



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2026 – 05:00 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 : 0.0.1.dev133
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 : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

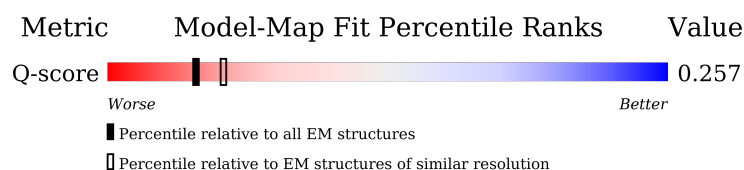
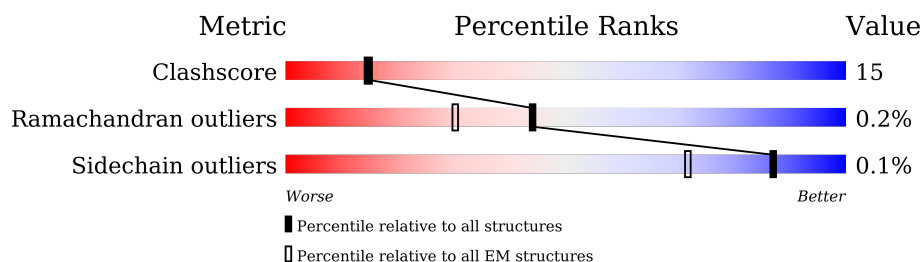
1 Overall quality at a glance

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.



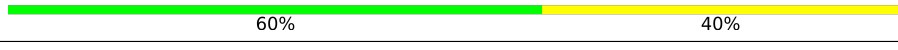
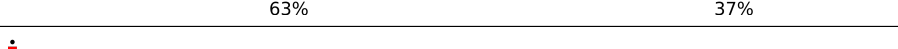
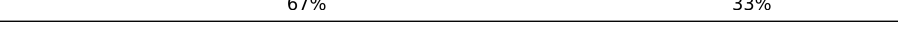
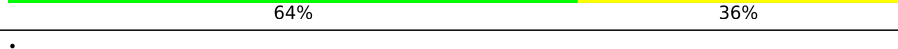
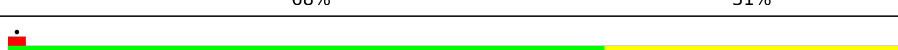
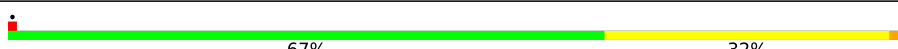
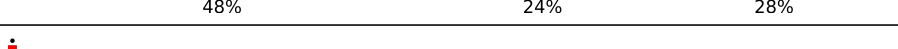
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	682	
1	11	682	
1	12	682	
1	13	682	

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Mol	Chain	Length	Quality of chain
1	14	682	
1	15	682	
1	16	682	
1	17	682	
1	18	682	
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	

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Mol	Chain	Length	Quality of chain
4	i	933	
5	J	466	
5	j	466	
6	K	163	
6	k	163	
7	O	147	
7	o	147	
8	P	782	
8	Q	782	
8	p	782	
8	q	782	
9	R	55	
9	r	55	
10	N	966	
10	n	966	
11	L	445	
11	l	445	
12	M	445	
12	m	445	
13	A	963	
13	F	963	
13	a	963	
13	f	963	
14	B	436	
14	G	436	

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Mol	Chain	Length	Quality of chain
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		

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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.

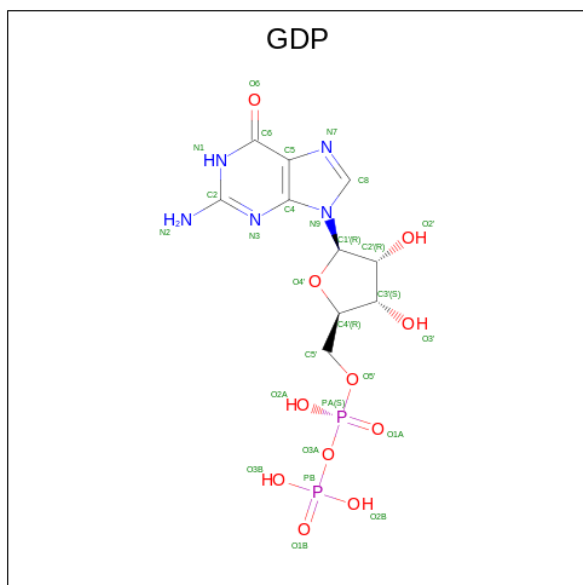
Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	333	Total	C	N	O	S	0	0
			2626	1666	462	479	19		
14	G	366	Total	C	N	O	S	0	0
			2890	1833	507	530	20		
14	b	333	Total	C	N	O	S	0	0
			2626	1666	462	479	19		

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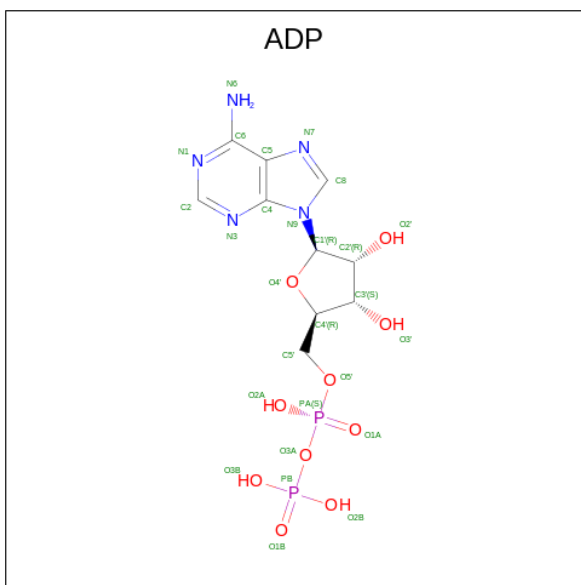
Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	366	Total	C	N	O	S	0	0
			2890	1833	507	530	20		

- 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
15	L	1	Total	C	N	O	P	0
			28	10	5	11	2	
15	M	1	Total	C	N	O	P	0
			28	10	5	11	2	
15	l	1	Total	C	N	O	P	0
			28	10	5	11	2	
15	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

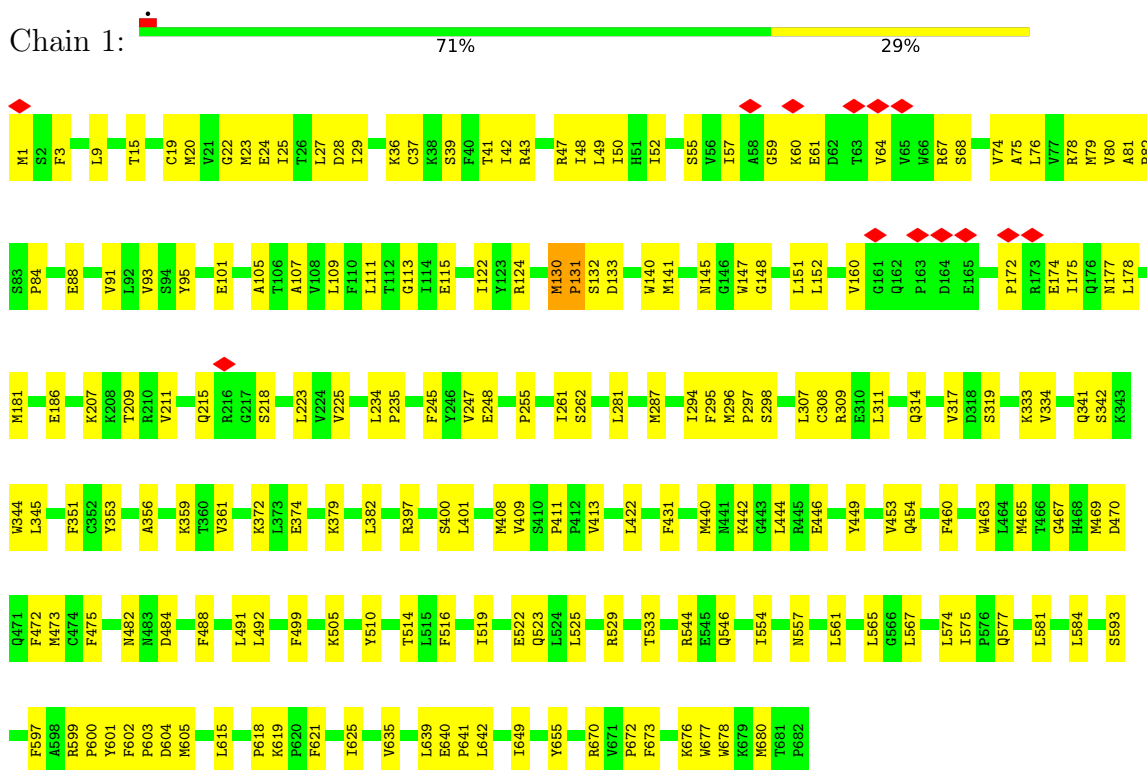


Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 27	C 10	N 5	O 10	P 2	0
16	F	1	Total 27	C 10	N 5	O 10	P 2	0
16	a	1	Total 27	C 10	N 5	O 10	P 2	0
16	f	1	Total 27	C 10	N 5	O 10	P 2	0

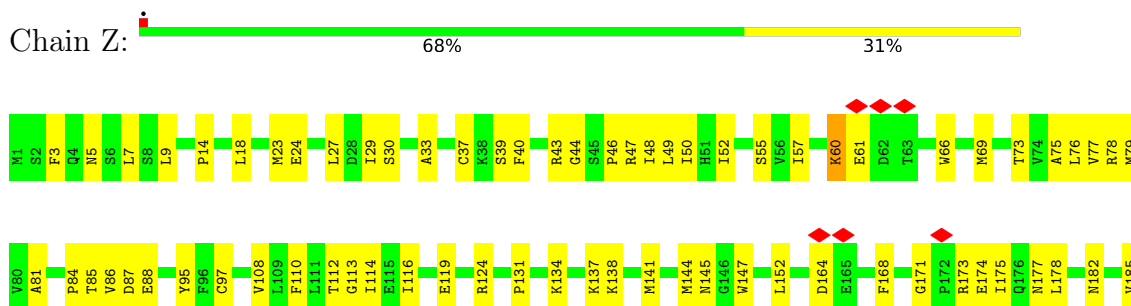
3 Residue-property plots

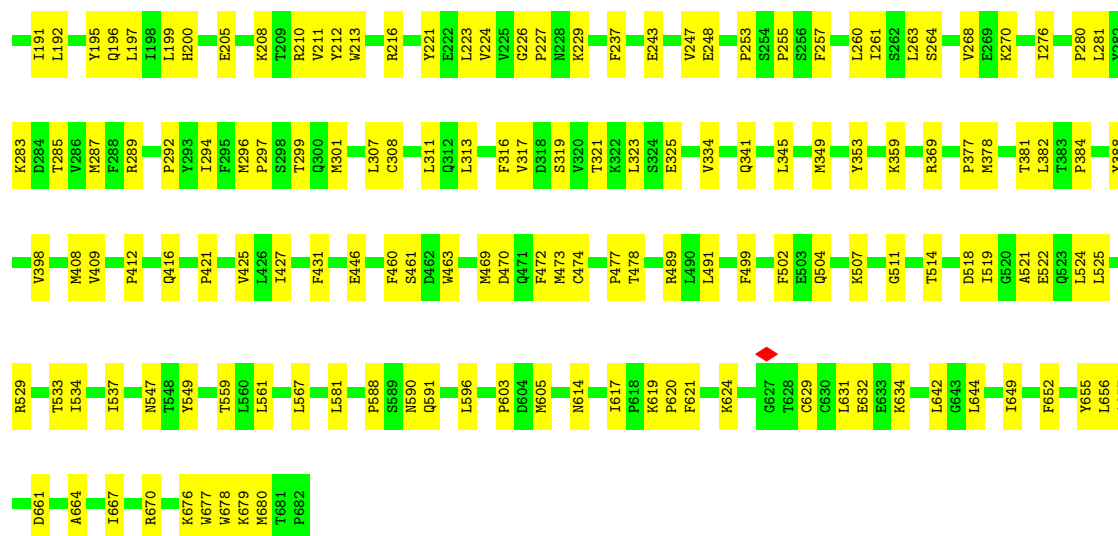
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

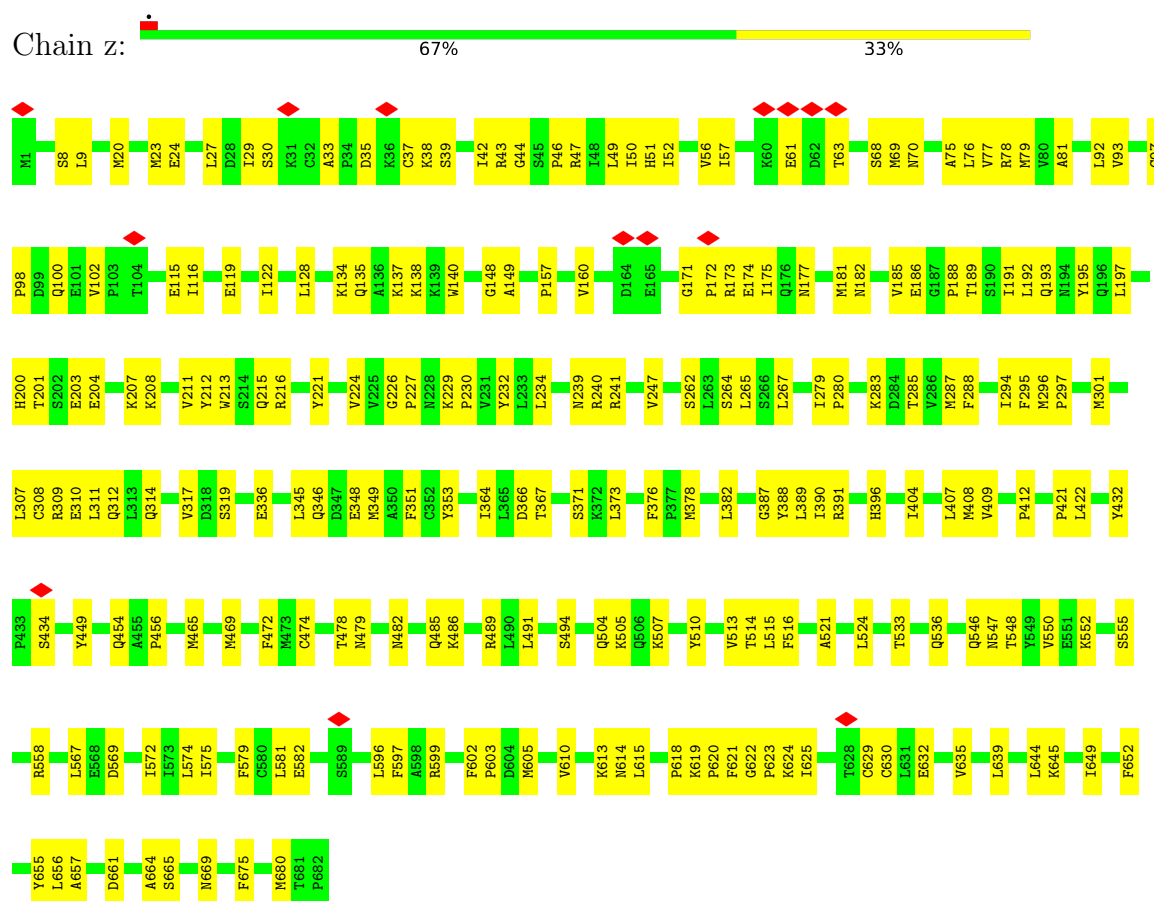


- Molecule 1: Inactive protein-arginine deiminase type-6



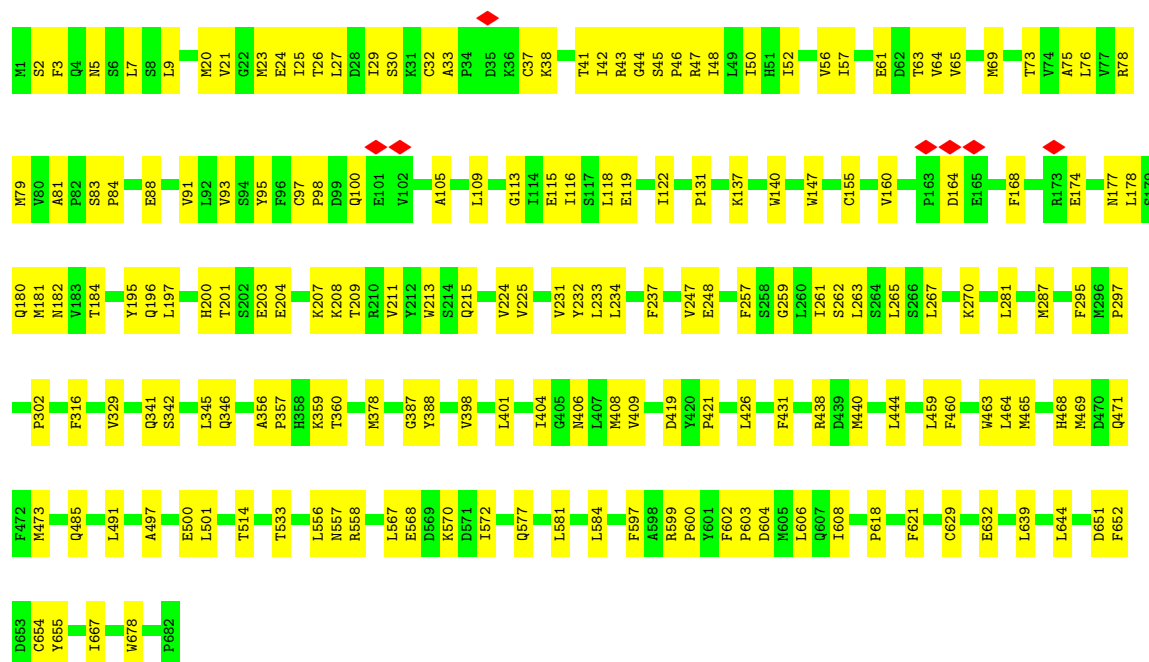


- Molecule 1: Inactive protein-arginine deiminase type-6

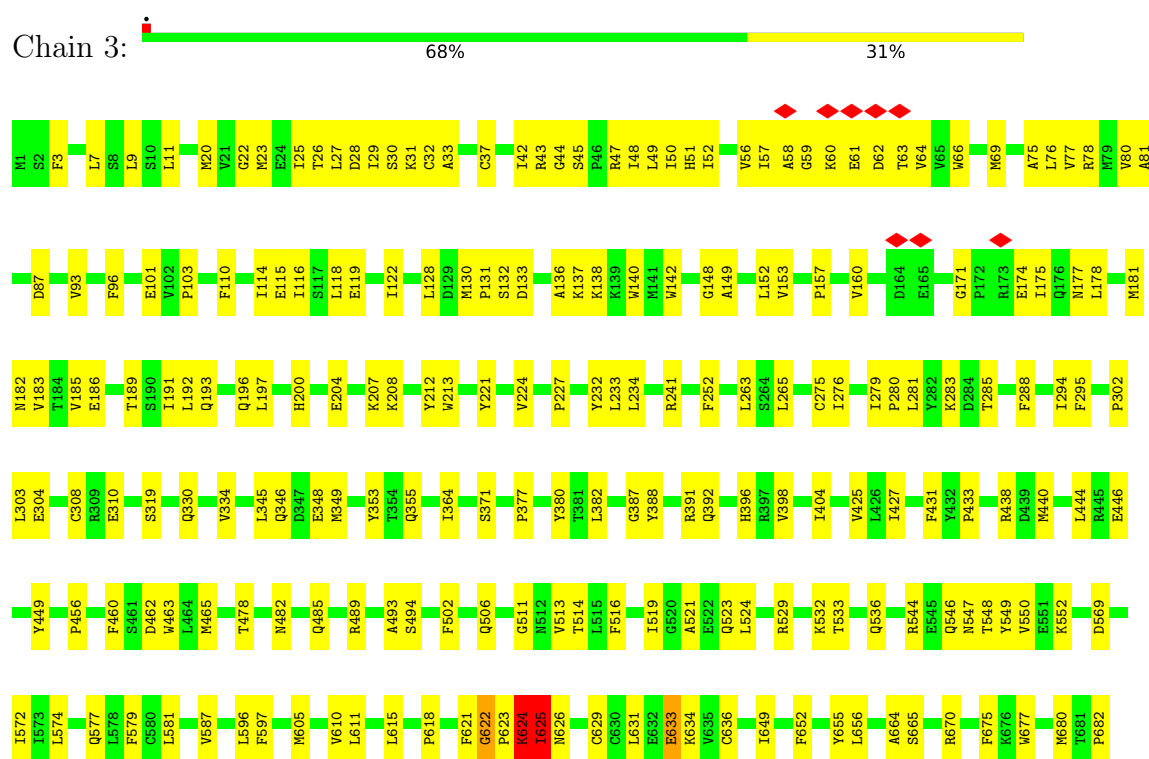


- Molecule 1: Inactive protein-arginine deiminase type-6

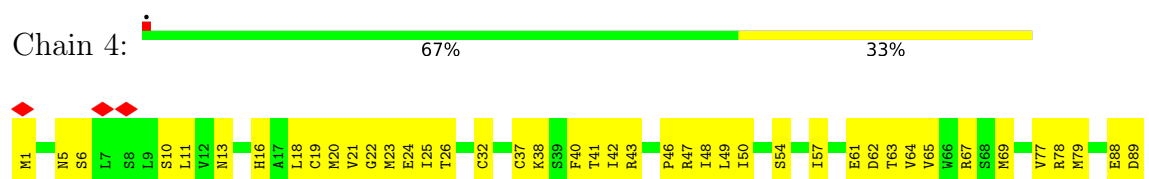


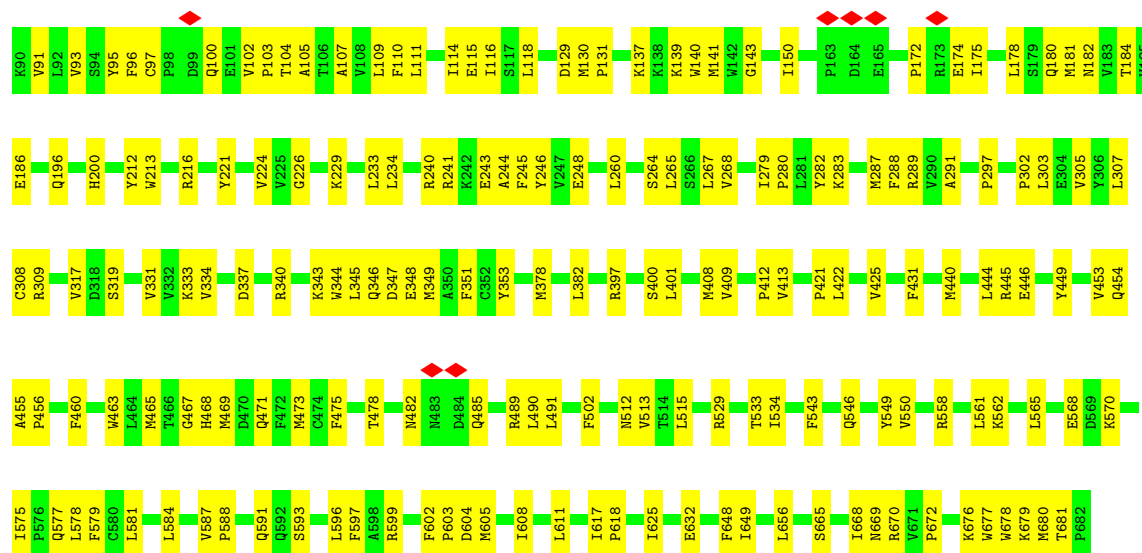


- Molecule 1: Inactive protein-arginine deiminase type-6



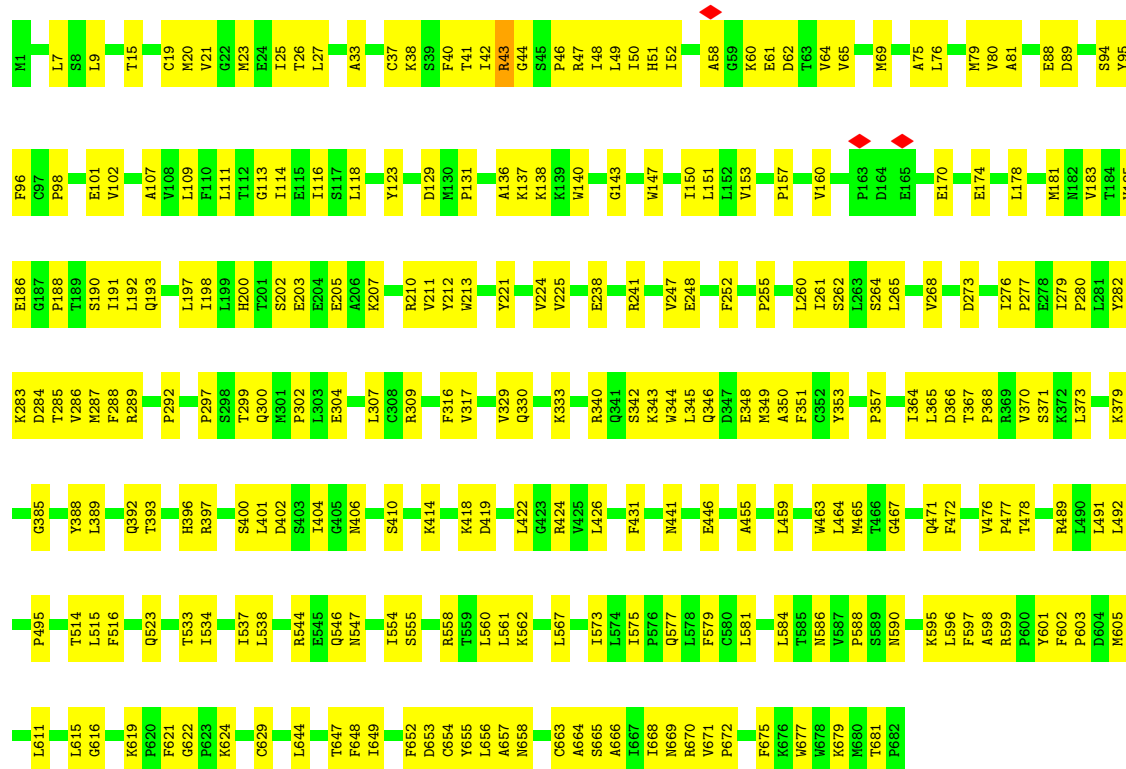
- Molecule 1: Inactive protein-arginine deiminase type-6





