



wwPDB EM Validation Summary Report ⓘ

Jun 14, 2026 – 01:43 AM JST

PDB ID : 9W2M / pdb_00009w2m
EMDB ID : EMD-65575
Title : Cryo-EM structure of the Cytoplasmic lattice(CPL) from mouse oocyte
Authors : Liu, S.X.; Xue, J.C.; Zhang, Y.; Liu, Y.S.; Gao, H.S.; Shen, E.Z.
Deposited on : 2025-07-28
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

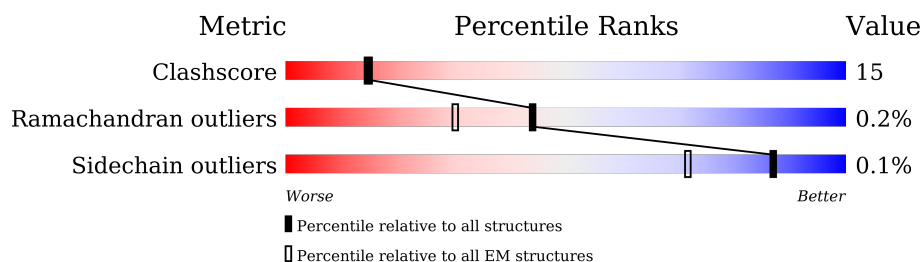
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	682	71% 29%
1	11	682	69% 30%
1	12	682	74% 26%
1	13	682	67% 33%
1	14	682	66% 34%
1	15	682	60% 40%
1	16	682	63% 37%
1	17	682	71% 29%
1	18	682	67% 33%

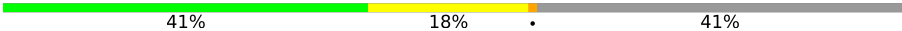
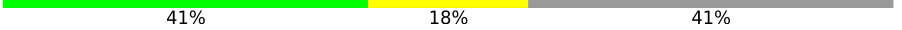
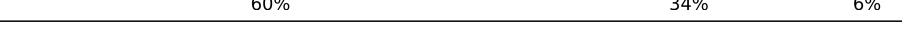
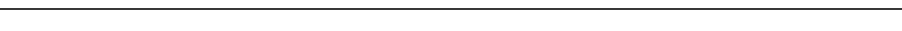
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	19	682	
1	2	682	
1	3	682	
1	4	682	
1	5	682	
1	6	682	
1	7	682	
1	8	682	
1	9	682	
1	Z	682	
1	z	682	
2	C	125	
2	H	125	
2	c	125	
2	h	125	
3	D	128	
3	d	128	
4	E	933	
4	I	933	
4	e	933	
4	i	933	
5	J	466	
5	j	466	
6	K	163	
6	k	163	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	O	147	 65% 35% .
7	o	147	 67% 33% .
8	P	782	 41% 18% 41% .
8	Q	782	 5% 8% 87%
8	p	782	 41% 18% 41%
8	q	782	 6% 7% 87%
9	R	55	 51% 44% 5%
9	r	55	 56% 42% .
10	N	966	 67% 33%
10	n	966	 68% 31%
11	L	445	 60% 34% 6%
11	l	445	 59% 35% 6%
12	M	445	 58% 36% 6%
12	m	445	 60% 34% 6%
13	A	963	 70% 29% .
13	F	963	 67% 31% .
13	a	963	 71% 28% .
13	f	963	 68% 31% .
14	B	436	 55% 22% 24%
14	G	436	 58% 26% 16%
14	b	436	 54% 22% 24%
14	g	436	 58% 26% 16%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 234055 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	682	Total	C	N	O	S	0	0
			5386	3440	888	1019	39		
1	Z	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	z	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	2	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	3	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	4	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	5	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	6	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	7	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	8	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	9	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	12	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	11	682	Total	C	N	O	S	0	0
			5386	3440	888	1019	39		
1	19	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	15	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	16	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	14	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	13	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	17	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		
1	18	682	Total	C	N	O	S	0	0
			5388	3442	888	1019	39		

- Molecule 2 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	125	Total	C	N	O	S	0	0
			1003	642	174	182	5		
2	H	90	Total	C	N	O	S	0	0
			726	465	124	132	5		
2	c	125	Total	C	N	O	S	0	0
			1003	642	174	182	5		
2	h	90	Total	C	N	O	S	0	0
			726	465	124	132	5		

- Molecule 3 is a protein called KH domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	128	Total	C	N	O	S	0	0
			1069	690	191	179	9		
3	d	128	Total	C	N	O	S	0	0
			1069	690	191	179	9		

- Molecule 4 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	933	Total	C	N	O	S	0	0
			7519	4801	1254	1394	70		
4	I	847	Total	C	N	O	S	0	0
			6805	4340	1131	1267	67		
4	e	933	Total	C	N	O	S	0	0
			7519	4801	1254	1394	70		
4	i	847	Total	C	N	O	S	0	0
			6805	4340	1131	1267	67		

- Molecule 5 is a protein called FBXW24.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	466	Total	C	N	O	S	0	0
			3747	2411	627	676	33		
5	j	466	Total	C	N	O	S	0	0
			3747	2411	627	676	33		

- Molecule 6 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	158	Total	C	N	O	S	0	0
			1261	791	204	260	6		
6	k	158	Total	C	N	O	S	0	0
			1261	791	204	260	6		

- Molecule 7 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	147	Total	C	N	O	S	0	0
			1174	751	200	215	8		
7	o	147	Total	C	N	O	S	0	0
			1174	751	200	215	8		

- Molecule 8 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	104	Total	C	N	O	S	0	0
			856	537	164	150	5		
8	q	104	Total	C	N	O	S	0	0
			856	537	164	150	5		
8	P	464	Total	C	N	O	S	0	0
			3704	2313	673	691	27		
8	p	460	Total	C	N	O	S	0	0
			3675	2297	669	683	26		

- Molecule 9 is a protein called Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	55	Total	C	N	O	S	0	0
			445	282	83	74	6		
9	r	55	Total	C	N	O	S	0	0
			445	282	83	74	6		

- Molecule 10 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	962	Total	C	N	O	S	0	0
			7689	4887	1317	1421	64		
10	n	962	Total	C	N	O	S	0	0
			7689	4887	1317	1421	64		

- Molecule 11 is a protein called Tubulin beta-2A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	420	Total	C	N	O	S	0	0
			3288	2061	564	638	25		
11	l	420	Total	C	N	O	S	0	0
			3288	2061	564	638	25		

- Molecule 12 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	420	Total	C	N	O	S	0	0
			3290	2062	564	638	26		
12	m	420	Total	C	N	O	S	0	0
			3290	2062	564	638	26		

- Molecule 13 is a protein called Isoform 4 of NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	949	Total	C	N	O	S	0	0
			7481	4760	1267	1388	66		
13	F	949	Total	C	N	O	S	0	0
			7481	4760	1267	1388	66		
13	a	949	Total	C	N	O	S	0	0
			7481	4760	1267	1388	66		
13	f	949	Total	C	N	O	S	0	0
			7481	4760	1267	1388	66		

- Molecule 14 is a protein called Transducin-like enhancer protein 6.

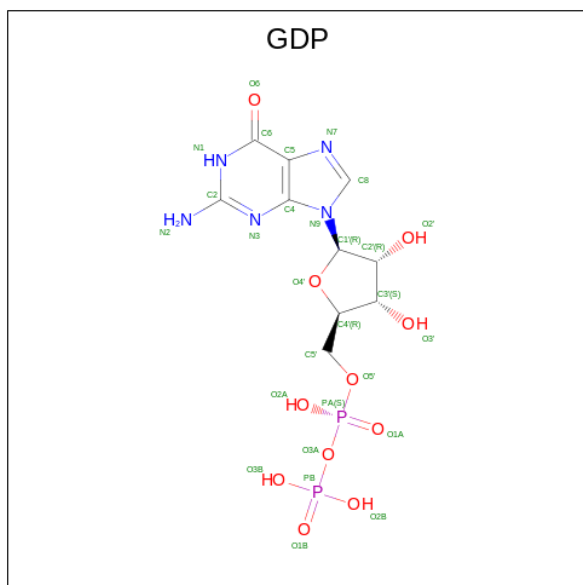
Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	333	Total	C	N	O	S	0	0
			2626	1666	462	479	19		
14	G	366	Total	C	N	O	S	0	0
			2890	1833	507	530	20		
14	b	333	Total	C	N	O	S	0	0
			2626	1666	462	479	19		

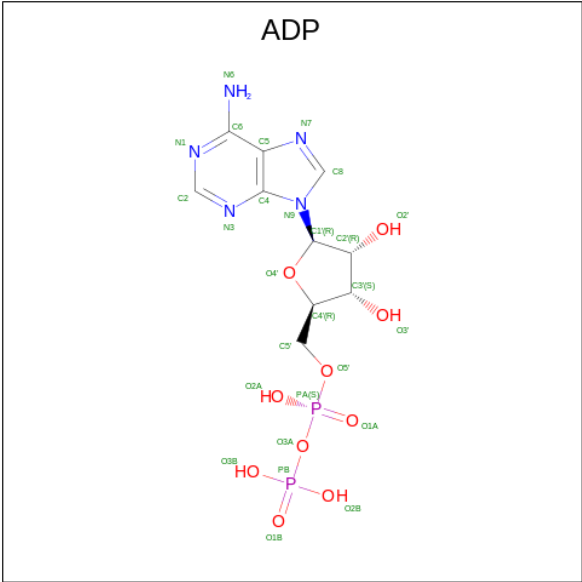
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	366	Total	C	N	O	S	0	0
			2890	1833	507	530	20		

- Molecule 15 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



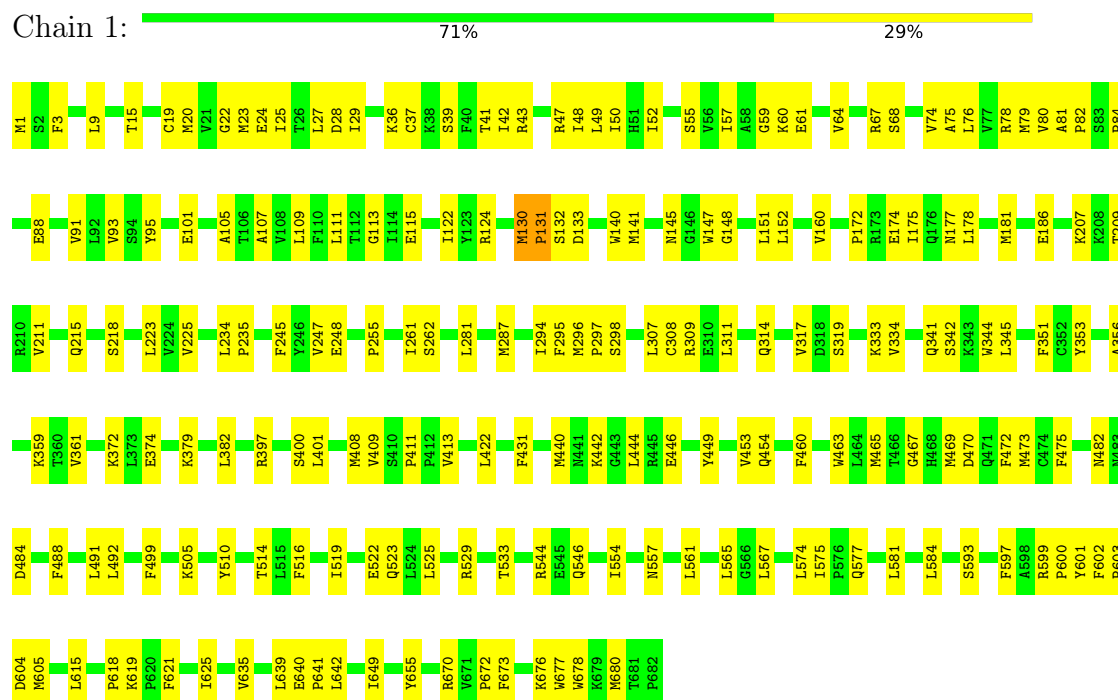


Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
16	f	1	Total	C	N	O	P	0
			27	10	5	10	2	

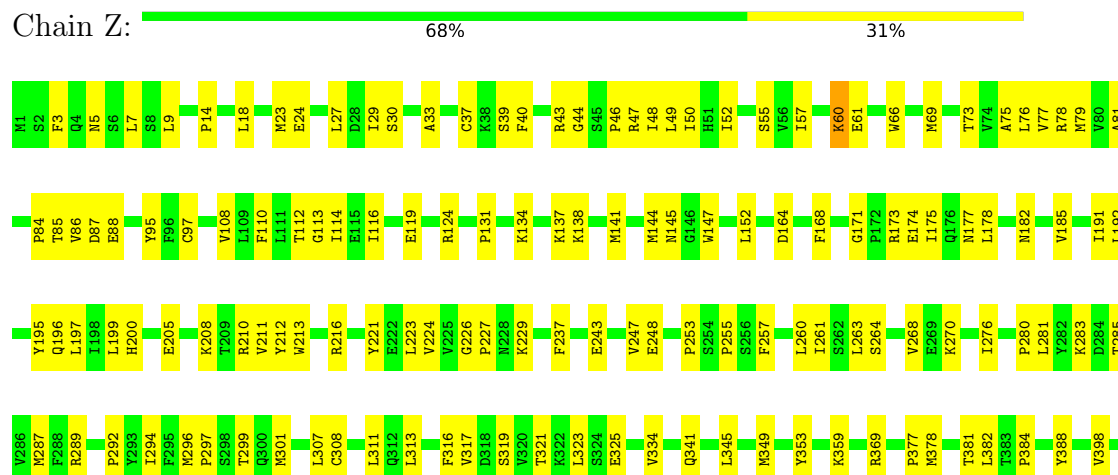
3 Residue-property plots

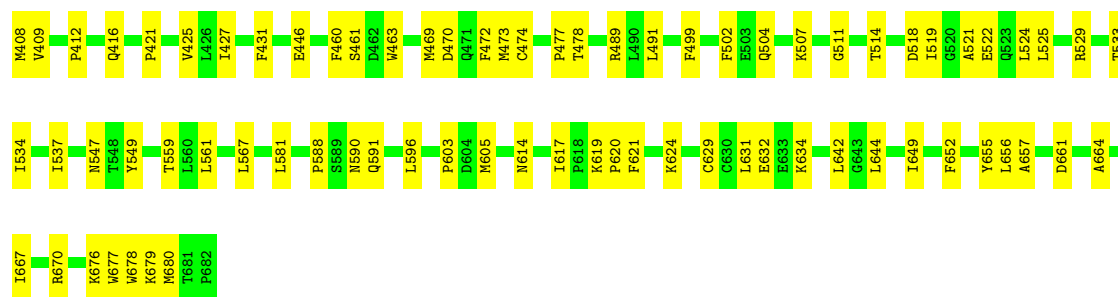
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Inactive protein-arginine deiminase type-6



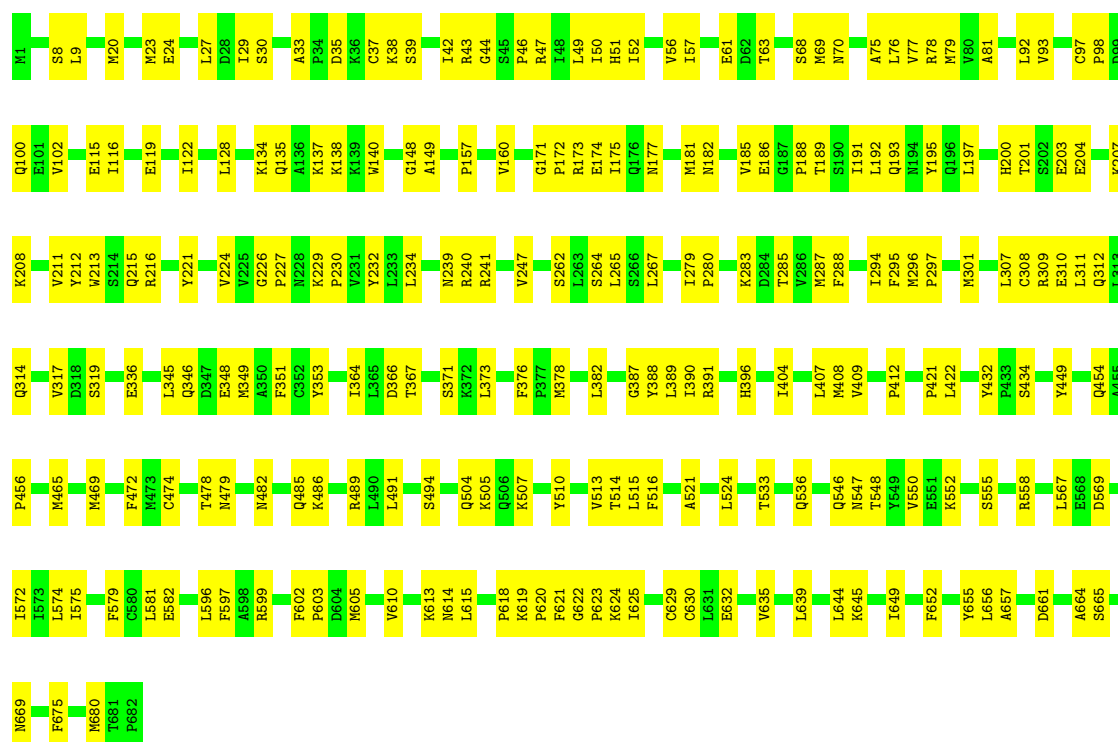
- Molecule 1: Inactive protein-arginine deiminase type-6





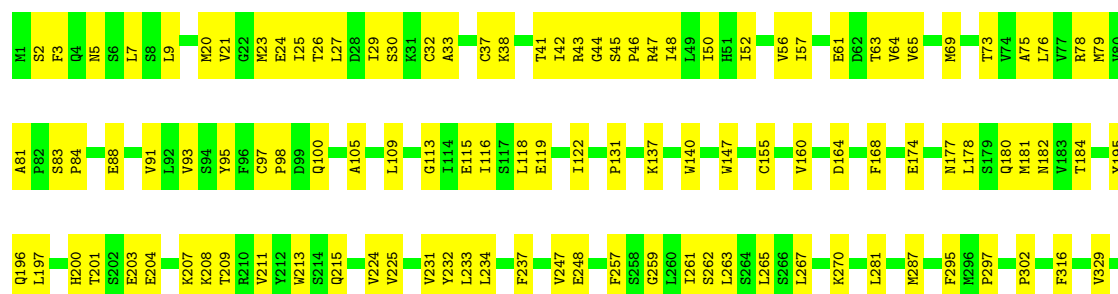
- Molecule 1: Inactive protein-arginine deiminase type-6

