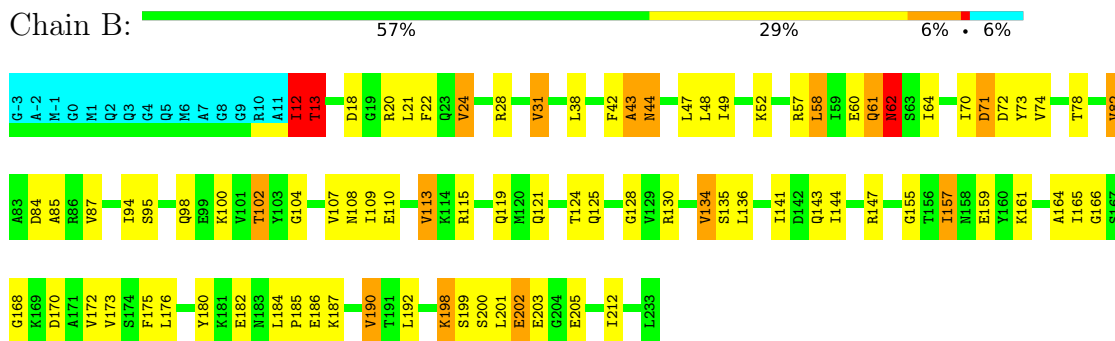
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

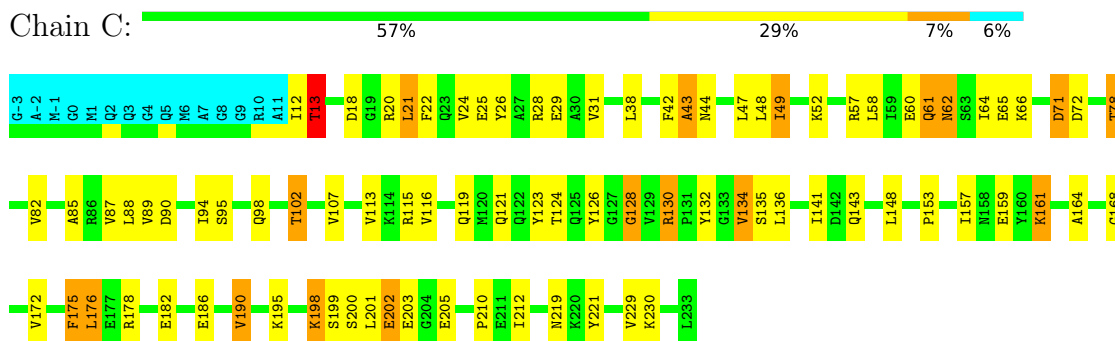
- Molecule 1: Proteasome subunit alpha



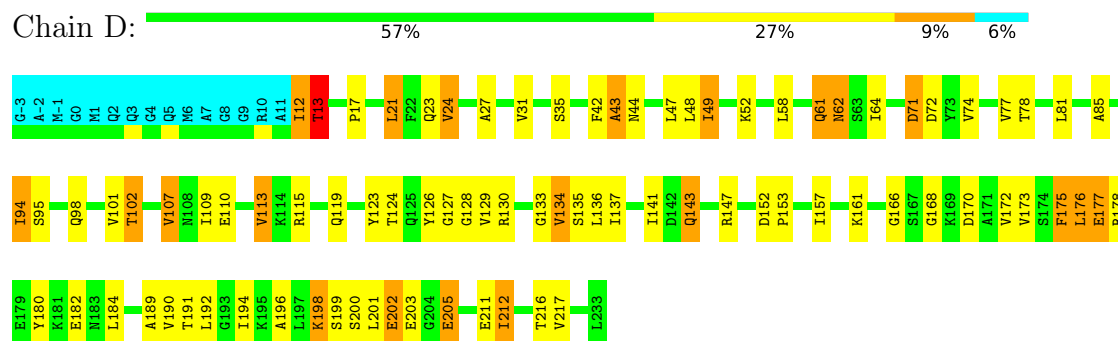
- Molecule 1: Proteasome subunit alpha



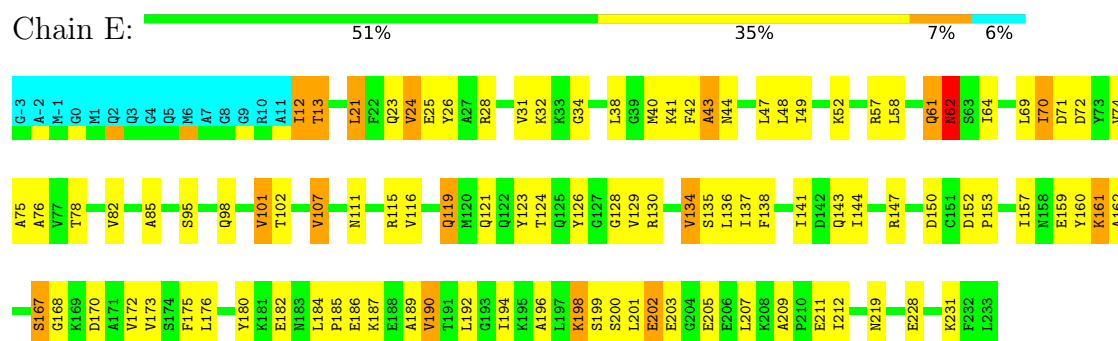
- Molecule 1: Proteasome subunit alpha



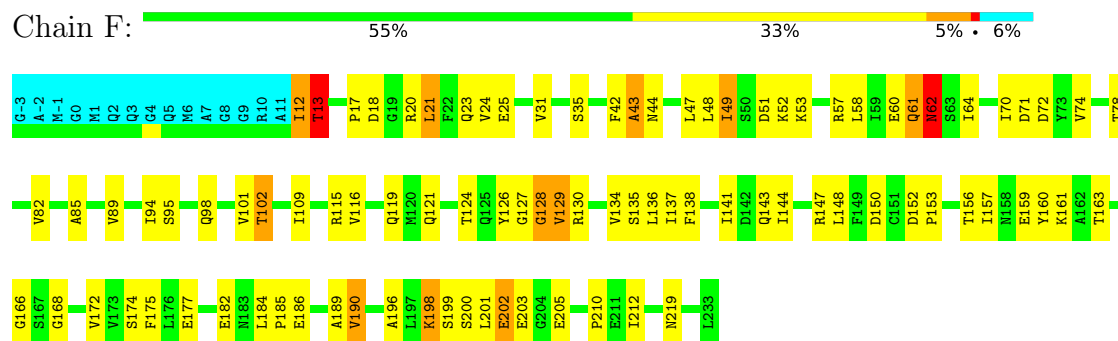
- Molecule 1: Proteasome subunit alpha



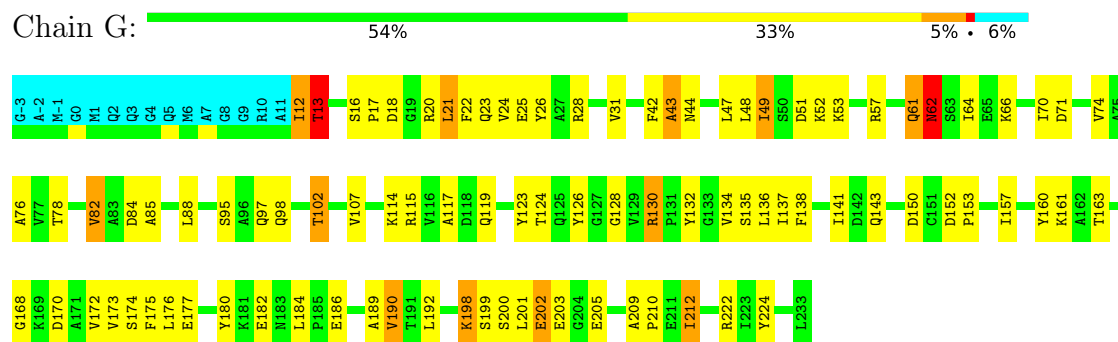
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

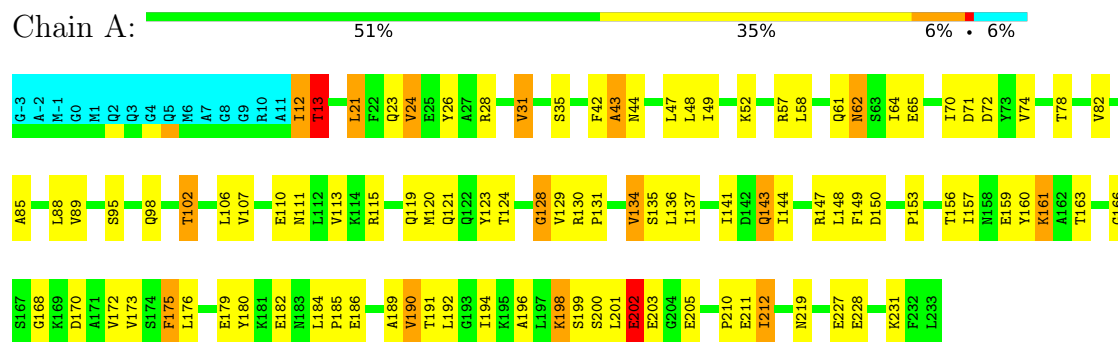


- Molecule 1: Proteasome subunit alpha

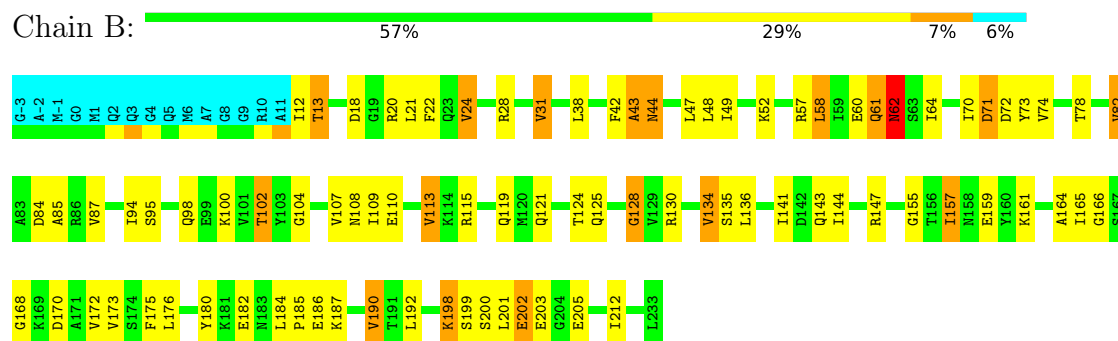


4.2.2 Score per residue for model 2

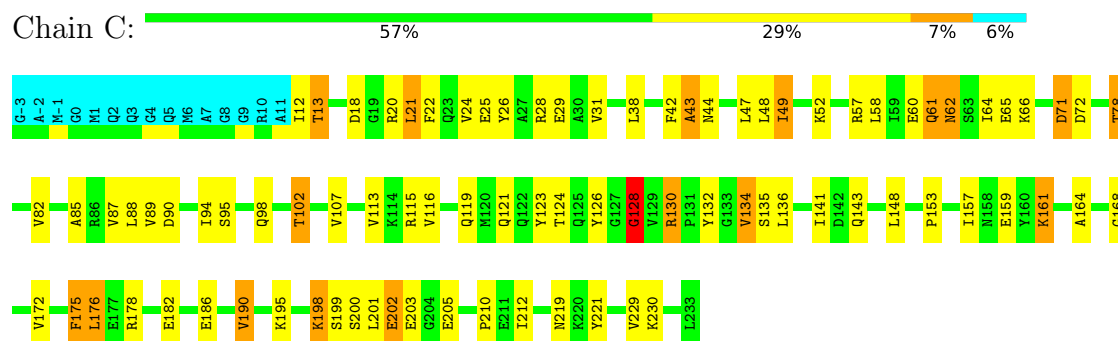
• Molecule 1: Proteasome subunit alpha



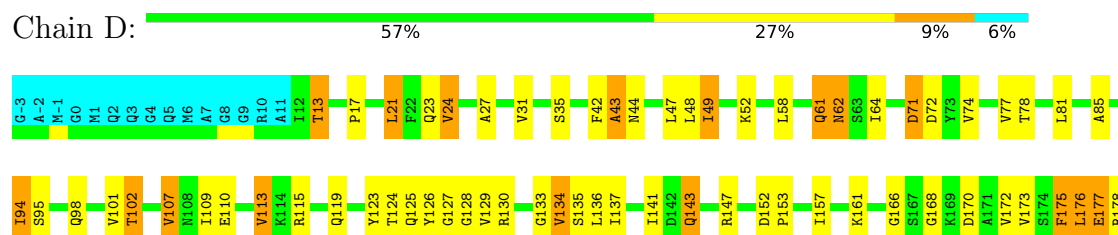
• Molecule 1: Proteasome subunit alpha

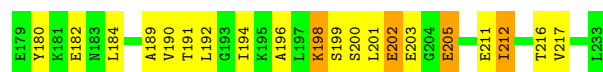


• Molecule 1: Proteasome subunit alpha

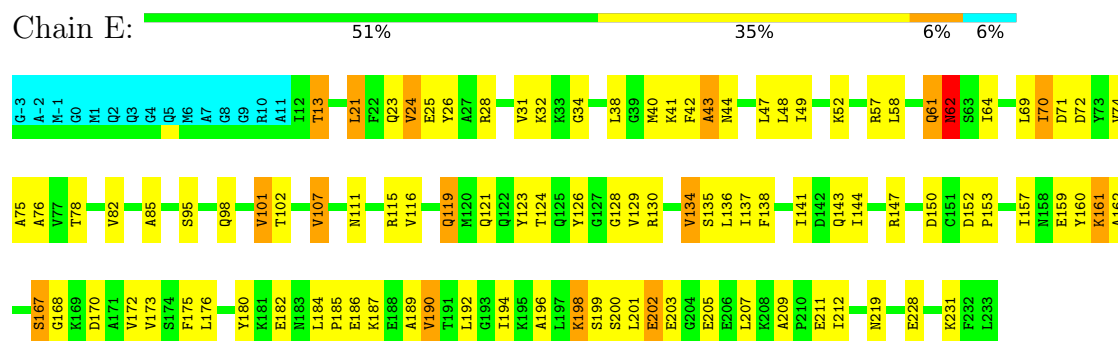


• Molecule 1: Proteasome subunit alpha

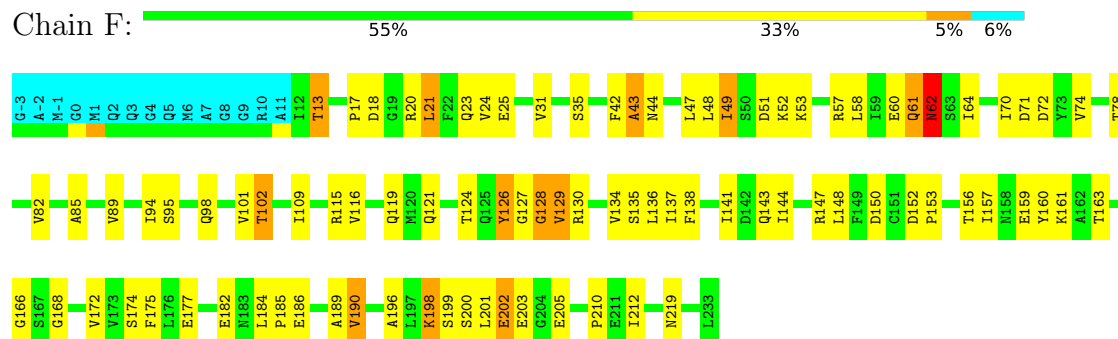




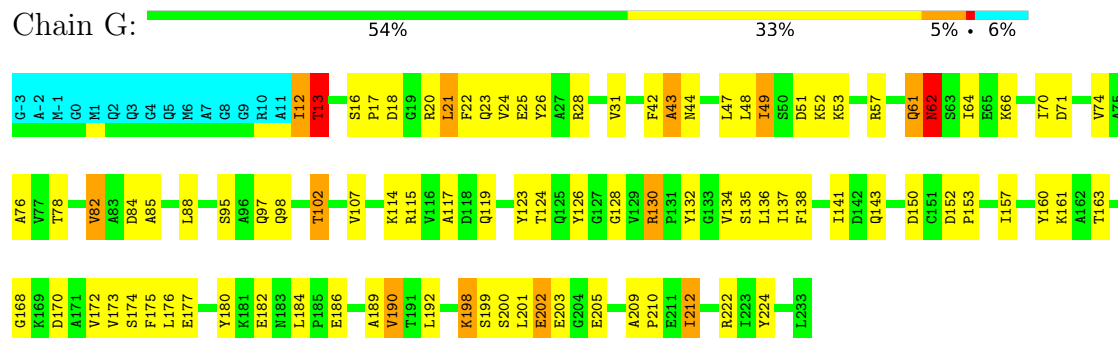
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

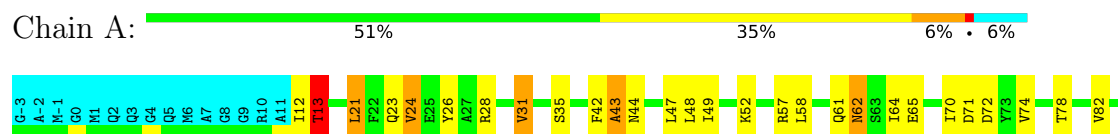


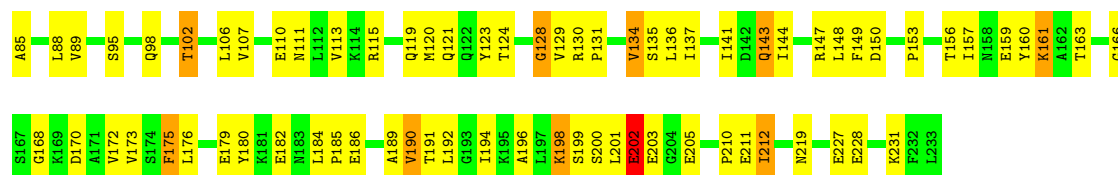
- Molecule 1: Proteasome subunit alpha



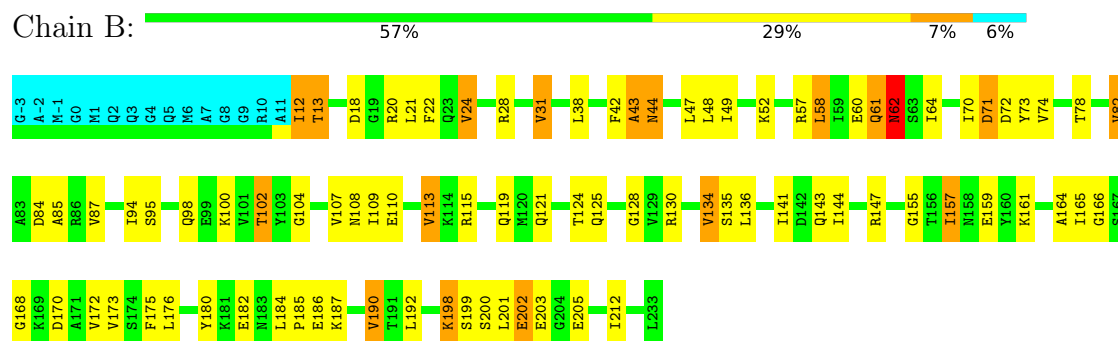
4.2.3 Score per residue for model 3

- Molecule 1: Proteasome subunit alpha

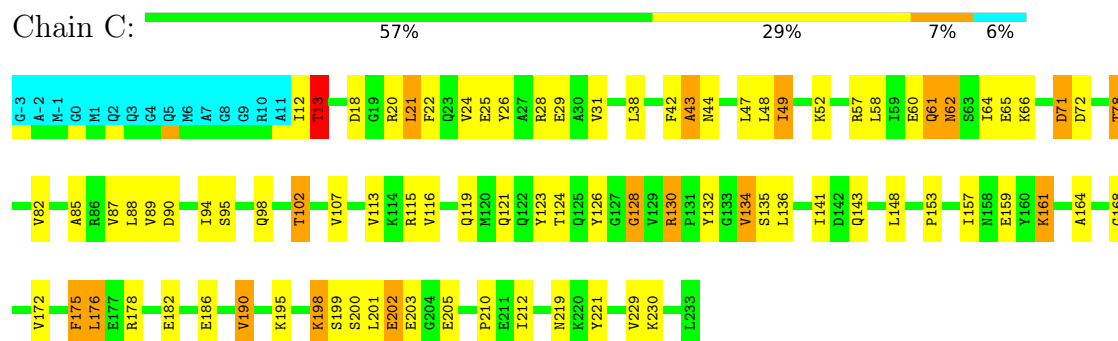




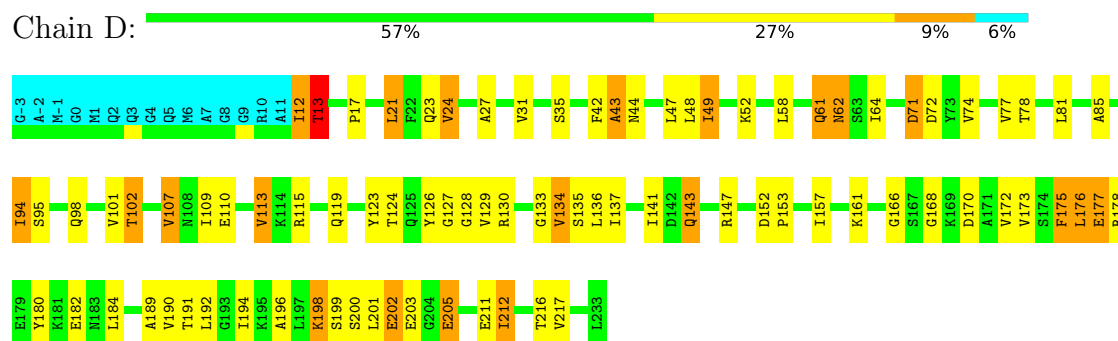
• Molecule 1: Proteasome subunit alpha



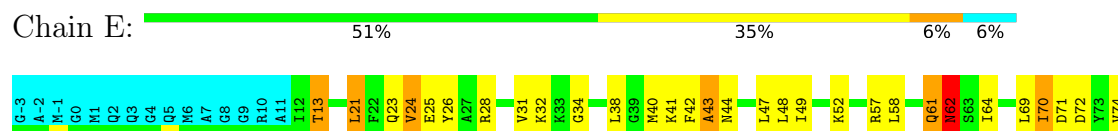
• Molecule 1: Proteasome subunit alpha

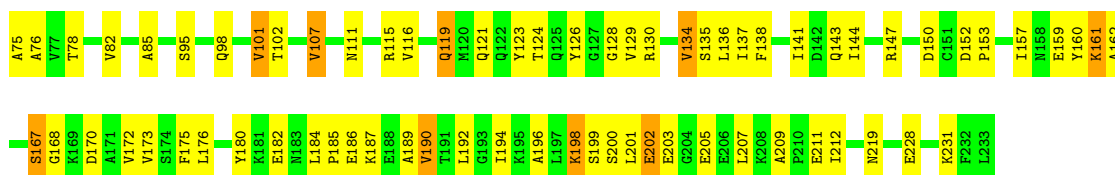


• Molecule 1: Proteasome subunit alpha



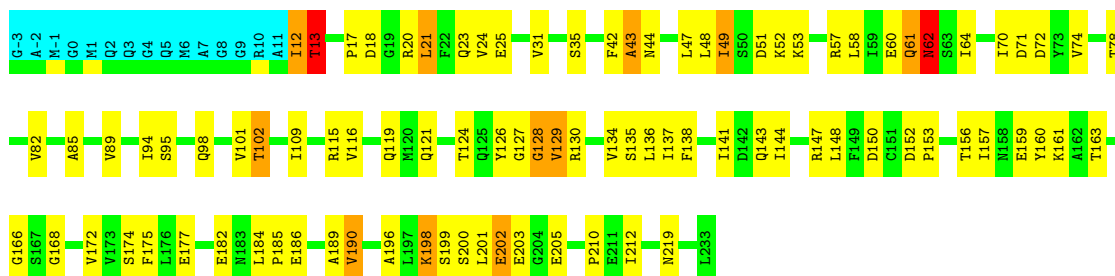
• Molecule 1: Proteasome subunit alpha





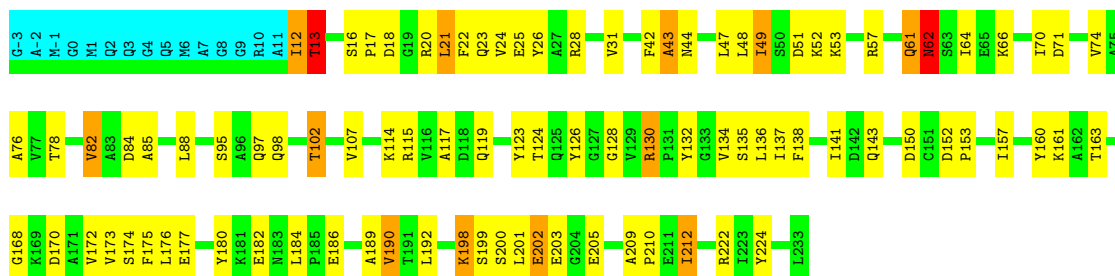
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% • 6%



• Molecule 1: Proteasome subunit alpha

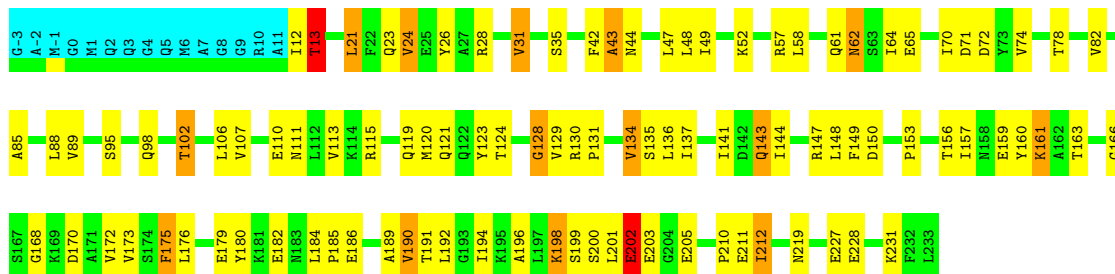
Chain G: 54% 33% 5% • 6%



4.2.4 Score per residue for model 4

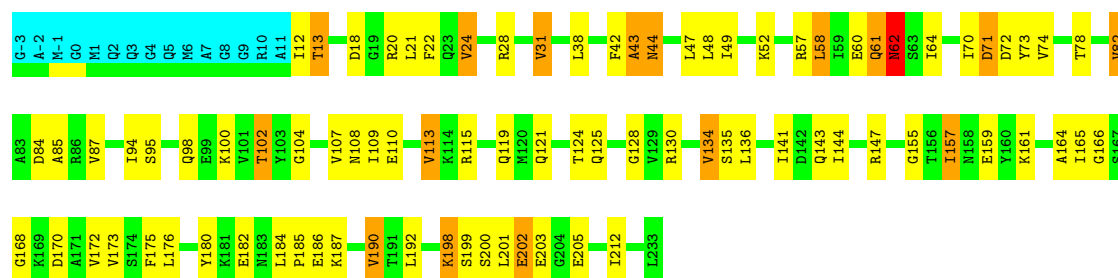
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% • 6%



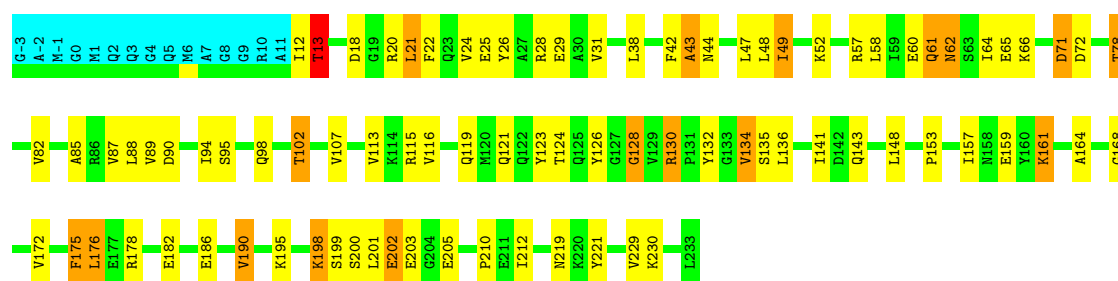
• Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 7% • 6%



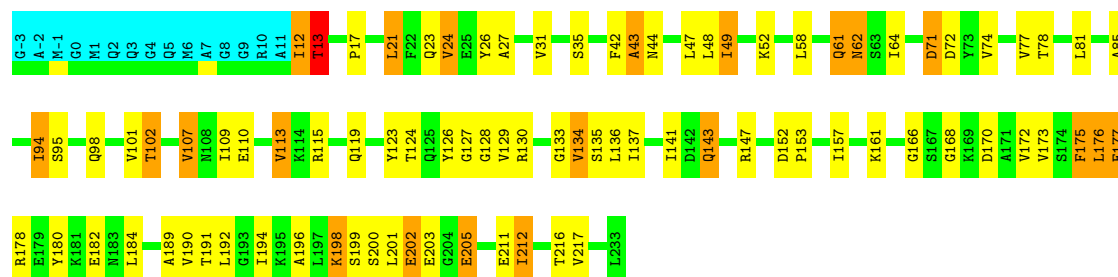
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 29% 7% 6%



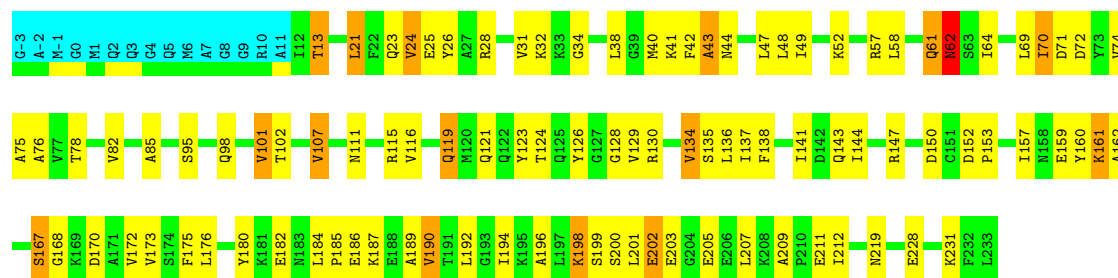
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



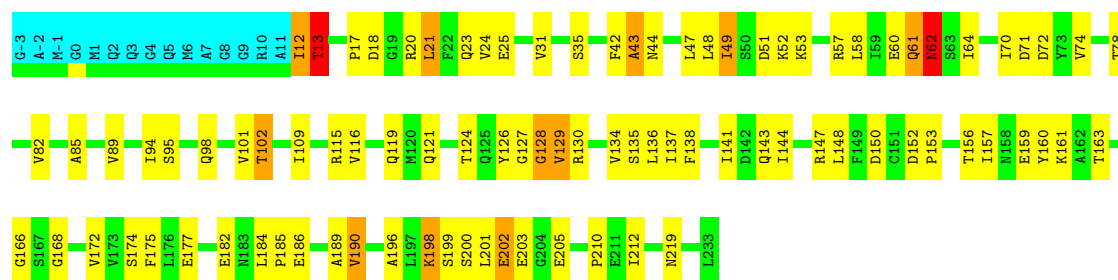
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% 6%



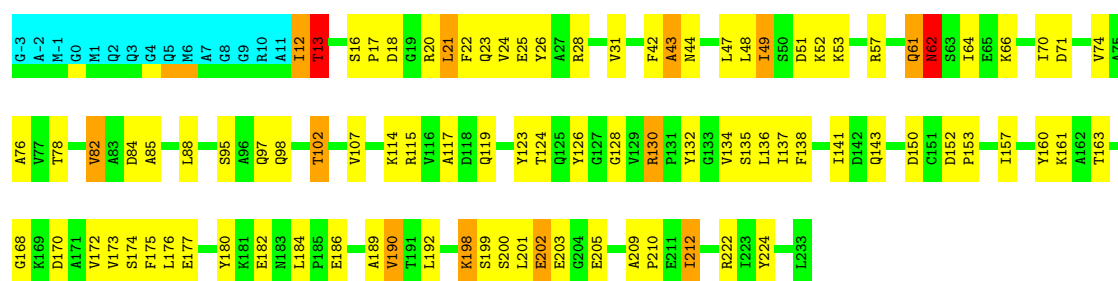
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

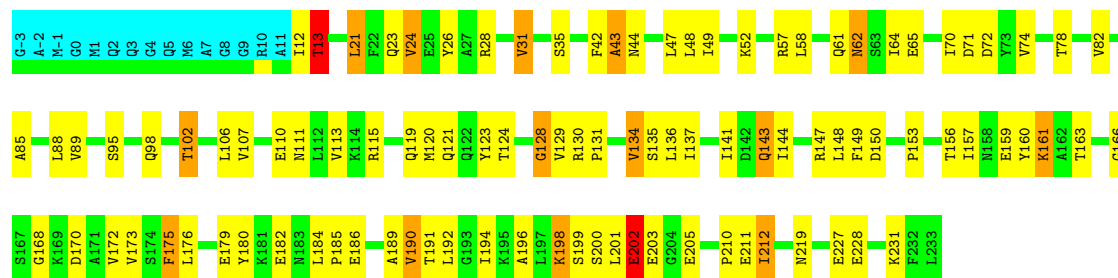
Chain G: 54% 33% 5% • 6%



4.2.5 Score per residue for model 5

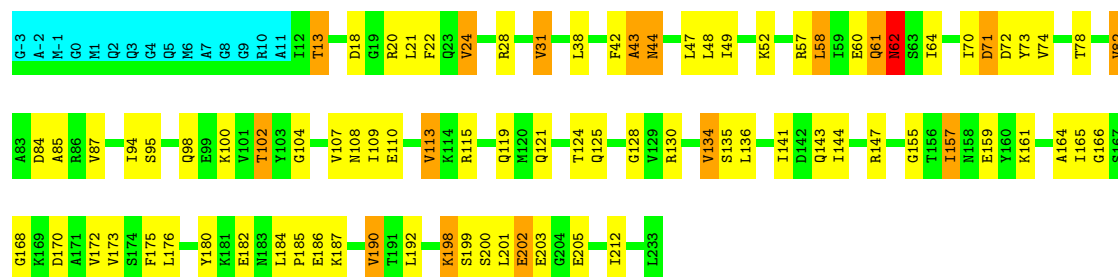
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% • 6%

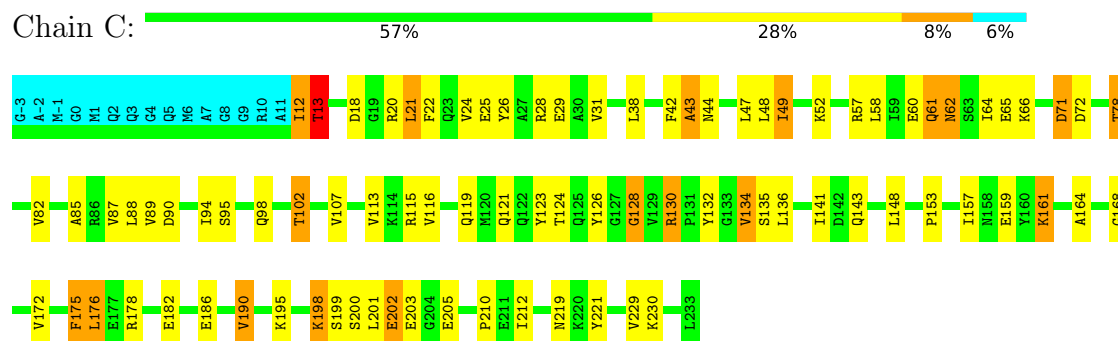


• Molecule 1: Proteasome subunit alpha

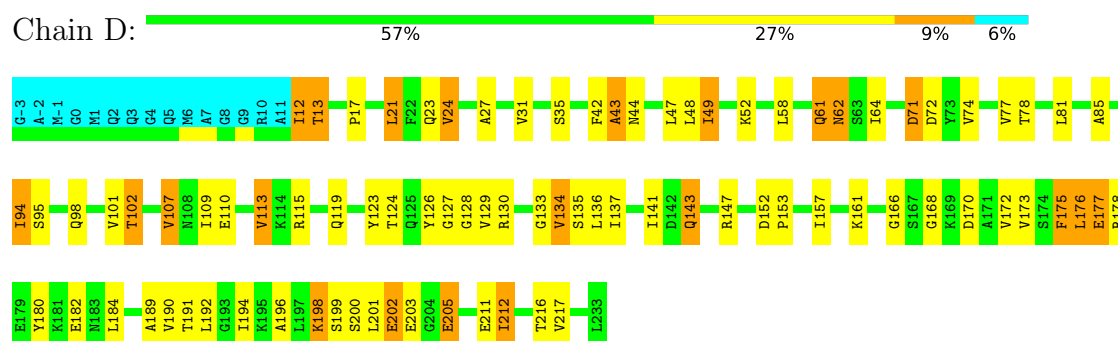
Chain B: 57% 29% 7% 6%



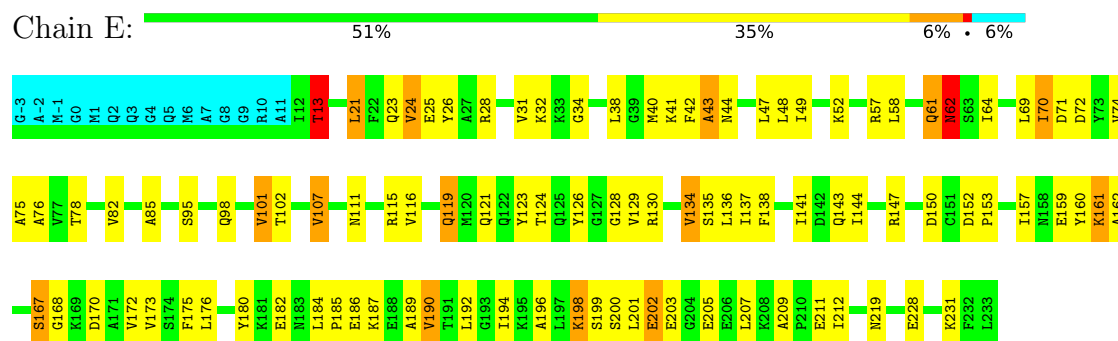
- Molecule 1: Proteasome subunit alpha



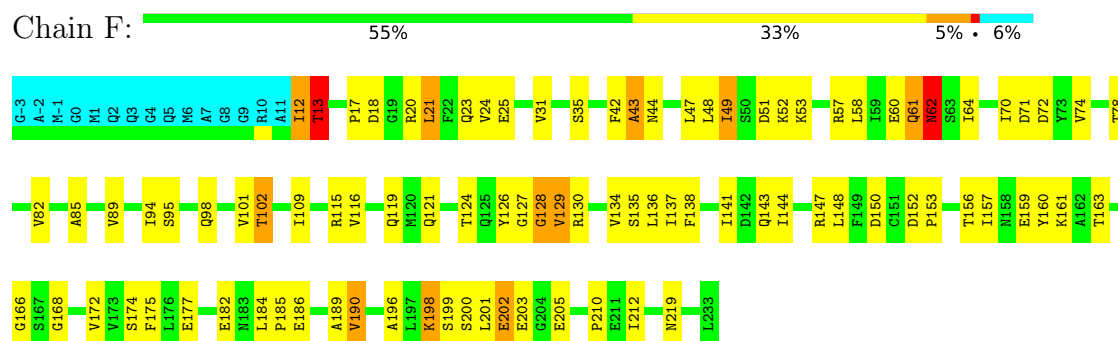
- Molecule 1: Proteasome subunit alpha



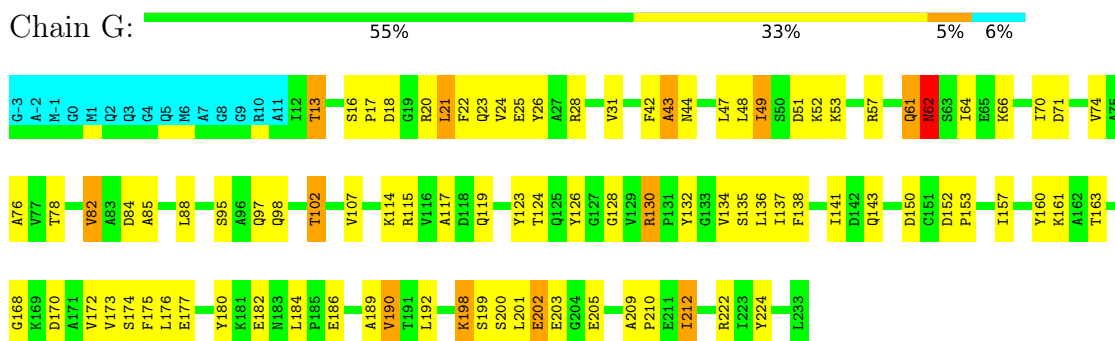
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

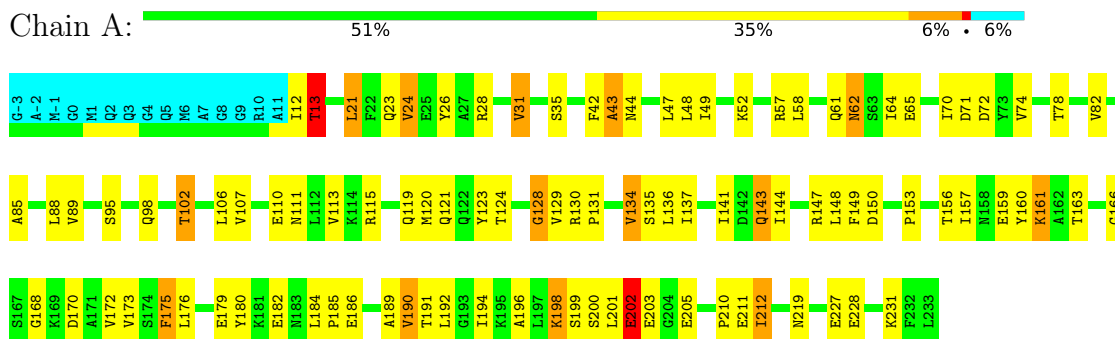


- Molecule 1: Proteasome subunit alpha

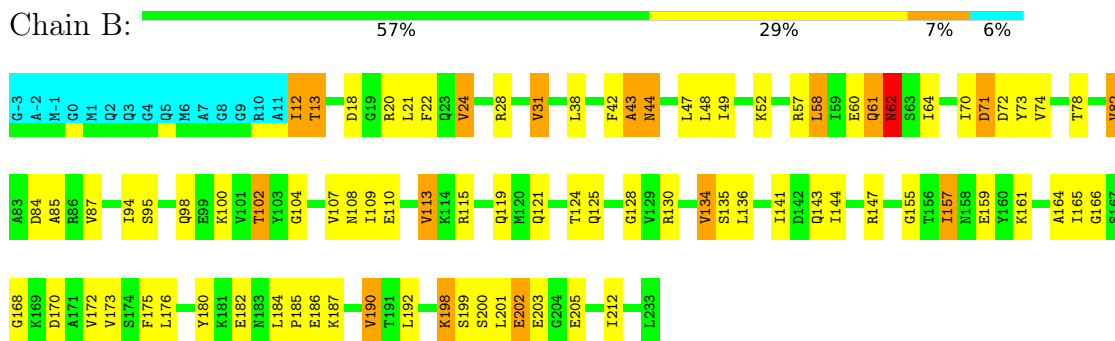


4.2.6 Score per residue for model 6

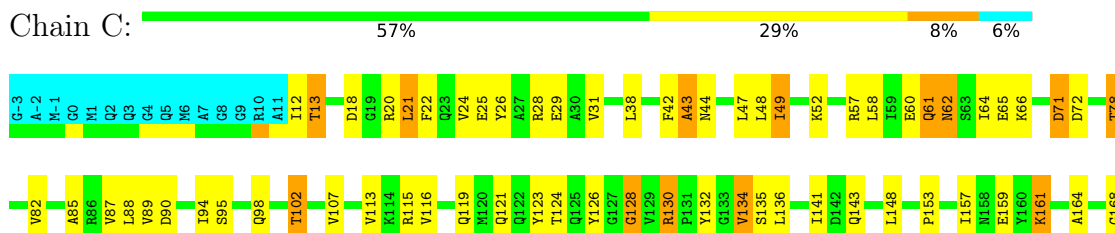
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



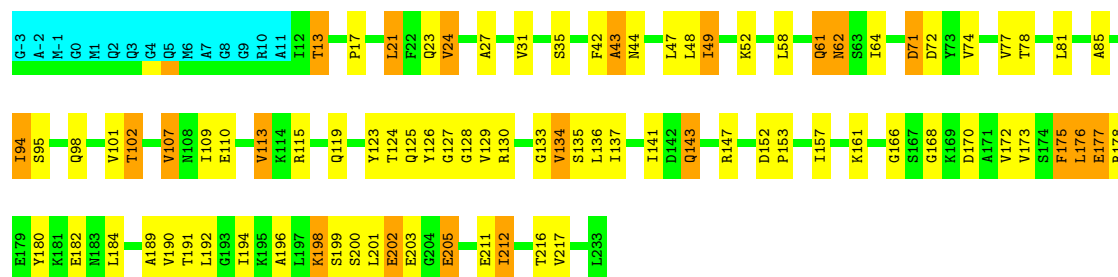
- Molecule 1: Proteasome subunit alpha





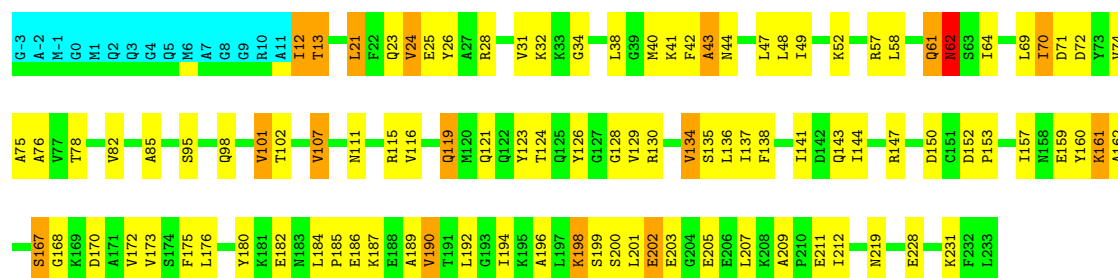
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



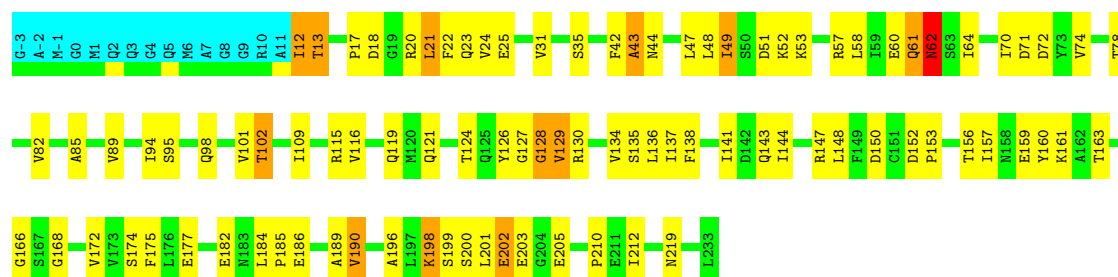
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



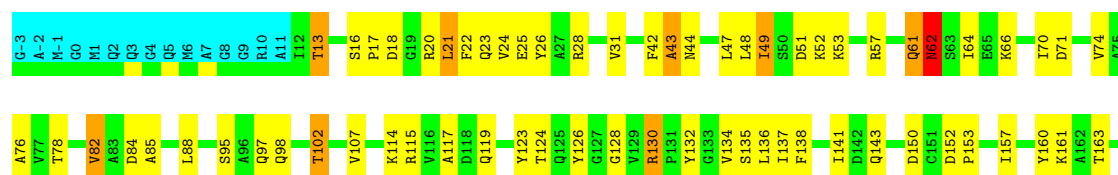
• Molecule 1: Proteasome subunit alpha

Chain F: 54% 34% 5% 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 55% 33% 5% 6%

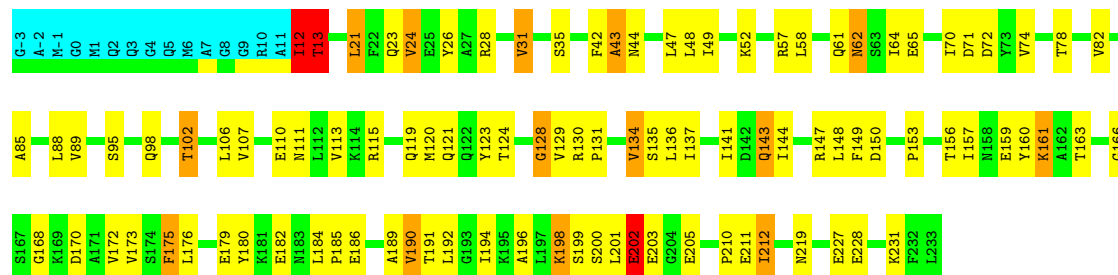




4.2.7 Score per residue for model 7

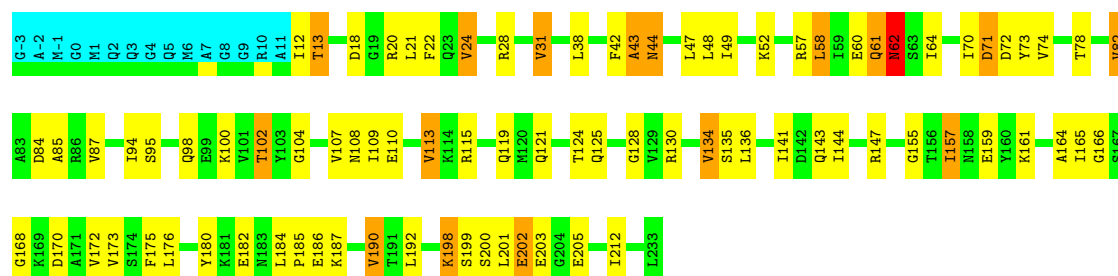
- Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



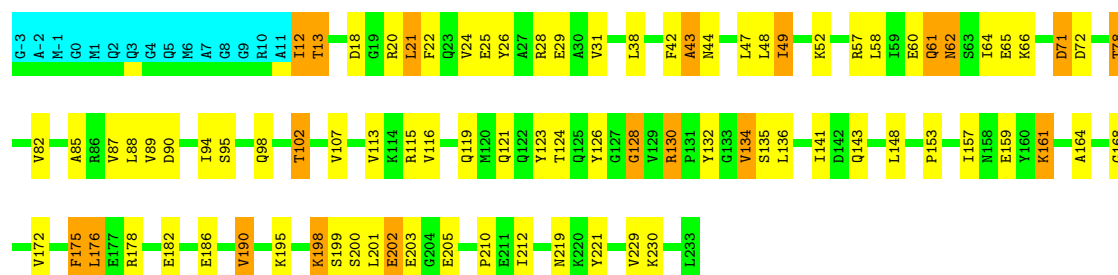
- Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 7% 6%