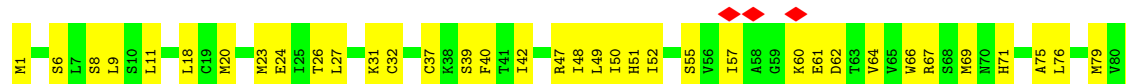
• Molecule 1: Inactive protein-arginine deiminase type-6

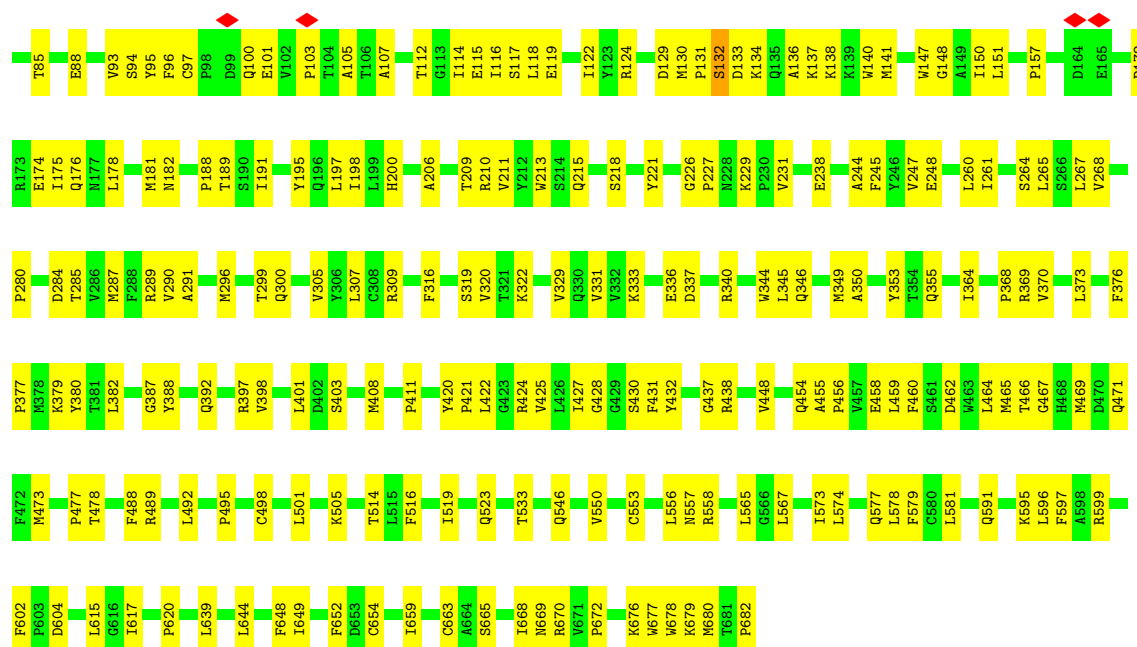
Chain 5: 62% 37%



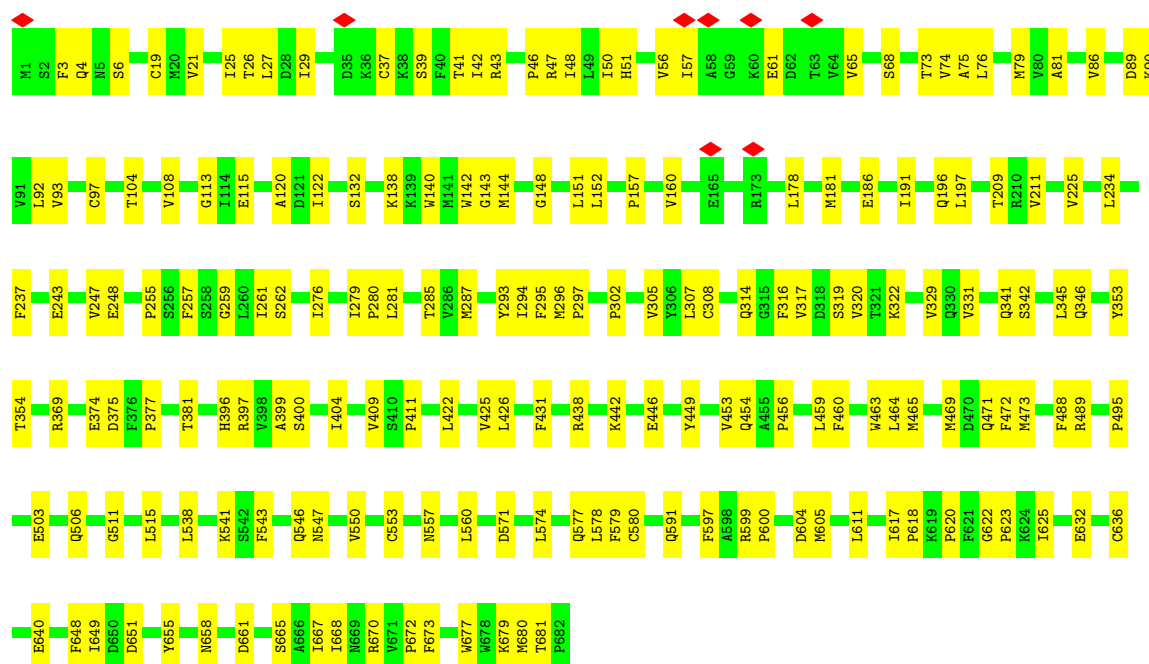
• Molecule 1: Inactive protein-arginine deiminase type-6

Chain 6: 64% 36%



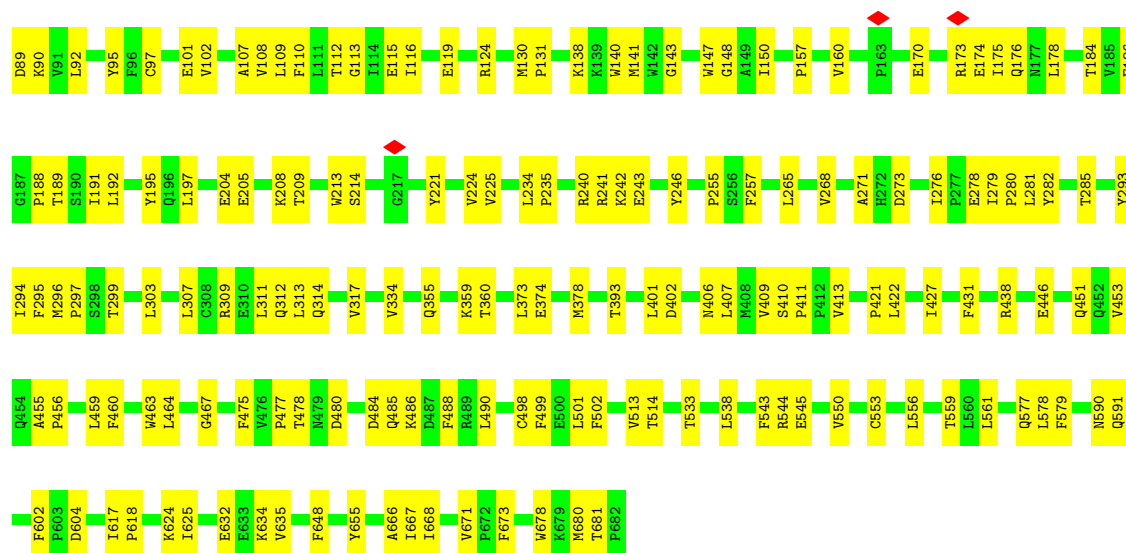


- Molecule 1: Inactive protein-arginine deiminase type-6



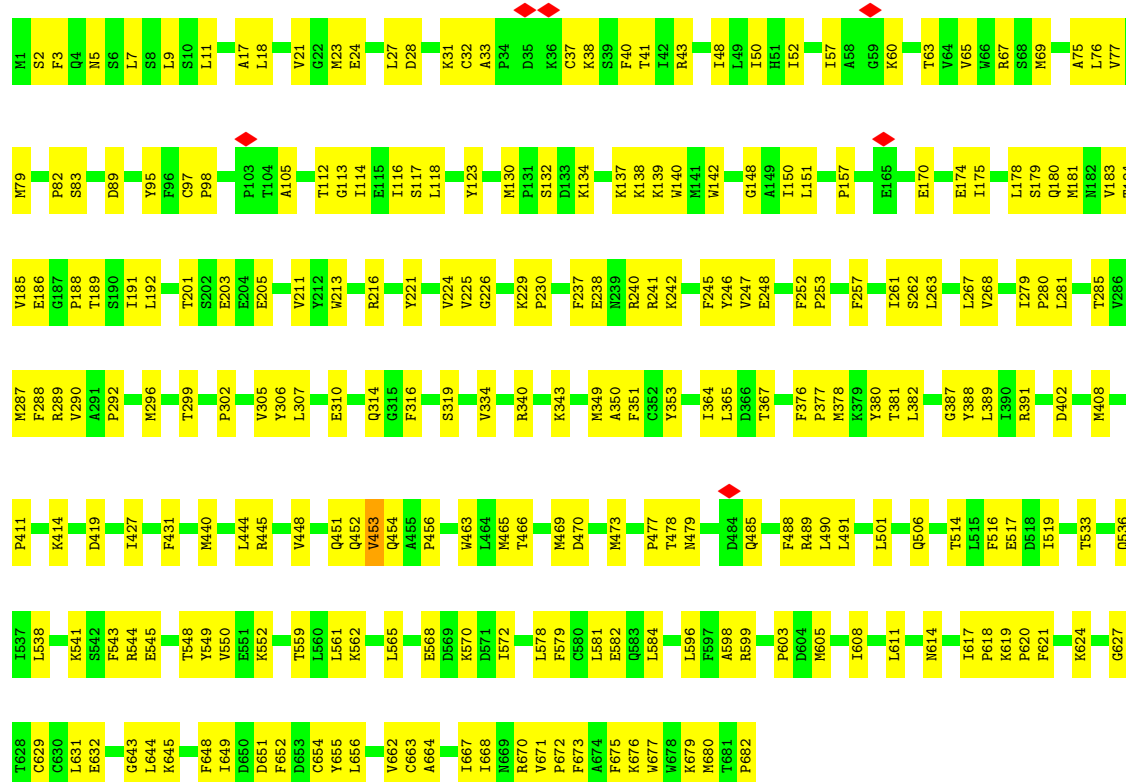
- Molecule 1: Inactive protein-arginine deiminase type-6





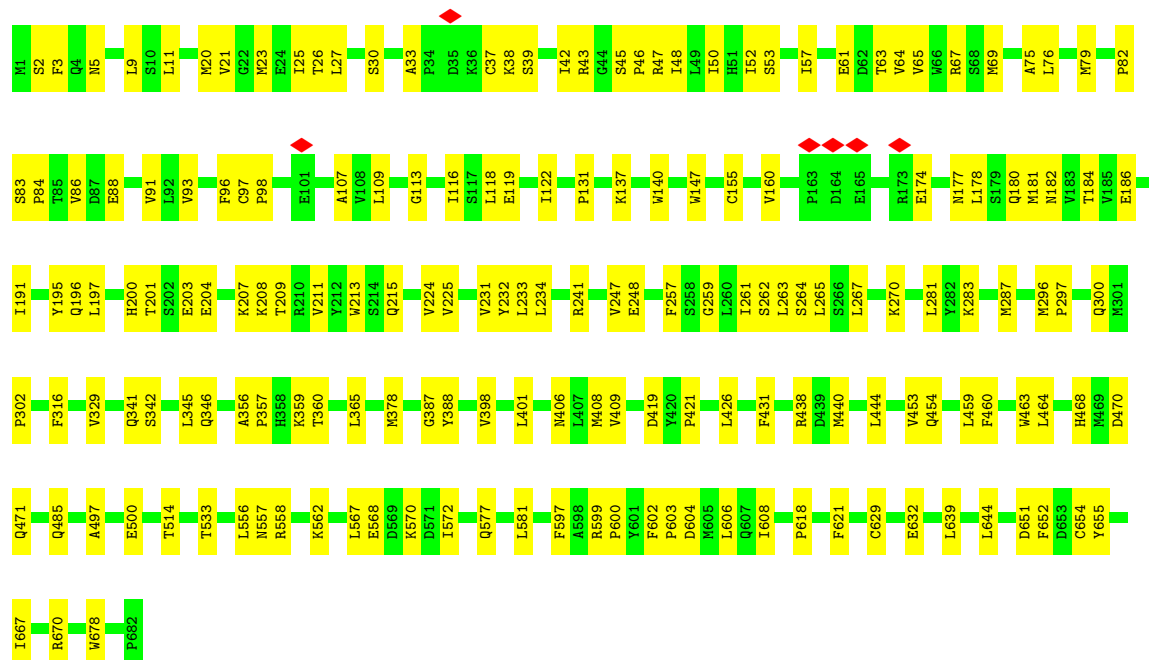
• Molecule 1: Inactive protein-arginine deiminase type-6

Chain 9: 64% 36%

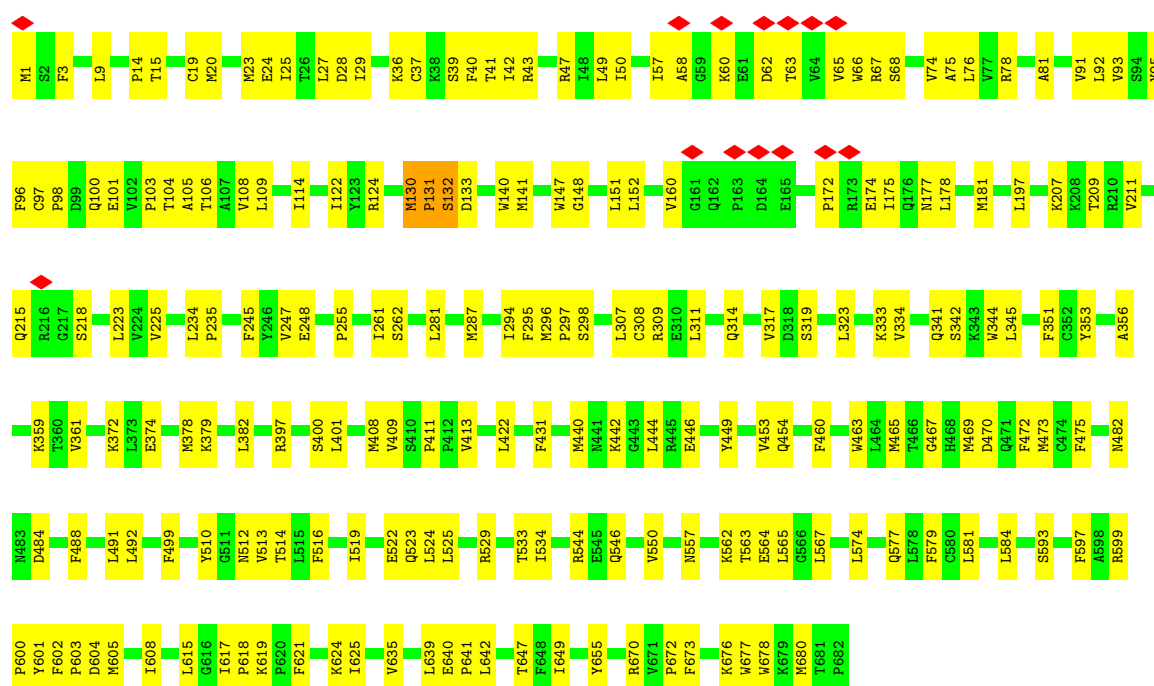


• Molecule 1: Inactive protein-arginine deiminase type-6

Chain 12: 74% 26%

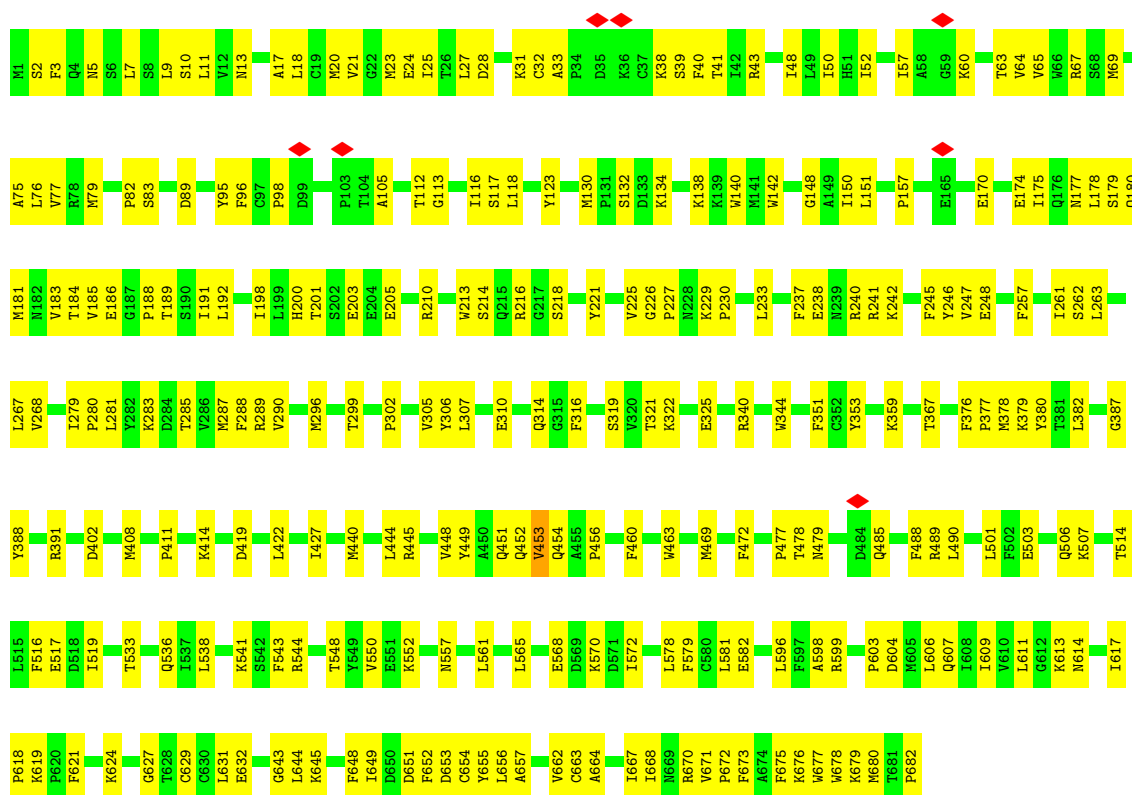


- Molecule 1: Inactive protein-arginine deiminase type-6



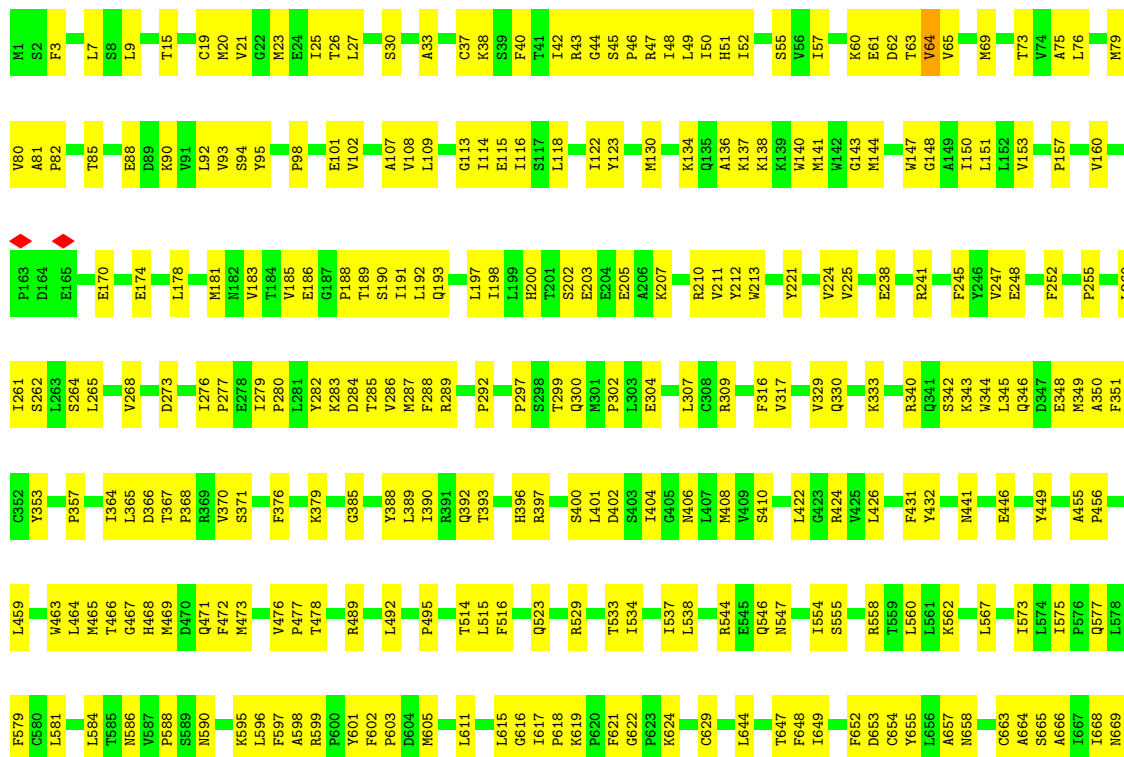
- Molecule 1: Inactive protein-arginine deiminase type-6