Chain z: 67% 33%



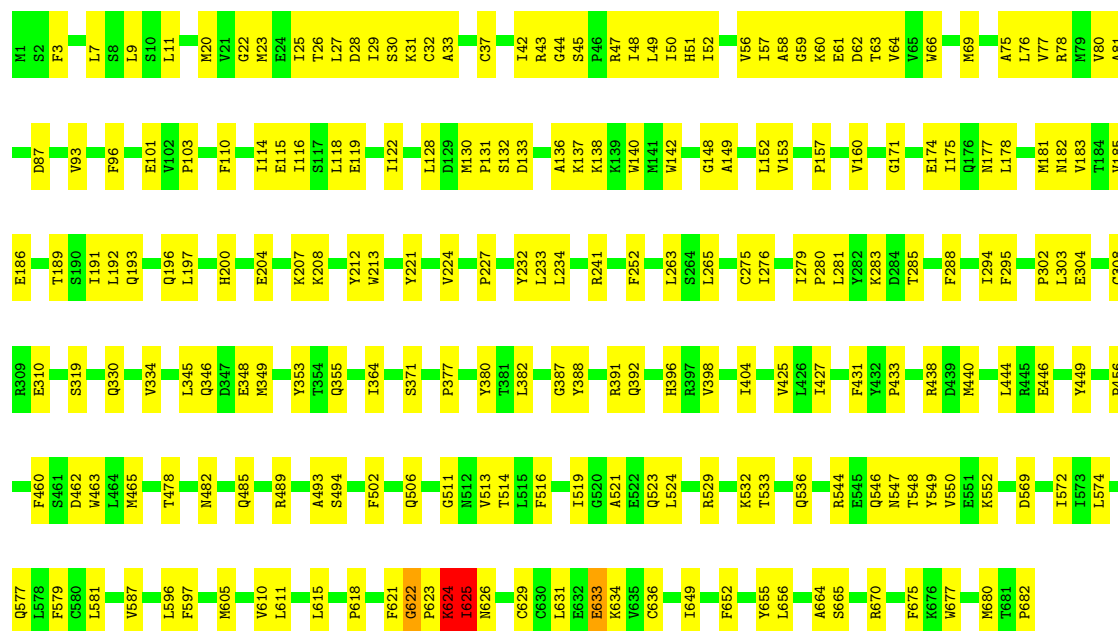
- Molecule 1: Inactive protein-arginine deiminase type-6

Chain 2: 74% 26%

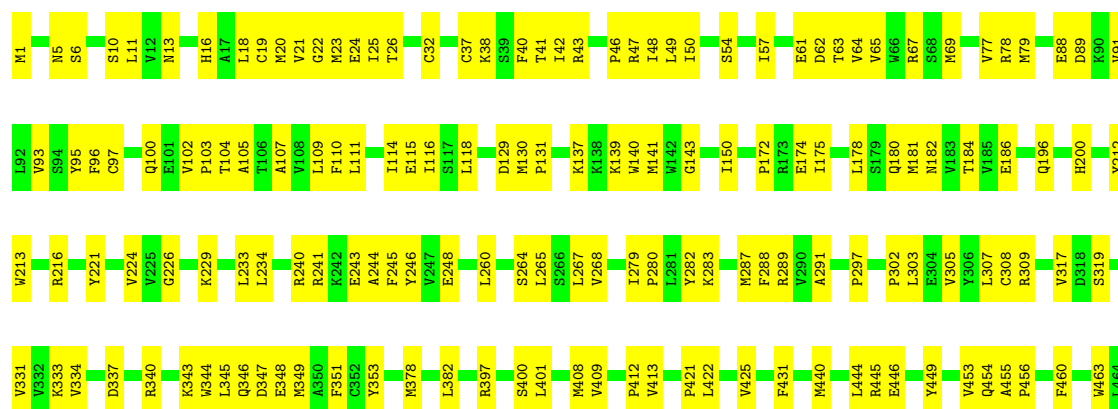


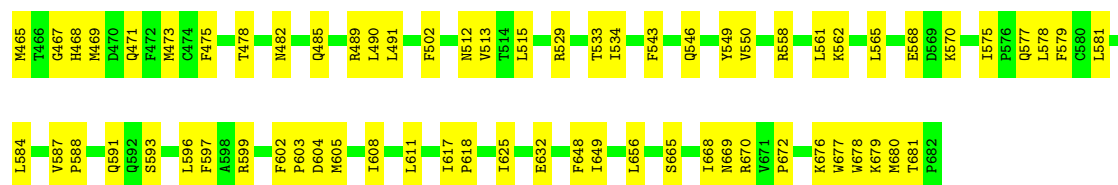


- Molecule 1: Inactive protein-arginine deiminase type-6

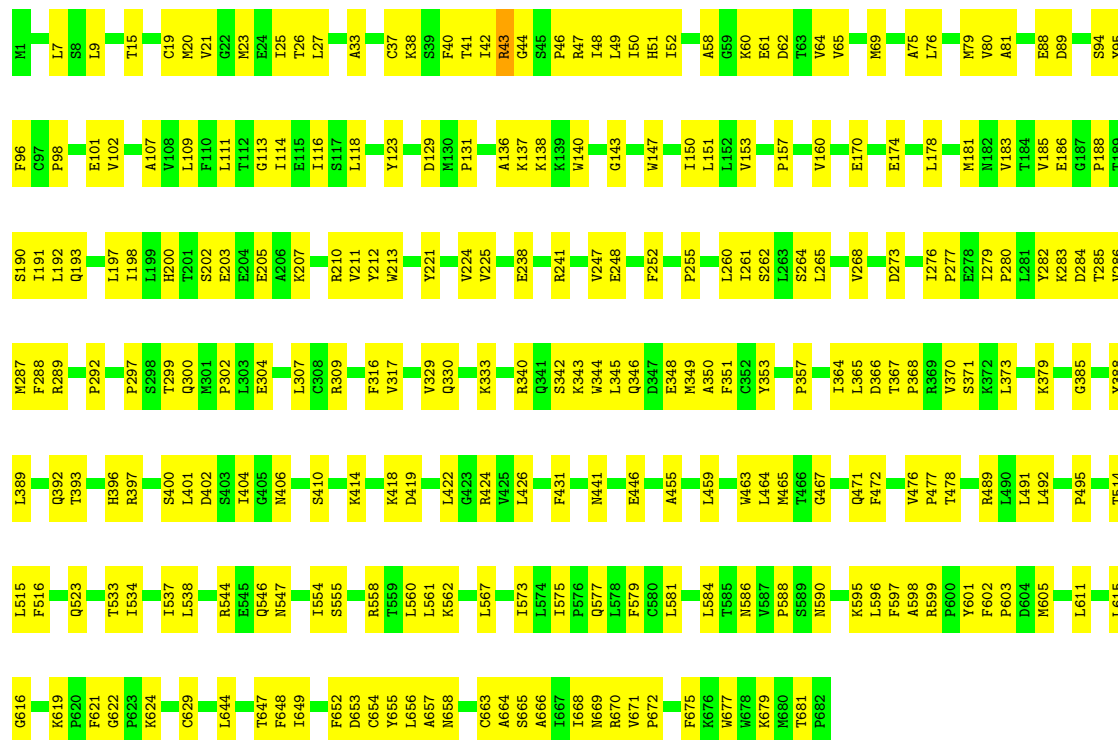


- Molecule 1: Inactive protein-arginine deiminase type-6

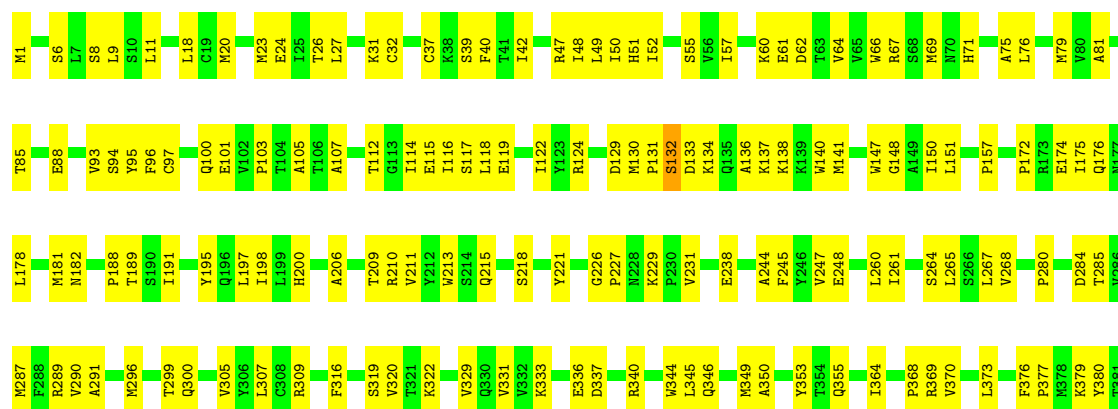


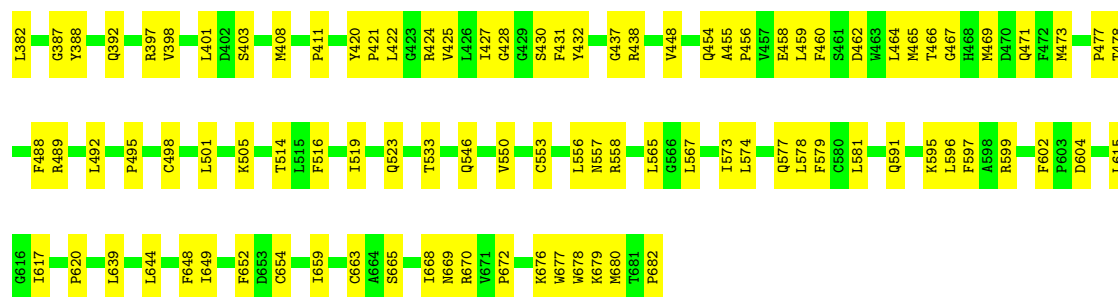


• Molecule 1: Inactive protein-arginine deiminase type-6



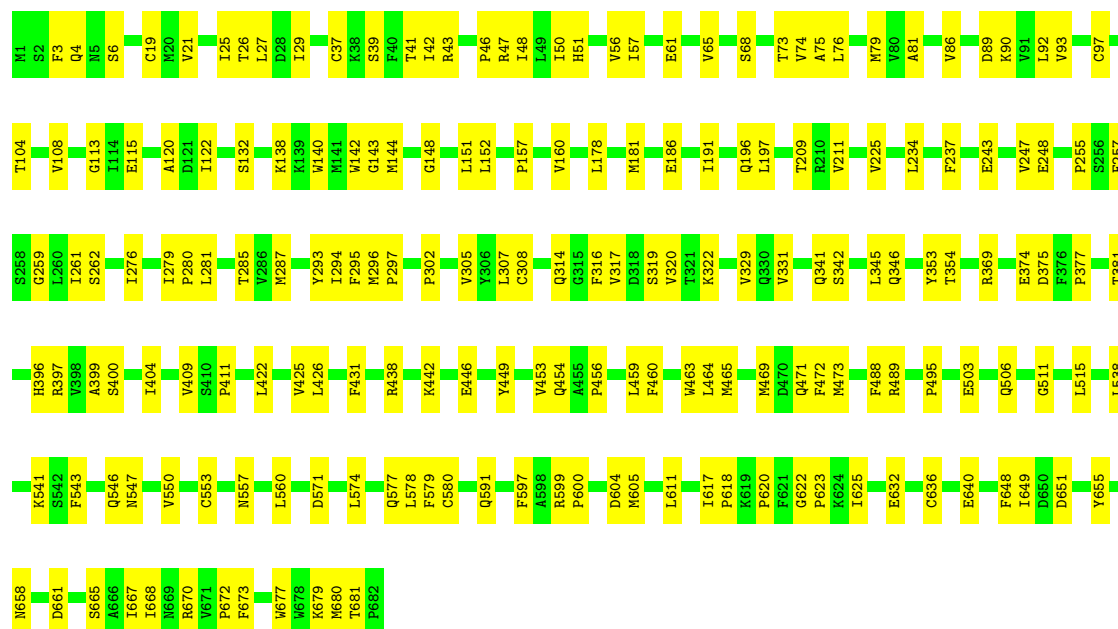
• Molecule 1: Inactive protein-arginine deiminase type-6





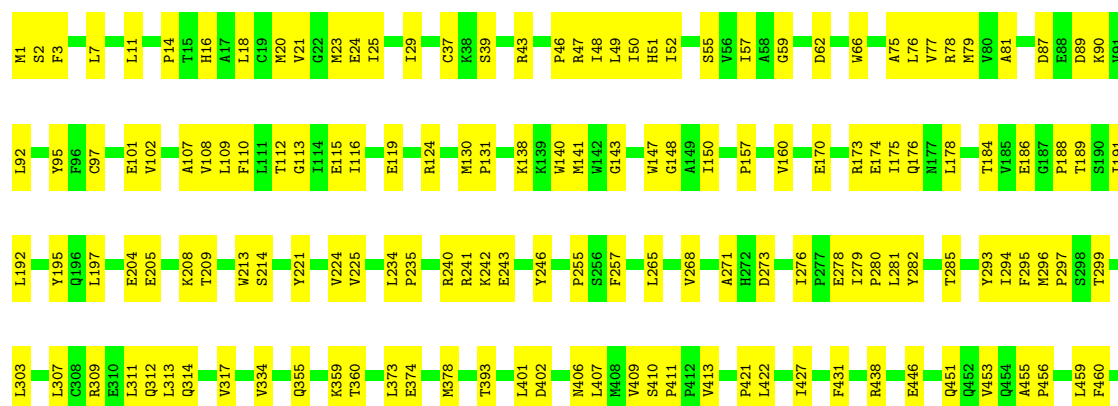
• Molecule 1: Inactive protein-arginine deiminase type-6

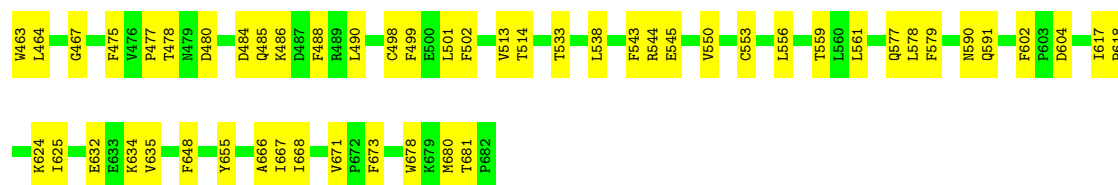
Chain 7: 73% 27%



• Molecule 1: Inactive protein-arginine deiminase type-6

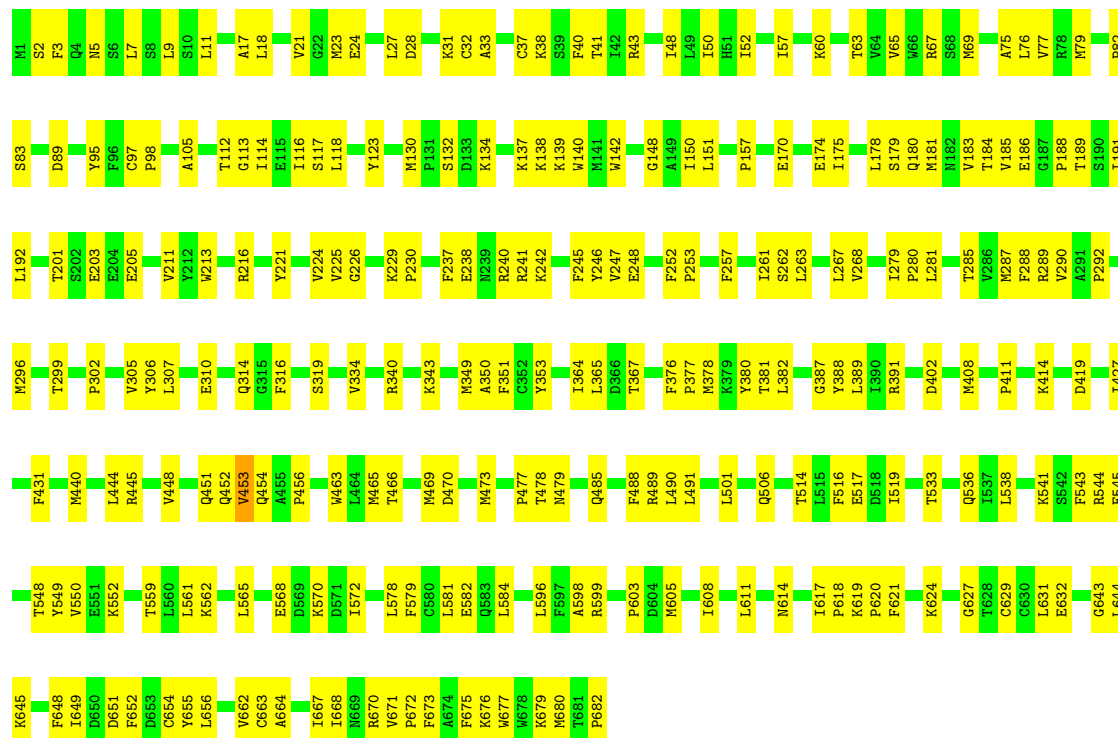
Chain 8: 71% 29%





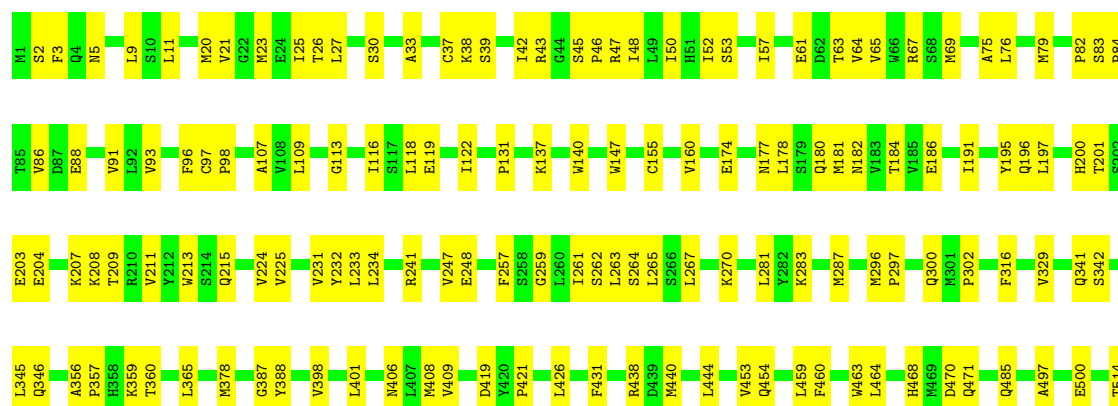
- Molecule 1: Inactive protein-arginine deiminase type-6