- Molecule 1: Proteasome subunit alpha

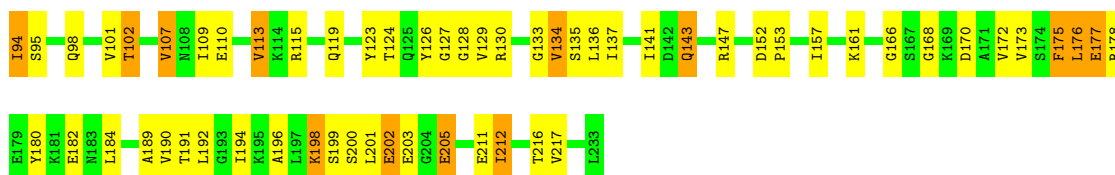
Chain C: 57% 28% 8% 6%



- Molecule 1: Proteasome subunit alpha

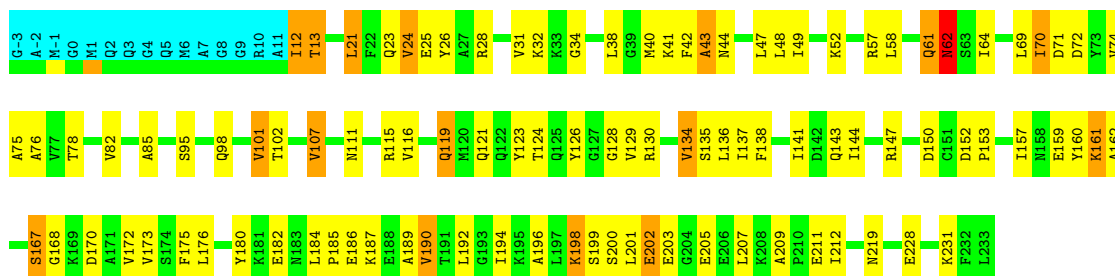
Chain D: 57% 27% 9% 6%





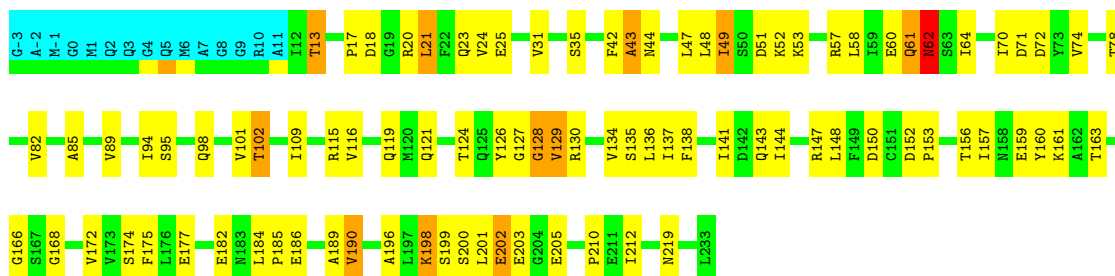
- Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



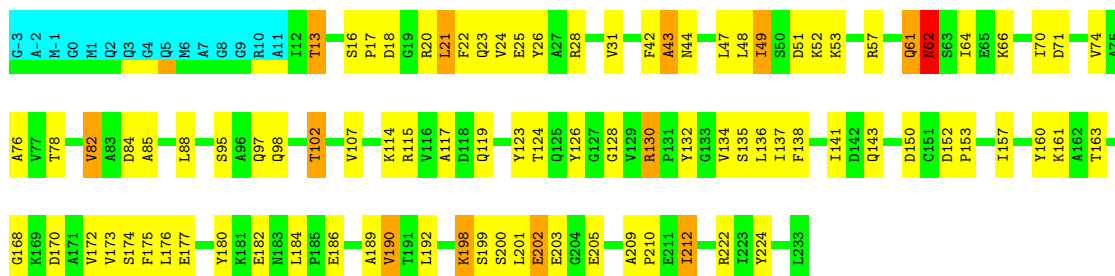
- Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



- Molecule 1: Proteasome subunit alpha

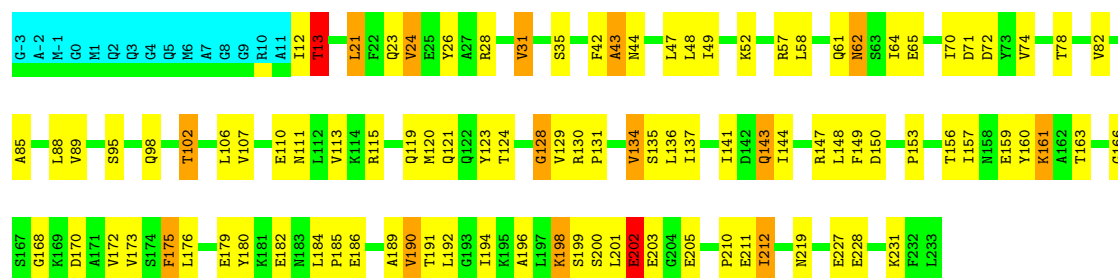
Chain G: 55% 33% 5% 6%



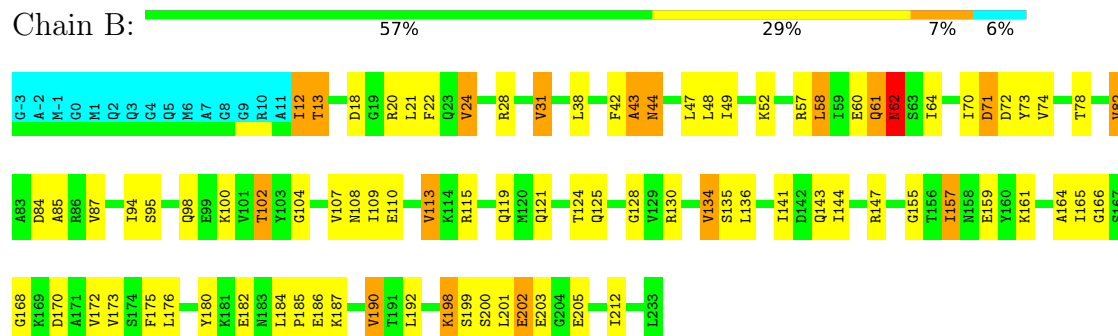
4.2.8 Score per residue for model 8

- Molecule 1: Proteasome subunit alpha

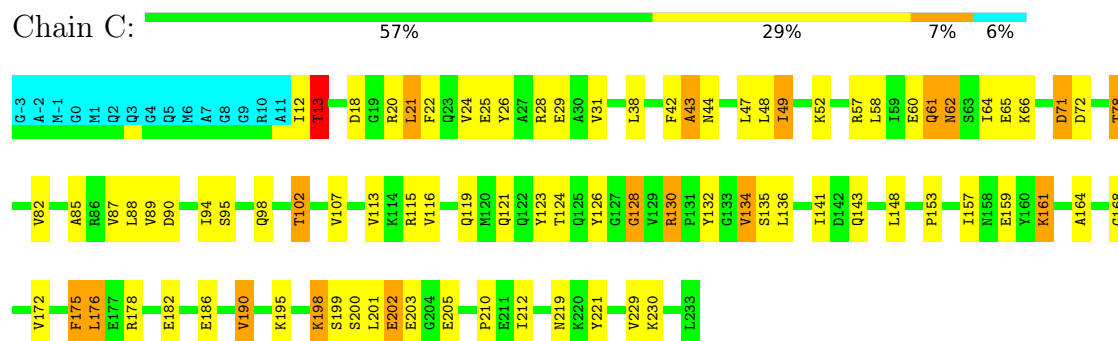
Chain A: 51% 35% 6% 6%



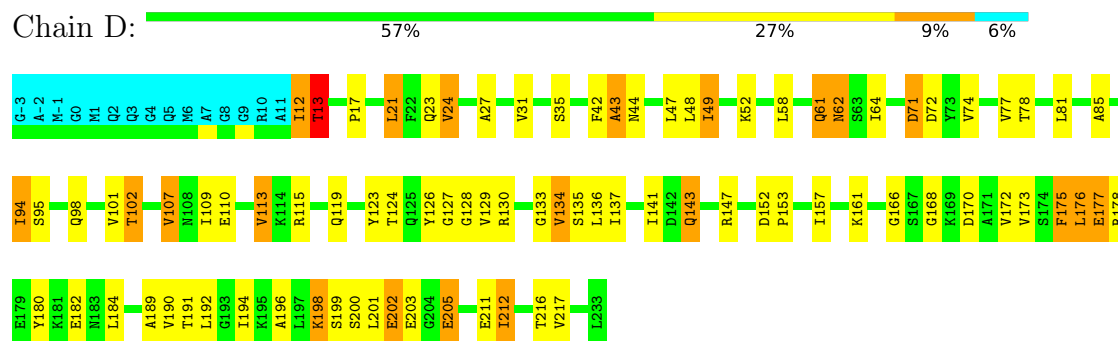
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

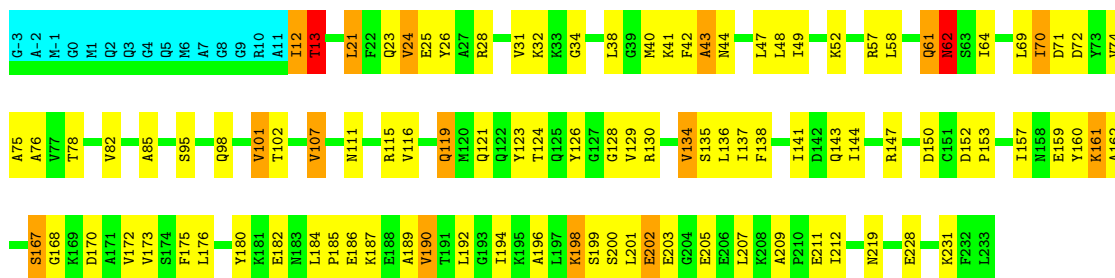


• Molecule 1: Proteasome subunit alpha



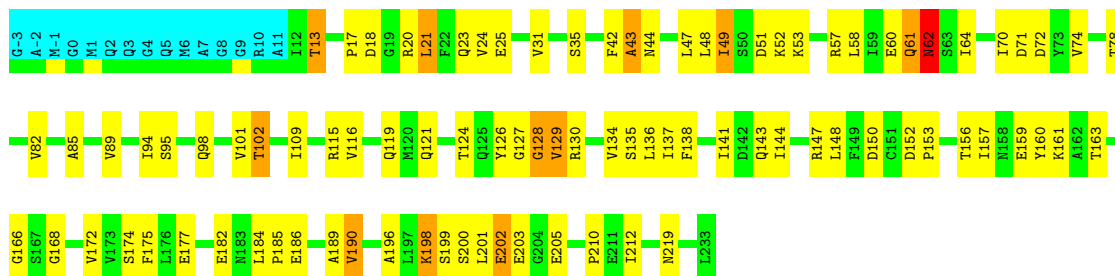
• Molecule 1: Proteasome subunit alpha





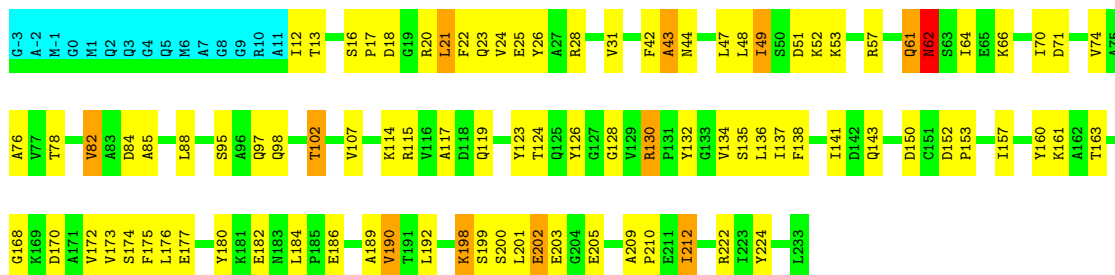
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

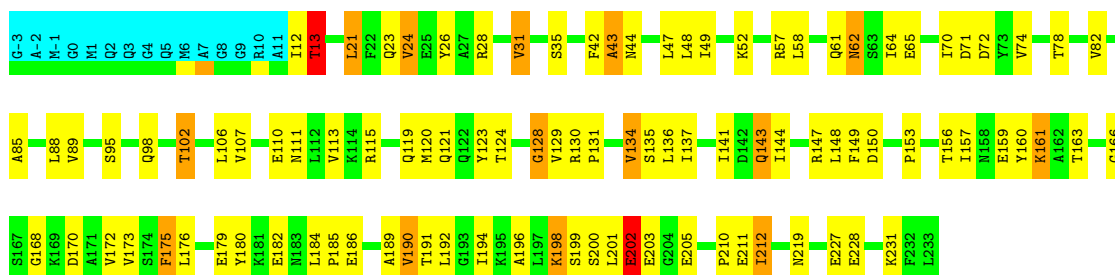
Chain G: 54% 34% 5% 6%



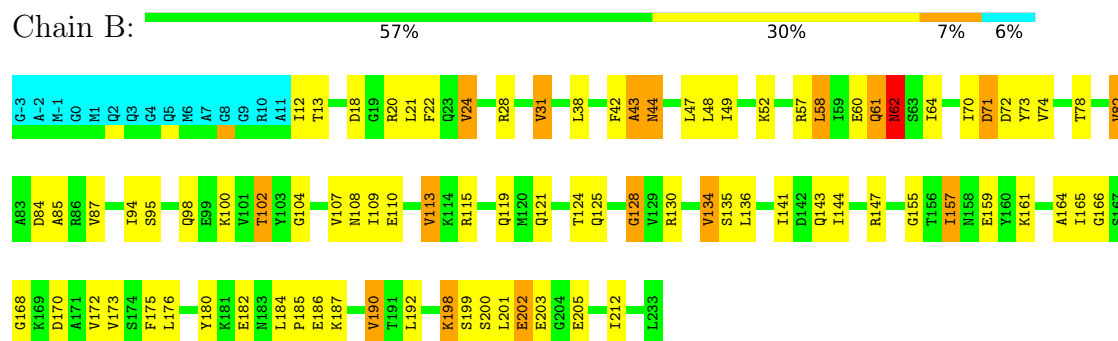
4.2.9 Score per residue for model 9

• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



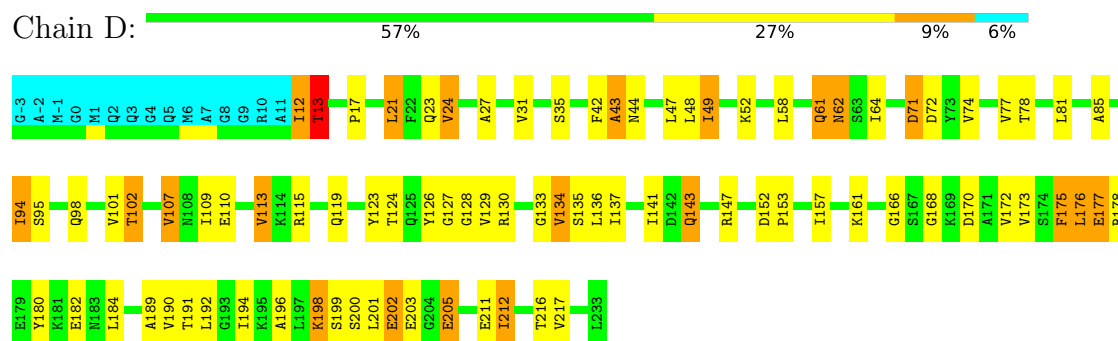
- Molecule 1: Proteasome subunit alpha



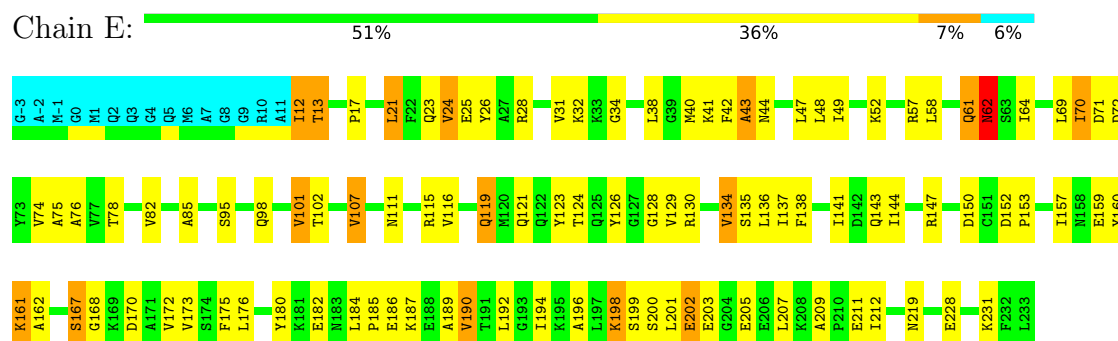
- Molecule 1: Proteasome subunit alpha



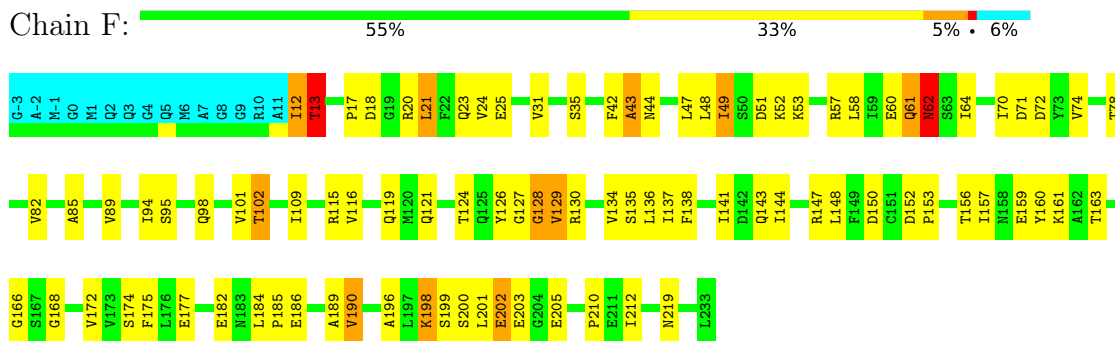
- Molecule 1: Proteasome subunit alpha



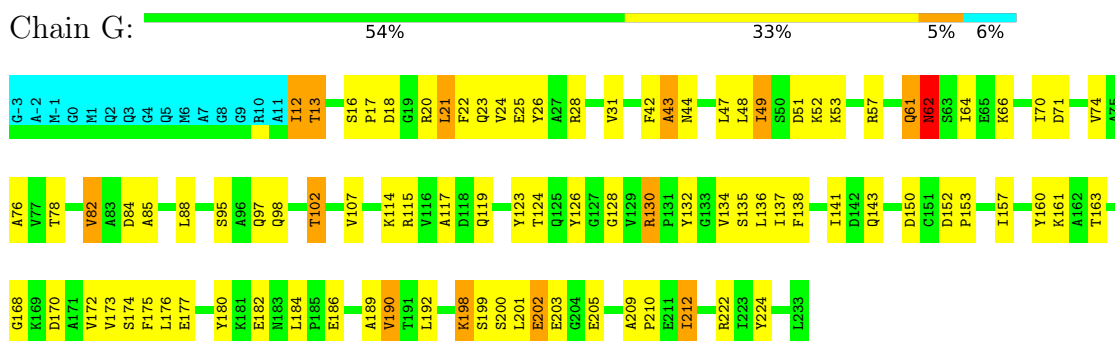
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

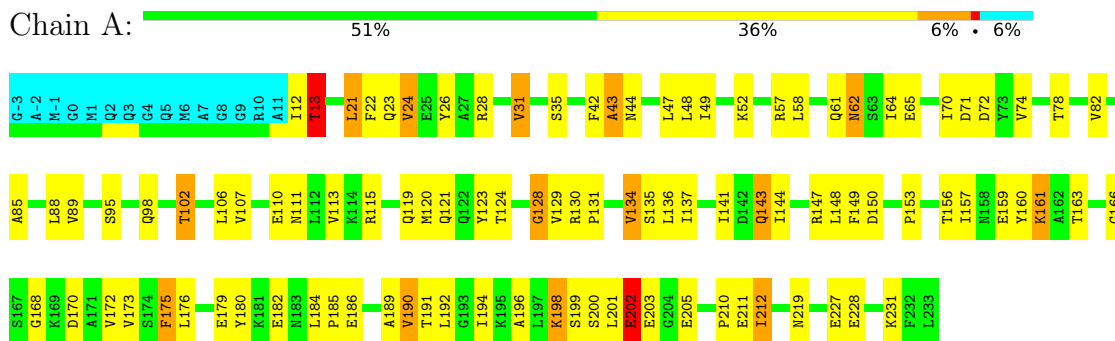


- Molecule 1: Proteasome subunit alpha

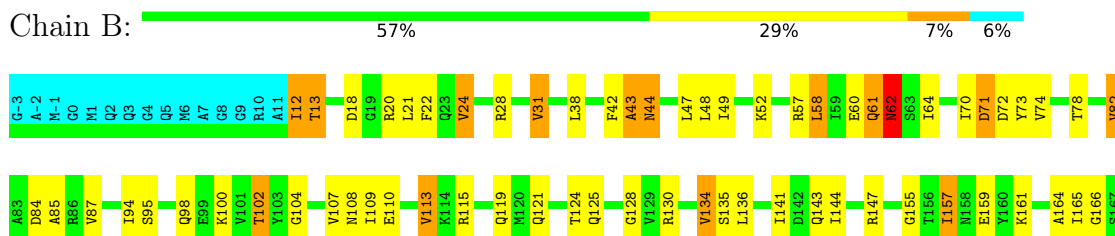


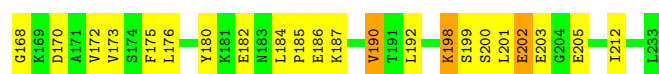
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha





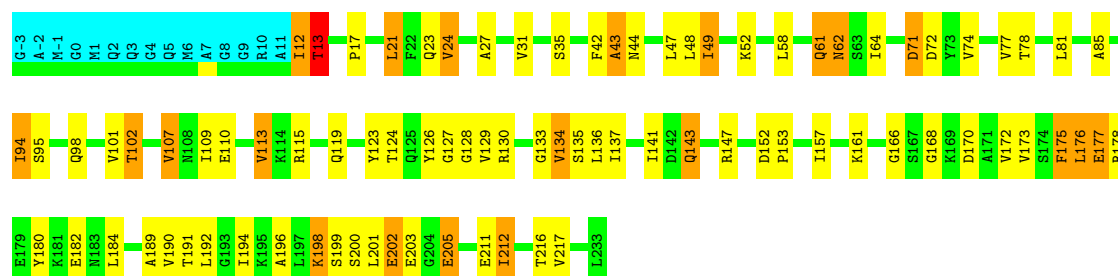
• Molecule 1: Proteasome subunit alpha

Chain C: 58% 28% 8% 6%



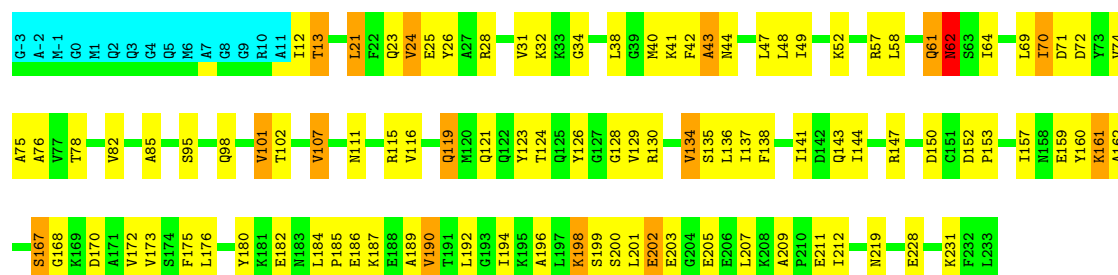
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



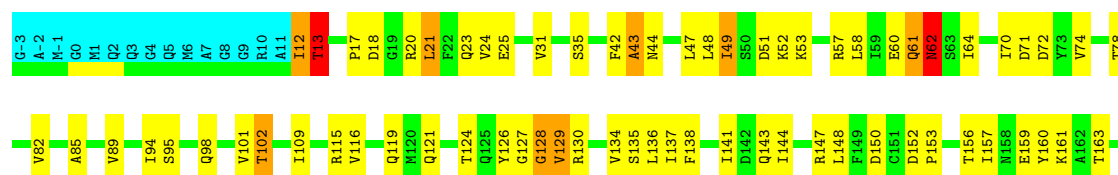
• Molecule 1: Proteasome subunit alpha

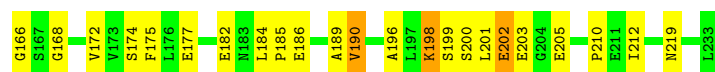
Chain E: 51% 36% 6% 6%



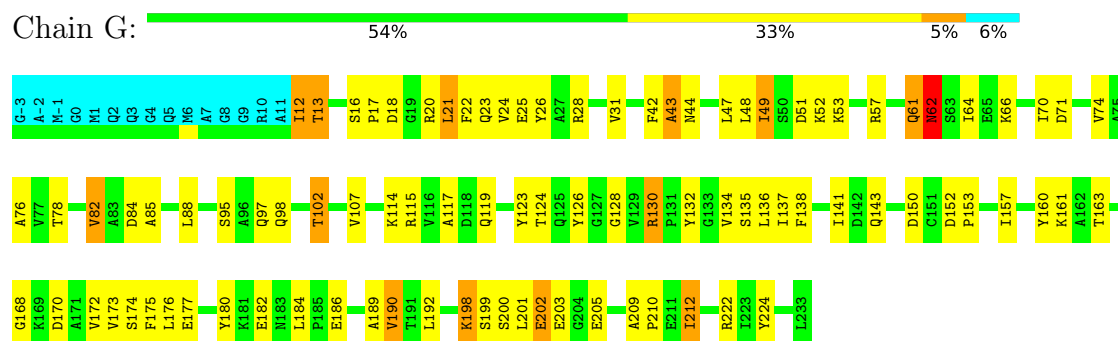
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



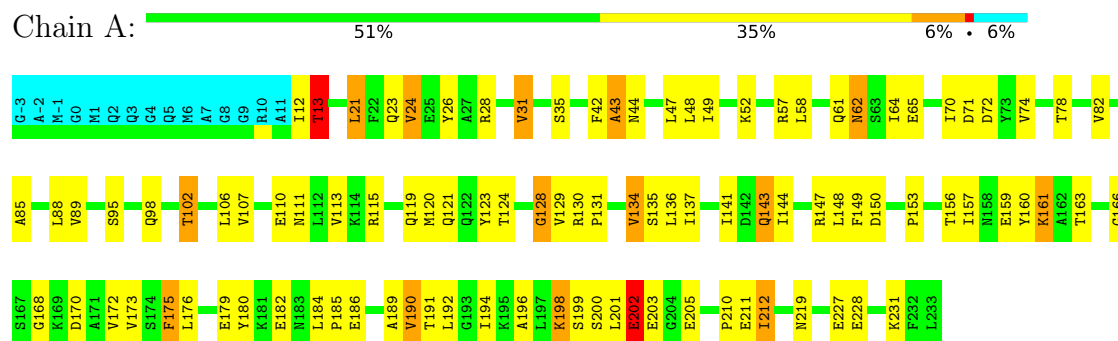


• Molecule 1: Proteasome subunit alpha

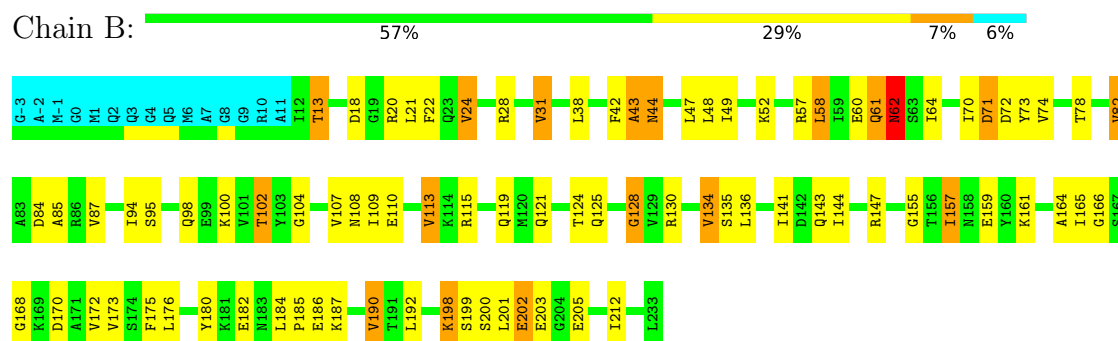


4.2.11 Score per residue for model 11

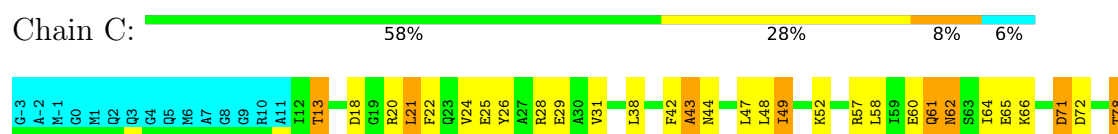
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



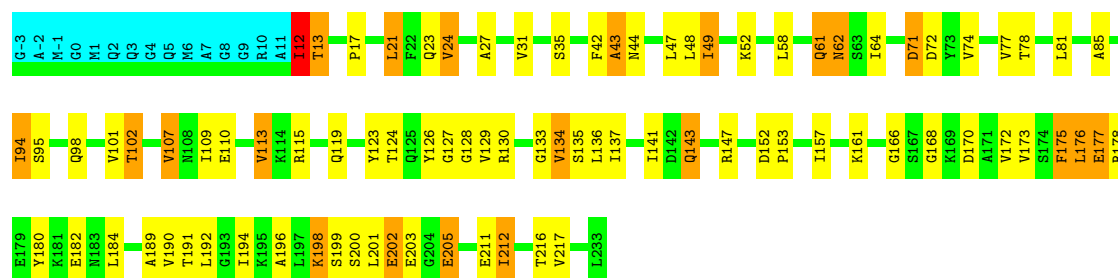
• Molecule 1: Proteasome subunit alpha





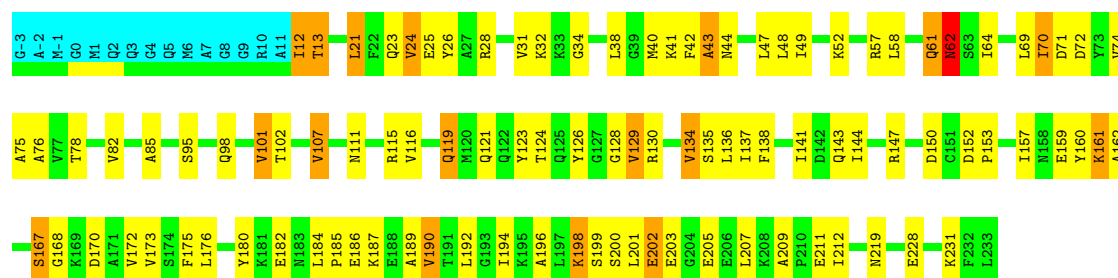
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



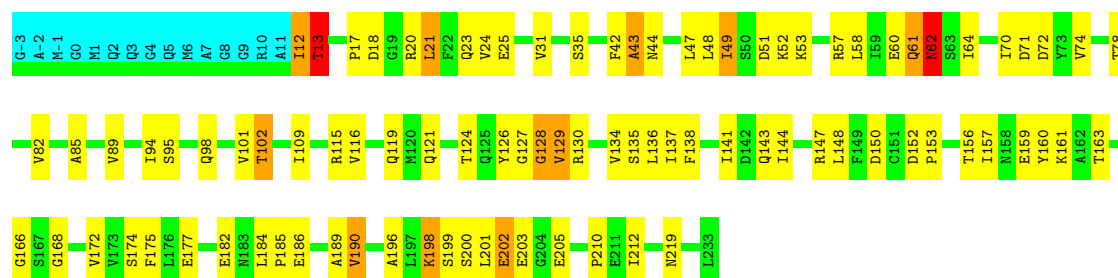
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



• Molecule 1: Proteasome subunit alpha

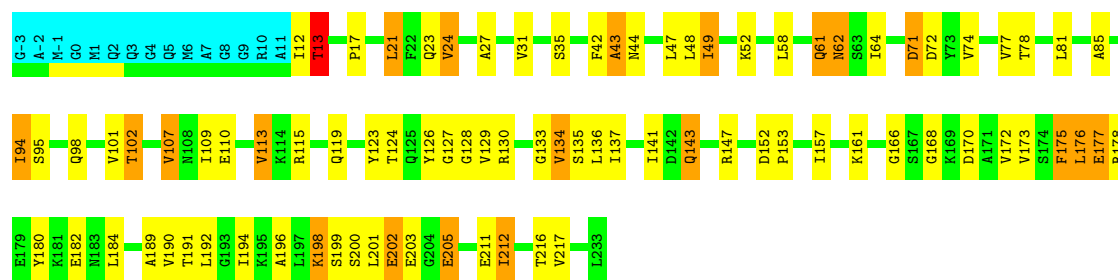
Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

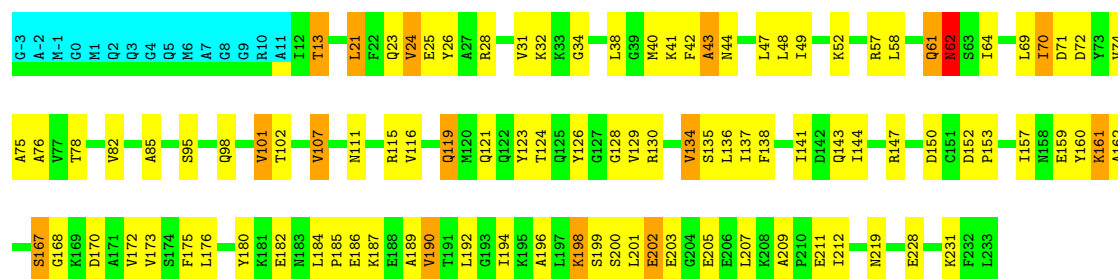
Chain G: 54% 33% 5% 6%





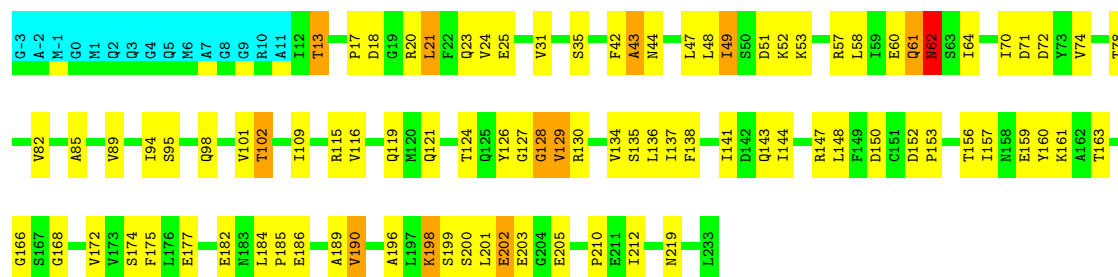
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% 6%



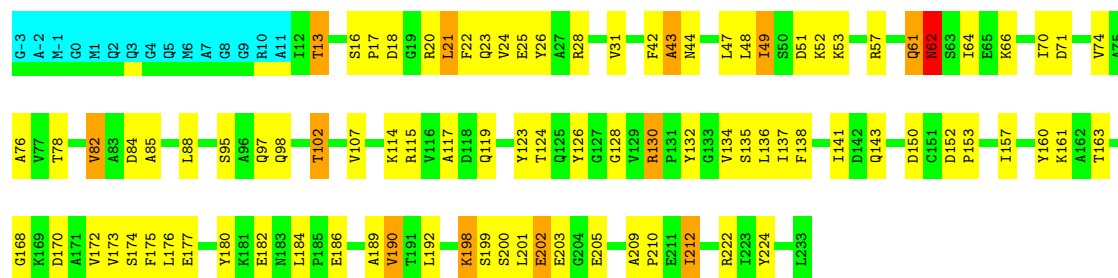
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



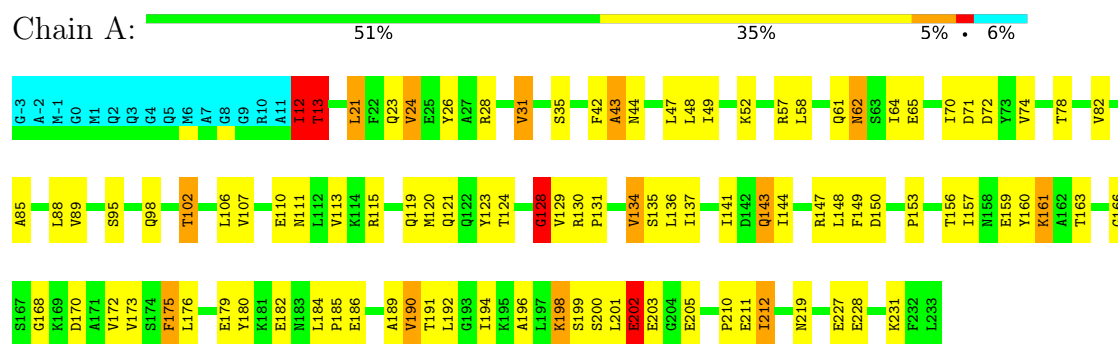
• Molecule 1: Proteasome subunit alpha

Chain G: 55% 33% 5% 6%

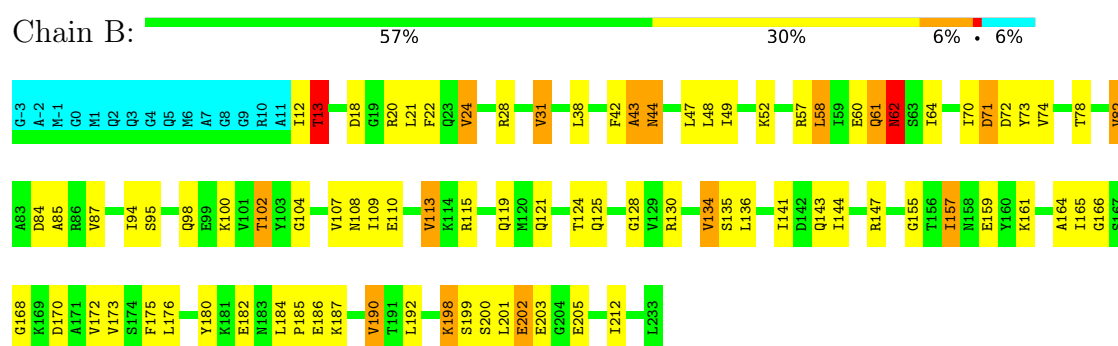


4.2.13 Score per residue for model 13

• Molecule 1: Proteasome subunit alpha



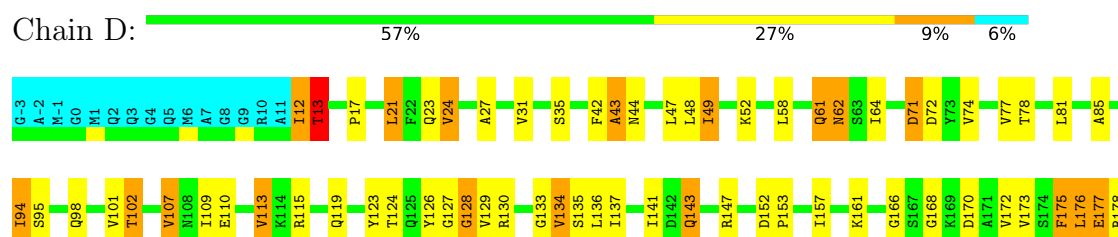
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

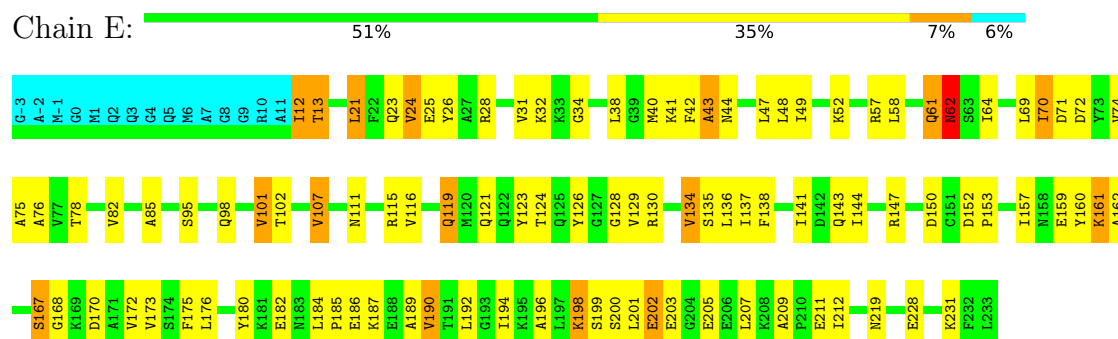


• Molecule 1: Proteasome subunit alpha

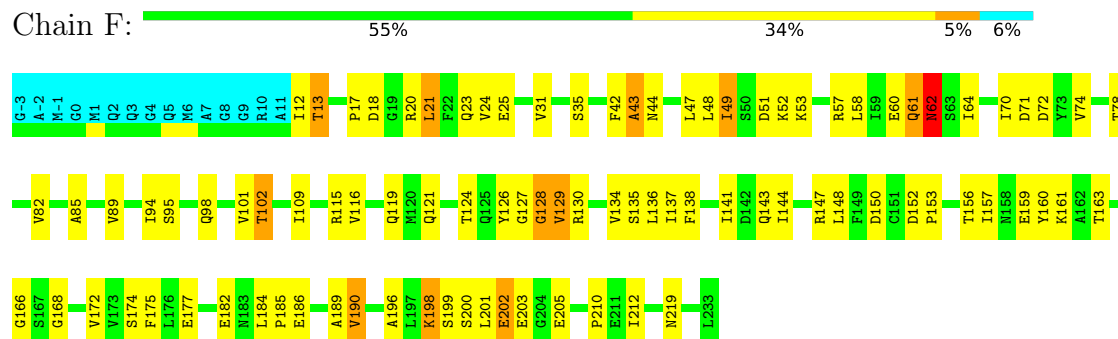




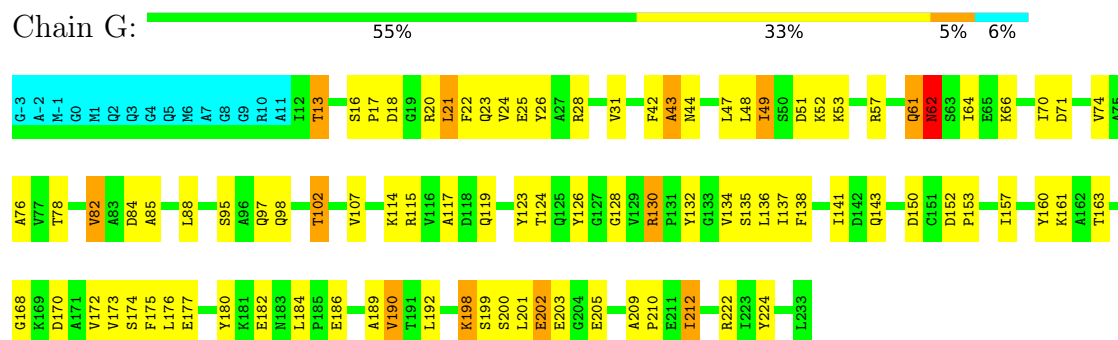
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

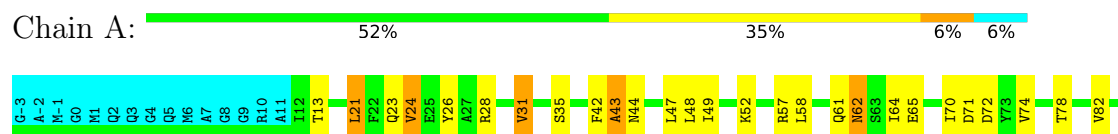


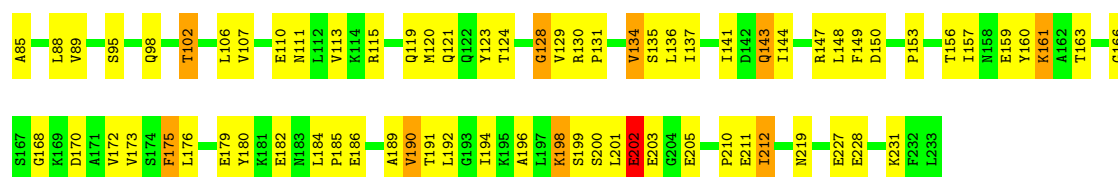
• Molecule 1: Proteasome subunit alpha



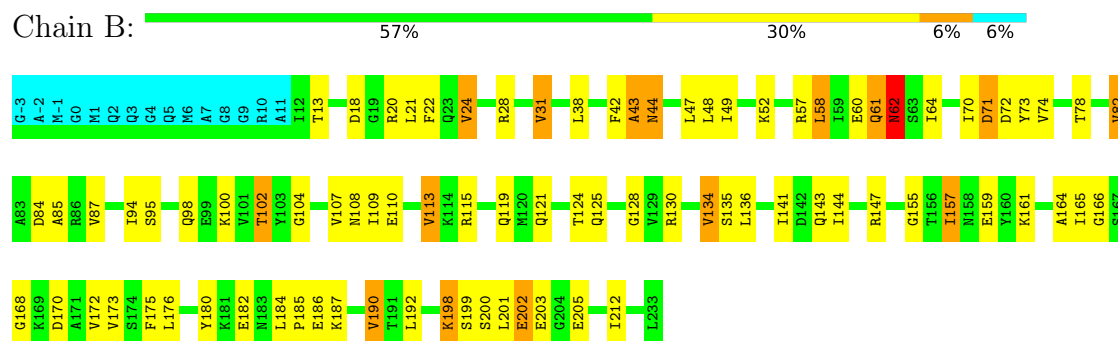
4.2.14 Score per residue for model 14

• Molecule 1: Proteasome subunit alpha

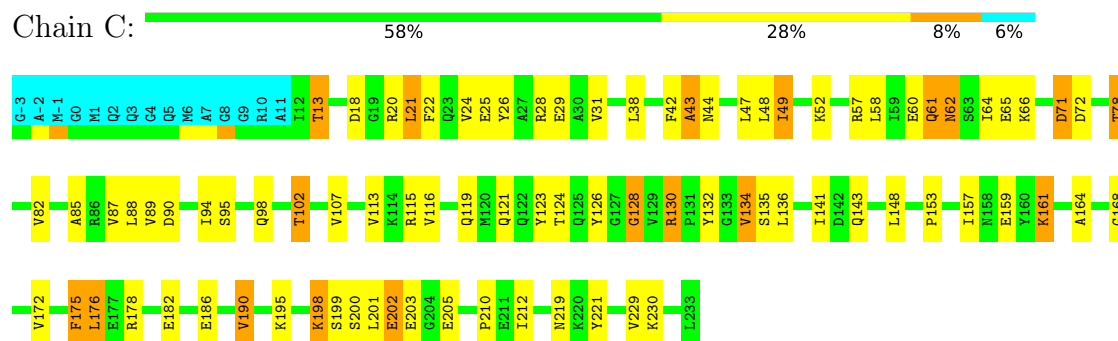




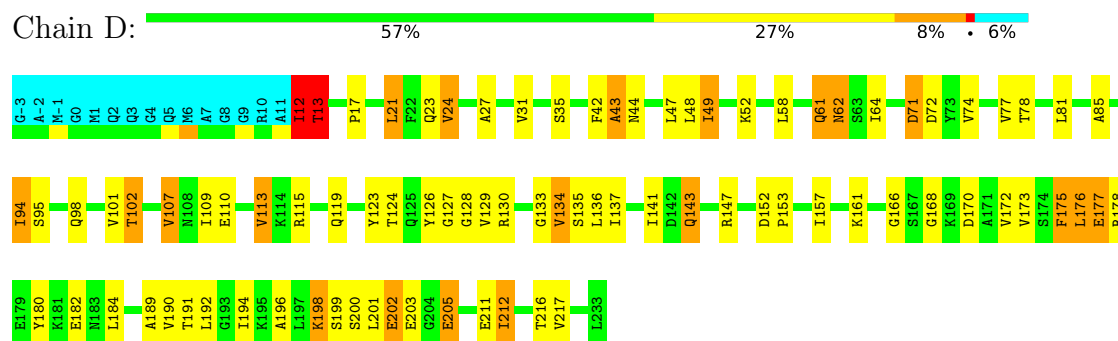
• Molecule 1: Proteasome subunit alpha



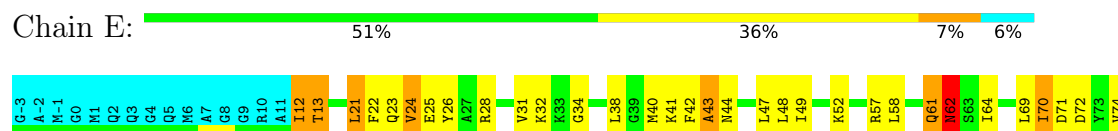
• Molecule 1: Proteasome subunit alpha

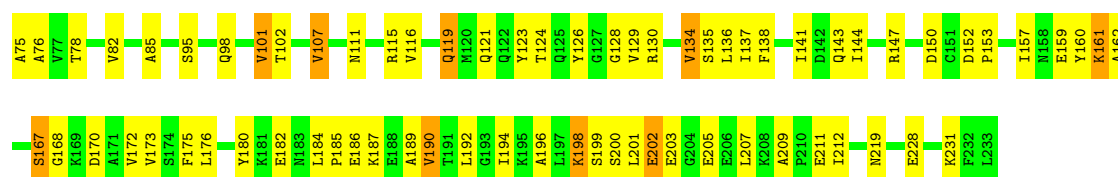


• Molecule 1: Proteasome subunit alpha

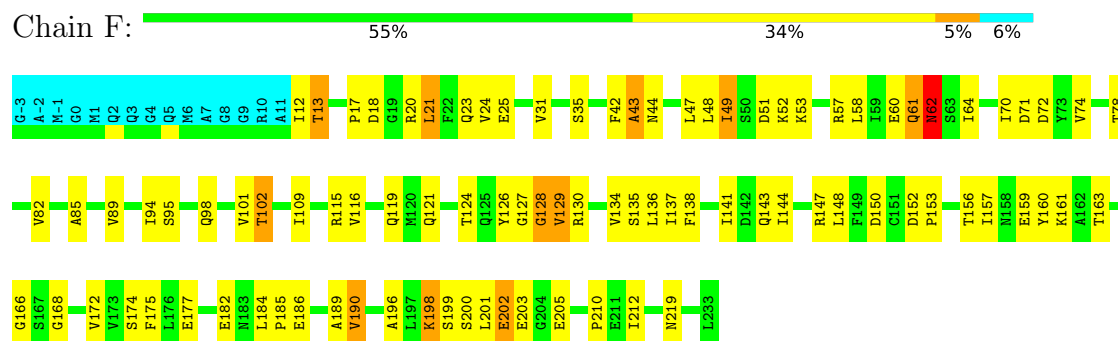


• Molecule 1: Proteasome subunit alpha

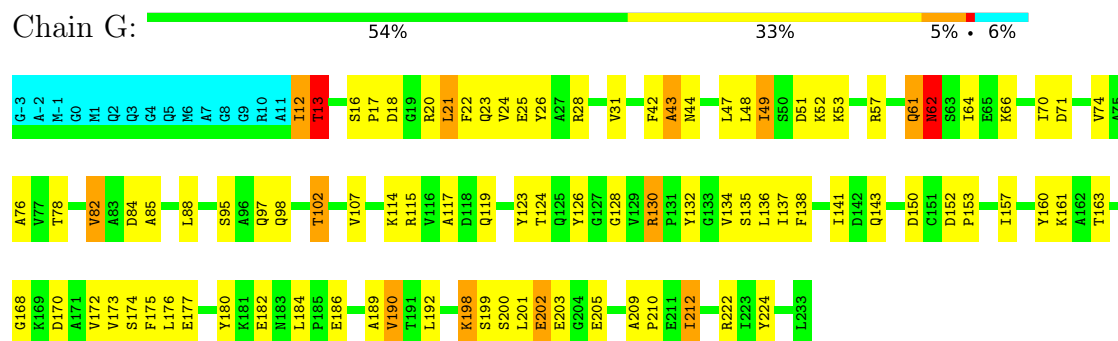




• Molecule 1: Proteasome subunit alpha

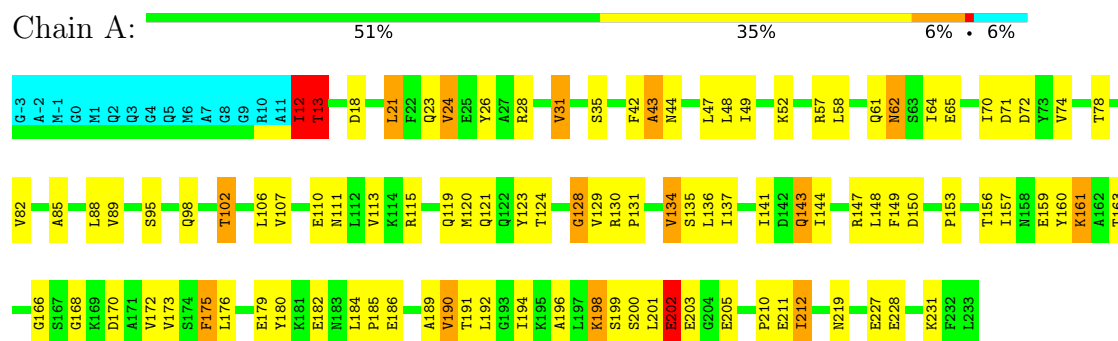


• Molecule 1: Proteasome subunit alpha



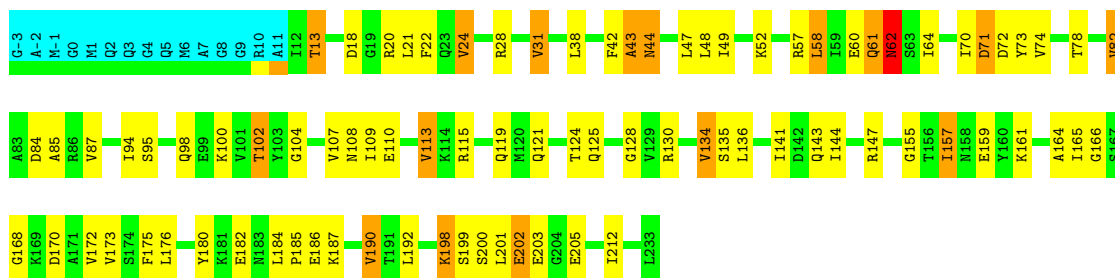
4.2.15 Score per residue for model 15

• Molecule 1: Proteasome subunit alpha

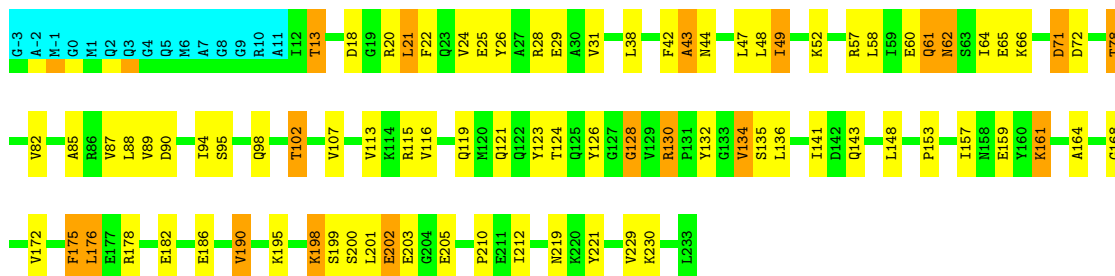


• Molecule 1: Proteasome subunit alpha

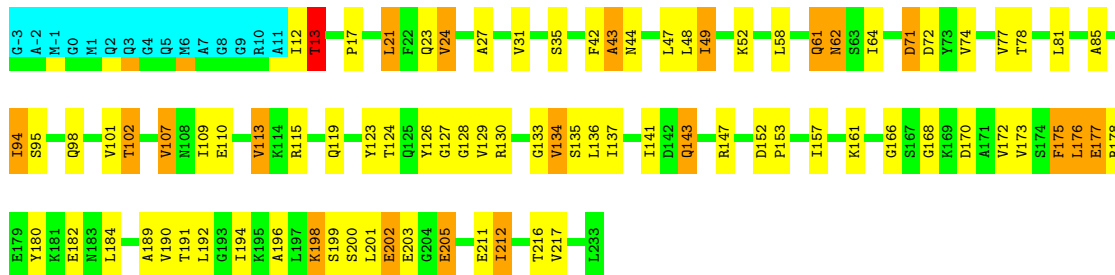




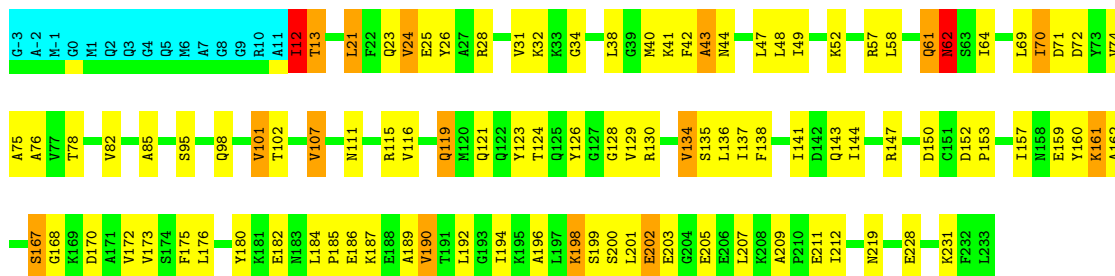
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