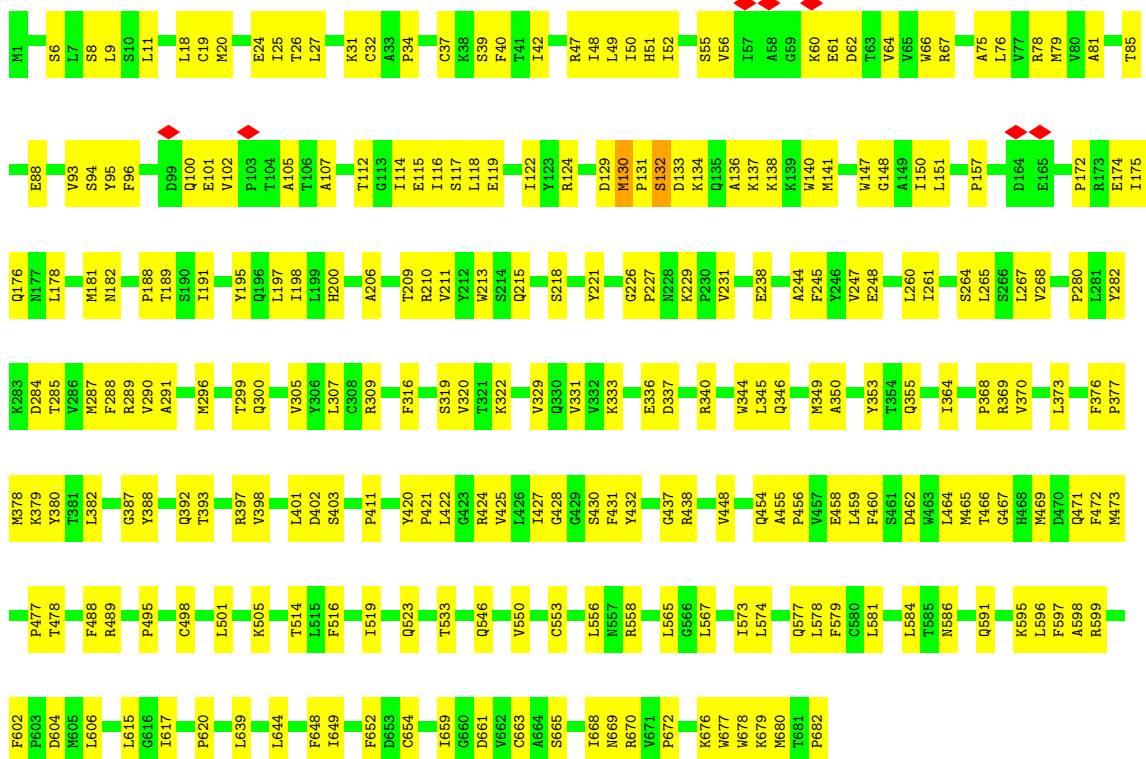




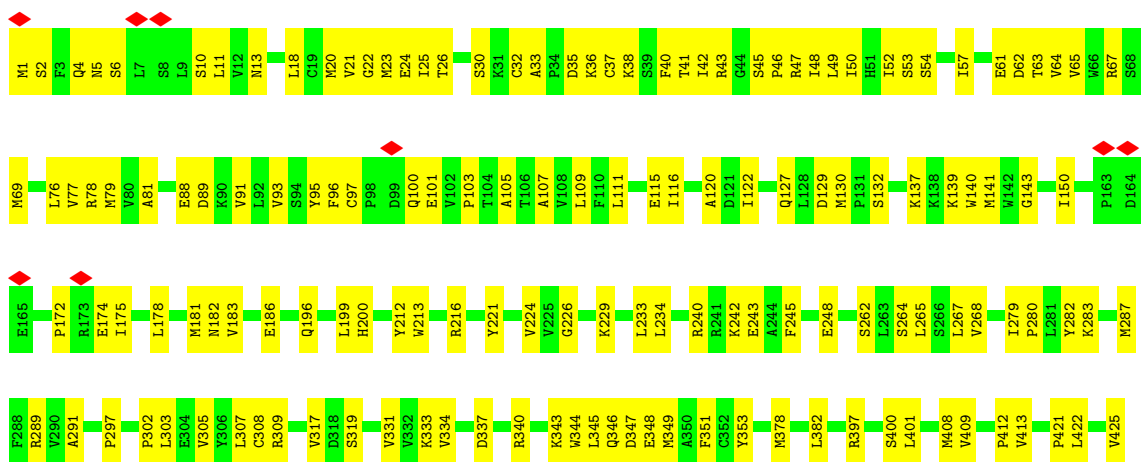
• Molecule 1: Inactive protein-arginine deiminase type-6

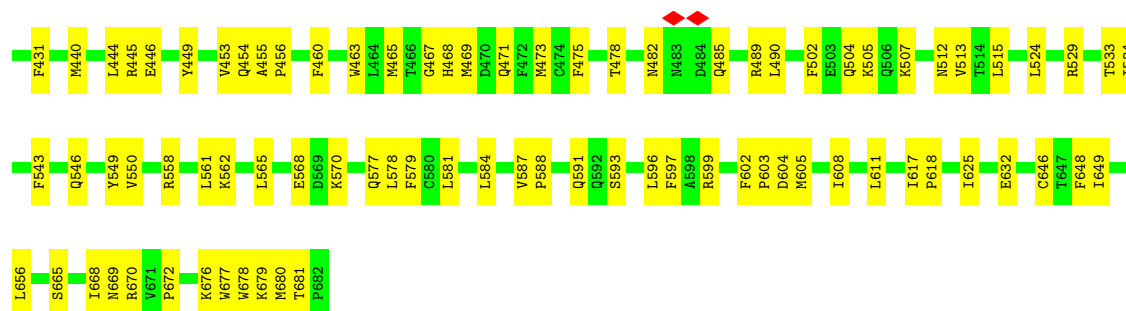
Chain 15: 60% 40%





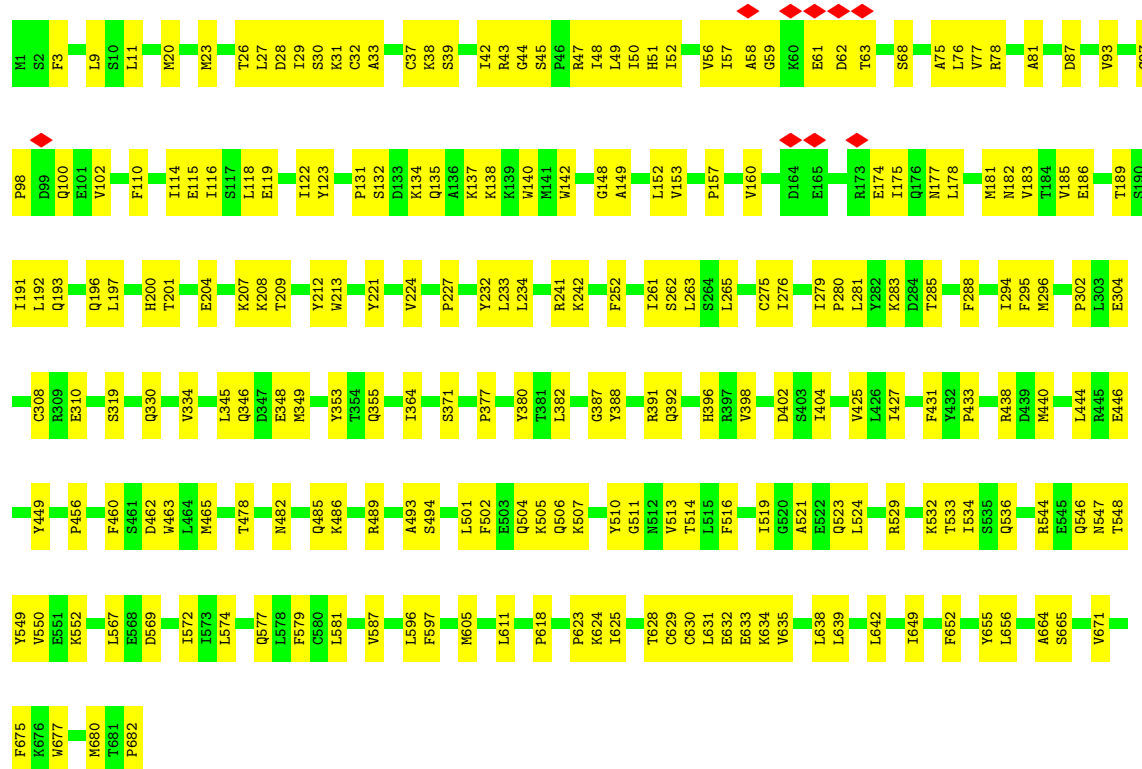
- Molecule 1: Inactive protein-arginine deiminase type-6





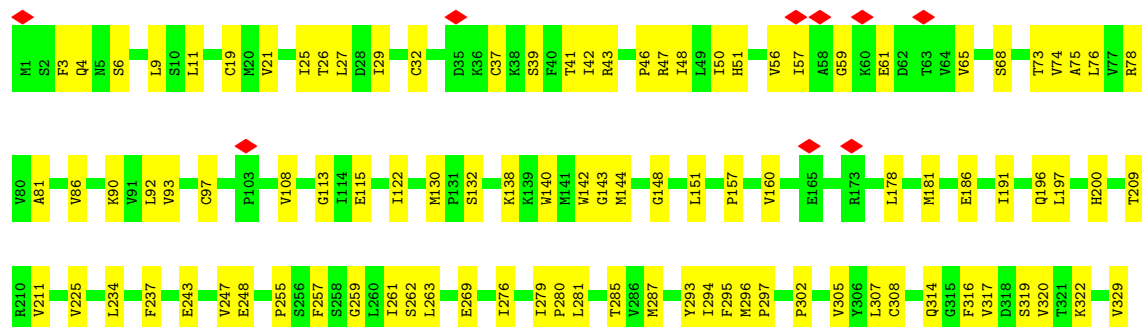
- Molecule 1: Inactive protein-arginine deiminase type-6

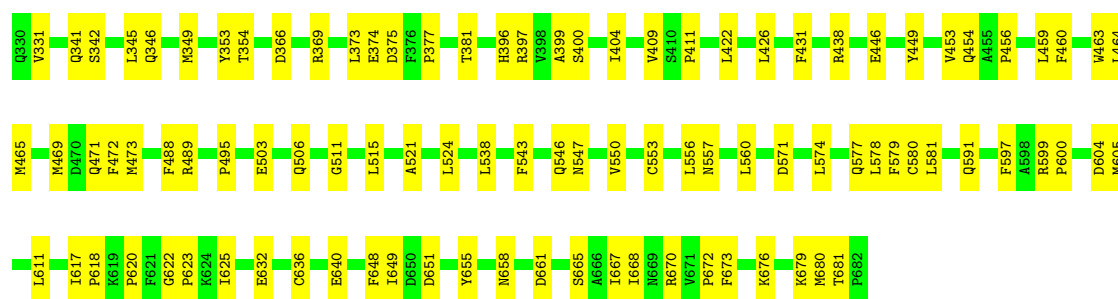
Chain 13: 67% 33%



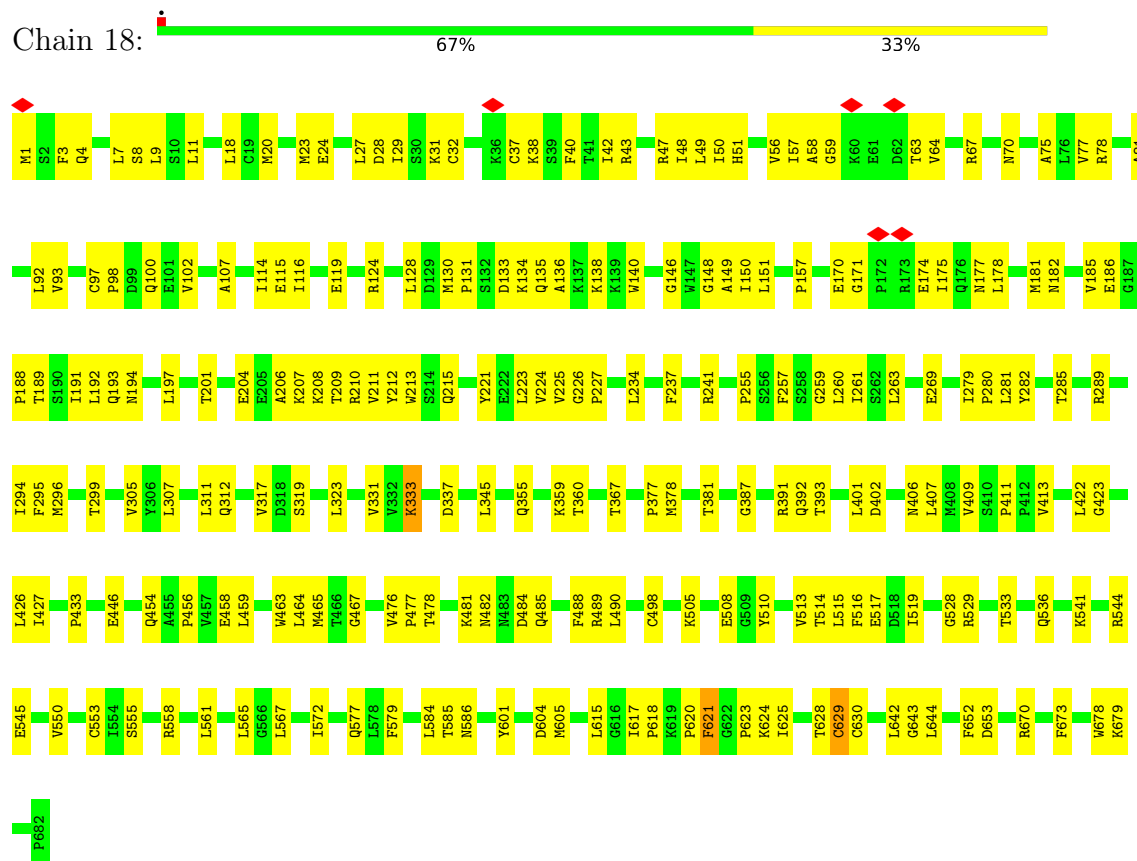
- Molecule 1: Inactive protein-arginine deiminase type-6

Chain 17: 71% 29%

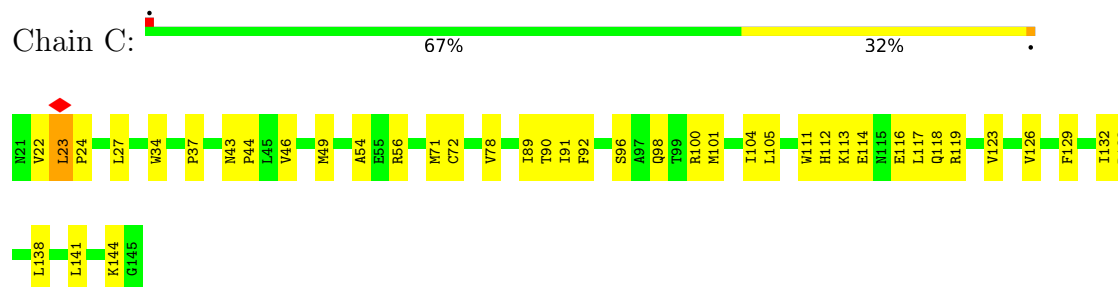




• Molecule 1: Inactive protein-arginine deiminase type-6



• Molecule 2: Oocyte-expressed protein homolog

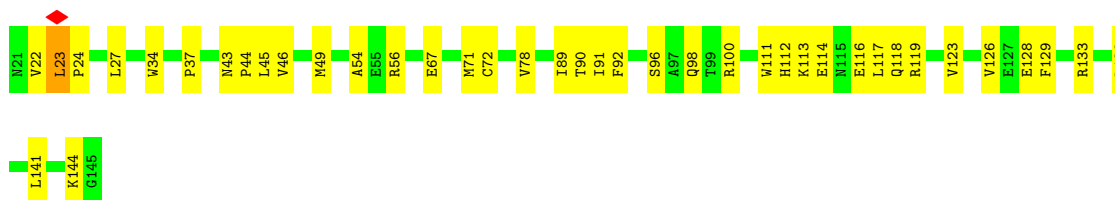


• Molecule 2: Oocyte-expressed protein homolog

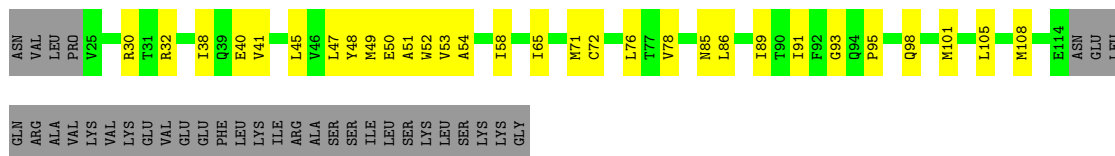




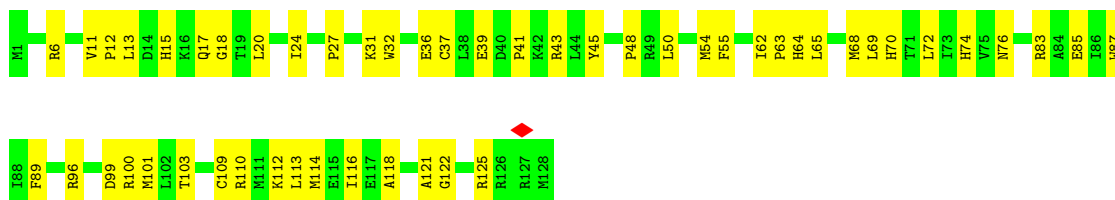
• Molecule 2: Oocyte-expressed protein homolog



• Molecule 2: Oocyte-expressed protein homolog



• Molecule 3: KH domain-containing protein 3

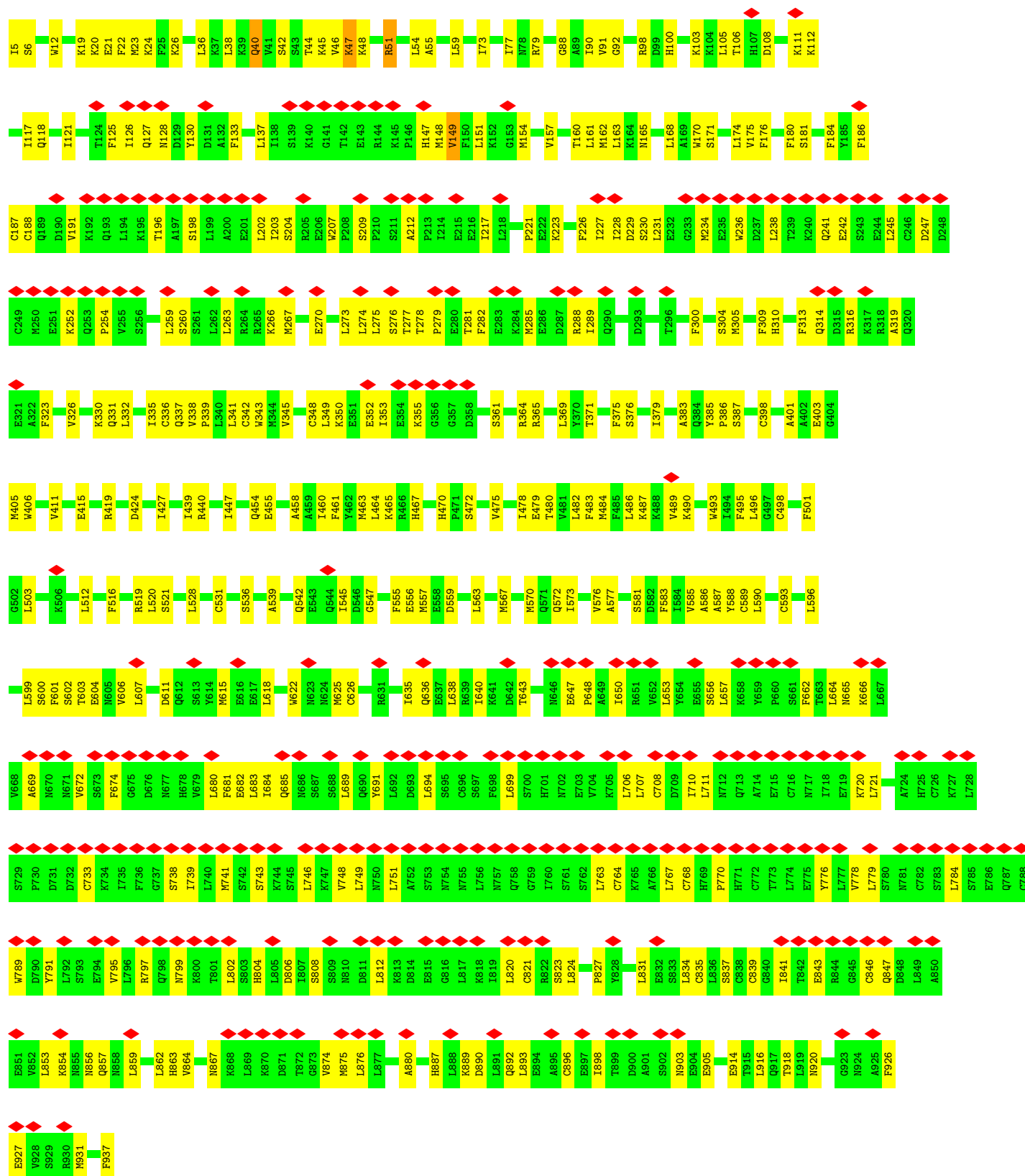


• Molecule 3: KH domain-containing protein 3



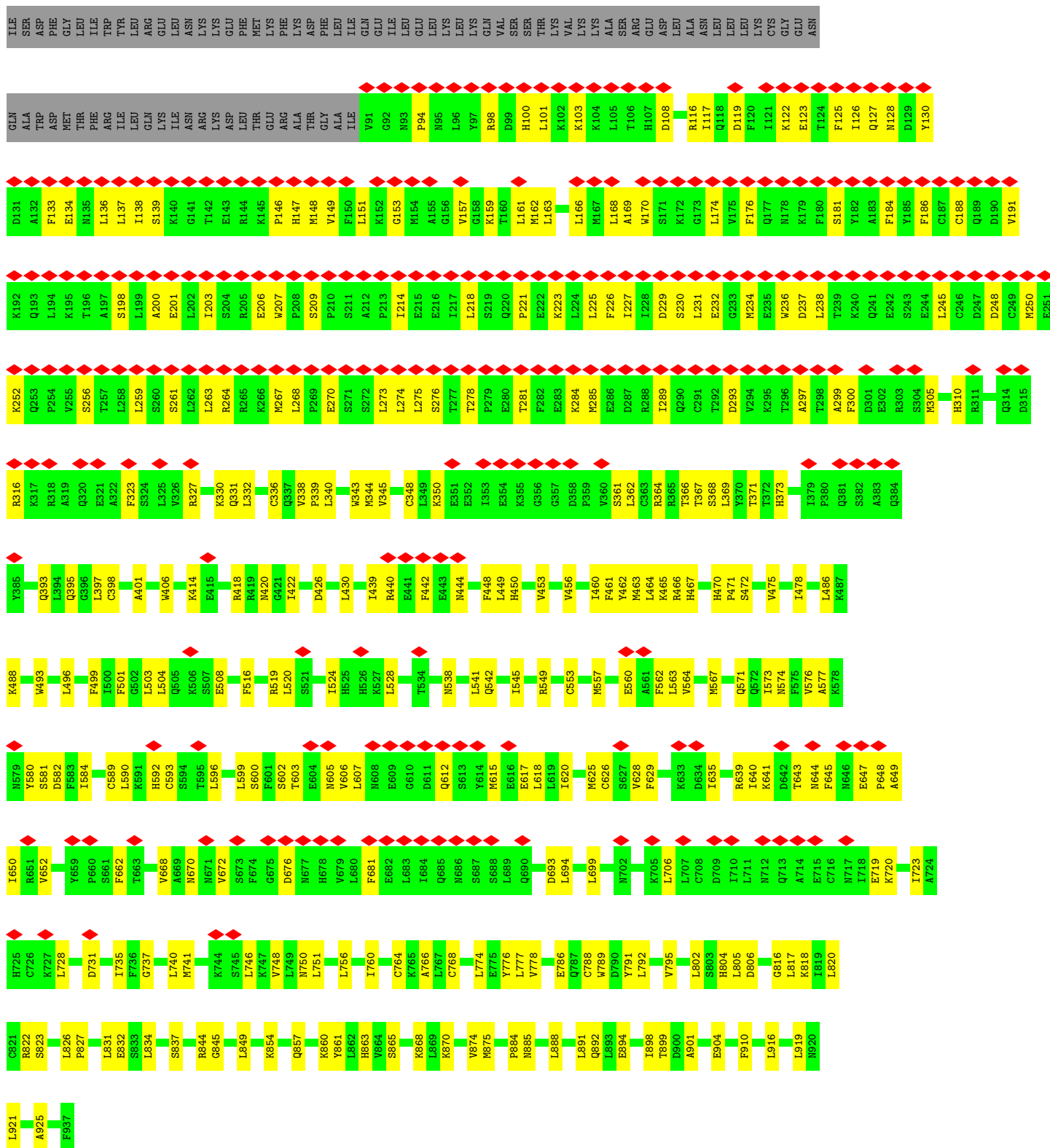
• Molecule 4: NLR family, pyrin domain containing 4F