Chain 9: 64% 36%



- Molecule 1: Inactive protein-arginine deiminase type-6

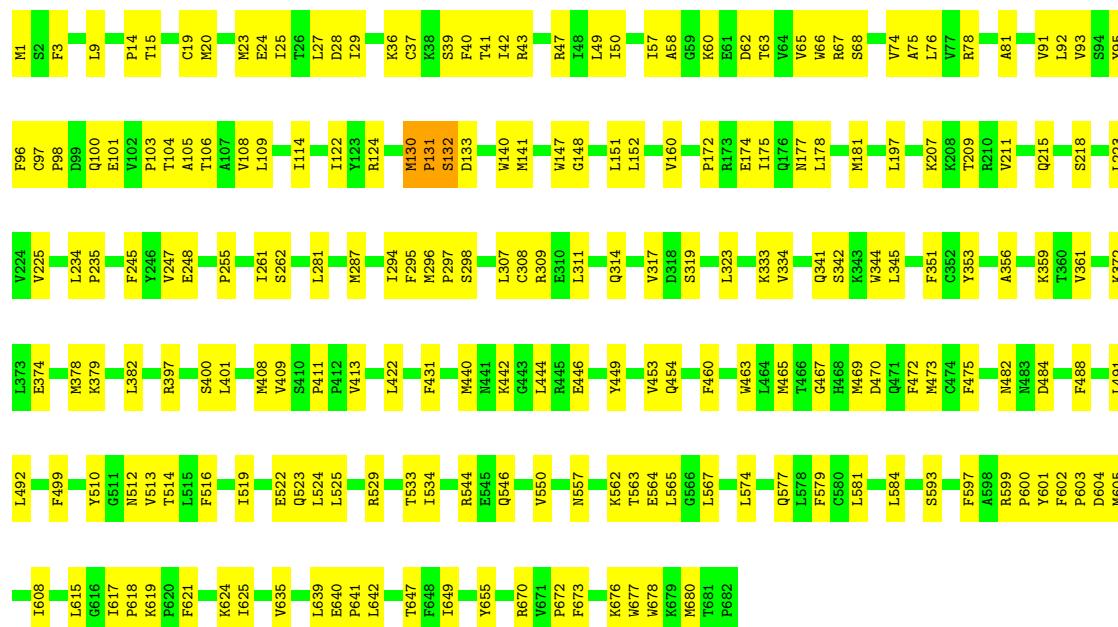
Chain 12: 74% 26%





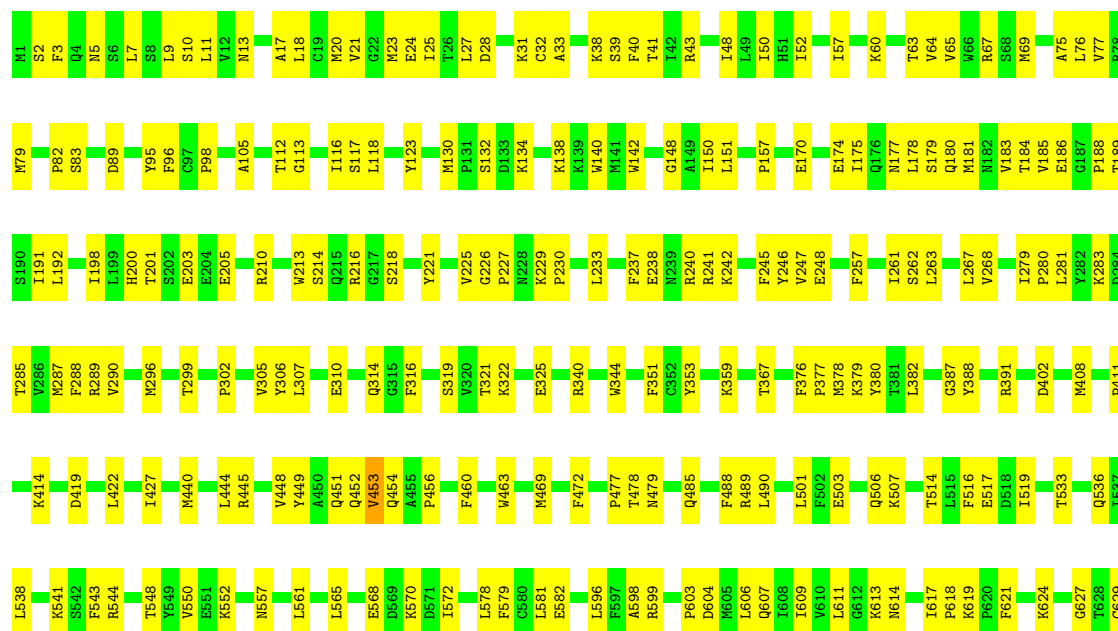
• Molecule 1: Inactive protein-arginine deiminase type-6

Chain 11: 69% 30%



• Molecule 1: Inactive protein-arginine deiminase type-6

Chain 19: 63% 37%





Satisfaction Level	Percentage
Very satisfied	60%
Satisfied	40%



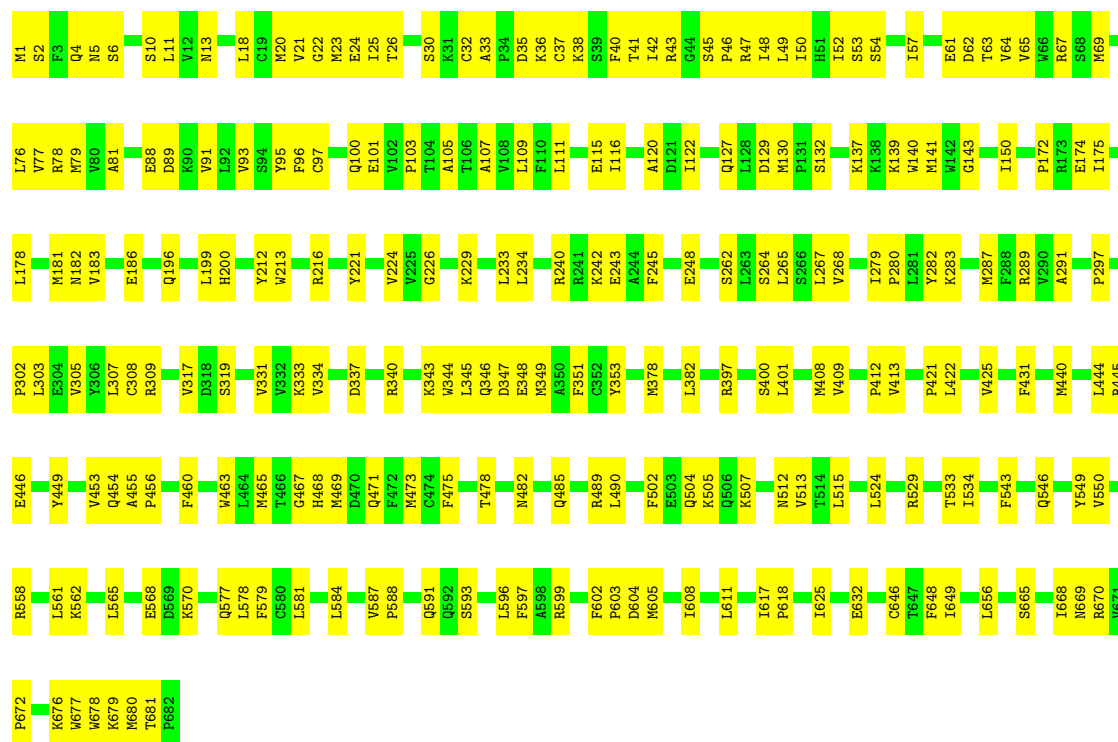
Category	Percentage
Very satisfied	63%
Satisfied	37%





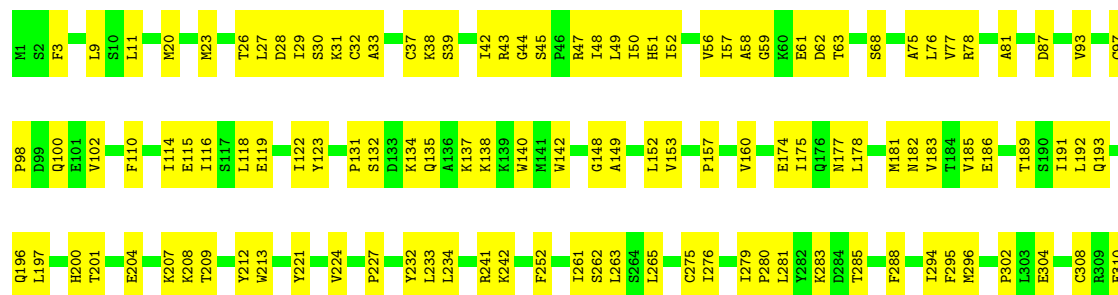
- Molecule 1: Inactive protein-arginine deiminase type-6

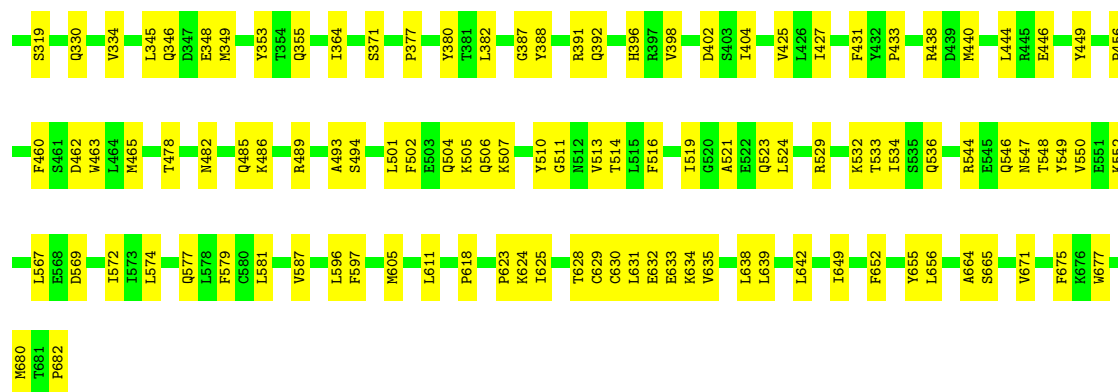
Chain 14: 66% 34%

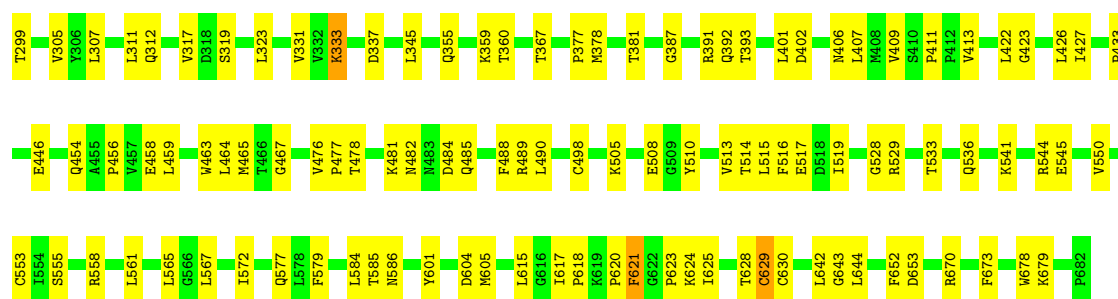


- Molecule 1: Inactive protein-arginine deiminase type-6

Chain 13: 67% 33%

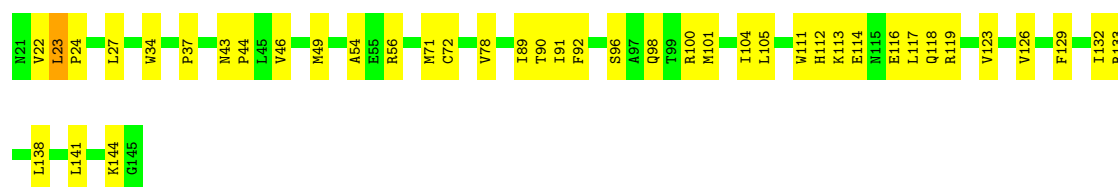






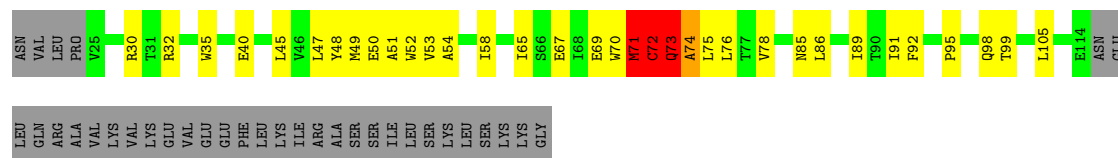
- Molecule 2: Oocyte-expressed protein homolog

Chain C: 67% 32%



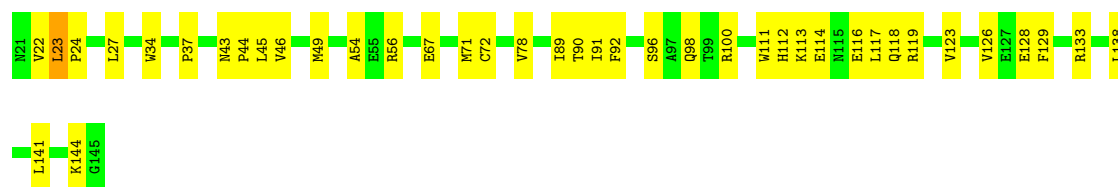
- Molecule 2: Oocyte-expressed protein homolog

Chain H: 45% 24% 28%



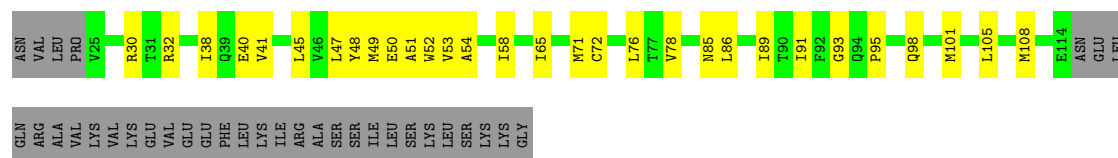
- Molecule 2: Oocyte-expressed protein homolog

Chain c: 68% 31%



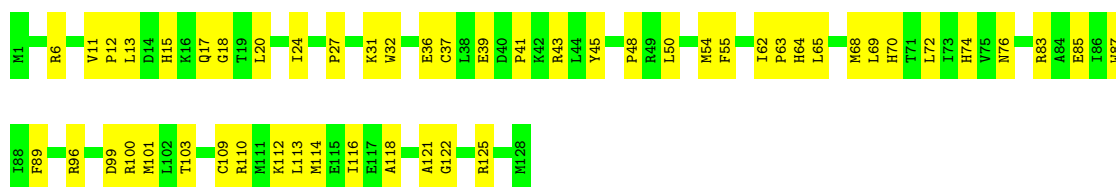
- Molecule 2: Oocyte-expressed protein homolog

Chain h: 48% 24% 28%



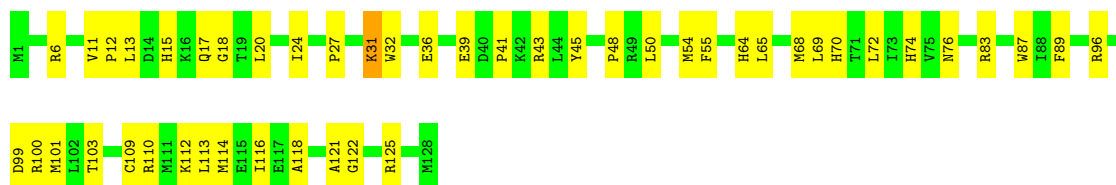
- Molecule 3: KH domain-containing protein 3

Chain D:  60% 40%



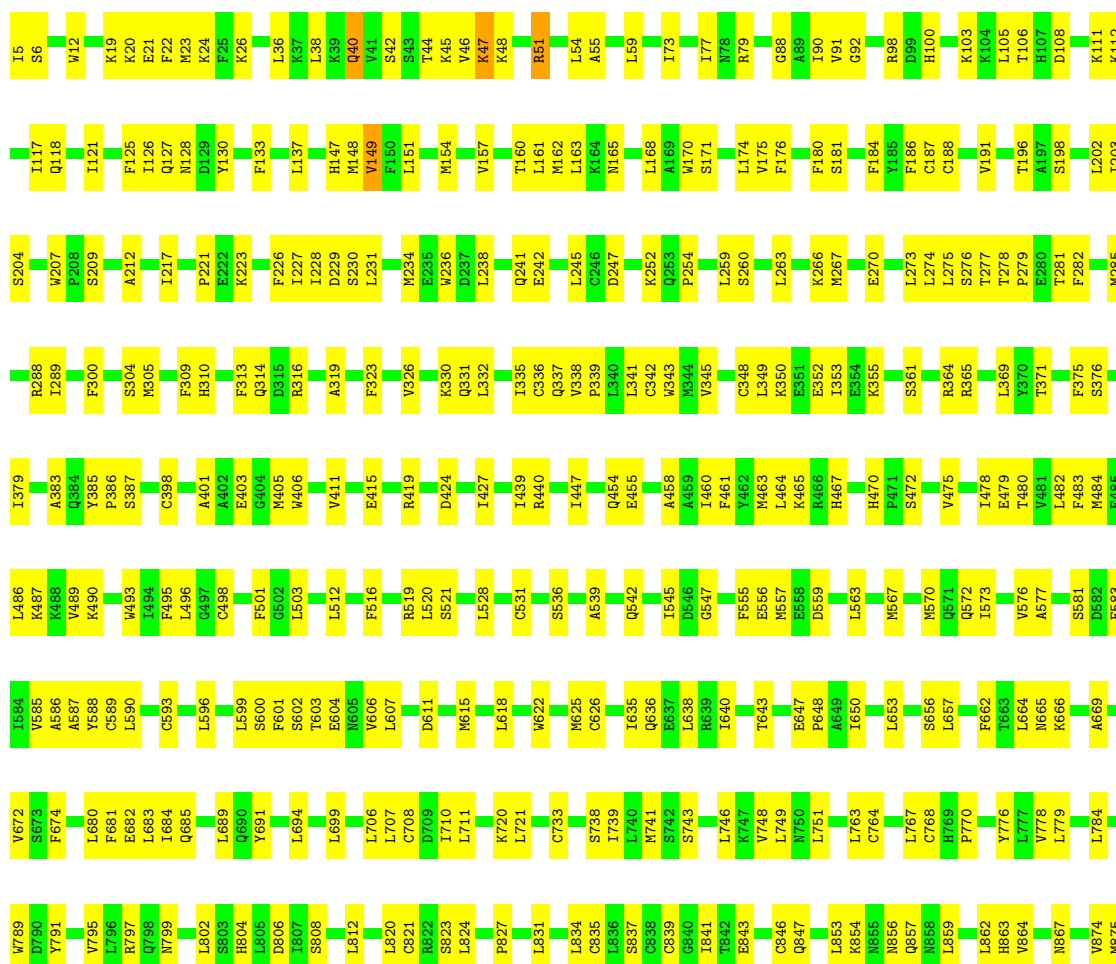
• Molecule 3: KH domain-containing protein 3