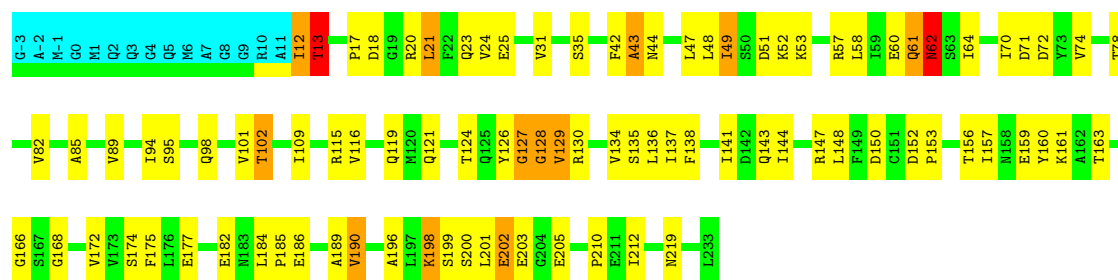


- Molecule 1: Proteasome subunit alpha



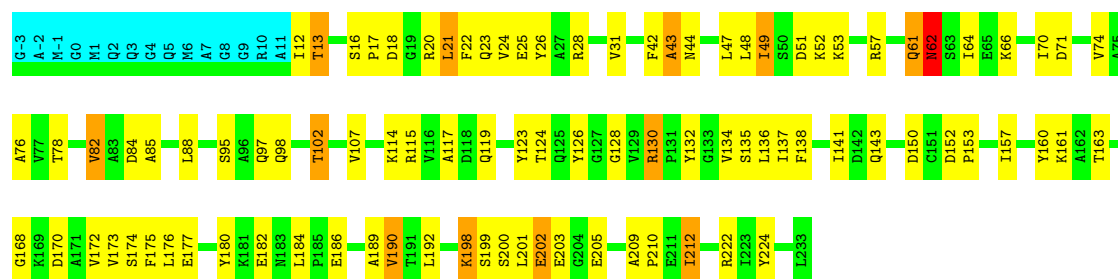
- Molecule 1: Proteasome subunit alpha





• Molecule 1: Proteasome subunit alpha

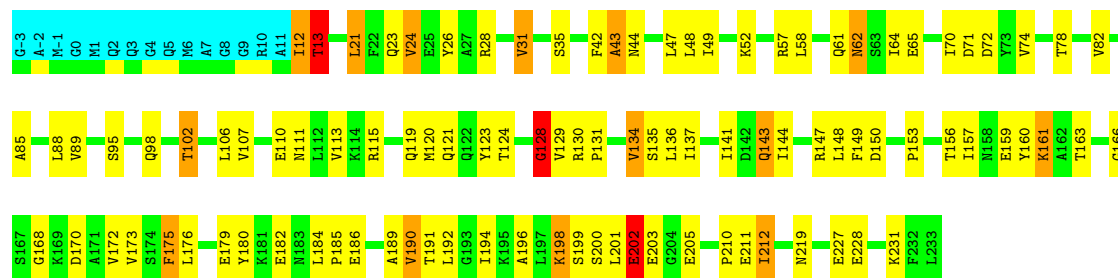
Chain G: 54% 34% 5% 6%



4.2.16 Score per residue for model 16

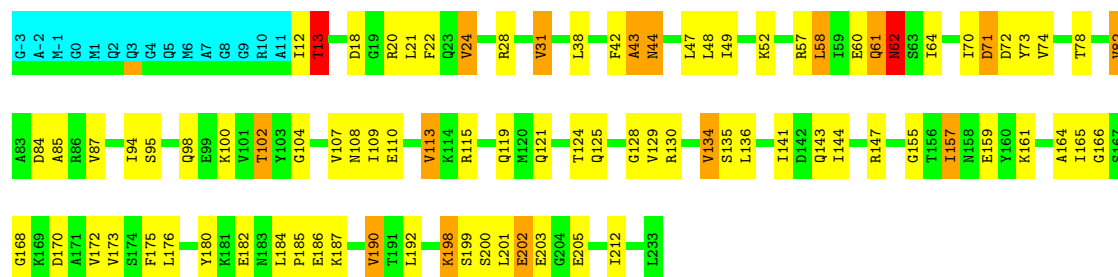
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%

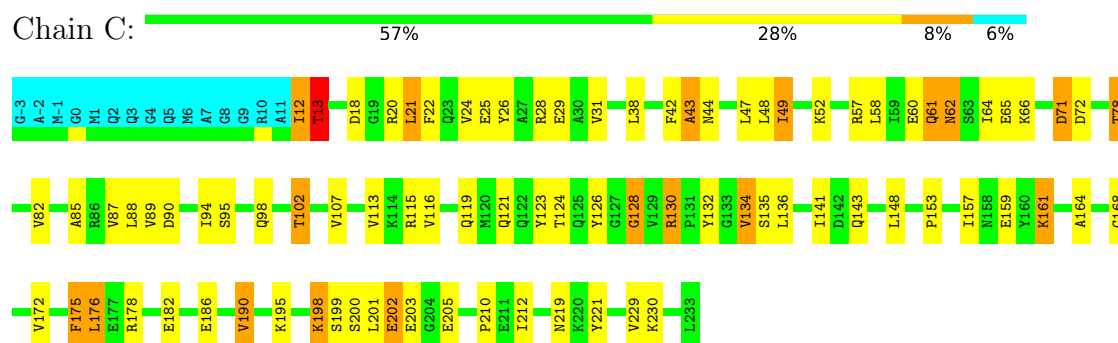


• Molecule 1: Proteasome subunit alpha

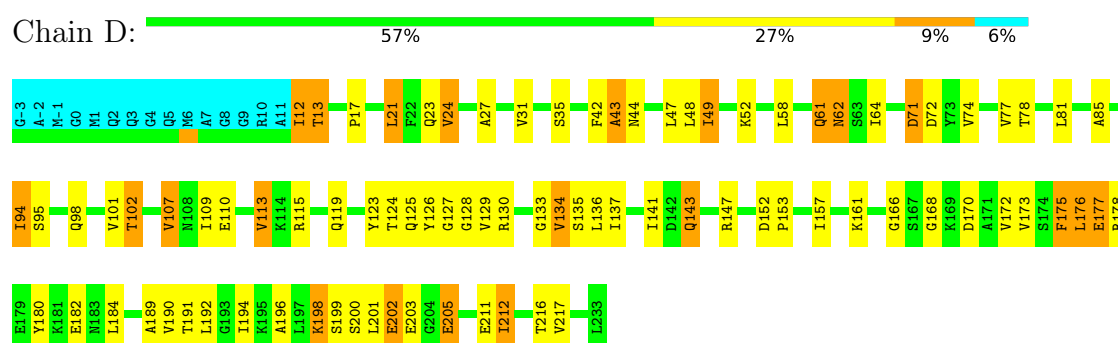
Chain B: 57% 30% 6% 6%



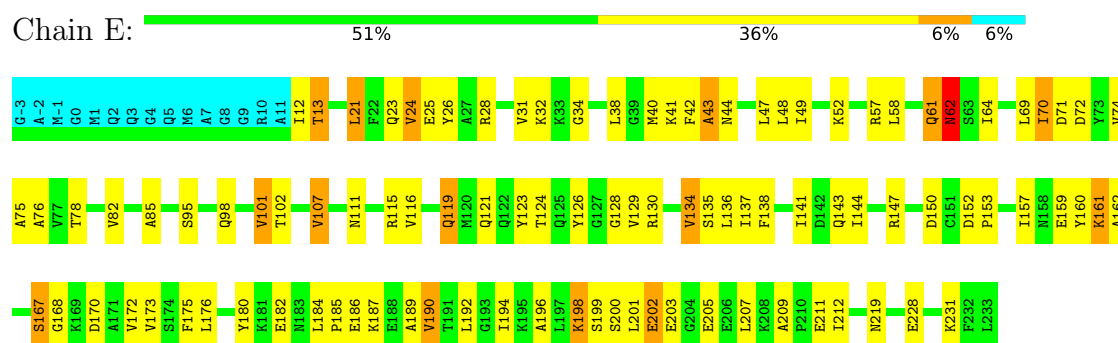
- Molecule 1: Proteasome subunit alpha



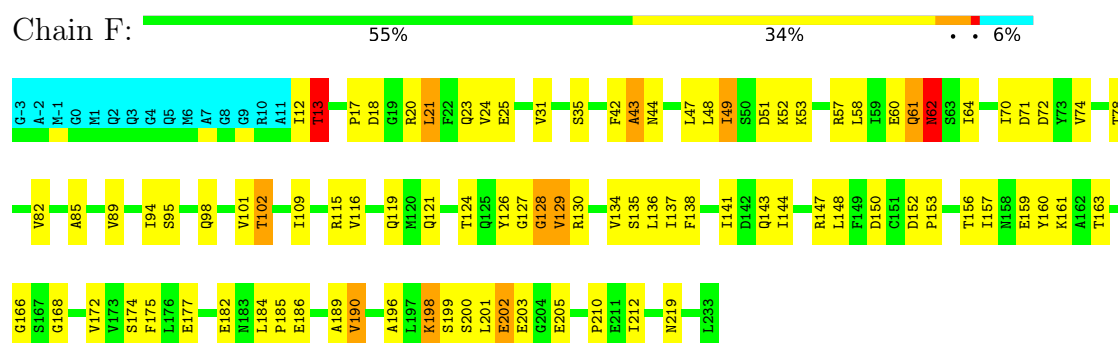
- Molecule 1: Proteasome subunit alpha



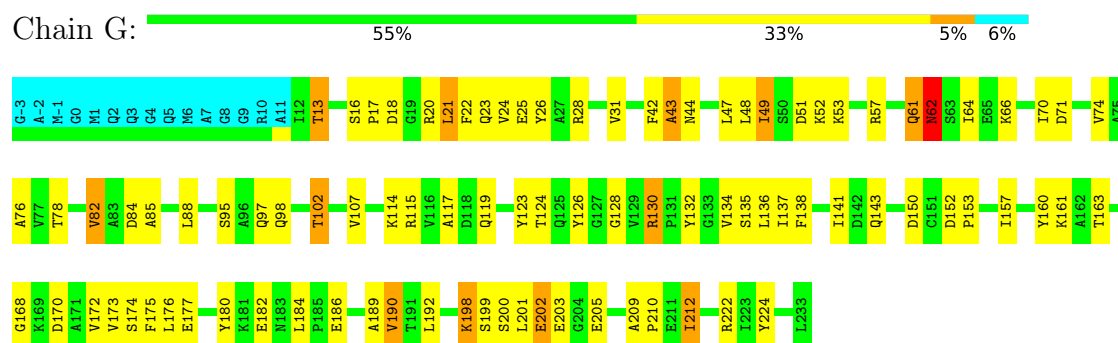
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

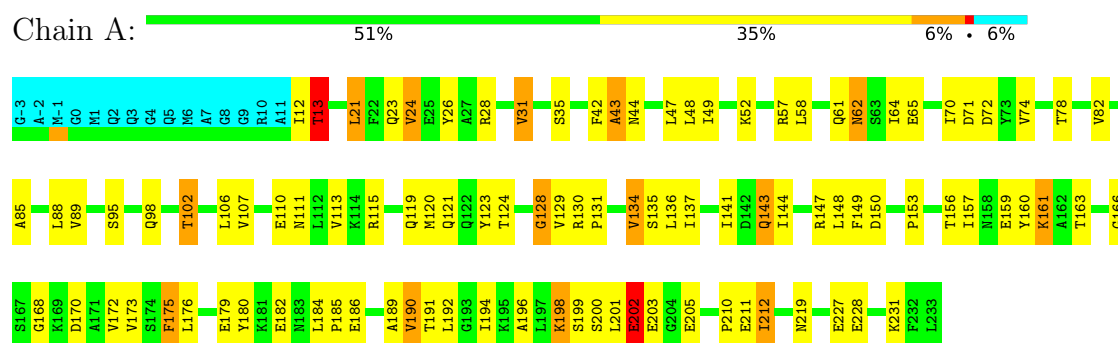


- Molecule 1: Proteasome subunit alpha

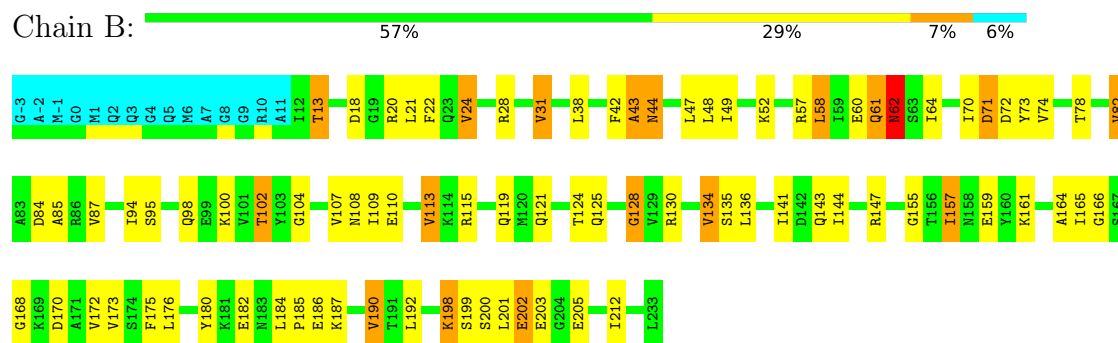


4.2.17 Score per residue for model 17

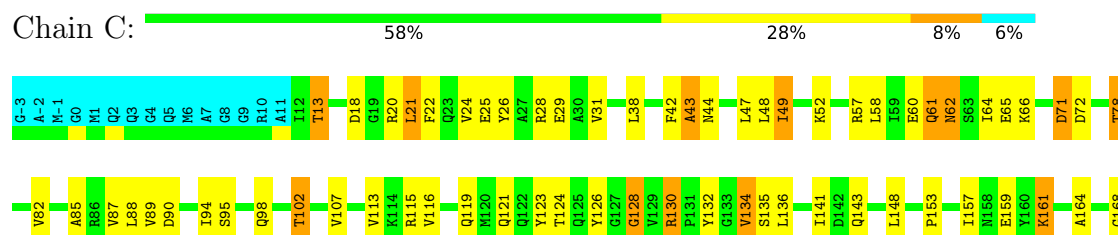
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



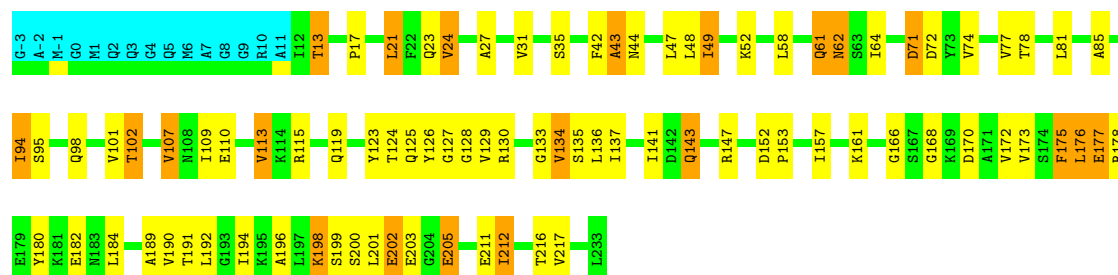
- Molecule 1: Proteasome subunit alpha





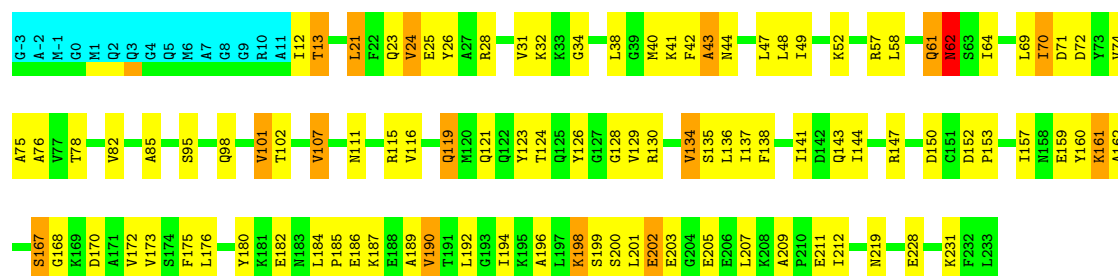
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



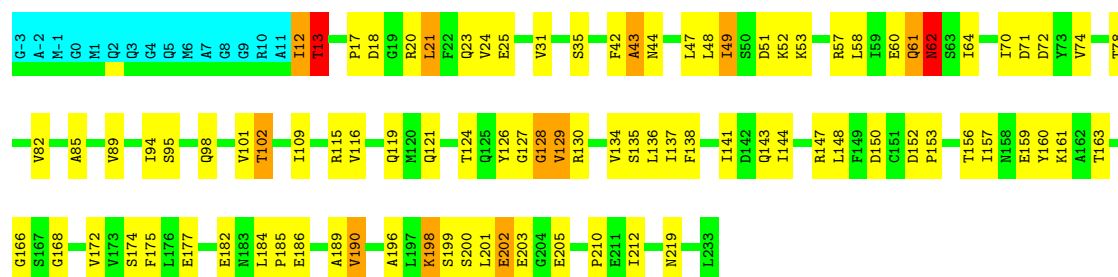
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 36% 6% 6%



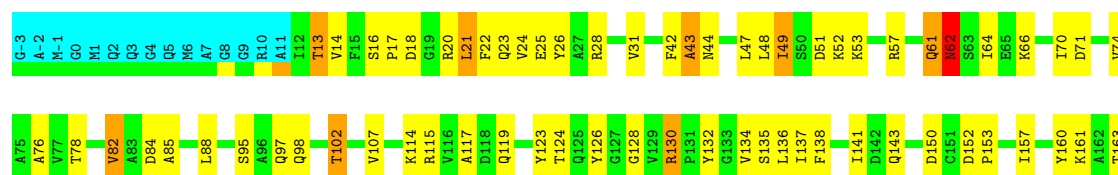
• Molecule 1: Proteasome subunit alpha

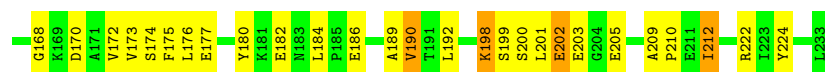
Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 54% 34% 5% 6%

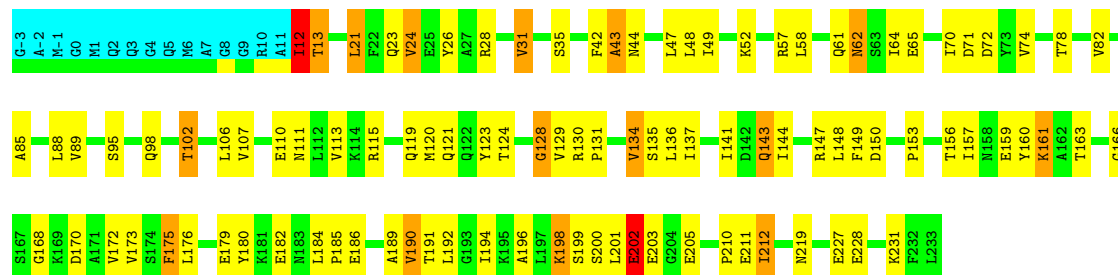




4.2.18 Score per residue for model 18

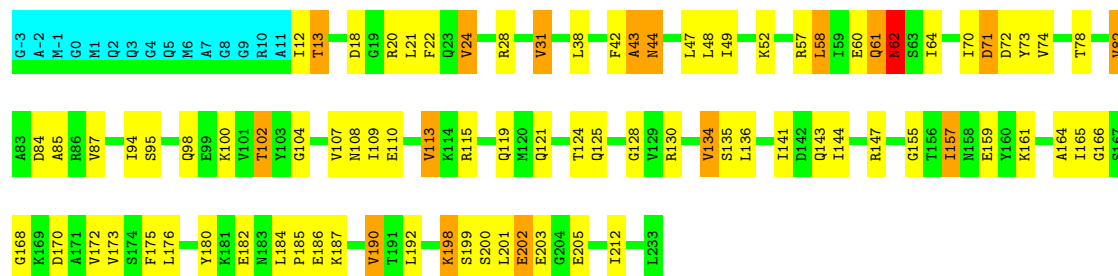
- Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



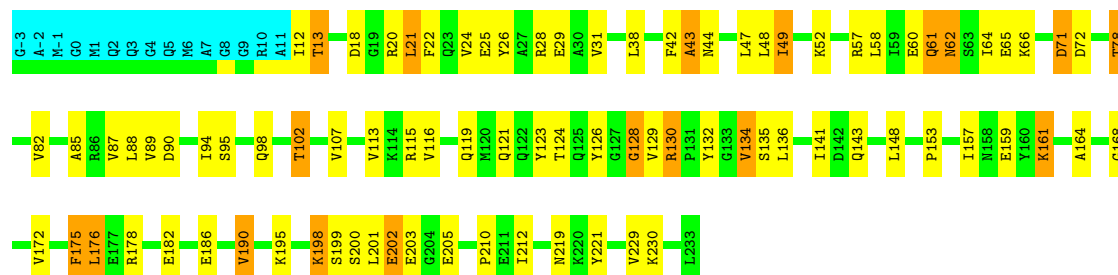
- Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 7% 6%



- Molecule 1: Proteasome subunit alpha

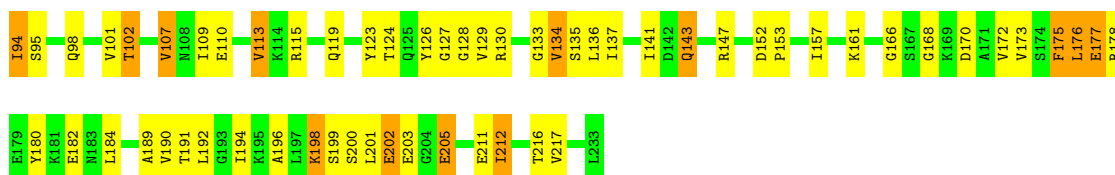
Chain C: 57% 29% 8% 6%



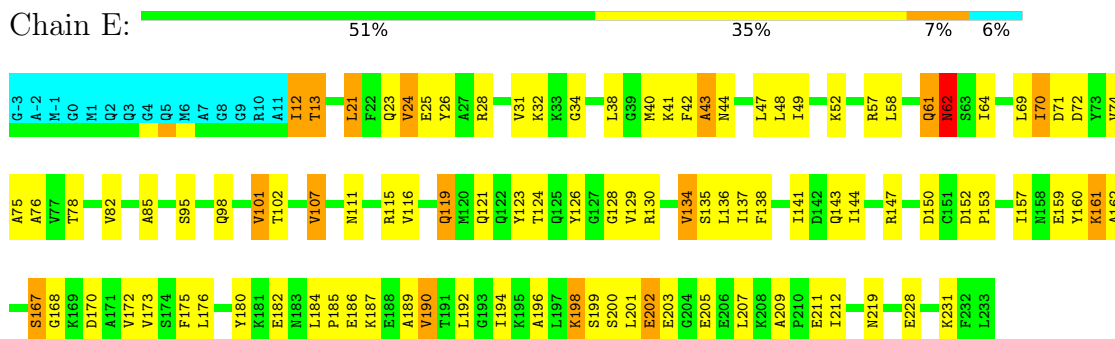
- Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 8% 6%





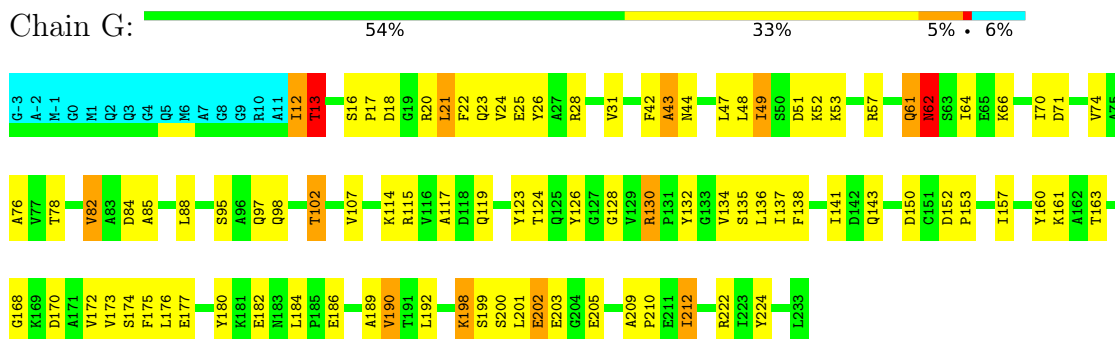
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



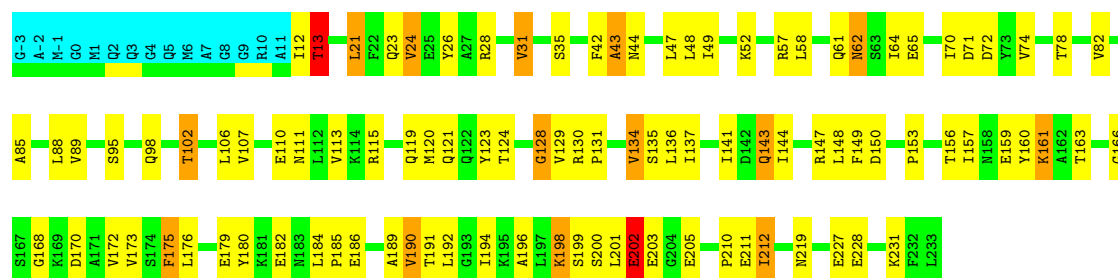
• Molecule 1: Proteasome subunit alpha



4.2.19 Score per residue for model 19

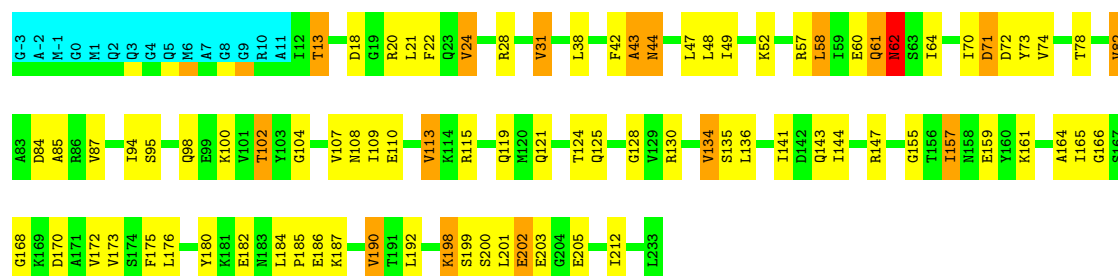
• Molecule 1: Proteasome subunit alpha





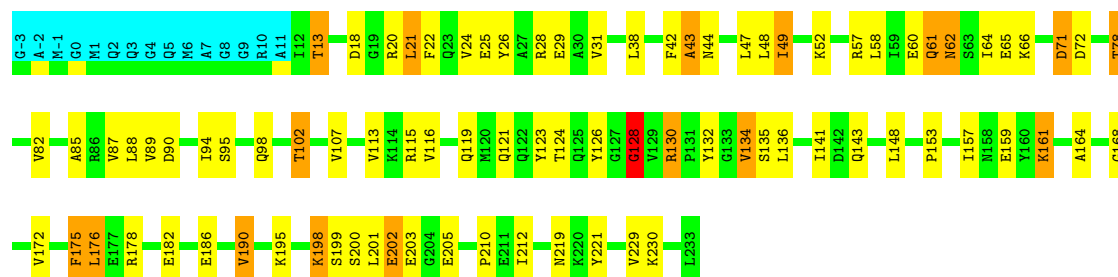
• Molecule 1: Proteasome subunit alpha

Chain B: 57% 29% 7% 6%



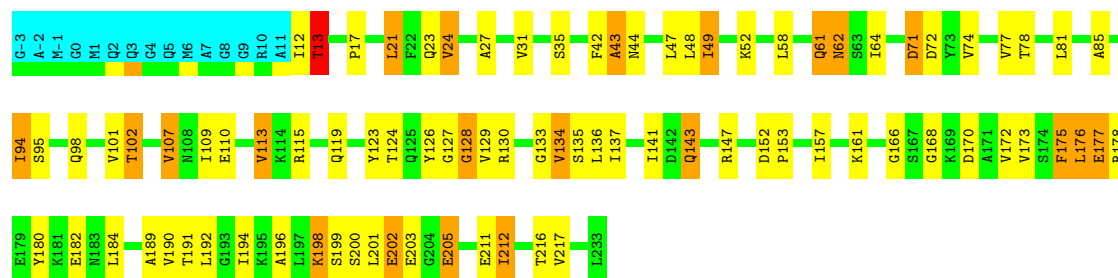
• Molecule 1: Proteasome subunit alpha

Chain C: 58% 28% 7% 6%



• Molecule 1: Proteasome subunit alpha

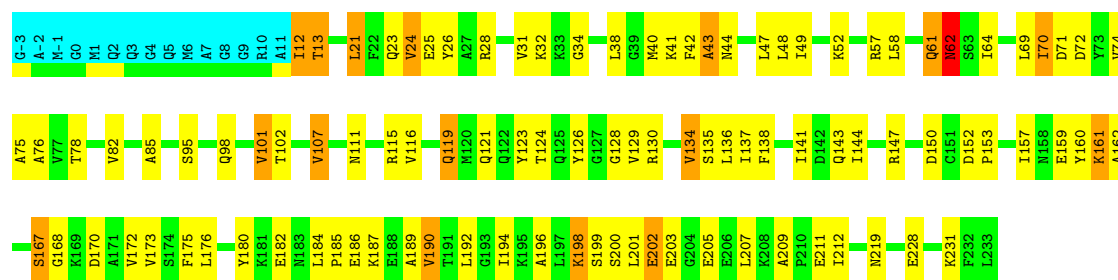
Chain D: 57% 27% 9% 6%



• Molecule 1: Proteasome subunit alpha

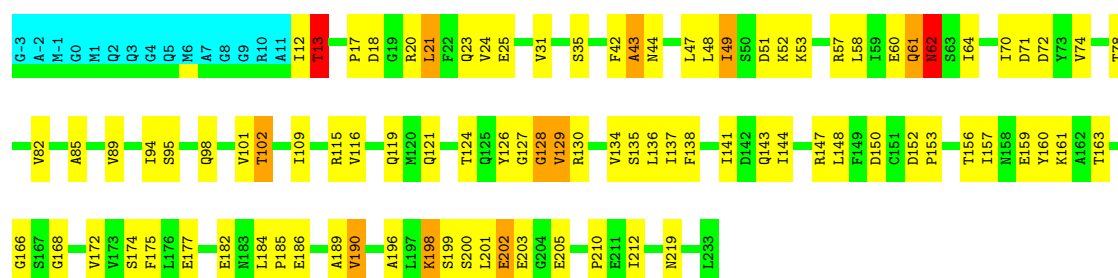
Chain E: 51% 35% 7% 6%





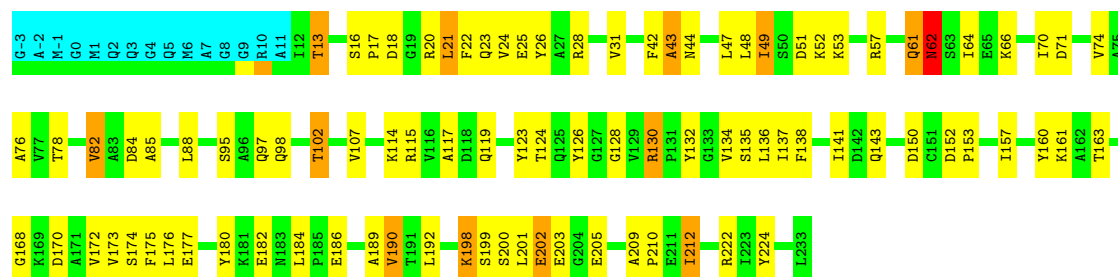
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 34% 6%



• Molecule 1: Proteasome subunit alpha

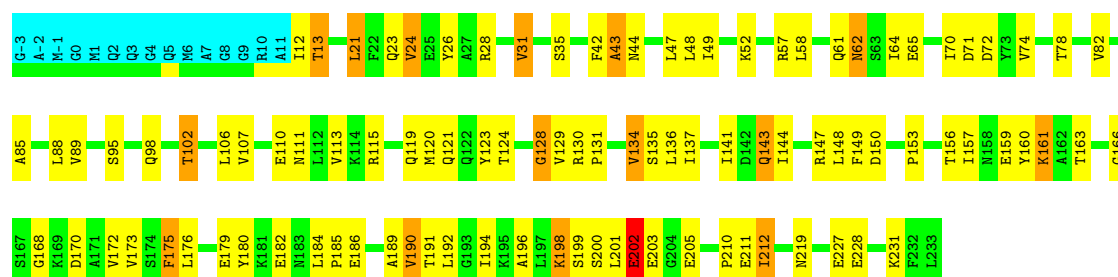
Chain G: 55% 33% 5% 6%



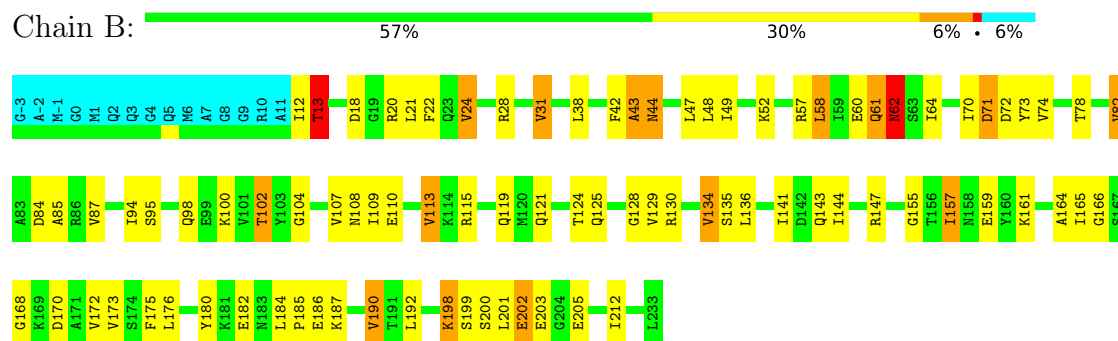
4.2.20 Score per residue for model 20

• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



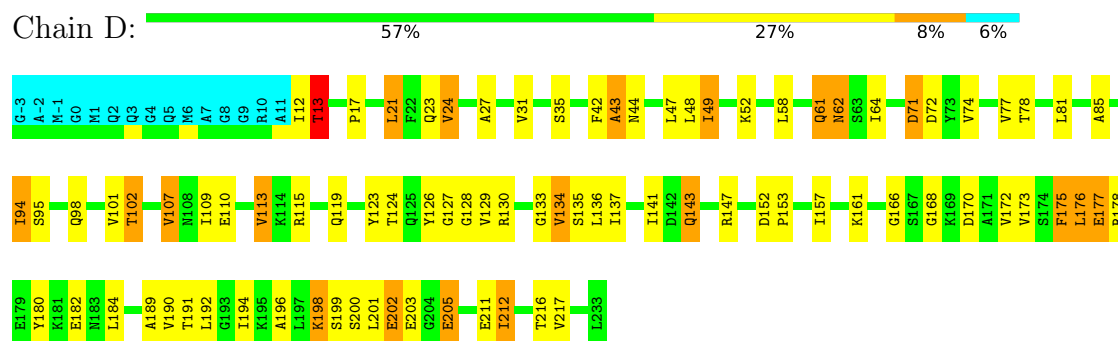
- Molecule 1: Proteasome subunit alpha



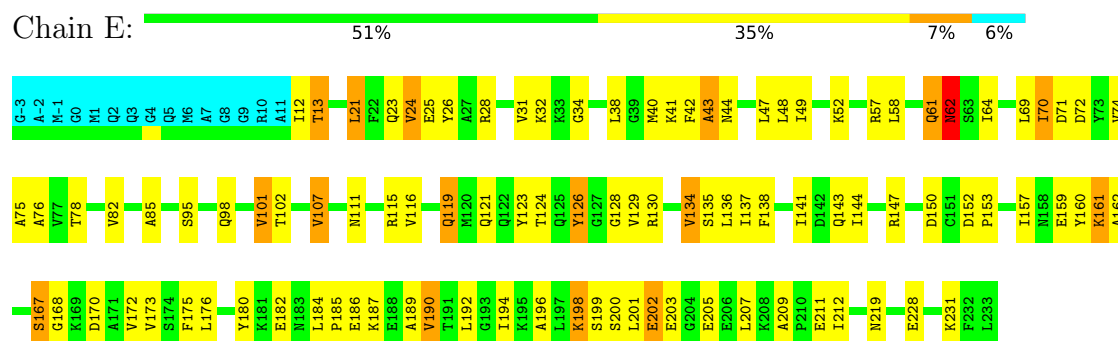
- Molecule 1: Proteasome subunit alpha



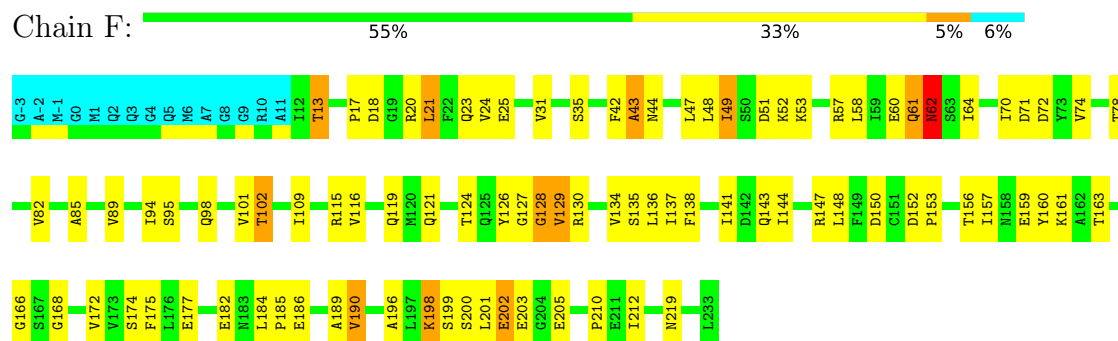
- Molecule 1: Proteasome subunit alpha



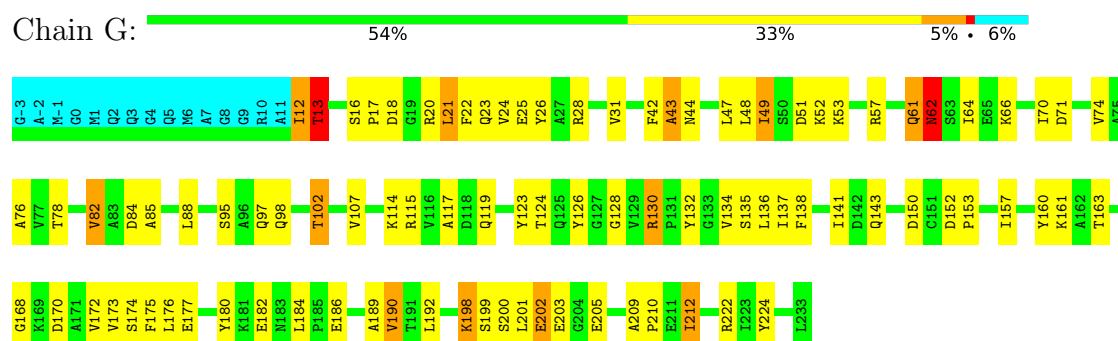
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

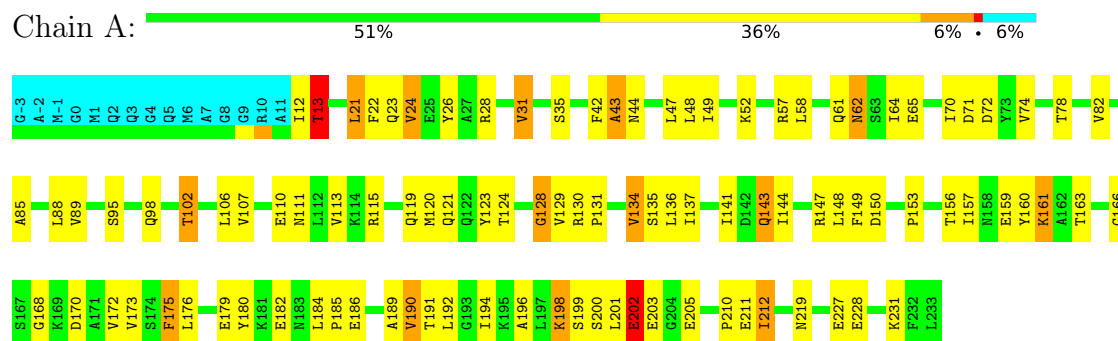


- Molecule 1: Proteasome subunit alpha

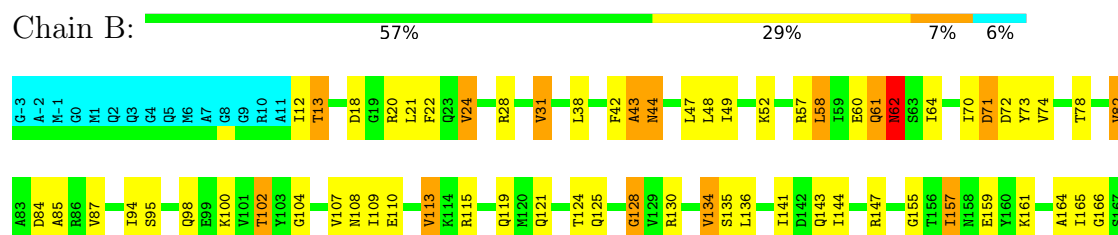


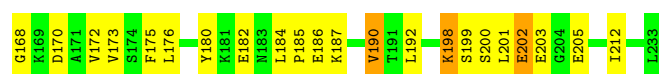
4.2.21 Score per residue for model 21

- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha





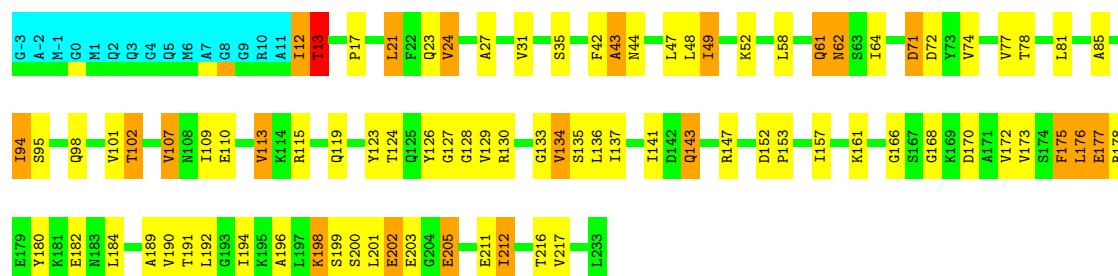
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 29% 8% 6%



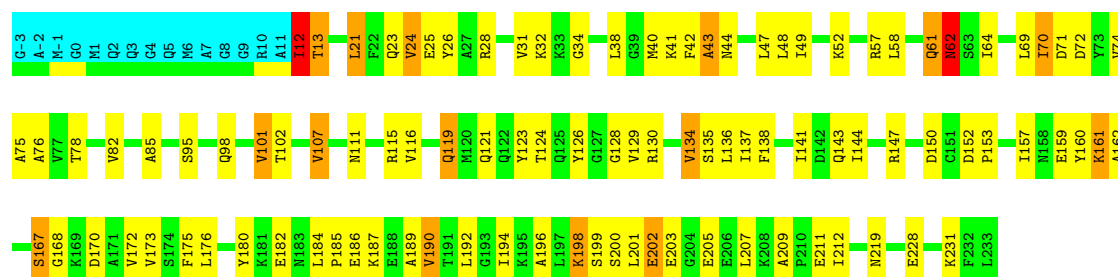
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