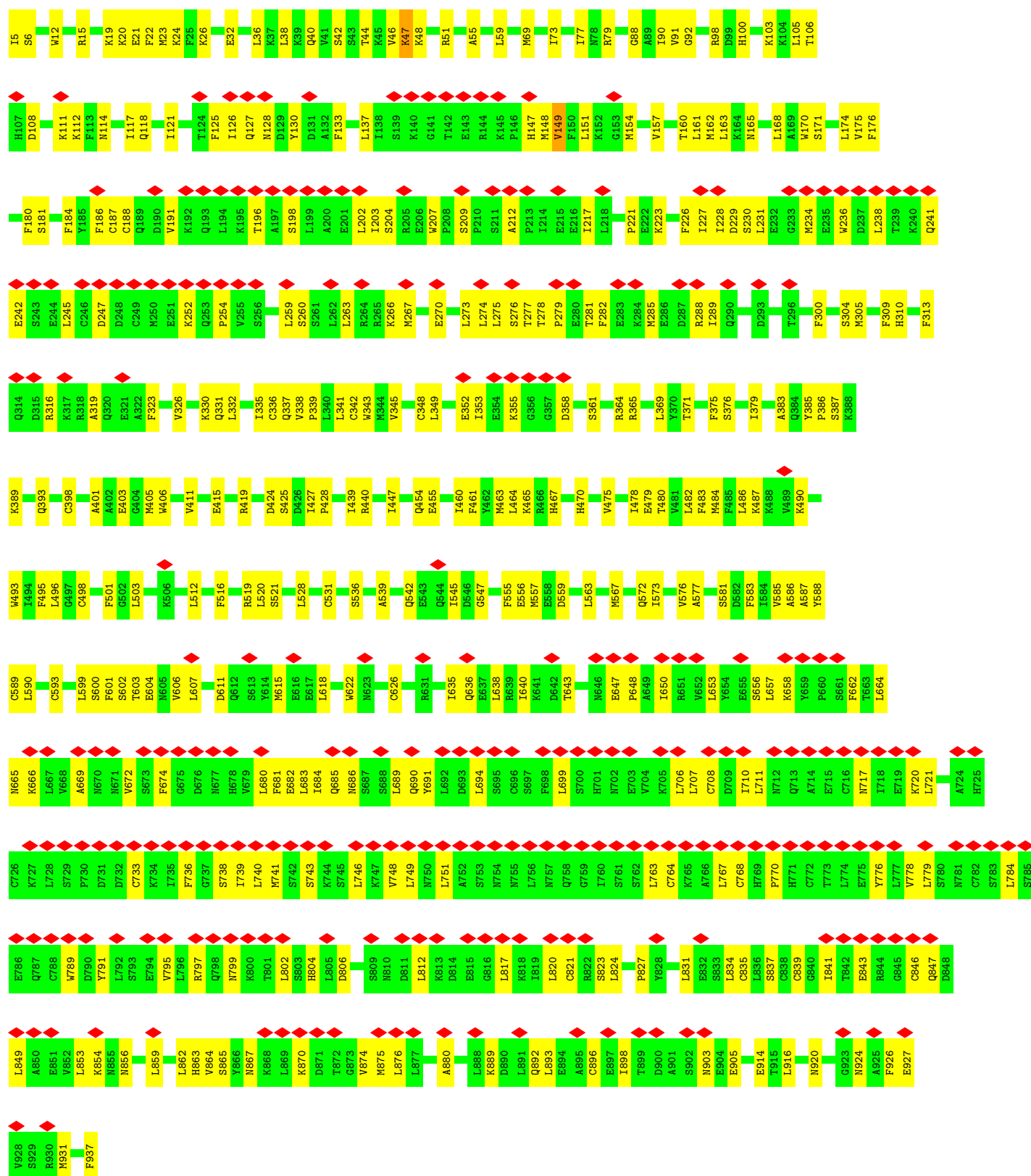
• Molecule 4: NLR family, pyrin domain containing 4F

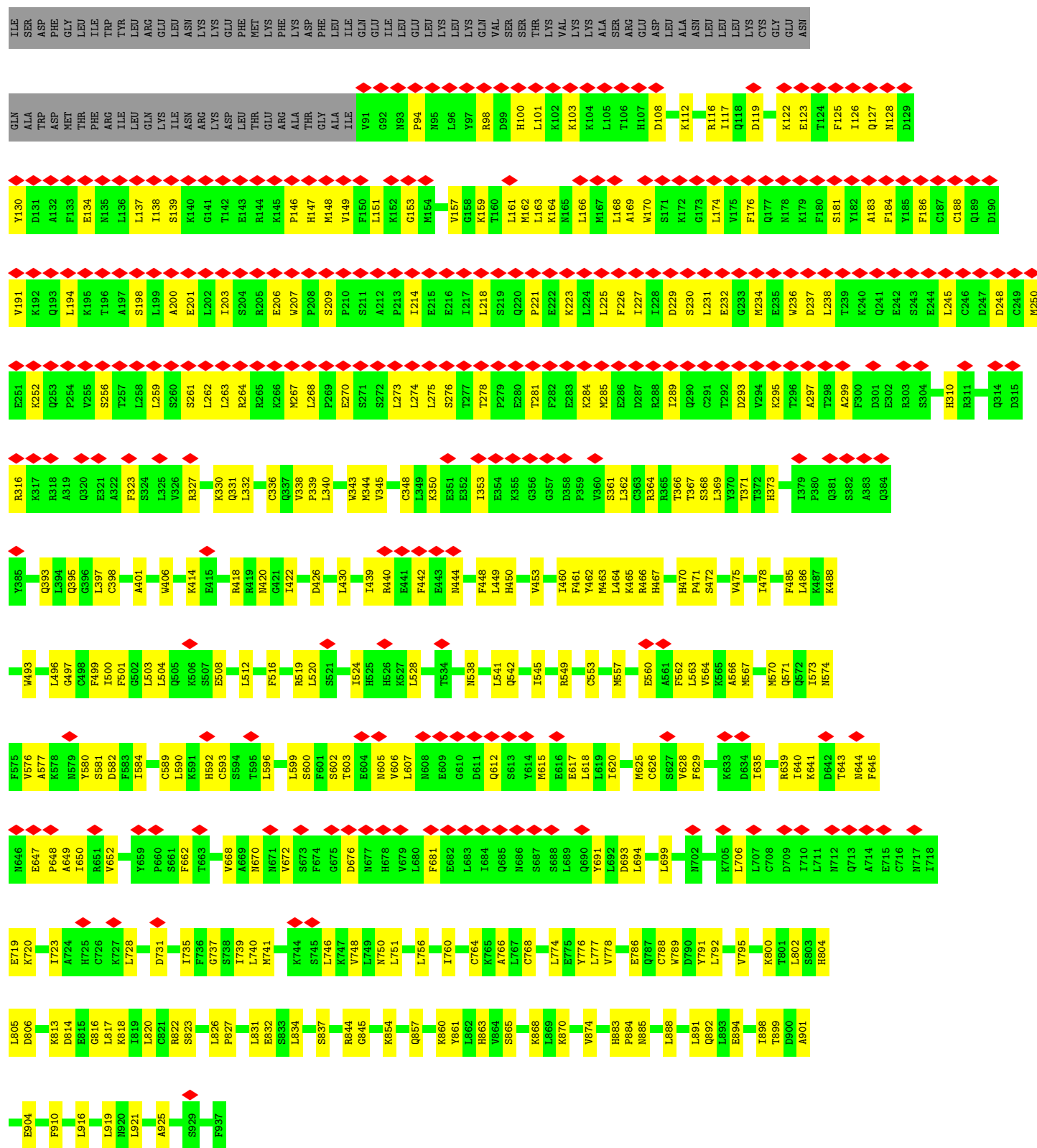




- Molecule 4: NLR family, pyrin domain containing 4F

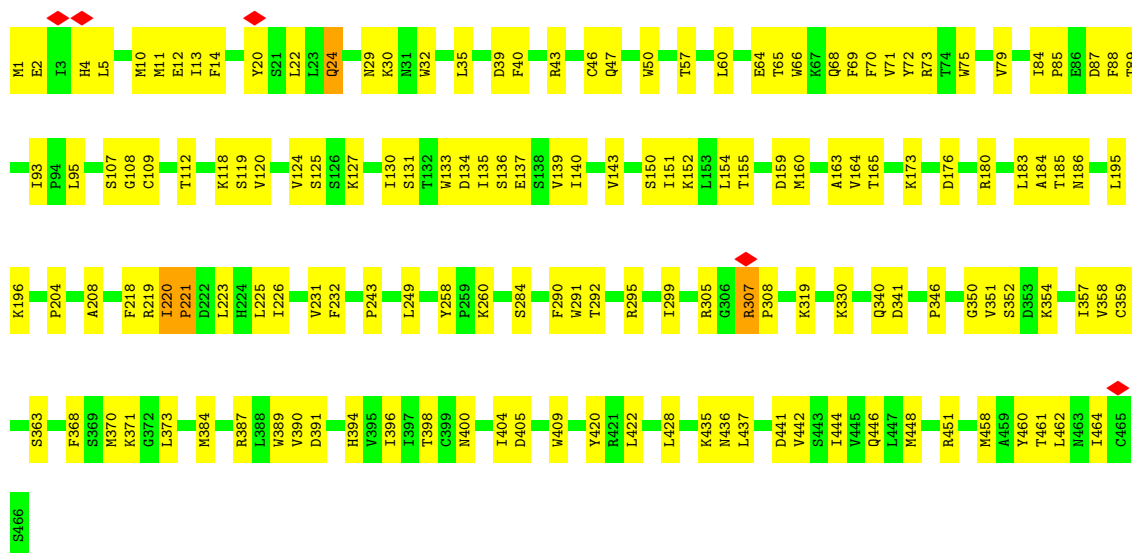






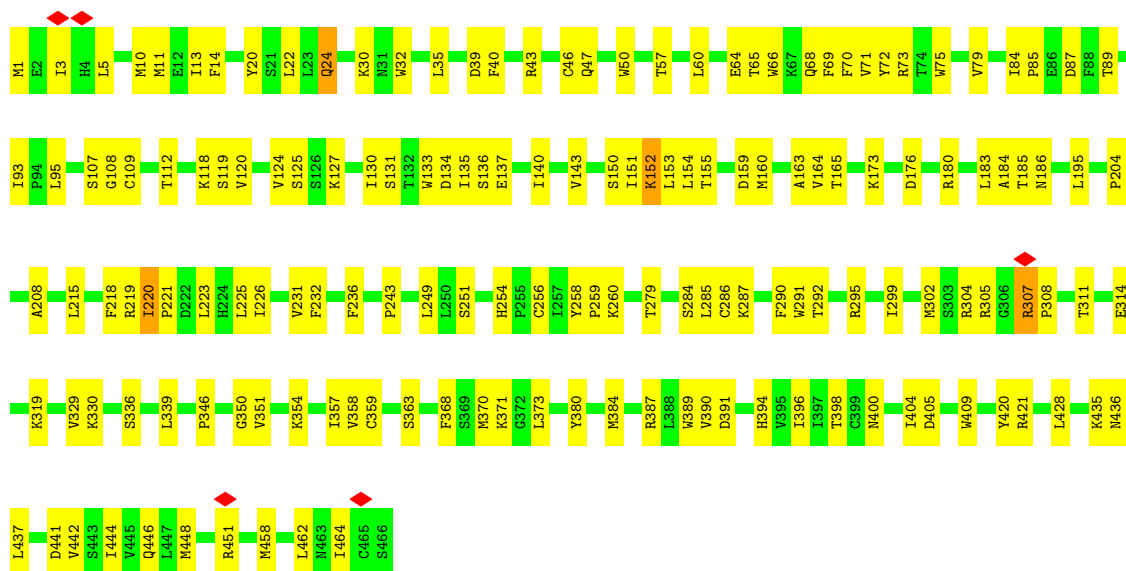
• Molecule 5: FBXW24

Chain J: 68% 32%



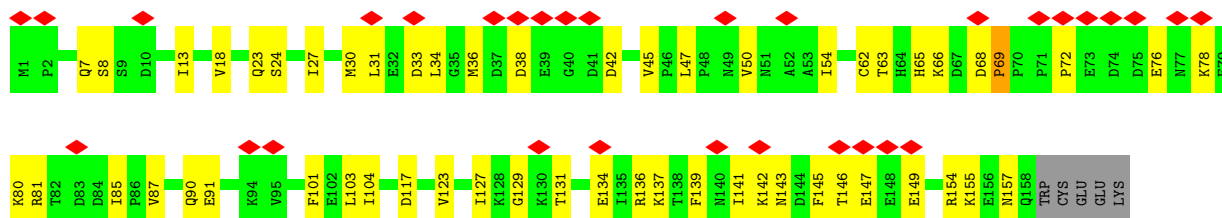
• Molecule 5: FBXW24

Chain j: 66% 33%

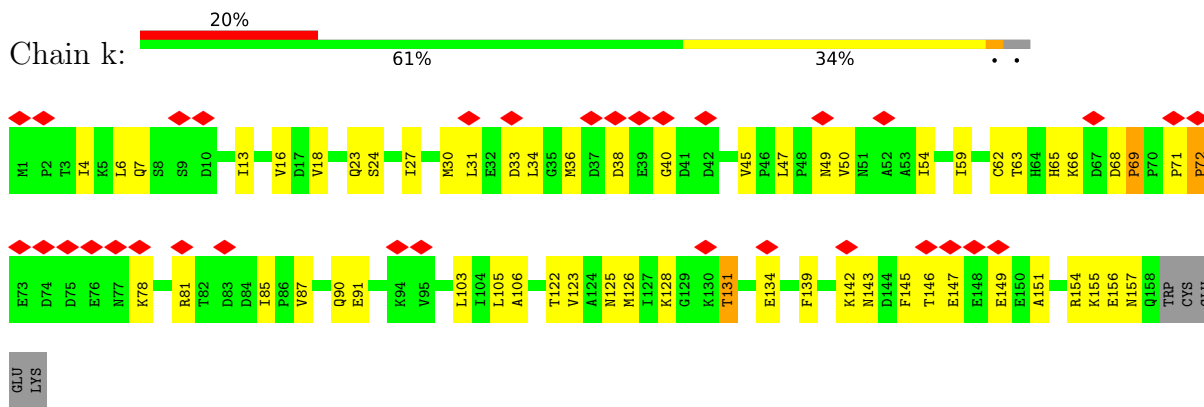


• Molecule 6: S-phase kinase-associated protein 1

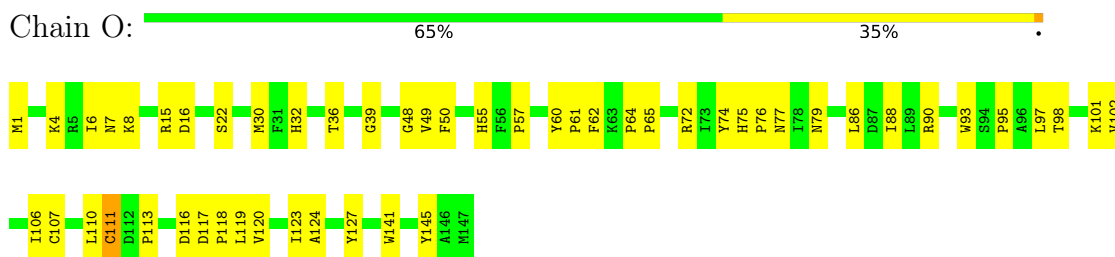
Chain K: 19% 63% 33%



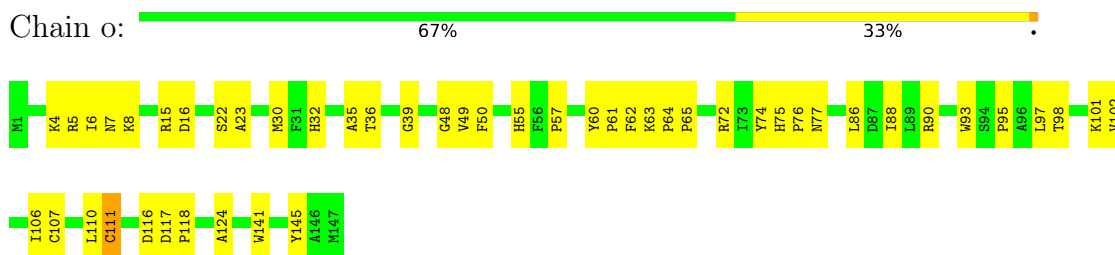
• Molecule 6: S-phase kinase-associated protein 1



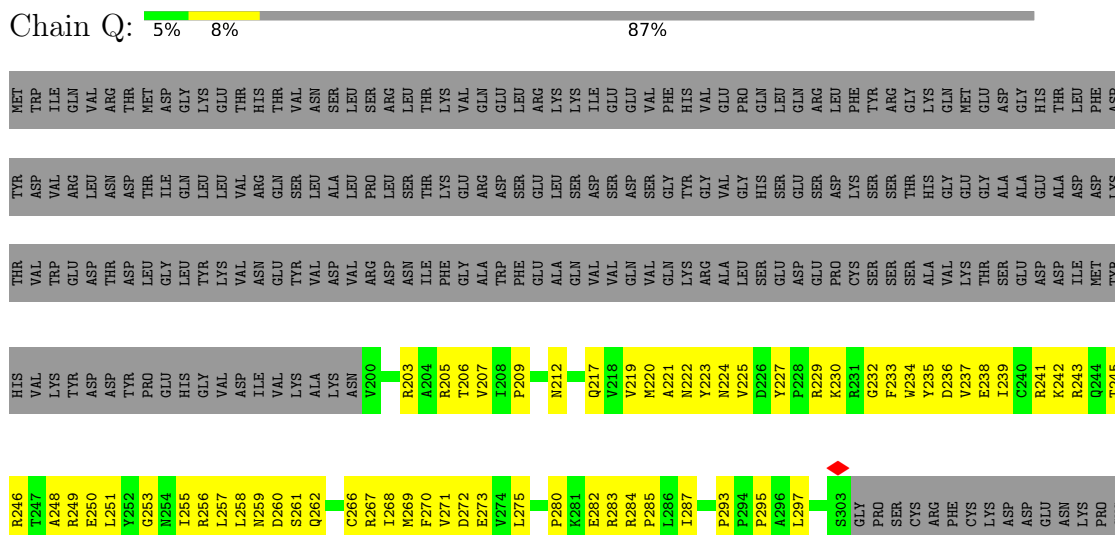
- Molecule 7: Ubiquitin-conjugating enzyme E2 D3



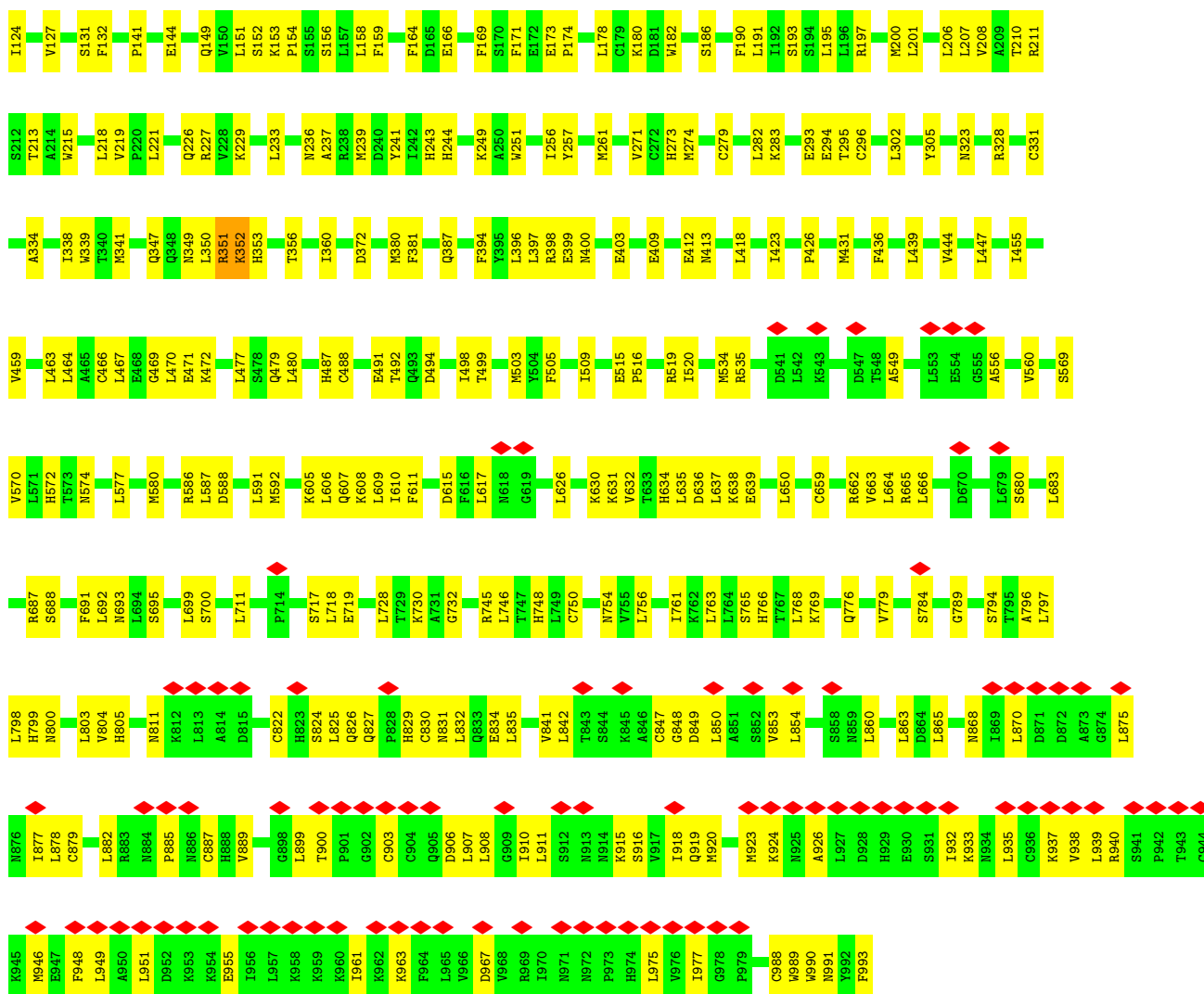
- Molecule 7: Ubiquitin-conjugating enzyme E2 D3



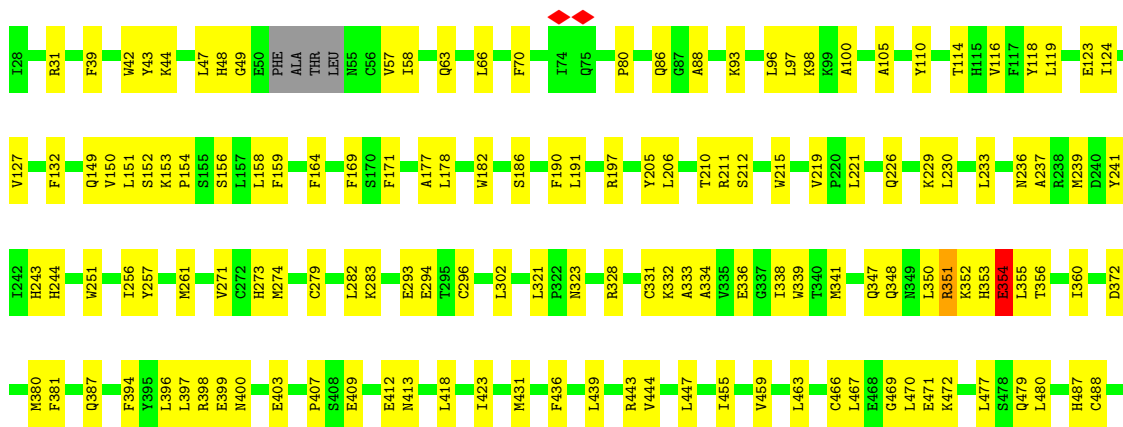
- Molecule 8: E3 ubiquitin-protein ligase UHRF1

