



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 11:06 AM EST

PDB ID : 3JBL
EMDB ID : EMD-6458
Title : Cryo-EM Structure of the Activated NAIP2/NLRC4 Inflammasome Reveals Nucleated Polymerization
Authors : Zhang, L.; Chen, S.; Ruan, J.; Wu, J.; Tong, A.B.; Yin, Q.; Li, Y.; David, L.; Lu, A.; Wang, W.L.; Marks, C.; Ouyang, Q.; Zhang, X.; Mao, Y.; Wu, H.
Deposited on : 2015-09-05
Resolution : 4.70 Å(reported)

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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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

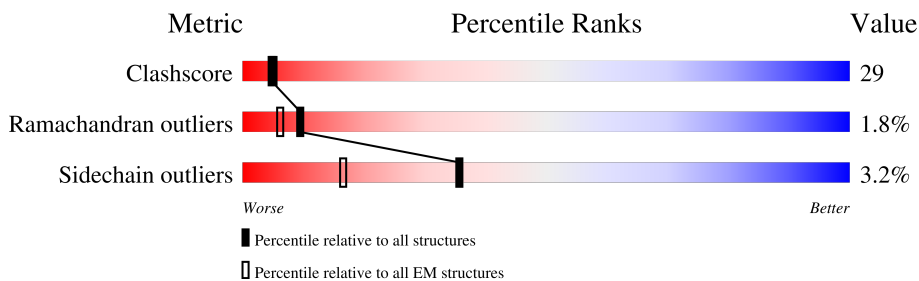
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	932	55% 43% 51% ..
1	B	932	55% 43% 51% ..
1	C	932	55% 44% 50% ..
1	D	932	54% 44% 50% ..
1	E	932	55% 44% 50% ..
1	F	932	54% 44% 50% ..
1	G	932	55% 44% 50% ..
1	H	932	55% 43% 50% ..

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Mol	Chain	Length	Quality of chain
1	I	932	
1	J	932	
1	K	932	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 80124 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.

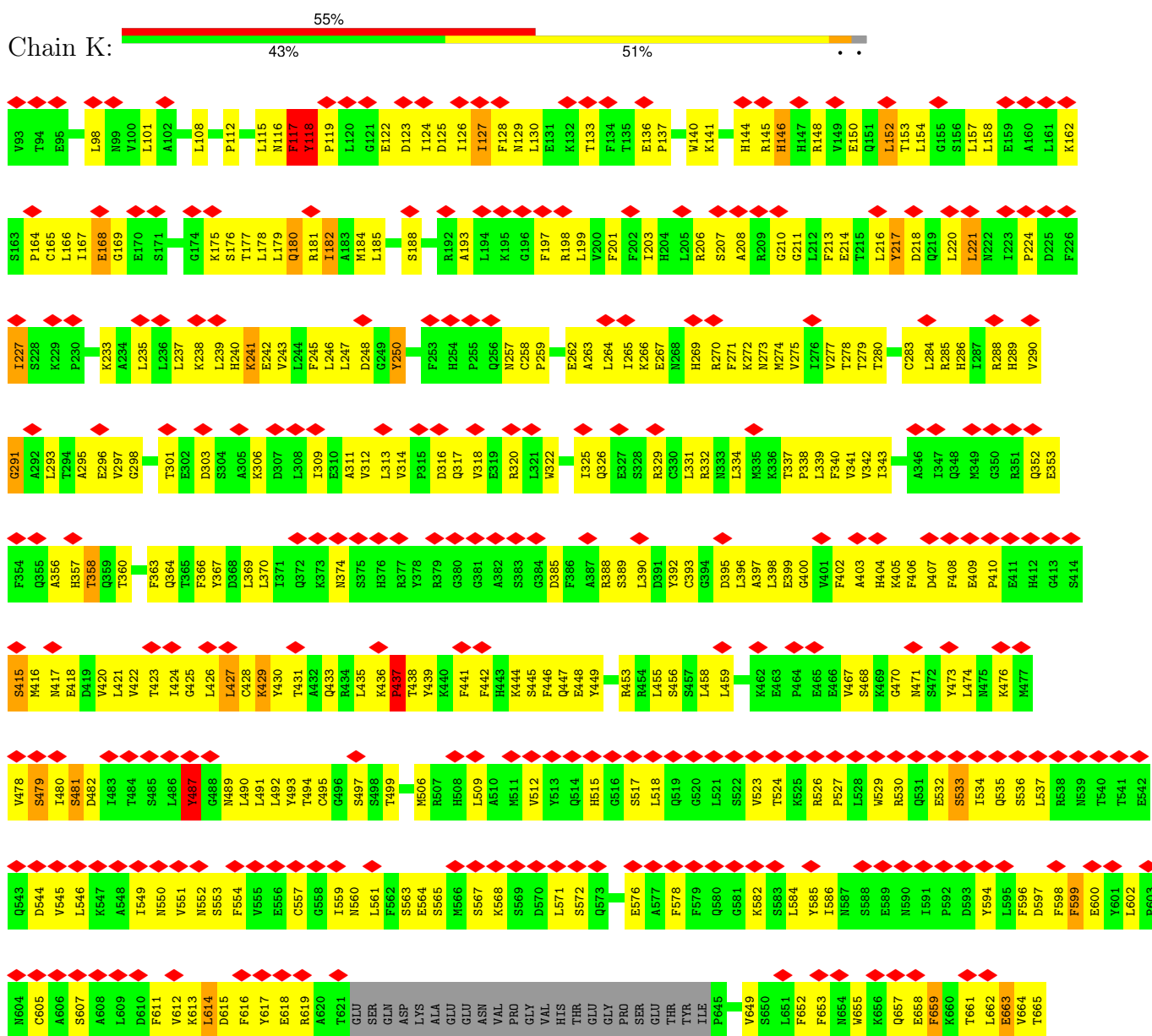
- Molecule 1 is a protein called NLR family CARD domain-containing protein 4.

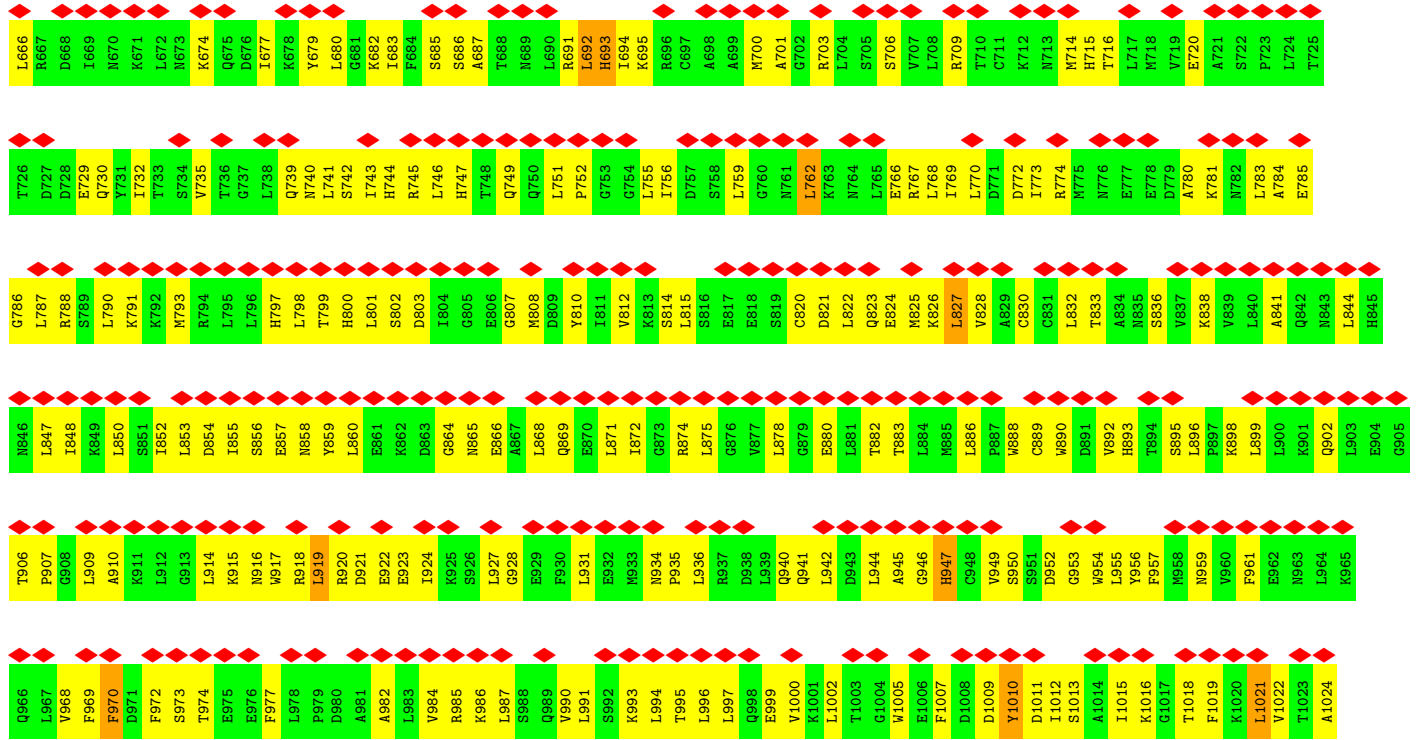
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	K	909	7284	4647	1233	1363	1	40	0	0
1	A	909	7284	4647	1233	1363	1	40	0	0
1	B	909	7284	4647	1233	1363	1	40	0	0
1	C	909	7284	4647	1233	1363	1	40	0	0
1	D	909	7284	4647	1233	1363	1	40	0	0
1	E	909	7284	4647	1233	1363	1	40	0	0
1	F	909	7284	4647	1233	1363	1	40	0	0
1	G	909	7284	4647	1233	1363	1	40	0	0
1	H	909	7284	4647	1233	1363	1	40	0	0
1	I	909	7284	4647	1233	1363	1	40	0	0
1	J	909	7284	4647	1233	1363	1	40	0	0

3 Residue-property plots

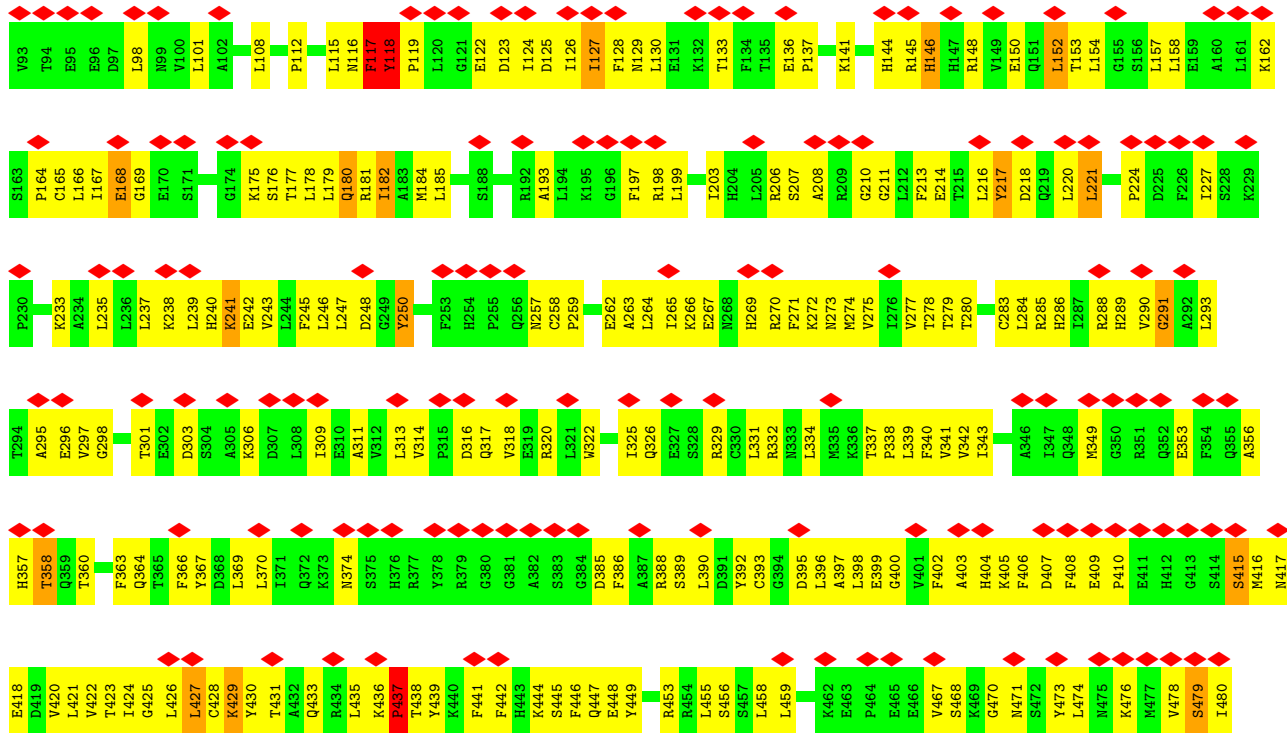
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