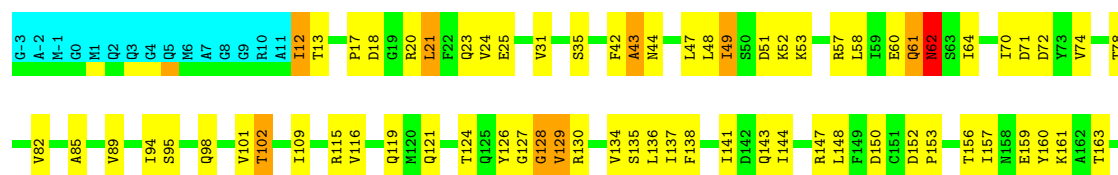
• Molecule 1: Proteasome subunit alpha

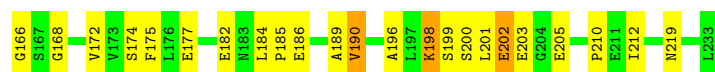
Chain E: 51% 35% 6% 6%



• Molecule 1: Proteasome subunit alpha

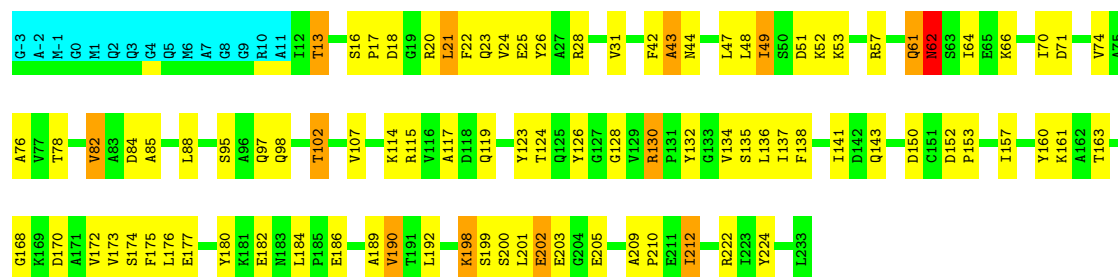
Chain F: 55% 34% 5% 6%





- Molecule 1: Proteasome subunit alpha

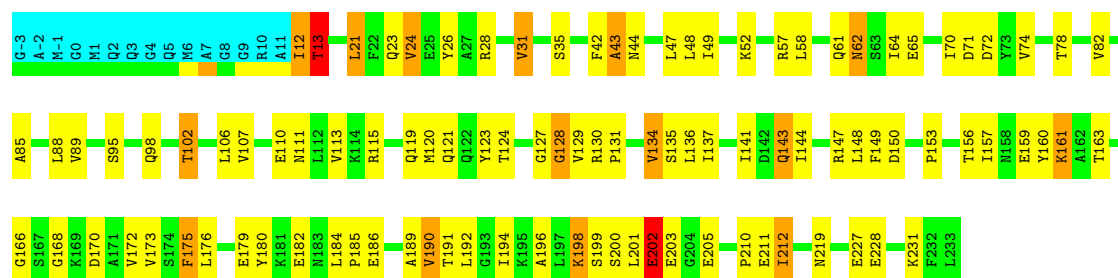
Chain G: 55% 33% 5% 6%



4.2.22 Score per residue for model 22

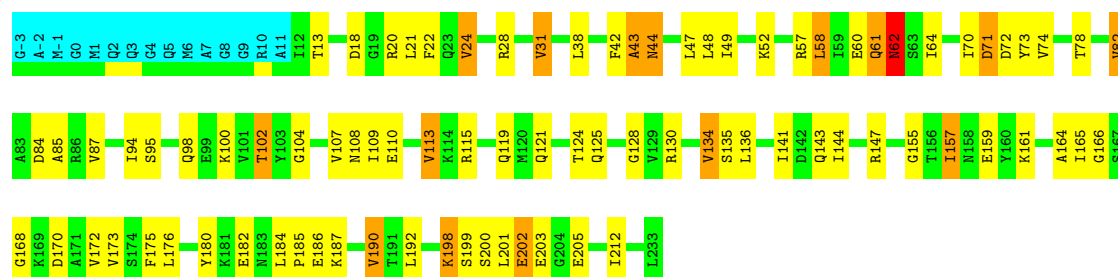
- Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



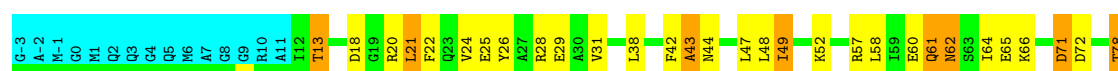
- Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 6% 6%



- Molecule 1: Proteasome subunit alpha

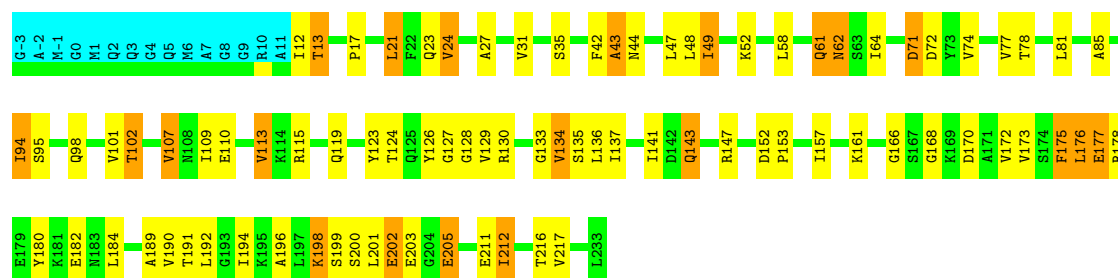
Chain C: 57% 29% 8% 6%





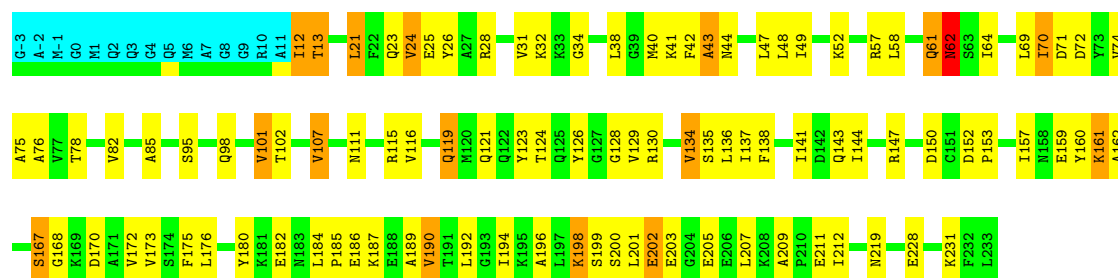
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



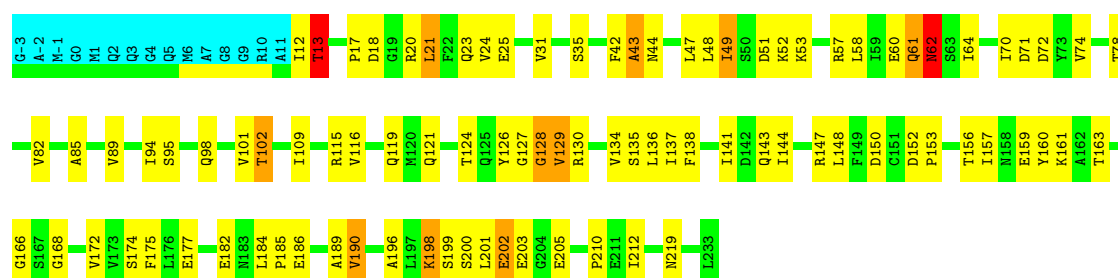
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



• Molecule 1: Proteasome subunit alpha

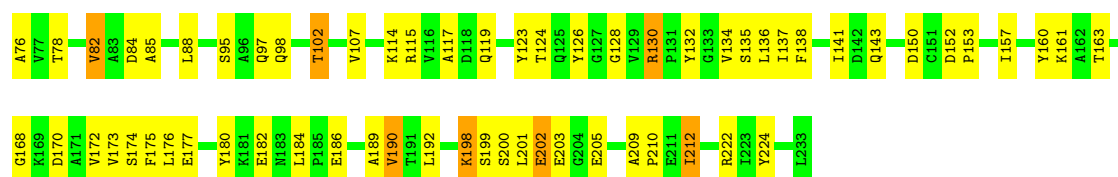
Chain F: 55% 34% 6%



• Molecule 1: Proteasome subunit alpha

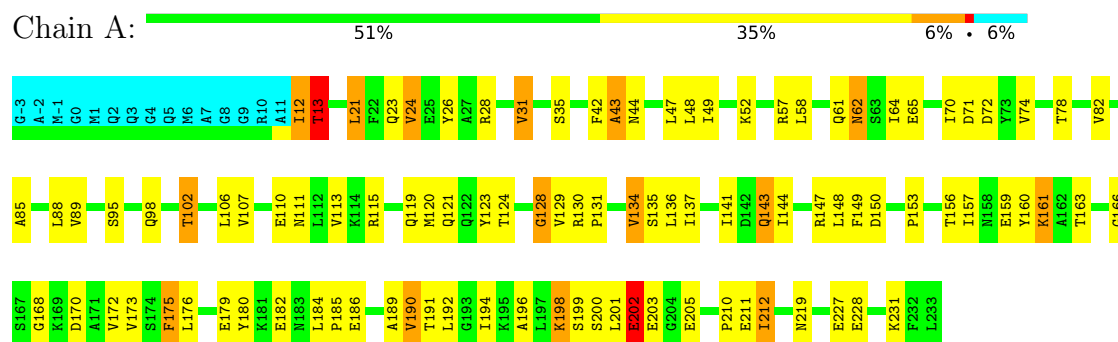
Chain G: 54% 33% 5% 6%



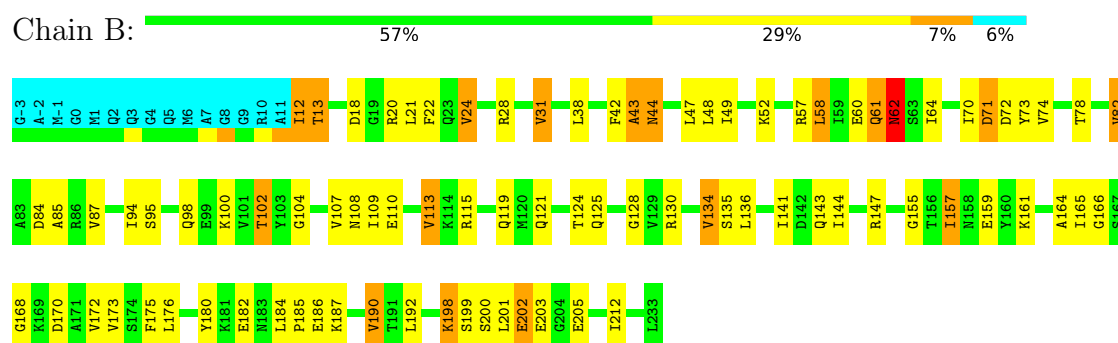


4.2.23 Score per residue for model 23

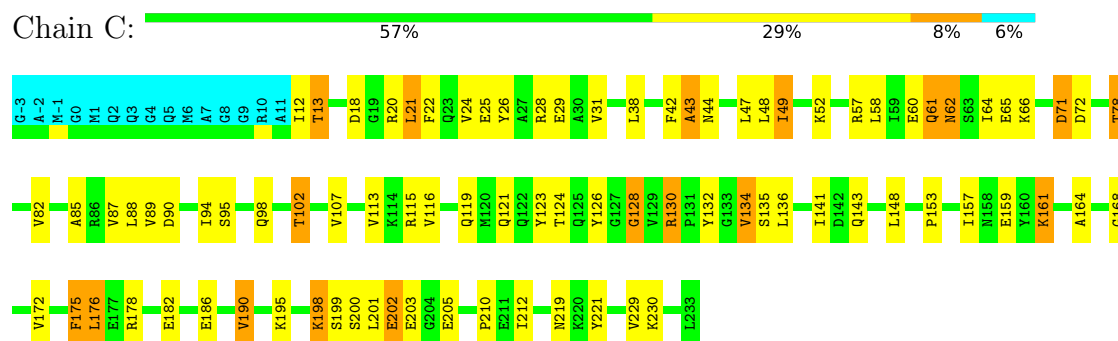
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

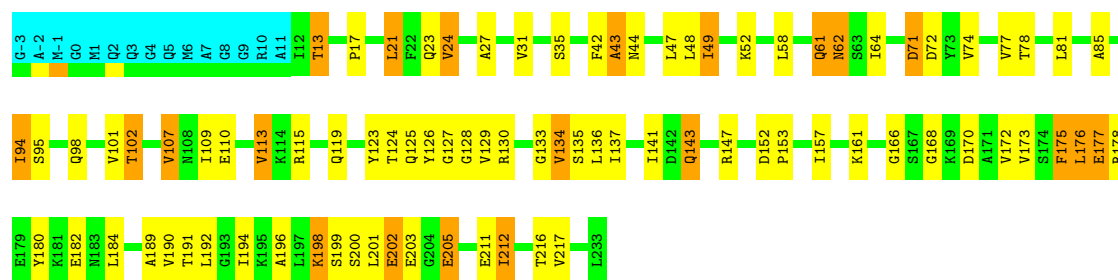


- Molecule 1: Proteasome subunit alpha



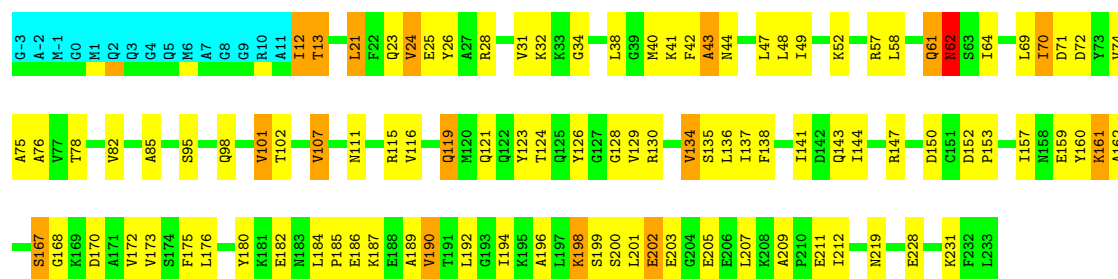
- Molecule 1: Proteasome subunit alpha





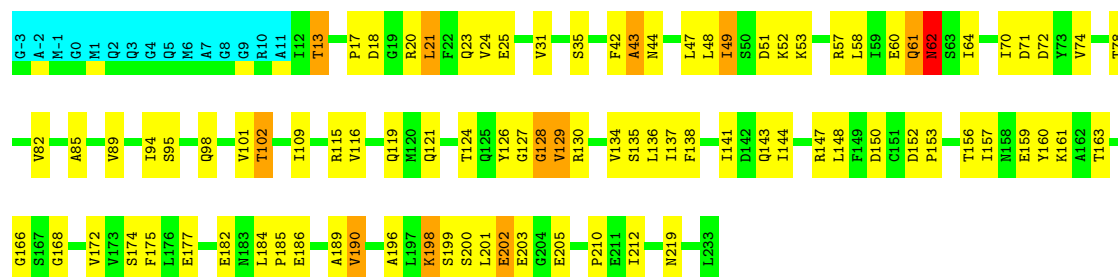
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



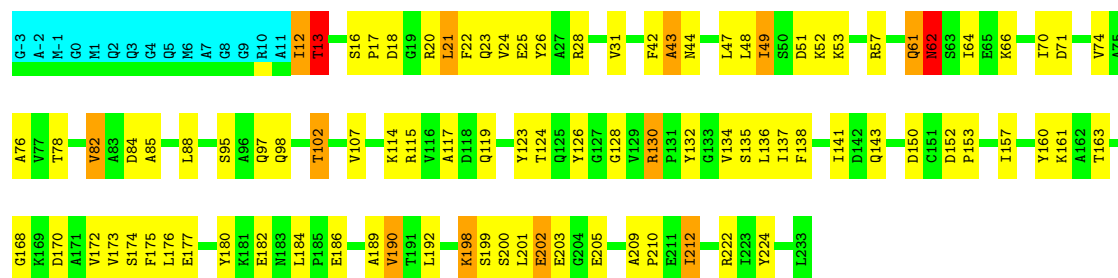
• Molecule 1: Proteasome subunit alpha

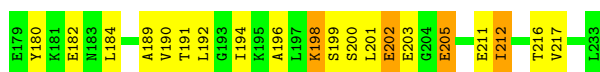
Chain F: 55% 33% 5% 6%



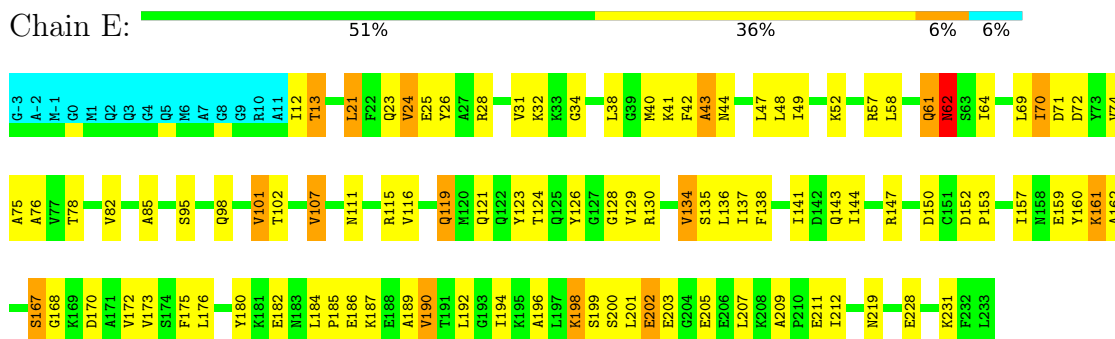
• Molecule 1: Proteasome subunit alpha

Chain G: 54% 33% 5% 6%





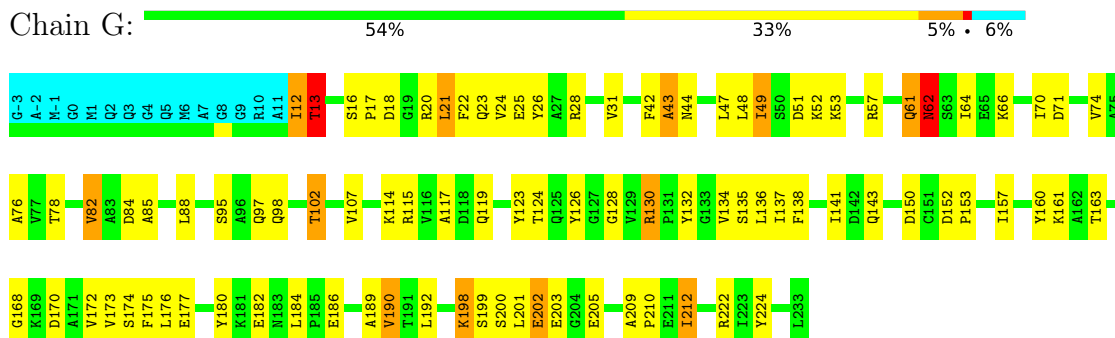
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

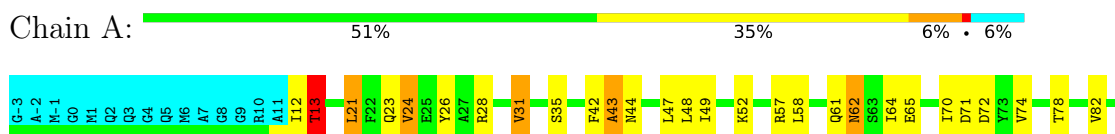


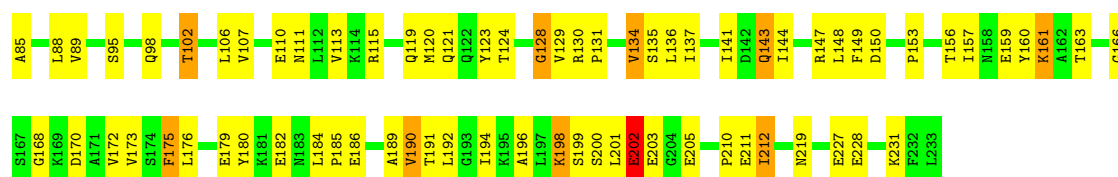
• Molecule 1: Proteasome subunit alpha



4.2.25 Score per residue for model 25

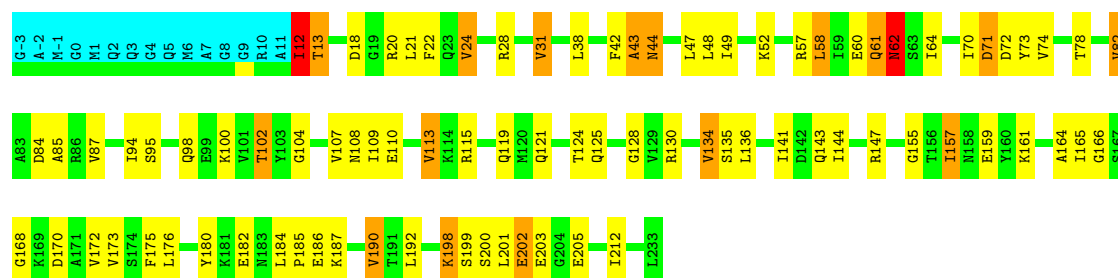
• Molecule 1: Proteasome subunit alpha





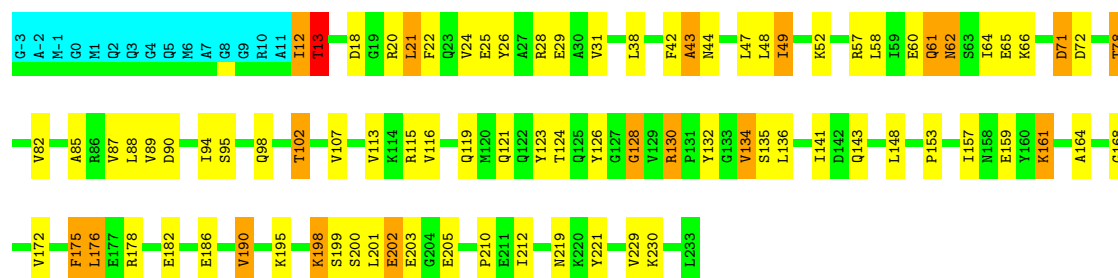
• Molecule 1: Proteasome subunit alpha

Chain B: 57% 29% 7% 6%



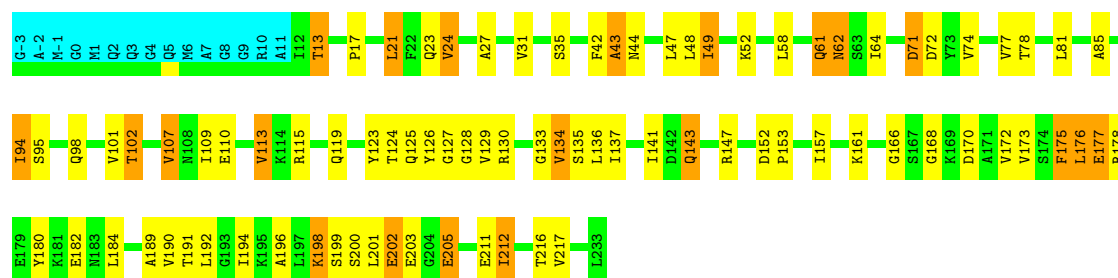
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 28% 8% 6%



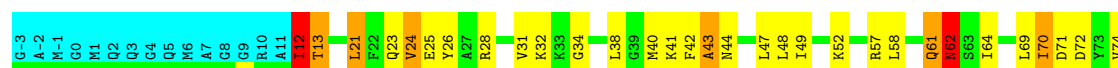
• Molecule 1: Proteasome subunit alpha

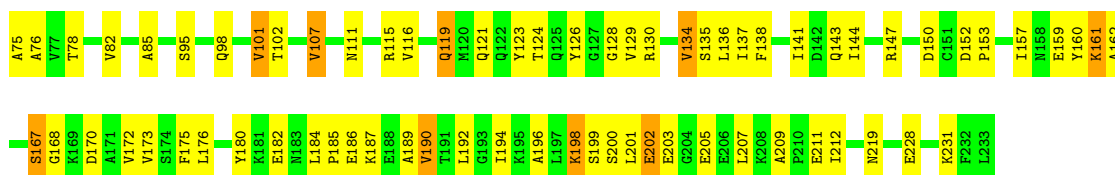
Chain D: 57% 27% 9% 6%



• Molecule 1: Proteasome subunit alpha

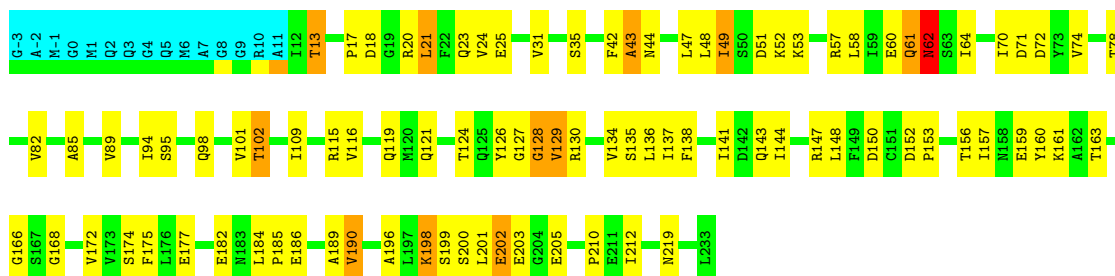
Chain E: 51% 35% 6% 6%





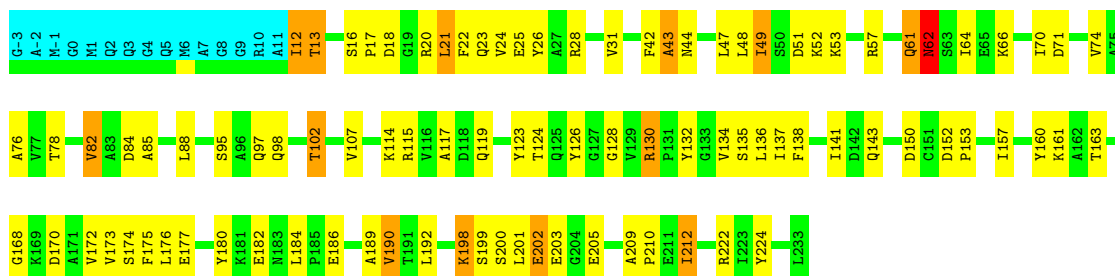
- Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



- Molecule 1: Proteasome subunit alpha

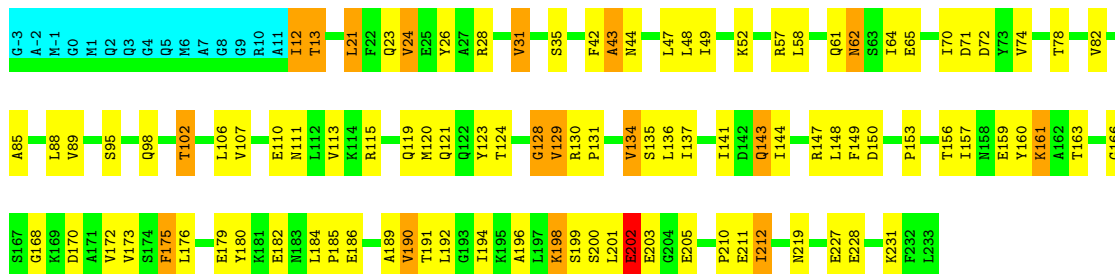
Chain G: 54% 33% 5% 6%



4.2.26 Score per residue for model 26

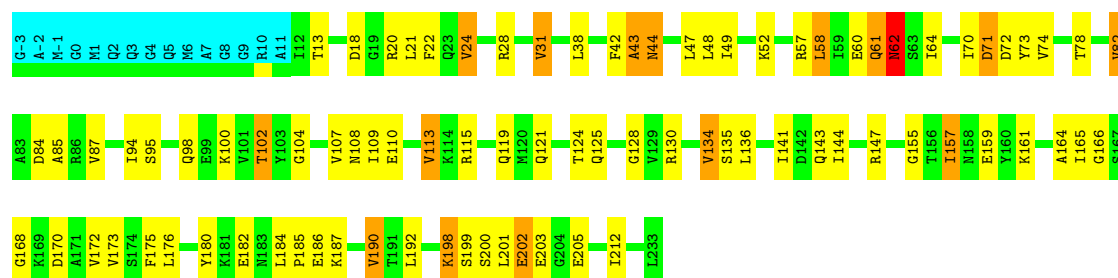
- Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 7% 6%

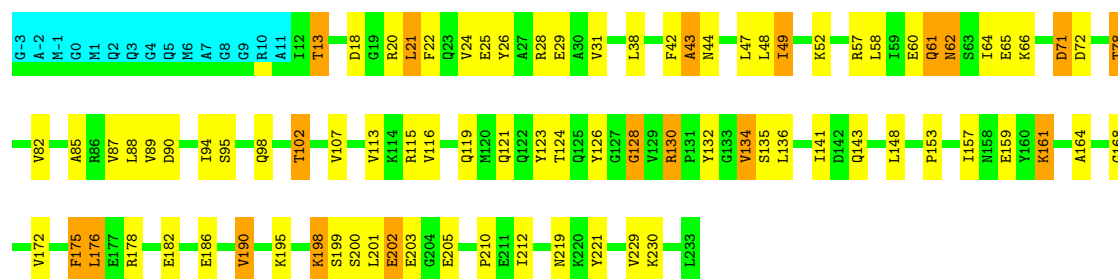


- Molecule 1: Proteasome subunit alpha

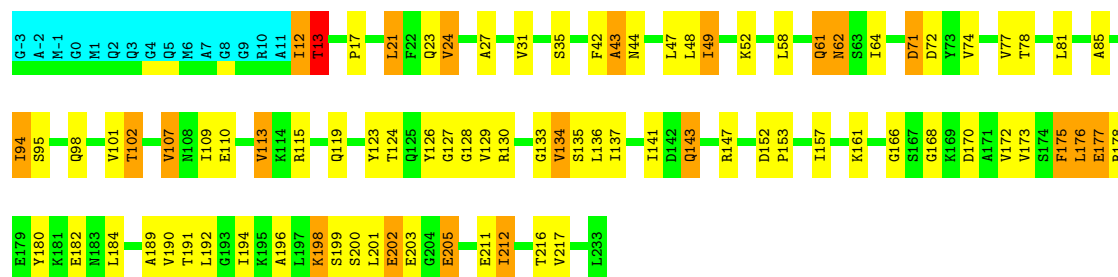
Chain B: 57% 30% 6% 6%



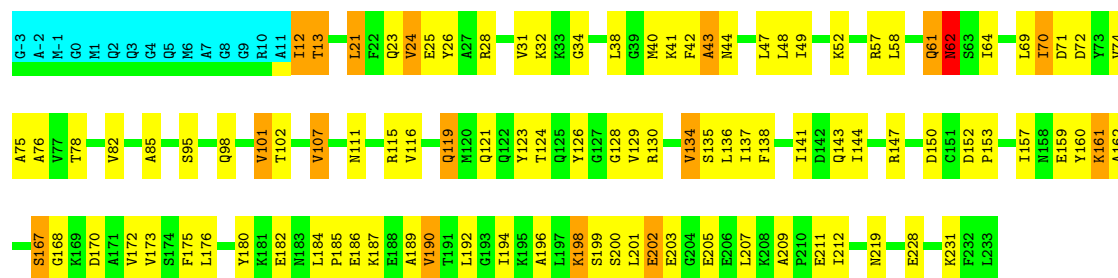
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

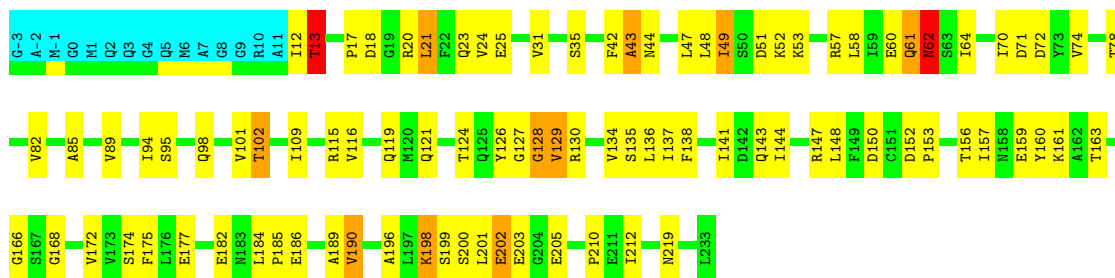


- Molecule 1: Proteasome subunit alpha



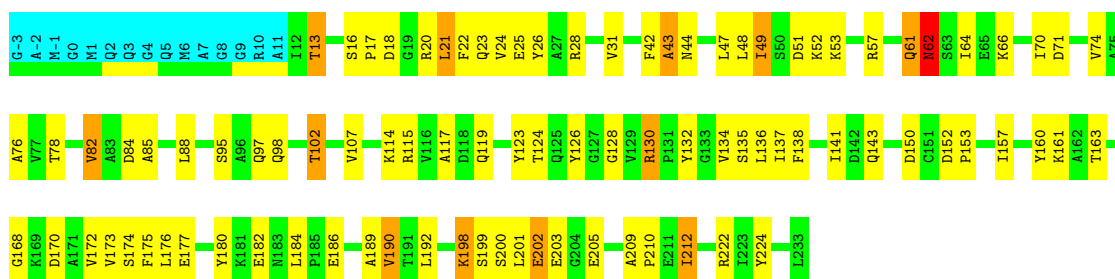
- Molecule 1: Proteasome subunit alpha





• Molecule 1: Proteasome subunit alpha

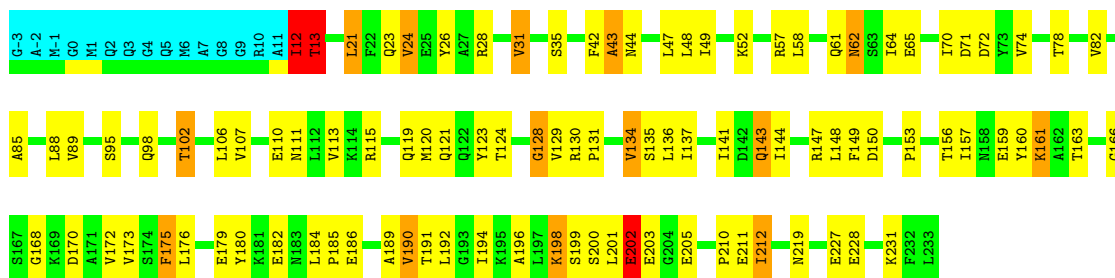
Chain G: 55% 33% 5% 6%



4.2.27 Score per residue for model 27

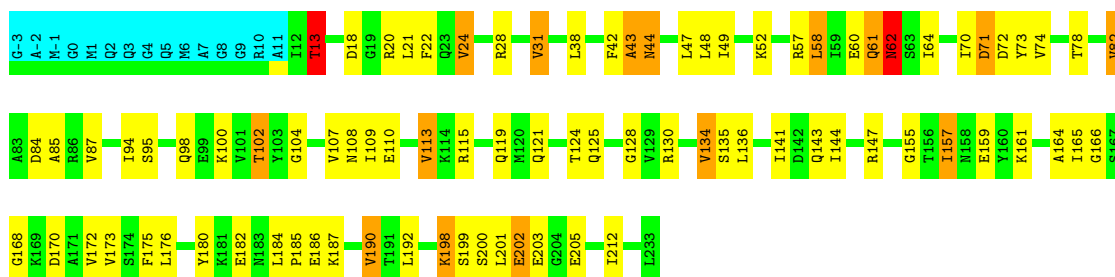
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%

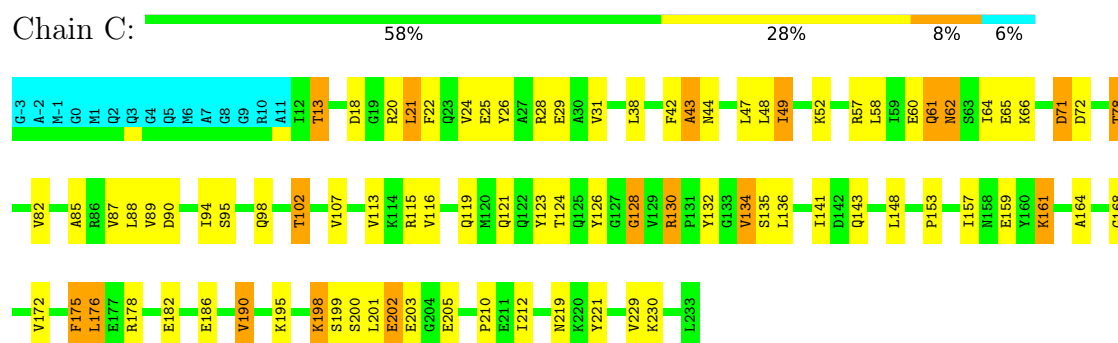


• Molecule 1: Proteasome subunit alpha

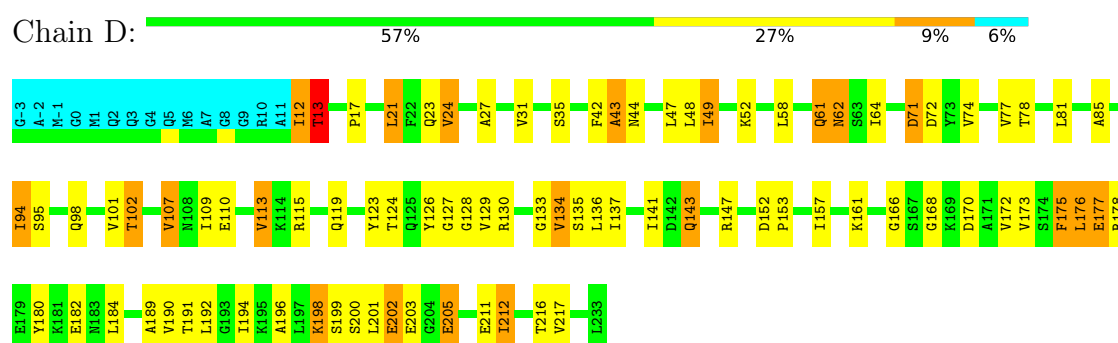
Chain B: 57% 29% 6% 6%



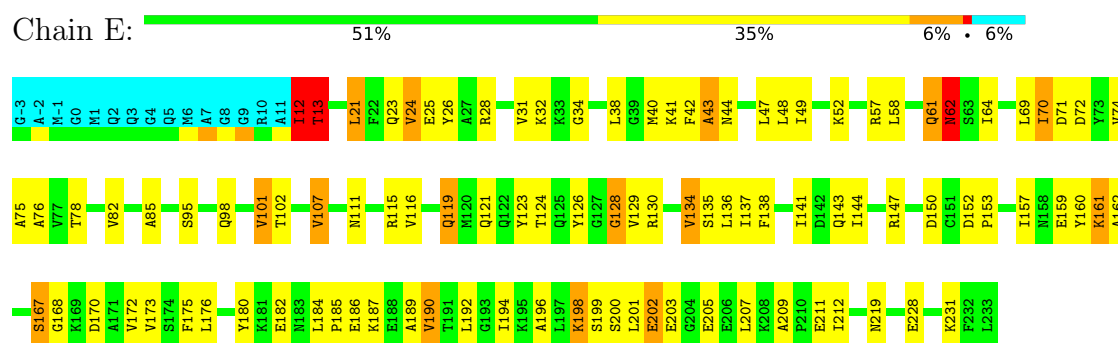
- Molecule 1: Proteasome subunit alpha



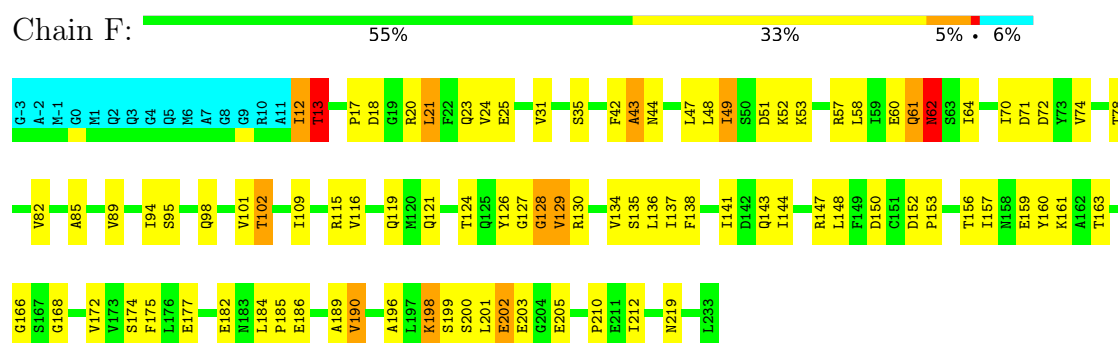
- Molecule 1: Proteasome subunit alpha



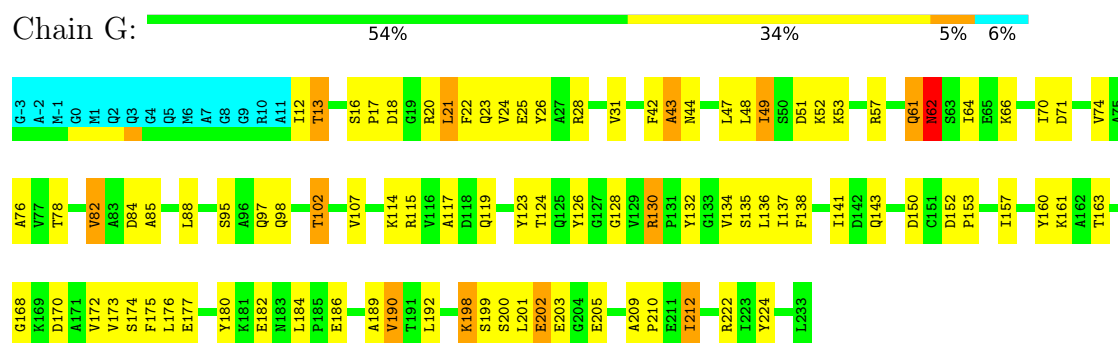
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

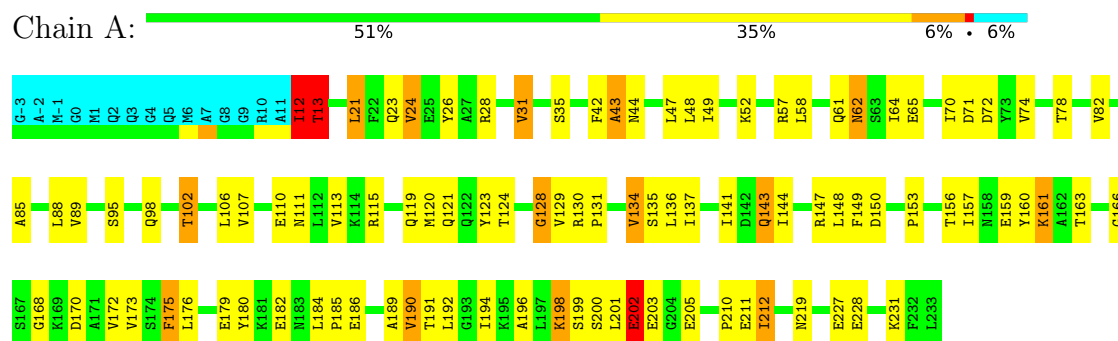


- Molecule 1: Proteasome subunit alpha

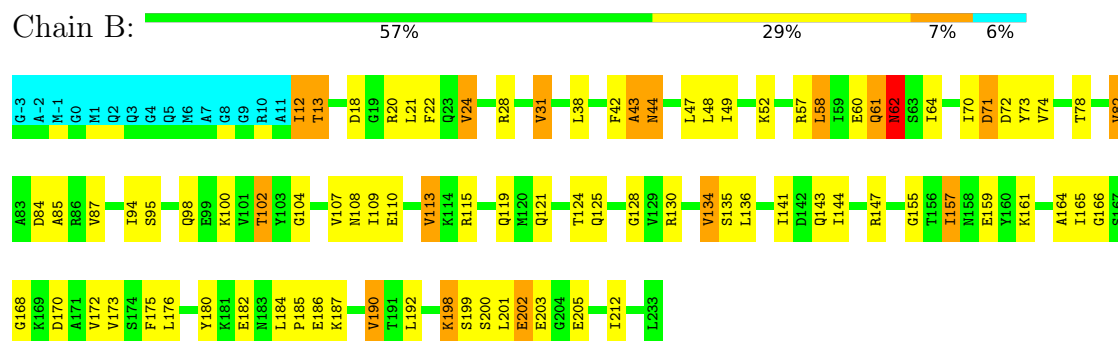


4.2.28 Score per residue for model 28

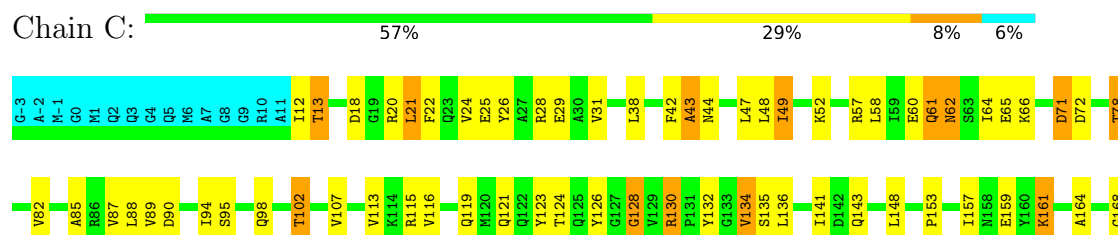
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



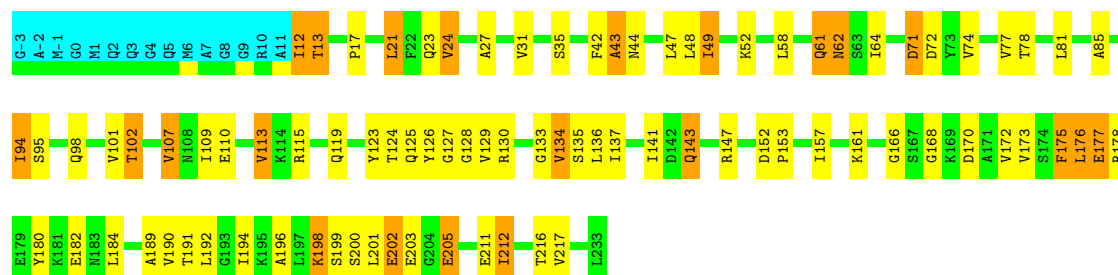
- Molecule 1: Proteasome subunit alpha





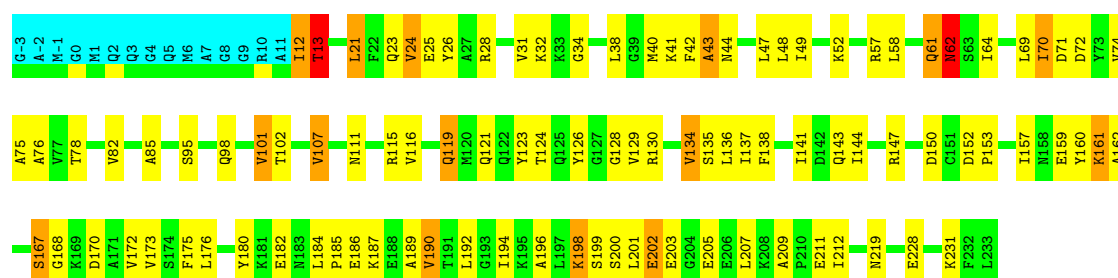
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



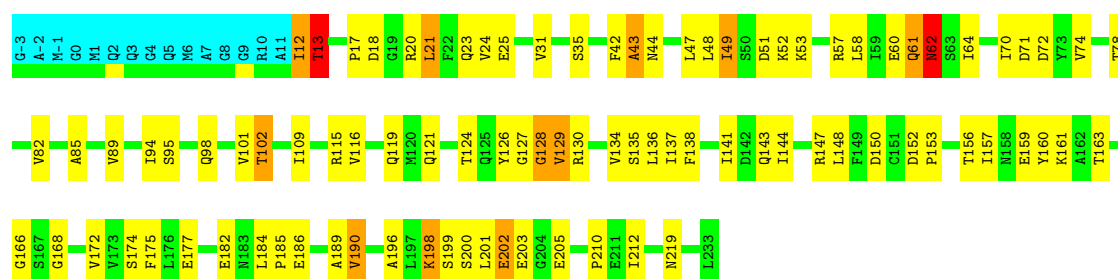
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% • 6%



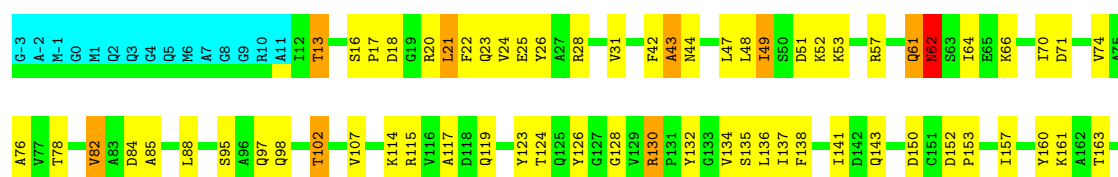
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% • 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 55% 33% 5% 6%

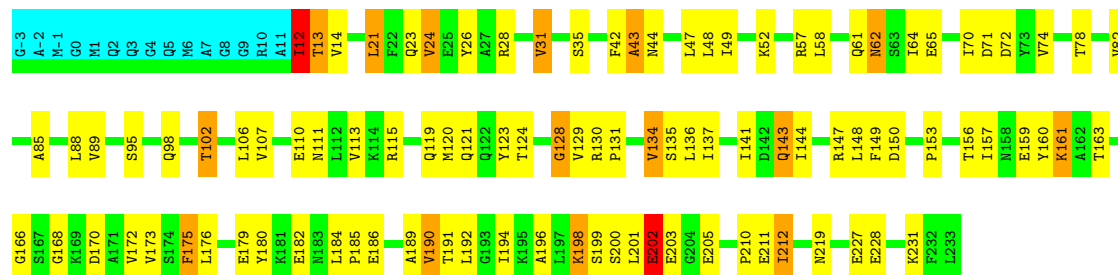




4.2.29 Score per residue for model 29

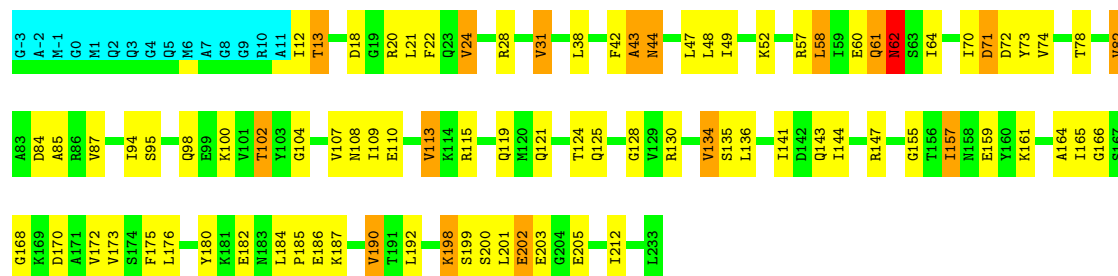
- Molecule 1: Proteasome subunit alpha

Chain A:



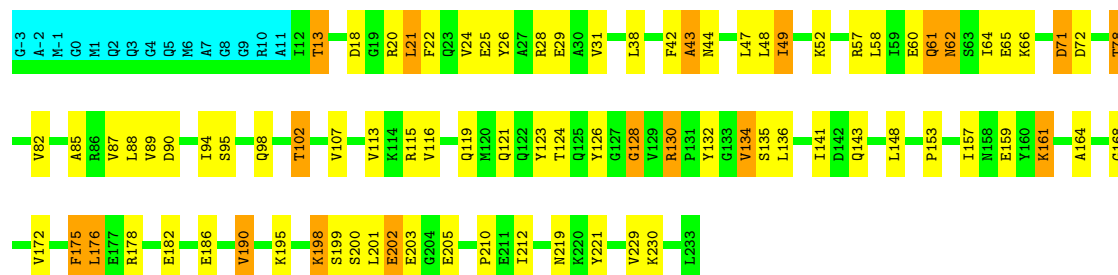
- Molecule 1: Proteasome subunit alpha

Chain B:



- Molecule 1: Proteasome subunit alpha

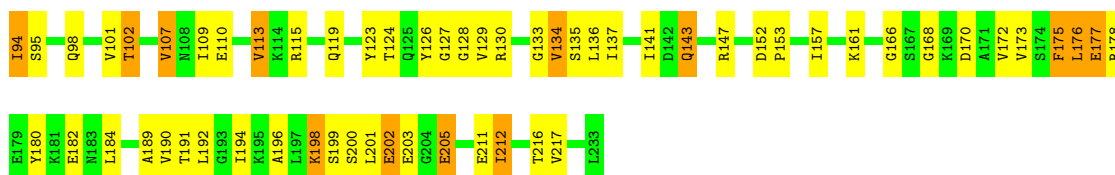
Chain C:



- Molecule 1: Proteasome subunit alpha

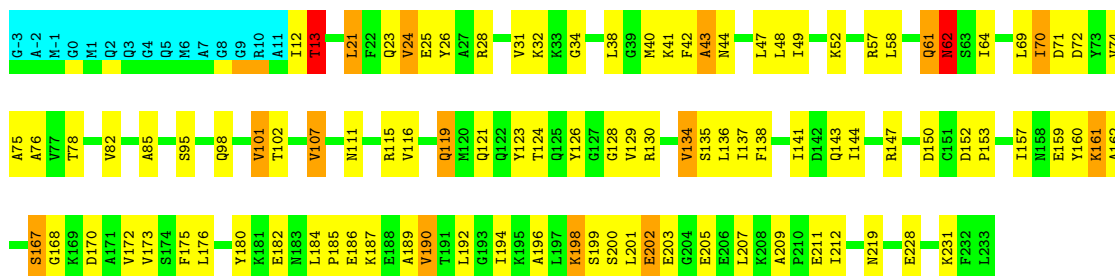
Chain D:





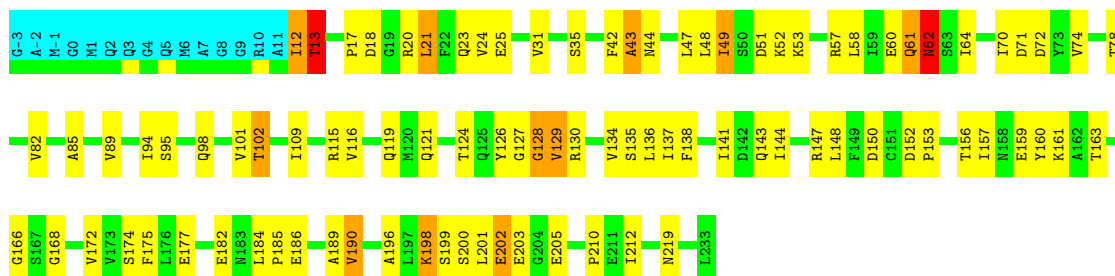
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 36% 6% • 6%



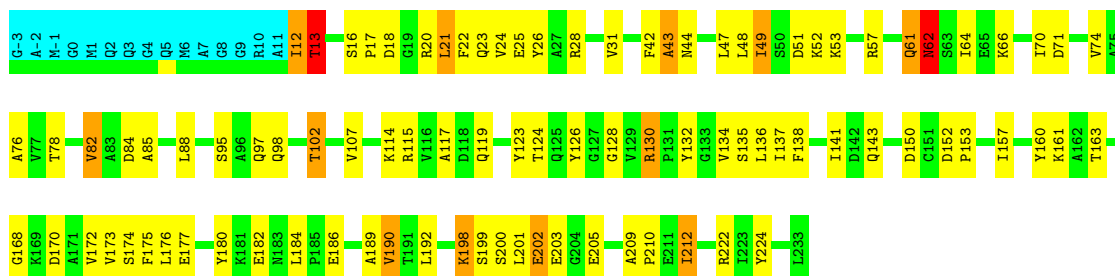
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% • 6%



• Molecule 1: Proteasome subunit alpha

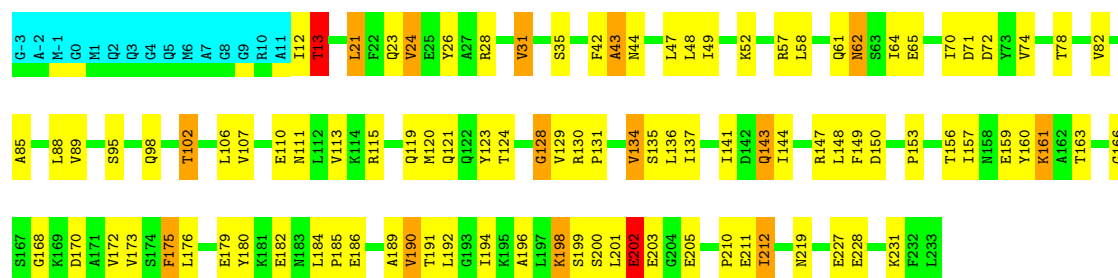
Chain G: 54% 33% 5% • 6%



4.2.30 Score per residue for model 30

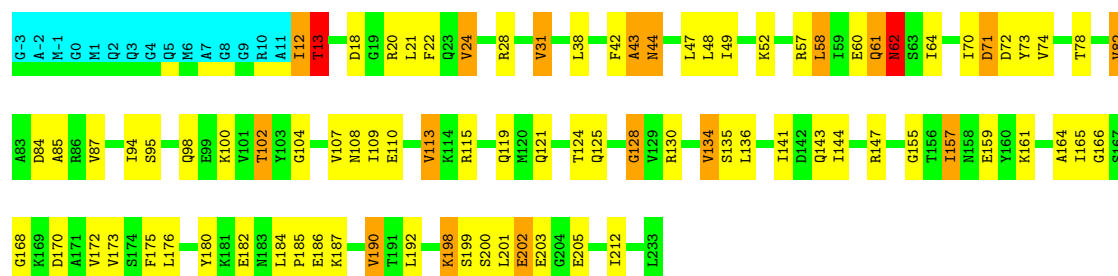
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% • 6%



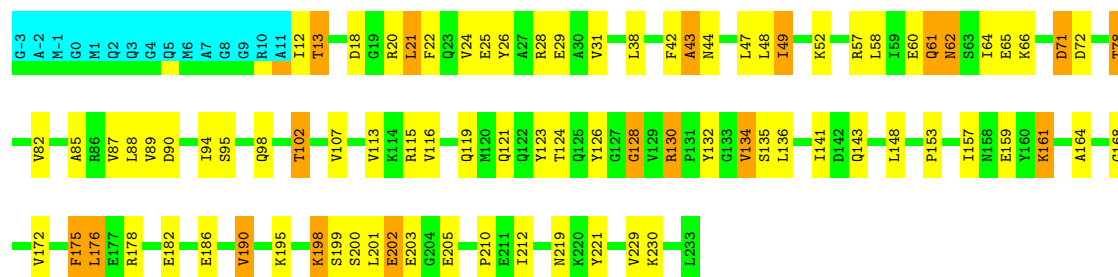
• Molecule 1: Proteasome subunit alpha

Chain B: 57% 29% 7% 6%



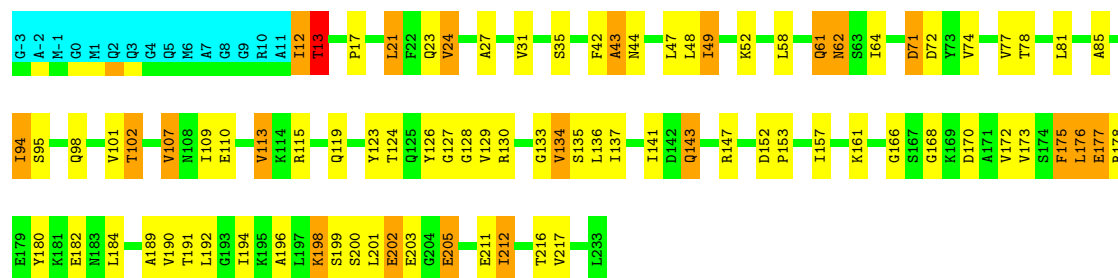
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 29% 8% 6%



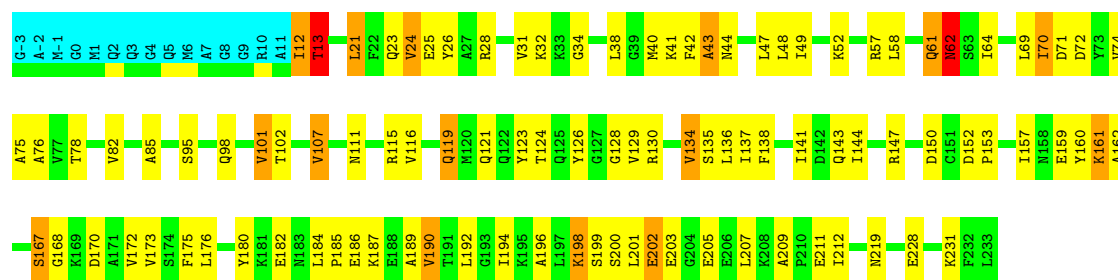
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



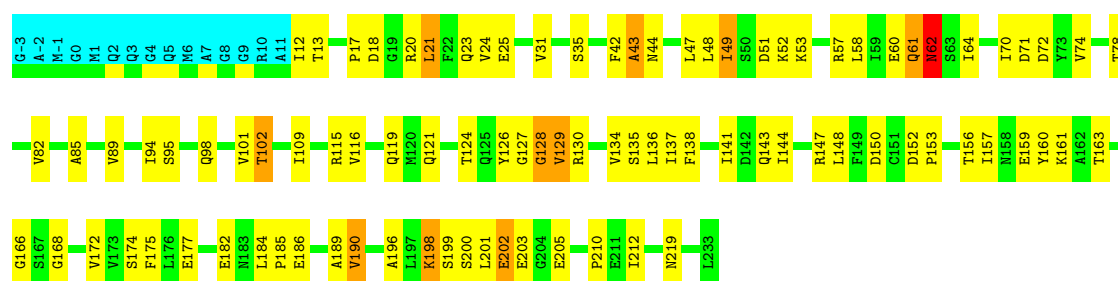
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% 6%



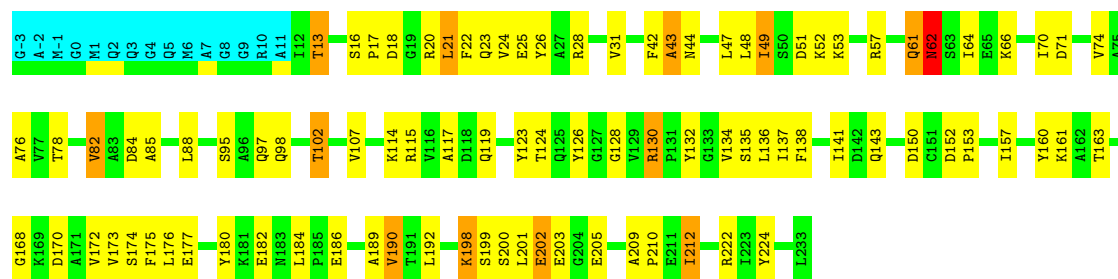
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 34% 6%



• Molecule 1: Proteasome subunit alpha

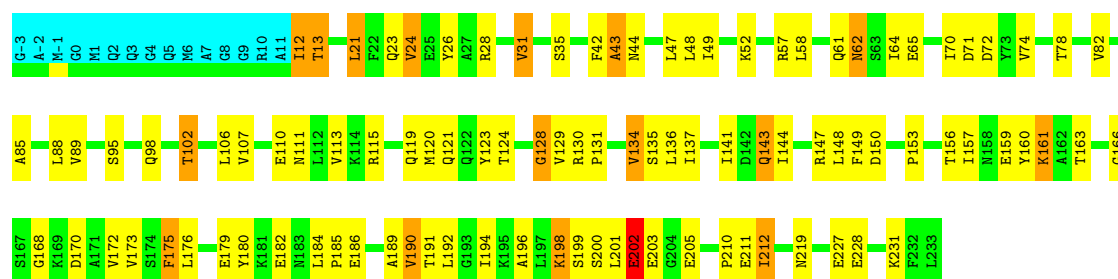
Chain G: 55% 33% 5% 6%



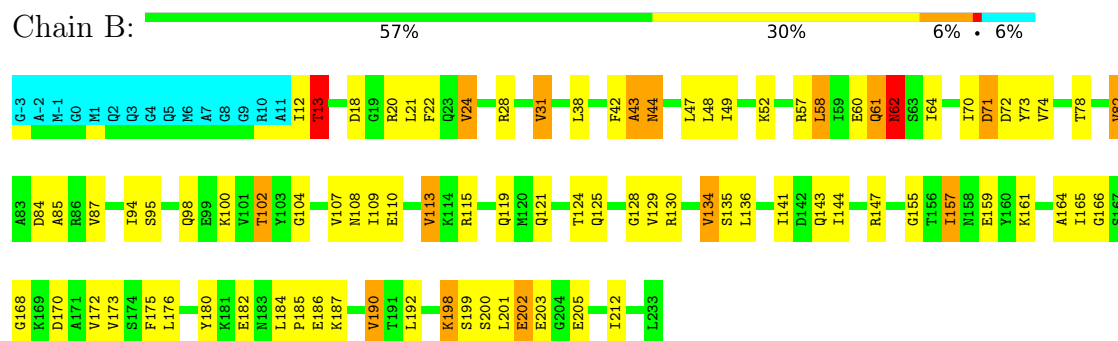
4.2.31 Score per residue for model 31

• Molecule 1: Proteasome subunit alpha

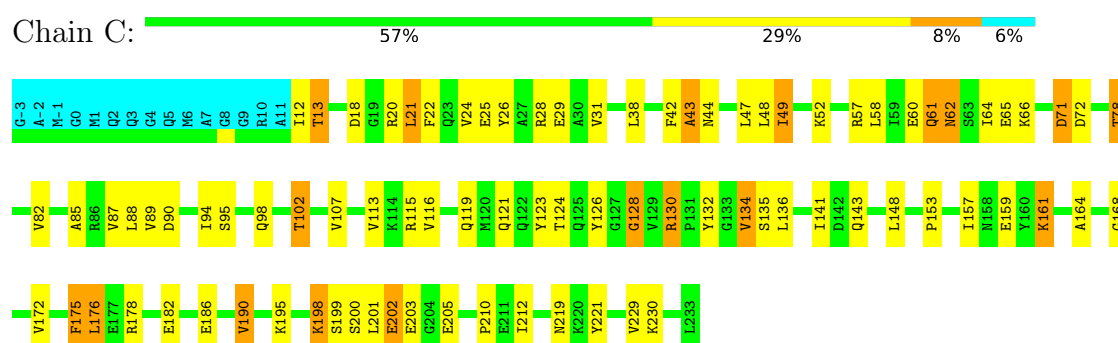
Chain A: 51% 35% 7% 6%



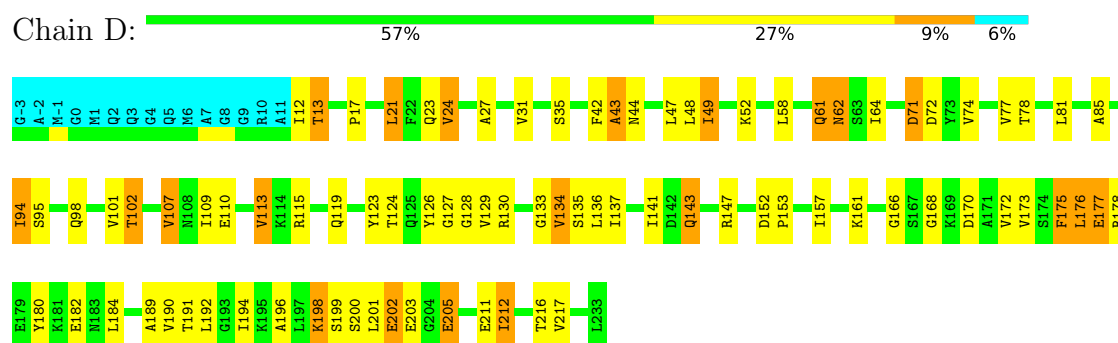
- Molecule 1: Proteasome subunit alpha



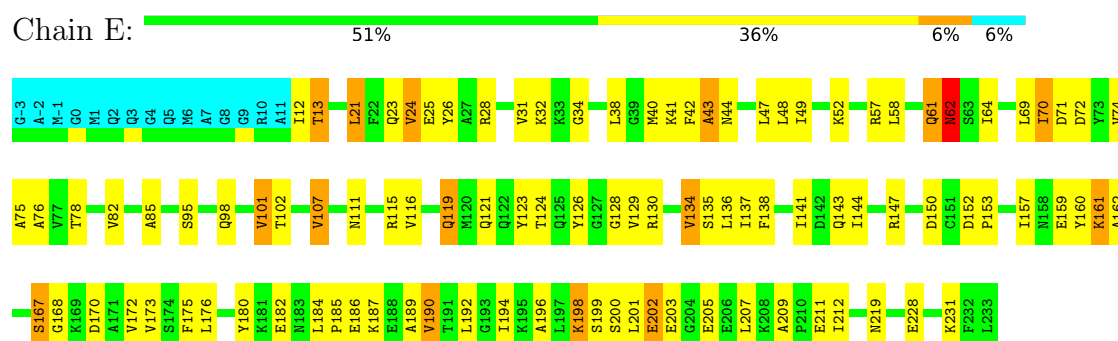
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



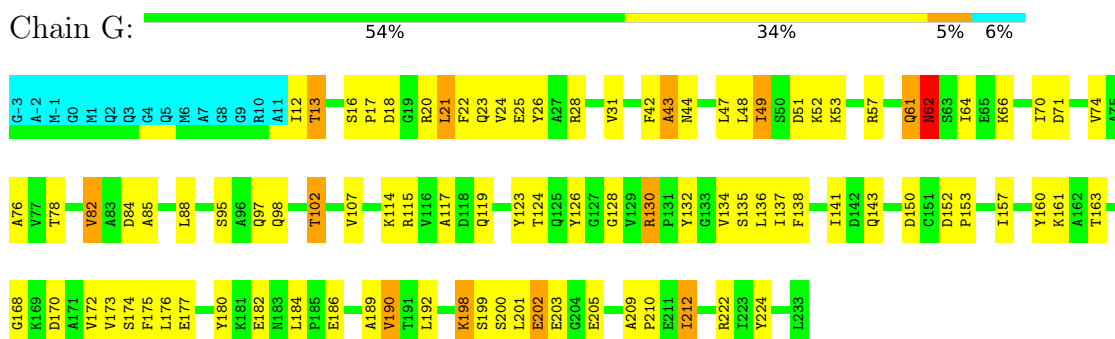
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

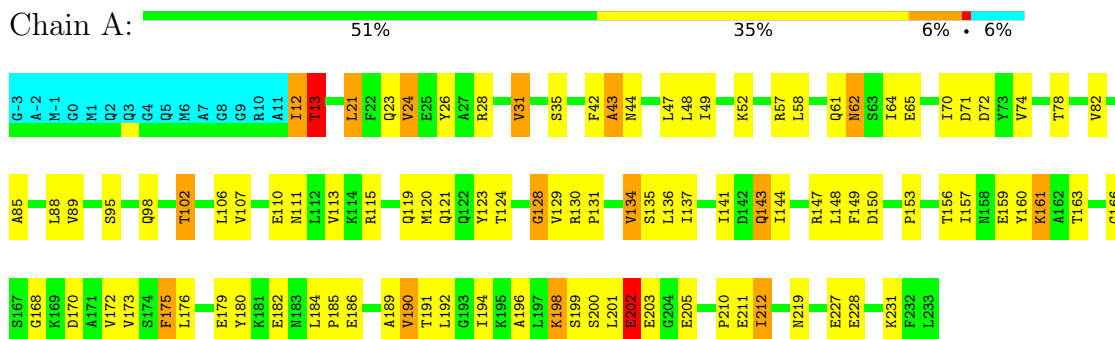


- Molecule 1: Proteasome subunit alpha

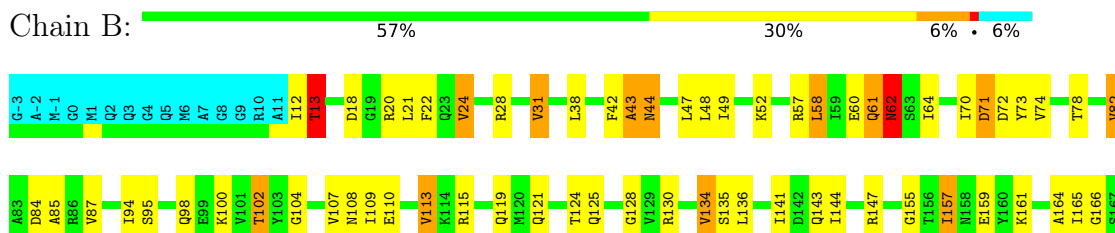


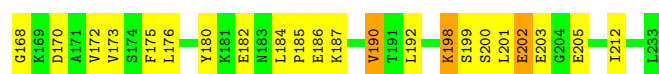
4.2.32 Score per residue for model 32

- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha





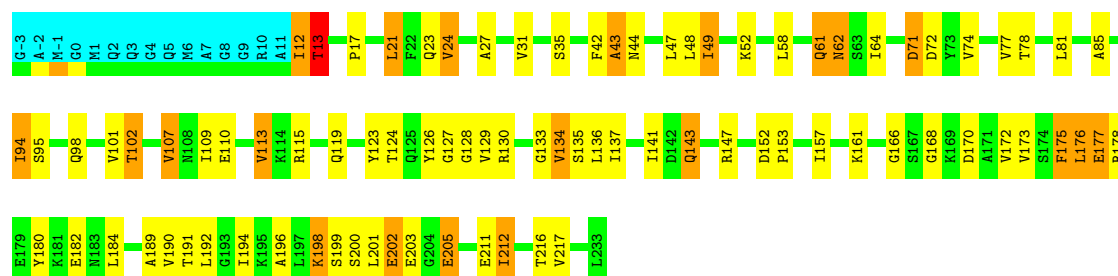
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 28% 8% 6%



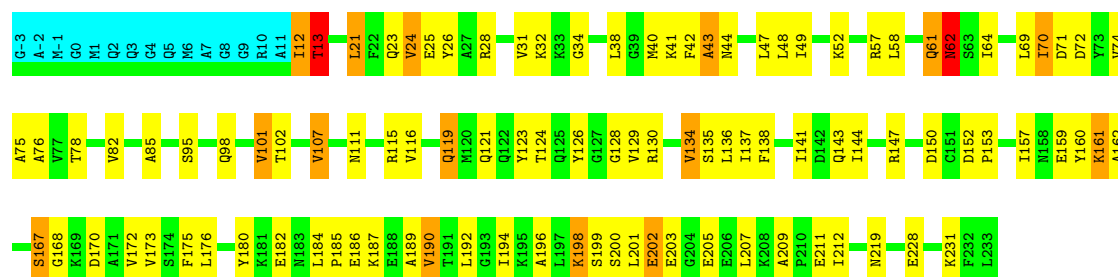
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



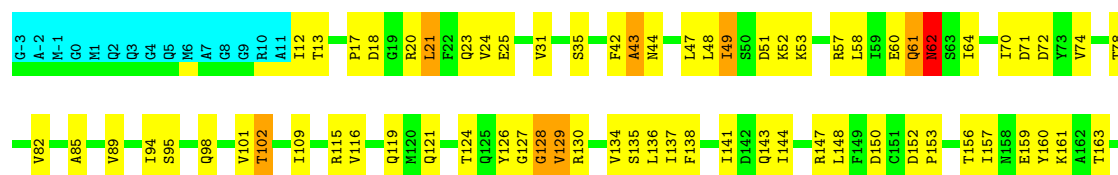
• Molecule 1: Proteasome subunit alpha

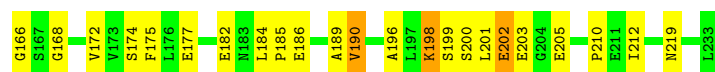
Chain E: 51% 35% 6% 6%



• Molecule 1: Proteasome subunit alpha

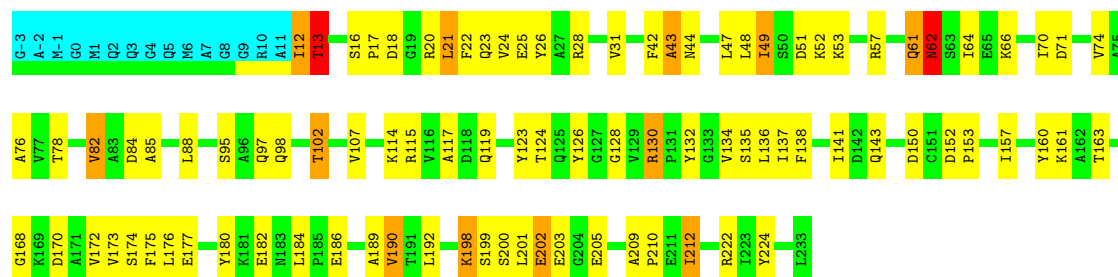
Chain F: 55% 34% 6%





• Molecule 1: Proteasome subunit alpha

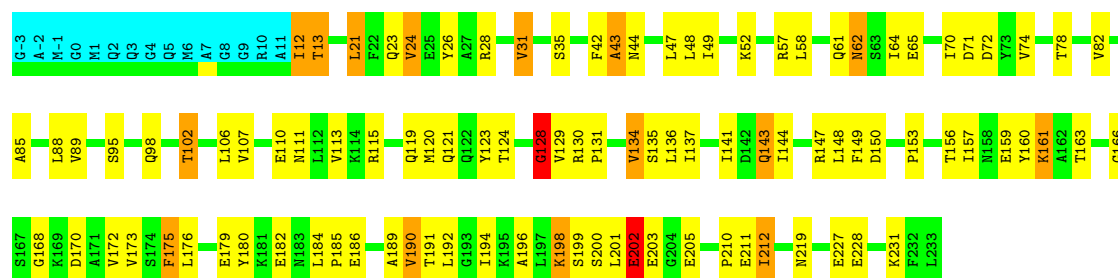
Chain G: 54% 33% 5% • 6%



4.2.33 Score per residue for model 33

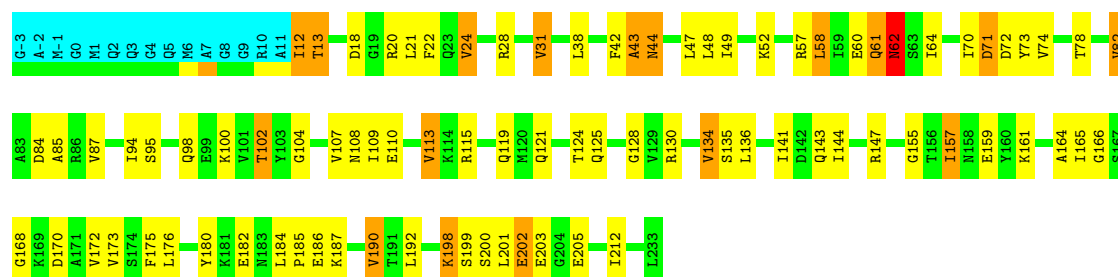
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% • 6%



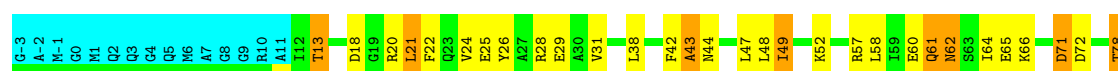
• Molecule 1: Proteasome subunit alpha

Chain B: 57% 29% 7% 6%



• Molecule 1: Proteasome subunit alpha

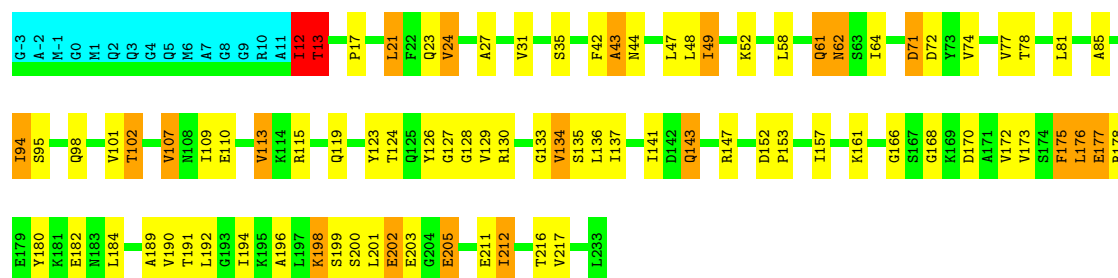
Chain C: 58% 28% 8% 6%





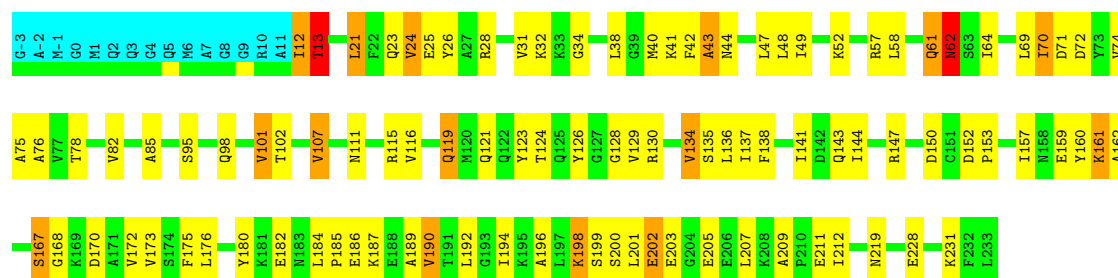
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 8% • 6%



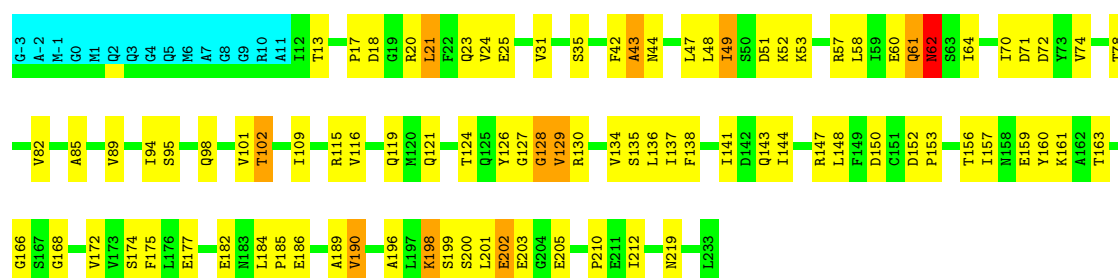
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% • 6%



• Molecule 1: Proteasome subunit alpha

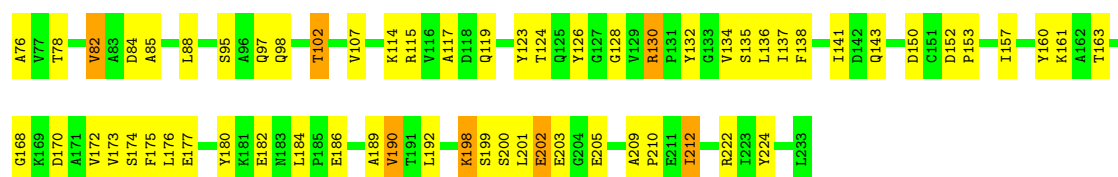
Chain F: 55% 34% • 6%



• Molecule 1: Proteasome subunit alpha

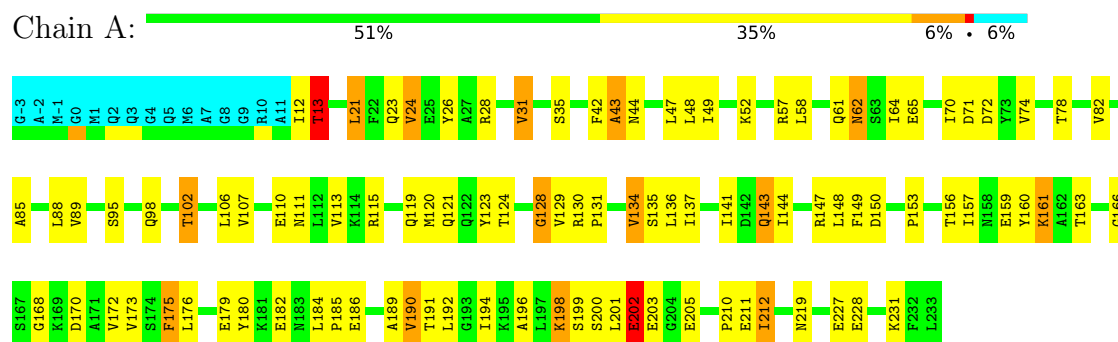
Chain G: 55% 33% 5% 6%



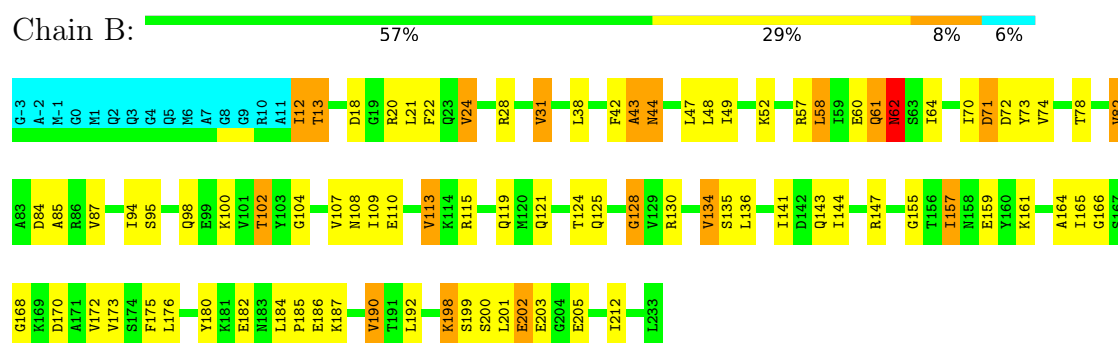


4.2.34 Score per residue for model 34

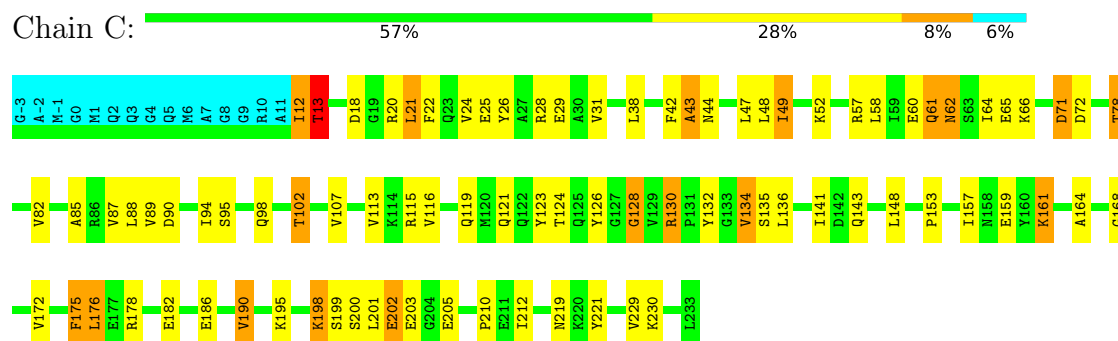
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

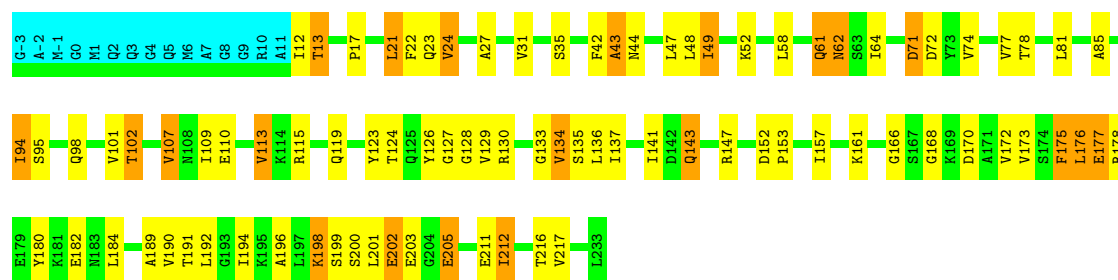


- Molecule 1: Proteasome subunit alpha



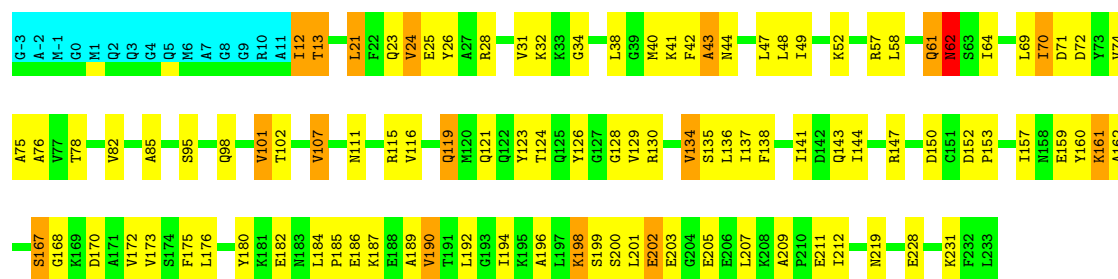
- Molecule 1: Proteasome subunit alpha





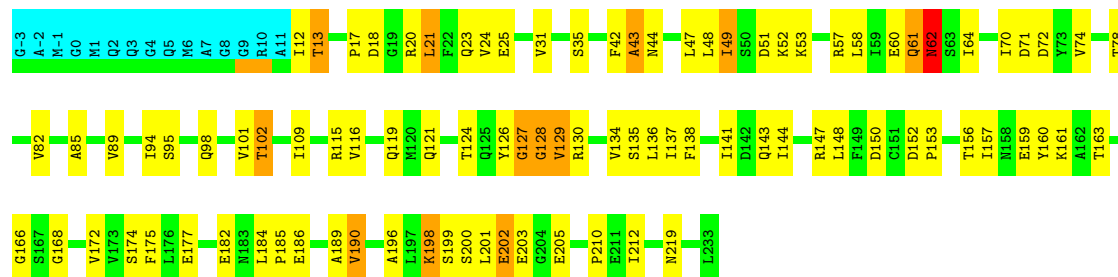
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



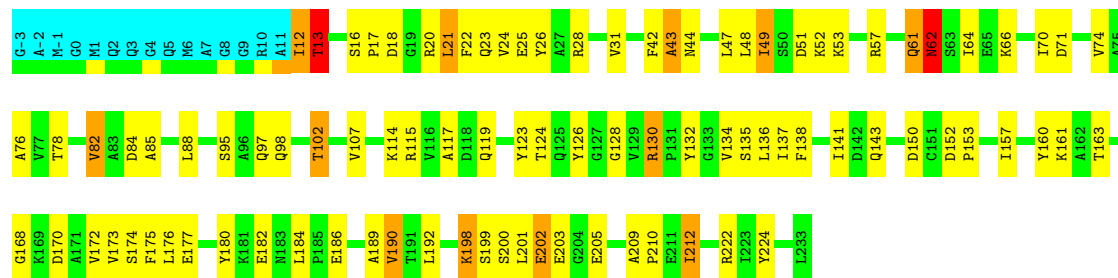
• Molecule 1: Proteasome subunit alpha

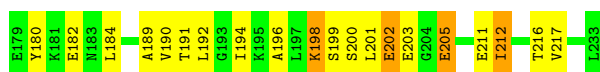
Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 54% 33% 5% 6%





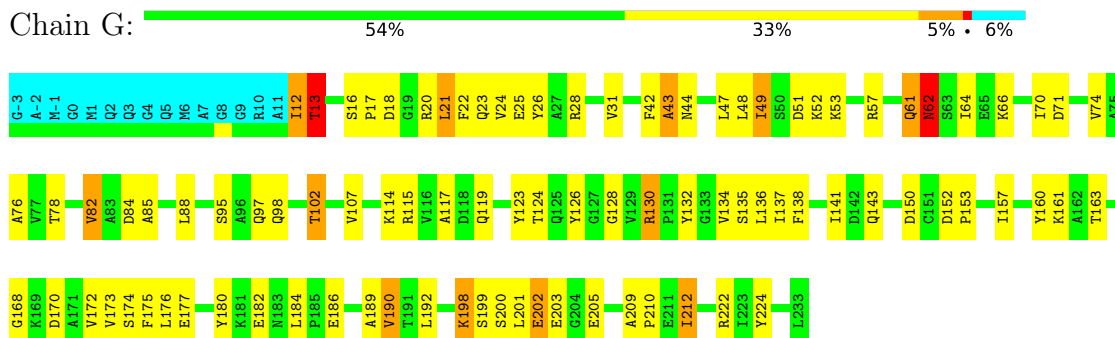
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

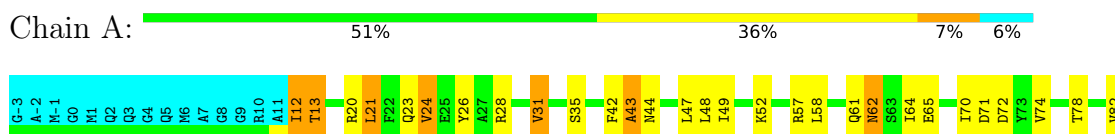


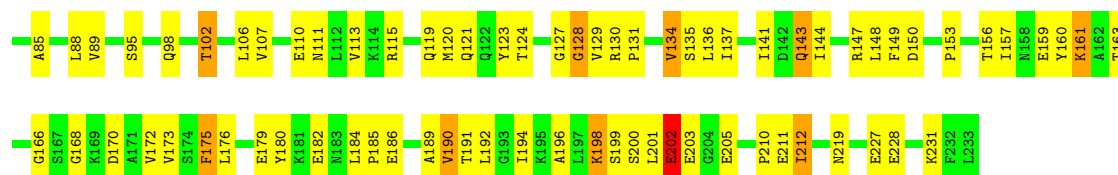
• Molecule 1: Proteasome subunit alpha



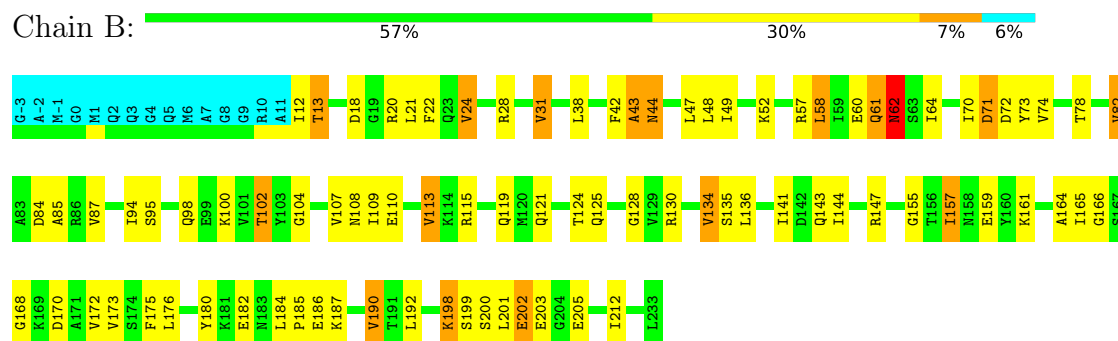
4.2.36 Score per residue for model 36

• Molecule 1: Proteasome subunit alpha

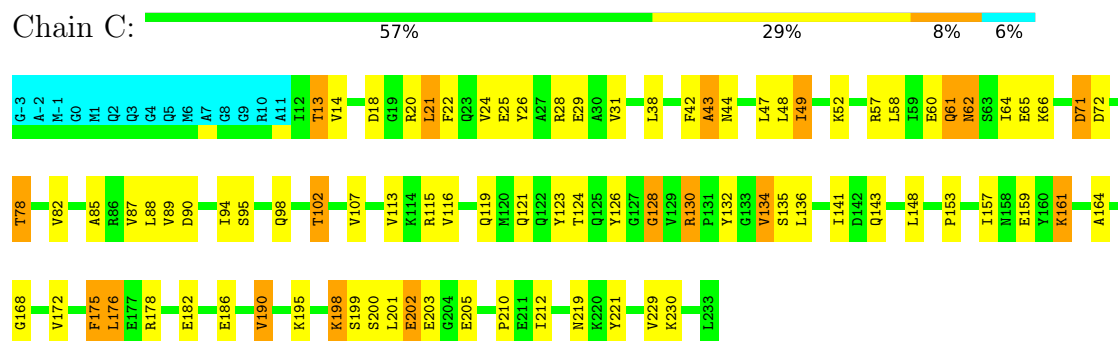




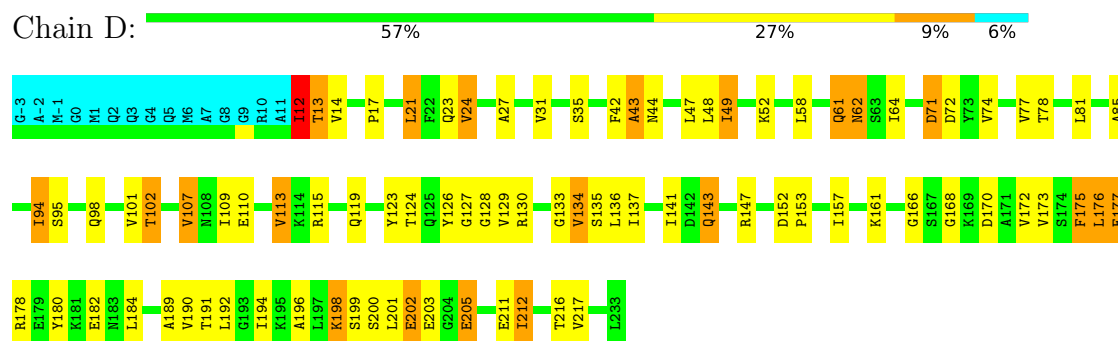
• Molecule 1: Proteasome subunit alpha



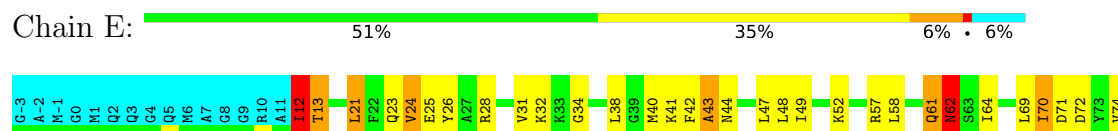
• Molecule 1: Proteasome subunit alpha

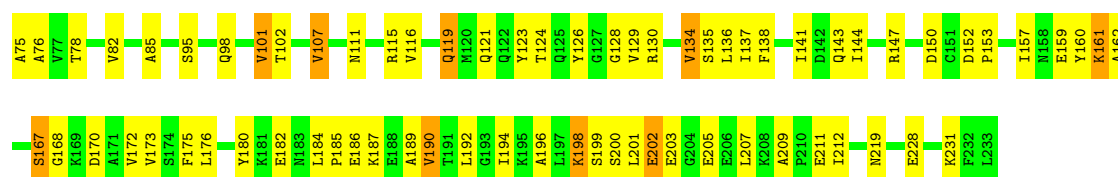


• Molecule 1: Proteasome subunit alpha



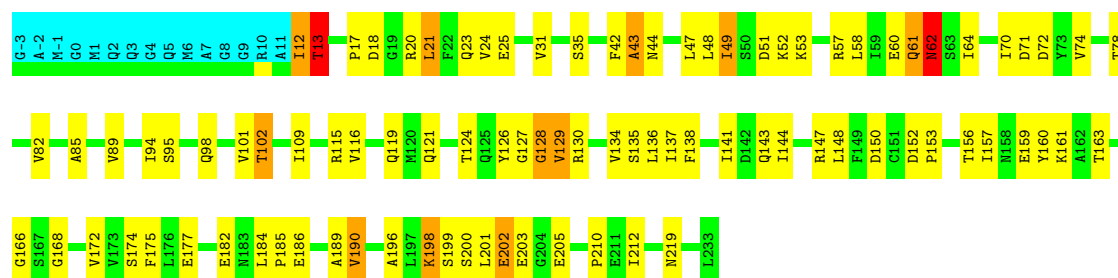
• Molecule 1: Proteasome subunit alpha





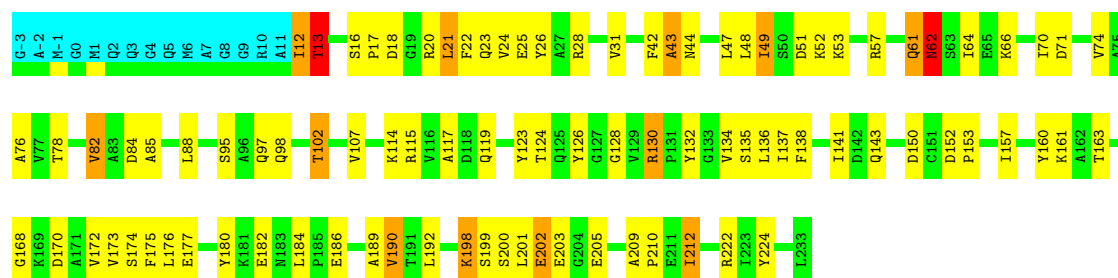
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% • 6%



• Molecule 1: Proteasome subunit alpha

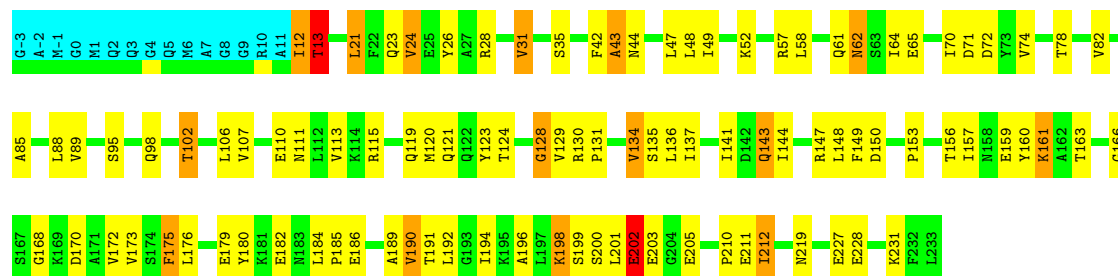
Chain G: 54% 33% 5% • 6%



4.2.37 Score per residue for model 37

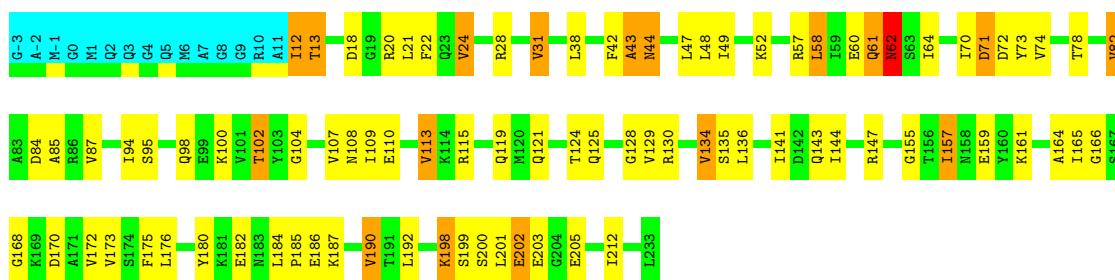
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% • 6%