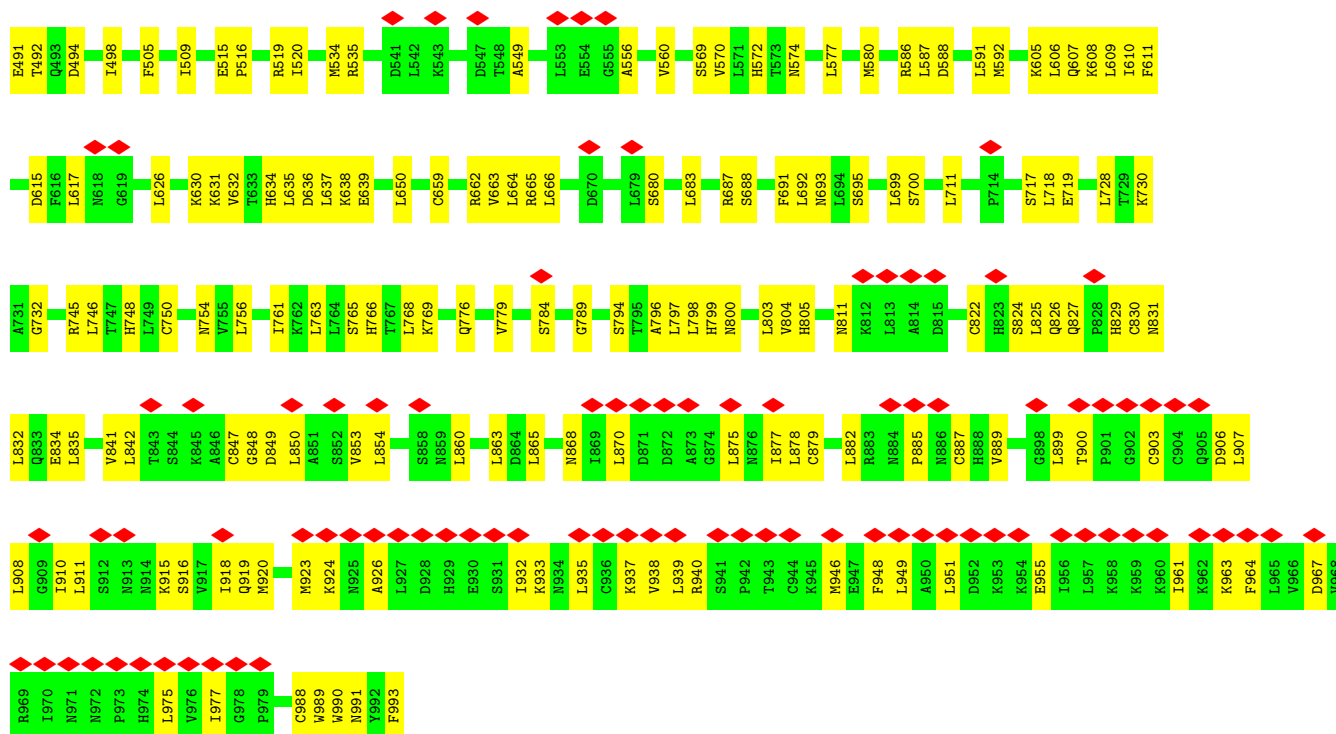






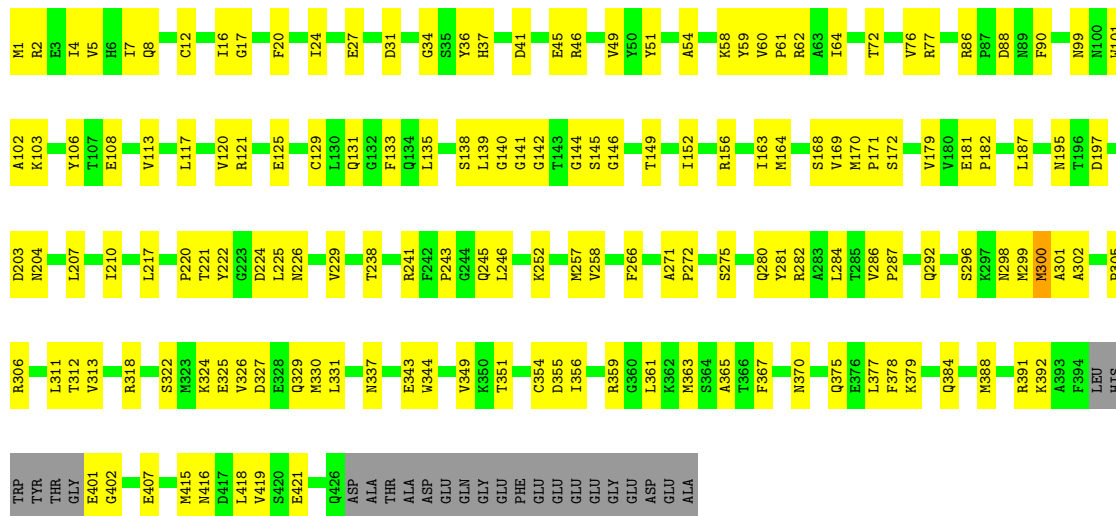
• Molecule 10: NACHT, LRR and PYD domains-containing protein 14





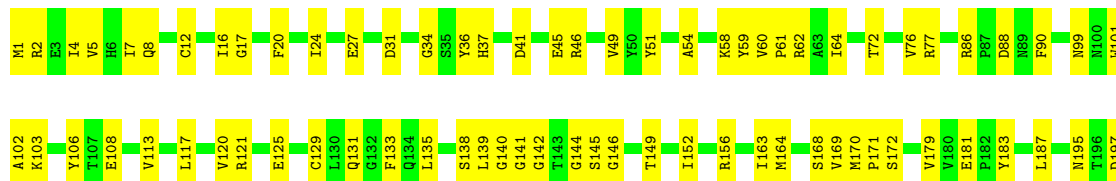
• Molecule 11: Tubulin beta-2A chain

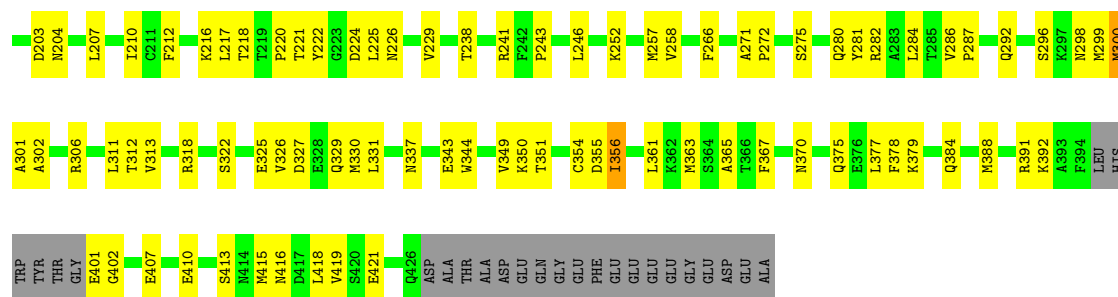
Chain L: 60% 34% 6%



• Molecule 11: Tubulin beta-2A chain

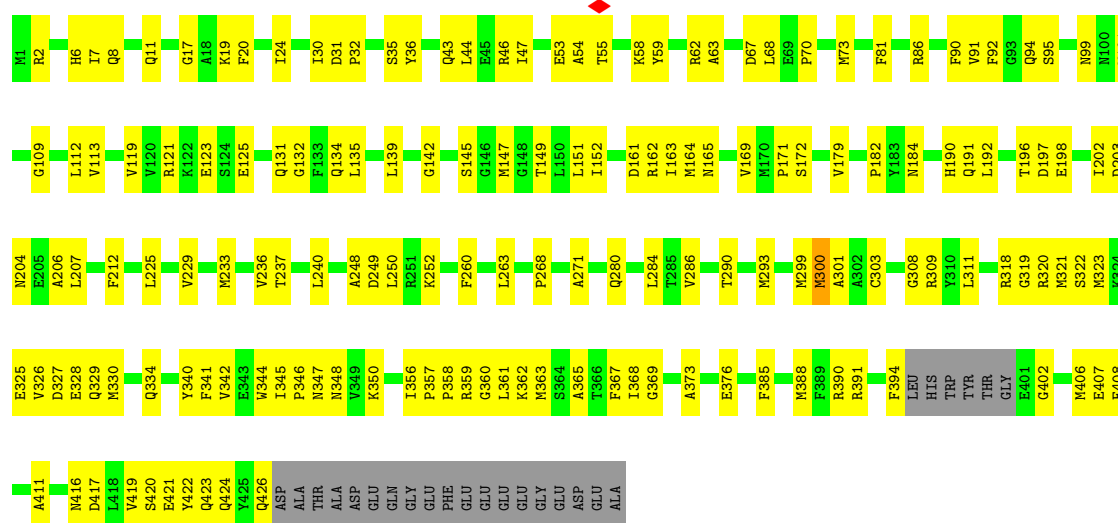
Chain L: 59% 35% 6%





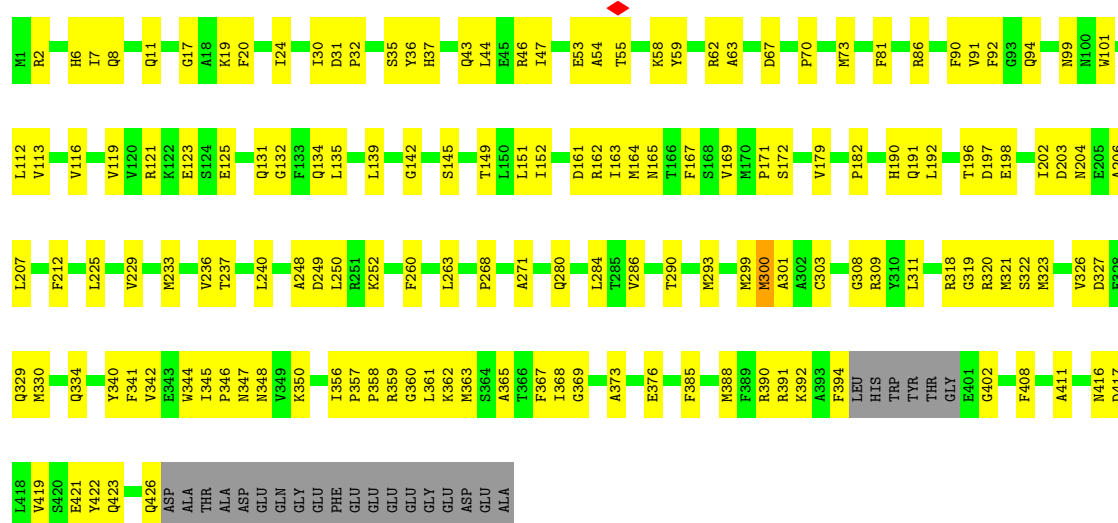
• Molecule 12: Tubulin beta-2B chain

Chain M: 58% 36% 6%



• Molecule 12: Tubulin beta-2B chain

Chain m: 60% 34% 6%

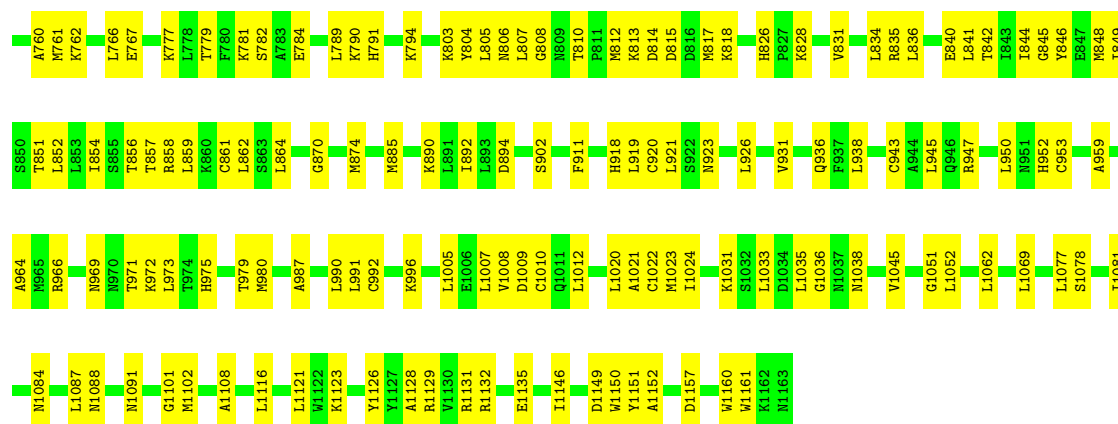


• Molecule 13: Isoform 4 of NACHT, LRR and PYD domains-containing protein 5

T1070	L853	F962	R853	A697	C573	Q416	V322	D201
S1071	R854	F966	R854	R699	I1E	V417	I323	P224
C1074	R860	R966	R860	R703	ASN	L421	G32E	K227
L1077	R864	T971	R864	D704	GLN	H425	R329	F233
S1078	R865	K972	R865	N710	ARG	Q426	K234	K234
A1080	R866	H975	R866	N720	I1E	F428	L333	P235
L1090	R868	T979	R868	V720	GLU	MET	Q334	Y236
N1091	R880	H980	R880	L729	VAL	D429	R335	Q237
N1092	R870	N981	R870	L737	LYS	Q430	S341	T244
F1097	R871	P982	R871	C737	ARG	C431	R342	I245
L1079	R872	P983	R872	S738	THR	Q432	K343	R250
F1098	R873	G984	R873	W739	ASP	V436	K344	R251
T1099	R874	D985	R874	L740	P589	C437	K345	P251
S1100	R875	R989	R875	L743	T590	V440	Q348	G254
G1101	R885	C992	R885	L746	R591	K448	P349	K255
L1103	R886	C992	R886	K747	F600	K448	I350	L258
K1104	R887	L995	R887	E748	G601	K452	Y351	A259
L1105	R888	K996	R888	L749	L602		L357	V263
A1108	R890	V1008	R890	D750	T607	L461	L359	W266
F1109	L891	D1009	L891	C765	L611	L468	A361	F272
Q1110	L893	C1010	L893	K777	V623	V469	L362	M275
L1116	L898	Q1011	L898	L778	K626	F470	L368	T278
I1119	L906	C1016	L906	T779	L627	Q472	I369	I279
Q1124	L918	L1020	L918	E784	V630	L475	T370	F280
A1128	L919	A1021	L919	V785	L633	K476	R373	F281
R1129	C1022	C1022	C920	W786	I634	V492	K374	S282
V1130	N923	N1023	N923	L792	Q493	G493	T375	V283
R1131	G1036	G1036	N924	W923	A635	L494	R377	I286
R1132	N1037	N1037	S925	K794	Q636	C495	K379	K287
Q1133	N1038	N1038	L926	L795	L666	V496	C379	W288
V1137	G1041	G1041	Q927	L796	E671	N497	L380	S293
V1144	V1045	V1045	T928	F797	K520	L519	K381	L297
W1150	E1050	E1050	V931	L802	T676	K520	K383	I298
N1159	G1051	G1051	C935	K303	K679	L527	L388	E301
W1160	L1052	L1052	R939	Y804	V680	F528	H529	L308
W1161	Q1054	Q1054	R806	N806	D681	H529	V392	V309
K1162	L1059	L1059	R947	A823	V684	I532	R400	T310
N1163	R1060	R1060	L950	T833	S685	Y559	V404	K311
	R1061	R1061	N951	L834	V687	L562	L405	I312
	L1062	L1062	H952	R895	C688	L565	I408	K313
	K1063	K1063	C953	L836	L689	L565	S409	L319
	C1067	C1067	N954	D837	H691	W568	N410	L320
	T1069	T1069	L959	S850	C692		T41E	E263

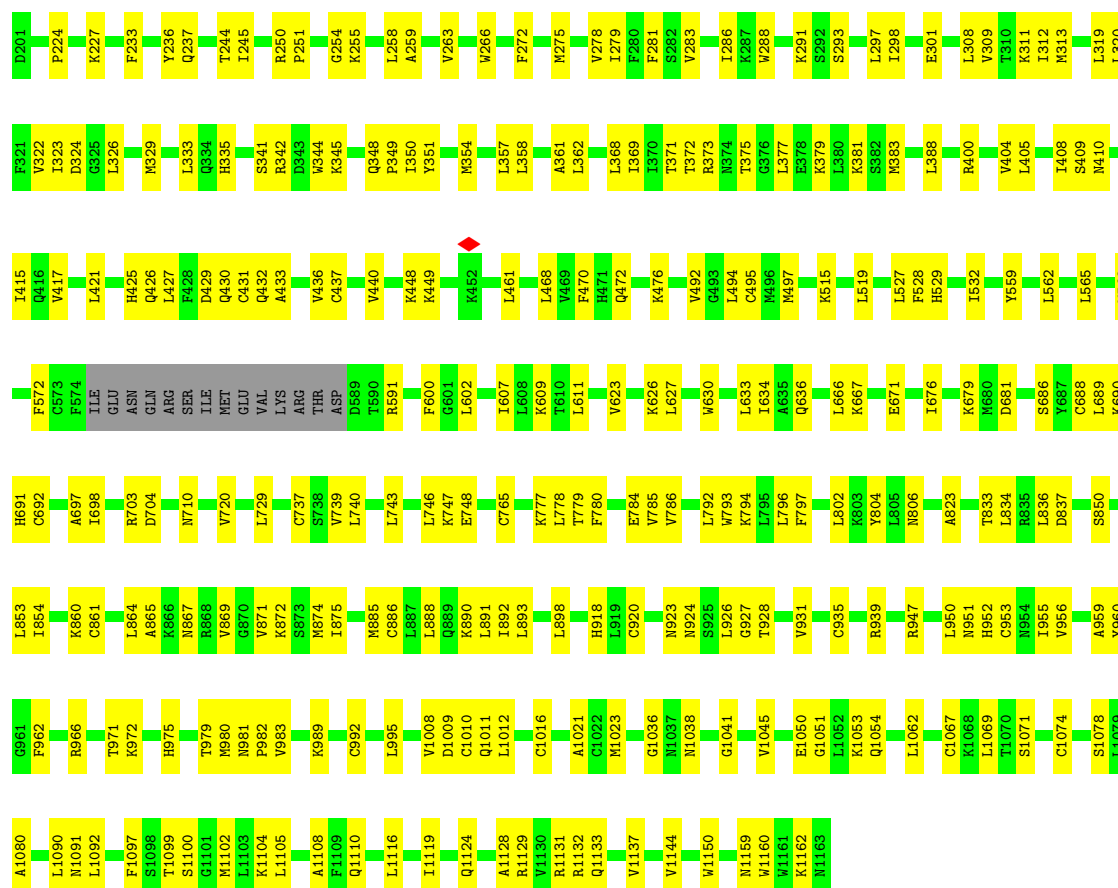
- Chain F:  67% 31% .

F650	F651	C652	L653	F654	E655	F661	L666	I676	D681	V684	C688	L689	K690	H691	C692	Q693	V700	D701	T702	R703	L704	L705	L706	S707	L714	C715	F716	F717	T718	T719	V720	Q721	E722	T723	K726	F727	L728	L729	M730	N735	F736	C737	S738	F739	L740	L743										
H548	L549	S550	L551	A557	L558	Y559	Y560	E566	E567	W568	N569	F572	C573	F574	I575	GLU	ASN	GLN	ASN	ARG	SER	I576	I577	MET	GLU	VAL	LYS	ARG	THR	ASP	D589	T590	B591		R597	F600	G601	L602	M603		L607	L614		V623	E624	Q625	K626	L627	Q628		V638	M644	D645	T646		
L308	H419	S420	L421	Q426	L427	V440		K452	Q459	T460	L461	L464	F470	H471	Q472	L473	R477	P478	S479		L483	S484	Q488		V492	Q493	L494	C495	M496	M497	V508	F509		Y517	K520	E521	S522	M530		L533	L534	Q535		E541	Y544	V545	F546									
D201	L202	K212	F213	S216		L219		F233	K234	G325	L326	H335	M338	T339	L340	H248	G249	R250	F251	G252	V253		S256		R260		V263		I369	L370	T371	F272	Q273	K274	V278	L279	V283	K284	E285	L286	K287	V288		K291	S292	S293	L294		L297	L298	A299	K300				



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

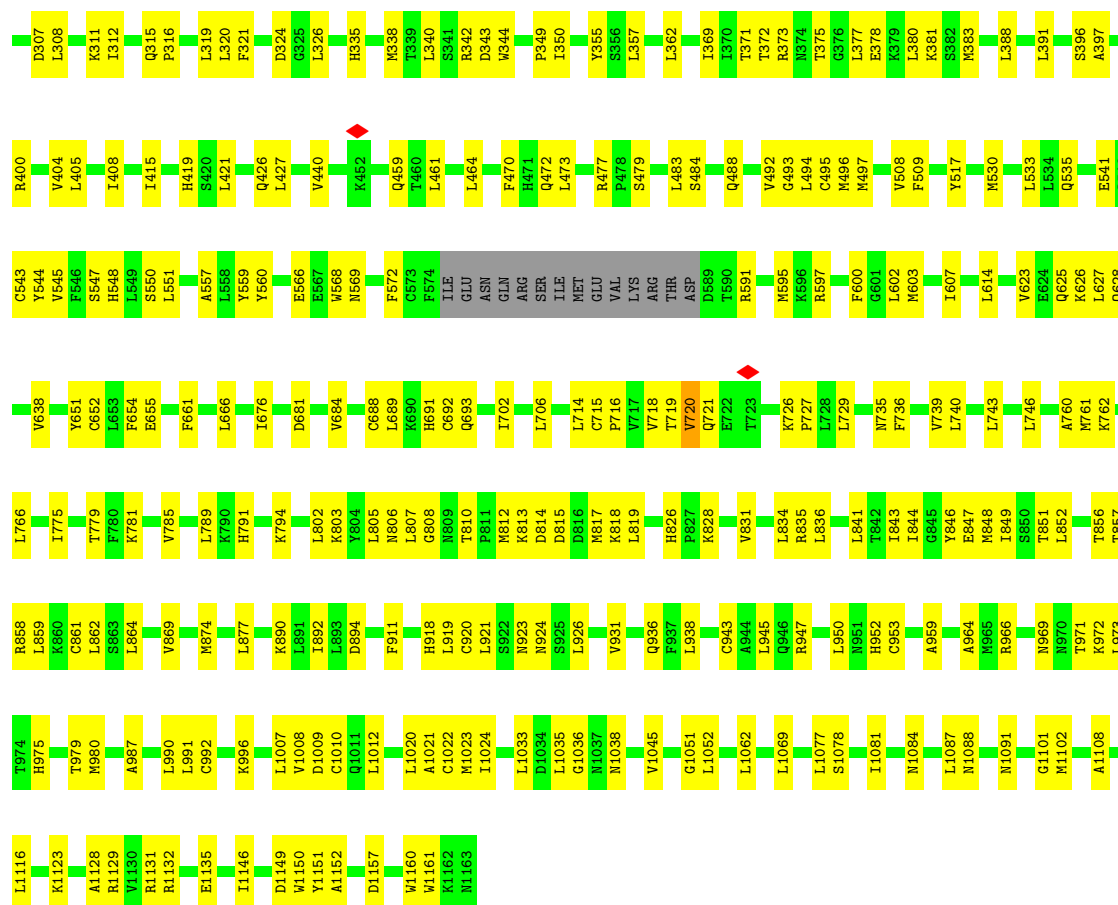
Chain a: 71% 28% .