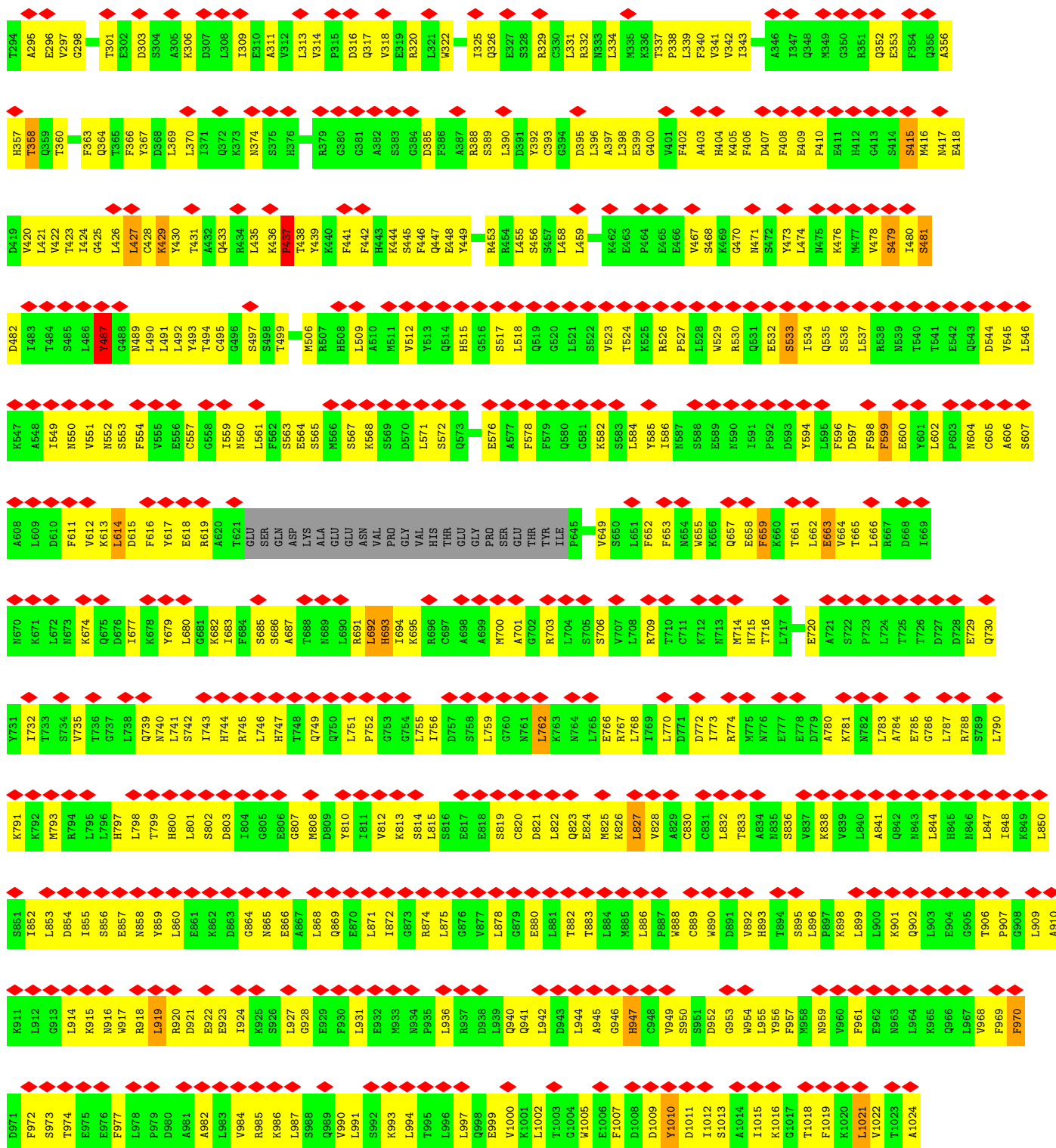
- Molecule 1: NLR family CARD domain-containing protein 4





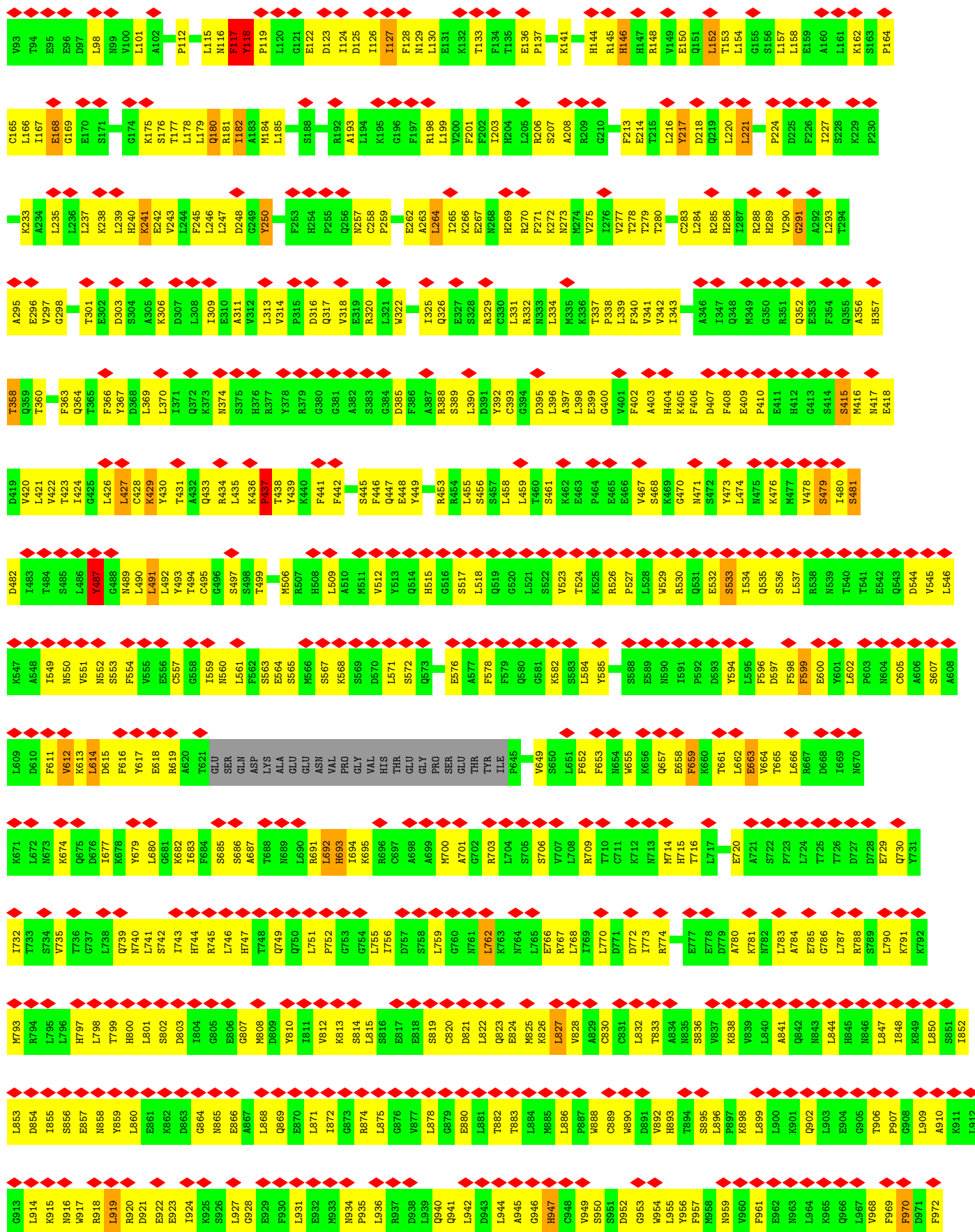
• Molecule 1: NLR family CARD domain-containing protein 4

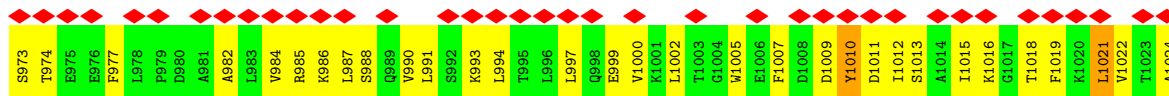




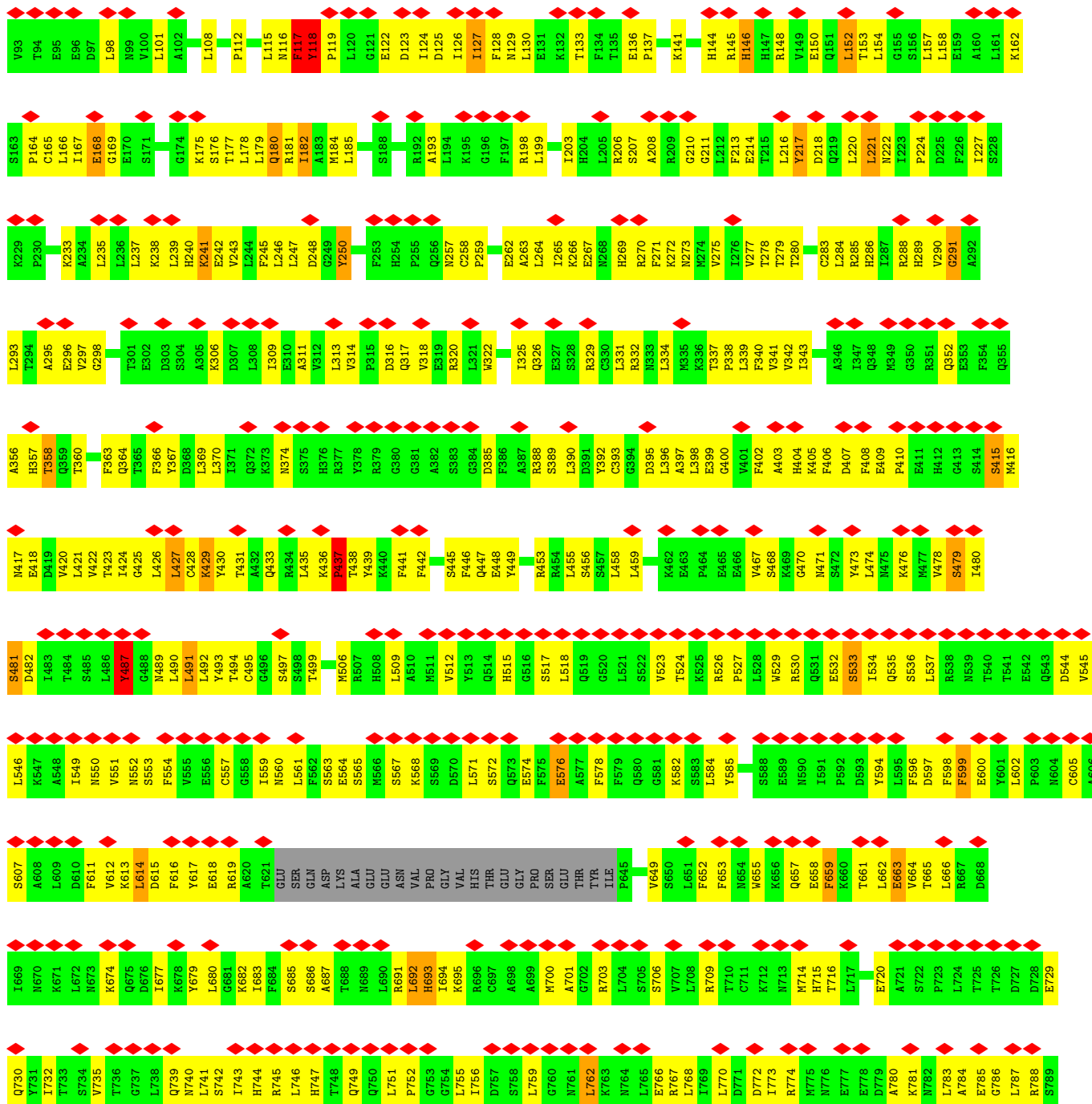
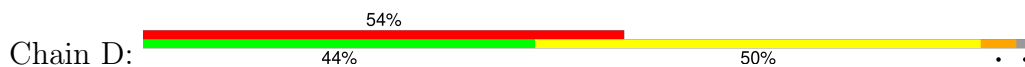
● Molecule 1: NLR family CARD domain-containing protein 4