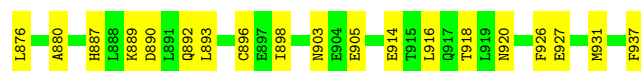
Chain d:  63% 36%



• Molecule 4: NLR family, pyrin domain containing 4F

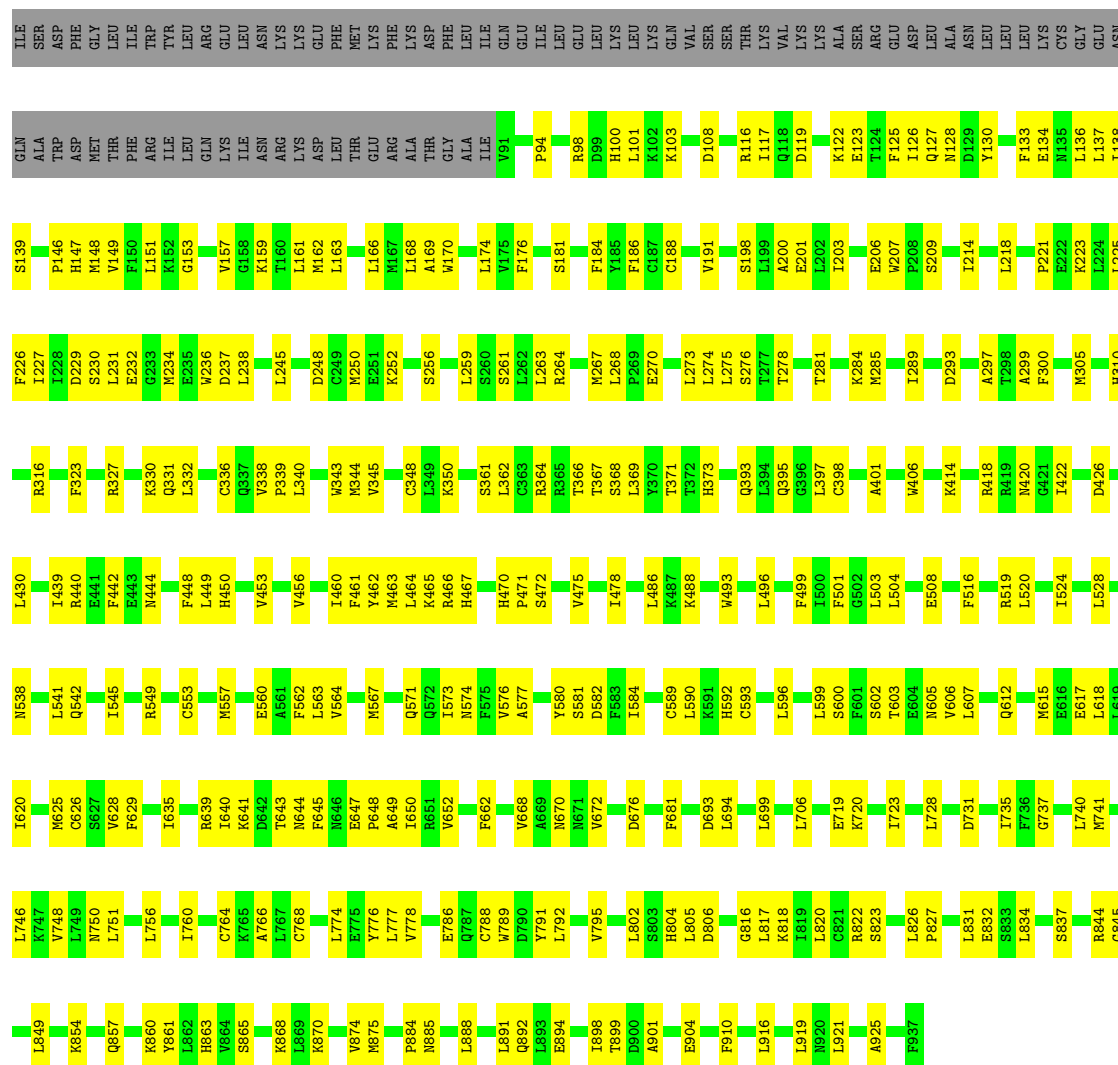
Chain E:  62% 37%





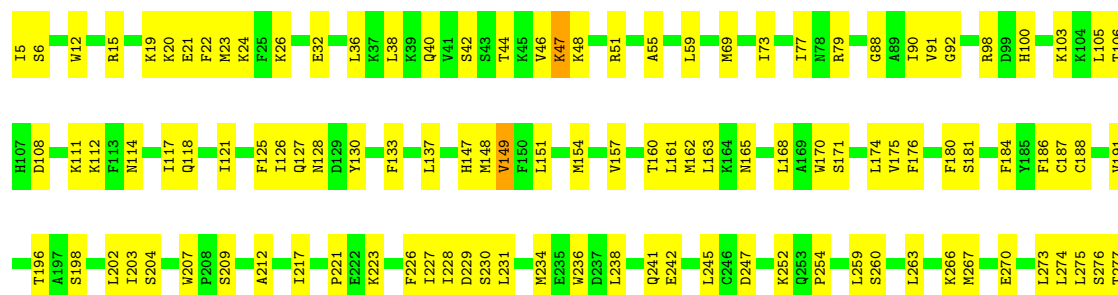
- Molecule 4: NLR family, pyrin domain containing 4F

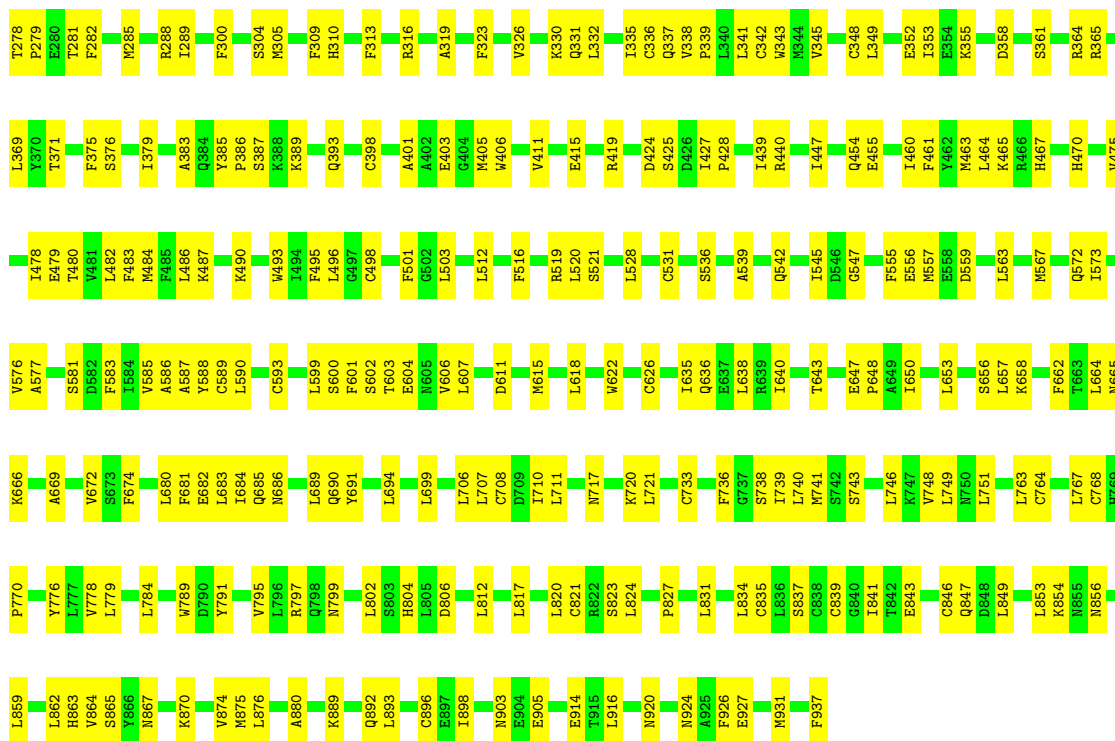
Chain I: 59% 32% 9%



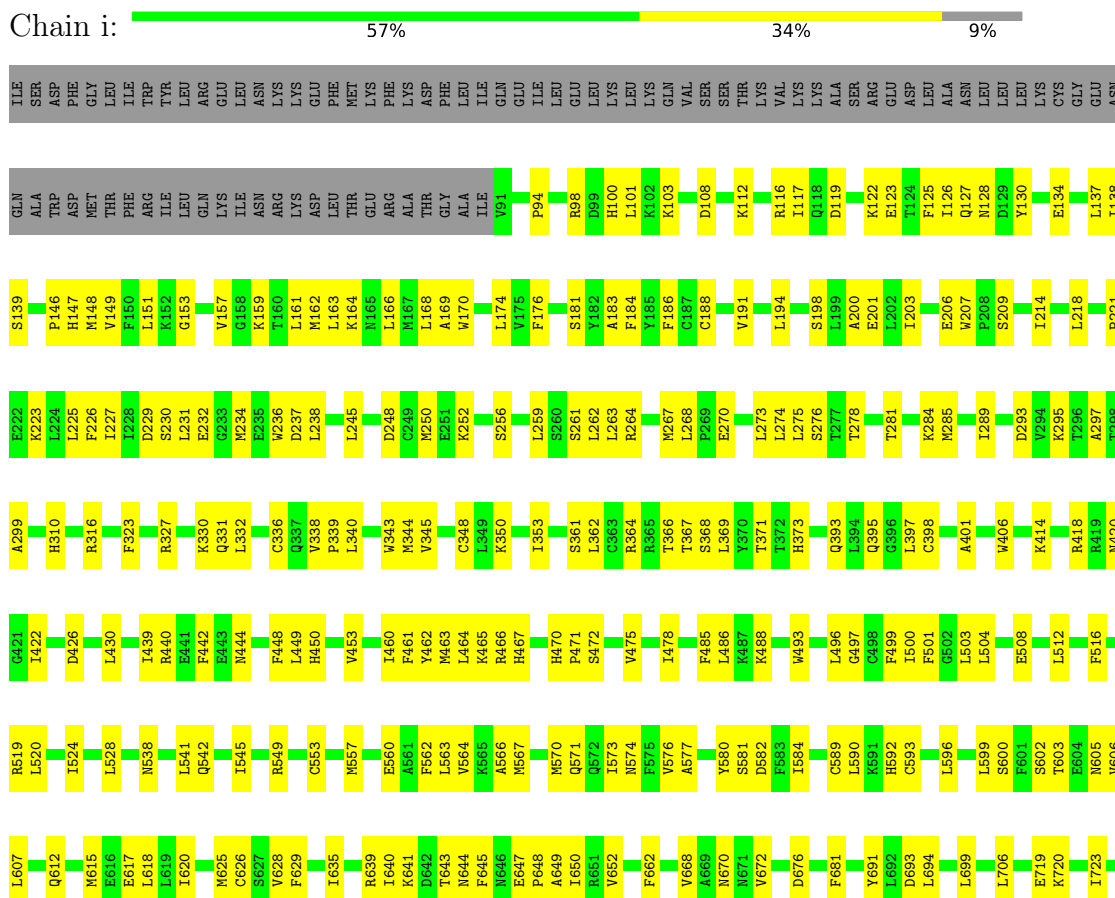
- Molecule 4: NLR family, pyrin domain containing 4F

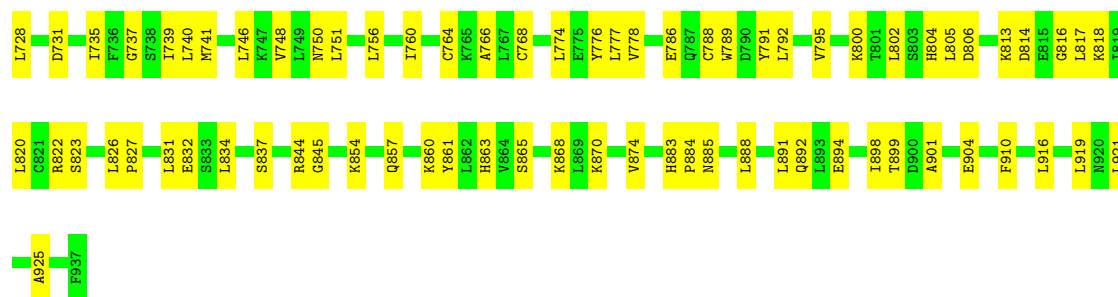
Chain e: 62% 38%





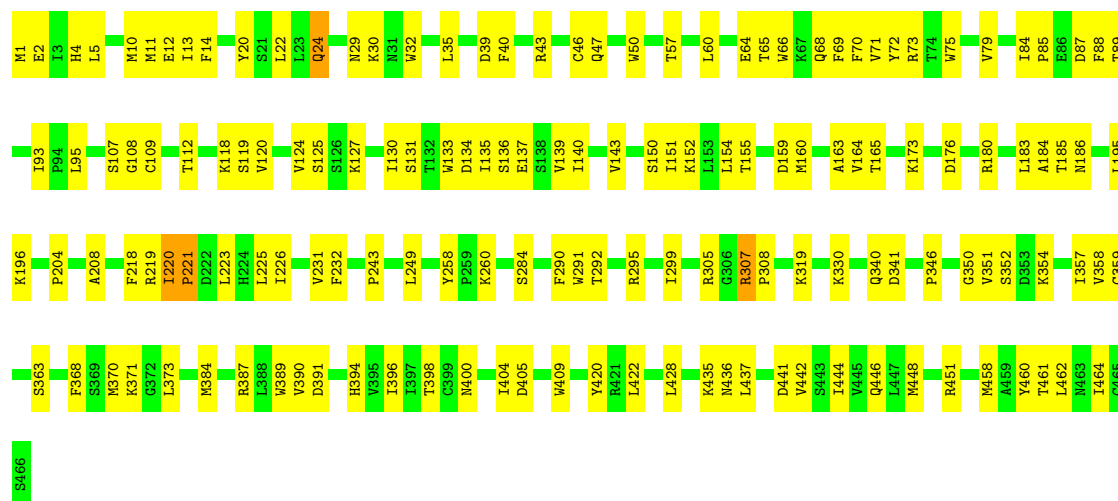
- Molecule 4: NLR family, pyrin domain containing 4F