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

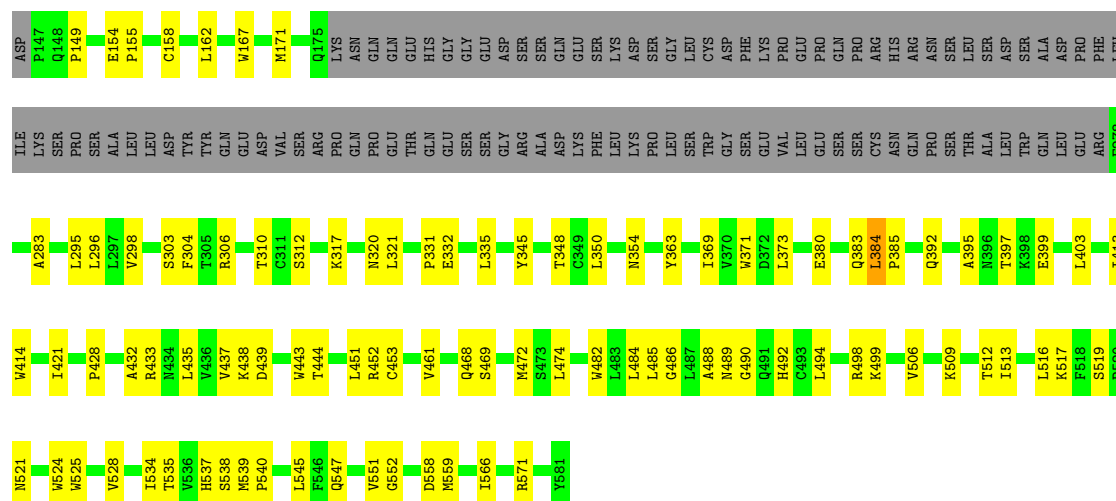
Chain f: 68% 31% .





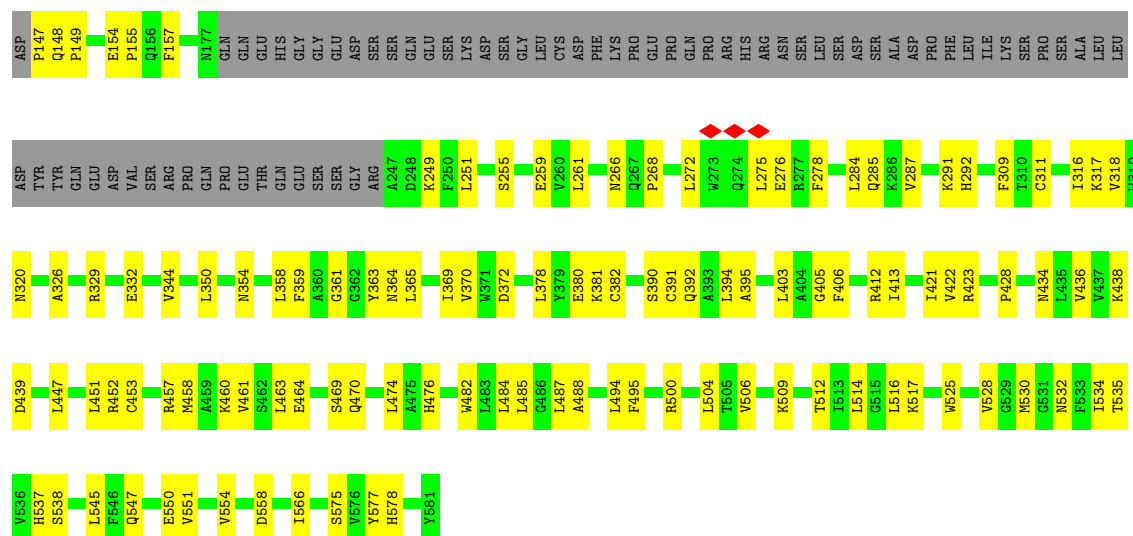
• Molecule 14: Transducin-like enhancer protein 6

Chain B: 55% 22% 24%



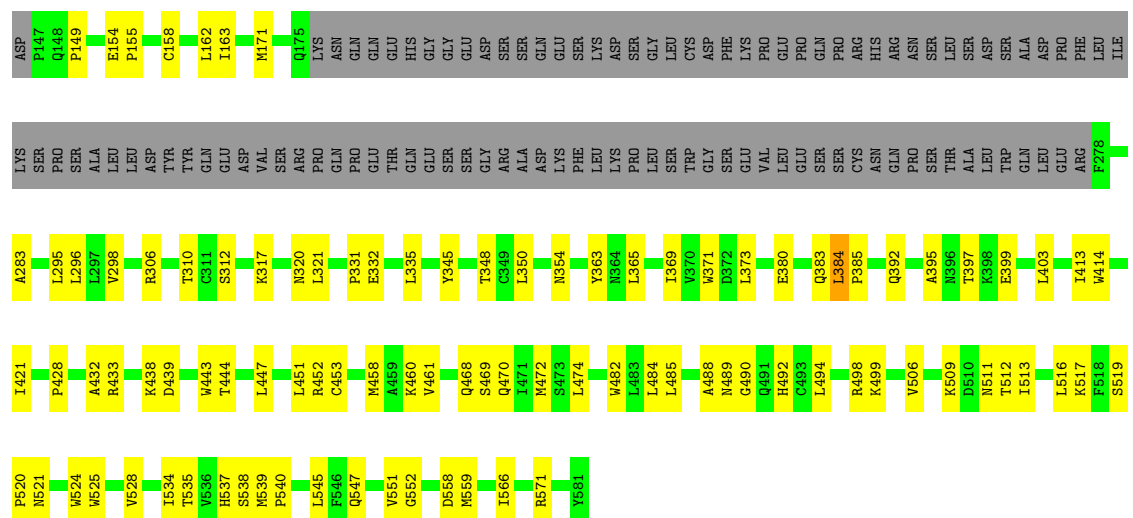
• Molecule 14: Transducin-like enhancer protein 6

Chain G: 58% 26% 16%



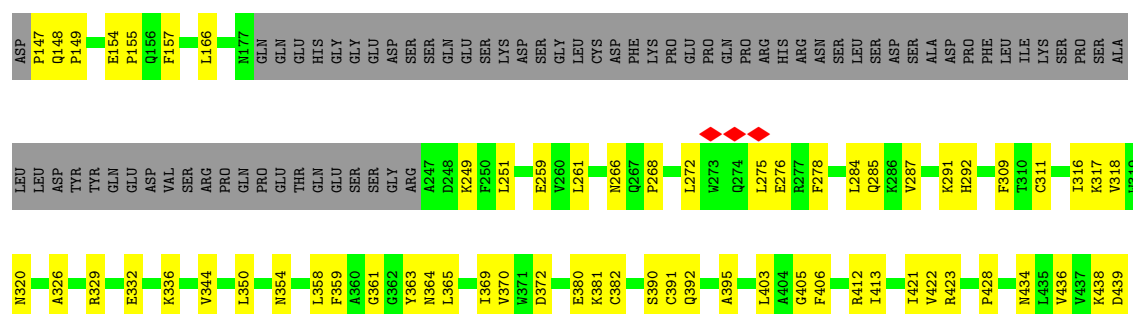
- Molecule 14: Transducin-like enhancer protein 6

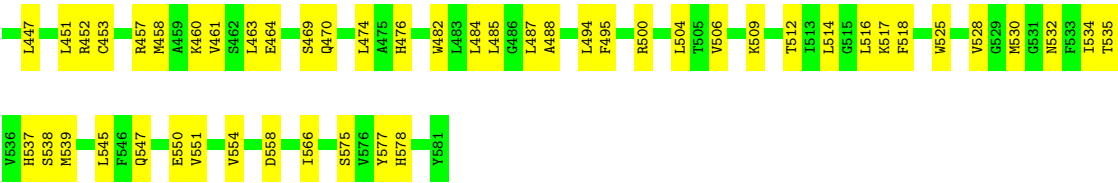
Chain b: 54% 22% 24%



- Molecule 14: Transducin-like enhancer protein 6

Chain g: 58% 26% 16%





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
Maximum map value	1.057	Depositor
Minimum map value	-0.503	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.085	Depositor
Map size ($\text{\AA}$)	689.472, 689.472, 689.472	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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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

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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

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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

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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

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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	m	501	-	28,30,30	1.15	3 (10%)	44,47,47	1.91	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	1.17	3 (10%)	44,47,47	1.95	8 (18%)
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	1.98	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	F	1201	-	27,29,29	1.36	4 (14%)	42,45,45	1.97	9 (21%)
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	m	501	-	-	2/16/32/32	0/3/3/3
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	A	1201	-	-	4/16/32/32	0/3/3/3
16	ADP	F	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

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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:

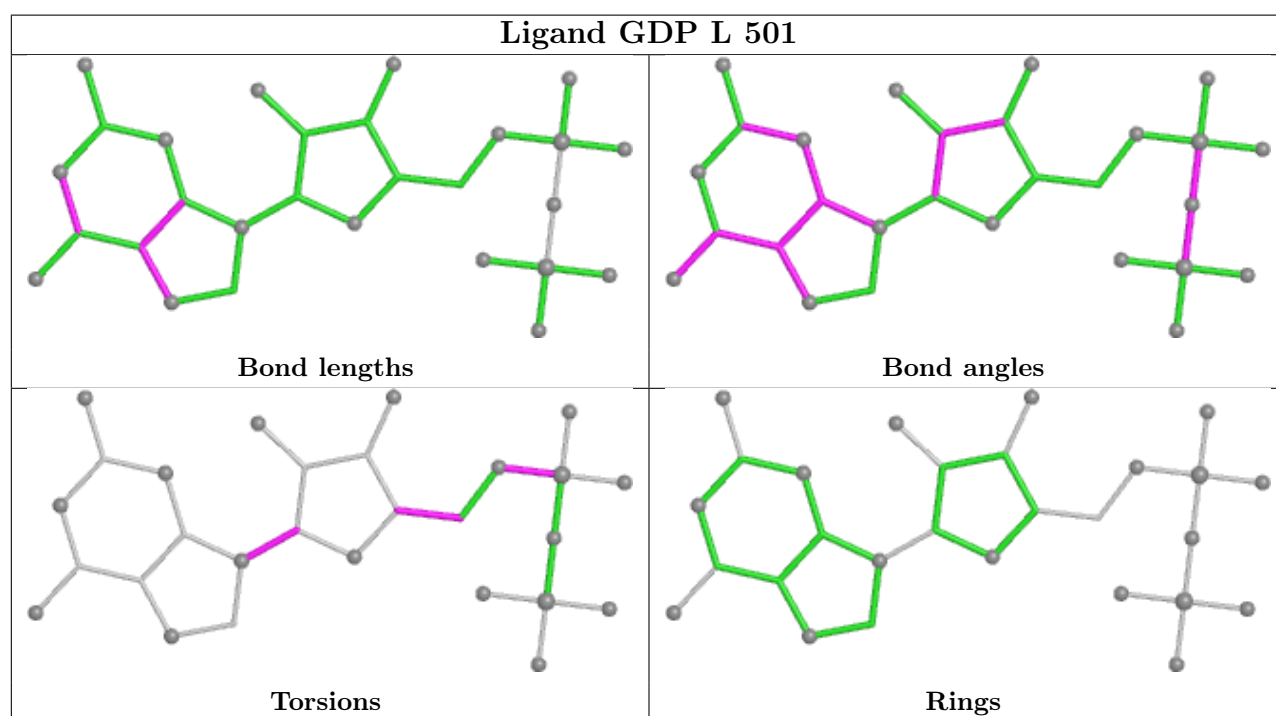
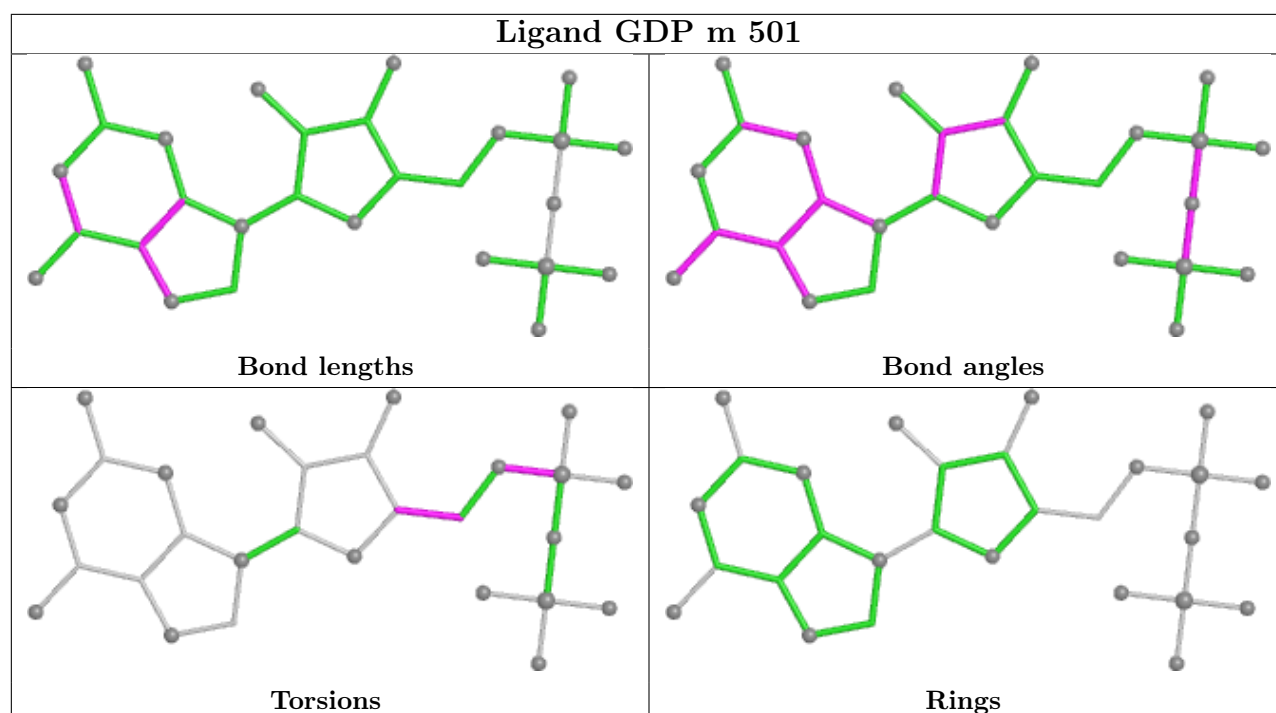
Mol	Chain	Res	Type	Atoms
15	L	501	GDP	O4'-C4'-C5'-O5'
15	l	501	GDP	O4'-C4'-C5'-O5'
16	A	1201	ADP	C5'-O5'-PA-O3A
16	F	1201	ADP	PA-O3A-PB-O3B
16	F	1201	ADP	PB-O3A-PA-O5'

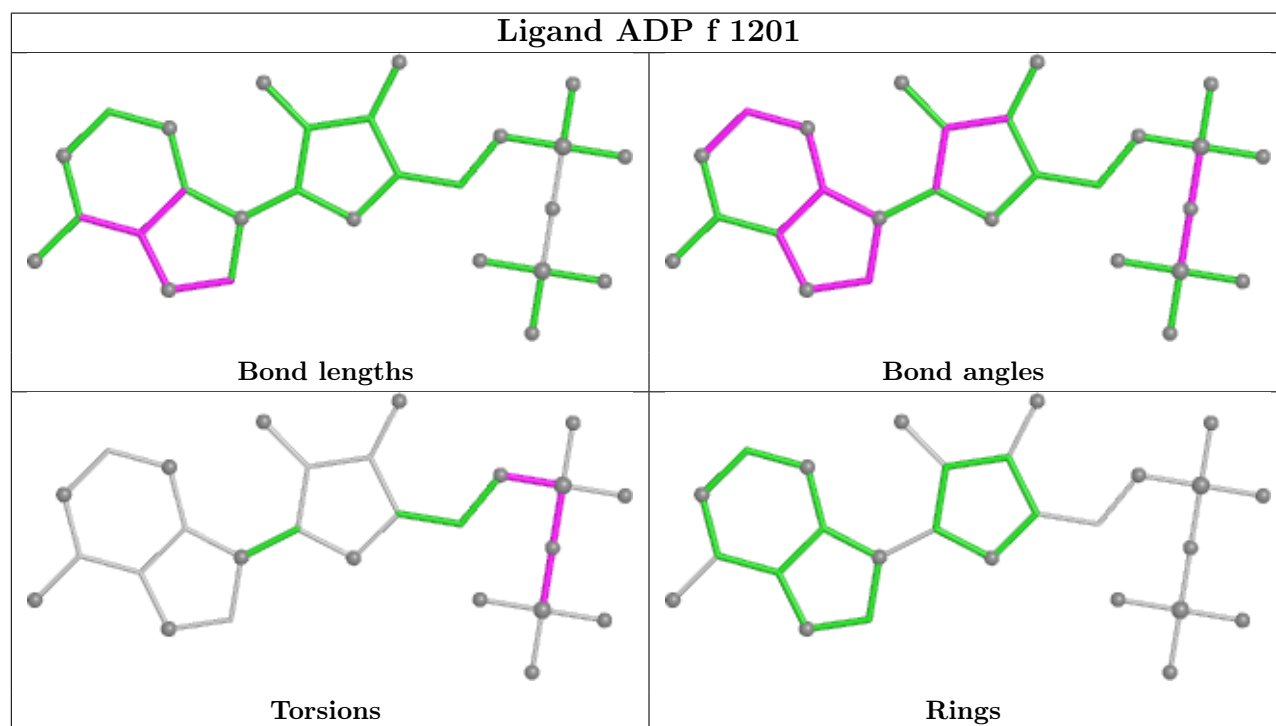
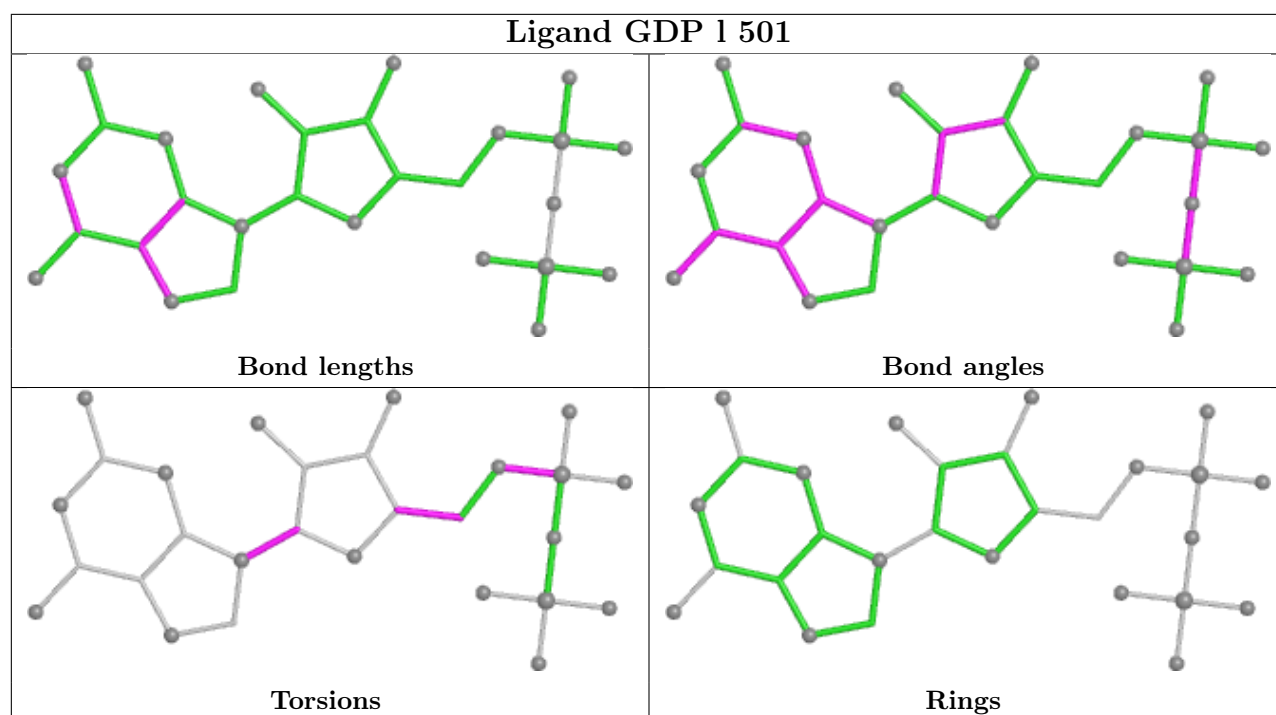
There are no ring outliers.

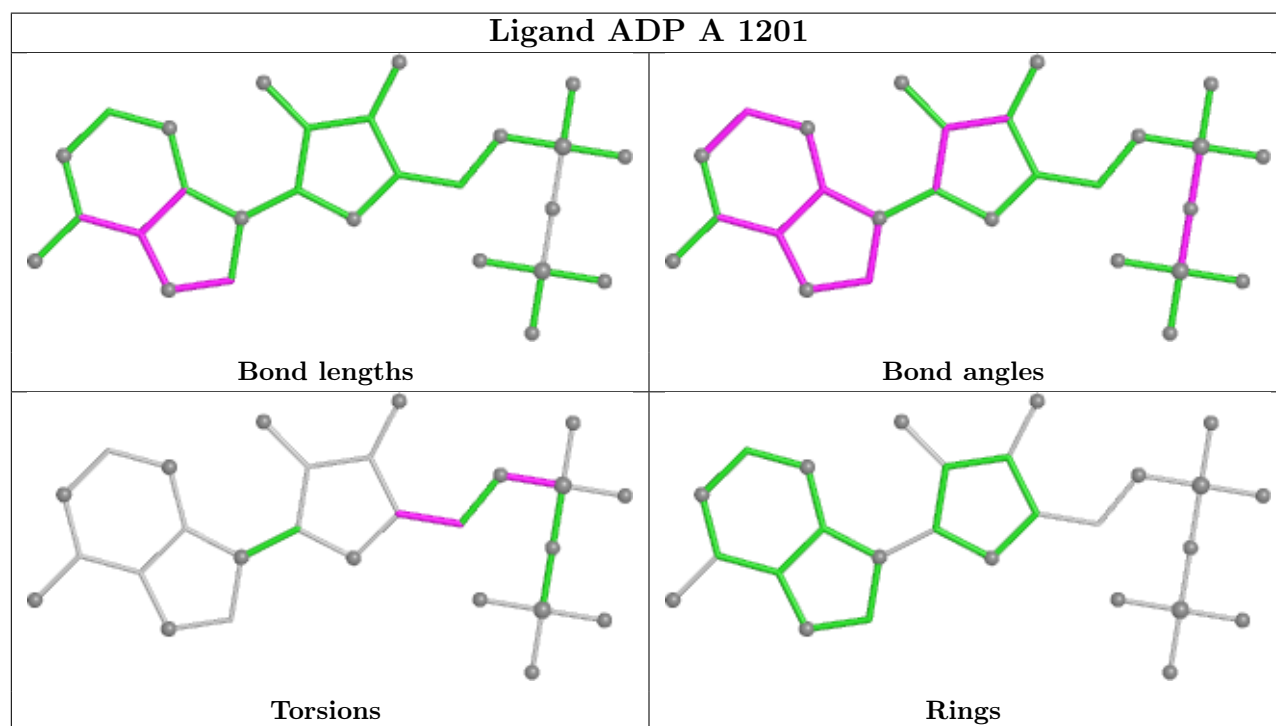
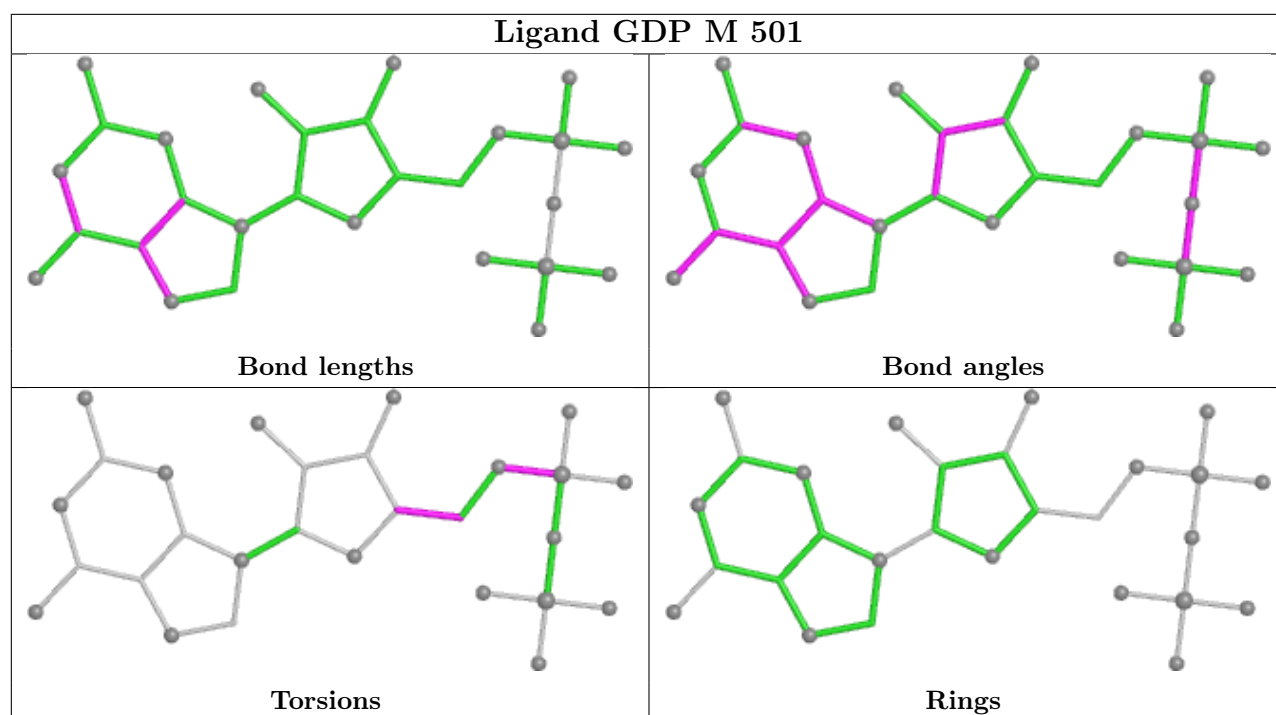
8 monomers are involved in 12 short contacts:

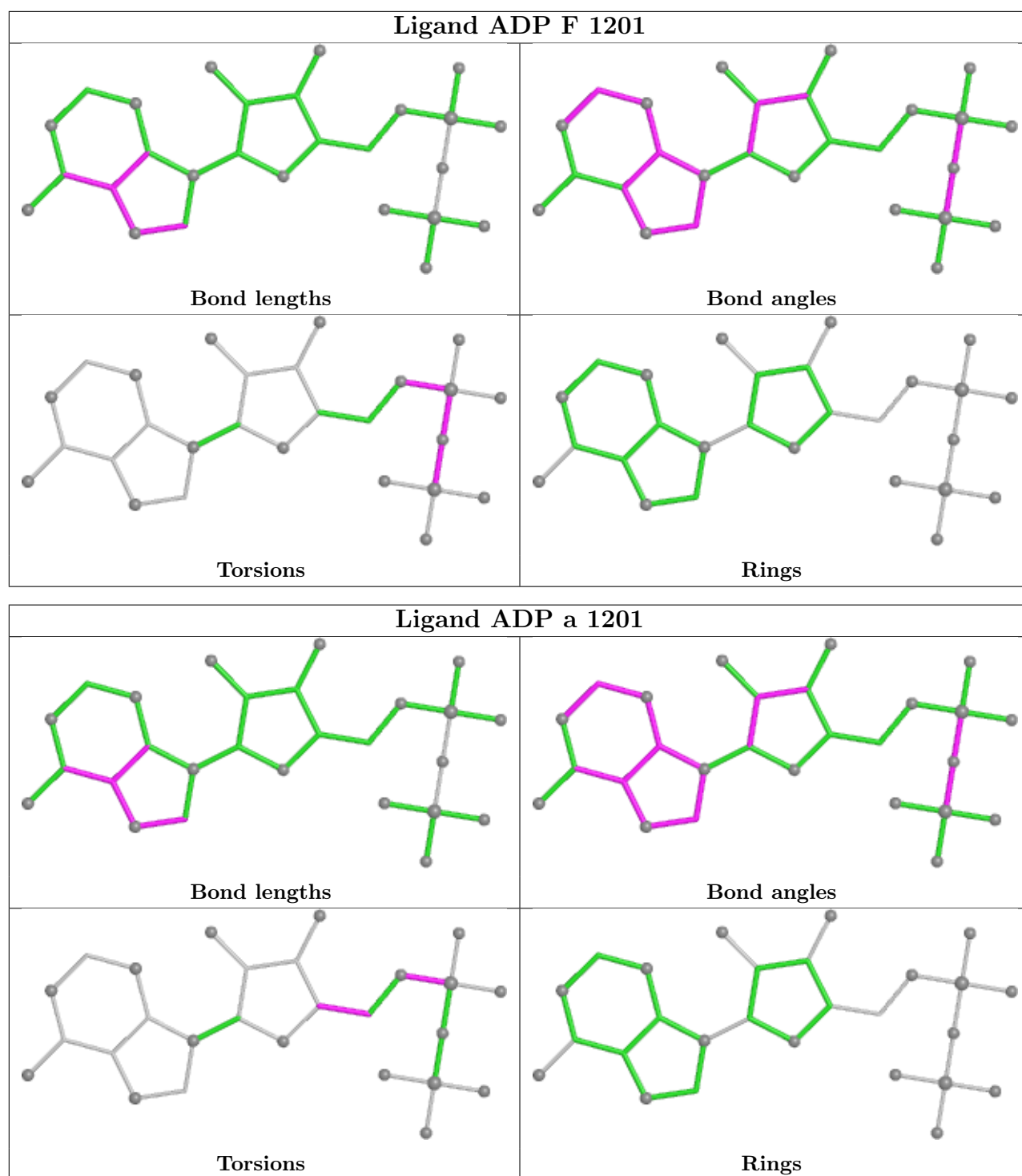
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	m	501	GDP	1	0
15	L	501	GDP	2	0
15	l	501	GDP	2	0
16	f	1201	ADP	1	0
15	M	501	GDP	1	0
16	A	1201	ADP	2	0
16	F	1201	ADP	1	0
16	a	1201	ADP	2	0

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.

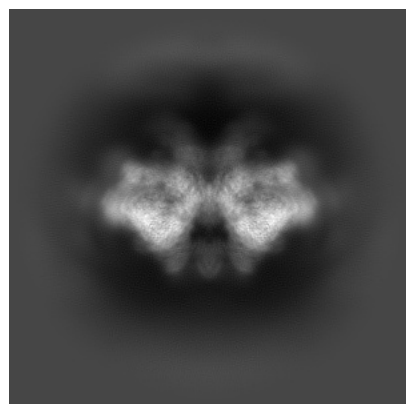
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65575. These allow visual inspection of the internal detail of the map and identification of artifacts.

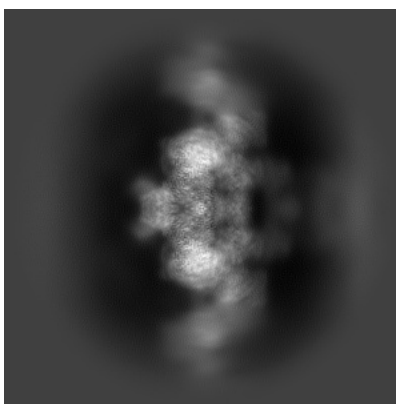
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

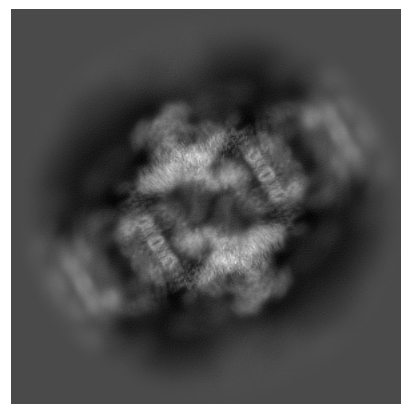
6.1.1 Primary map



X

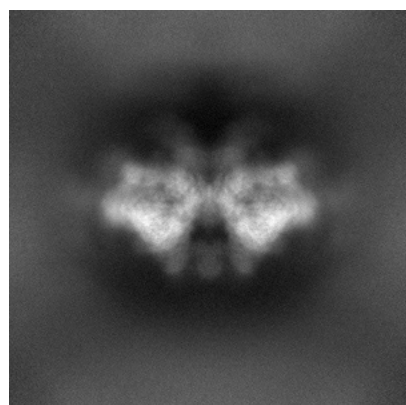


Y

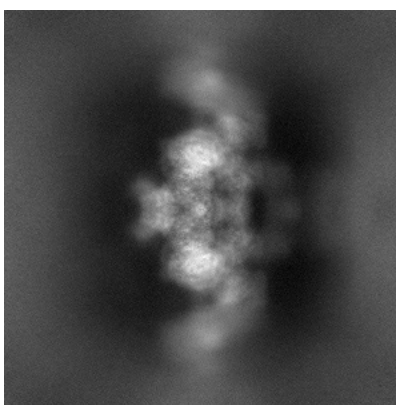


Z

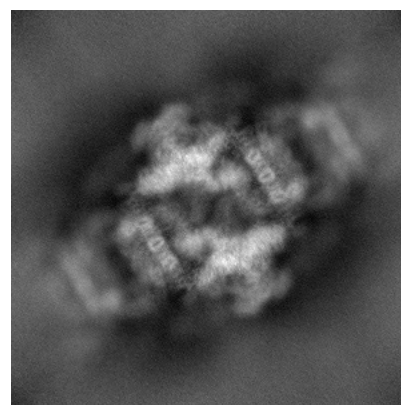
6.1.2 Raw map



X



Y

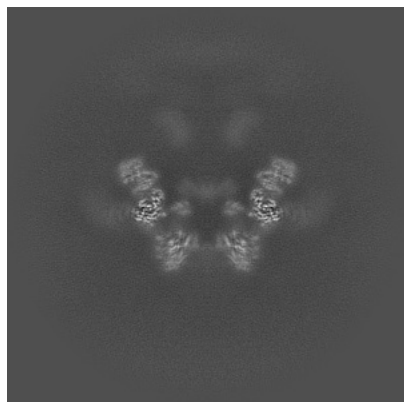


Z

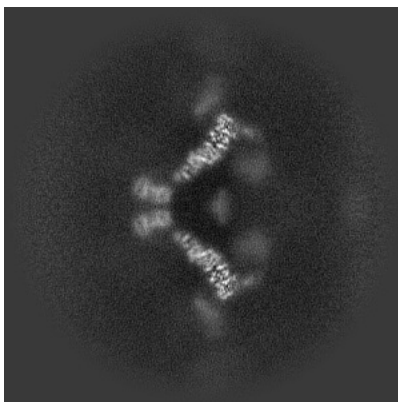
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

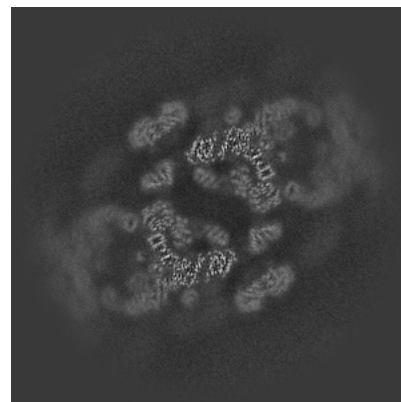
6.2.1 Primary map



X Index: 320

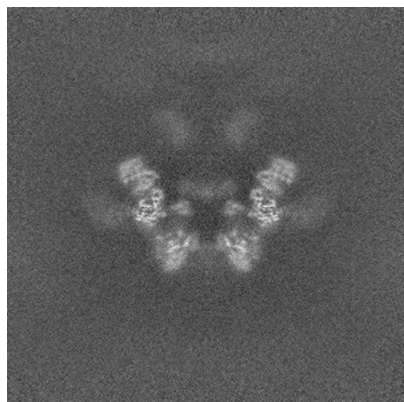


Y Index: 320

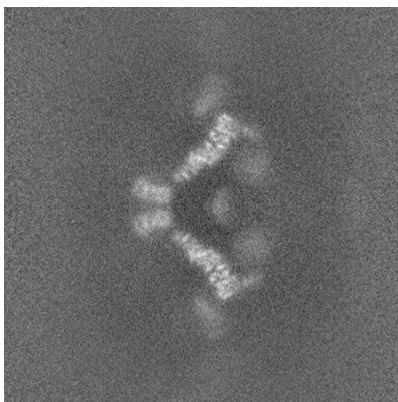


Z Index: 320

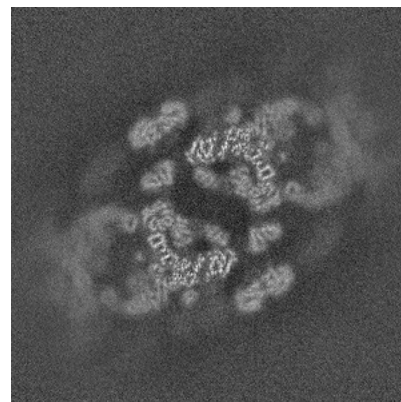
6.2.2 Raw map



X Index: 320



Y Index: 320

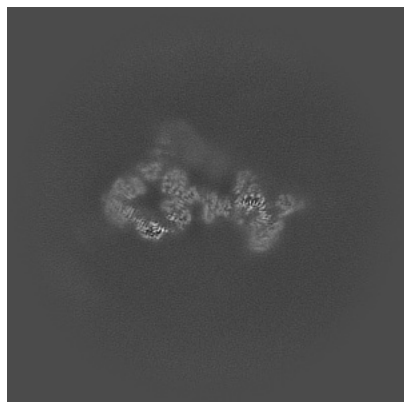


Z Index: 320

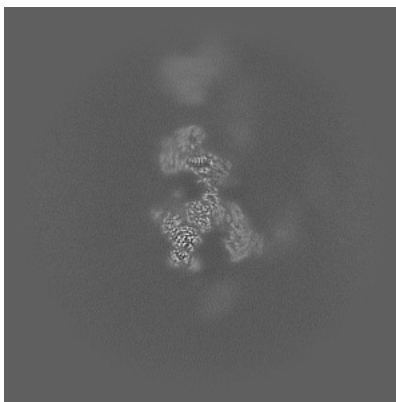
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

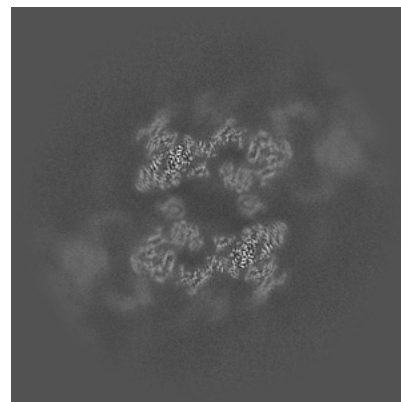
6.3.1 Primary map



X Index: 396

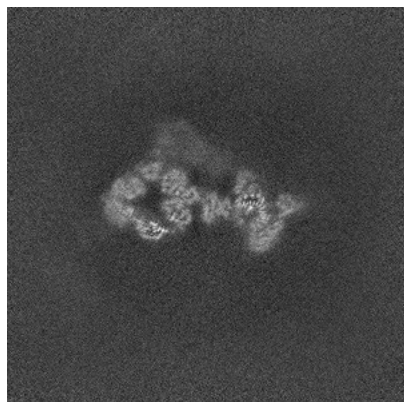


Y Index: 405

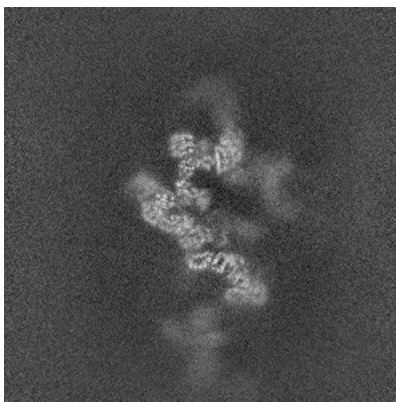


Z Index: 297

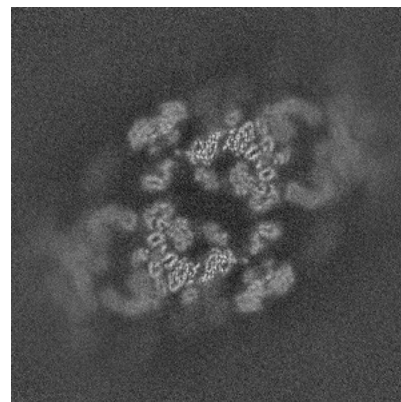
6.3.2 Raw map



X Index: 396



Y Index: 271

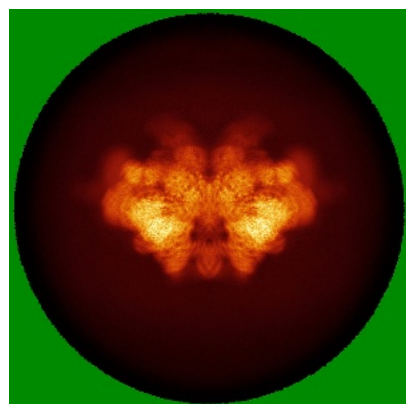


Z Index: 315

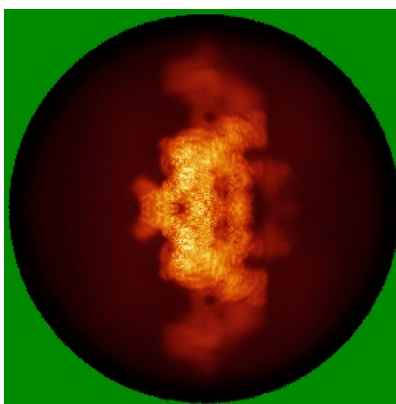
The images above show the largest variance slices of the map in three orthogonal directions.

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

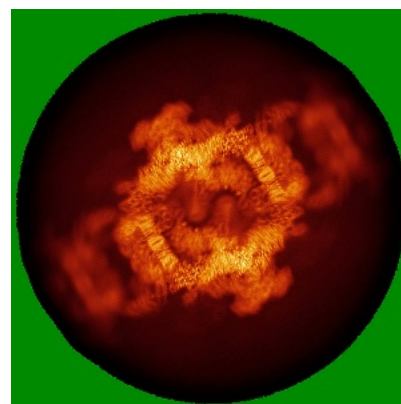
6.4.1 Primary map



X

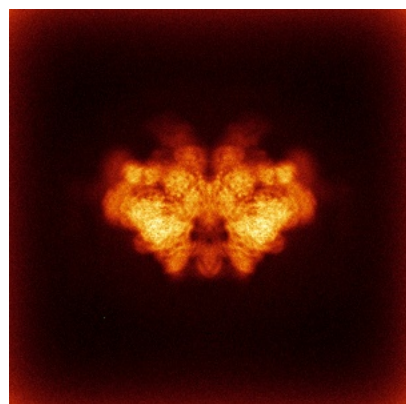


Y

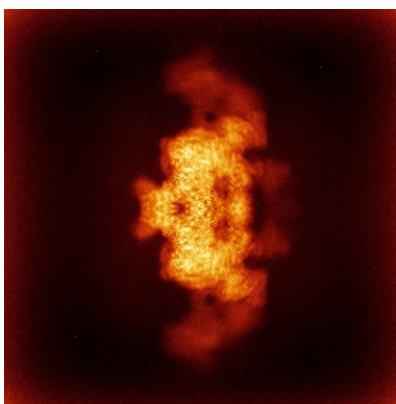


Z

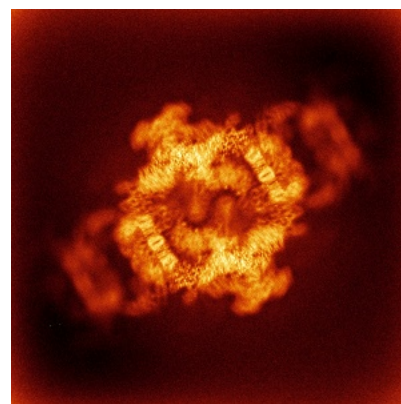
6.4.2 Raw map



X



Y



Z

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

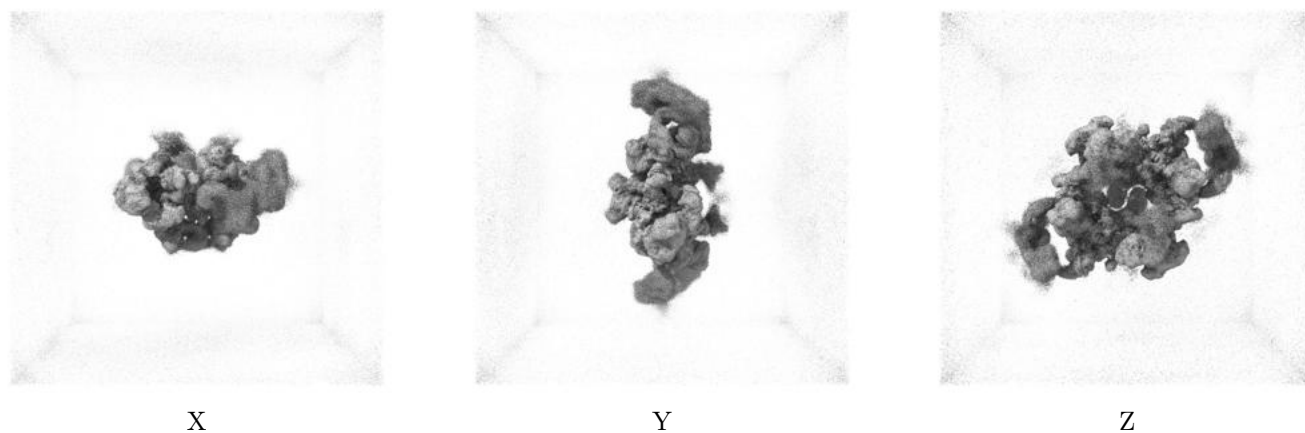
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

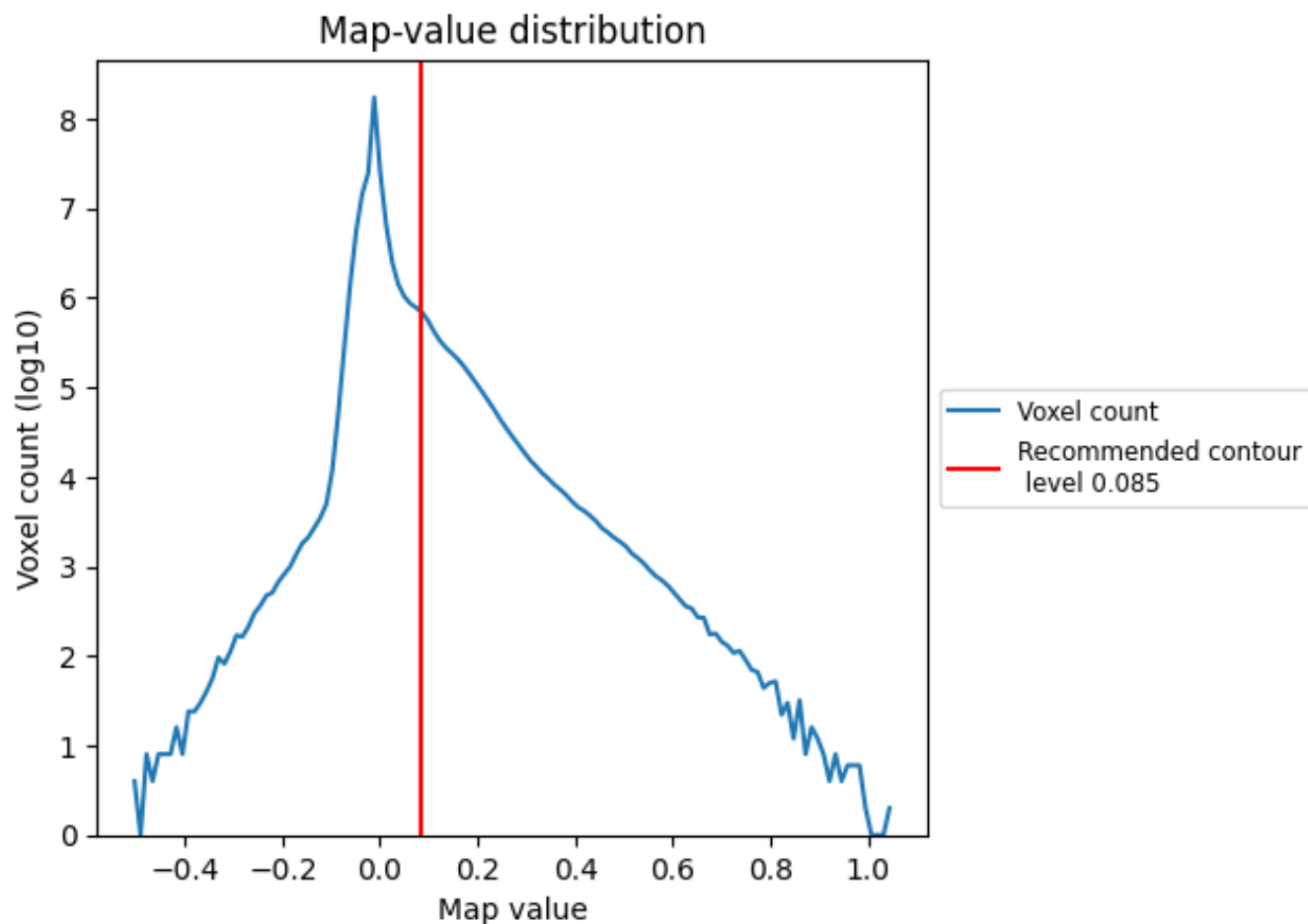
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