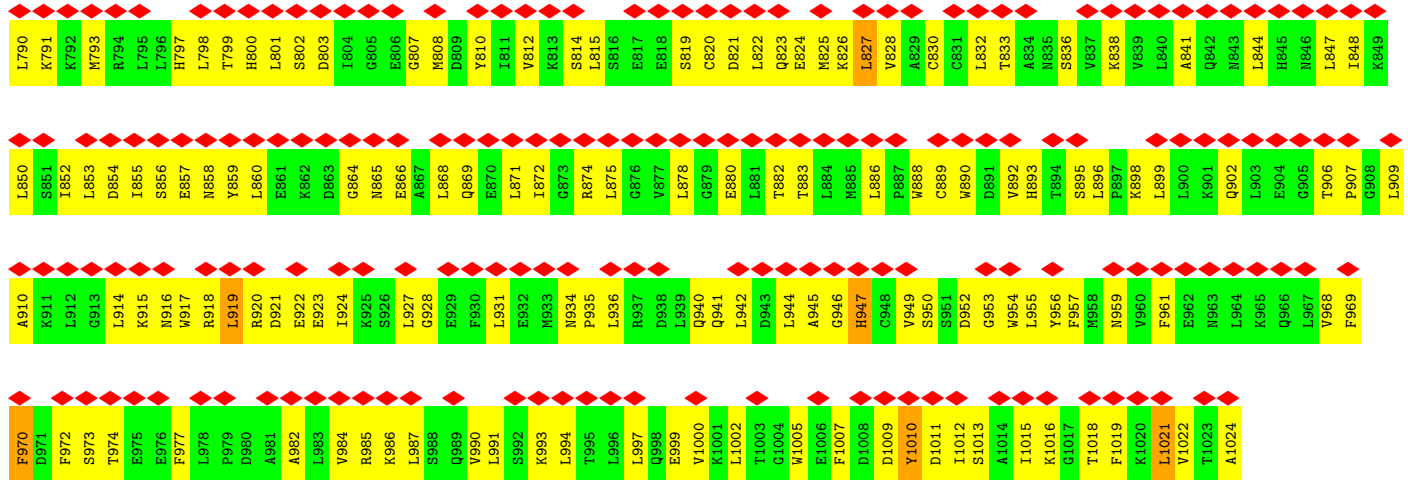




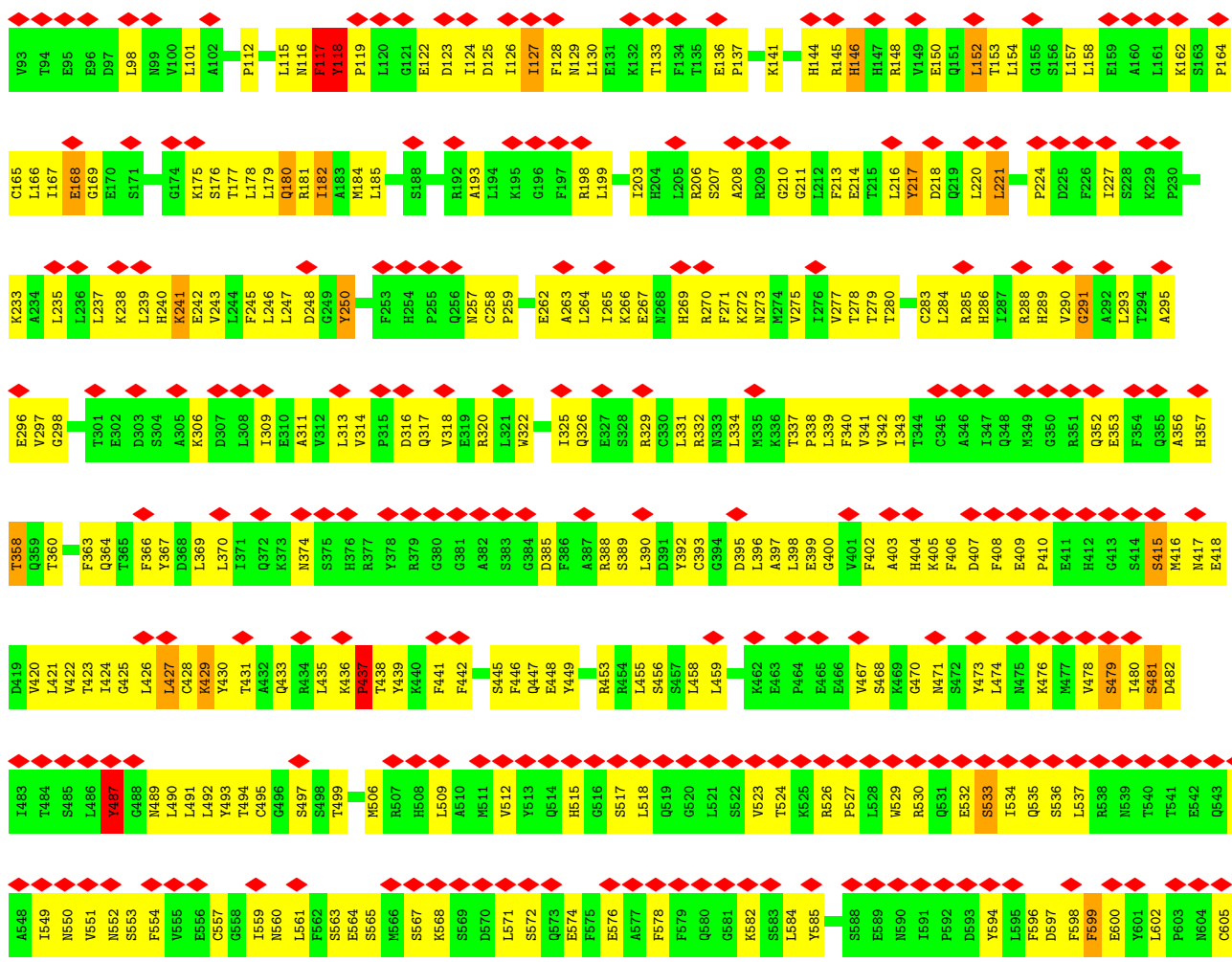
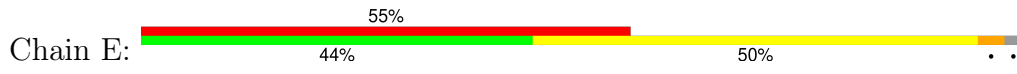


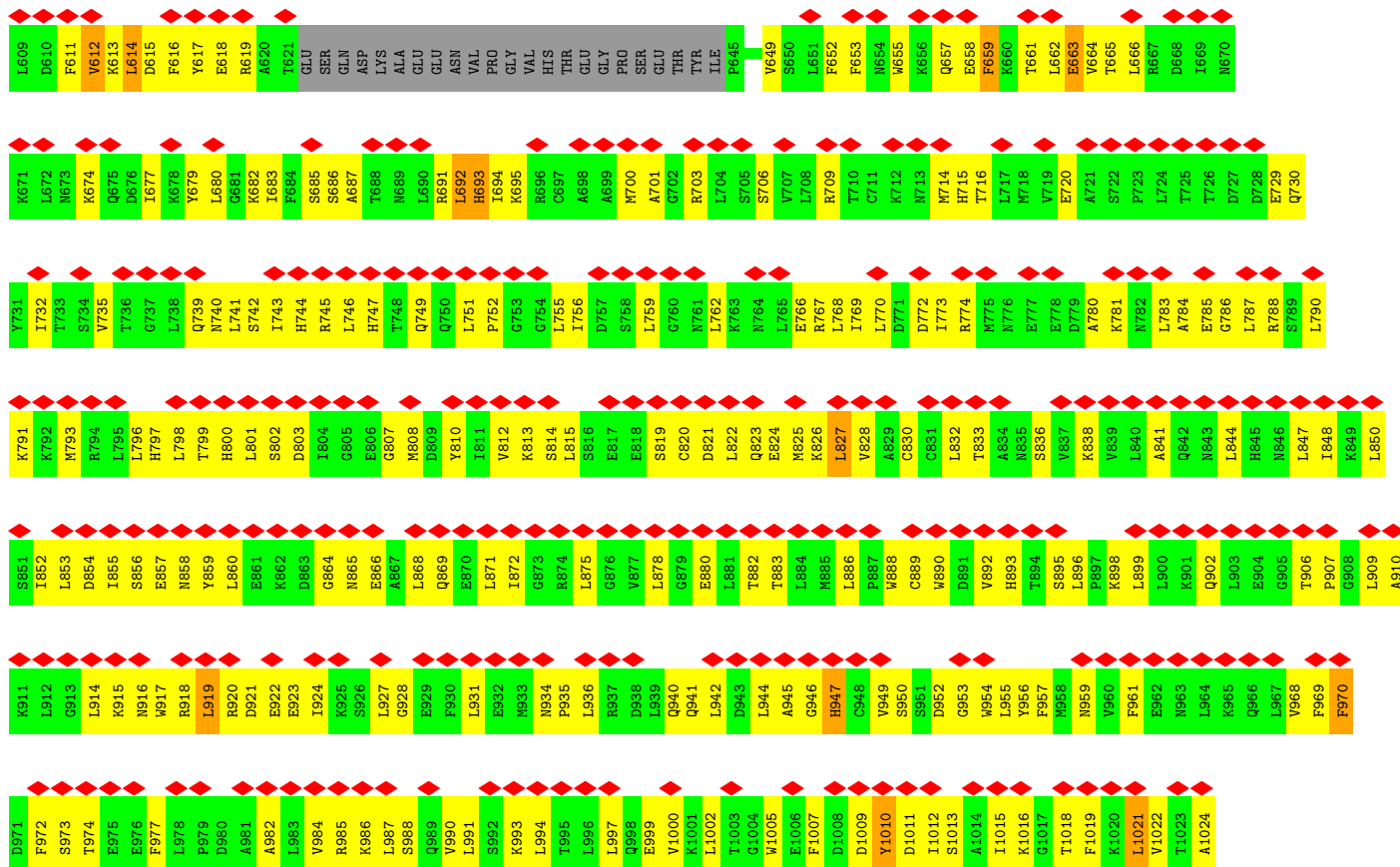
• Molecule 1: NLR family CARD domain-containing protein 4