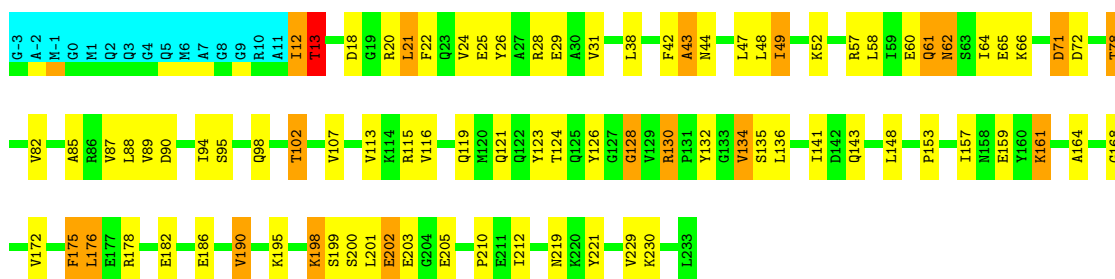
• Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 7% 6%



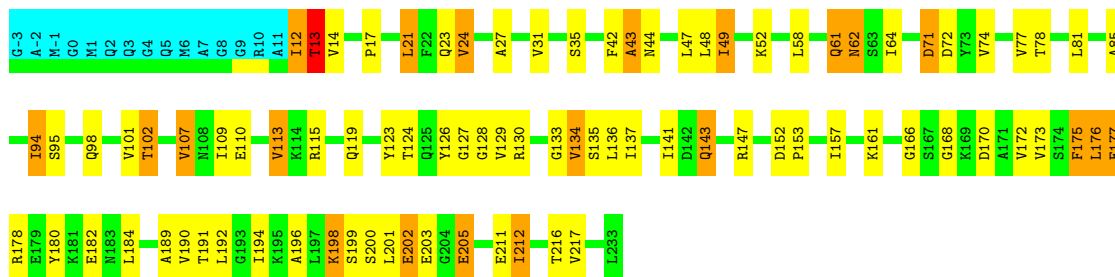
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 28% 8% 6%



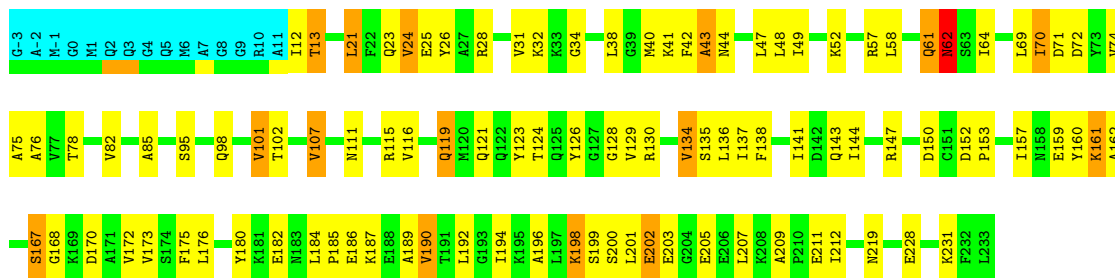
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



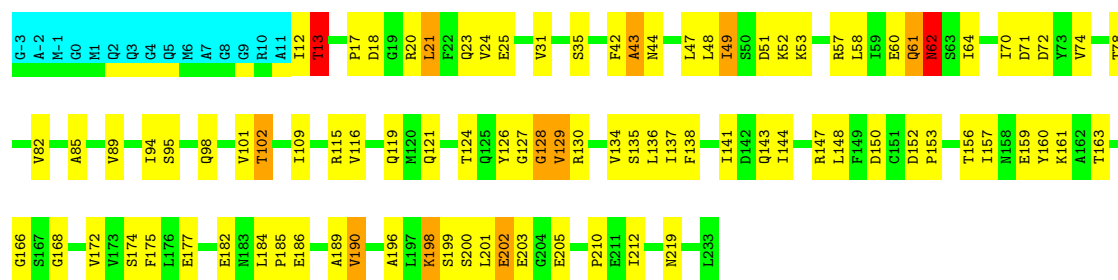
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 36% 6% 6%



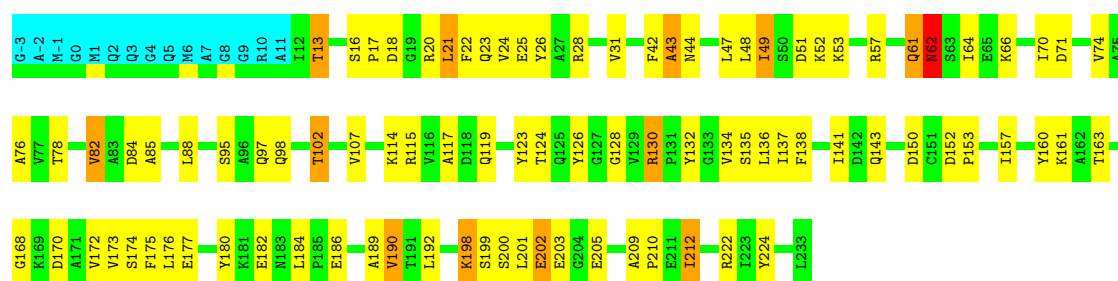
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 34% 6%



- Molecule 1: Proteasome subunit alpha

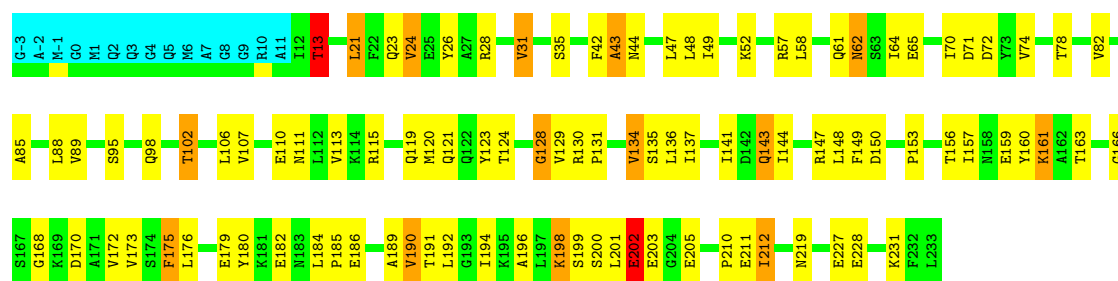
Chain G: 55% 33% 5% 6%



4.2.38 Score per residue for model 38

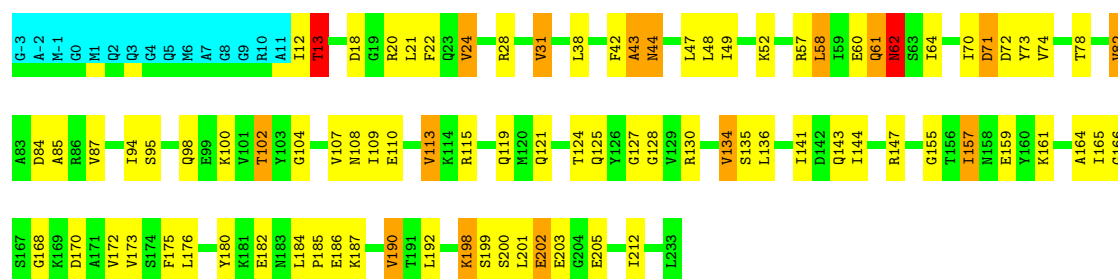
- Molecule 1: Proteasome subunit alpha

Chain A: 52% 35% 6% 6%

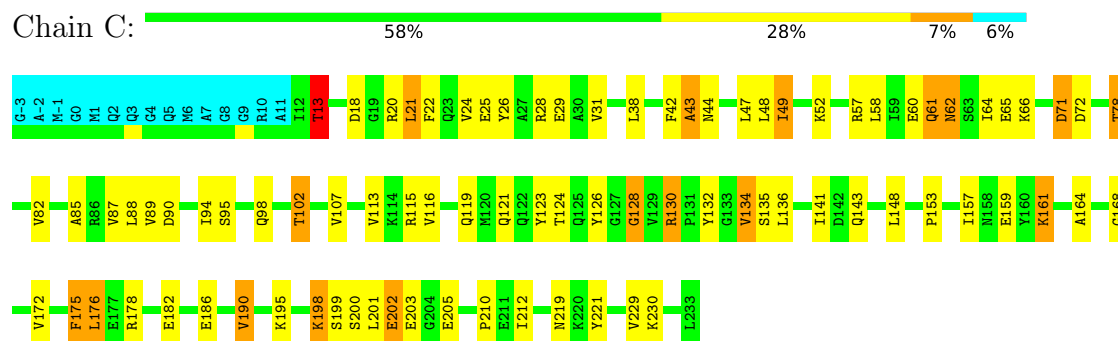


- Molecule 1: Proteasome subunit alpha

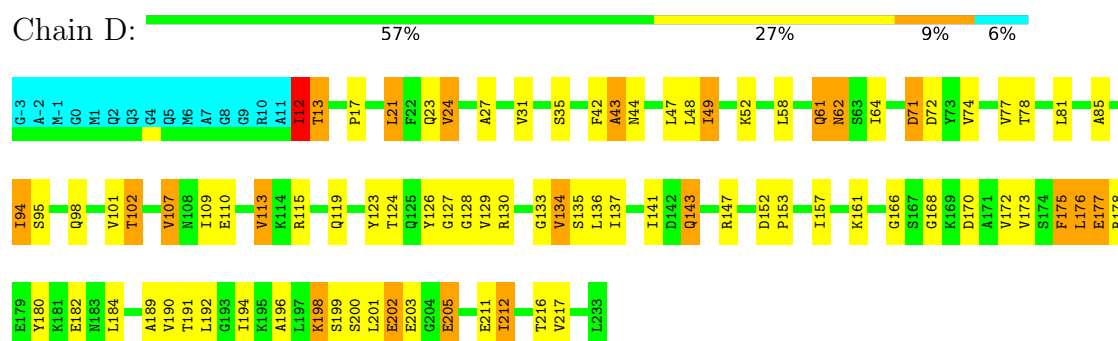
Chain B: 57% 30% 6% 6%



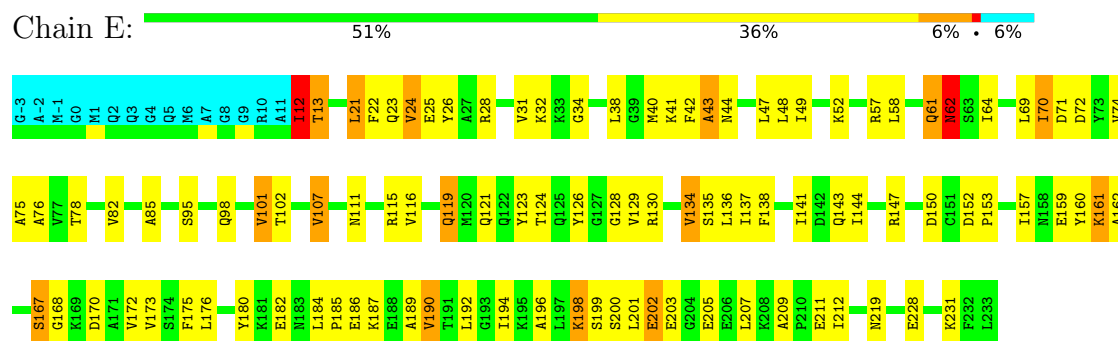
- Molecule 1: Proteasome subunit alpha



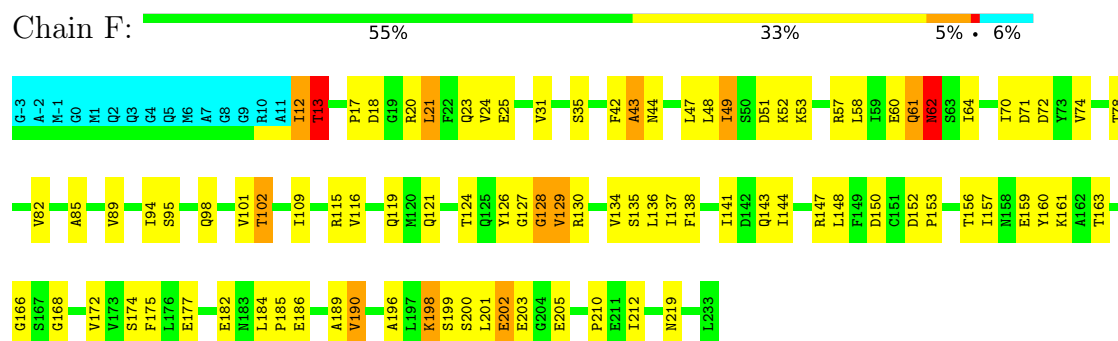
- Molecule 1: Proteasome subunit alpha



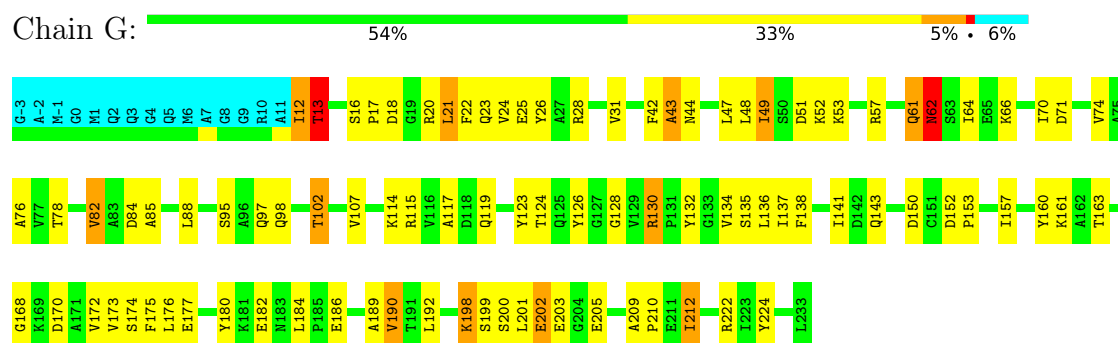
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

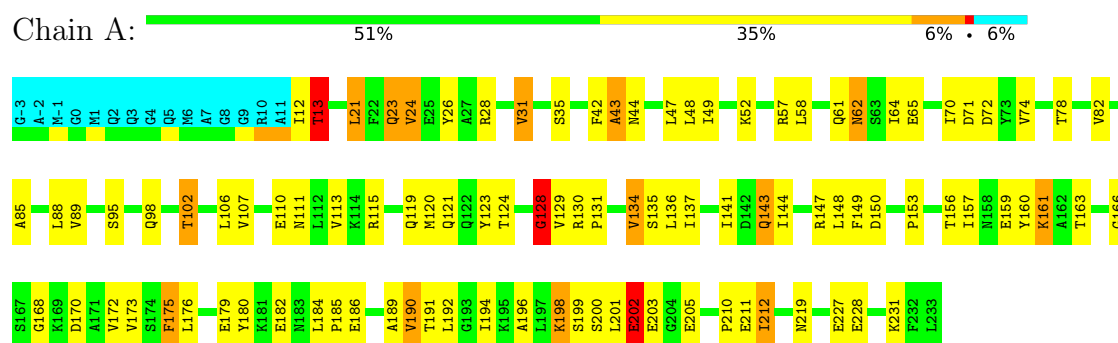


- Molecule 1: Proteasome subunit alpha

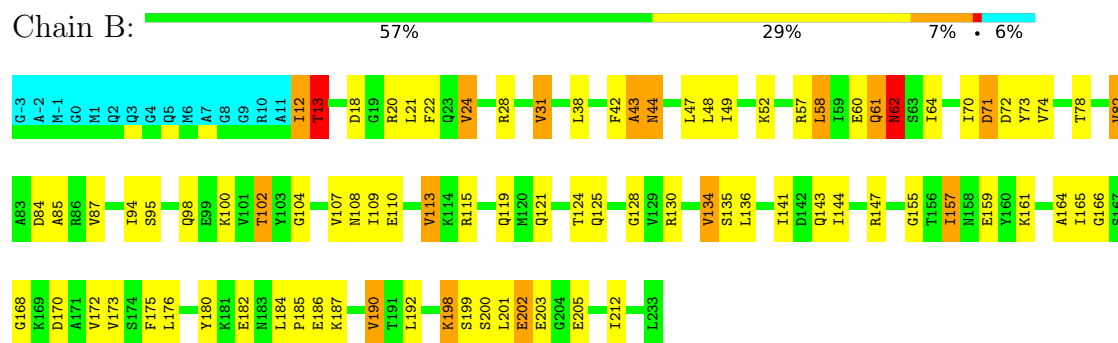


4.2.39 Score per residue for model 39

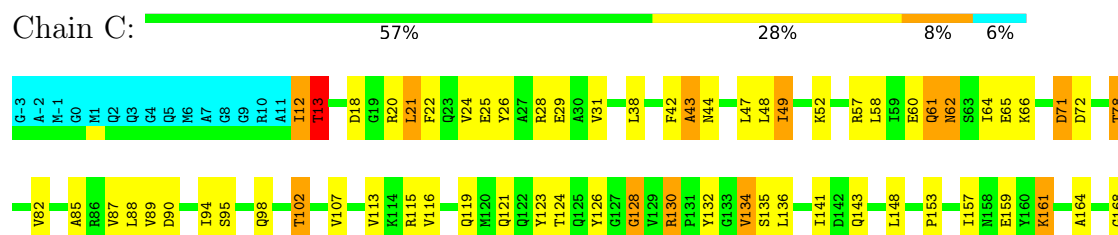
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha





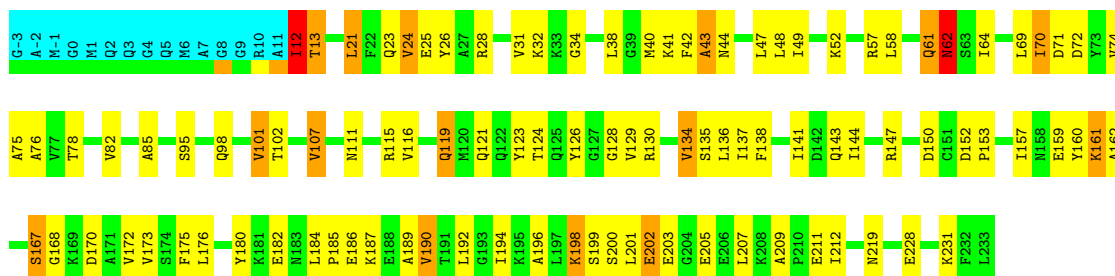
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



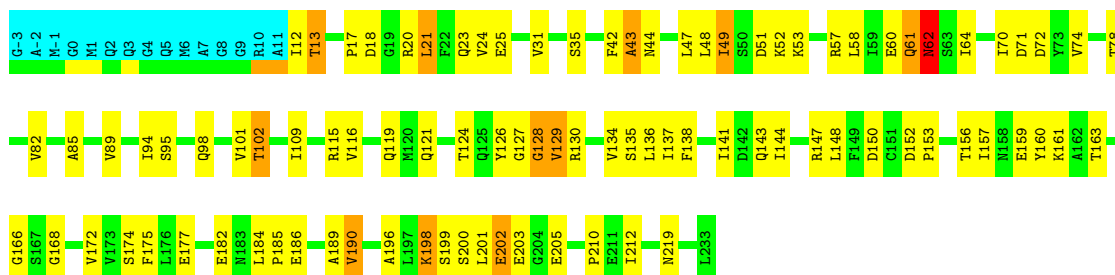
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% 6%



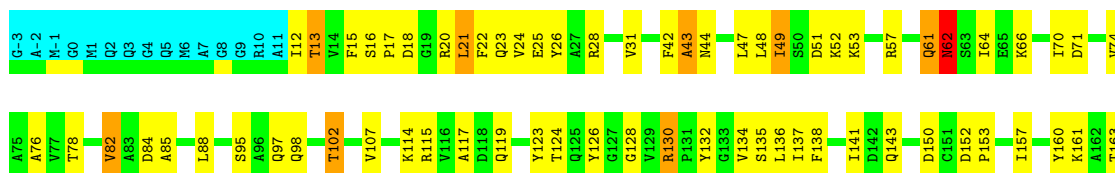
• Molecule 1: Proteasome subunit alpha

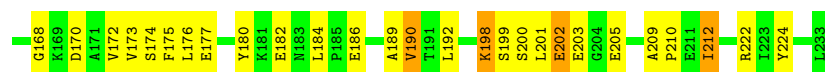
Chain F: 55% 34% 5% 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 54% 34% 5% 6%

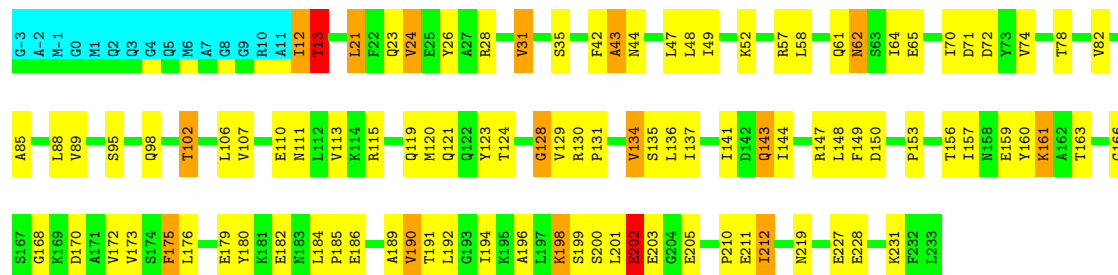




4.2.40 Score per residue for model 40

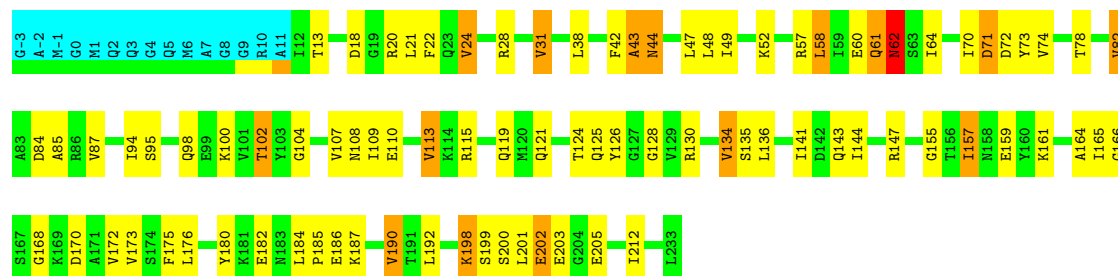
- Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



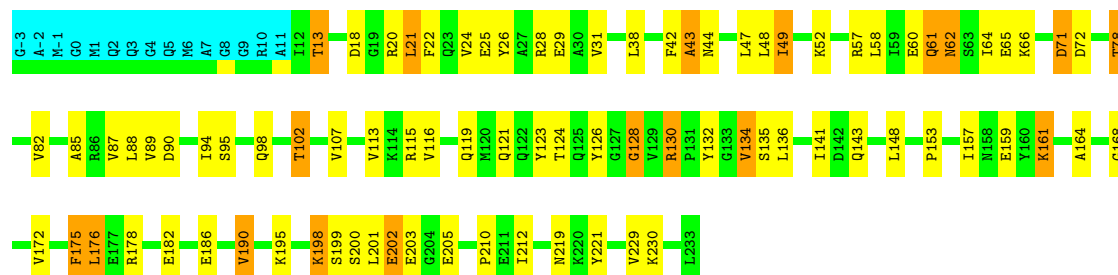
- Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 6% 6%



- Molecule 1: Proteasome subunit alpha

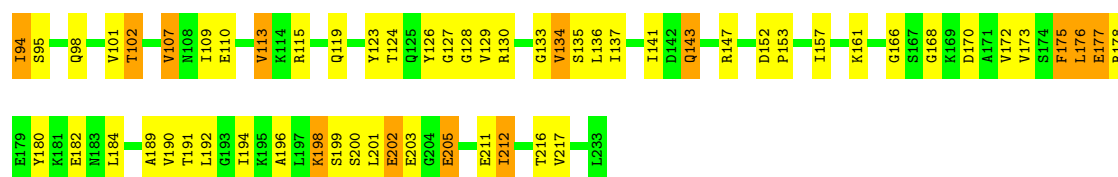
Chain C: 58% 28% 8% 6%



- Molecule 1: Proteasome subunit alpha

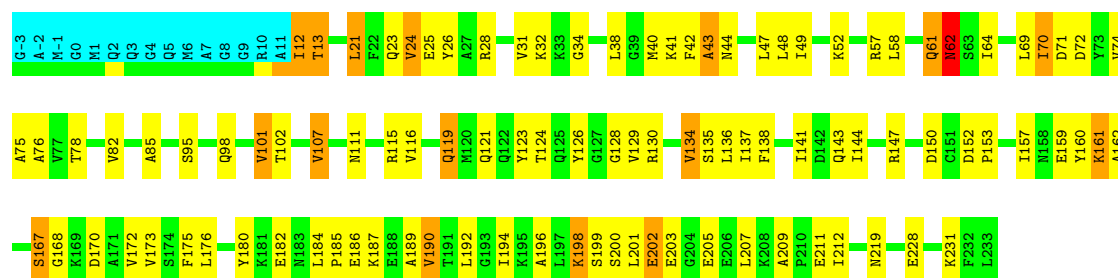
Chain D: 57% 27% 9% 6%





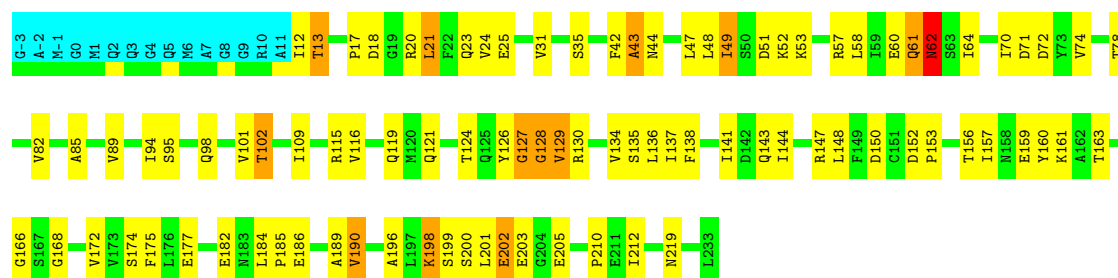
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



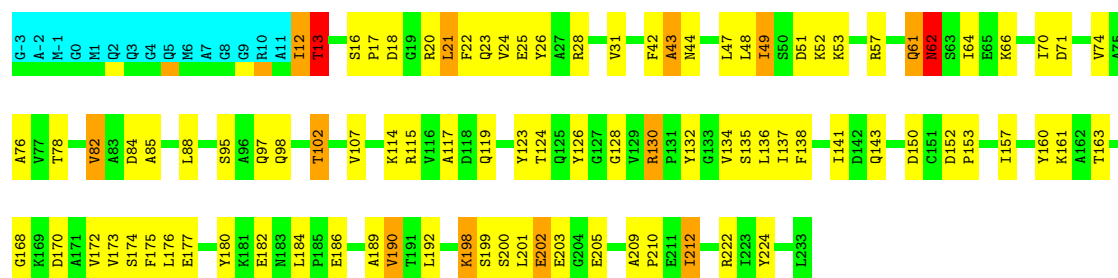
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

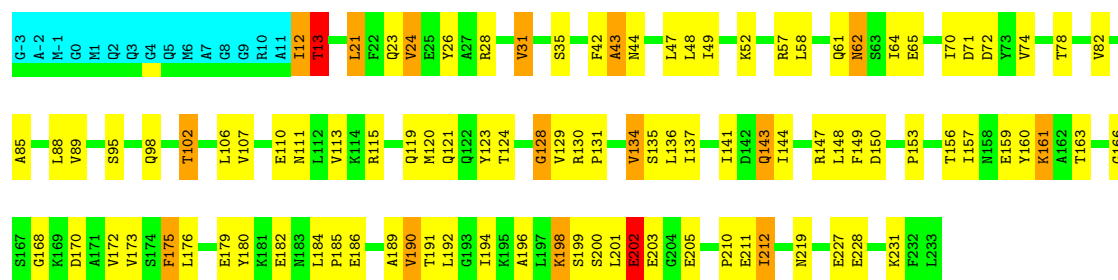
Chain G: 54% 33% 5% 6%



4.2.41 Score per residue for model 41

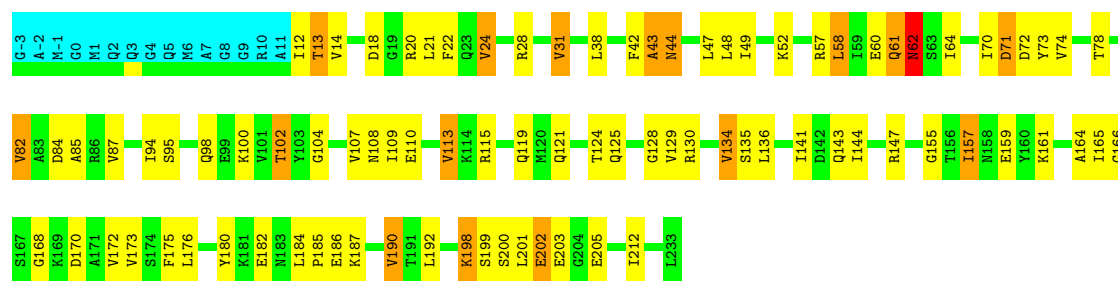
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



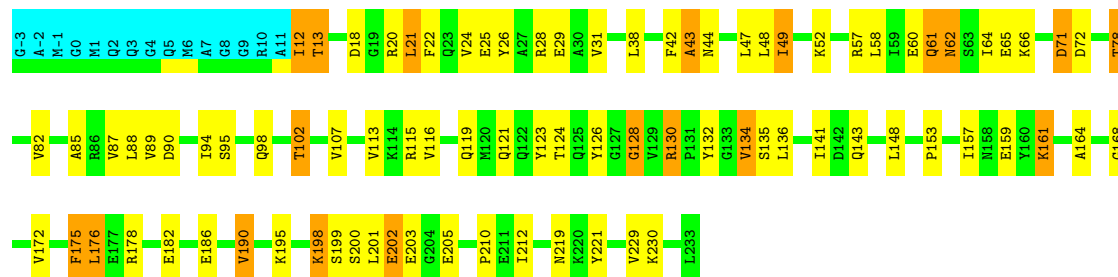
- Molecule 1: Proteasome subunit alpha

Chain B: 56% 30% 7% 6%



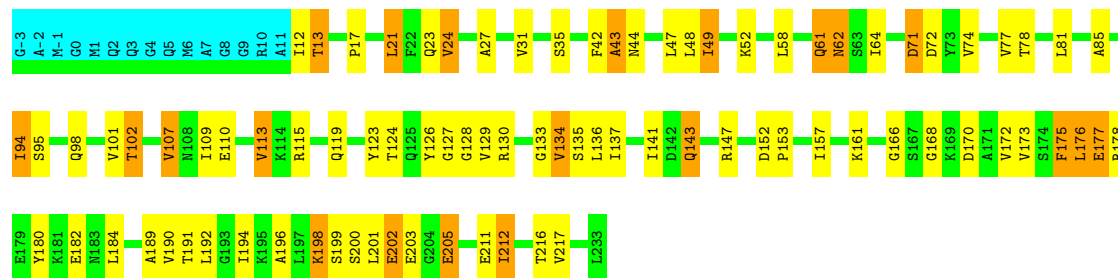
- Molecule 1: Proteasome subunit alpha

Chain C: 57% 28% 8% 6%



- Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%

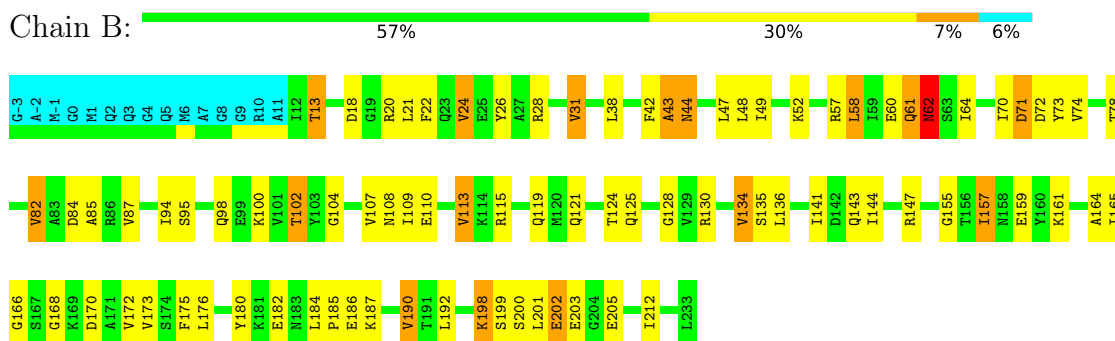


- Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% 6%



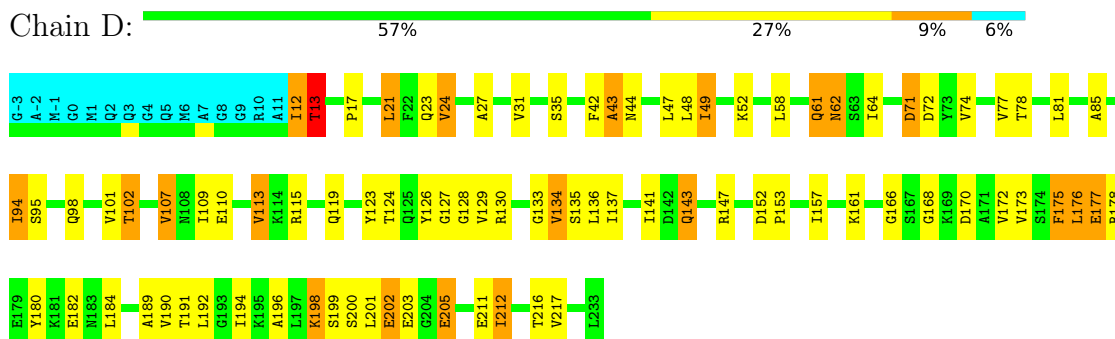
- Molecule 1: Proteasome subunit alpha



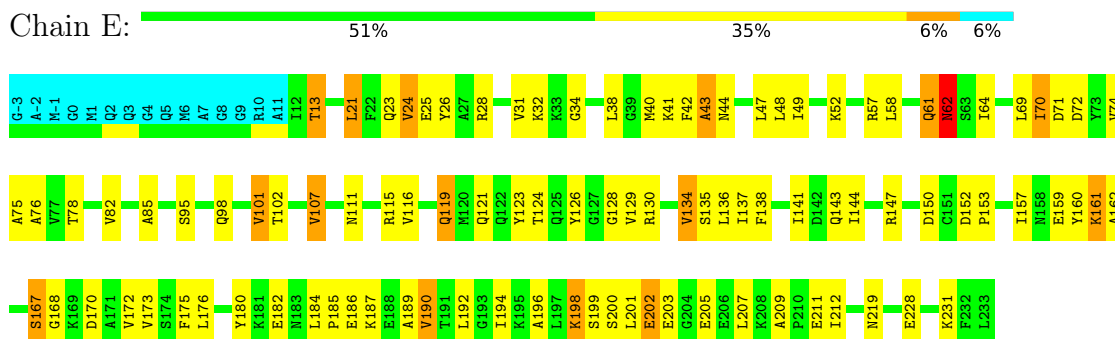
- Molecule 1: Proteasome subunit alpha



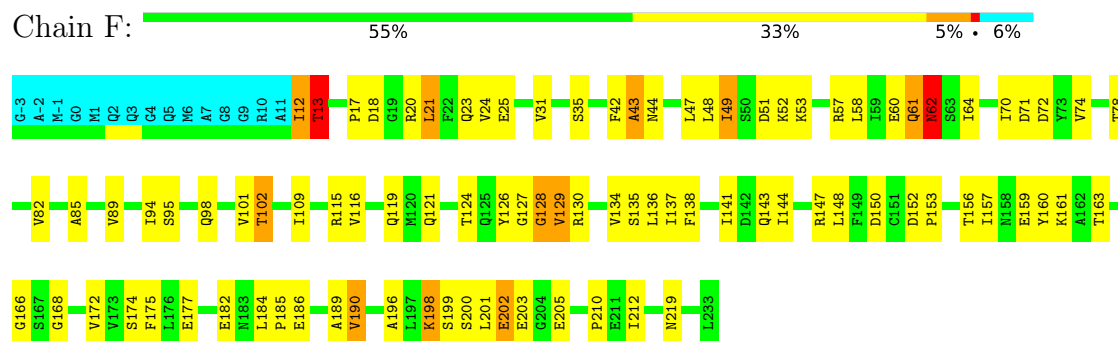
- Molecule 1: Proteasome subunit alpha



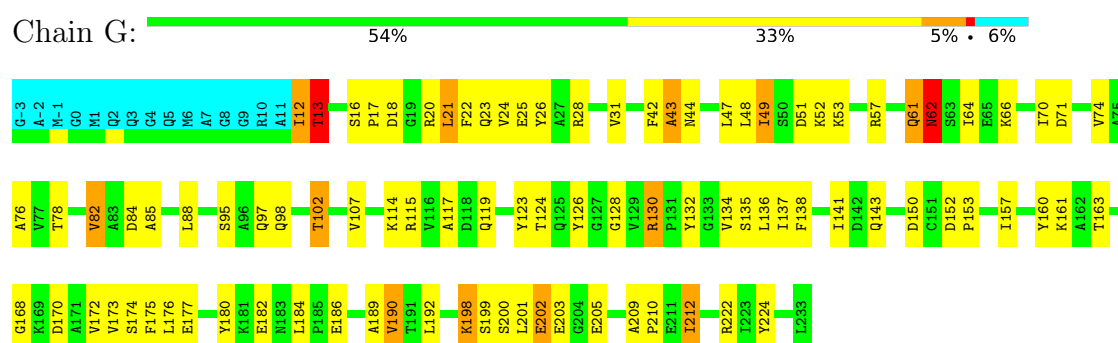
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

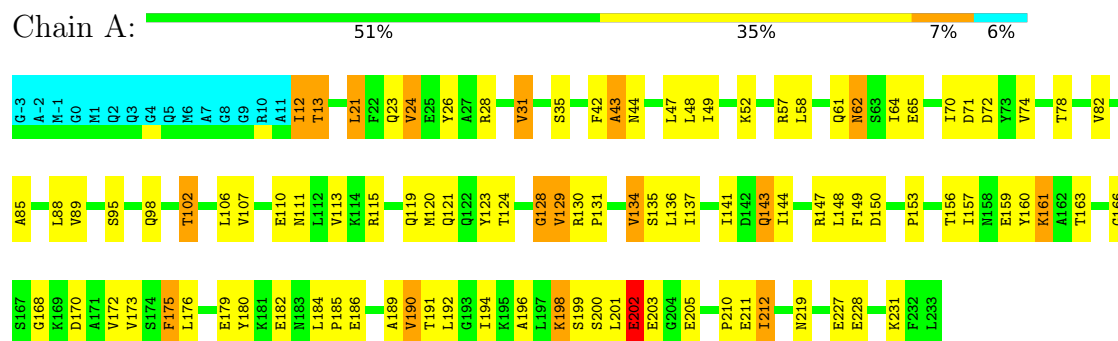


- Molecule 1: Proteasome subunit alpha

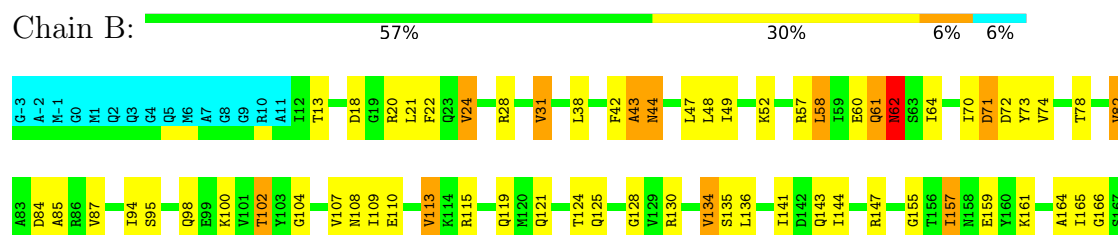


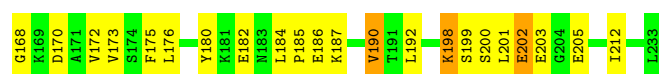
4.2.43 Score per residue for model 43

- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha





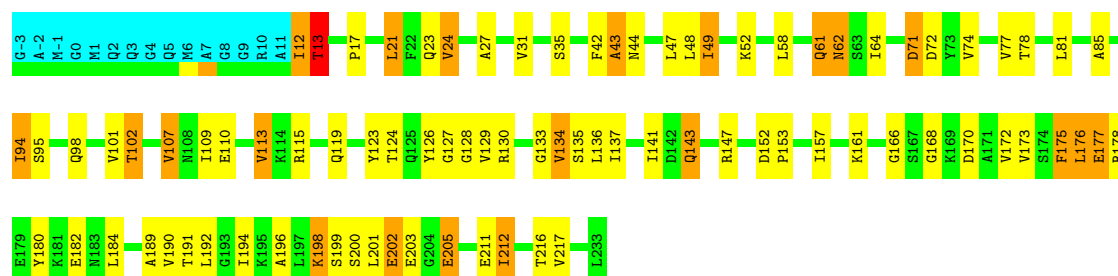
• Molecule 1: Proteasome subunit alpha

Chain C: 58% 28% 7% 6%



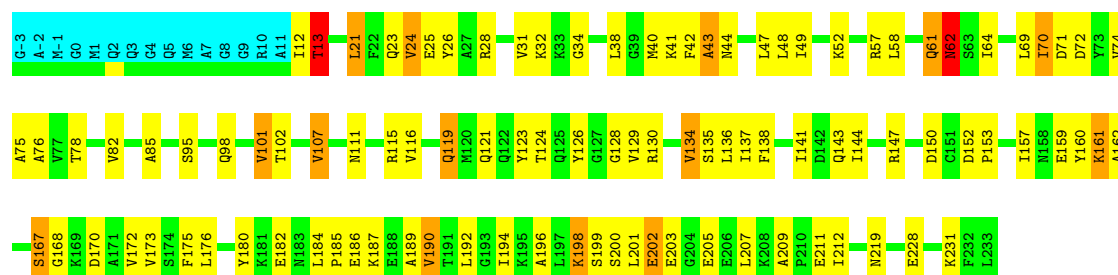
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



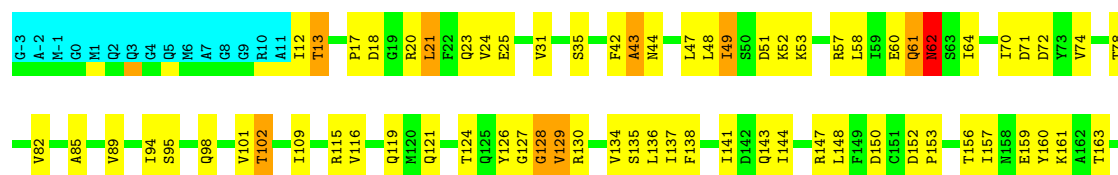
• Molecule 1: Proteasome subunit alpha

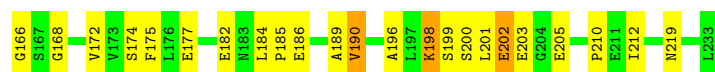
Chain E: 51% 36% 6% 6%



• Molecule 1: Proteasome subunit alpha

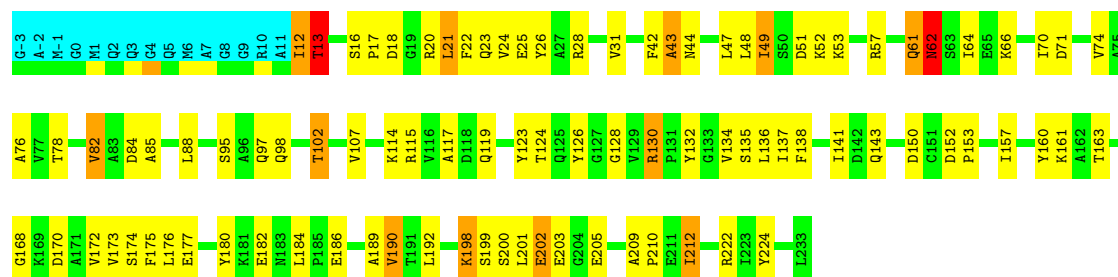
Chain F: 55% 34% 5% 6%





• Molecule 1: Proteasome subunit alpha

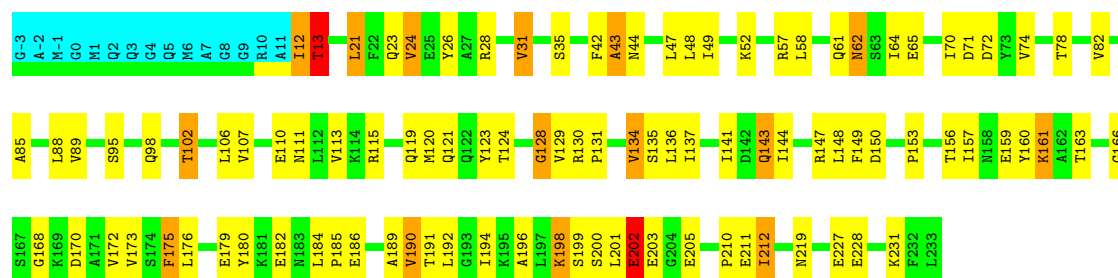
Chain G: 54% 33% 5% • 6%



4.2.44 Score per residue for model 44

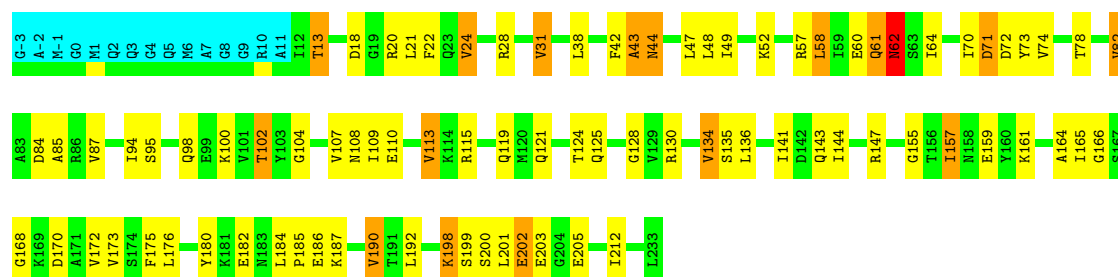
• Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% • 6%



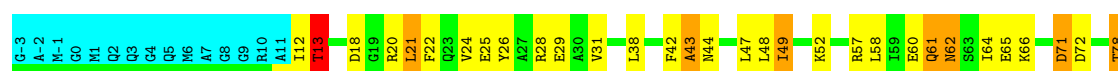
• Molecule 1: Proteasome subunit alpha

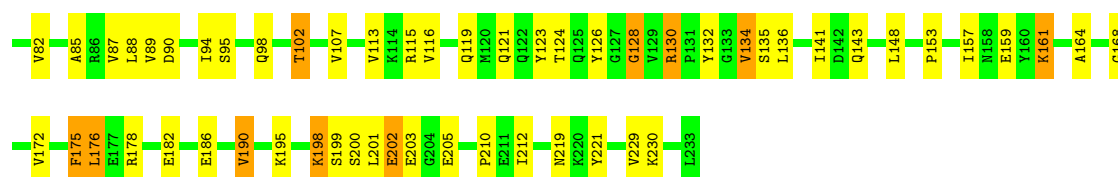
Chain B: 57% 29% 7% 6%



• Molecule 1: Proteasome subunit alpha

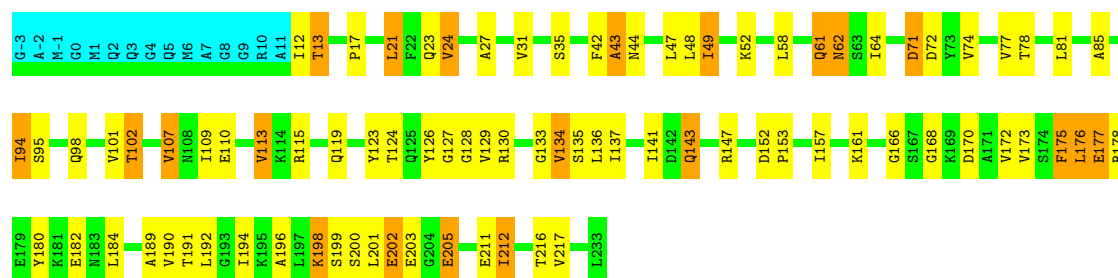
Chain C: 57% 29% 7% 6%





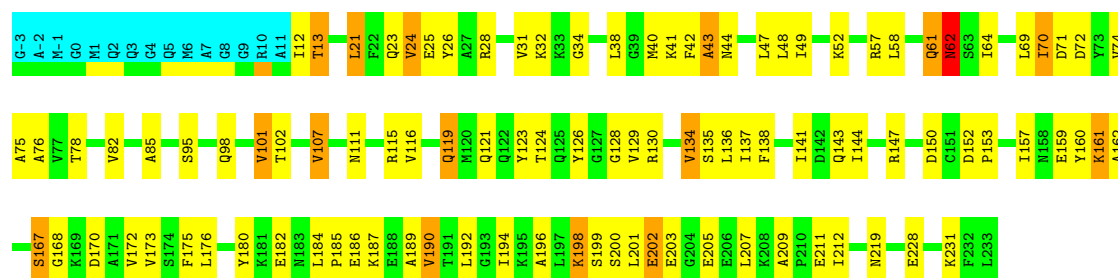
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



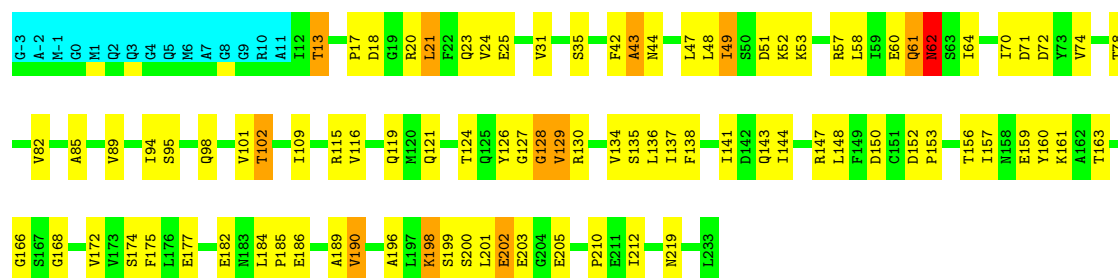
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 36% 6% 6%