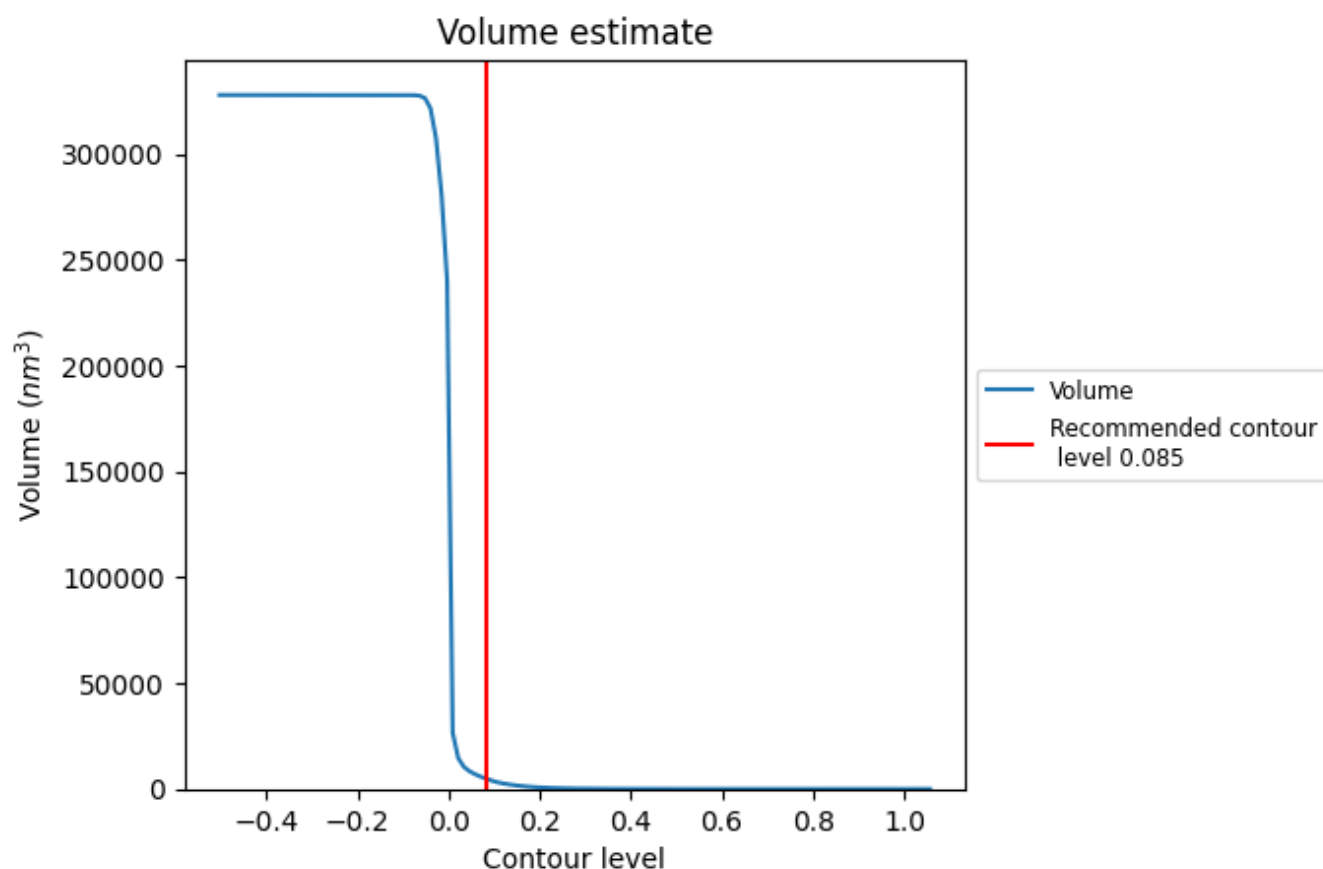
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

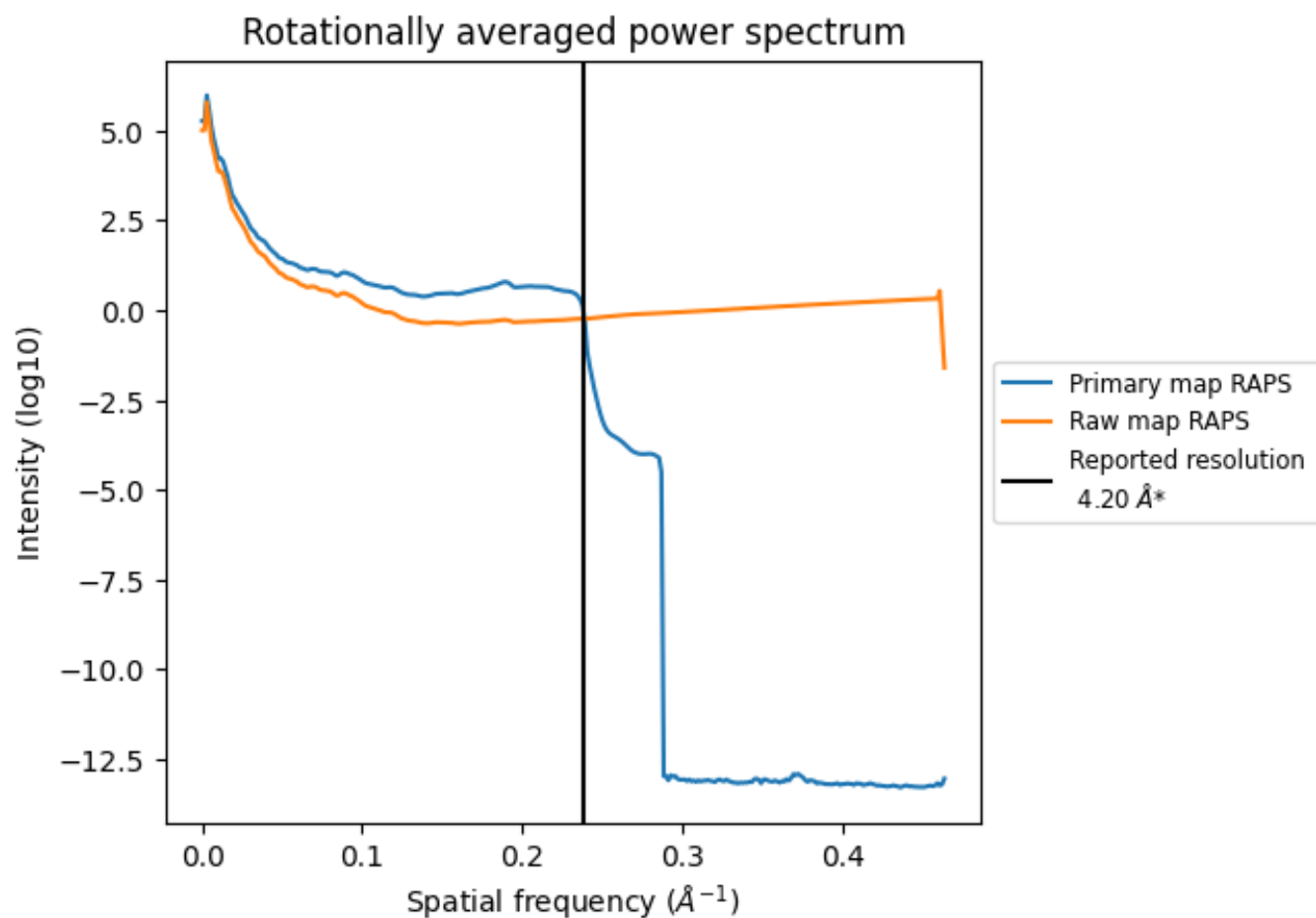
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4642 nm^3 ; this corresponds to an approximate mass of 4193 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

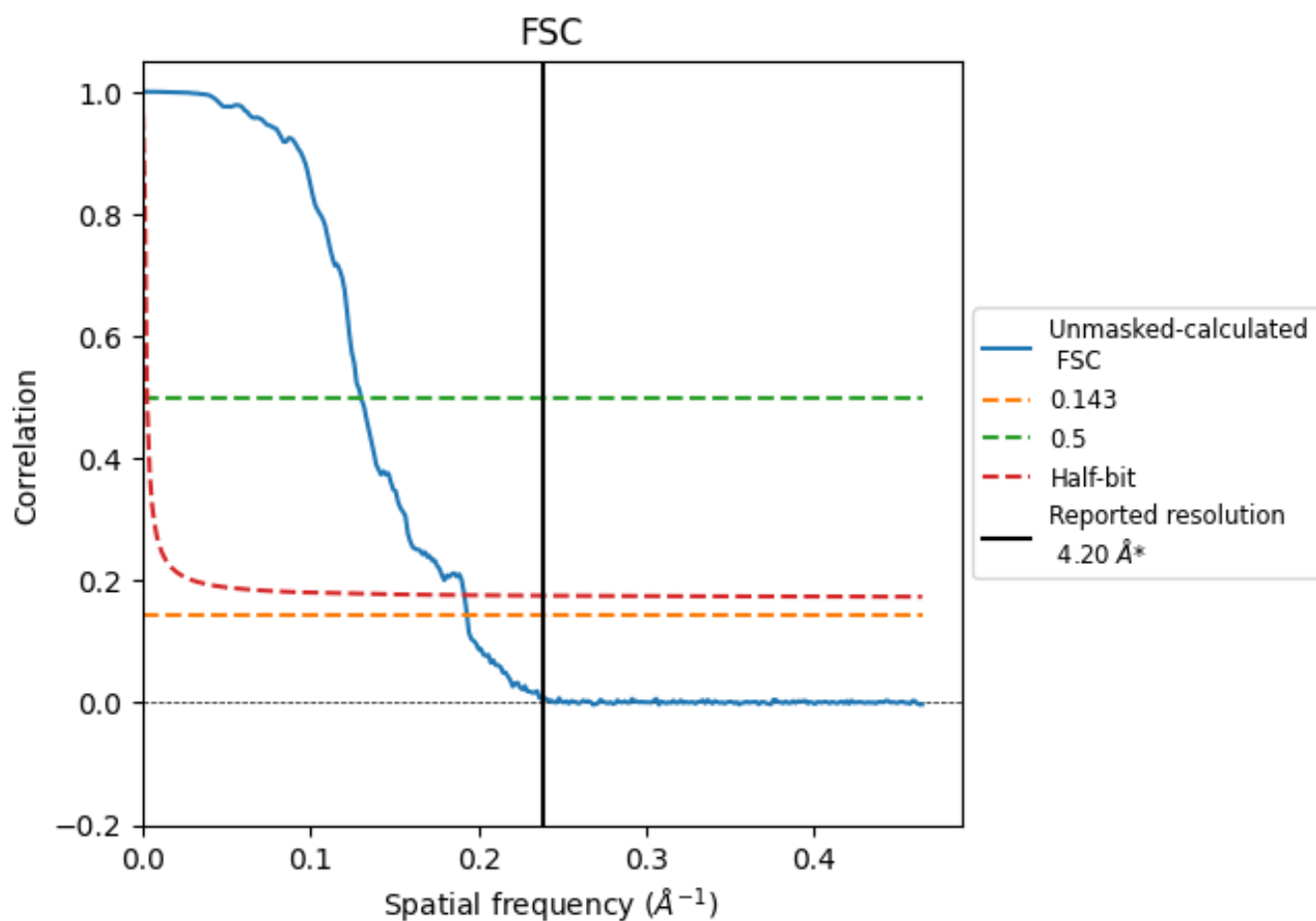


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

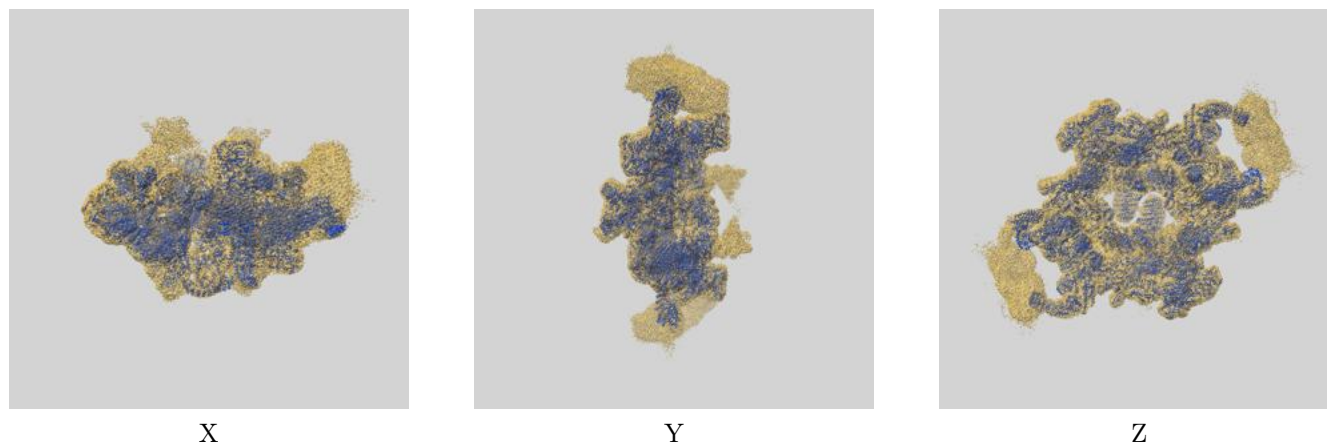
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.18	7.68	5.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.18 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

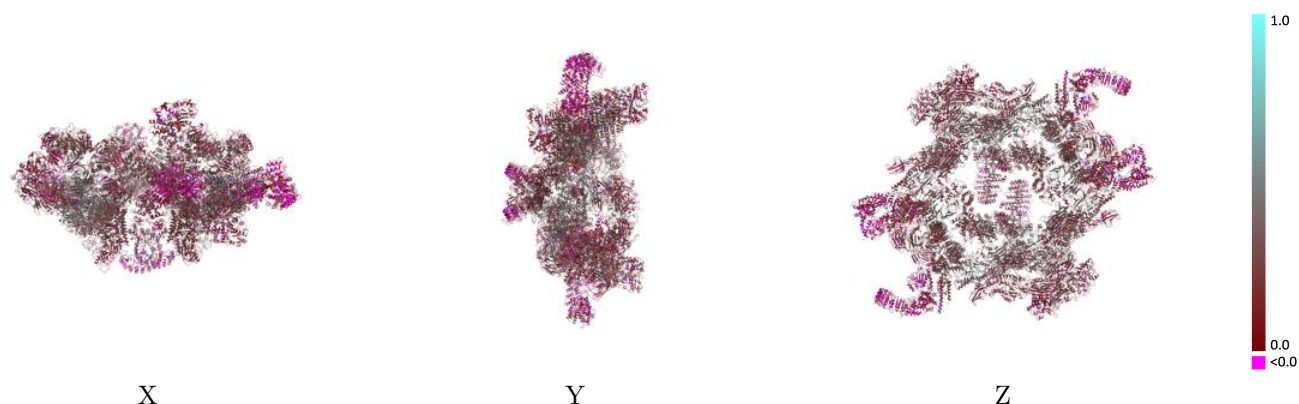
This section contains information regarding the fit between EMDB map EMD-65575 and PDB model 9W2M. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



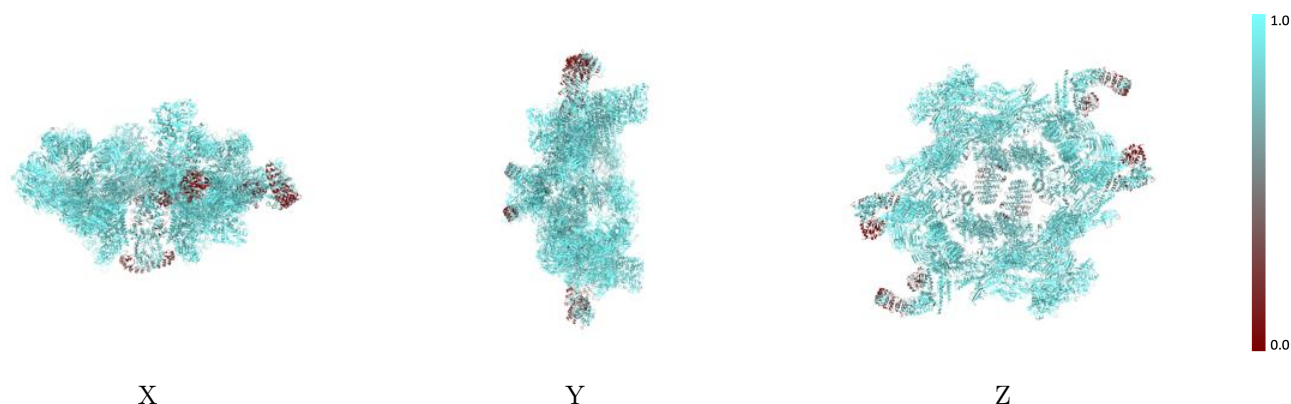
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



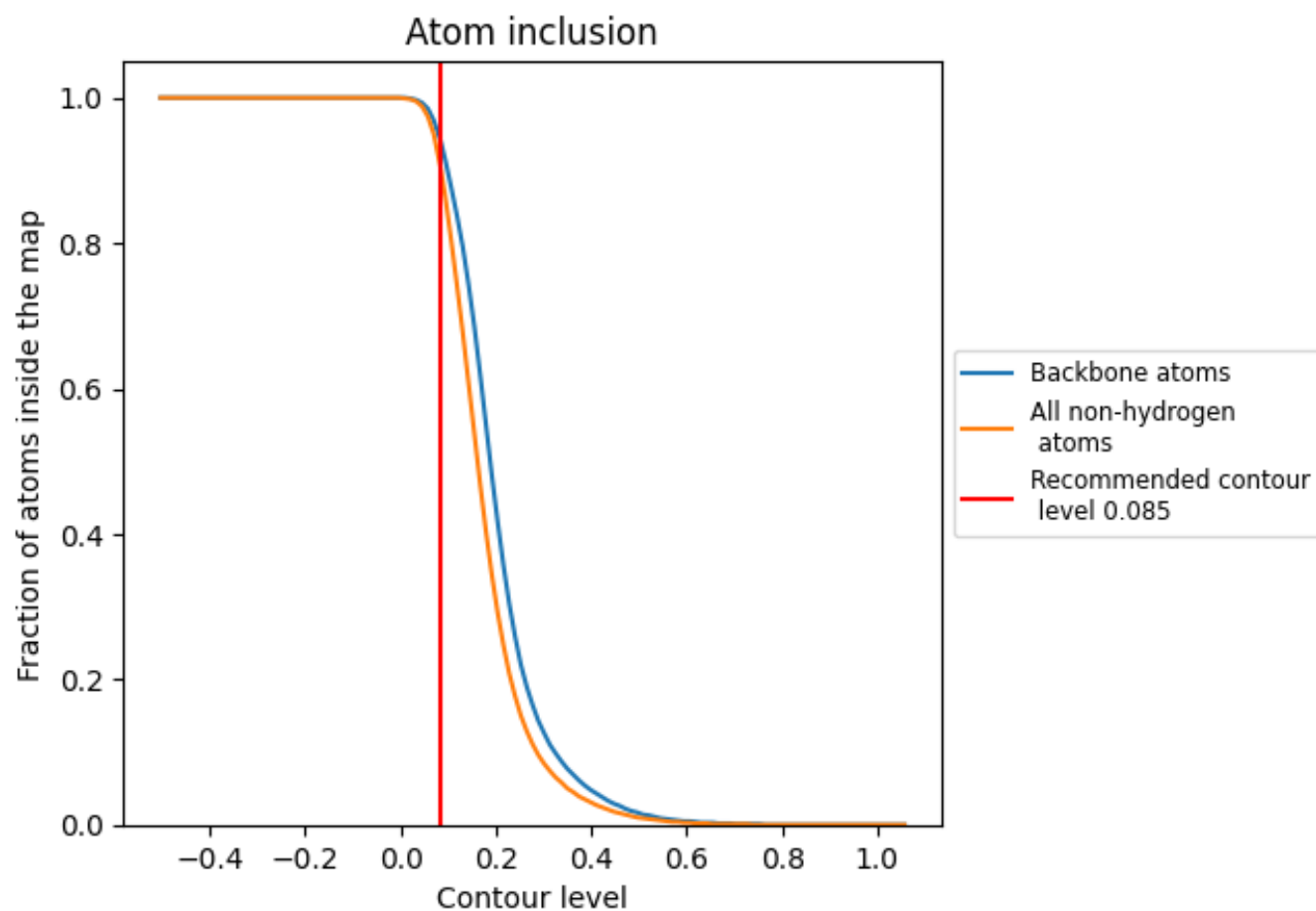
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.2570
1	 0.9450	 0.3770
11	 0.9430	 0.3760
12	 0.9590	 0.3780
13	 0.9530	 0.2890
14	 0.9600	 0.2450
15	 0.9700	 0.2180
16	 0.9660	 0.2230
17	 0.9550	 0.3400
18	 0.9490	 0.3660
19	 0.9560	 0.2670
2	 0.9580	 0.3760
3	 0.9530	 0.2910
4	 0.9620	 0.2460
5	 0.9690	 0.2190
6	 0.9680	 0.2240
7	 0.9550	 0.3410
8	 0.9590	 0.3880
9	 0.9540	 0.2680
A	 0.9680	 0.2770
B	 0.9850	 0.2510
C	 0.9440	 0.2590
D	 0.8920	 0.2360
E	 0.6420	 0.1090
F	 0.9420	 0.2570
G	 0.9600	 0.2550
H	 0.9800	 0.2720
I	 0.5840	 0.1160
J	 0.9160	 0.2920
K	 0.6710	 0.1630
L	 0.9660	 0.2480
M	 0.9340	 0.2610
N	 0.8510	 0.1930
O	 0.9570	 0.3490
P	 0.9290	 0.2970



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Chain	Atom inclusion	Q-score
Q	 0.9830	 0.1160
R	 0.9880	 0.2560
Z	 0.9380	 0.3090
a	 0.9670	 0.2790
b	 0.9850	 0.2500
c	 0.9430	 0.2580
d	 0.8920	 0.2320
e	 0.6410	 0.1070
f	 0.9410	 0.2580
g	 0.9590	 0.2540
h	 0.9800	 0.2700
i	 0.5840	 0.1160
j	 0.9150	 0.2950
k	 0.6690	 0.1610
l	 0.9670	 0.2490
m	 0.9350	 0.2610
n	 0.8510	 0.1940
o	 0.9570	 0.3500
p	 0.9300	 0.2980
q	 0.9830	 0.1220
r	 0.9930	 0.2610
z	 0.9120	 0.2640