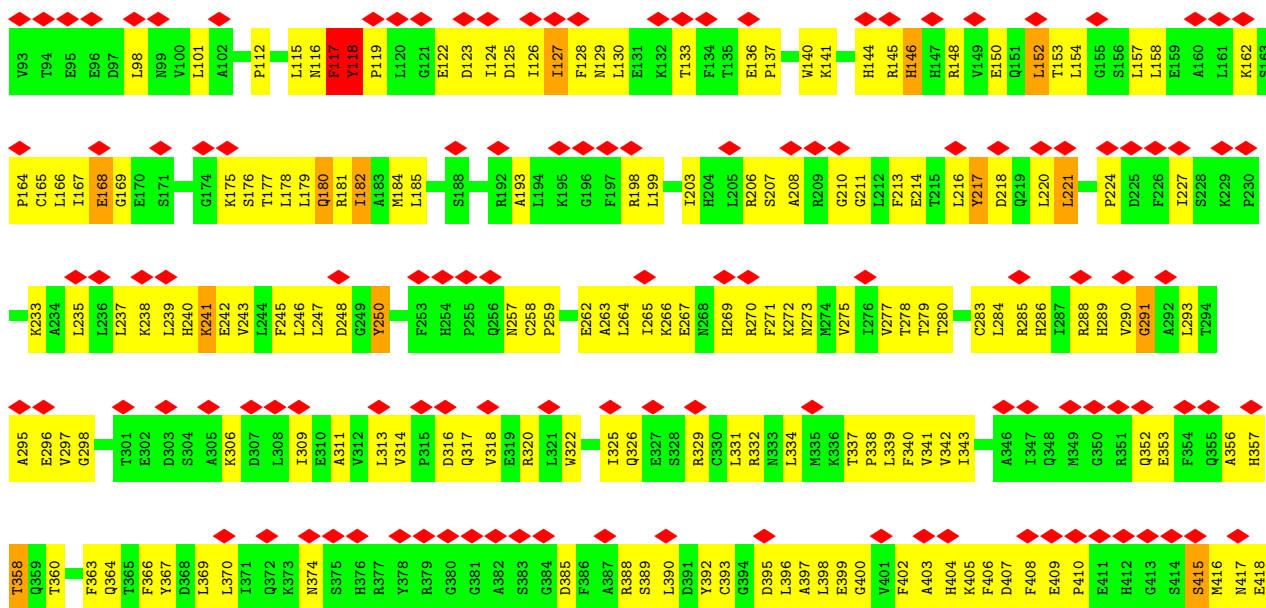


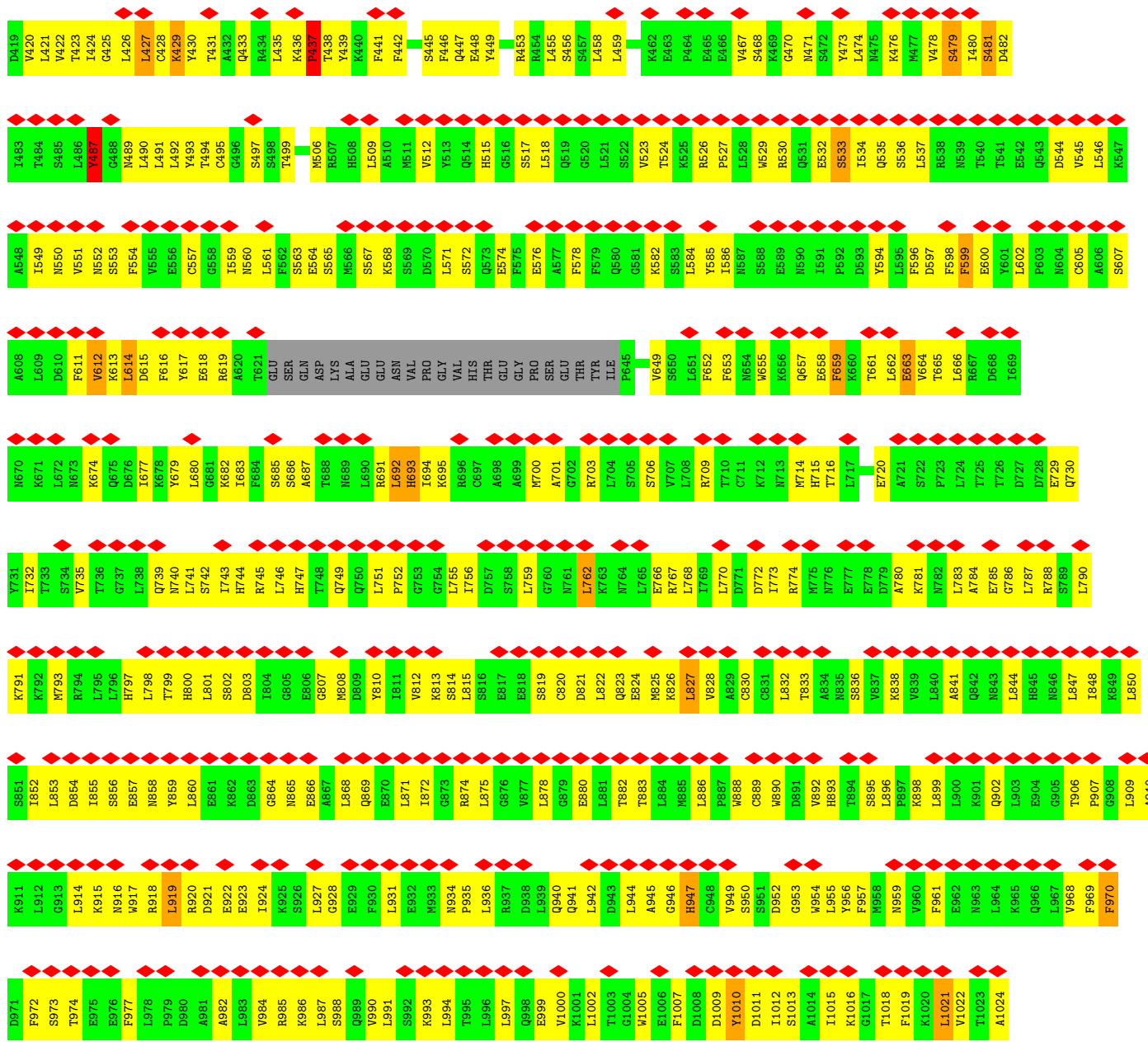
• Molecule 1: NLR family CARD domain-containing protein 4



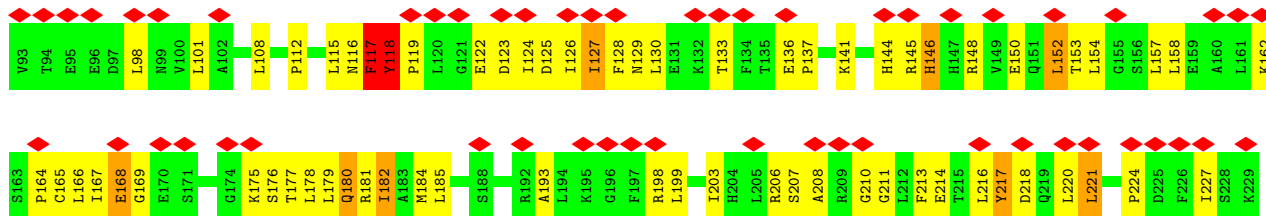
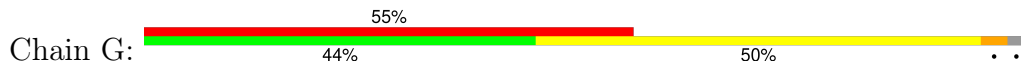


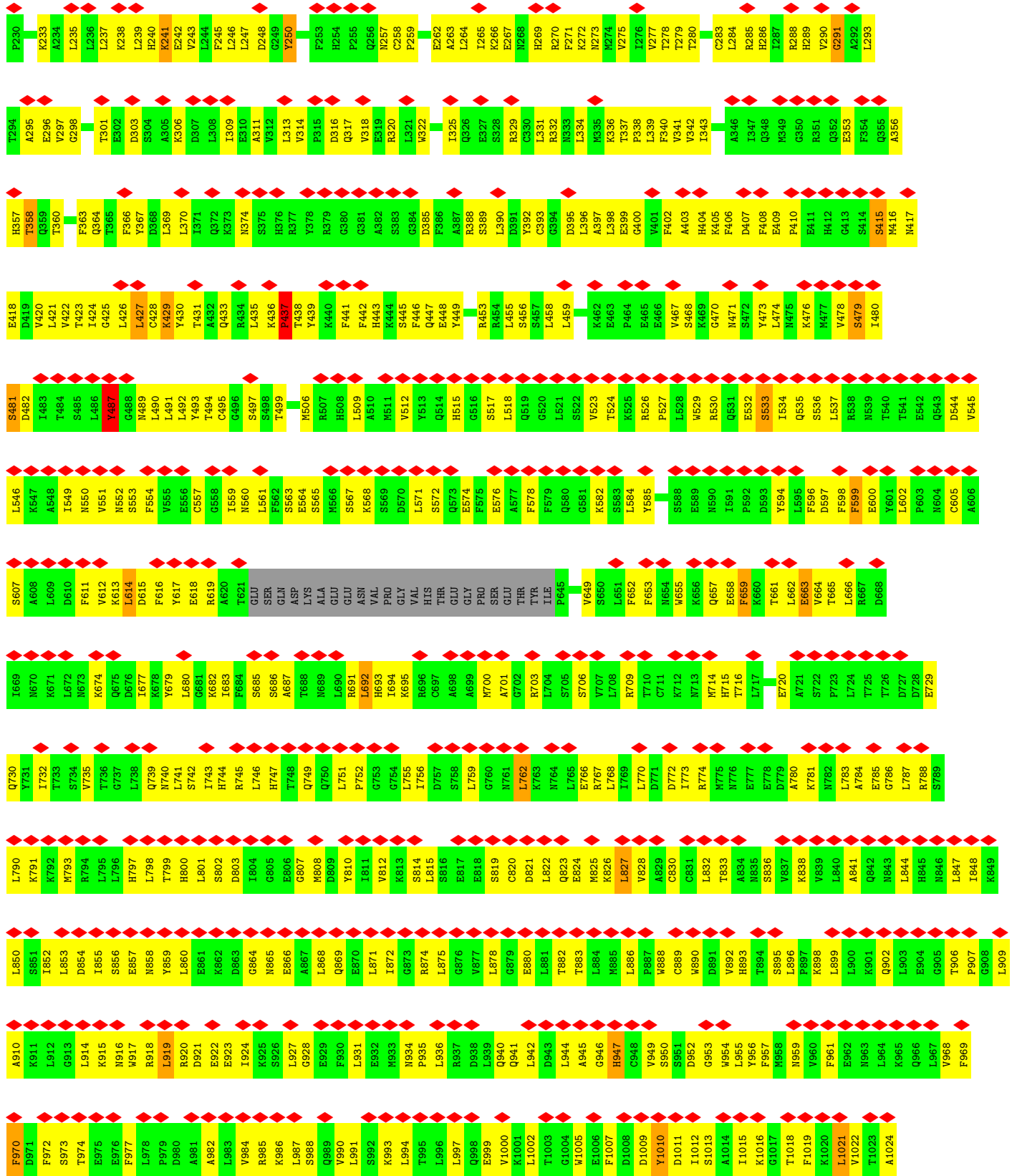
● Molecule 1: NLR family CARD domain-containing protein 4



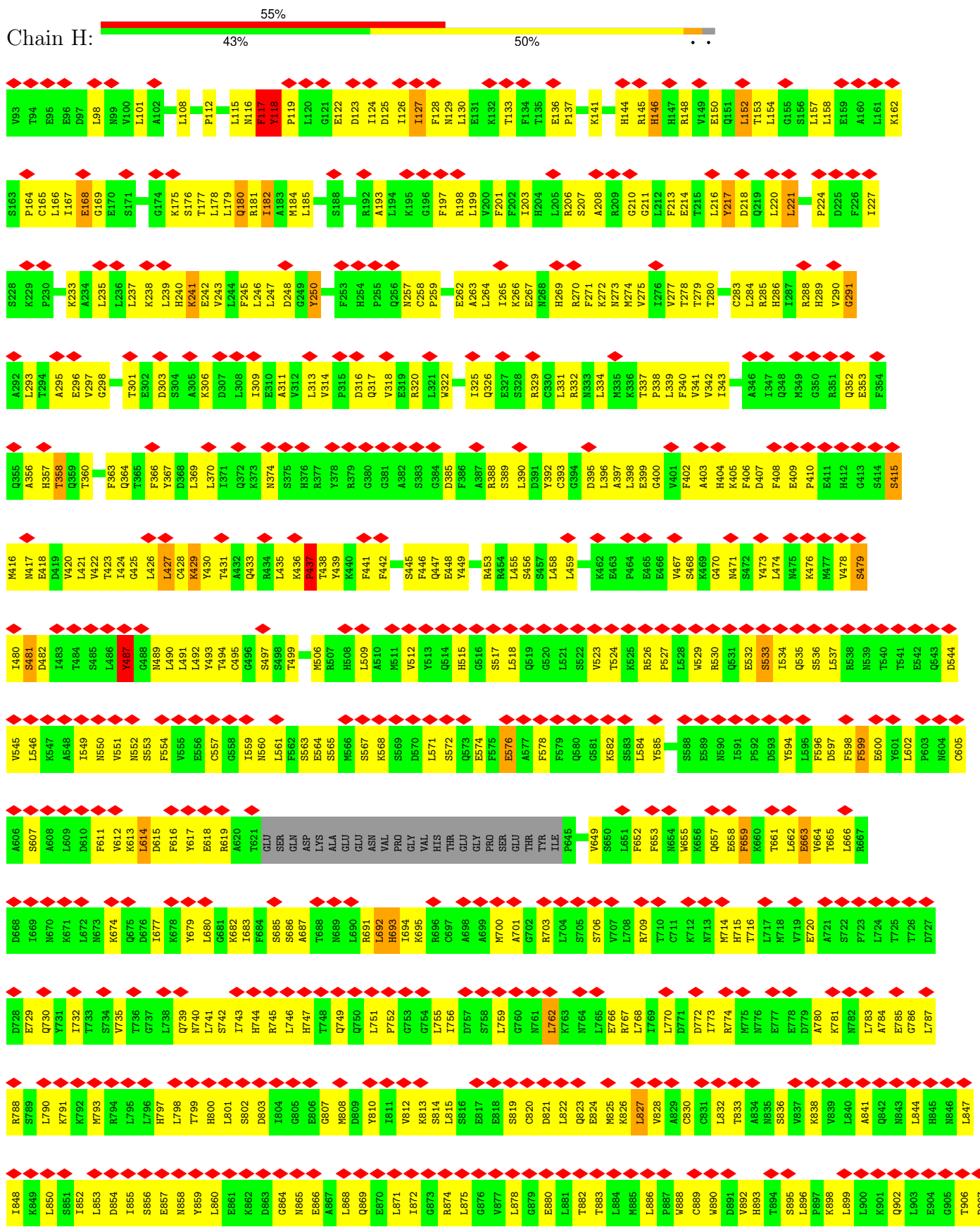


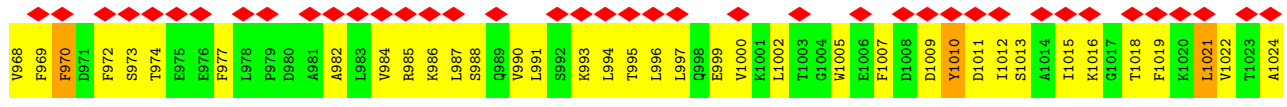
● Molecule 1: NLR family CARD domain-containing protein 4



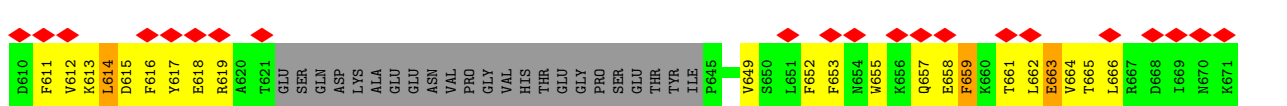
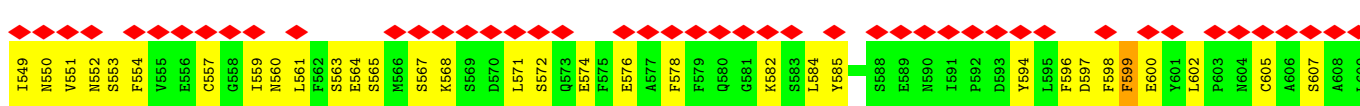
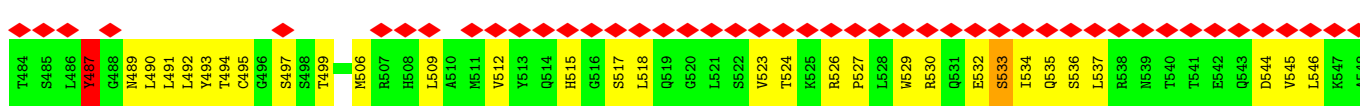
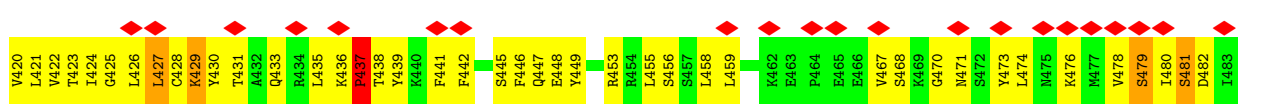
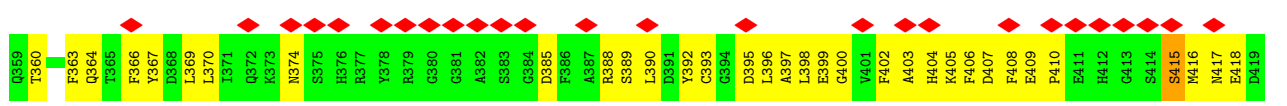
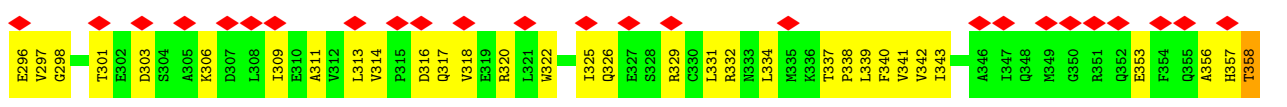
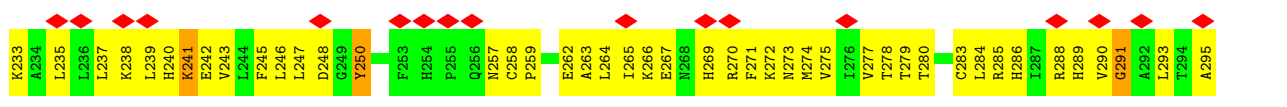
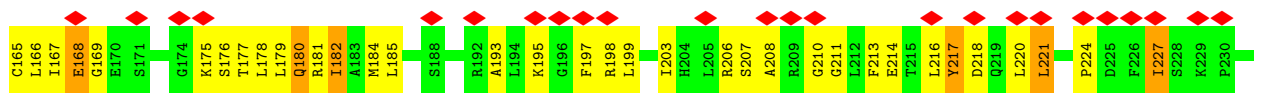
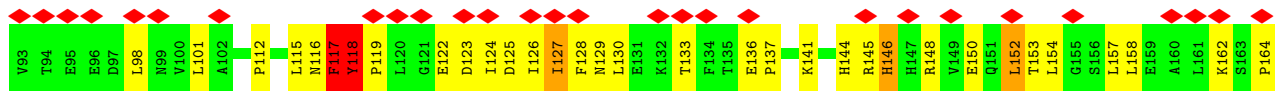
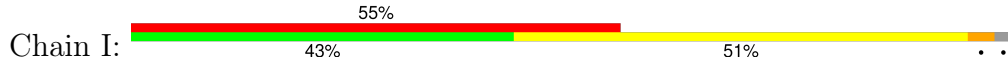


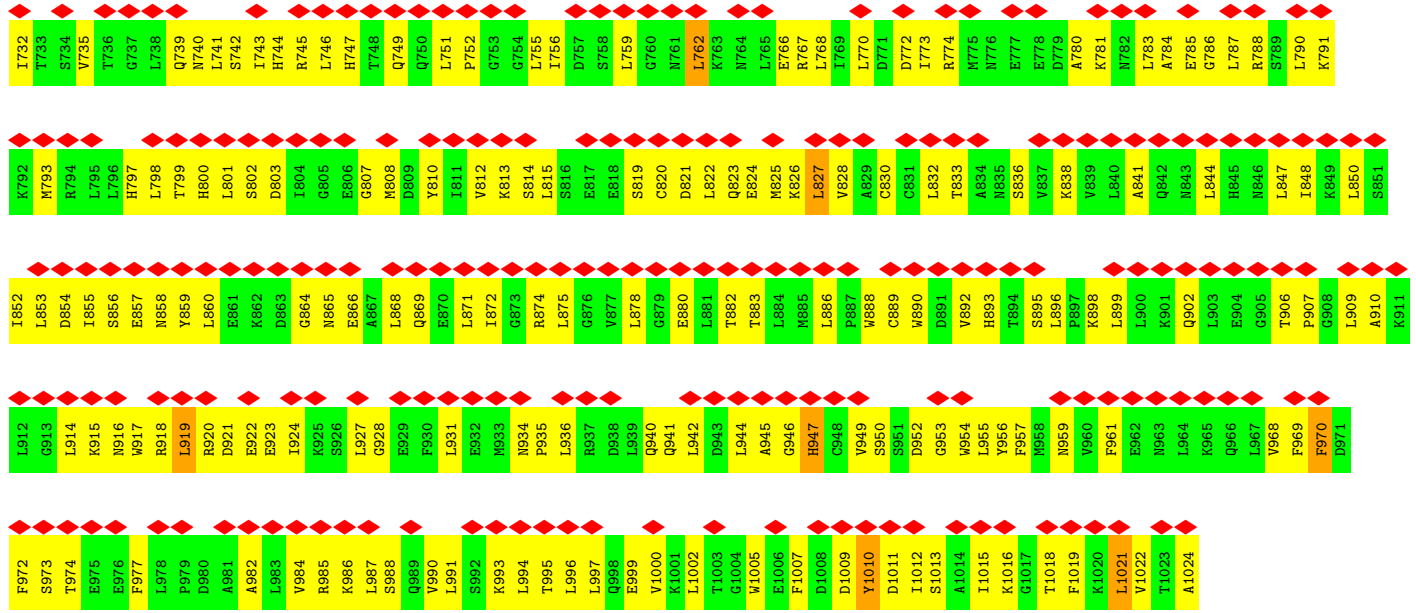
• Molecule 1: NLR family CARD domain-containing protein 4



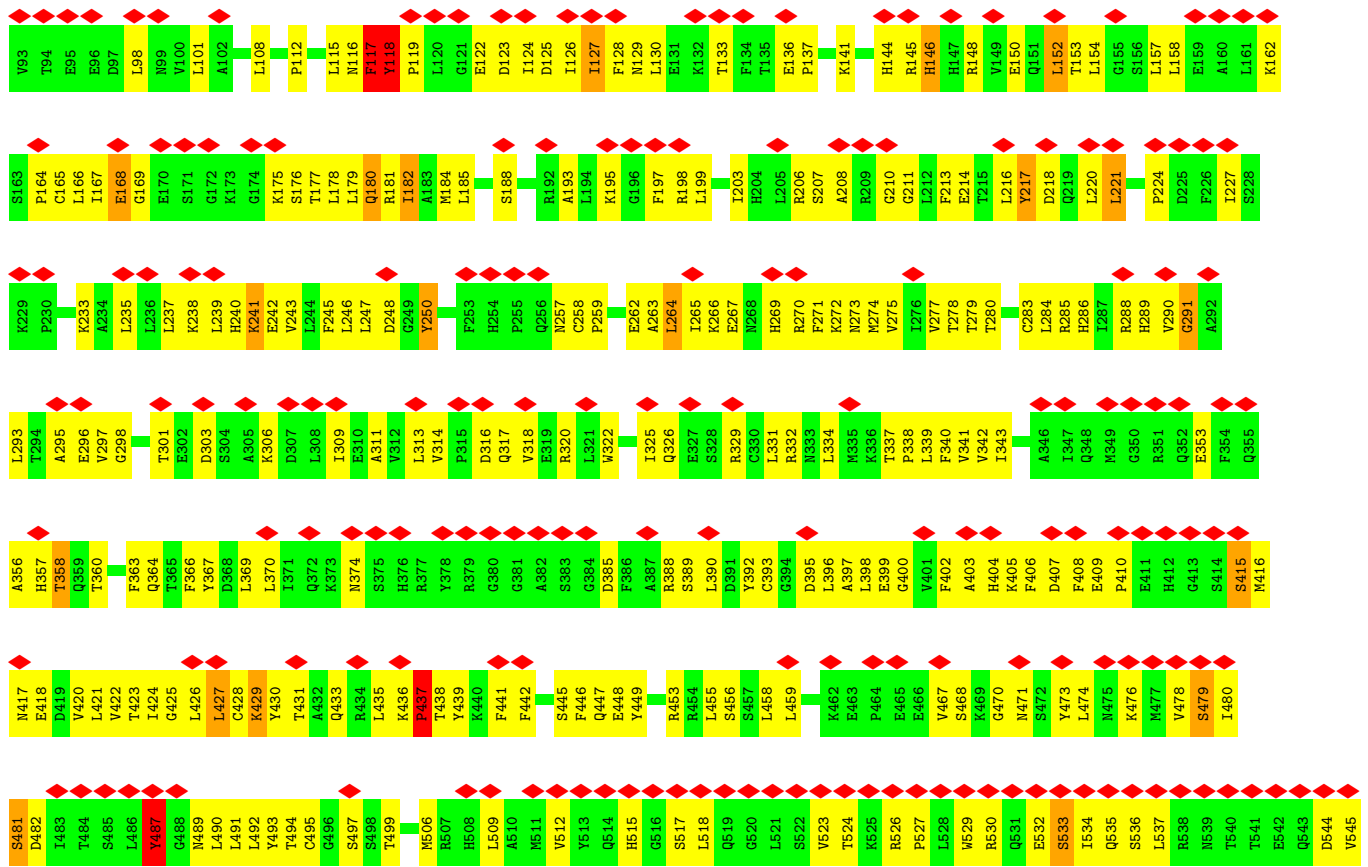


● Molecule 1: NLR family CARD domain-containing protein 4





• Molecule 1: NLR family CARD domain-containing protein 4



L546	K647	A548	I649	N650	V651	N652	S653	F654	V655	E656	C657	G658	I659	N660	L661	F662	S663	E664	S665	M666	S667	K668	S669	D670	L671	S672	Q673	E674	F675	E676	A677	F678	F679	Q680	G681	K682	L683	L684	Y685	S688	E689	N690	I691	F692	D693	Y694	L695	F696	D697	F698	F699	E600	L602	F603	N604	C605	A606			
S607	A608	L609	D610	F611	V612	K613	L614	D615	F616	Y617	E618	R619	A620	T621	GLU	SER	GLN	ASP	LYS	ALA	GLU	GLU	ASN	VAL	PRO	GLY	VAL	HIS	THR	GLY	PRO	A701	THR	TYR	THR	ILE	P645	V649	S650	L651	F652	F653	N654	W655	K656	Q657	E658	F659	K660	T661	L662	E663	V664	T665	L666	R667	D668			
I669	N670	K671	L672	N673	K674	Q675	D676	I677	K678	Y679	L680	G681	K682	I683	F684	S685	S686	A687	T688	N689	L690	R691	L692	H693	I694	K695	R696	C697	A698	Q699	M700	A701	G702	R703	L704	S705	S706	V707	L708	R709	T710	C711	K712	N713	M714	H715	T716	L717	M718	V719	E720	A721	S722	F723	L724	T725	T726	D727	D728	
E729	Q730	Y731	I732	T733	S734	V735	T736	G737	L738	N740	L741	S742	I743	H744	R745	L746	H747	T748	Q749	Q750	L751	P752	G753	G754	L755	I756	D757	S758	L759	G760	N761	L762	K763	N764	L765	E766	R767	L768	I769	L770	D771	D772	I773	R774	M775	N776	E777	E778	D779	A780	K781	M782	L783	A784	E785	G786	L787	R788		
S789	L790	K791	K792	M793	R794	L795	L796	H797	L798	T799	H800	L801	S802	I803	D804	I804	G805	E806	H807	M808	D809	Y810	I811	V812	K813	S814	L815	S816	E817	E818	S819	C820	D821	L822	Q823	E824	M825	K826	L827	V828	A829	C830	C831	L832	T833	A834	N835	S836	V837	K838	V839	L840	A841	Q842	N843	L844	H845	M846	L847	I848
K849	L850	S851	I852	L853	D854	L855	S856	E857	N858	Y859	L860	E861	K862	D863	G864	N865	E866	A867	L868	Q869	E870	L871	I872	G873	R874	L875	G876	V877	L878	G879	E880	L881	T882	T883	L884	M885	L886	P887	W888	C889	W890	D891	V892	H893	T894	S895	L896	K897	K898	L899	L900	K901	Q902	L903	E904	G905	P907	G908		
L909	A910	K911	L912	G913	L914	K915	N916	H917	R918	L919	R920	D921	E922	E923	I924	K925	S926	L927	G928	E929	F930	L931	E932	N933	N934	P935	L936	R937	Q938	L939	Q940	L942	D943	L944	A945	G946	H947	C948	V949	S950	S951	D952	G953	N954	L955	Y956	F957	N958	N959	V960	F961	E962	N963	L964	K965	Q966	L967	Y968		
F969	F970	D971	F972	S973	T974	E975	E976	F977	L978	P979	D980	A981	A982	L983	V984	R985	K986	L987	S988	Q989	V990	L991	S992	K993	L994	T995	L996	L997	Q998	E999	V1000	K1001	L1002	T1003	G1004	W1005	E1006	F1007	D1008	D1009	Y1010	D1011	I1012	S1013	A1014	I1015	K1016	G1017	T1018	F1019	K1020	L1021	V1022	T1023	A1024					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	75114	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Wiener-type filter	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	28736	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.012	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0045	Depositor
Map size (\AA)	385.28, 385.28, 385.28	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/7412	0.93	18/10004 (0.2%)
1	B	0.37	0/7412	0.93	18/10004 (0.2%)
1	C	0.37	0/7412	0.93	18/10004 (0.2%)
1	D	0.37	0/7412	0.93	18/10004 (0.2%)
1	E	0.37	0/7412	0.93	18/10004 (0.2%)
1	F	0.37	0/7412	0.93	18/10004 (0.2%)
1	G	0.37	0/7412	0.93	17/10004 (0.2%)
1	H	0.37	0/7412	0.93	18/10004 (0.2%)
1	I	0.37	0/7412	0.93	17/10004 (0.2%)
1	J	0.37	0/7412	0.93	18/10004 (0.2%)
1	K	0.37	0/7412	0.93	18/10004 (0.2%)
All	All	0.37	0/81532	0.93	196/110044 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
All	All	0	22

There are no bond length outliers.

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	280	THR	N-CA-C	-8.11	89.11	111.00
1	G	280	THR	N-CA-C	-8.11	89.11	111.00
1	K	280	THR	N-CA-C	-8.10	89.12	111.00
1	B	280	THR	N-CA-C	-8.10	89.12	111.00
1	C	280	THR	N-CA-C	-8.10	89.13	111.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	PHE	Peptide
1	A	441	PHE	Peptide
1	B	117	PHE	Peptide
1	K	117	PHE	Peptide
1	K	441	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7284	0	7329	442	0
1	B	7284	0	7329	440	0
1	C	7284	0	7329	440	0
1	D	7284	0	7329	442	0
1	E	7284	0	7329	437	0
1	F	7284	0	7329	442	0
1	G	7284	0	7329	436	0
1	H	7284	0	7329	444	0
1	I	7284	0	7329	442	0
1	J	7284	0	7329	457	0
1	K	7284	0	7329	454	0
All	All	80124	0	80619	4740	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 29.

The worst 5 of 4740 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)
1:K:125:ASP:H	1:J:433:GLN:HG2	1.28	0.95
1:A:433:GLN:HG2	1:B:125:ASP:H	1.33	0.94
1:F:433:GLN:HG2	1:G:125:ASP:H	1.33	0.93
1:G:433:GLN:HG2	1:H:125:ASP:H	1.33	0.93
1:D:433:GLN:HG2	1:E:125:ASP:H	1.34	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	B	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	C	904/932 (97%)	822 (91%)	66 (7%)	16 (2%)	7	34
1	D	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	E	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	F	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	G	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	H	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
1	I	904/932 (97%)	822 (91%)	66 (7%)	16 (2%)	7	34
1	J	904/932 (97%)	822 (91%)	66 (7%)	16 (2%)	7	34
1	K	904/932 (97%)	823 (91%)	65 (7%)	16 (2%)	7	34
All	All	9944/10252 (97%)	9050 (91%)	718 (7%)	176 (2%)	9	34

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	146	HIS
1	K	241	LYS
1	K	272	LYS
1	K	442	PHE
1	K	481	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	B	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	C	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	D	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	E	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	F	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	G	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	H	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	I	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	J	810/830 (98%)	784 (97%)	26 (3%)	34	54
1	K	810/830 (98%)	784 (97%)	26 (3%)	34	54
All	All	8910/9130 (98%)	8624 (97%)	286 (3%)	36	54

5 of 286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	970	PHE
1	I	182	ILE
1	J	117	PHE
1	C	663	GLU
1	C	585	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	693	HIS
1	H	257	ASN
1	F	869	GLN
1	G	433	GLN
1	H	693	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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
1	SEP	A	533	1	8,9,10	1.60	1 (12%)	7,12,14	0.99	0
1	SEP	E	533	1	8,9,10	1.60	1 (12%)	7,12,14	0.99	0
1	SEP	G	533	1	8,9,10	1.60	1 (12%)	7,12,14	0.98	0
1	SEP	H	533	1	8,9,10	1.60	1 (12%)	7,12,14	0.99	0
1	SEP	C	533	1	8,9,10	1.60	1 (12%)	7,12,14	1.00	0
1	SEP	I	533	1	8,9,10	1.60	1 (12%)	7,12,14	1.00	0
1	SEP	J	533	1	8,9,10	1.60	1 (12%)	7,12,14	1.00	0
1	SEP	D	533	1	8,9,10	1.59	1 (12%)	7,12,14	0.99	0
1	SEP	K	533	1	8,9,10	1.60	1 (12%)	7,12,14	0.99	0
1	SEP	F	533	1	8,9,10	1.60	1 (12%)	7,12,14	0.98	0
1	SEP	B	533	1	8,9,10	1.61	1 (12%)	7,12,14	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	533	1	-	0/6/8/10	-
1	SEP	E	533	1	-	0/6/8/10	-
1	SEP	G	533	1	-	0/6/8/10	-
1	SEP	H	533	1	-	0/6/8/10	-
1	SEP	C	533	1	-	0/6/8/10	-
1	SEP	I	533	1	-	0/6/8/10	-
1	SEP	J	533	1	-	0/6/8/10	-
1	SEP	D	533	1	-	0/6/8/10	-
1	SEP	K	533	1	-	0/6/8/10	-
1	SEP	F	533	1	-	0/6/8/10	-
1	SEP	B	533	1	-	0/6/8/10	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	533	SEP	P-O1P	3.54	1.61	1.50
1	F	533	SEP	P-O1P	3.54	1.61	1.50
1	C	533	SEP	P-O1P	3.54	1.61	1.50
1	B	533	SEP	P-O1P	3.53	1.61	1.50
1	K	533	SEP	P-O1P	3.53	1.61	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	533	SEP	2	0
1	E	533	SEP	2	0
1	G	533	SEP	2	0
1	H	533	SEP	2	0
1	C	533	SEP	2	0
1	I	533	SEP	2	0
1	J	533	SEP	2	0
1	D	533	SEP	2	0
1	K	533	SEP	2	0
1	F	533	SEP	3	0
1	B	533	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

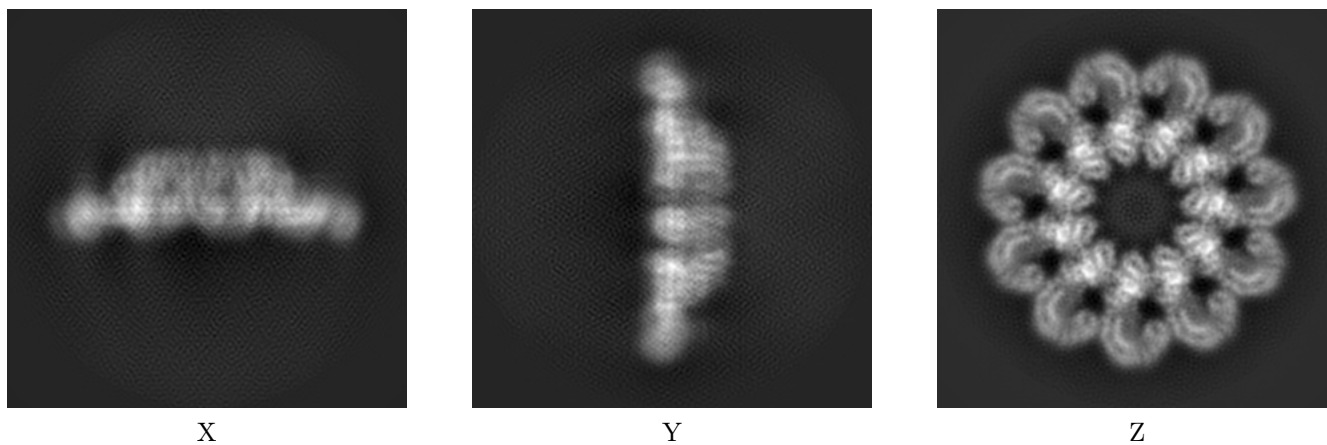
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6458. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

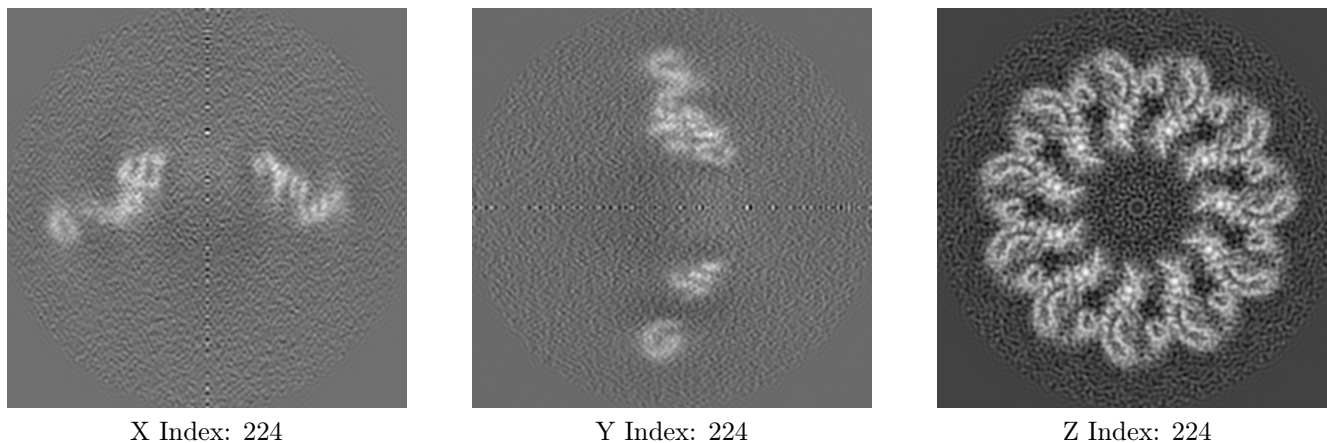
6.1.1 Primary map



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

6.2 Central slices [i](#)

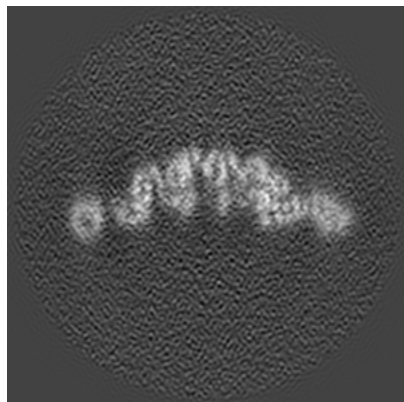
6.2.1 Primary map



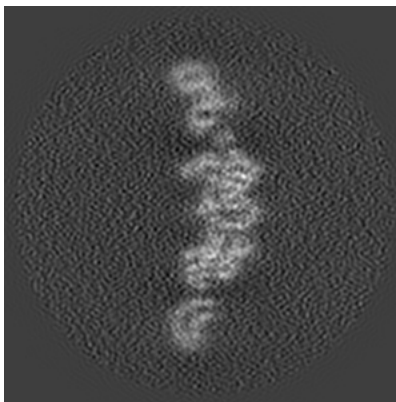
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

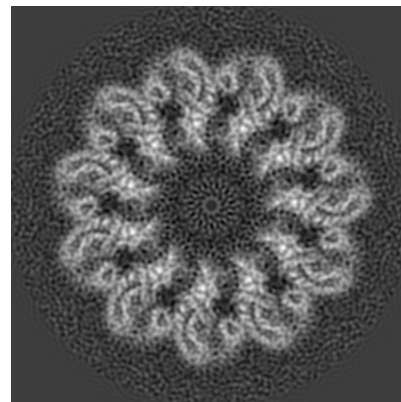
6.3.1 Primary map



X Index: 157



Y Index: 148

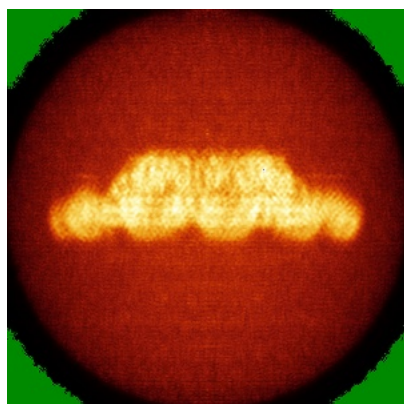


Z Index: 223

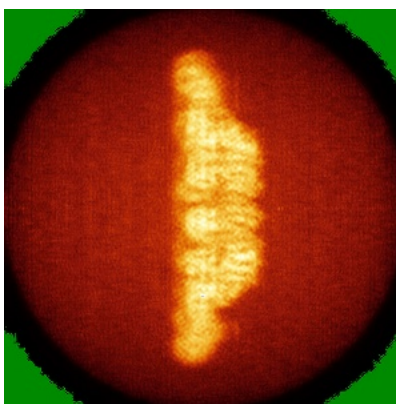
The images above show the largest variance slices of the map in three orthogonal directions.

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

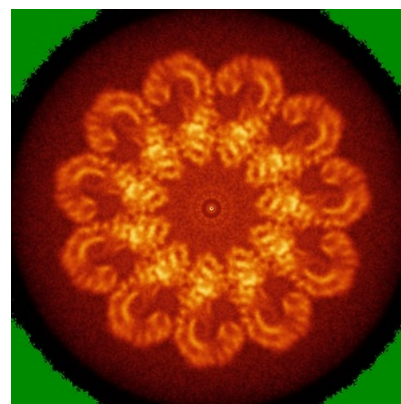
6.4.1 Primary map



X



Y

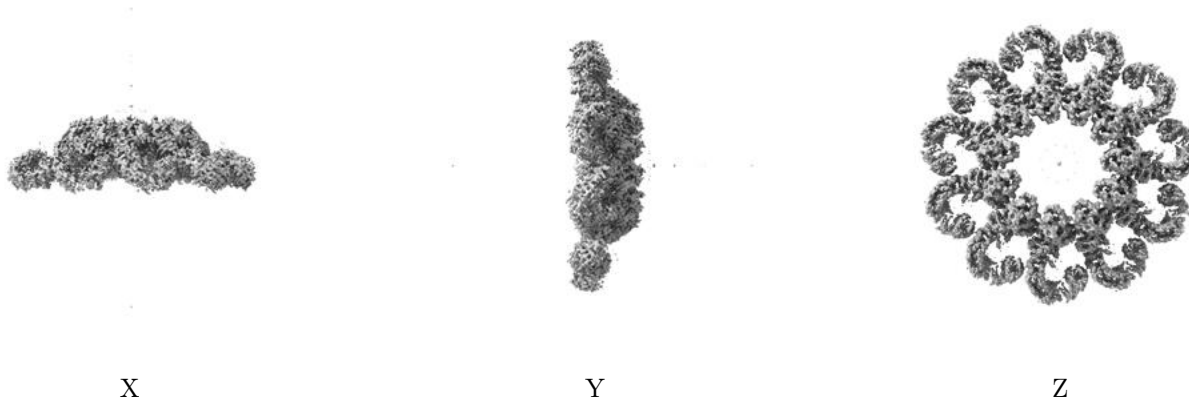


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

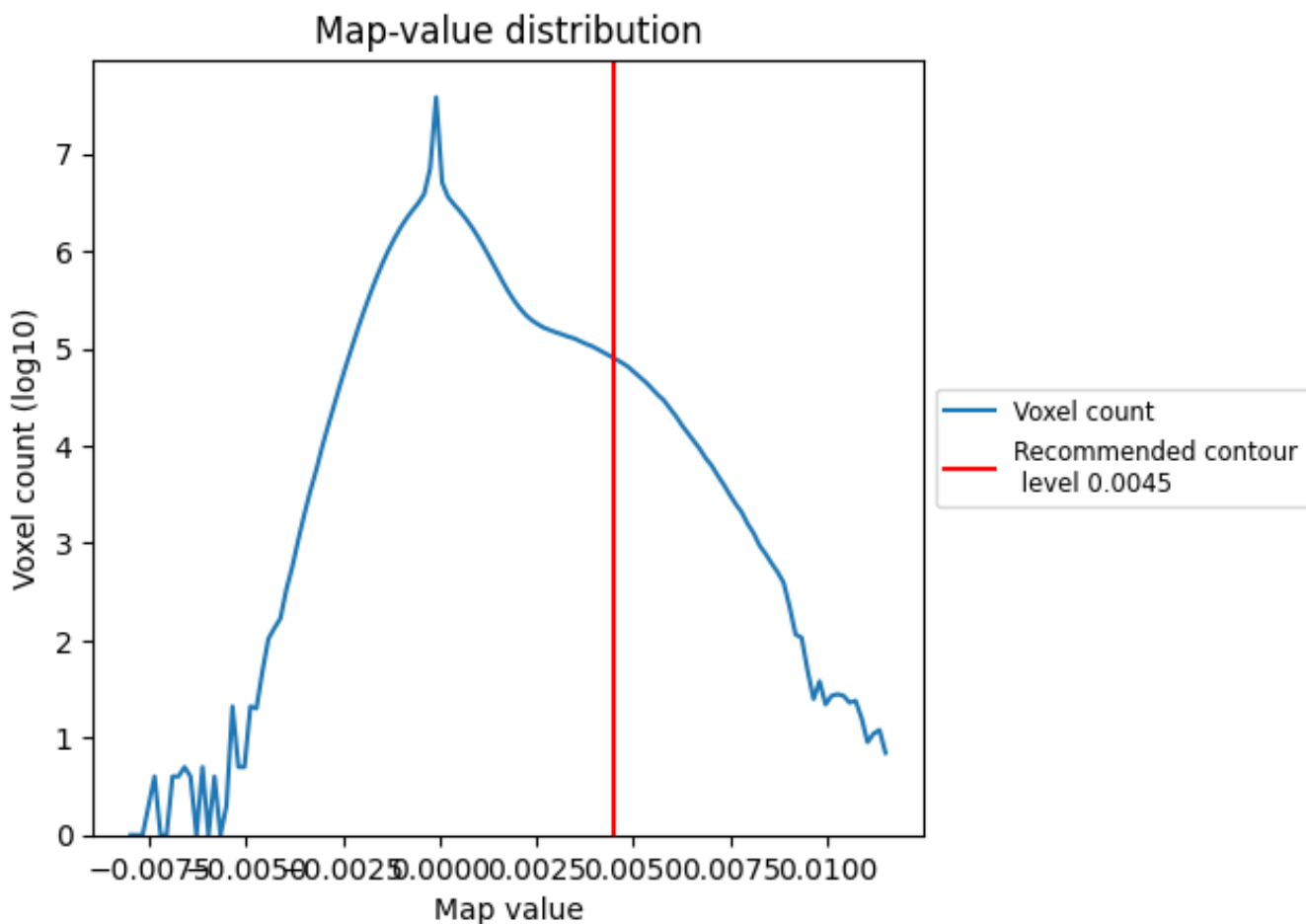
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

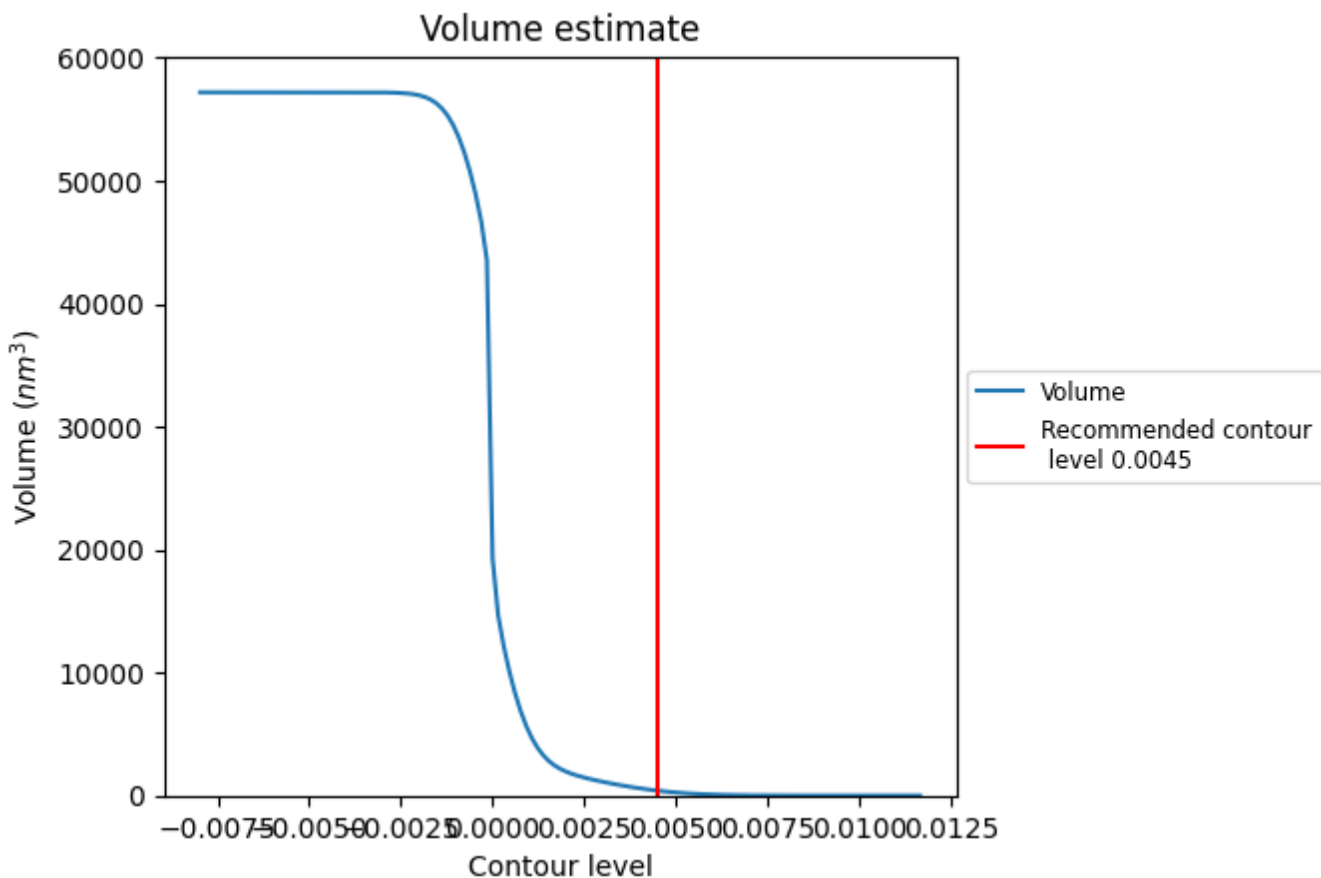
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

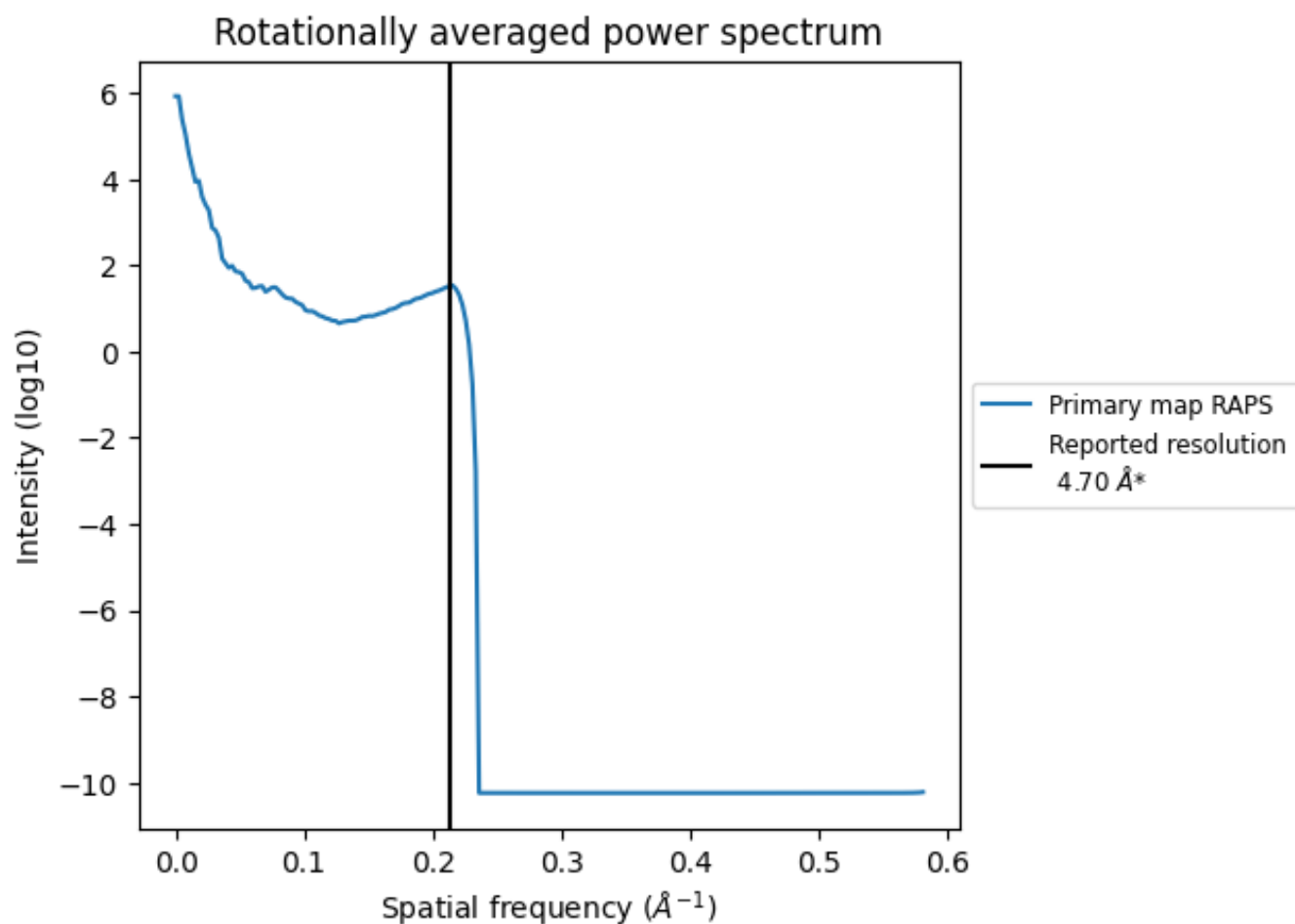
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 399 nm³; this corresponds to an approximate mass of 361 kDa.

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

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



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

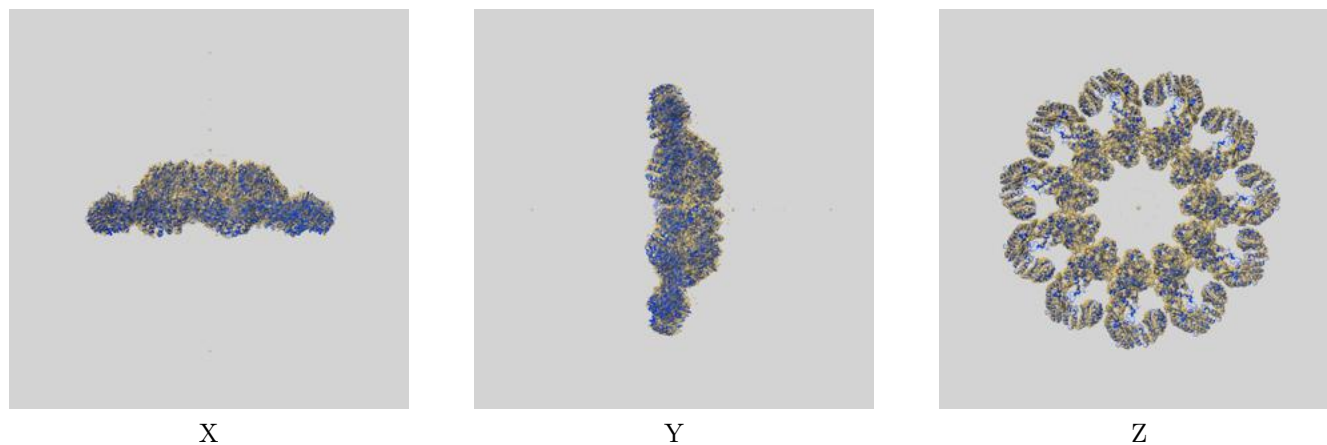
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

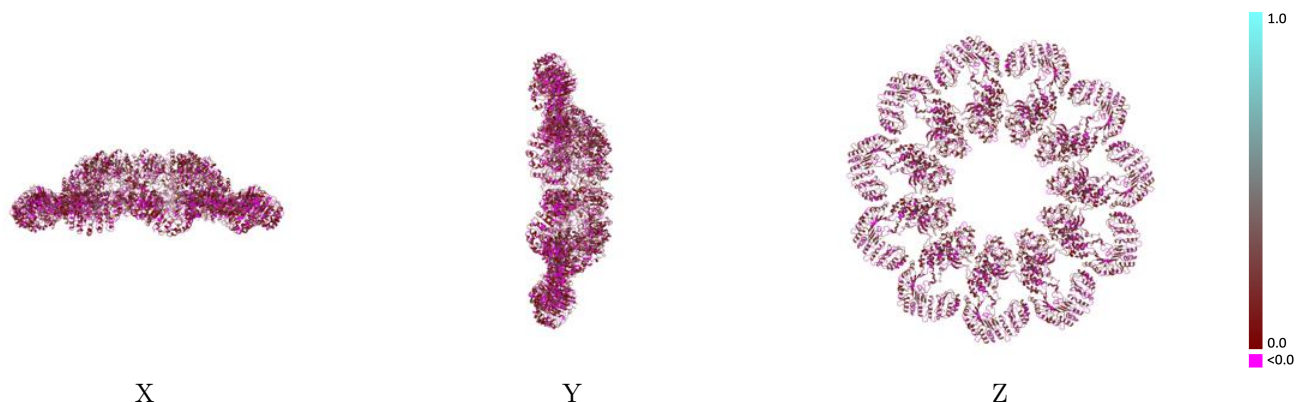
This section contains information regarding the fit between EMDB map EMD-6458 and PDB model 3JBL. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



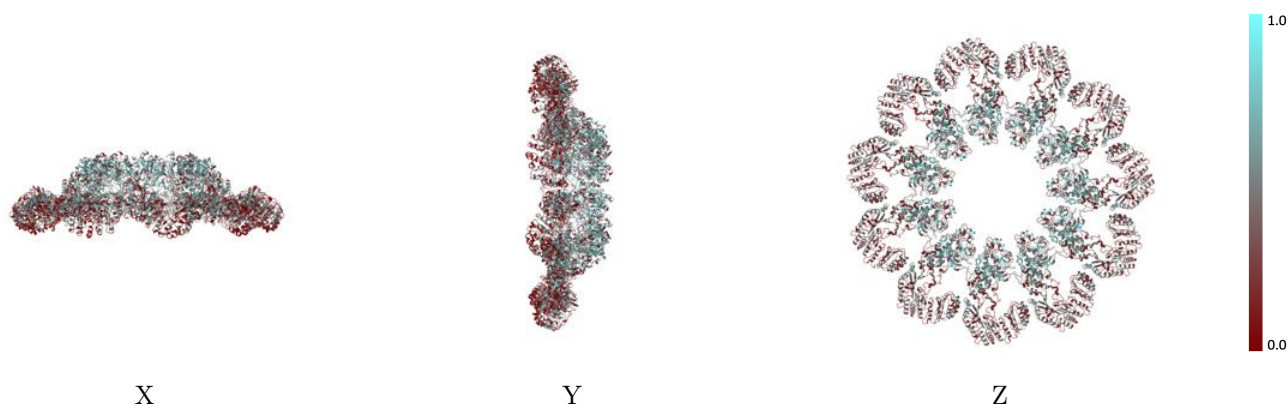
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



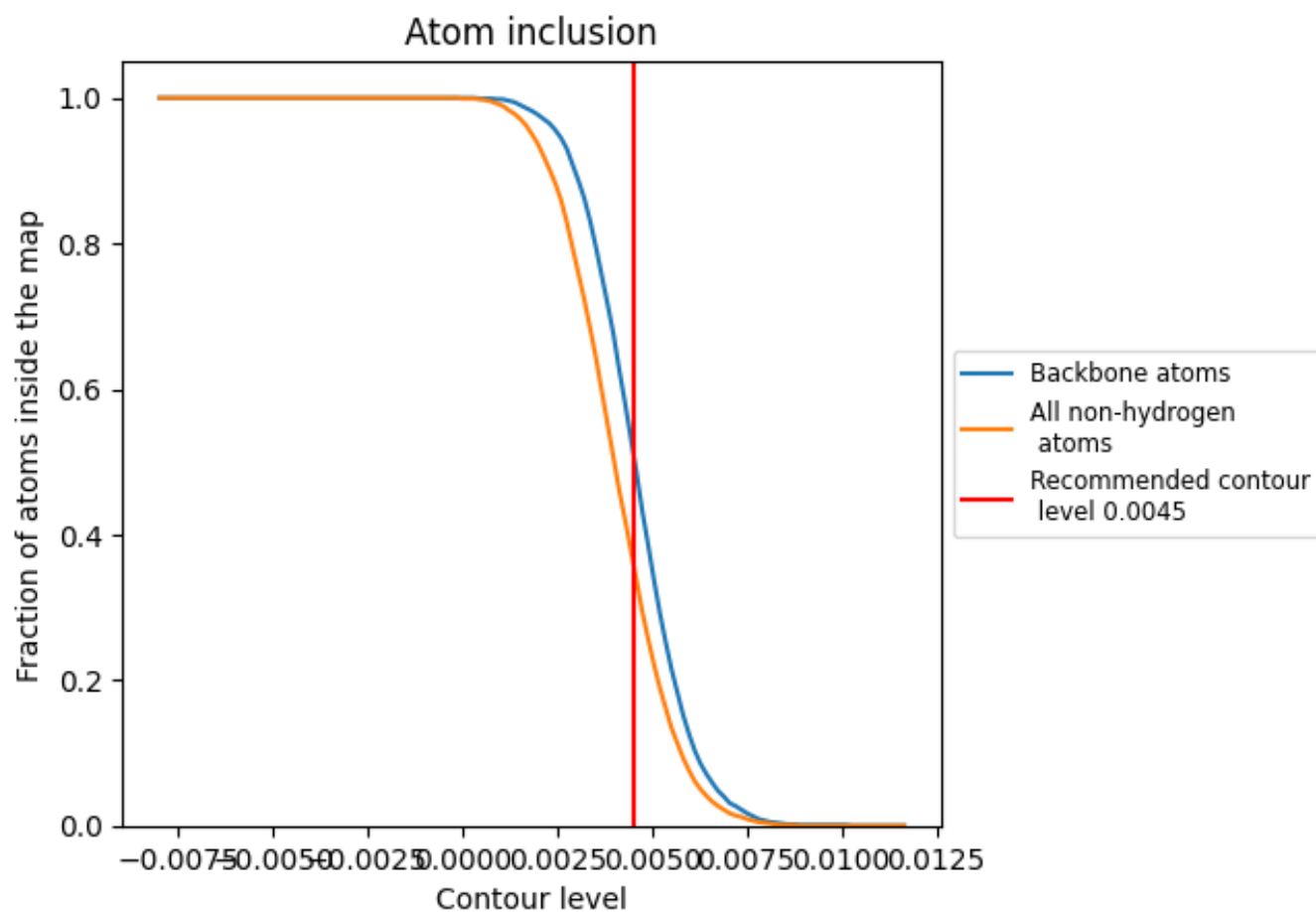
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3640	0.1160
A	0.3660	0.1160
B	0.3630	0.1170
C	0.3650	0.1160
D	0.3660	0.1170
E	0.3630	0.1160
F	0.3650	0.1170
G	0.3640	0.1170
H	0.3640	0.1170
I	0.3670	0.1160
J	0.3620	0.1160
K	0.3620	0.1160