• Molecule 1: Proteasome subunit alpha

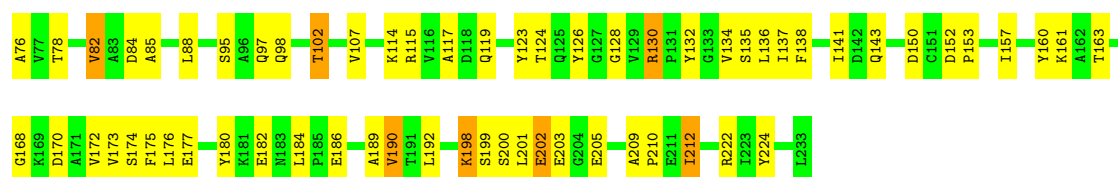
Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

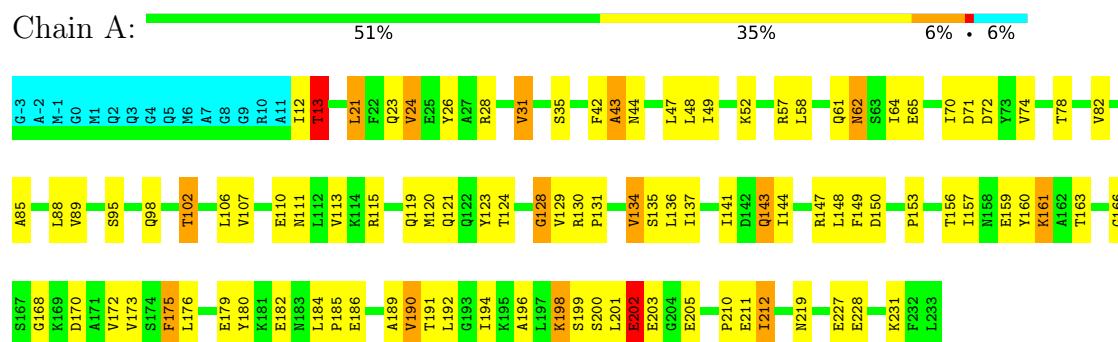
Chain G: 54% 34% 5% 6%



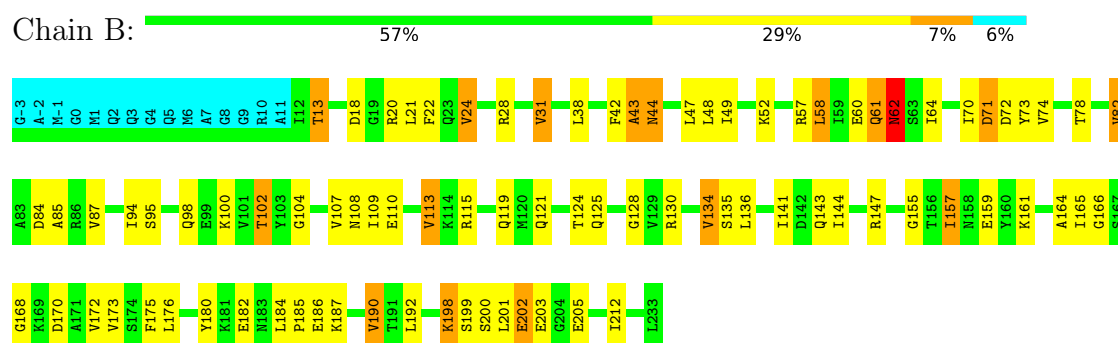


4.2.45 Score per residue for model 45

- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

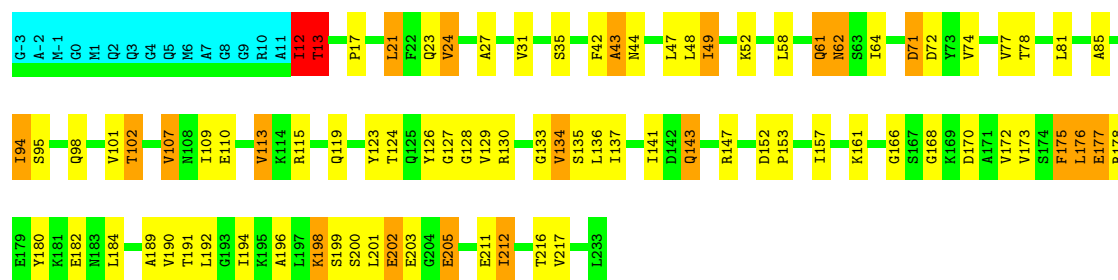


- Molecule 1: Proteasome subunit alpha



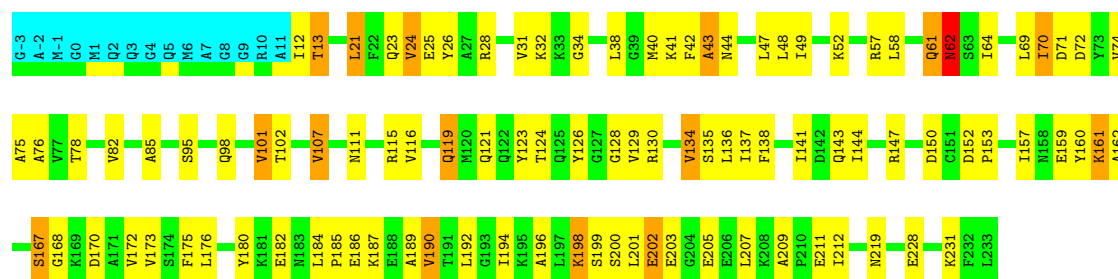
- Molecule 1: Proteasome subunit alpha





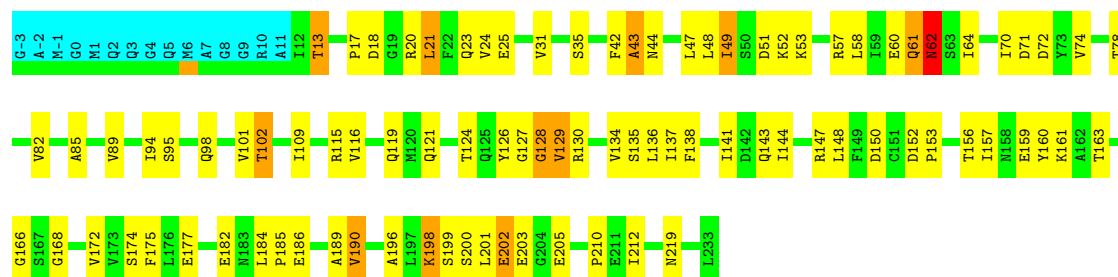
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 36% 6% 6%



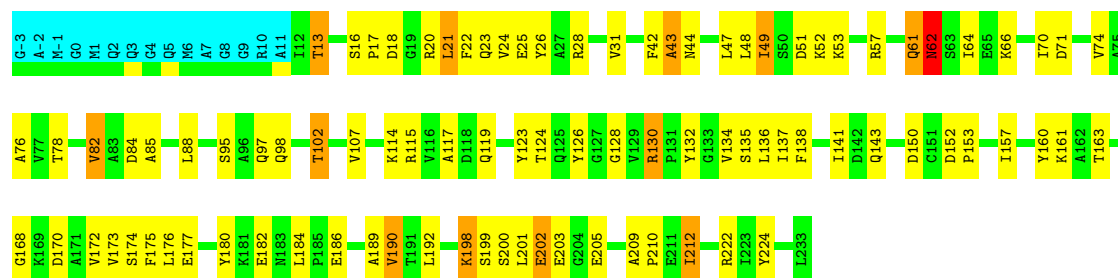
• Molecule 1: Proteasome subunit alpha

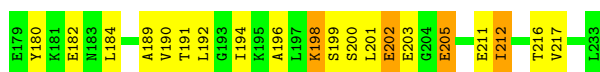
Chain F: 55% 33% 5% 6%



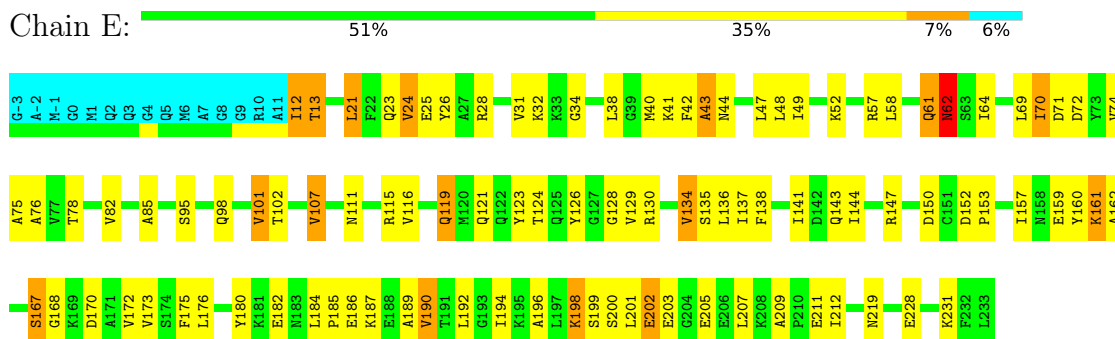
• Molecule 1: Proteasome subunit alpha

Chain G: 55% 33% 5% 6%





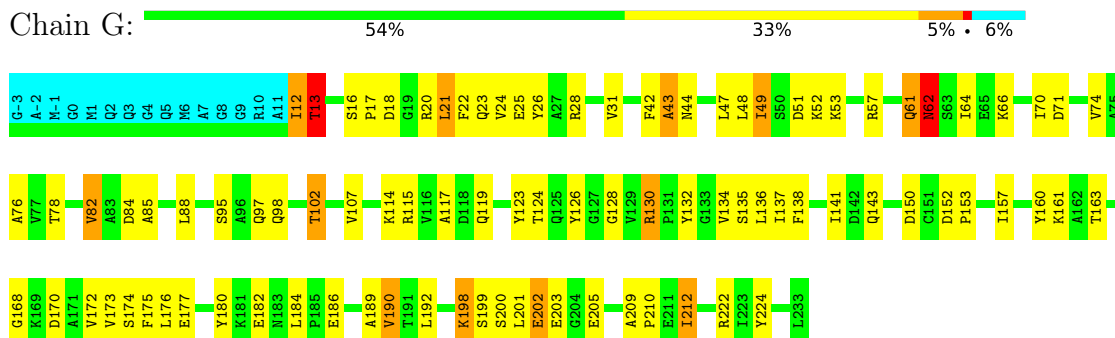
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

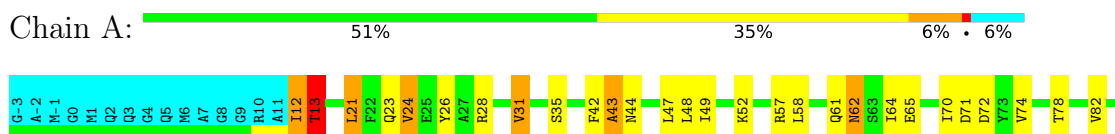


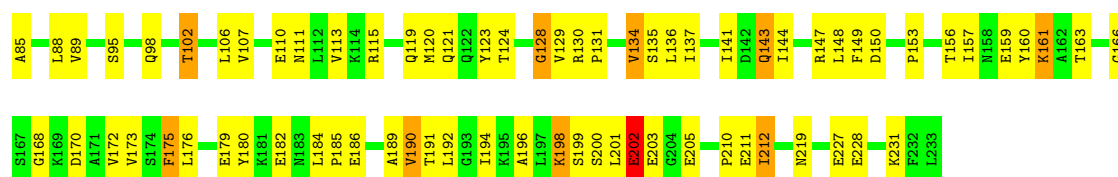
• Molecule 1: Proteasome subunit alpha



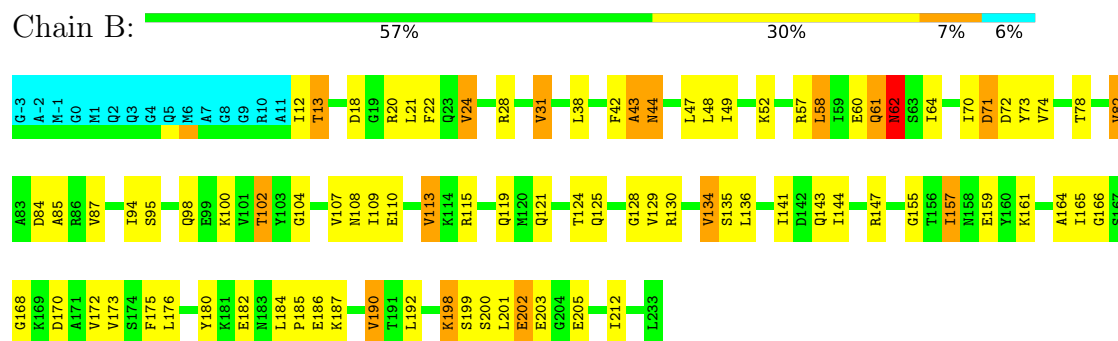
4.2.47 Score per residue for model 47

• Molecule 1: Proteasome subunit alpha

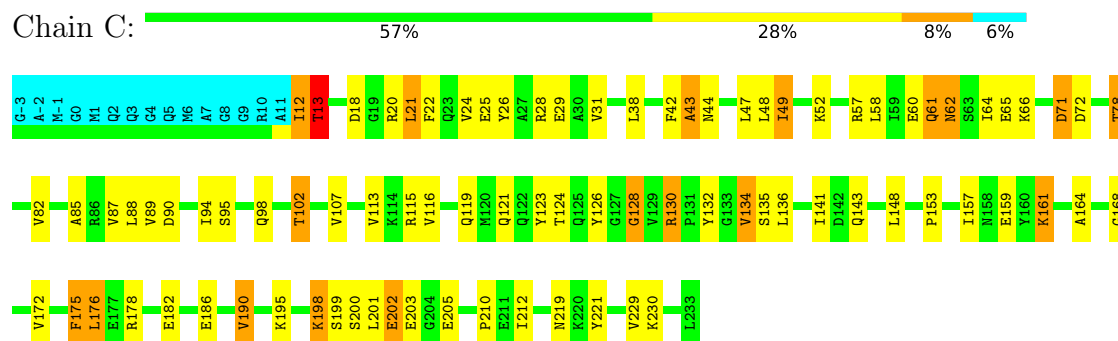




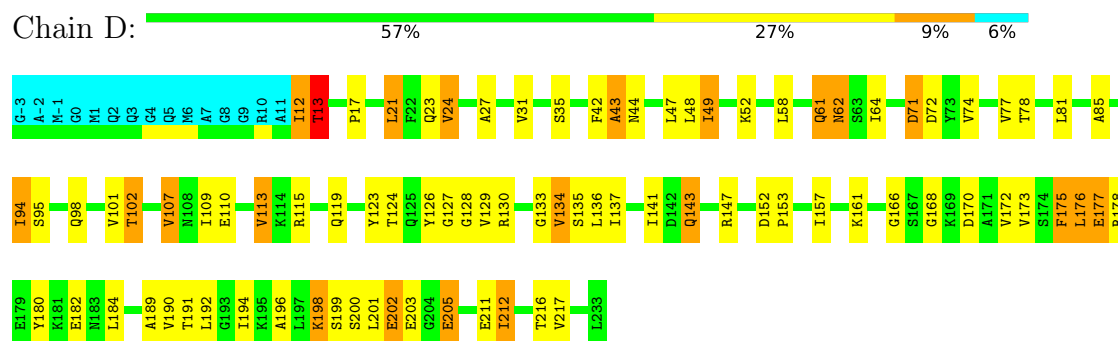
• Molecule 1: Proteasome subunit alpha



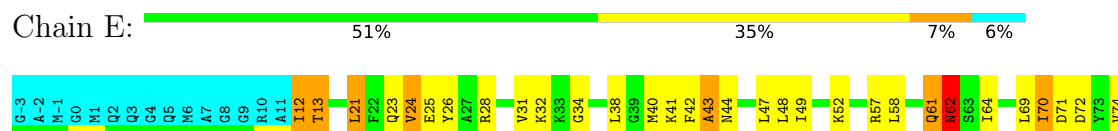
• Molecule 1: Proteasome subunit alpha

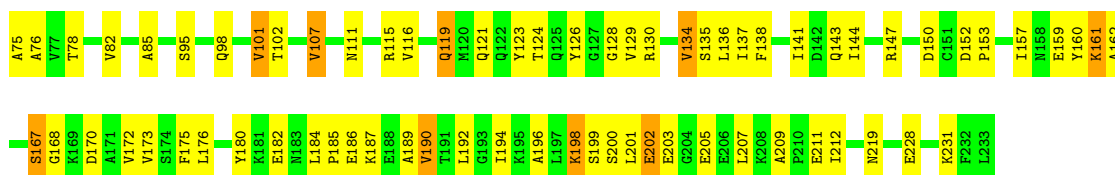


• Molecule 1: Proteasome subunit alpha



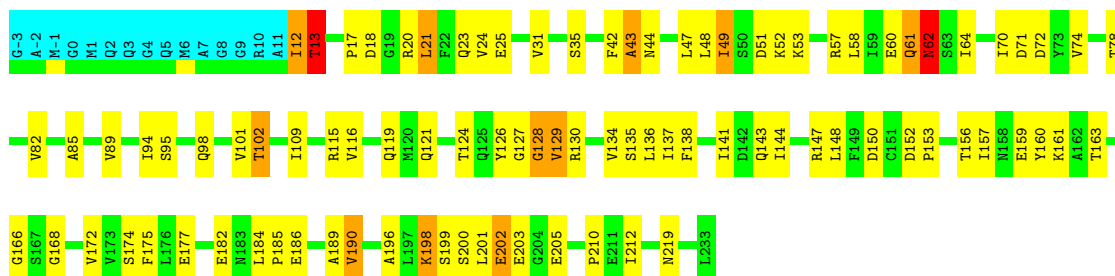
• Molecule 1: Proteasome subunit alpha





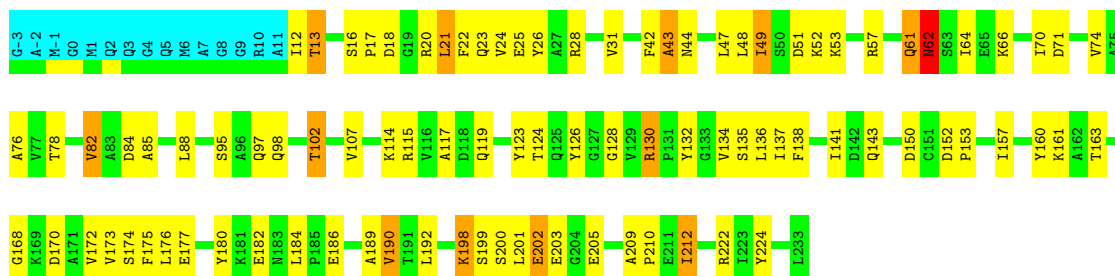
- Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



- Molecule 1: Proteasome subunit alpha

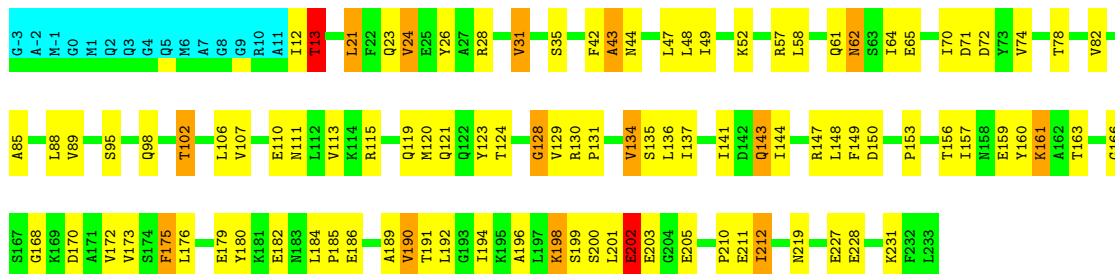
Chain G: 54% 34% 5% 6%



4.2.48 Score per residue for model 48

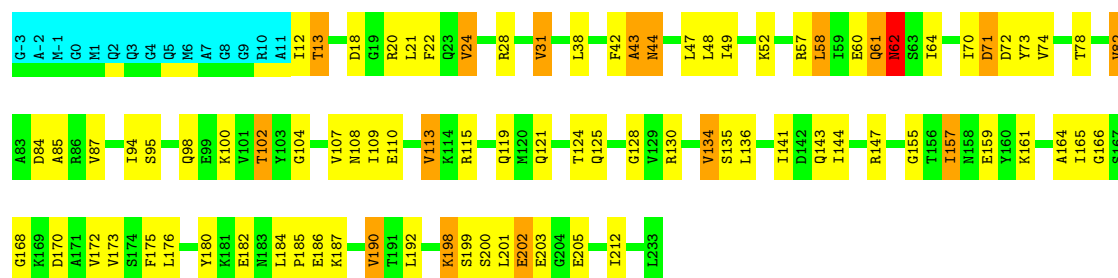
- Molecule 1: Proteasome subunit alpha

Chain A: 51% 35% 6% 6%



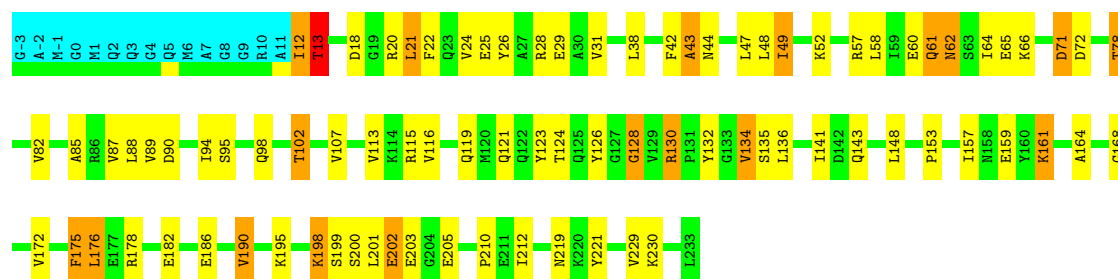
- Molecule 1: Proteasome subunit alpha

Chain B: 57% 30% 7% 6%



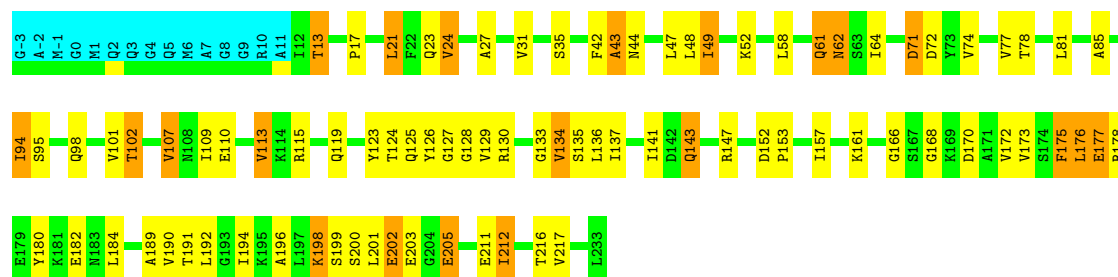
• Molecule 1: Proteasome subunit alpha

Chain C: 57% 28% 8% 6%



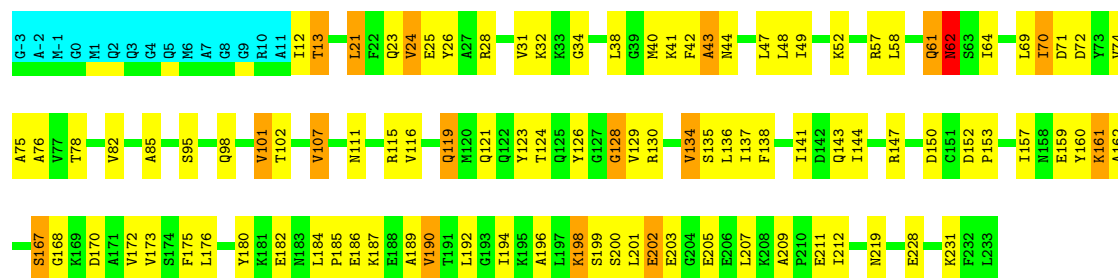
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 9% 6%



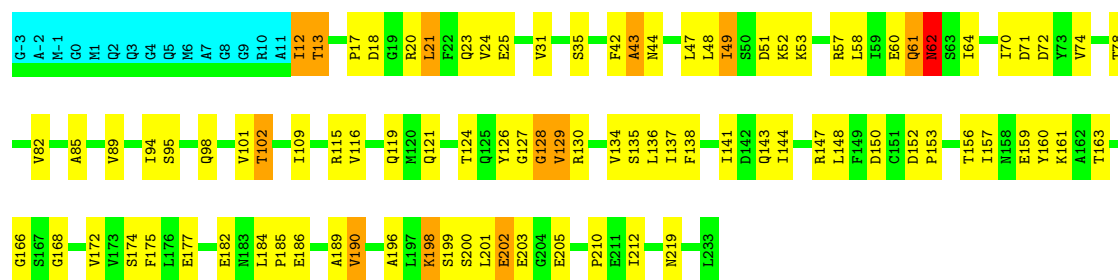
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 7% 6%



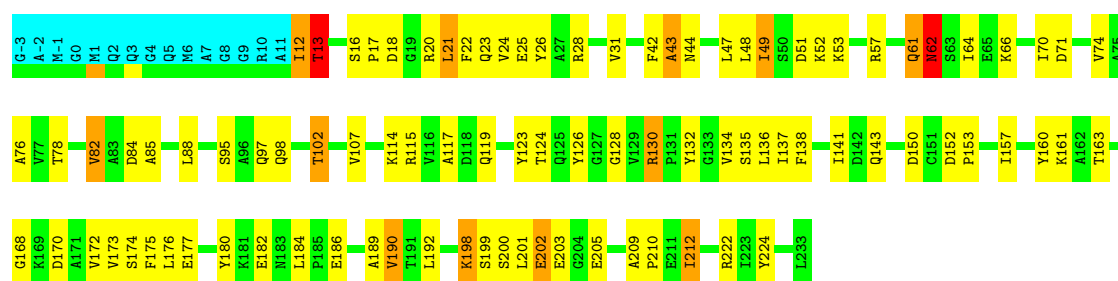
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



- Molecule 1: Proteasome subunit alpha

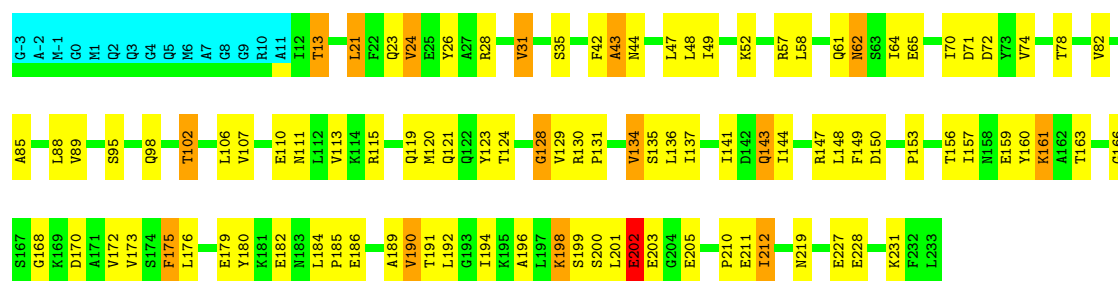
Chain G: 54% 33% 5% • 6%



4.2.49 Score per residue for model 49

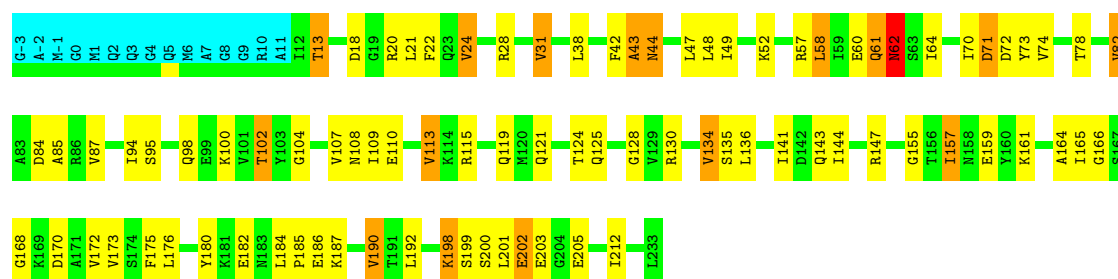
- Molecule 1: Proteasome subunit alpha

Chain A: 52% 35% 6% 6%

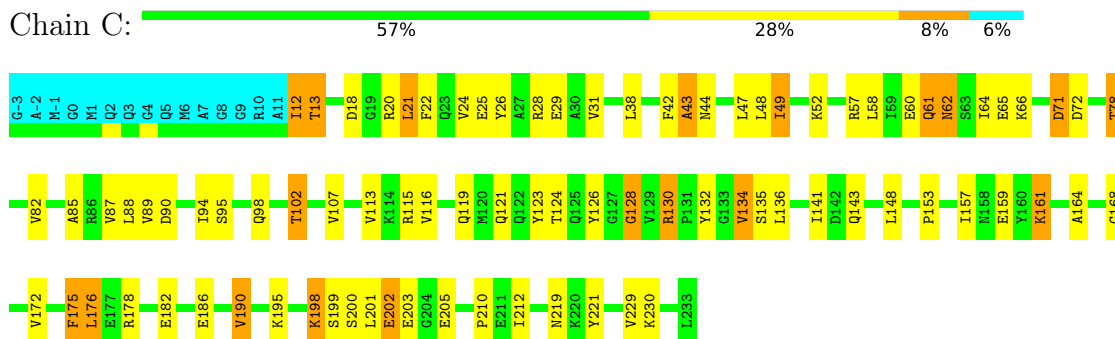


- Molecule 1: Proteasome subunit alpha

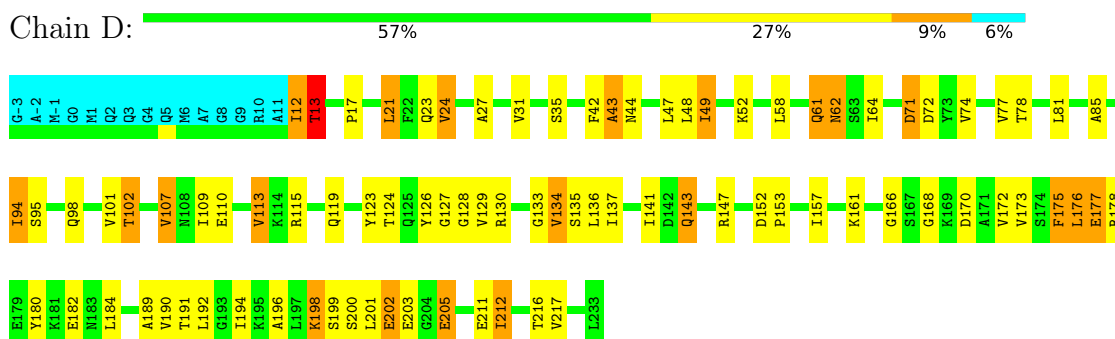
Chain B: 57% 29% 7% 6%



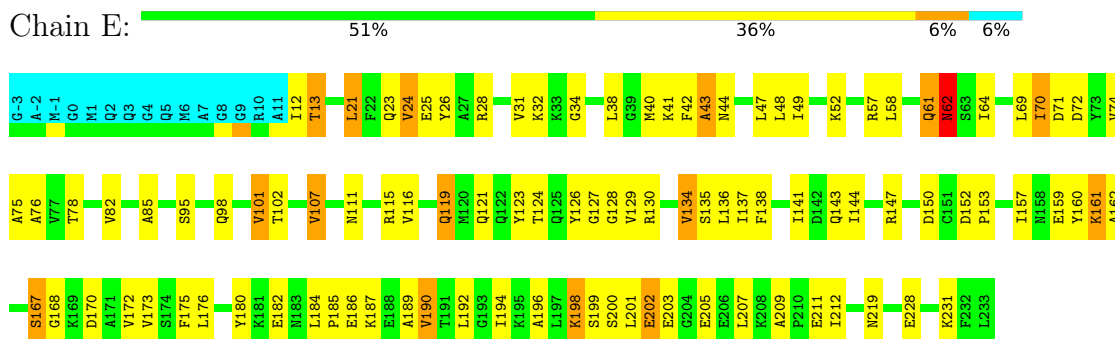
- Molecule 1: Proteasome subunit alpha



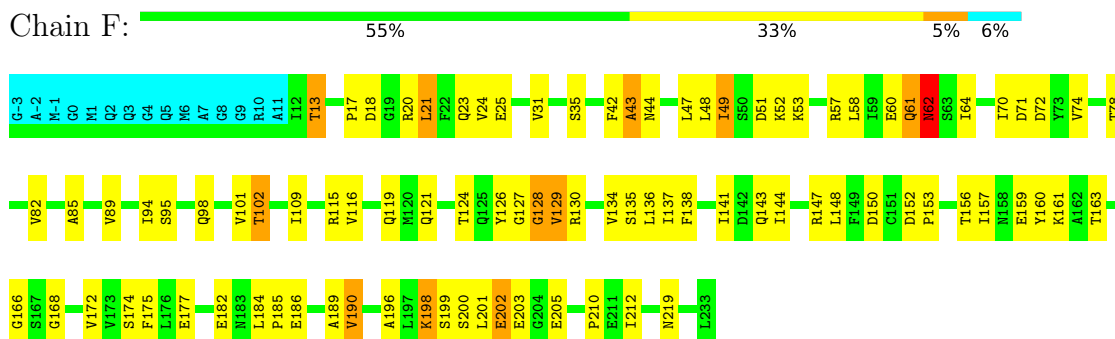
- Molecule 1: Proteasome subunit alpha



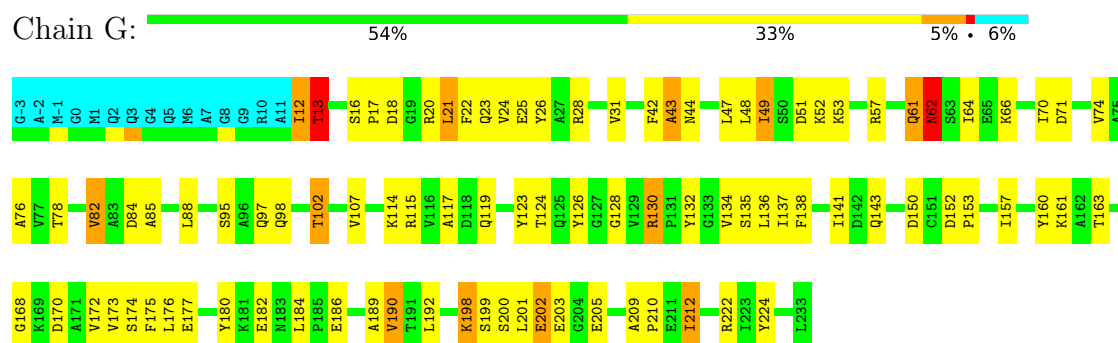
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

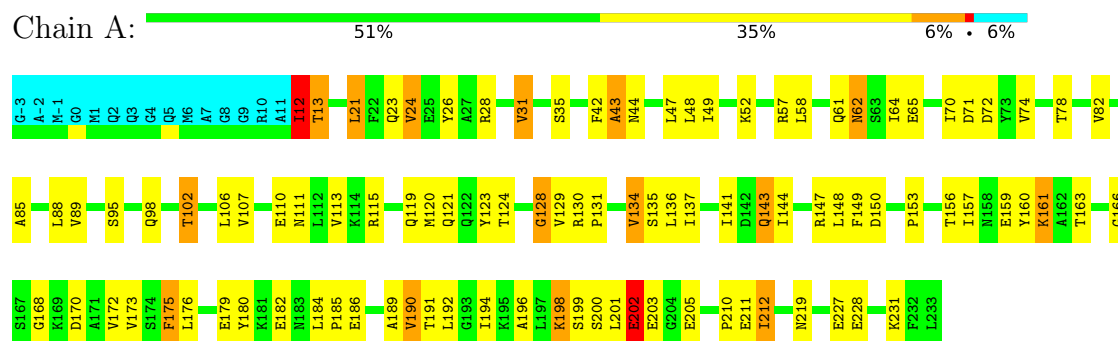


- Molecule 1: Proteasome subunit alpha

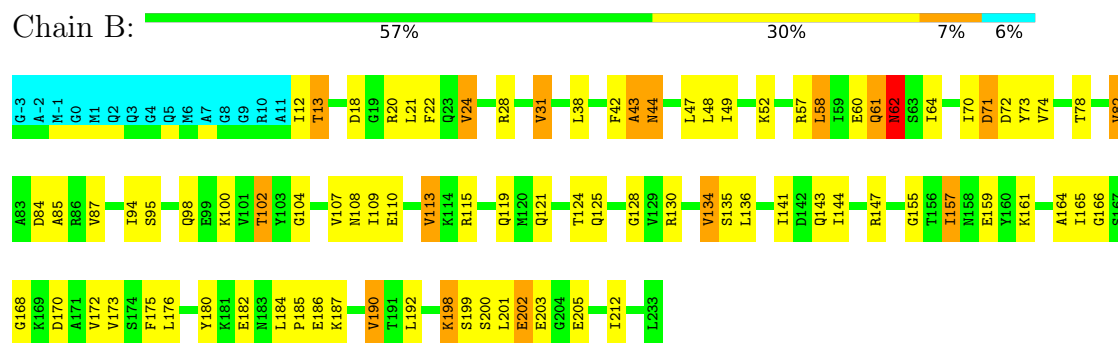


4.2.50 Score per residue for model 50

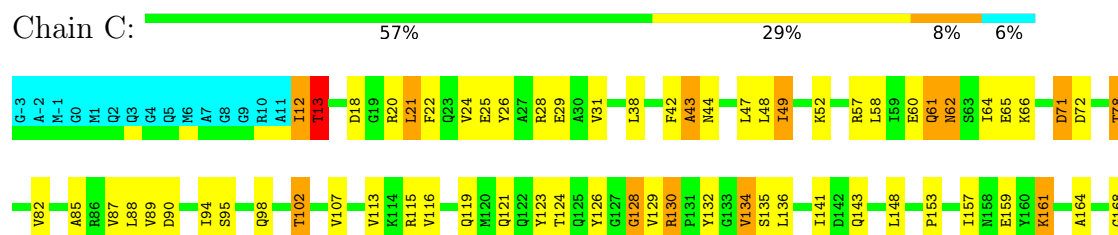
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



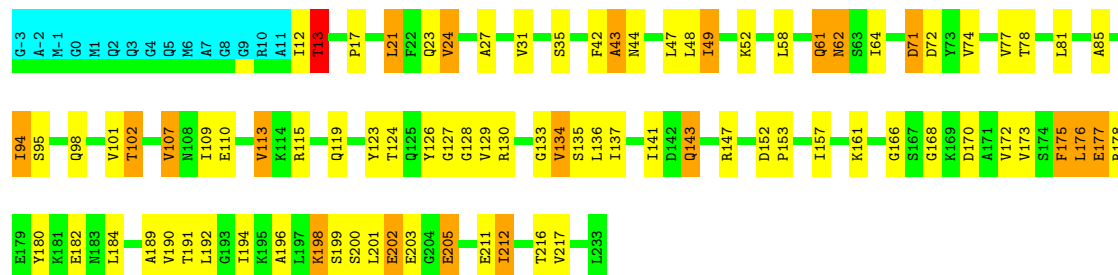
- Molecule 1: Proteasome subunit alpha





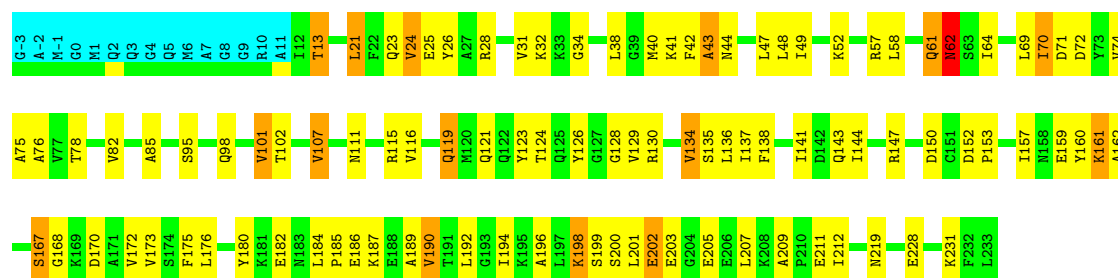
• Molecule 1: Proteasome subunit alpha

Chain D: 57% 27% 8% 6%



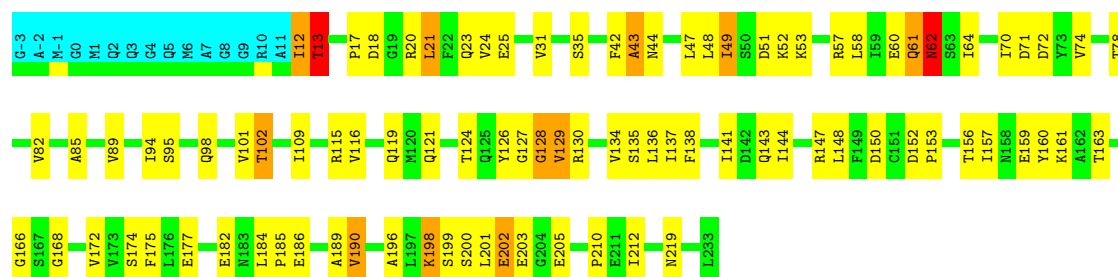
• Molecule 1: Proteasome subunit alpha

Chain E: 51% 35% 6% 6%



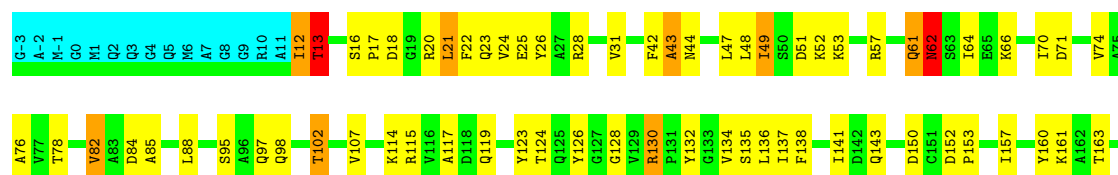
• Molecule 1: Proteasome subunit alpha

Chain F: 55% 33% 5% 6%



• Molecule 1: Proteasome subunit alpha

Chain G: 54% 33% 5% 6%



G168	K169	D170	A171	V172	S173	S174	F175	L176	E177	Y180	K181	E182	R183	L184	P185	E186	A189	V190	T191	L192	K198	S199	S200	L201	E202	E203	G204	E205	A209	P210	E211	I212	R222	I223	Y224	L233
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 166 calculated structures, 50 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	2.23
X-PLOR NIH	refinement	2.23

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 (average) 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	0.63±0.00	0±0/1751 (0.0± 0.0%)	0.99±0.00	6±0/2359 (0.3± 0.0%)
1	B	0.66±0.00	0±0/1751 (0.0± 0.0%)	1.04±0.00	5±0/2359 (0.2± 0.0%)
1	C	0.66±0.00	0±0/1751 (0.0± 0.0%)	1.04±0.00	11±0/2359 (0.5± 0.0%)
1	D	0.67±0.00	0±0/1751 (0.0± 0.0%)	1.01±0.00	6±0/2359 (0.3± 0.0%)
1	E	0.66±0.00	0±0/1751 (0.0± 0.0%)	1.03±0.00	8±0/2359 (0.3± 0.0%)
1	F	0.65±0.00	0±0/1751 (0.0± 0.0%)	1.04±0.00	7±0/2359 (0.3± 0.0%)
1	G	0.65±0.00	0±0/1751 (0.0± 0.0%)	1.03±0.00	7±0/2359 (0.3± 0.0%)
All	All	0.65	0/612850 (0.0%)	1.03	2506/825650 (0.3%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	F	161	LYS	N-CA-C	-11.21	98.21	112.90	1	50
1	C	203	GLU	N-CA-C	-10.53	98.96	112.23	1	50
1	E	203	GLU	N-CA-C	-10.21	99.36	112.23	1	50
1	F	203	GLU	N-CA-C	-10.10	99.51	112.23	1	50
1	B	203	GLU	N-CA-C	-10.09	99.52	112.23	1	50
1	B	161	LYS	N-CA-C	-10.01	101.19	113.41	1	50
1	G	203	GLU	N-CA-C	-9.96	100.26	111.82	1	50
1	A	203	GLU	N-CA-C	-9.88	100.35	111.82	1	50
1	D	203	GLU	N-CA-C	-9.64	100.09	112.23	1	50
1	G	161	LYS	N-CA-C	-9.42	101.92	113.41	1	50
1	D	161	LYS	N-CA-C	-9.04	102.38	113.41	1	50
1	C	161	LYS	N-CA-C	-8.69	102.81	113.50	1	50
1	E	70	ILE	N-CA-C	-8.66	104.30	112.96	1	50
1	A	161	LYS	N-CA-C	-8.42	103.14	113.41	1	50
1	E	161	LYS	N-CA-C	-7.27	103.37	112.90	1	50
1	G	126	TYR	N-CA-C	7.07	121.67	110.70	1	50
1	C	219	ASN	N-CA-C	6.58	116.97	108.34	1	50
1	A	57	ARG	N-CA-C	-6.55	104.76	112.89	1	50

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	126	TYR	N-CA-C	6.53	120.82	110.70	1	50
1	C	57	ARG	N-CA-C	-6.40	104.96	112.89	1	50
1	G	57	ARG	N-CA-C	-6.38	104.42	111.82	1	50
1	B	57	ARG	N-CA-C	-6.36	104.44	111.82	1	50
1	E	107	VAL	N-CA-C	6.26	116.41	110.53	1	50
1	C	82	VAL	N-CA-C	6.13	117.61	110.62	1	50
1	F	57	ARG	N-CA-C	-6.03	104.64	112.23	1	50
1	F	219	ASN	N-CA-C	5.89	116.86	108.74	1	50
1	C	78	THR	N-CA-C	5.81	118.24	109.41	1	50
1	E	119	GLN	N-CA-C	-5.72	104.95	111.07	1	50
1	E	57	ARG	N-CA-C	-5.71	105.81	112.89	1	50
1	D	107	VAL	N-CA-C	5.70	115.89	110.42	1	50
1	D	126	TYR	N-CA-C	5.67	122.88	110.80	1	50
1	C	13	THR	N-CA-C	-5.67	106.17	112.57	30	2
1	C	128	GLY	N-CA-C	5.62	126.49	113.18	1	50
1	A	219	ASN	N-CA-C	5.59	116.45	108.74	1	50
1	A	179	GLU	N-CA-C	5.52	119.12	112.93	1	50
1	F	126	TYR	N-CA-C	5.49	122.49	110.80	1	50
1	D	130	ARG	CA-C-N	5.44	126.64	119.84	1	50
1	D	130	ARG	C-N-CA	5.44	126.64	119.84	1	50
1	C	195	LYS	N-CA-C	-5.35	105.36	111.14	1	50
1	C	130	ARG	CA-C-N	5.35	125.64	119.92	1	50
1	C	130	ARG	C-N-CA	5.35	125.64	119.92	1	50
1	F	127	GLY	N-CA-C	5.33	120.93	111.02	1	50
1	A	128	GLY	N-CA-C	5.32	125.78	113.18	1	50
1	E	13	THR	N-CA-C	-5.30	105.50	112.72	43	1
1	B	155	GLY	N-CA-C	-5.30	107.91	115.64	1	50
1	G	70	ILE	N-CA-C	-5.24	105.69	113.39	1	50
1	A	13	THR	N-CA-C	-5.17	107.49	112.97	46	2
1	E	126	TYR	N-CA-C	5.15	121.77	110.80	1	50
1	E	219	ASN	N-CA-C	5.14	116.11	108.86	1	50
1	D	13	THR	N-CA-C	-5.08	104.42	110.41	34	1
1	G	130	ARG	N-CA-C	5.07	116.04	109.65	1	50
1	G	82	VAL	N-CA-C	5.06	115.68	110.36	1	50
1	B	82	VAL	N-CA-C	5.03	115.64	110.36	1	50
1	F	82	VAL	N-CA-C	5.00	115.61	110.36	1	50

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1728	1765	1765	61±1
1	B	1728	1765	1765	52±2
1	C	1728	1765	1765	42±1
1	D	1728	1765	1765	50±1
1	E	1728	1765	1765	58±1
1	F	1728	1765	1765	58±1
1	G	1728	1765	1765	51±1
All	All	604800	617750	617750	17309