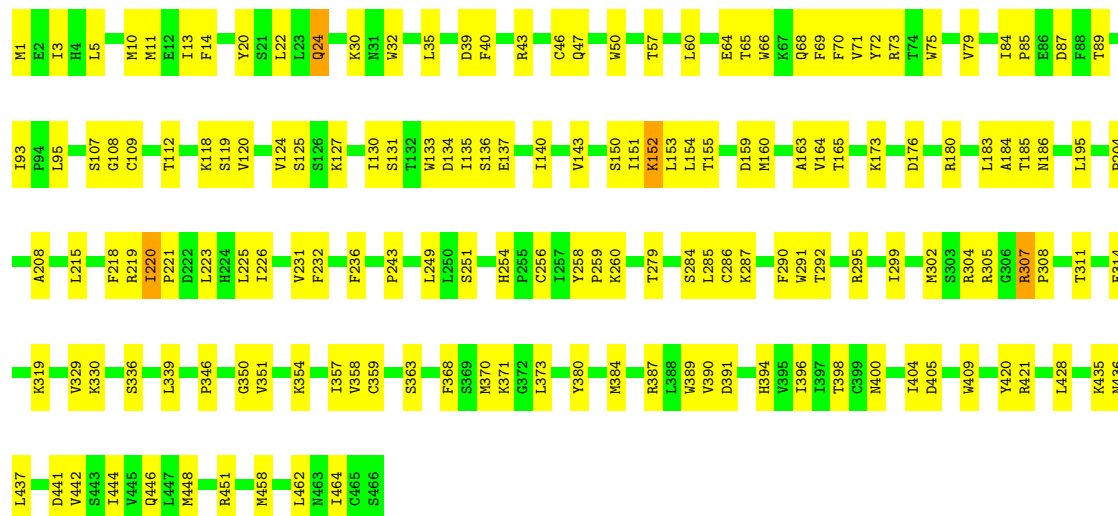
• Molecule 5: FBXW24

Chain J: 68% 32%



• Molecule 5: FBXW24

Chain j: 66% 33%



• Molecule 6: S-phase kinase-associated protein 1

- Molecule 6: S-phase kinase-associated protein 1

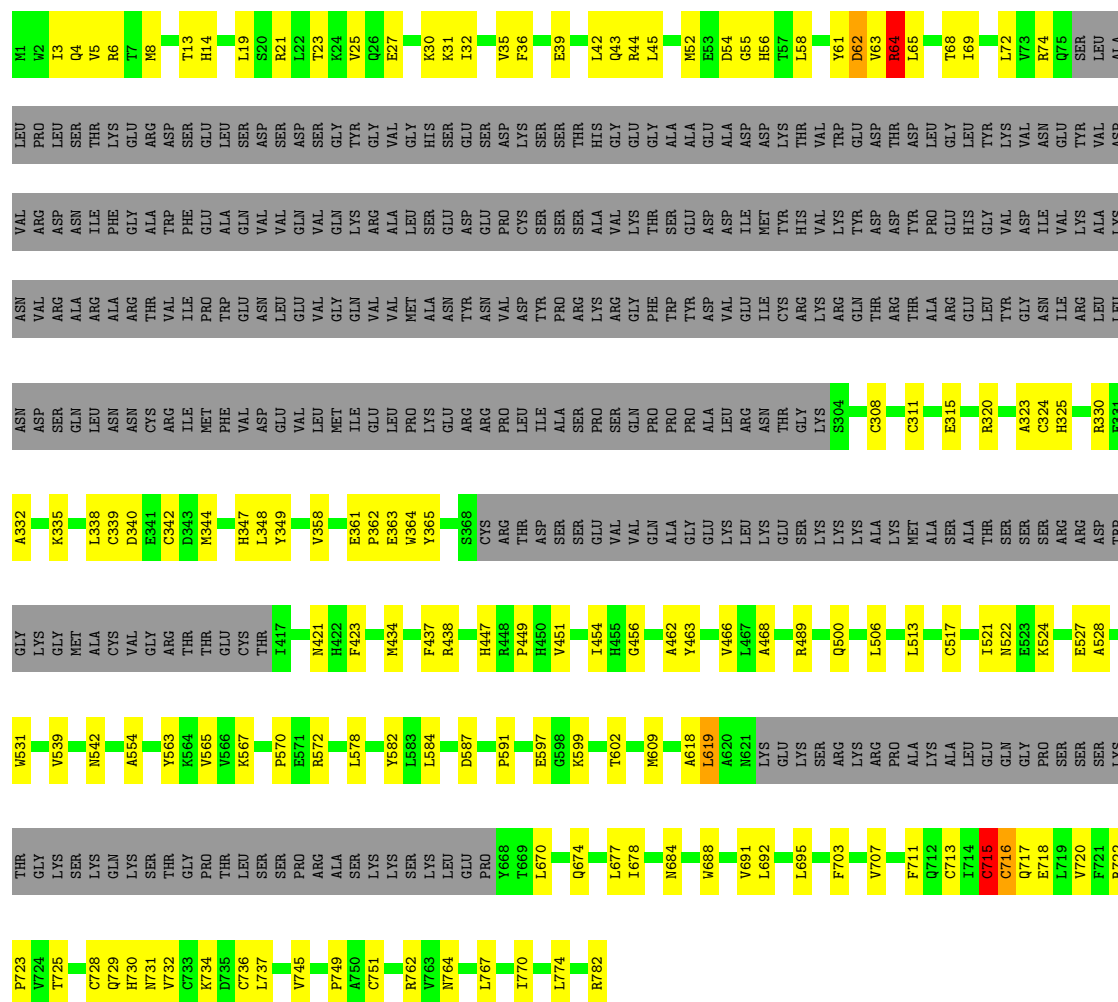
- Molecule 7: Ubiquitin-conjugating enzyme E2 D3

- Molecule 7: Ubiquitin-conjugating enzyme E2 D3

- Molecule 8: E3 ubiquitin-protein ligase UHRF1







- Molecule 9: Zinc finger BED domain-containing protein 3

Chain R: 51% 44% 5%



- Molecule 9: Zinc finger BED domain-containing protein 3

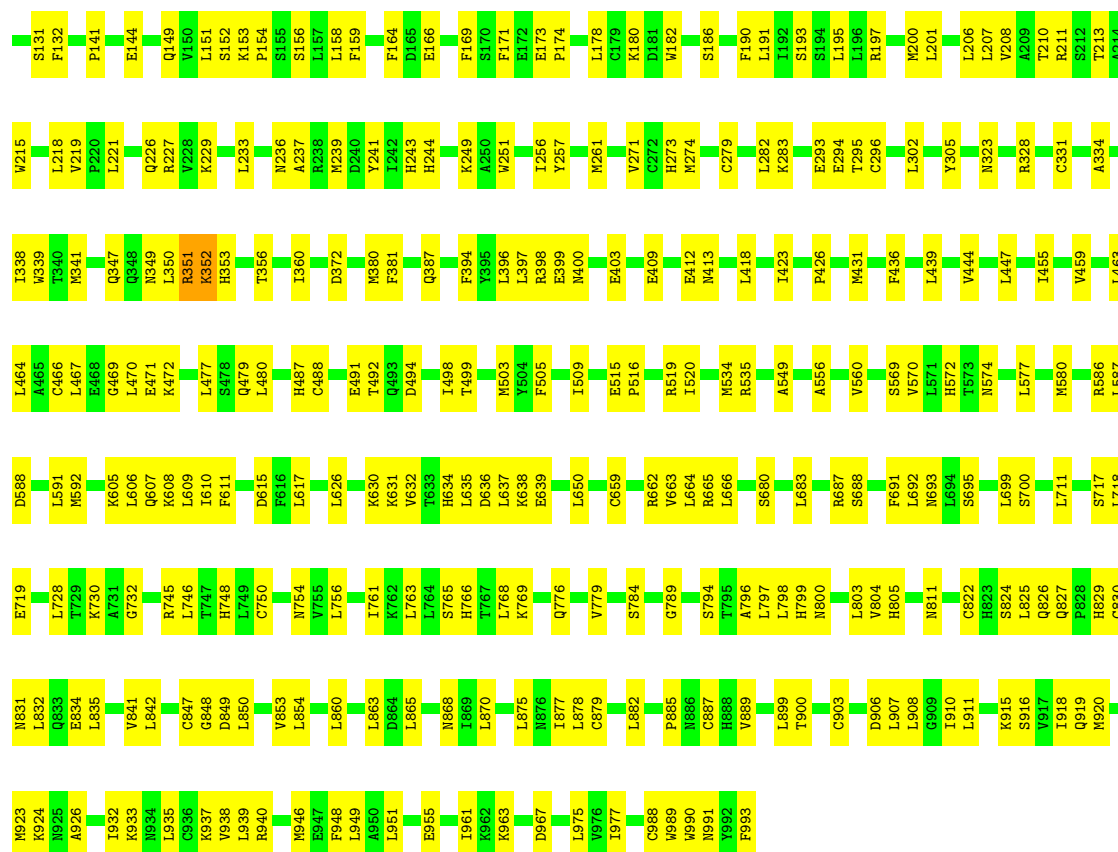
Chain r: 56% 42% 2%



- Molecule 10: NACHT, LRR and PYD domains-containing protein 14

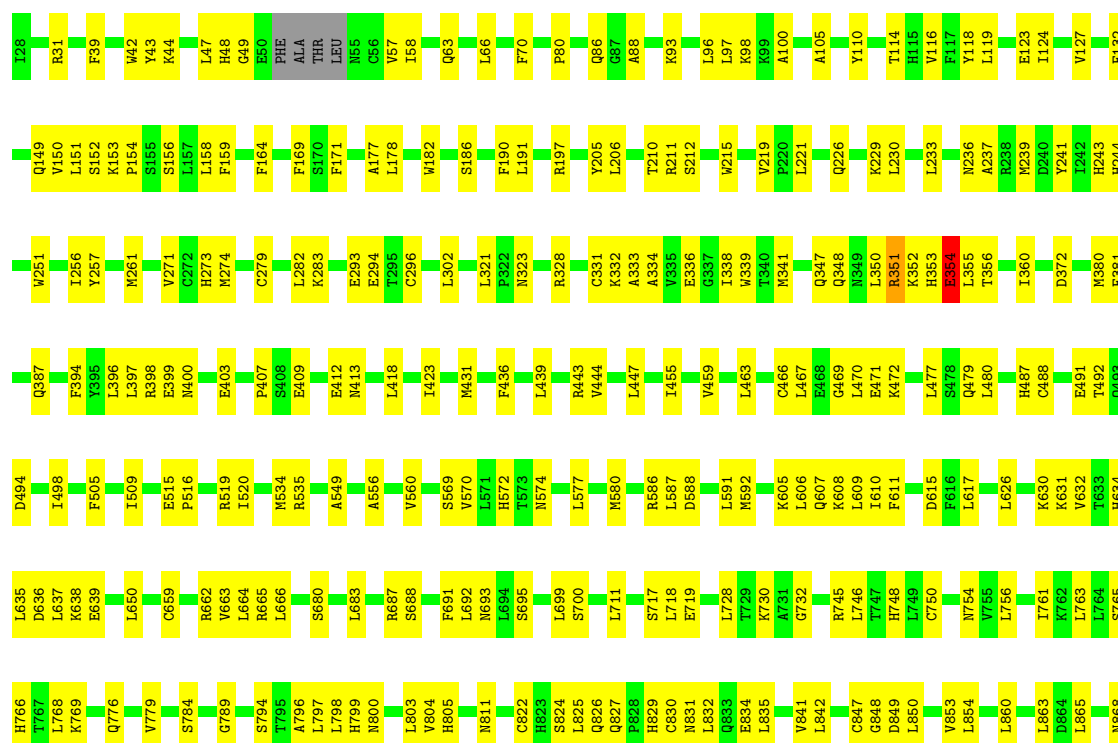
Chain N: 67% 33% 0%





- Molecule 10: NACHT, LRR and PYD domains-containing protein 14

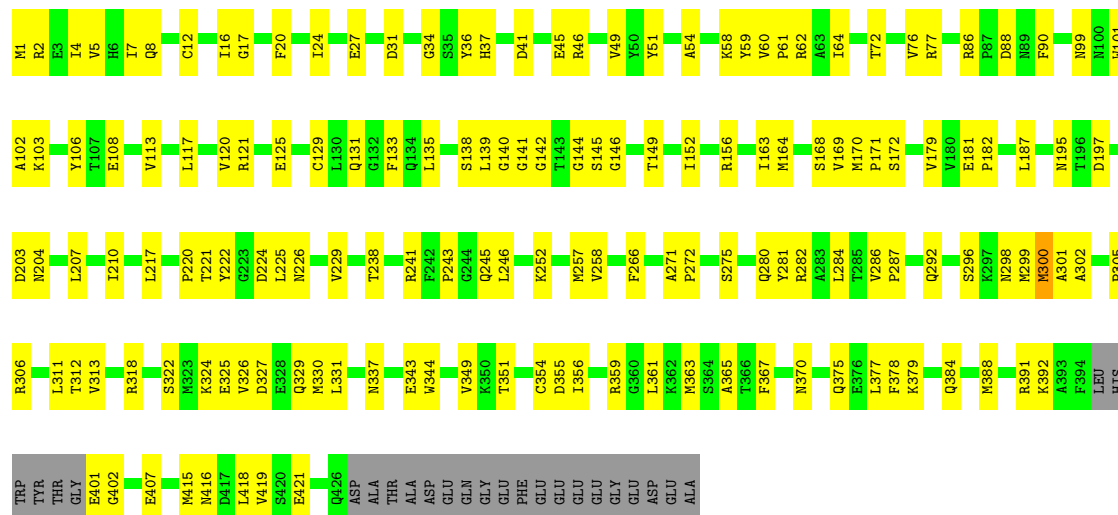
Chain n: 68% 31%





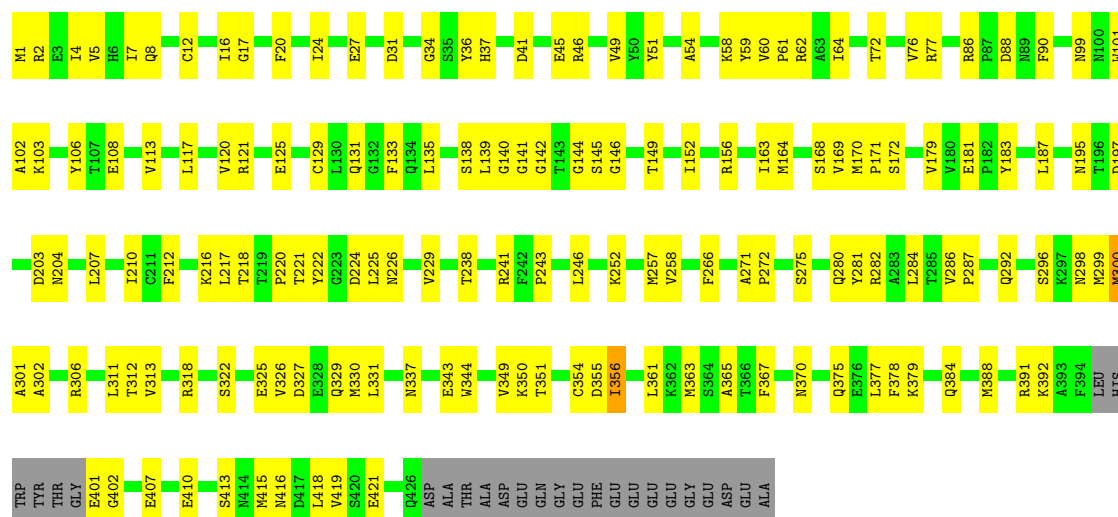
• Molecule 11: Tubulin beta-2A chain

Chain L: 60% 34% 6%



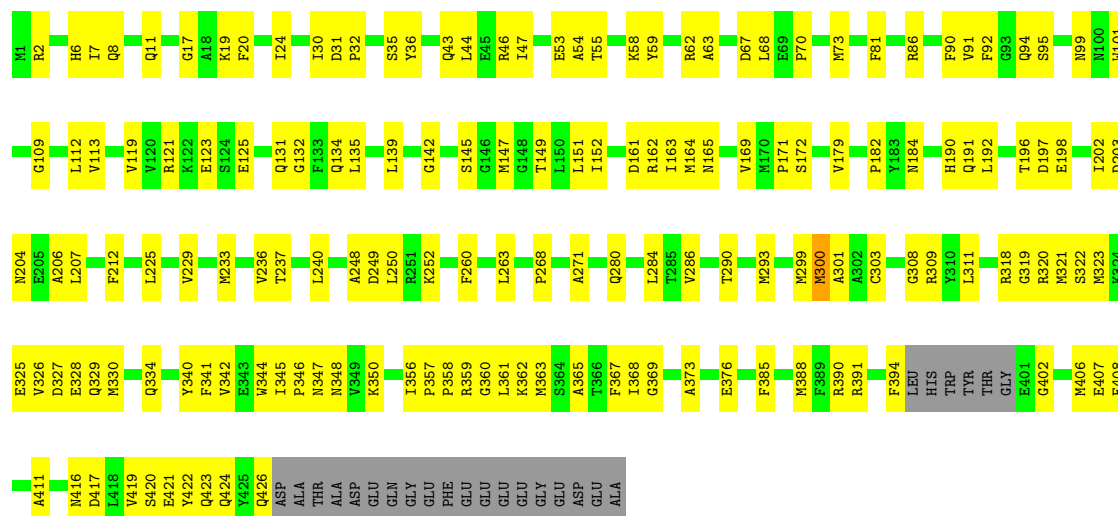
• Molecule 11: Tubulin beta-2A chain

Chain l: 59% 35% 6%

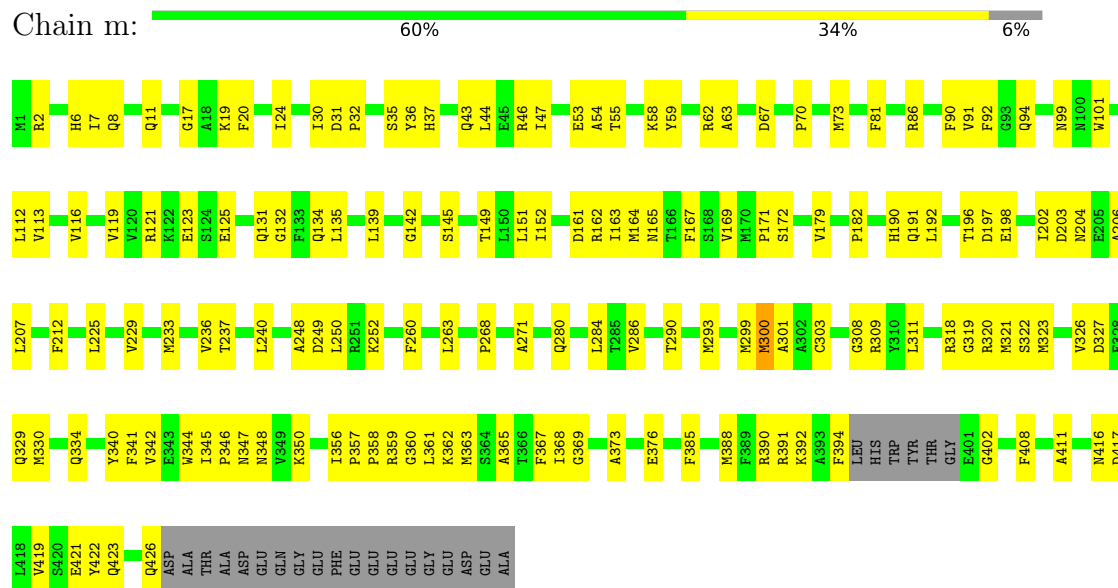


• Molecule 12: Tubulin beta-2B chain

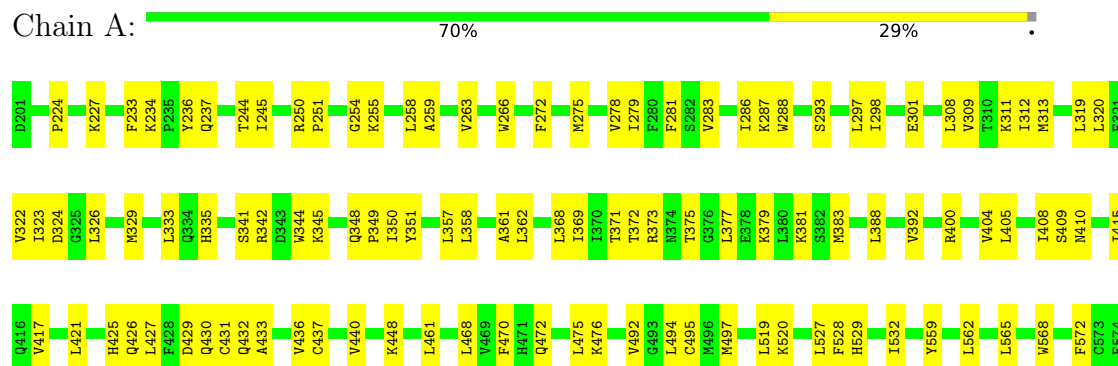
Chain M: 58% 36% 6%



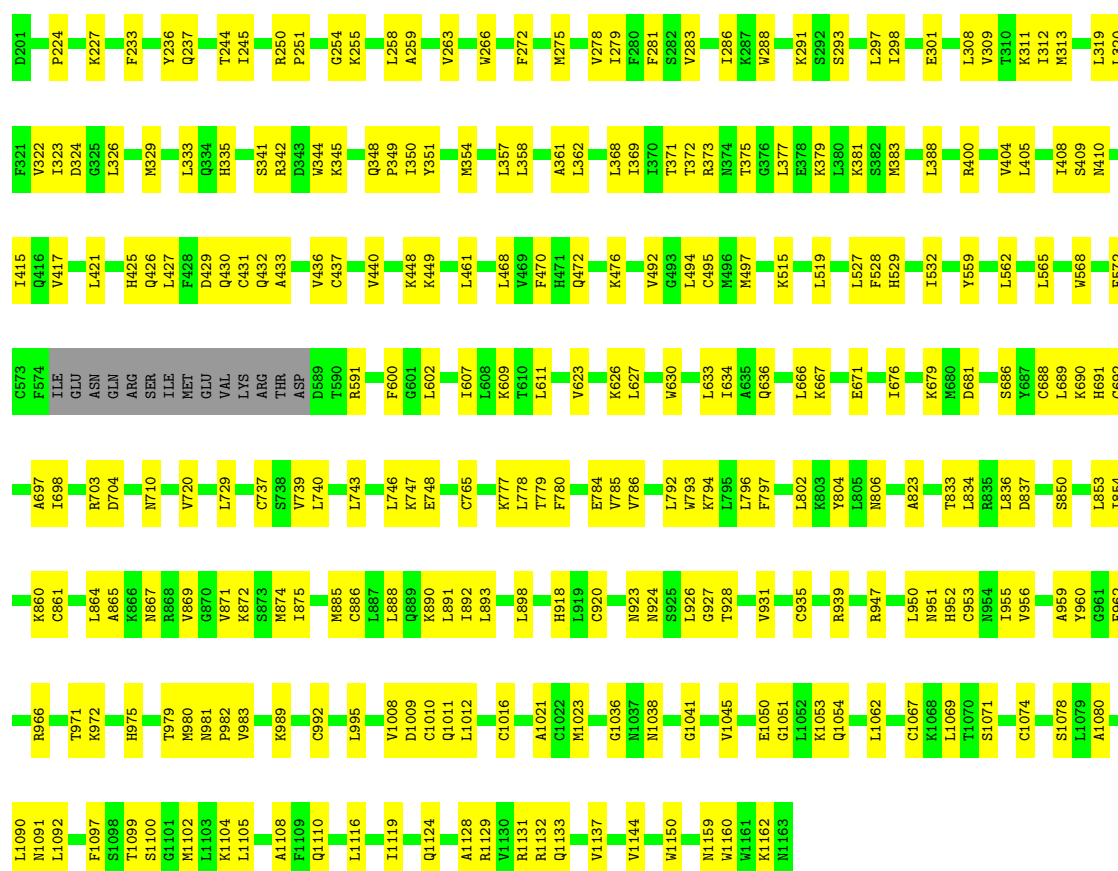
• Molecule 12: Tubulin beta-2B chain



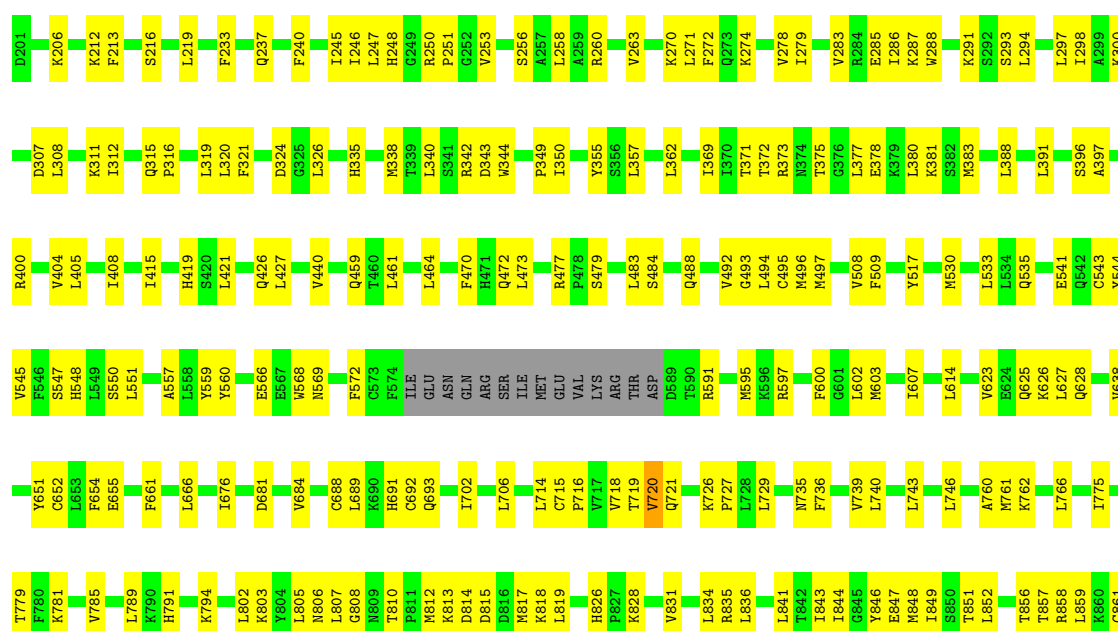
• Molecule 13: Isoform 4 of NACHT, LRR and PYD domains-containing protein 5

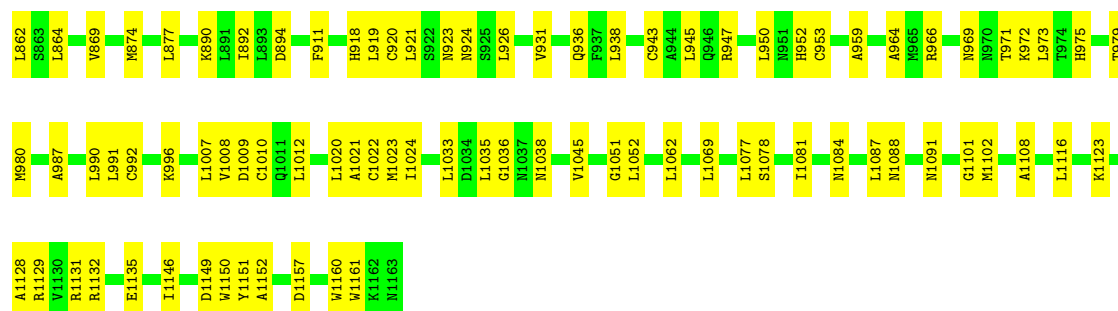




Chain a:  71% 28%

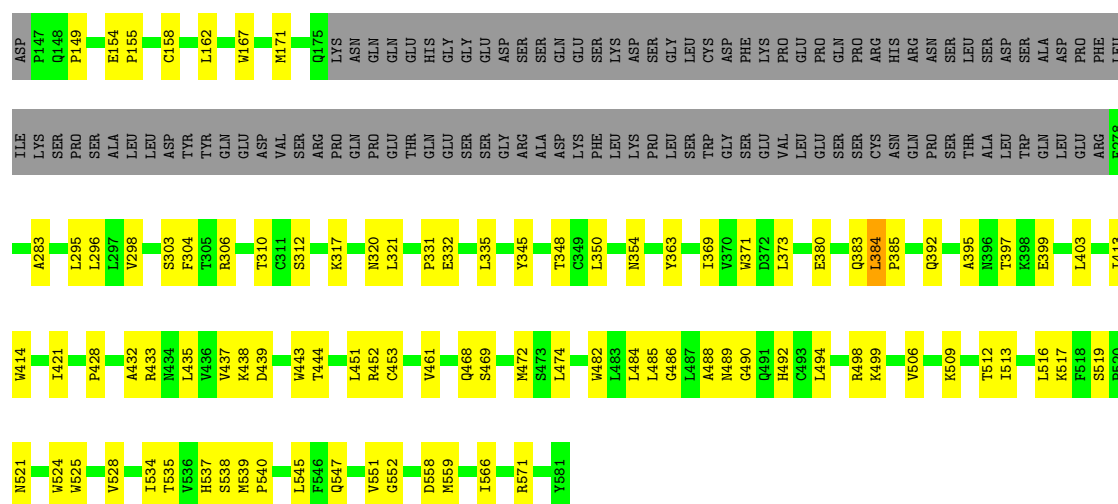
- Molecule 13: Isoform 4 of NACHT, LRR and PYD domains-containing protein 5

Chain f:  68% 31%



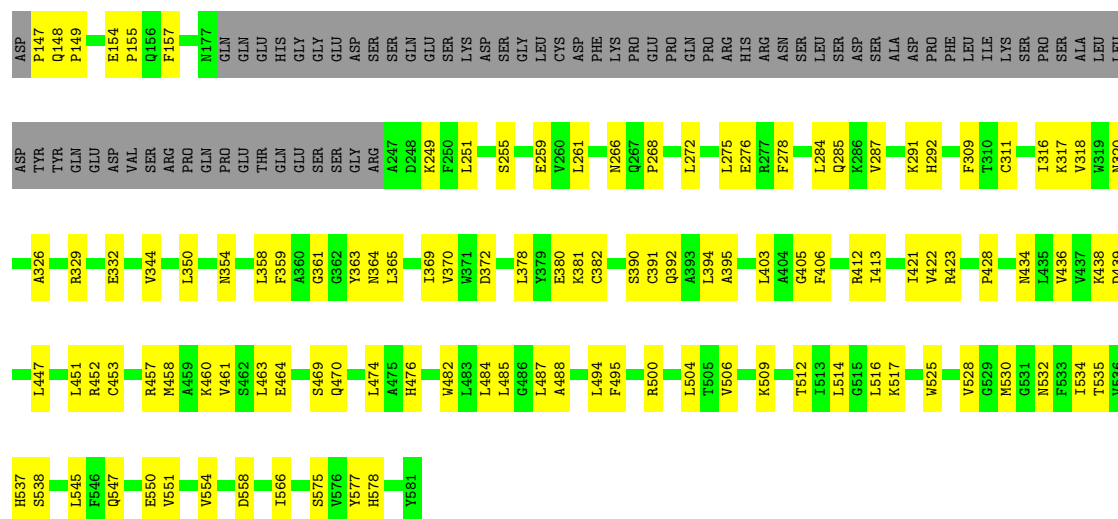
- Molecule 14: Transducin-like enhancer protein 6

Chain B: 55% 22% 24%

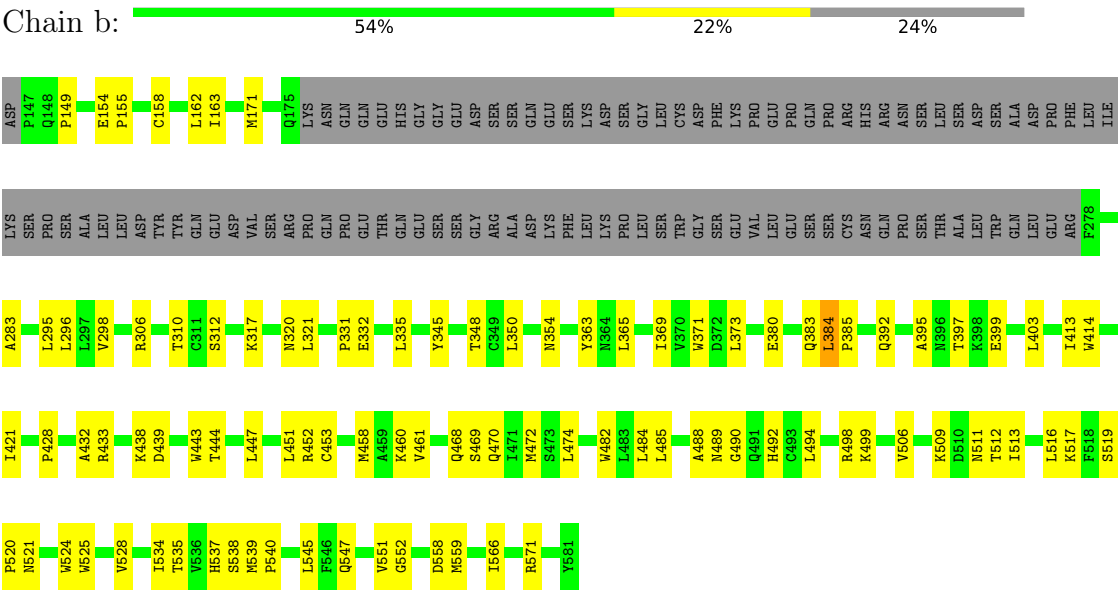


- Molecule 14: Transducin-like enhancer protein 6

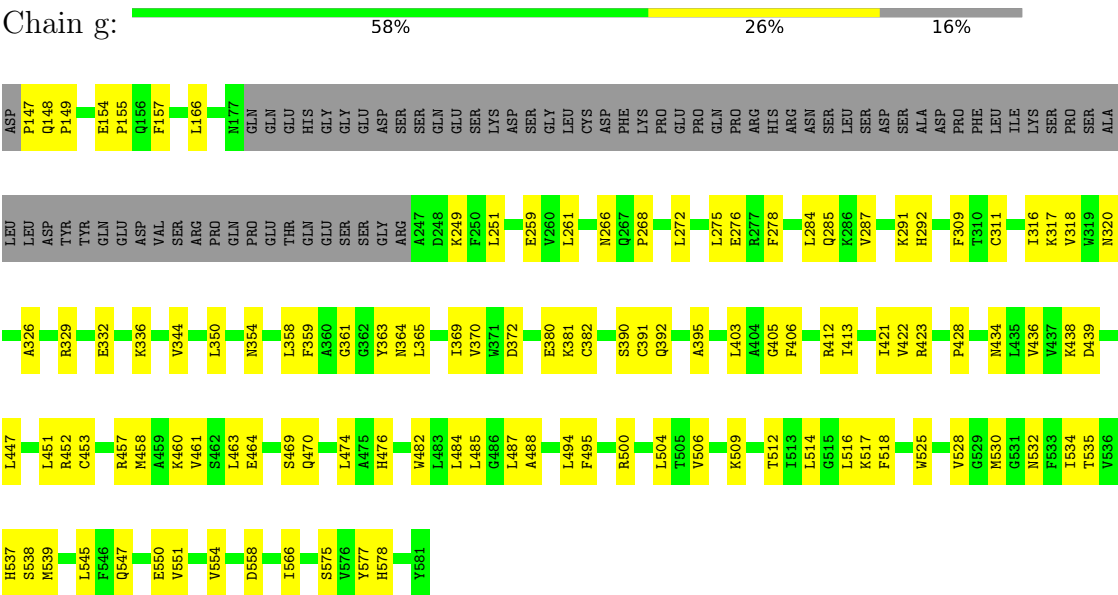
Chain G: 58% 26% 16%



- Molecule 14: Transducin-like enhancer protein 6



● Molecule 14: Transducin-like enhancer protein 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	676923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.19	0/5508	0.41	1/7470 (0.0%)
1	11	0.19	0/5508	0.40	1/7470 (0.0%)
1	12	0.18	0/5511	0.35	0/7475
1	13	0.13	0/5511	0.32	0/7475
1	14	0.12	0/5511	0.32	0/7475
1	15	0.14	0/5511	0.34	0/7475
1	16	0.13	0/5511	0.34	0/7475
1	17	0.18	0/5511	0.37	0/7475
1	18	0.25	0/5511	0.47	0/7475
1	19	0.13	0/5511	0.34	0/7475
1	2	0.18	0/5511	0.36	0/7475
1	3	0.14	0/5511	0.33	0/7475
1	4	0.12	0/5511	0.31	0/7475
1	5	0.14	0/5511	0.34	0/7475
1	6	0.13	0/5511	0.33	0/7475
1	7	0.18	0/5511	0.38	0/7475
1	8	0.23	0/5511	0.40	0/7475
1	9	0.13	0/5511	0.35	0/7475
1	Z	0.14	0/5511	0.35	1/7475 (0.0%)
1	z	0.16	0/5511	0.38	0/7475
2	C	0.17	0/1022	0.44	0/1385
2	H	0.22	0/743	0.49	2/1013 (0.2%)
2	c	0.16	0/1022	0.44	0/1385
2	h	0.14	0/743	0.39	0/1013
3	D	0.16	0/1099	0.37	0/1483
3	d	0.15	0/1099	0.36	0/1483
4	E	0.13	0/7660	0.33	0/10315
4	I	0.12	0/6936	0.31	0/9348
4	e	0.13	0/7660	0.33	0/10315
4	i	0.12	0/6936	0.31	0/9348
5	J	0.15	0/3839	0.43	0/5207
5	j	0.15	0/3839	0.41	0/5207

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	K	0.13	0/1282	0.38	0/1737
6	k	0.14	0/1282	0.40	0/1737
7	O	0.21	0/1209	0.47	1/1647 (0.1%)
7	o	0.21	0/1209	0.47	1/1647 (0.1%)
8	P	0.17	0/3791	0.40	0/5124
8	Q	0.20	0/873	0.40	0/1182
8	p	0.20	0/3762	0.44	2/5084 (0.0%)
8	q	0.16	0/873	0.38	0/1182
9	R	0.19	0/461	0.46	0/626
9	r	0.17	0/461	0.42	0/626
10	N	0.14	0/7832	0.34	1/10586 (0.0%)
10	n	0.14	0/7832	0.34	1/10586 (0.0%)
11	L	0.15	0/3358	0.41	1/4547 (0.0%)
11	l	0.16	0/3358	0.42	1/4547 (0.0%)
12	M	0.16	0/3360	0.42	0/4550
12	m	0.15	0/3360	0.41	0/4550
13	A	0.15	0/7613	0.36	0/10294
13	F	0.16	0/7613	0.38	0/10294
13	a	0.15	0/7613	0.36	0/10294
13	f	0.16	0/7613	0.39	0/10294
14	B	0.13	0/2685	0.35	0/3643
14	G	0.13	0/2956	0.35	0/4011
14	b	0.13	0/2685	0.33	0/3643
14	g	0.13	0/2956	0.35	0/4011
All	All	0.16	0/238849	0.37	13/323434 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	16	0	1
5	J	0	3
5	j	0	3
8	p	0	1
9	R	0	1
9	r	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	p	716	CYS	CA-CB-SG	8.10	133.03	114.40
1	1	131	PRO	N-CA-CB	7.01	110.61	103.25
1	11	131	PRO	N-CA-CB	6.99	110.59	103.25
7	O	111	CYS	CA-CB-SG	6.67	129.74	114.40
2	H	71	MET	N-CA-C	-6.67	101.69	110.43

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	J	220	ILE	Peptide
5	J	221	PRO	Peptide
5	J	307	ARG	Peptide
9	R	62	LEU	Peptide
5	j	220	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5386	0	5383	152	0
1	11	5386	0	5383	161	0
1	12	5388	0	5389	111	0
1	13	5388	0	5389	171	0
1	14	5388	0	5389	172	0
1	15	5388	0	5389	226	0
1	16	5388	0	5389	196	0
1	17	5388	0	5389	147	0
1	18	5388	0	5389	164	0
1	19	5388	0	5389	169	0
1	2	5388	0	5389	123	0
1	3	5388	0	5389	177	0
1	4	5388	0	5389	159	0
1	5	5388	0	5389	206	0
1	6	5388	0	5389	185	0
1	7	5388	0	5389	141	0
1	8	5388	0	5389	145	0
1	9	5388	0	5389	172	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	5388	0	5389	159	0
1	z	5388	0	5389	178	0
2	C	1003	0	1032	48	0
2	H	726	0	722	28	0
2	c	1003	0	1032	47	0
2	h	726	0	722	21	0
3	D	1069	0	1084	49	0
3	d	1069	0	1084	48	0
4	E	7519	0	7583	271	0
4	I	6805	0	6831	236	0
4	e	7519	0	7583	266	0
4	i	6805	0	6831	236	0
5	J	3747	0	3770	119	0
5	j	3747	0	3770	131	0
6	K	1261	0	1243	43	0
6	k	1261	0	1243	52	0
7	O	1174	0	1159	39	0
7	o	1174	0	1159	35	0
8	P	3704	0	3591	112	0
8	Q	856	0	874	50	0
8	p	3675	0	3563	113	0
8	q	856	0	874	47	0
9	R	445	0	413	46	0
9	r	445	0	413	33	0
10	N	7689	0	7791	227	0
10	n	7689	0	7791	224	0
11	L	3288	0	3162	118	0
11	l	3288	0	3162	117	0
12	M	3290	0	3164	113	0
12	m	3290	0	3164	111	0
13	A	7481	0	7567	191	0
13	F	7481	0	7569	222	0
13	a	7481	0	7567	186	0
13	f	7481	0	7569	215	0
14	B	2626	0	2613	66	0
14	G	2890	0	2872	70	0
14	b	2626	0	2613	66	0
14	g	2890	0	2872	70	0
15	L	28	0	12	2	0
15	M	28	0	12	1	0
15	l	28	0	12	2	0
15	m	28	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	27	0	12	2	0
16	F	27	0	12	1	0
16	a	27	0	12	2	0
16	f	27	0	12	1	0
All	All	234055	0	233916	7049	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7049 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:904:GLU:HB2	9:r:66:GLN:OE1	1.28	1.30
4:I:904:GLU:N	9:R:66:GLN:OE1	1.63	1.28
4:i:904:GLU:CB	9:r:66:GLN:OE1	1.84	1.26
7:O:107:CYS:O	7:O:111:CYS:HB3	1.32	1.23
7:o:107:CYS:O	7:o:111:CYS:HB3	1.31	1.22

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	680/682 (100%)	629 (92%)	49 (7%)	2 (0%)	36	71
1	11	680/682 (100%)	634 (93%)	44 (6%)	2 (0%)	36	71
1	12	680/682 (100%)	641 (94%)	39 (6%)	0	100	100
1	13	680/682 (100%)	648 (95%)	32 (5%)	0	100	100
1	14	680/682 (100%)	654 (96%)	26 (4%)	0	100	100
1	15	680/682 (100%)	640 (94%)	39 (6%)	1 (0%)	48	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	16	680/682 (100%)	638 (94%)	41 (6%)	1 (0%)	48	82
1	17	680/682 (100%)	642 (94%)	38 (6%)	0	100	100
1	18	680/682 (100%)	632 (93%)	46 (7%)	2 (0%)	36	71
1	19	680/682 (100%)	641 (94%)	38 (6%)	1 (0%)	48	82
1	2	680/682 (100%)	636 (94%)	44 (6%)	0	100	100
1	3	680/682 (100%)	646 (95%)	30 (4%)	4 (1%)	21	58
1	4	680/682 (100%)	659 (97%)	21 (3%)	0	100	100
1	5	680/682 (100%)	642 (94%)	38 (6%)	0	100	100
1	6	680/682 (100%)	638 (94%)	41 (6%)	1 (0%)	48	82
1	7	680/682 (100%)	643 (95%)	37 (5%)	0	100	100
1	8	680/682 (100%)	629 (92%)	51 (8%)	0	100	100
1	9	680/682 (100%)	642 (94%)	37 (5%)	1 (0%)	48	82
1	Z	680/682 (100%)	645 (95%)	35 (5%)	0	100	100
1	z	680/682 (100%)	654 (96%)	26 (4%)	0	100	100
2	C	123/125 (98%)	111 (90%)	11 (9%)	1 (1%)	16	52
2	H	88/125 (70%)	79 (90%)	7 (8%)	2 (2%)	5	29
2	c	123/125 (98%)	111 (90%)	11 (9%)	1 (1%)	16	52
2	h	88/125 (70%)	82 (93%)	6 (7%)	0	100	100
3	D	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
3	d	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
4	E	931/933 (100%)	881 (95%)	48 (5%)	2 (0%)	43	77
4	I	845/933 (91%)	813 (96%)	32 (4%)	0	100	100
4	e	931/933 (100%)	882 (95%)	47 (5%)	2 (0%)	43	77
4	i	845/933 (91%)	816 (97%)	29 (3%)	0	100	100
5	J	464/466 (100%)	416 (90%)	47 (10%)	1 (0%)	43	77
5	j	464/466 (100%)	419 (90%)	44 (10%)	1 (0%)	43	77
6	K	156/163 (96%)	135 (86%)	18 (12%)	3 (2%)	6	32
6	k	156/163 (96%)	137 (88%)	16 (10%)	3 (2%)	6	32
7	O	145/147 (99%)	132 (91%)	13 (9%)	0	100	100
7	o	145/147 (99%)	133 (92%)	12 (8%)	0	100	100
8	P	456/782 (58%)	404 (89%)	49 (11%)	3 (1%)	18	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Q	102/782 (13%)	86 (84%)	15 (15%)	1 (1%)	12	47
8	p	452/782 (58%)	403 (89%)	45 (10%)	4 (1%)	14	49
8	q	102/782 (13%)	86 (84%)	15 (15%)	1 (1%)	12	47
9	R	53/55 (96%)	41 (77%)	11 (21%)	1 (2%)	6	32
9	r	53/55 (96%)	41 (77%)	12 (23%)	0	100	100
10	N	958/966 (99%)	894 (93%)	62 (6%)	2 (0%)	43	77
10	n	958/966 (99%)	888 (93%)	67 (7%)	3 (0%)	36	71
11	L	416/445 (94%)	378 (91%)	35 (8%)	3 (1%)	18	54
11	l	416/445 (94%)	379 (91%)	34 (8%)	3 (1%)	18	54
12	M	416/445 (94%)	374 (90%)	40 (10%)	2 (0%)	24	62
12	m	416/445 (94%)	371 (89%)	42 (10%)	3 (1%)	18	54
13	A	945/963 (98%)	882 (93%)	62 (7%)	1 (0%)	48	82
13	F	945/963 (98%)	865 (92%)	76 (8%)	4 (0%)	30	66
13	a	945/963 (98%)	883 (93%)	61 (6%)	1 (0%)	48	82
13	f	945/963 (98%)	863 (91%)	80 (8%)	2 (0%)	43	77
14	B	329/436 (76%)	310 (94%)	18 (6%)	1 (0%)	36	71
14	G	362/436 (83%)	334 (92%)	28 (8%)	0	100	100
14	b	329/436 (76%)	311 (94%)	17 (5%)	1 (0%)	36	71
14	g	362/436 (83%)	334 (92%)	28 (8%)	0	100	100
All	All	29316/32226 (91%)	27351 (93%)	1898 (6%)	67 (0%)	44	77

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	131	PRO
2	C	23	LEU
6	K	72	PRO
2	c	23	LEU
6	k	72	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	612/613 (100%)	612 (100%)	0	100	100
1	11	612/613 (100%)	611 (100%)	1 (0%)	87	85
1	12	613/613 (100%)	613 (100%)	0	100	100
1	13	613/613 (100%)	613 (100%)	0	100	100
1	14	613/613 (100%)	613 (100%)	0	100	100
1	15	613/613 (100%)	613 (100%)	0	100	100
1	16	613/613 (100%)	613 (100%)	0	100	100
1	17	613/613 (100%)	613 (100%)	0	100	100
1	18	613/613 (100%)	611 (100%)	2 (0%)	86	84
1	19	613/613 (100%)	613 (100%)	0	100	100
1	2	613/613 (100%)	613 (100%)	0	100	100
1	3	613/613 (100%)	609 (99%)	4 (1%)	76	78
1	4	613/613 (100%)	613 (100%)	0	100	100
1	5	613/613 (100%)	612 (100%)	1 (0%)	87	85
1	6	613/613 (100%)	613 (100%)	0	100	100
1	7	613/613 (100%)	613 (100%)	0	100	100
1	8	613/613 (100%)	613 (100%)	0	100	100
1	9	613/613 (100%)	613 (100%)	0	100	100
1	Z	613/613 (100%)	613 (100%)	0	100	100
1	z	613/613 (100%)	612 (100%)	1 (0%)	87	85
2	C	111/111 (100%)	111 (100%)	0	100	100
2	H	79/111 (71%)	76 (96%)	3 (4%)	29	51
2	c	111/111 (100%)	111 (100%)	0	100	100
2	h	79/111 (71%)	79 (100%)	0	100	100
3	D	116/116 (100%)	115 (99%)	1 (1%)	70	75
3	d	116/116 (100%)	115 (99%)	1 (1%)	70	75
4	E	859/859 (100%)	856 (100%)	3 (0%)	86	84
4	I	781/859 (91%)	781 (100%)	0	100	100
4	e	859/859 (100%)	858 (100%)	1 (0%)	88	88
4	i	781/859 (91%)	781 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	429/429 (100%)	428 (100%)	1 (0%)	87	85
5	j	429/429 (100%)	428 (100%)	1 (0%)	87	85
6	K	145/150 (97%)	145 (100%)	0	100	100
6	k	145/150 (97%)	145 (100%)	0	100	100
7	O	132/132 (100%)	132 (100%)	0	100	100
7	o	132/132 (100%)	132 (100%)	0	100	100
8	P	405/682 (59%)	399 (98%)	6 (2%)	57	70
8	Q	94/682 (14%)	94 (100%)	0	100	100
8	p	401/682 (59%)	399 (100%)	2 (0%)	81	81
8	q	94/682 (14%)	94 (100%)	0	100	100
9	R	46/46 (100%)	44 (96%)	2 (4%)	26	48
9	r	46/46 (100%)	46 (100%)	0	100	100
10	N	881/884 (100%)	879 (100%)	2 (0%)	87	85
10	n	881/884 (100%)	878 (100%)	3 (0%)	86	84
11	L	360/382 (94%)	360 (100%)	0	100	100
11	l	360/382 (94%)	360 (100%)	0	100	100
12	M	361/383 (94%)	360 (100%)	1 (0%)	86	84
12	m	361/383 (94%)	360 (100%)	1 (0%)	86	84
13	A	849/875 (97%)	849 (100%)	0	100	100
13	F	849/875 (97%)	847 (100%)	2 (0%)	87	85
13	a	849/875 (97%)	849 (100%)	0	100	100
13	f	849/875 (97%)	849 (100%)	0	100	100
14	B	292/386 (76%)	292 (100%)	0	100	100
14	G	322/386 (83%)	322 (100%)	0	100	100
14	b	292/386 (76%)	292 (100%)	0	100	100
14	g	322/386 (83%)	322 (100%)	0	100	100
All	All	26476/28956 (91%)	26437 (100%)	39 (0%)	87	88

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	F	703	ARG
12	m	280	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	F	705	LEU
10	n	354	GLU
1	18	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 304 such sidechains are listed below:

Mol	Chain	Res	Type
13	a	693	GLN
1	14	346	GLN
14	b	334	HIS
1	11	215	GLN
1	18	416	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GDP	L	501	-	28,30,30	1.17	3 (10%)	44,47,47	1.95	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GDP	l	501	-	28,30,30	1.16	3 (10%)	44,47,47	1.95	8 (18%)
16	ADP	F	1201	-	27,29,29	1.36	4 (14%)	42,45,45	1.97	9 (21%)
15	GDP	m	501	-	28,30,30	1.15	3 (10%)	44,47,47	1.91	8 (18%)
16	ADP	f	1201	-	27,29,29	1.36	4 (14%)	42,45,45	1.98	9 (21%)
15	GDP	M	501	-	28,30,30	1.15	3 (10%)	44,47,47	1.90	8 (18%)
16	ADP	A	1201	-	27,29,29	1.36	4 (14%)	42,45,45	1.96	10 (23%)
16	ADP	a	1201	-	27,29,29	1.37	4 (14%)	42,45,45	1.97	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GDP	L	501	-	-	3/16/32/32	0/3/3/3
15	GDP	l	501	-	-	3/16/32/32	0/3/3/3
16	ADP	F	1201	-	-	4/16/32/32	0/3/3/3
15	GDP	m	501	-	-	2/16/32/32	0/3/3/3
16	ADP	f	1201	-	-	4/16/32/32	0/3/3/3
15	GDP	M	501	-	-	2/16/32/32	0/3/3/3
16	ADP	A	1201	-	-	4/16/32/32	0/3/3/3
16	ADP	a	1201	-	-	4/16/32/32	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	1201	ADP	C5-C4	4.58	1.47	1.39
16	f	1201	ADP	C5-C4	4.58	1.47	1.39
16	a	1201	ADP	C5-C4	4.56	1.47	1.39
16	A	1201	ADP	C5-C4	4.53	1.47	1.39
15	L	501	GDP	C5-C4	3.17	1.47	1.38

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	l	501	GDP	C5-C4-N3	-6.72	117.56	128.46
15	L	501	GDP	C5-C4-N3	-6.72	117.56	128.46
15	m	501	GDP	C5-C4-N3	-6.56	117.81	128.46
15	M	501	GDP	C5-C4-N3	-6.54	117.84	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	f	1201	ADP	C5-C4-N3	-6.47	118.31	126.75

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

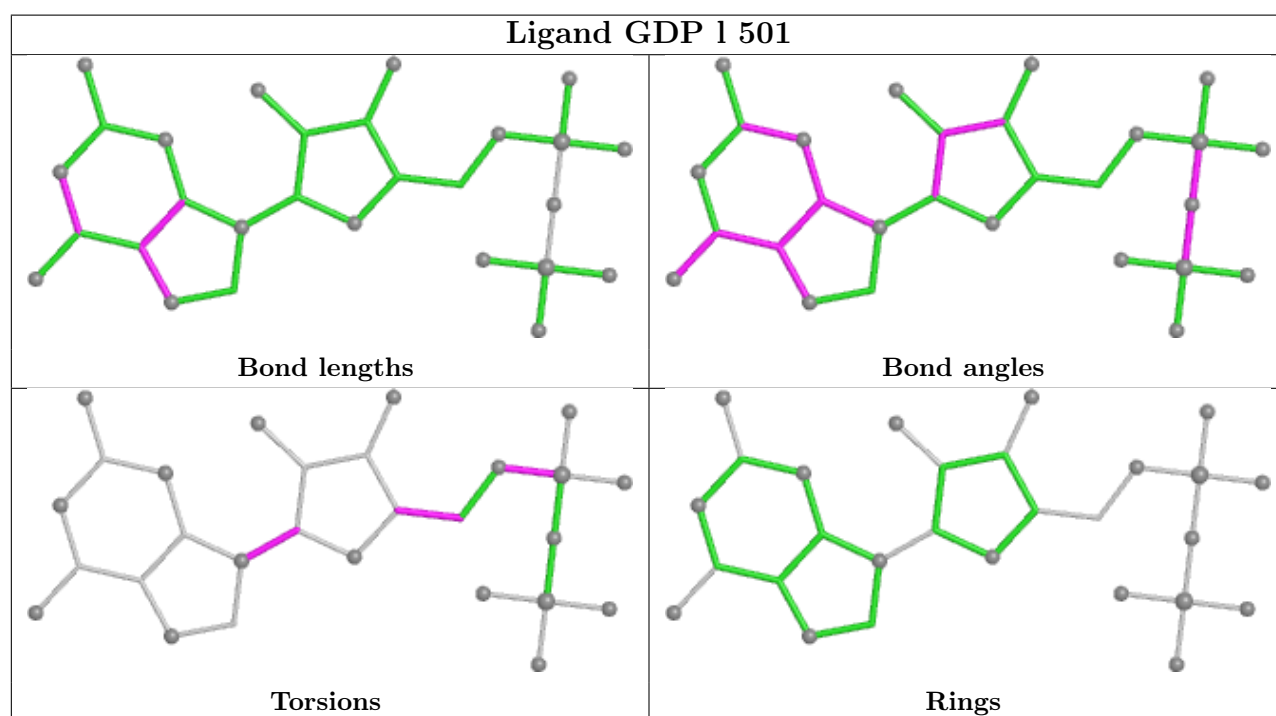
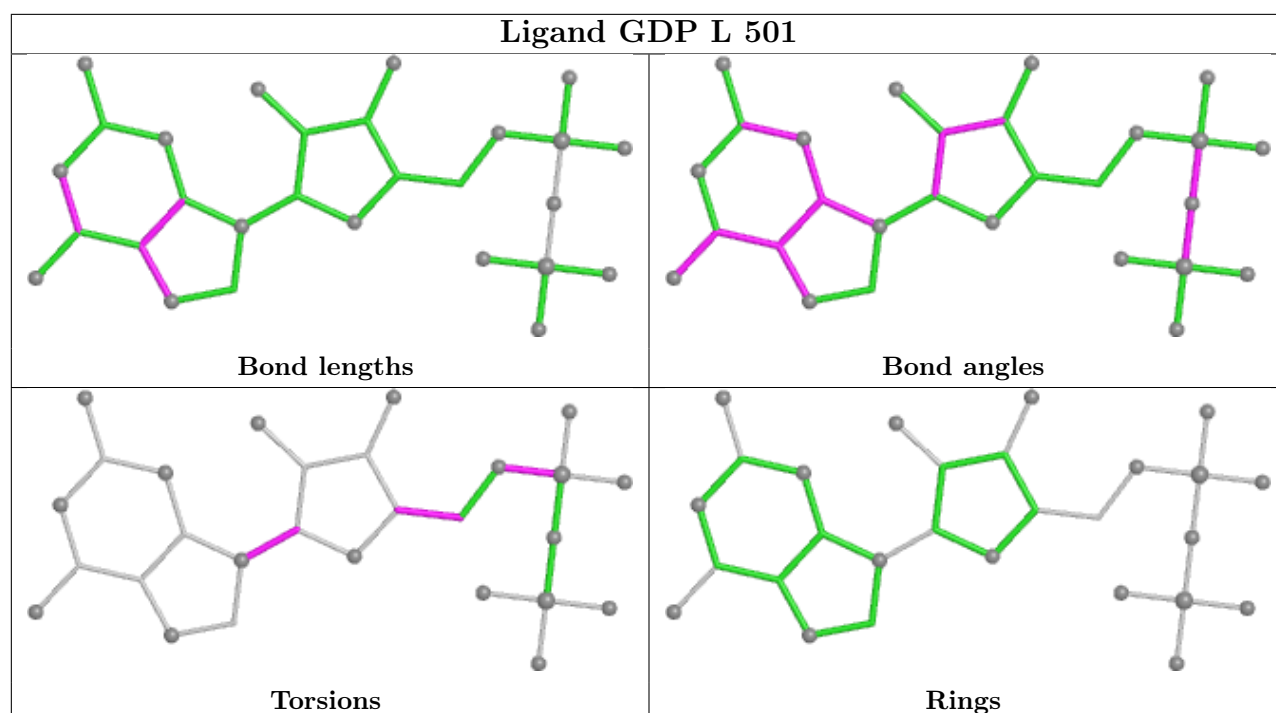
Mol	Chain	Res	Type	Atoms
15	L	501	GDP	O4'-C4'-C5'-O5'
15	l	501	GDP	O4'-C4'-C5'-O5'
16	A	1201	ADP	C5'-O5'-PA-O3A
16	F	1201	ADP	PA-O3A-PB-O3B
16	F	1201	ADP	PB-O3A-PA-O5'

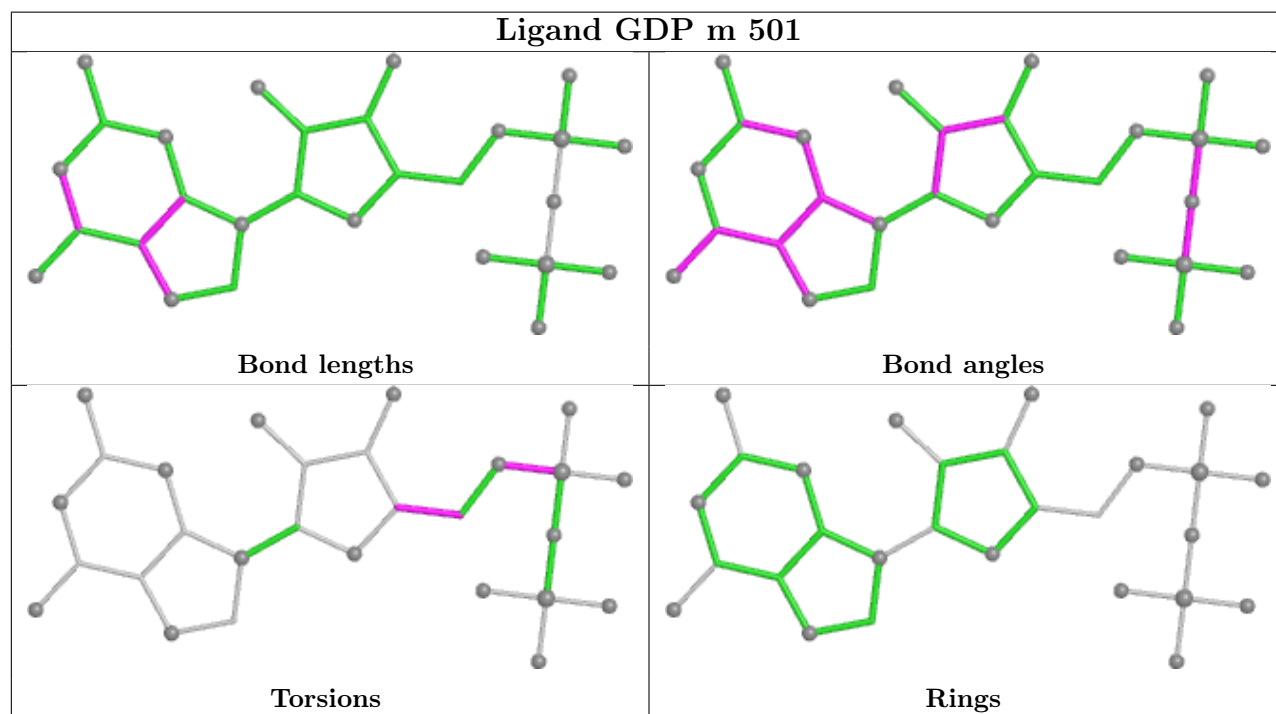
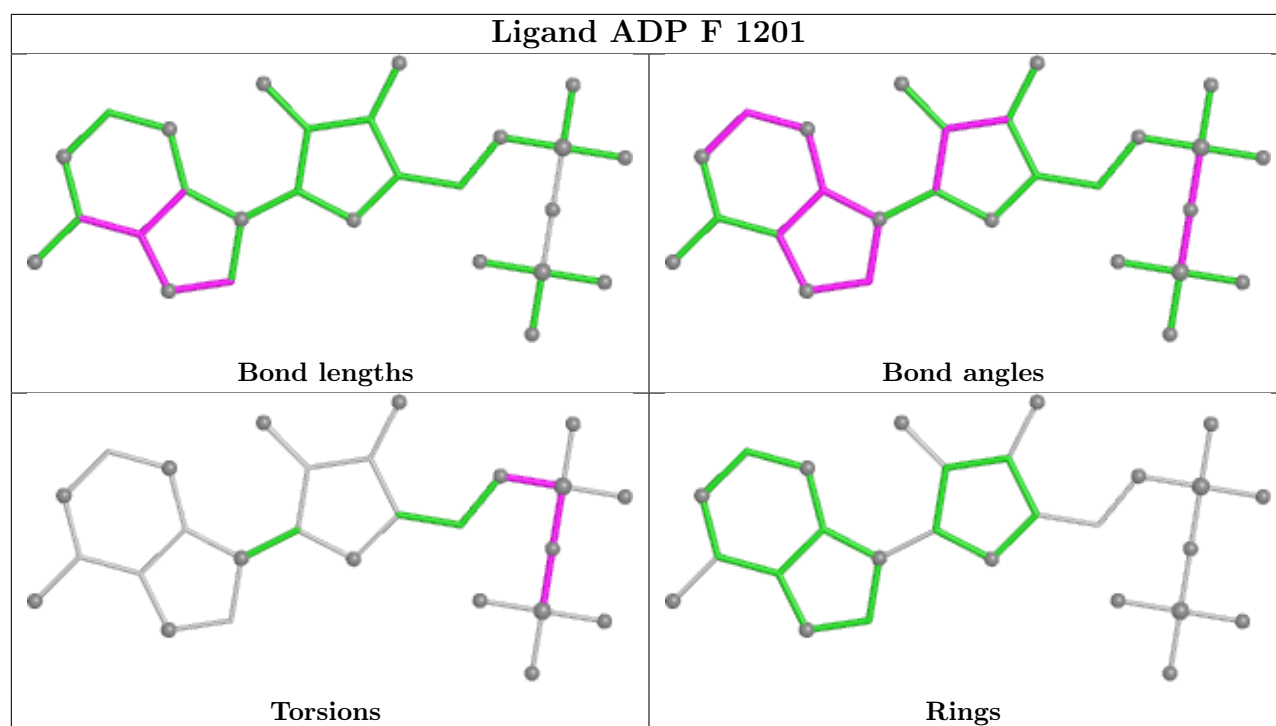
There are no ring outliers.

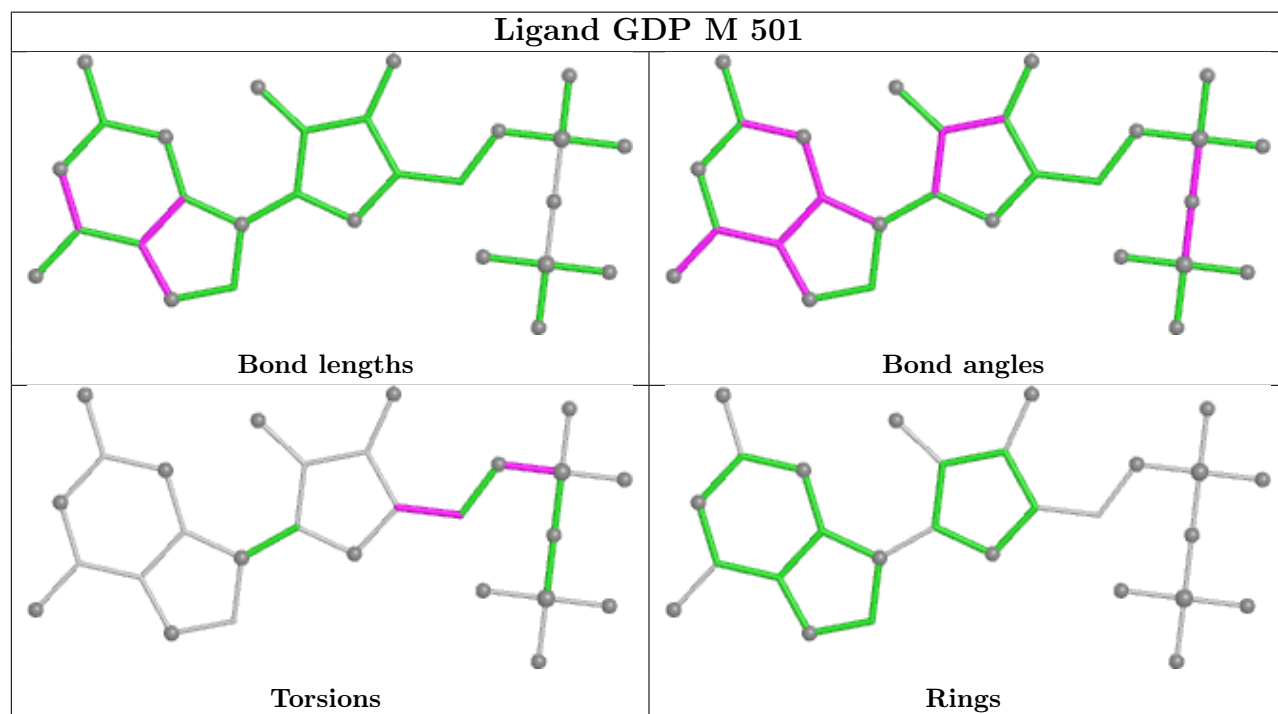
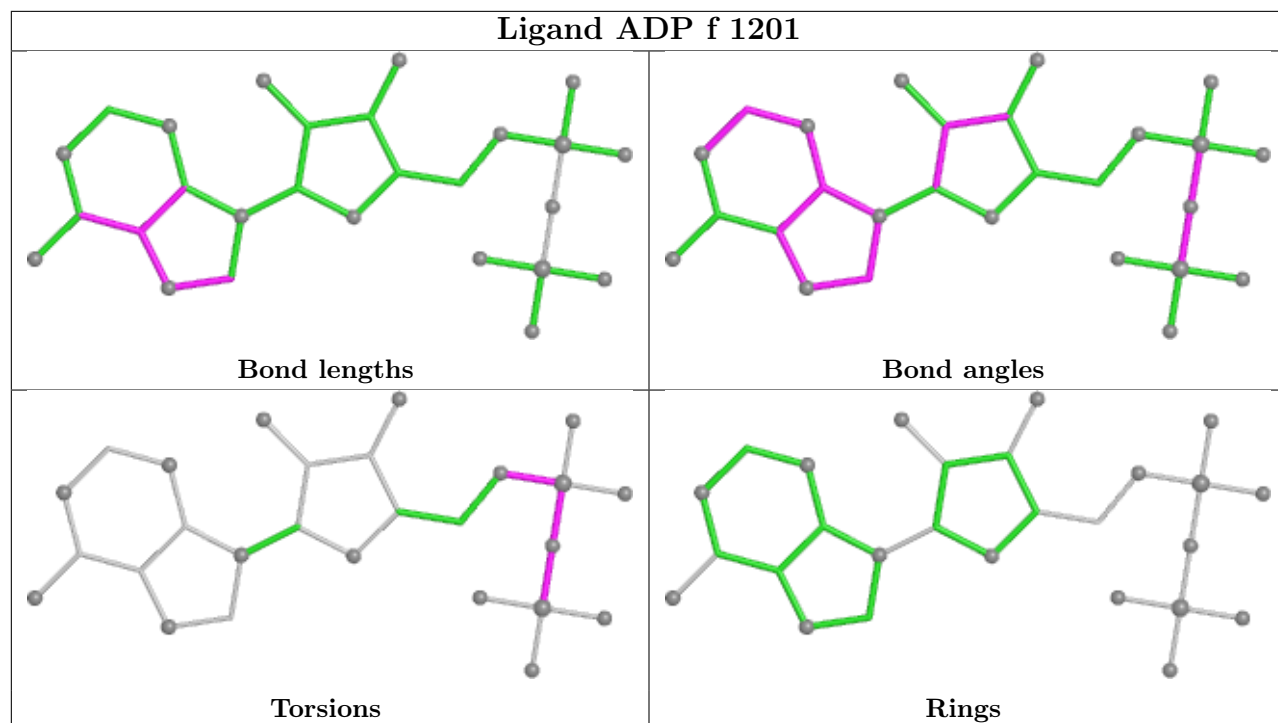
8 monomers are involved in 12 short contacts:

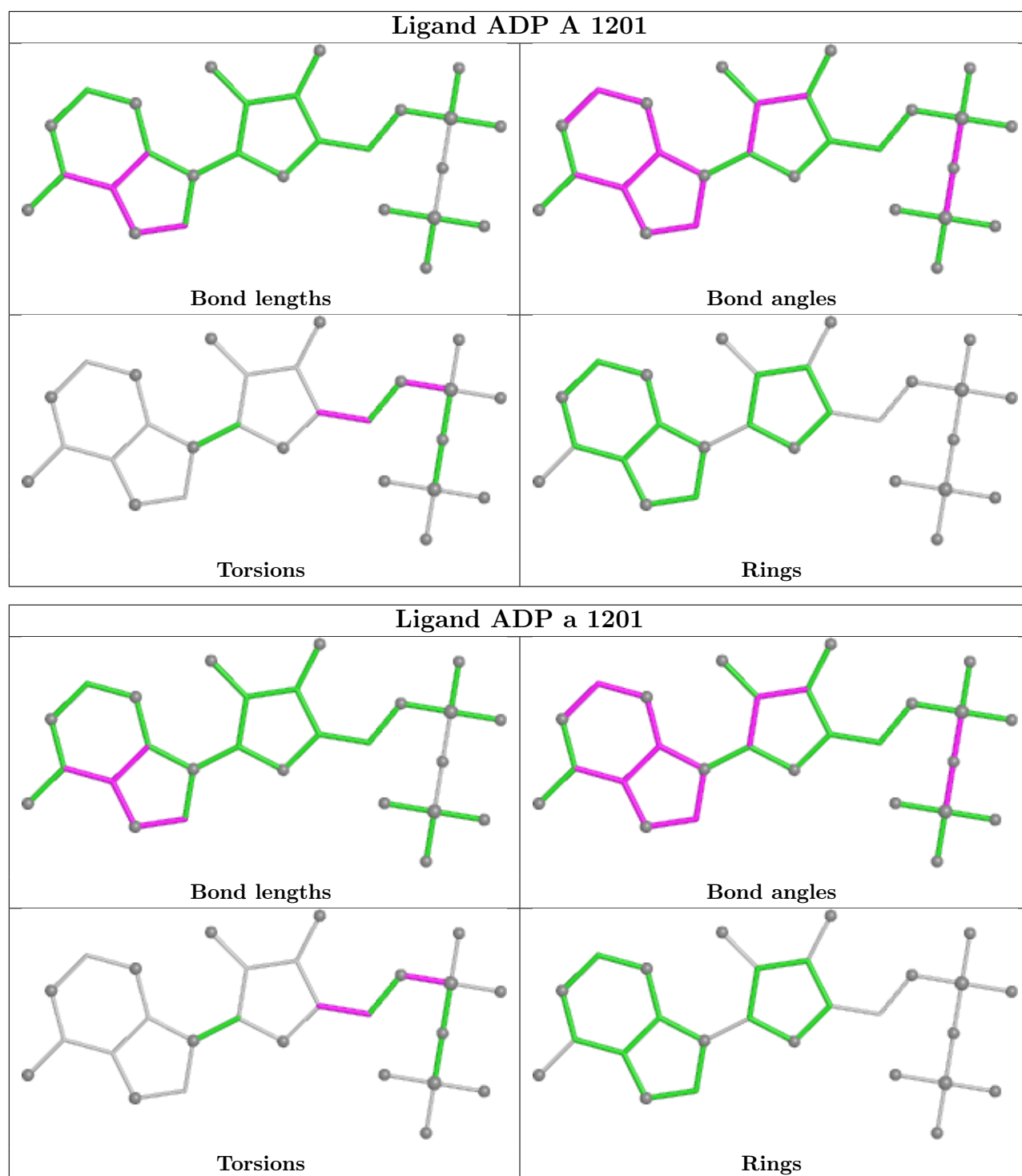
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	501	GDP	2	0
15	l	501	GDP	2	0
16	F	1201	ADP	1	0
15	m	501	GDP	1	0
16	f	1201	ADP	1	0
15	M	501	GDP	1	0
16	A	1201	ADP	2	0
16	a	1201	ADP	2	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.