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ILE:HD12	1:A:12:ILE:N	0.77	1.94	4	2
1:F:12:ILE:HD13	1:F:12:ILE:H	0.76	1.39	21	1
1:A:52:LYS:NZ	1:A:62:ASN:HA	0.76	1.96	1	50
1:C:12:ILE:HD13	1:C:12:ILE:H	0.74	1.41	50	2
1:A:12:ILE:HD12	1:A:12:ILE:O	0.73	1.83	6	10
1:A:186:GLU:O	1:A:190:VAL:HG12	0.73	1.84	1	50
1:F:124:THR:HG22	1:G:130:ARG:HH21	0.72	1.44	1	50
1:B:18:ASP:OD2	1:B:20:ARG:HD3	0.71	1.85	1	50
1:E:124:THR:HG22	1:F:130:ARG:HH21	0.71	1.45	1	50
1:E:12:ILE:O	1:E:12:ILE:HD12	0.71	1.85	7	2
1:F:12:ILE:HD11	1:F:127:GLY:O	0.71	1.85	34	2
1:C:12:ILE:HD11	1:C:129:VAL:H	0.71	1.46	50	1
1:B:12:ILE:HG22	1:B:12:ILE:O	0.71	1.85	16	9
1:G:168:GLY:O	1:G:172:VAL:HG12	0.71	1.85	1	50
1:A:12:ILE:C	1:A:12:ILE:HD13	0.69	2.13	15	1
1:B:12:ILE:HD13	1:B:12:ILE:N	0.69	2.02	1	4
1:F:21:LEU:O	1:F:24:VAL:HG12	0.69	1.87	1	50
1:D:135:SER:OG	1:D:153:PRO:HD3	0.68	1.88	1	50
1:F:12:ILE:HD13	1:F:12:ILE:N	0.68	2.04	21	1
1:A:168:GLY:O	1:A:172:VAL:HG12	0.67	1.89	1	50
1:D:12:ILE:HD12	1:D:12:ILE:O	0.67	1.88	20	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:12:ILE:HD13	1:E:12:ILE:C	0.67	2.15	39	4
1:A:12:ILE:C	1:A:13:THR:HG22	0.66	2.16	44	31
1:C:52:LYS:NZ	1:C:62:ASN:HA	0.66	2.04	1	50
1:C:12:ILE:HD13	1:C:12:ILE:N	0.66	2.06	50	2
1:E:52:LYS:NZ	1:E:62:ASN:HA	0.65	2.06	1	50
1:A:12:ILE:HD11	1:A:127:GLY:O	0.65	1.91	1	2
1:F:52:LYS:NZ	1:F:62:ASN:HA	0.65	2.06	1	50
1:G:21:LEU:O	1:G:24:VAL:HG12	0.65	1.92	1	50
1:C:12:ILE:C	1:C:13:THR:HG22	0.65	2.17	4	17
1:A:124:THR:HG22	1:B:130:ARG:HH21	0.65	1.50	1	50
1:C:98:GLN:O	1:C:102:THR:HG22	0.65	1.91	1	50
1:F:198:LYS:O	1:F:202:GLU:HB2	0.64	1.92	1	50
1:E:12:ILE:HG23	1:E:13:THR:N	0.64	2.08	11	6
1:E:12:ILE:HG23	1:E:13:THR:H	0.64	1.53	32	5
1:B:42:PHE:HB2	1:B:184:LEU:O	0.64	1.92	1	50
1:C:135:SER:OG	1:C:153:PRO:HD3	0.64	1.92	1	50
1:A:12:ILE:HG21	1:A:129:VAL:O	0.64	1.93	43	2
1:E:21:LEU:HD11	1:F:130:ARG:HD2	0.63	1.68	1	50
1:A:78:THR:HG21	1:A:85:ALA:HB1	0.63	1.70	1	50
1:C:198:LYS:O	1:C:202:GLU:HB2	0.63	1.94	1	50
1:G:95:SER:OG	1:G:115:ARG:HD3	0.62	1.94	1	50
1:E:12:ILE:HD13	1:E:12:ILE:O	0.62	1.94	14	4
1:E:13:THR:HG23	1:E:13:THR:O	0.62	1.94	20	28
1:G:198:LYS:O	1:G:202:GLU:HB2	0.62	1.95	1	50
1:D:52:LYS:NZ	1:D:62:ASN:HA	0.62	2.10	1	50
1:B:12:ILE:N	1:B:12:ILE:HD12	0.61	2.10	2	13
1:C:21:LEU:O	1:C:25:GLU:HG2	0.61	1.95	1	50
1:D:12:ILE:O	1:D:13:THR:HG22	0.61	1.95	29	2
1:B:168:GLY:O	1:B:172:VAL:HG12	0.61	1.95	1	50
1:F:186:GLU:O	1:F:190:VAL:HG12	0.61	1.95	1	50
1:F:12:ILE:HD12	1:F:12:ILE:O	0.61	1.96	37	3
1:A:198:LYS:O	1:A:202:GLU:HB2	0.61	1.96	1	50
1:D:198:LYS:O	1:D:202:GLU:HB2	0.61	1.95	1	50
1:G:12:ILE:HD13	1:G:13:THR:N	0.61	2.10	10	1
1:F:121:GLN:O	1:F:124:THR:HB	0.61	1.96	1	50
1:A:61:GLN:O	1:A:64:ILE:HG22	0.60	1.95	1	50
1:E:168:GLY:O	1:E:172:VAL:HG12	0.60	1.96	1	50
1:G:12:ILE:HG23	1:G:12:ILE:O	0.60	1.97	47	4
1:G:12:ILE:C	1:G:13:THR:HG22	0.60	2.20	34	25
1:E:186:GLU:O	1:E:190:VAL:HG12	0.60	1.96	1	50
1:F:52:LYS:HZ1	1:F:62:ASN:HA	0.60	1.56	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:12:ILE:C	1:E:13:THR:HG22	0.60	2.22	23	6
1:E:198:LYS:O	1:E:202:GLU:HB2	0.60	1.97	1	50
1:E:21:LEU:O	1:E:24:VAL:HG12	0.59	1.98	1	50
1:F:12:ILE:C	1:F:13:THR:HG22	0.59	2.21	42	28
1:B:78:THR:HG21	1:B:85:ALA:HB1	0.59	1.74	1	50
1:G:61:GLN:O	1:G:64:ILE:HG22	0.59	1.96	1	50
1:D:12:ILE:C	1:D:13:THR:HG22	0.59	2.22	8	29
1:G:12:ILE:O	1:G:13:THR:HG22	0.59	1.97	9	1
1:C:61:GLN:O	1:C:64:ILE:HG22	0.58	1.98	1	50
1:E:13:THR:O	1:E:13:THR:CG2	0.58	2.51	30	29
1:F:135:SER:OG	1:F:153:PRO:HD3	0.58	1.98	1	50
1:F:52:LYS:HE3	1:F:64:ILE:HG23	0.58	1.75	1	50
1:G:13:THR:HG23	1:G:13:THR:O	0.58	1.99	45	20
1:C:12:ILE:C	1:C:12:ILE:HD12	0.58	2.23	48	9
1:A:184:LEU:HD23	1:A:189:ALA:HA	0.58	1.75	1	50
1:B:12:ILE:N	1:B:12:ILE:CD1	0.58	2.66	33	11
1:F:21:LEU:HD11	1:G:130:ARG:HD2	0.58	1.76	1	50
1:F:168:GLY:O	1:F:172:VAL:HG12	0.58	1.99	1	50
1:G:52:LYS:NZ	1:G:62:ASN:HA	0.58	2.14	1	50
1:C:21:LEU:O	1:C:24:VAL:HG12	0.57	2.00	1	50
1:B:94:ILE:HG13	1:B:95:SER:N	0.57	2.14	1	50
1:B:186:GLU:O	1:B:190:VAL:HG12	0.57	1.99	1	50
1:A:121:GLN:O	1:A:124:THR:HB	0.57	2.00	1	50
1:C:52:LYS:HZ3	1:C:62:ASN:HA	0.57	1.60	1	50
1:A:52:LYS:HZ1	1:A:62:ASN:HA	0.57	1.59	1	50
1:D:78:THR:HG21	1:D:85:ALA:HB1	0.57	1.75	1	50
1:C:52:LYS:HA	1:C:66:LYS:HZ2	0.57	1.59	2	50
1:D:13:THR:O	1:D:13:THR:HG23	0.57	2.00	24	10
1:F:12:ILE:HD12	1:F:12:ILE:N	0.57	2.14	31	1
1:B:13:THR:HG23	1:B:13:THR:O	0.56	2.00	23	3
1:D:124:THR:HG22	1:E:130:ARG:HH21	0.56	1.58	1	50
1:E:170:ASP:O	1:E:173:VAL:HG12	0.56	1.99	1	50
1:D:13:THR:O	1:D:13:THR:CG2	0.56	2.53	17	10
1:F:78:THR:HG21	1:F:85:ALA:HB1	0.56	1.76	1	50
1:F:18:ASP:OD2	1:F:20:ARG:HD3	0.56	2.00	1	50
1:F:124:THR:HG22	1:G:130:ARG:NH2	0.56	2.16	1	50
1:C:13:THR:HG23	1:C:13:THR:O	0.56	2.01	33	23
1:D:61:GLN:O	1:D:64:ILE:HG22	0.56	2.00	1	50
1:F:12:ILE:HD12	1:F:12:ILE:C	0.56	2.25	18	1
1:A:49:ILE:HD12	1:A:211:GLU:O	0.56	2.01	1	50
1:A:88:LEU:HD21	1:A:120:MET:SD	0.56	2.41	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:186:GLU:O	1:C:190:VAL:HG12	0.56	2.01	1	50
1:E:13:THR:CG2	1:E:13:THR:O	0.56	2.54	22	2
1:A:61:GLN:OE1	1:A:62:ASN:HB3	0.55	2.01	1	50
1:A:12:ILE:HD11	1:G:13:THR:O	0.55	2.01	34	1
1:F:12:ILE:N	1:F:12:ILE:CD1	0.55	2.69	21	1
1:D:175:PHE:CD1	1:D:175:PHE:C	0.55	2.83	1	50
1:F:13:THR:HG23	1:F:13:THR:O	0.55	2.00	20	9
1:D:24:VAL:O	1:D:27:ALA:HB3	0.55	2.02	1	50
1:G:170:ASP:O	1:G:173:VAL:HG12	0.55	2.01	1	50
1:A:159:GLU:HG2	1:B:60:GLU:HG3	0.55	1.79	1	50
1:B:198:LYS:O	1:B:202:GLU:HB2	0.55	2.01	1	50
1:G:12:ILE:C	1:G:12:ILE:HD12	0.55	2.26	44	24
1:G:98:GLN:O	1:G:102:THR:HG22	0.55	2.01	1	50
1:E:13:THR:O	1:E:13:THR:HG23	0.55	2.00	22	3
1:C:12:ILE:HG23	1:C:12:ILE:O	0.55	2.02	23	2
1:C:168:GLY:O	1:C:172:VAL:HG12	0.55	2.02	1	50
1:C:52:LYS:HA	1:C:66:LYS:NZ	0.55	2.17	1	50
1:E:69:LEU:HD23	1:E:75:ALA:HB2	0.55	1.79	1	50
1:E:12:ILE:O	1:E:13:THR:HG22	0.55	2.02	23	7
1:A:42:PHE:HD1	1:A:43:ALA:N	0.54	2.00	1	50
1:F:61:GLN:O	1:F:64:ILE:HG22	0.54	2.01	1	50
1:B:12:ILE:HD12	1:B:12:ILE:H	0.54	1.63	50	2
1:C:175:PHE:C	1:C:175:PHE:CD1	0.54	2.85	1	50
1:D:12:ILE:HD12	1:D:12:ILE:C	0.54	2.27	11	5
1:F:184:LEU:HD23	1:F:189:ALA:HA	0.54	1.77	1	50
1:G:13:THR:O	1:G:13:THR:CG2	0.54	2.55	33	20
1:A:175:PHE:CD1	1:A:175:PHE:C	0.54	2.84	1	50
1:B:12:ILE:O	1:B:12:ILE:CG2	0.54	2.56	16	9
1:E:121:GLN:O	1:E:124:THR:HB	0.54	2.03	1	50
1:A:12:ILE:N	1:A:12:ILE:CD1	0.54	2.66	4	2
1:A:12:ILE:CD1	1:G:13:THR:O	0.54	2.55	34	1
1:A:28:ARG:O	1:A:31:VAL:HG22	0.54	2.02	1	50
1:F:95:SER:OG	1:F:115:ARG:HD3	0.54	2.03	1	50
1:F:148:LEU:O	1:F:159:GLU:HG3	0.54	2.03	1	50
1:D:12:ILE:O	1:D:12:ILE:CD1	0.54	2.56	36	6
1:E:95:SER:OG	1:E:115:ARG:HD3	0.54	2.03	1	50
1:B:12:ILE:HD13	1:B:129:VAL:O	0.54	2.03	41	2
1:A:12:ILE:N	1:A:12:ILE:HD13	0.53	2.18	29	2
1:D:13:THR:OG1	1:E:130:ARG:N	0.53	2.41	18	40
1:B:13:THR:O	1:B:13:THR:CG2	0.53	2.56	3	3
1:C:12:ILE:HD12	1:C:12:ILE:O	0.53	2.04	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:42:PHE:HB2	1:F:184:LEU:O	0.53	2.03	1	50
1:A:135:SER:OG	1:A:153:PRO:HD3	0.53	2.04	1	50
1:B:84:ASP:O	1:B:87:VAL:HG12	0.53	2.02	1	50
1:E:12:ILE:HD11	1:E:123:TYR:O	0.53	2.04	7	1
1:F:137:ILE:HG22	1:F:150:ASP:HB2	0.53	1.78	1	50
1:F:175:PHE:CD1	1:F:175:PHE:C	0.53	2.87	1	50
1:B:52:LYS:HE3	1:B:64:ILE:HG23	0.53	1.81	1	50
1:C:49:ILE:HD11	1:C:210:PRO:HB3	0.53	1.80	1	50
1:E:52:LYS:HZ3	1:E:62:ASN:HA	0.53	1.64	1	50
1:C:13:THR:O	1:C:13:THR:CG2	0.53	2.57	18	23
1:A:35:SER:O	1:A:166:GLY:HA3	0.52	2.03	1	50
1:E:175:PHE:CD2	1:E:196:ALA:HA	0.52	2.39	1	50
1:B:175:PHE:CD1	1:B:175:PHE:C	0.52	2.88	1	50
1:A:42:PHE:CD1	1:A:43:ALA:N	0.52	2.78	1	50
1:E:180:TYR:HA	1:E:192:LEU:HD21	0.52	1.80	1	50
1:E:61:GLN:O	1:E:64:ILE:HG22	0.52	2.05	1	50
1:E:78:THR:HG21	1:E:85:ALA:HB1	0.52	1.81	1	50
1:F:12:ILE:O	1:F:13:THR:HG22	0.52	2.04	48	4
1:A:21:LEU:HD11	1:B:130:ARG:HD2	0.52	1.79	1	50
1:F:98:GLN:O	1:F:102:THR:HG22	0.52	2.04	1	50
1:F:13:THR:O	1:F:13:THR:CG2	0.52	2.58	7	9
1:B:43:ALA:HB2	1:B:185:PRO:HA	0.52	1.82	1	50
1:G:76:ALA:HB2	1:G:138:PHE:CD1	0.52	2.40	1	50
1:A:12:ILE:HD12	1:A:12:ILE:C	0.52	2.30	7	5
1:D:94:ILE:HG13	1:D:95:SER:N	0.52	2.20	1	50
1:E:124:THR:HG22	1:F:130:ARG:NH2	0.52	2.18	1	50
1:F:42:PHE:HD1	1:F:43:ALA:N	0.52	2.03	1	50
1:E:144:ILE:HD12	1:E:147:ARG:NH1	0.52	2.19	1	50
1:B:13:THR:O	1:C:12:ILE:HD11	0.52	2.05	5	1
1:C:13:THR:O	1:C:13:THR:OG1	0.51	2.25	7	21
1:F:13:THR:CG2	1:F:13:THR:O	0.51	2.57	2	2
1:E:12:ILE:C	1:E:12:ILE:HD12	0.51	2.30	25	2
1:E:12:ILE:O	1:E:12:ILE:CD1	0.51	2.58	14	2
1:A:12:ILE:C	1:A:12:ILE:CD1	0.51	2.84	15	1
1:G:78:THR:HG21	1:G:85:ALA:HB1	0.51	1.82	1	50
1:G:175:PHE:CD1	1:G:175:PHE:C	0.51	2.88	1	50
1:F:13:THR:O	1:F:13:THR:HG23	0.51	2.05	2	2
1:D:49:ILE:HD12	1:D:211:GLU:O	0.51	2.05	1	50
1:E:70:ILE:HD12	1:E:74:VAL:HG22	0.51	1.82	1	50
1:F:13:THR:O	1:F:13:THR:OG1	0.51	2.26	34	30
1:G:42:PHE:HB2	1:G:184:LEU:O	0.51	2.06	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:121:GLN:O	1:B:124:THR:HB	0.51	2.06	1	50
1:C:198:LYS:O	1:C:199:SER:C	0.51	2.54	1	50
1:A:52:LYS:HZ3	1:A:62:ASN:HA	0.51	1.66	1	50
1:F:85:ALA:O	1:F:89:VAL:HG23	0.51	2.06	1	50
1:D:175:PHE:C	1:D:175:PHE:HD1	0.50	2.14	1	50
1:E:123:TYR:CD1	1:E:123:TYR:N	0.50	2.78	1	50
1:D:12:ILE:O	1:D:13:THR:CG2	0.50	2.58	29	2
1:B:12:ILE:C	1:B:13:THR:HG22	0.50	2.30	39	2
1:D:12:ILE:C	1:D:12:ILE:HD12	0.50	2.32	13	21
1:A:13:THR:O	1:A:13:THR:OG1	0.50	2.27	11	26
1:D:198:LYS:O	1:D:199:SER:C	0.50	2.54	1	50
1:F:175:PHE:CD2	1:F:196:ALA:HA	0.50	2.41	1	50
1:A:13:THR:HG23	1:A:13:THR:O	0.50	2.06	1	1
1:B:109:ILE:CG2	1:B:147:ARG:HD3	0.50	2.37	1	50
1:E:52:LYS:HE3	1:E:64:ILE:HG23	0.50	1.82	1	50
1:E:12:ILE:CG2	1:E:13:THR:N	0.50	2.74	11	3
1:G:12:ILE:HD13	1:G:13:THR:H	0.50	1.64	10	1
1:E:12:ILE:C	1:E:12:ILE:CD1	0.50	2.84	39	4
1:D:12:ILE:O	1:D:13:THR:CB	0.50	2.59	29	10
1:E:12:ILE:O	1:E:13:THR:CB	0.50	2.59	23	5
1:D:170:ASP:O	1:D:173:VAL:HG12	0.50	2.07	1	50
1:F:12:ILE:HG23	1:F:12:ILE:O	0.50	2.07	43	1
1:A:95:SER:OG	1:A:115:ARG:HD3	0.49	2.07	1	50
1:B:198:LYS:O	1:B:199:SER:C	0.49	2.55	1	50
1:B:198:LYS:HG2	1:B:202:GLU:HG2	0.49	1.82	1	50
1:F:12:ILE:C	1:F:12:ILE:HD12	0.49	2.31	29	14
1:G:52:LYS:HB3	1:G:209:ALA:O	0.49	2.05	1	50
1:G:186:GLU:O	1:G:190:VAL:HG12	0.49	2.06	1	50
1:B:13:THR:OG1	1:C:12:ILE:CD1	0.49	2.60	5	1
1:E:12:ILE:O	1:E:12:ILE:CG1	0.49	2.59	30	2
1:F:12:ILE:HG23	1:F:127:GLY:O	0.49	2.06	15	1
1:A:49:ILE:HD11	1:A:210:PRO:HB3	0.49	1.85	1	50
1:G:21:LEU:O	1:G:25:GLU:HG2	0.49	2.08	1	50
1:B:61:GLN:O	1:B:64:ILE:HG22	0.49	2.08	1	50
1:C:26:TYR:O	1:C:29:GLU:HB2	0.49	2.06	1	50
1:A:12:ILE:O	1:A:12:ILE:CD1	0.49	2.59	19	6
1:E:12:ILE:O	1:E:12:ILE:HG23	0.49	2.06	40	4
1:A:175:PHE:C	1:A:175:PHE:HD1	0.49	2.15	1	50
1:E:134:VAL:CG2	1:E:135:SER:N	0.49	2.76	1	50
1:G:174:SER:O	1:G:177:GLU:HB3	0.49	2.08	1	50
1:B:95:SER:OG	1:B:115:ARG:HD3	0.49	2.08	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:42:PHE:CD1	1:F:43:ALA:N	0.49	2.81	1	50
1:G:42:PHE:HD1	1:G:43:ALA:N	0.49	2.04	1	50
1:D:12:ILE:O	1:D:12:ILE:CG1	0.49	2.60	36	3
1:A:42:PHE:HB2	1:A:184:LEU:O	0.48	2.08	1	50
1:E:187:LYS:O	1:E:190:VAL:HG13	0.48	2.08	1	50
1:G:42:PHE:CD1	1:G:43:ALA:N	0.48	2.81	1	50
1:A:12:ILE:C	1:A:12:ILE:HD12	0.48	2.32	13	5
1:A:14:VAL:HG23	1:A:14:VAL:O	0.48	2.08	29	1
1:A:13:THR:O	1:B:12:ILE:HD11	0.48	2.08	18	3
1:B:13:THR:O	1:B:13:THR:OG1	0.48	2.28	18	29
1:D:71:ASP:OD2	1:D:74:VAL:HG12	0.48	2.08	1	50
1:F:12:ILE:O	1:F:13:THR:CB	0.48	2.62	24	7
1:G:12:ILE:O	1:G:13:THR:CB	0.48	2.60	9	12
1:C:88:LEU:HD13	1:C:132:TYR:CD2	0.48	2.44	1	50
1:G:97:GLN:OE1	1:G:97:GLN:HA	0.48	2.07	1	50
1:A:13:THR:OG1	1:B:12:ILE:HD11	0.48	2.09	9	1
1:E:41:LYS:HE3	1:E:160:TYR:O	0.48	2.09	1	50
1:G:12:ILE:O	1:G:13:THR:CG2	0.48	2.61	9	1
1:C:12:ILE:O	1:C:13:THR:HG22	0.48	2.08	25	2
1:F:61:GLN:OE1	1:F:62:ASN:HB3	0.48	2.09	1	50
1:E:12:ILE:HG23	1:E:13:THR:HG22	0.48	1.85	15	2
1:E:12:ILE:CD1	1:E:129:VAL:O	0.48	2.61	11	2
1:A:12:ILE:O	1:A:13:THR:CB	0.48	2.61	41	9
1:B:165:ILE:HG13	1:B:166:GLY:N	0.48	2.24	1	50
1:G:180:TYR:HA	1:G:192:LEU:HD21	0.48	1.85	1	50
1:D:21:LEU:HD11	1:E:130:ARG:HD2	0.48	1.85	1	50
1:D:127:GLY:O	1:D:129:VAL:N	0.48	2.47	1	50
1:D:109:ILE:CG2	1:D:147:ARG:HD3	0.48	2.38	1	50
1:B:144:ILE:HD12	1:B:147:ARG:NH1	0.48	2.24	1	50
1:D:175:PHE:CD2	1:D:196:ALA:HA	0.48	2.44	1	50
1:E:12:ILE:HD13	1:E:13:THR:N	0.48	2.23	6	1
1:E:13:THR:O	1:E:13:THR:OG1	0.48	2.32	34	10
1:E:12:ILE:CG2	1:E:13:THR:H	0.47	2.21	11	1
1:A:13:THR:O	1:A:13:THR:CG2	0.47	2.62	1	1
1:D:134:VAL:CG2	1:D:135:SER:N	0.47	2.76	1	50
1:D:176:LEU:HB3	1:E:58:LEU:HD21	0.47	1.85	1	50
1:A:130:ARG:N	1:G:13:THR:OG1	0.47	2.47	44	28
1:A:144:ILE:HD12	1:A:147:ARG:NH1	0.47	2.24	1	50
1:C:78:THR:HG21	1:C:85:ALA:HB1	0.47	1.85	1	50
1:B:159:GLU:HG2	1:C:60:GLU:HG3	0.47	1.85	1	50
1:G:198:LYS:O	1:G:199:SER:C	0.47	2.56	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:94:ILE:CG1	1:B:95:SER:N	0.47	2.78	1	50
1:C:24:VAL:O	1:C:28:ARG:HG3	0.47	2.09	1	50
1:C:175:PHE:C	1:C:175:PHE:HD1	0.47	2.18	1	50
1:F:94:ILE:HG13	1:F:95:SER:N	0.47	2.24	1	50
1:A:143:GLN:HA	1:A:143:GLN:HE21	0.47	1.70	1	50
1:A:160:TYR:CD2	1:A:163:THR:HB	0.47	2.45	1	50
1:C:12:ILE:C	1:C:13:THR:CG2	0.47	2.88	32	7
1:D:81:LEU:HD23	1:D:133:GLY:HA3	0.47	1.85	1	50
1:F:21:LEU:O	1:F:25:GLU:HG2	0.47	2.09	1	50
1:F:137:ILE:HG22	1:F:150:ASP:CB	0.47	2.40	1	50
1:F:198:LYS:O	1:F:199:SER:C	0.47	2.57	1	50
1:G:61:GLN:OE1	1:G:62:ASN:HB3	0.47	2.09	1	50
1:G:160:TYR:CD2	1:G:163:THR:HB	0.47	2.44	1	50
1:D:13:THR:OG1	1:D:13:THR:O	0.47	2.31	22	11
1:F:144:ILE:HD12	1:F:147:ARG:NH1	0.47	2.24	1	50
1:G:135:SER:OG	1:G:153:PRO:HD3	0.47	2.10	1	50
1:D:14:VAL:O	1:D:14:VAL:HG13	0.47	2.10	36	2
1:C:12:ILE:N	1:C:12:ILE:CD1	0.47	2.75	50	1
1:B:58:LEU:N	1:B:58:LEU:CD1	0.47	2.78	1	50
1:D:110:GLU:O	1:D:113:VAL:HG13	0.47	2.10	1	50
1:B:165:ILE:HG13	1:B:166:GLY:H	0.46	1.70	1	50
1:G:137:ILE:HG22	1:G:150:ASP:HB2	0.46	1.86	1	50
1:A:21:LEU:O	1:A:24:VAL:HG12	0.46	2.10	1	50
1:G:18:ASP:OD2	1:G:20:ARG:HD3	0.46	2.11	1	50
1:C:12:ILE:O	1:C:13:THR:CB	0.46	2.62	25	4
1:A:85:ALA:O	1:A:89:VAL:HG23	0.46	2.11	1	50
1:C:42:PHE:O	1:C:43:ALA:C	0.46	2.59	1	50
1:E:21:LEU:O	1:E:25:GLU:HG2	0.46	2.09	1	50
1:D:49:ILE:HD13	1:D:212:ILE:HB	0.46	1.87	1	50
1:B:12:ILE:HG21	1:B:129:VAL:O	0.46	2.10	16	4
1:A:191:THR:O	1:A:194:ILE:HG22	0.46	2.11	1	50
1:E:34:GLY:O	1:E:167:SER:HB2	0.46	2.11	1	50
1:F:156:THR:HG23	1:G:82:VAL:HG11	0.46	1.88	1	50
1:E:12:ILE:O	1:E:13:THR:HB	0.46	2.11	41	2
1:D:98:GLN:O	1:D:102:THR:HG22	0.46	2.11	1	50
1:G:24:VAL:O	1:G:28:ARG:HG3	0.46	2.09	1	50
1:C:12:ILE:HD12	1:C:13:THR:N	0.46	2.25	48	1
1:A:198:LYS:O	1:A:199:SER:C	0.46	2.59	1	50
1:F:17:PRO:HA	1:G:26:TYR:CD1	0.46	2.46	1	50
1:F:35:SER:O	1:F:166:GLY:HA3	0.46	2.11	1	50
1:D:42:PHE:CD1	1:D:43:ALA:N	0.46	2.84	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:160:TYR:CD2	1:F:163:THR:HB	0.46	2.45	1	50
1:D:12:ILE:HD11	1:D:127:GLY:O	0.46	2.11	16	1
1:B:170:ASP:O	1:B:173:VAL:HG12	0.46	2.10	1	50
1:E:24:VAL:O	1:E:28:ARG:HG3	0.46	2.11	1	50
1:F:49:ILE:HD11	1:F:210:PRO:HB3	0.46	1.86	1	50
1:C:62:ASN:O	1:C:65:GLU:HG2	0.45	2.11	1	50
1:E:12:ILE:HD11	1:E:127:GLY:O	0.45	2.11	49	1
1:E:198:LYS:O	1:E:199:SER:C	0.45	2.58	1	50
1:E:12:ILE:O	1:E:12:ILE:HG13	0.45	2.09	30	1
1:A:26:TYR:CD1	1:G:17:PRO:HA	0.45	2.45	1	50
1:D:95:SER:OG	1:D:115:ARG:HD3	0.45	2.11	1	50
1:A:12:ILE:C	1:A:13:THR:CG2	0.45	2.90	37	8
1:A:198:LYS:HG2	1:A:202:GLU:HG2	0.45	1.88	1	50
1:D:184:LEU:HD23	1:D:189:ALA:HA	0.45	1.87	1	50
1:G:13:THR:O	1:G:13:THR:OG1	0.45	2.31	7	3
1:E:13:THR:OG1	1:F:130:ARG:N	0.45	2.50	29	1
1:A:70:ILE:HD12	1:A:74:VAL:HG22	0.45	1.88	1	50
1:B:198:LYS:CG	1:B:202:GLU:HG2	0.45	2.42	1	50
1:C:95:SER:OG	1:C:115:ARG:HD3	0.45	2.10	1	50
1:D:61:GLN:OE1	1:D:62:ASN:HB3	0.45	2.12	1	50
1:G:123:TYR:N	1:G:123:TYR:CD1	0.45	2.85	1	50
1:G:12:ILE:C	1:G:13:THR:CG2	0.45	2.89	34	7
1:E:12:ILE:C	1:E:13:THR:CG2	0.45	2.90	23	2
1:C:123:TYR:CD1	1:C:123:TYR:N	0.45	2.85	1	50
1:B:12:ILE:H	1:B:12:ILE:CD1	0.45	2.23	2	2
1:A:49:ILE:HD13	1:A:212:ILE:HB	0.45	1.89	1	50
1:C:38:LEU:HA	1:C:164:ALA:HA	0.45	1.89	1	50
1:D:168:GLY:O	1:D:172:VAL:HG12	0.45	2.12	1	50
1:D:176:LEU:O	1:D:178:ARG:N	0.45	2.49	1	50
1:E:52:LYS:HB3	1:E:209:ALA:O	0.45	2.12	1	50
1:G:14:VAL:HG13	1:G:14:VAL:O	0.45	2.11	17	1
1:E:12:ILE:O	1:E:13:THR:CG2	0.45	2.64	23	1
1:D:12:ILE:HG23	1:D:13:THR:HG22	0.45	1.88	49	1
1:A:110:GLU:O	1:A:113:VAL:HG12	0.44	2.13	1	50
1:B:38:LEU:HA	1:B:164:ALA:HA	0.44	1.89	1	50
1:D:17:PRO:HA	1:E:26:TYR:CD1	0.44	2.48	1	50
1:F:116:VAL:HG11	1:F:138:PHE:CZ	0.44	2.46	1	50
1:G:61:GLN:CD	1:G:62:ASN:H	0.44	2.20	1	50
1:C:22:PHE:O	1:C:25:GLU:HB2	0.44	2.12	1	50
1:G:51:ASP:HB3	1:G:53:LYS:HZ3	0.44	1.72	1	50
1:A:43:ALA:HB2	1:A:185:PRO:HA	0.44	1.88	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ASP:O	1:A:173:VAL:HG12	0.44	2.13	1	50
1:A:137:ILE:HG22	1:A:150:ASP:CB	0.44	2.43	1	50
1:B:52:LYS:NZ	1:B:62:ASN:HA	0.44	2.26	1	50
1:D:135:SER:OG	1:D:152:ASP:HA	0.44	2.12	1	50
1:A:149:PHE:CE1	1:A:159:GLU:HB2	0.44	2.46	1	50
1:B:61:GLN:CD	1:B:62:ASN:H	0.44	2.21	1	50
1:A:130:ARG:HH21	1:G:124:THR:HG22	0.44	1.73	1	50
1:D:123:TYR:N	1:D:123:TYR:CD1	0.44	2.84	1	50
1:F:128:GLY:O	1:F:129:VAL:HB	0.44	2.13	1	50
1:D:13:THR:OG1	1:D:125:GLN:O	0.44	2.36	46	10
1:F:174:SER:O	1:F:177:GLU:HB3	0.44	2.12	1	50
1:F:12:ILE:CD1	1:F:127:GLY:O	0.44	2.65	40	1
1:B:20:ARG:CZ	1:B:22:PHE:CE1	0.44	3.01	1	50
1:D:42:PHE:HB2	1:D:184:LEU:O	0.44	2.13	1	50
1:B:134:VAL:CG2	1:B:135:SER:N	0.44	2.79	1	50
1:B:175:PHE:C	1:B:175:PHE:HD1	0.44	2.20	1	50
1:C:148:LEU:O	1:C:159:GLU:HG3	0.43	2.13	1	50
1:D:35:SER:O	1:D:166:GLY:HA3	0.43	2.13	1	50
1:E:32:LYS:O	1:E:167:SER:HA	0.43	2.14	1	50
1:B:13:THR:OG1	1:B:125:GLN:O	0.43	2.36	3	3
1:F:12:ILE:CD1	1:F:129:VAL:O	0.43	2.66	34	1
1:A:12:ILE:O	1:A:13:THR:HG22	0.43	2.12	41	2
1:G:12:ILE:HD12	1:G:12:ILE:O	0.43	2.13	44	1
1:D:52:LYS:HZ1	1:D:62:ASN:HA	0.43	1.71	1	50
1:E:175:PHE:CD1	1:E:175:PHE:C	0.43	2.96	1	50
1:F:152:ASP:HB2	1:F:153:PRO:CD	0.43	2.43	1	50
1:A:13:THR:OG1	1:A:13:THR:O	0.43	2.32	9	1
1:A:124:THR:HG22	1:B:130:ARG:NH2	0.43	2.23	1	50
1:B:180:TYR:HA	1:B:192:LEU:HD21	0.43	1.91	1	50
1:E:38:LEU:HG	1:E:49:ILE:HG23	0.43	1.89	1	50
1:F:70:ILE:HD12	1:F:74:VAL:HG22	0.43	1.88	1	50
1:G:88:LEU:HD13	1:G:132:TYR:CD2	0.43	2.47	1	50
1:G:175:PHE:C	1:G:175:PHE:HD1	0.43	2.22	1	50
1:A:130:ARG:NH1	1:A:131:PRO:O	0.43	2.51	1	50
1:B:187:LYS:O	1:B:190:VAL:HG13	0.43	2.14	1	50
1:A:148:LEU:O	1:A:159:GLU:HG3	0.43	2.14	1	50
1:C:85:ALA:O	1:C:89:VAL:HG23	0.43	2.14	1	50
1:D:180:TYR:HA	1:D:192:LEU:HD21	0.43	1.90	1	50
1:E:198:LYS:HG3	1:E:207:LEU:HD22	0.43	1.90	1	50
1:A:62:ASN:O	1:A:65:GLU:HG2	0.43	2.13	1	50
1:A:134:VAL:O	1:A:153:PRO:HG3	0.43	2.14	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:GLU:O	1:A:231:LYS:HB3	0.43	2.13	1	50
1:B:71:ASP:O	1:B:73:TYR:N	0.43	2.51	1	50
1:C:121:GLN:O	1:C:124:THR:HB	0.43	2.13	1	50
1:E:76:ALA:HB2	1:E:138:PHE:CD1	0.43	2.48	1	50
1:C:12:ILE:HG22	1:C:12:ILE:O	0.43	2.13	5	1
1:E:12:ILE:HD12	1:E:13:THR:H	0.43	1.73	13	1
1:B:28:ARG:O	1:B:31:VAL:HG22	0.43	2.13	1	50
1:D:191:THR:O	1:D:194:ILE:HG22	0.43	2.13	1	50
1:C:14:VAL:O	1:C:14:VAL:HG13	0.43	2.13	36	1
1:C:12:ILE:CD1	1:C:129:VAL:O	0.42	2.67	18	2
1:A:58:LEU:N	1:A:58:LEU:CD1	0.42	2.83	1	50
1:B:24:VAL:O	1:B:28:ARG:HG3	0.42	2.14	1	50
1:B:125:GLN:HB3	1:C:130:ARG:NH2	0.42	2.28	1	50
1:D:143:GLN:HE21	1:D:143:GLN:HA	0.42	1.75	1	50
1:G:52:LYS:HA	1:G:66:LYS:NZ	0.42	2.29	1	50
1:G:84:ASP:O	1:G:88:LEU:HB2	0.42	2.13	1	50
1:B:100:LYS:O	1:B:104:GLY:CA	0.42	2.68	1	50
1:D:176:LEU:C	1:D:178:ARG:N	0.42	2.75	1	50
1:D:202:GLU:HG3	1:D:205:GLU:O	0.42	2.14	1	50
1:E:49:ILE:HD12	1:E:211:GLU:O	0.42	2.14	1	50
1:A:12:ILE:HG23	1:A:127:GLY:O	0.42	2.15	22	1
1:B:12:ILE:HD13	1:B:23:GLN:HG3	0.42	1.92	24	1
1:G:16:SER:HB3	1:G:22:PHE:CE2	0.42	2.50	1	50
1:B:98:GLN:O	1:B:102:THR:HG23	0.42	2.15	1	50
1:F:51:ASP:HB3	1:F:53:LYS:HZ3	0.42	1.74	1	50
1:F:175:PHE:C	1:F:175:PHE:HD1	0.42	2.21	1	50
1:G:13:THR:OG1	1:G:13:THR:O	0.42	2.34	1	8
1:E:12:ILE:O	1:E:12:ILE:CG2	0.42	2.67	6	1
1:G:12:ILE:O	1:G:12:ILE:CG2	0.42	2.67	47	1
1:C:229:VAL:HG13	1:C:230:LYS:N	0.42	2.30	1	50
1:A:175:PHE:CD2	1:A:196:ALA:HA	0.42	2.50	1	50
1:B:113:VAL:HG22	1:B:157:ILE:HD12	0.42	1.92	1	50
1:E:159:GLU:HG2	1:F:60:GLU:HG3	0.42	1.91	1	50
1:F:12:ILE:O	1:F:13:THR:CG2	0.42	2.67	48	3
1:F:198:LYS:HG2	1:F:202:GLU:HG2	0.42	1.91	1	50
1:G:184:LEU:HD23	1:G:189:ALA:HA	0.42	1.92	1	50
1:C:12:ILE:O	1:C:12:ILE:CD1	0.42	2.67	7	1
1:F:12:ILE:O	1:F:12:ILE:HG23	0.42	2.14	13	1
1:F:12:ILE:O	1:F:12:ILE:CD1	0.42	2.67	37	1
1:C:176:LEU:C	1:C:178:ARG:N	0.42	2.74	1	50
1:E:58:LEU:CD1	1:E:58:LEU:N	0.42	2.83	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:12:ILE:C	1:F:13:THR:CG2	0.42	2.90	42	5
1:F:43:ALA:HB2	1:F:185:PRO:HA	0.42	1.91	1	50
1:A:156:THR:HG23	1:B:82:VAL:HG11	0.41	1.92	1	50
1:B:110:GLU:O	1:B:113:VAL:HG13	0.41	2.15	1	50
1:C:90:ASP:O	1:C:94:ILE:HG23	0.41	2.14	1	50
1:D:134:VAL:O	1:D:153:PRO:HG3	0.41	2.15	1	50
1:E:135:SER:OG	1:E:153:PRO:HD3	0.41	2.15	1	50
1:E:184:LEU:HD23	1:E:189:ALA:HA	0.41	1.92	1	50
1:G:114:LYS:O	1:G:117:ALA:HB3	0.41	2.15	1	50
1:A:98:GLN:O	1:A:102:THR:HG23	0.41	2.15	1	50
1:C:71:ASP:OD1	1:C:72:ASP:N	0.41	2.53	1	50
1:F:94:ILE:CG1	1:F:95:SER:N	0.41	2.82	1	50
1:F:198:LYS:CG	1:F:202:GLU:HG2	0.41	2.44	1	50
1:D:12:ILE:C	1:D:13:THR:CG2	0.41	2.93	39	2
1:E:38:LEU:CD2	1:E:49:ILE:HG23	0.41	2.44	1	50
1:E:42:PHE:HB2	1:E:184:LEU:O	0.41	2.14	1	50
1:A:61:GLN:CD	1:A:62:ASN:H	0.41	2.22	1	50
1:D:176:LEU:O	1:D:177:GLU:C	0.41	2.63	1	50
1:E:43:ALA:HB2	1:E:185:PRO:HA	0.41	1.92	1	50
1:E:160:TYR:C	1:F:60:GLU:HG2	0.41	2.40	1	50
1:C:172:VAL:O	1:C:176:LEU:HD22	0.41	2.16	1	50
1:E:228:GLU:O	1:E:231:LYS:HB3	0.41	2.15	1	50
1:A:70:ILE:HB	1:A:74:VAL:HG13	0.41	1.92	1	50
1:B:42:PHE:HD1	1:B:43:ALA:N	0.41	2.14	1	50
1:D:98:GLN:O	1:D:102:THR:CG2	0.41	2.69	1	50
1:E:40:MET:HA	1:E:162:ALA:HA	0.41	1.93	1	50
1:E:152:ASP:HB2	1:E:153:PRO:CD	0.41	2.46	1	50
1:G:135:SER:OG	1:G:152:ASP:HA	0.41	2.16	1	50
1:G:212:ILE:HG23	1:G:224:TYR:HB2	0.41	1.93	1	50
1:D:12:ILE:O	1:D:12:ILE:HG13	0.41	2.15	33	1
1:C:134:VAL:CG2	1:C:135:SER:N	0.41	2.83	1	50
1:E:194:ILE:O	1:E:198:LYS:HB2	0.41	2.16	1	50
1:D:12:ILE:HD12	1:D:13:THR:N	0.41	2.31	42	1
1:A:180:TYR:HA	1:A:192:LEU:HD21	0.41	1.93	1	50
1:A:227:GLU:N	1:A:227:GLU:CD	0.41	2.79	1	50
1:C:94:ILE:HG13	1:C:95:SER:N	0.41	2.29	1	50
1:D:77:VAL:CG1	1:D:137:ILE:HG12	0.41	2.46	1	50
1:F:109:ILE:CG2	1:F:147:ARG:HD3	0.41	2.46	1	50
1:E:137:ILE:HG22	1:E:150:ASP:HB2	0.40	1.92	1	50
1:B:44:ASN:HD22	1:B:44:ASN:HA	0.40	1.56	1	50
1:B:108:ASN:OD1	1:B:147:ARG:NH1	0.40	2.54	1	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:TYR:CD1	1:A:123:TYR:N	0.40	2.88	1	50
1:E:61:GLN:OE1	1:E:62:ASN:HB3	0.40	2.16	1	50
1:E:98:GLN:O	1:E:101:VAL:HG12	0.40	2.16	1	50
1:F:58:LEU:N	1:F:58:LEU:CD1	0.40	2.84	1	50
1:A:23:GLN:HE22	1:G:15:PHE:HB2	0.40	1.75	39	1
1:B:70:ILE:HD12	1:B:74:VAL:HG22	0.40	1.92	1	50
1:C:18:ASP:OD2	1:C:20:ARG:HD3	0.40	2.15	1	50
1:D:216:THR:O	1:D:217:VAL:C	0.40	2.64	1	50
1:G:49:ILE:HD11	1:G:210:PRO:HB3	0.40	1.92	1	50
1:G:222:ARG:NH2	1:G:224:TYR:CZ	0.40	2.89	1	50
1:C:12:ILE:C	1:C:12:ILE:CD1	0.40	2.90	48	1

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	221/237 (93%)	186±1 (84±0%)	25±1 (11±0%)	10±1 (5±0%)	3	26
1	B	221/237 (93%)	187±1 (84±0%)	25±1 (11±0%)	10±1 (4±0%)	3	28
1	C	221/237 (93%)	185±1 (84±0%)	28±1 (13±0%)	8±1 (3±0%)	4	34
1	D	221/237 (93%)	189±1 (85±0%)	22±1 (10±0%)	10±1 (4±0%)	3	27
1	E	221/237 (93%)	184±1 (83±0%)	26±1 (12±0%)	12±1 (5±0%)	3	23
1	F	221/237 (93%)	187±1 (85±0%)	23±0 (10±0%)	11±1 (5±0%)	3	25
1	G	221/237 (93%)	188±1 (85±0%)	24±1 (11±0%)	9±0 (4±0%)	4	30
All	All	77350/82950 (93%)	65258 (84%)	8702 (11%)	3390 (4%)	3	27

All 77 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	43	ALA	50
1	A	72	ASP	50
1	A	128	GLY	50

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Mol	Chain	Res	Type	Models (Total)
1	A	129	VAL	50
1	A	182	GLU	50
1	A	198	LYS	50
1	A	200	SER	50
1	A	202	GLU	50
1	A	205	GLU	50
1	B	43	ALA	50
1	B	61	GLN	50
1	B	62	ASN	50
1	B	72	ASP	50
1	B	128	GLY	50
1	B	182	GLU	50
1	B	198	LYS	50
1	B	200	SER	50
1	B	205	GLU	50
1	C	43	ALA	50
1	C	61	GLN	50
1	C	128	GLY	50
1	C	182	GLU	50
1	C	198	LYS	50
1	C	200	SER	50
1	C	205	GLU	50
1	D	43	ALA	50
1	D	61	GLN	50
1	D	72	ASP	50
1	D	128	GLY	50
1	D	177	GLU	50
1	D	182	GLU	50
1	D	198	LYS	50
1	D	200	SER	50
1	D	205	GLU	50
1	E	43	ALA	50
1	E	61	GLN	50
1	E	62	ASN	50
1	E	72	ASP	50
1	E	128	GLY	50
1	E	129	VAL	50
1	E	167	SER	50
1	E	182	GLU	50
1	E	198	LYS	50
1	E	200	SER	50
1	E	205	GLU	50

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Mol	Chain	Res	Type	Models (Total)
1	F	43	ALA	50
1	F	61	GLN	50
1	F	62	ASN	50
1	F	72	ASP	50
1	F	128	GLY	50
1	F	129	VAL	50
1	F	182	GLU	50
1	F	198	LYS	50
1	F	200	SER	50
1	F	205	GLU	50
1	G	43	ALA	50
1	G	61	GLN	50
1	G	62	ASN	50
1	G	128	GLY	50
1	G	182	GLU	50
1	G	198	LYS	50
1	G	200	SER	50
1	G	205	GLU	50
1	A	13	THR	36
1	D	13	THR	31
1	F	13	THR	29
1	G	13	THR	25
1	E	12	ILE	20
1	C	13	THR	19
1	B	13	THR	18
1	A	12	ILE	17
1	D	12	ILE	12
1	B	12	ILE	11
1	E	13	THR	10
1	C	12	ILE	7
1	F	12	ILE	4
1	G	12	ILE	1

6.3.2 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 NMR 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	185/192 (96%)	156±0 (85±0%)	29±0 (15±0%)	5	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	185/192 (96%)	160±0 (86±0%)	25±0 (14±0%)	6	45
1	C	185/192 (96%)	156±0 (84±0%)	29±0 (16±0%)	4	40
1	D	185/192 (96%)	155±1 (84±0%)	30±1 (16±0%)	4	40
1	E	185/192 (96%)	157±0 (85±0%)	28±0 (15±0%)	5	41
1	F	185/192 (96%)	163±0 (88±0%)	22±0 (12±0%)	7	49
1	G	185/192 (96%)	160±0 (87±0%)	25±0 (13±0%)	6	46
All	All	64750/67200 (96%)	55347 (85%)	9403 (15%)	5	43

All 193 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	13	THR	50
1	A	21	LEU	50
1	A	23	GLN	50
1	A	24	VAL	50
1	A	31	VAL	50
1	A	44	ASN	50
1	A	47	LEU	50
1	A	48	LEU	50
1	A	62	ASN	50
1	A	71	ASP	50
1	A	82	VAL	50
1	A	102	THR	50
1	A	106	LEU	50
1	A	107	VAL	50
1	A	111	ASN	50
1	A	119	GLN	50
1	A	134	VAL	50
1	A	136	LEU	50
1	A	141	ILE	50
1	A	143	GLN	50
1	A	157	ILE	50
1	A	161	LYS	50
1	A	175	PHE	50
1	A	176	LEU	50
1	A	190	VAL	50
1	A	201	LEU	50
1	A	202	GLU	50
1	A	212	ILE	50

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Mol	Chain	Res	Type	Models (Total)
1	B	13	THR	50
1	B	21	LEU	50
1	B	24	VAL	50
1	B	31	VAL	50
1	B	44	ASN	50
1	B	47	LEU	50
1	B	48	LEU	50
1	B	49	ILE	50
1	B	58	LEU	50
1	B	62	ASN	50
1	B	71	ASP	50
1	B	102	THR	50
1	B	107	VAL	50
1	B	113	VAL	50
1	B	119	GLN	50
1	B	134	VAL	50
1	B	136	LEU	50
1	B	141	ILE	50
1	B	143	GLN	50
1	B	157	ILE	50
1	B	176	LEU	50
1	B	190	VAL	50
1	B	201	LEU	50
1	B	202	GLU	50
1	B	212	ILE	50
1	C	13	THR	50
1	C	21	LEU	50
1	C	31	VAL	50
1	C	44	ASN	50
1	C	47	LEU	50
1	C	48	LEU	50
1	C	49	ILE	50
1	C	58	LEU	50
1	C	62	ASN	50
1	C	71	ASP	50
1	C	87	VAL	50
1	C	102	THR	50
1	C	107	VAL	50
1	C	113	VAL	50
1	C	116	VAL	50
1	C	119	GLN	50
1	C	134	VAL	50

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Mol	Chain	Res	Type	Models (Total)
1	C	136	LEU	50
1	C	141	ILE	50
1	C	143	GLN	50
1	C	157	ILE	50
1	C	161	LYS	50
1	C	175	PHE	50
1	C	176	LEU	50
1	C	190	VAL	50
1	C	201	LEU	50
1	C	202	GLU	50
1	C	212	ILE	50
1	C	221	TYR	50
1	D	21	LEU	50
1	D	23	GLN	50
1	D	24	VAL	50
1	D	31	VAL	50
1	D	44	ASN	50
1	D	47	LEU	50
1	D	48	LEU	50
1	D	49	ILE	50
1	D	58	LEU	50
1	D	62	ASN	50
1	D	71	ASP	50
1	D	94	ILE	50
1	D	101	VAL	50
1	D	102	THR	50
1	D	107	VAL	50
1	D	113	VAL	50
1	D	119	GLN	50
1	D	134	VAL	50
1	D	136	LEU	50
1	D	141	ILE	50
1	D	143	GLN	50
1	D	157	ILE	50
1	D	175	PHE	50
1	D	176	LEU	50
1	D	190	VAL	50
1	D	201	LEU	50
1	D	202	GLU	50
1	D	212	ILE	50
1	E	21	LEU	50
1	E	23	GLN	50

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Mol	Chain	Res	Type	Models (Total)
1	E	24	VAL	50
1	E	31	VAL	50
1	E	44	ASN	50
1	E	47	LEU	50
1	E	48	LEU	50
1	E	62	ASN	50
1	E	71	ASP	50
1	E	82	VAL	50
1	E	101	VAL	50
1	E	102	THR	50
1	E	107	VAL	50
1	E	111	ASN	50
1	E	116	VAL	50
1	E	119	GLN	50
1	E	134	VAL	50
1	E	136	LEU	50
1	E	141	ILE	50
1	E	143	GLN	50
1	E	157	ILE	50
1	E	161	LYS	50
1	E	176	LEU	50
1	E	190	VAL	50
1	E	201	LEU	50
1	E	202	GLU	50
1	E	212	ILE	50
1	F	21	LEU	50
1	F	23	GLN	50
1	F	31	VAL	50
1	F	44	ASN	50
1	F	47	LEU	50
1	F	48	LEU	50
1	F	49	ILE	50
1	F	62	ASN	50
1	F	71	ASP	50
1	F	101	VAL	50
1	F	102	THR	50
1	F	119	GLN	50
1	F	134	VAL	50
1	F	136	LEU	50
1	F	141	ILE	50
1	F	143	GLN	50
1	F	157	ILE	50

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Mol	Chain	Res	Type	Models (Total)
1	F	190	VAL	50
1	F	201	LEU	50
1	F	202	GLU	50
1	F	212	ILE	50
1	G	21	LEU	50
1	G	23	GLN	50
1	G	31	VAL	50
1	G	44	ASN	50
1	G	47	LEU	50
1	G	48	LEU	50
1	G	49	ILE	50
1	G	62	ASN	50
1	G	71	ASP	50
1	G	74	VAL	50
1	G	102	THR	50
1	G	107	VAL	50
1	G	119	GLN	50
1	G	134	VAL	50
1	G	136	LEU	50
1	G	141	ILE	50
1	G	143	GLN	50
1	G	157	ILE	50
1	G	176	LEU	50
1	G	190	VAL	50
1	G	201	LEU	50
1	G	202	GLU	50
1	G	212	ILE	50
1	G	13	THR	49
1	E	13	THR	48
1	F	13	THR	48
1	D	13	THR	47
1	D	12	ILE	32
1	G	12	ILE	29
1	A	12	ILE	26
1	F	12	ILE	24
1	E	12	ILE	22
1	C	12	ILE	15
1	B	12	ILE	12
1	B	14	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided