



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 09:40 pm BST

PDB ID : 9T64 / pdb_00009t64
EMDB ID : EMD-55604
Title : Cytoplasmic lattice filament repeat unit with the central FBXW-SKP1 complex
Authors : Singh, K.; Harasimov, K.; Carter, A.P.
Deposited on : 2025-11-06
Resolution : 7.30 Å(reported)

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

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

A user guide is available at

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

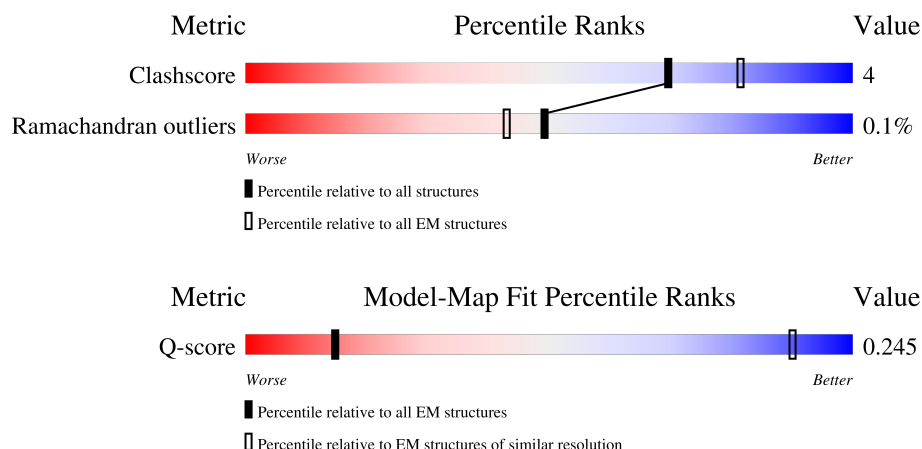
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.30 Å.

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



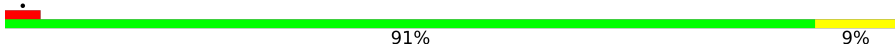
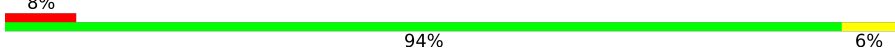
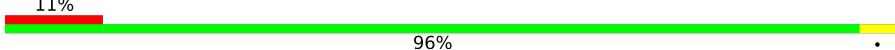
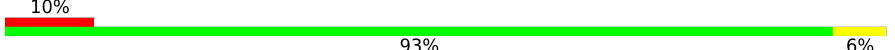
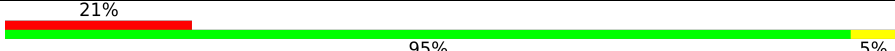
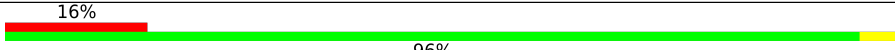
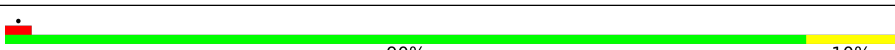
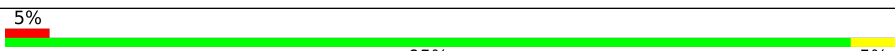
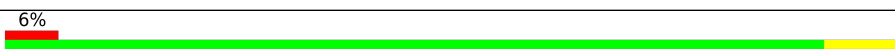
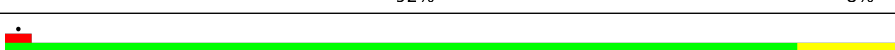
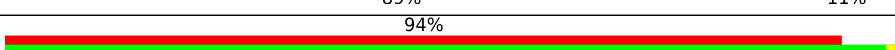
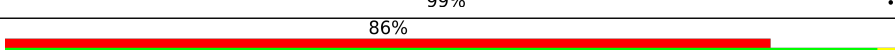
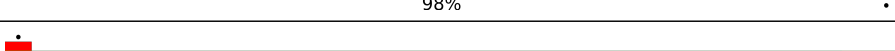
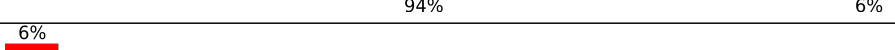
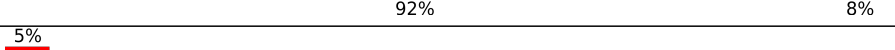
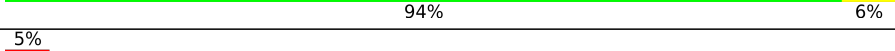
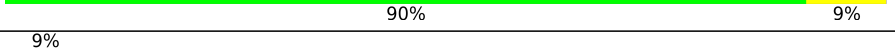
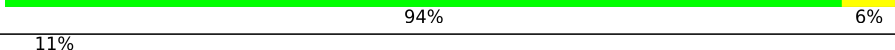
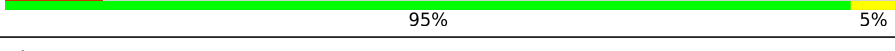
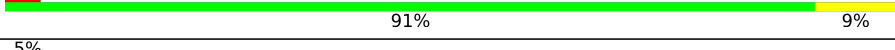
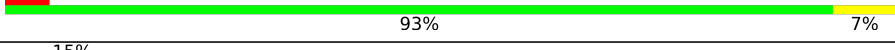
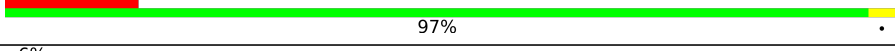
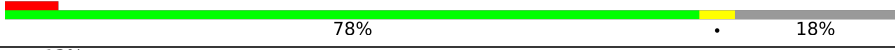
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	436 (6.80 - 7.80)

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

Mol	Chain	Length	Quality of chain
1	0	440	
1	S	440	
2	1	682	
2	2	682	
2	3	682	

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Mol	Chain	Length	Quality of chain
2	A	682	
2	B	682	
2	C	682	
2	D	682	
2	E	682	
2	F	682	
2	G	682	
2	H	682	
2	I	682	
2	J	682	
2	K	682	
2	L	682	
2	m	682	
2	s	682	
2	t	682	
2	u	682	
2	v	682	
2	w	682	
2	x	682	
2	y	682	
2	z	682	
3	4	1163	
3	7	1163	
3	M	1163	
3	P	1163	

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Mol	Chain	Length	Quality of chain
4	5	581	
4	8	581	
4	N	581	
4	Q	581	
5	6	164	
5	9	164	
5	O	164	
5	R	164	
6	AA	228	
6	T	228	
7	AE	937	
7	AF	937	
7	X	937	
7	Y	937	
8	AG	993	
8	Z	993	
8	n	993	
9	AH	782	
9	a	782	
9	o	782	
10	AI	147	
10	b	147	
10	p	147	
11	AJ	449	
11	c	449	

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Mol	Chain	Length	Quality of chain
11	q	449	
12	AK	445	
12	d	445	
12	r	445	
13	AL	466	
13	AN	466	
13	U	466	
13	e	466	
13	g	466	
14	AM	163	
14	AO	163	
14	f	163	
14	h	163	
14	j	163	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 183153 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 KH domain-containing protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	136	Total	C	N	O	0	0
			673	401	136	136		
1	S	136	Total	C	N	O	0	0
			673	401	136	136		

- Molecule 2 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	2	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	3	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	A	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	B	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	C	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	D	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	E	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	F	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	G	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	H	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	I	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	J	682	Total	C	N	O	0	0
			3373	2009	682	682		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	682	Total 3373	C 2009	N 682	O 682	0	0
2	L	682	Total 3373	C 2009	N 682	O 682	0	0
2	m	682	Total 3373	C 2009	N 682	O 682	0	0
2	s	682	Total 3373	C 2009	N 682	O 682	0	0
2	t	682	Total 3373	C 2009	N 682	O 682	0	0
2	u	682	Total 3373	C 2009	N 682	O 682	0	0
2	v	682	Total 3373	C 2009	N 682	O 682	0	0
2	w	682	Total 3373	C 2009	N 682	O 682	0	0
2	x	682	Total 3373	C 2009	N 682	O 682	0	0
2	y	682	Total 3373	C 2009	N 682	O 682	0	0
2	z	682	Total 3373	C 2009	N 682	O 682	0	0

- Molecule 3 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	949	Total 4702	C 2804	N 949	O 949	0	0
3	7	949	Total 4702	C 2804	N 949	O 949	0	0
3	M	949	Total 4702	C 2804	N 949	O 949	0	0
3	P	949	Total 4702	C 2804	N 949	O 949	0	0

- Molecule 4 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	367	Total 1812	C 1078	N 367	O 367	0	0
4	8	367	Total 1812	C 1078	N 367	O 367	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	Q	367	Total	C	N	O	0	0
			1812	1078	367	367		

- Molecule 5 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	6	119	Total	C	N	O	0	0
			592	354	119	119		
5	9	89	Total	C	N	O	0	0
			442	264	89	89		
5	O	119	Total	C	N	O	0	0
			592	354	119	119		
5	R	89	Total	C	N	O	0	0
			442	264	89	89		

- Molecule 6 is a protein called Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	AA	63	Total	C	N	O	0	0
			311	185	63	63		
6	T	63	Total	C	N	O	0	0
			311	185	63	63		

- Molecule 7 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AE	935	Total	C	N	O	0	0
			4643	2773	935	935		
7	AF	845	Total	C	N	O	0	0
			4196	2506	845	845		
7	X	935	Total	C	N	O	0	0
			4643	2773	935	935		
7	Y	845	Total	C	N	O	0	0
			4196	2506	845	845		

- Molecule 8 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AG	966	Total	C	N	O	0	0
			4794	2862	966	966		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	Z	966	Total	C	N	O	0	0
			4794	2862	966	966		
8	n	966	Total	C	N	O	0	0
			4794	2862	966	966		

- Molecule 9 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AH	635	Total	C	N	O	0	0
			3131	1861	635	635		
9	a	635	Total	C	N	O	0	0
			3131	1861	635	635		
9	o	635	Total	C	N	O	0	0
			3131	1861	635	635		

- Molecule 10 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AI	147	Total	C	N	O	0	0
			729	435	147	147		
10	b	147	Total	C	N	O	0	0
			729	435	147	147		
10	p	147	Total	C	N	O	0	0
			729	435	147	147		

- Molecule 11 is a protein called Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AJ	440	Total	C	N	O	0	0
			2167	1287	440	440		
11	c	440	Total	C	N	O	0	0
			2167	1287	440	440		
11	q	440	Total	C	N	O	0	0
			2167	1287	440	440		

- Molecule 12 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AK	431	Total	C	N	O	0	0
			2121	1259	431	431		
12	d	431	Total	C	N	O	0	0
			2121	1259	431	431		

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Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	431	Total	C	N	O	0	0
			2121	1259	431	431		

- Molecule 13 is a protein called F-box/WD repeat-containing protein.

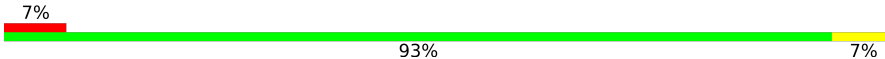
Mol	Chain	Residues	Atoms				AltConf	Trace
13	AL	466	Total	C	N	O	0	0
			2312	1380	466	466		
13	AN	466	Total	C	N	O	0	0
			2312	1380	466	466		
13	U	466	Total	C	N	O	0	0
			2312	1380	466	466		
13	e	466	Total	C	N	O	0	0
			2312	1380	466	466		
13	g	466	Total	C	N	O	0	0
			2312	1380	466	466		

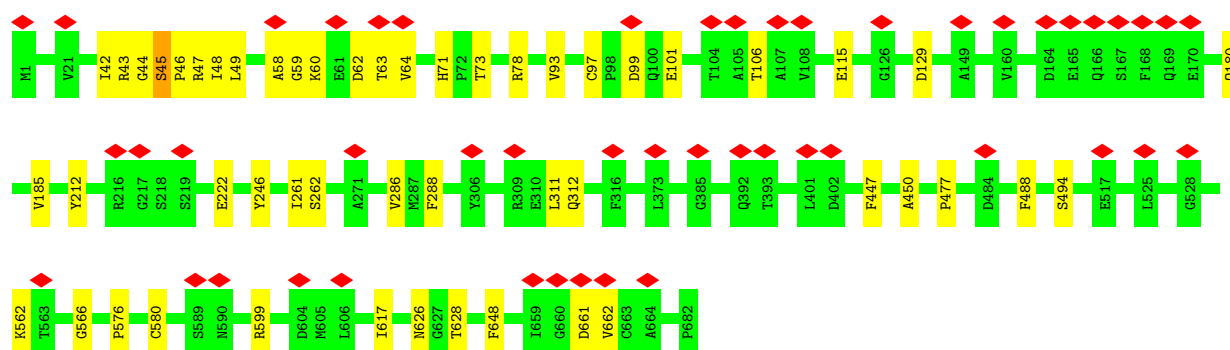
- Molecule 14 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AM	163	Total	C	N	O	0	0
			809	483	163	163		
14	AO	163	Total	C	N	O	0	0
			809	483	163	163		
14	f	163	Total	C	N	O	0	0
			809	483	163	163		
14	h	163	Total	C	N	O	0	0
			809	483	163	163		
14	j	163	Total	C	N	O	0	0
			809	483	163	163		

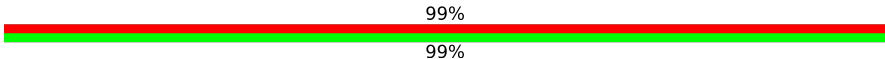
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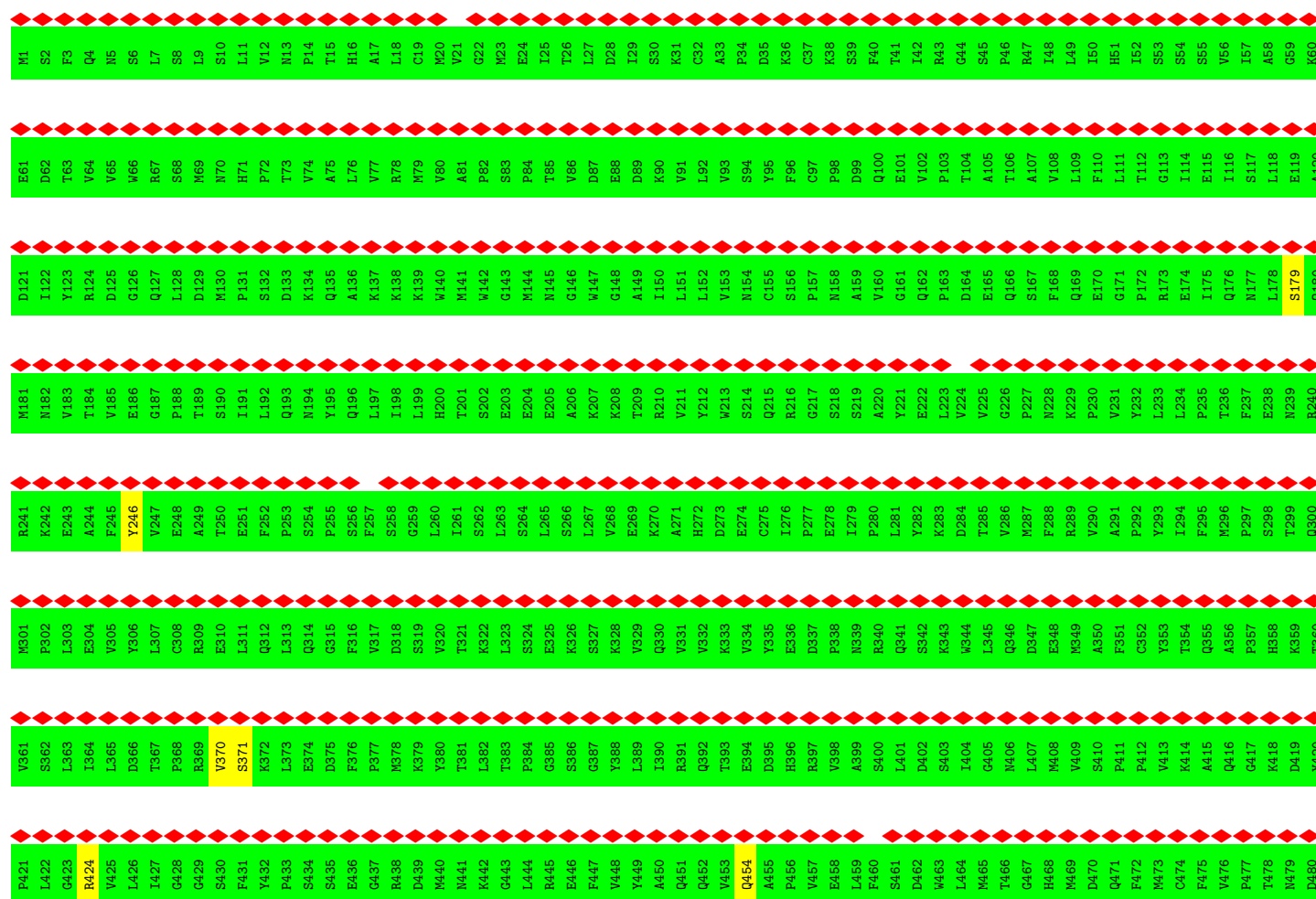
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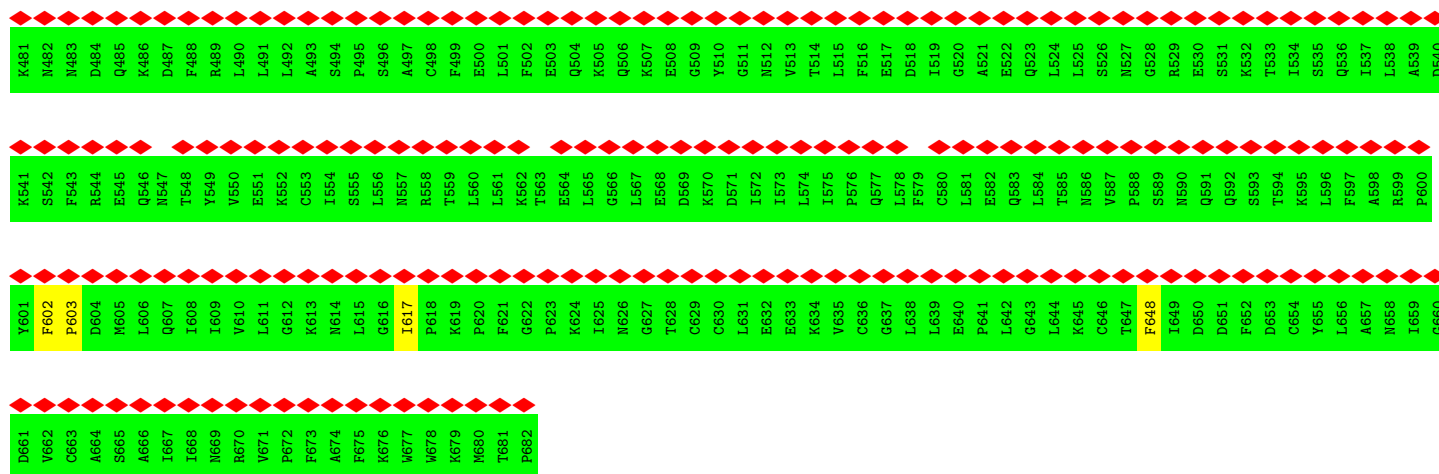
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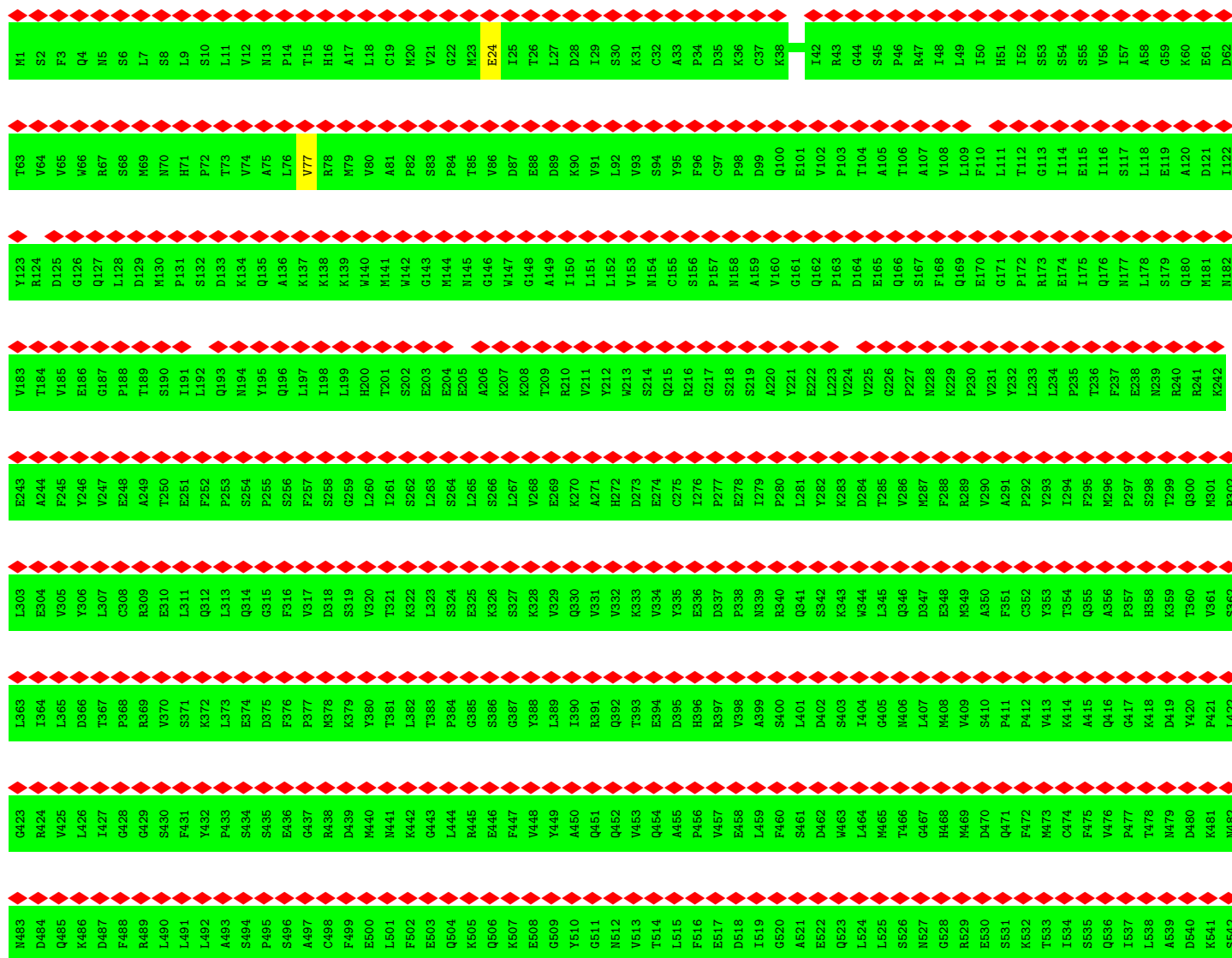
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain 2: 





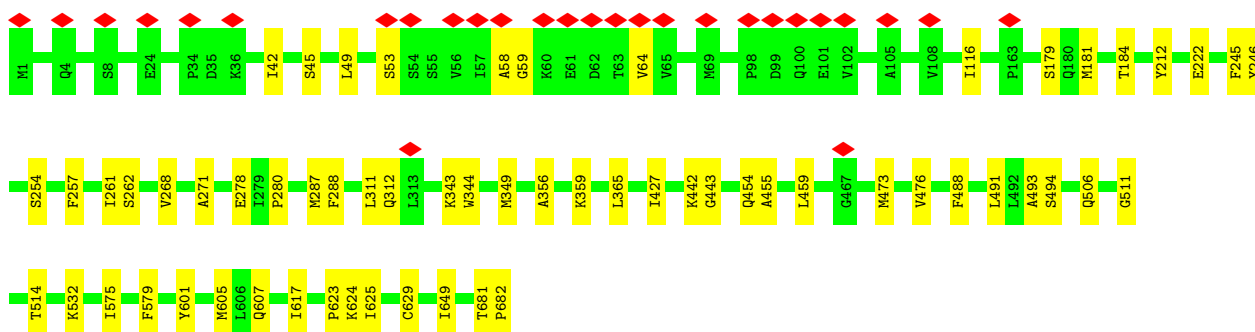
• Molecule 2: Inactive protein-arginine deiminase type-6





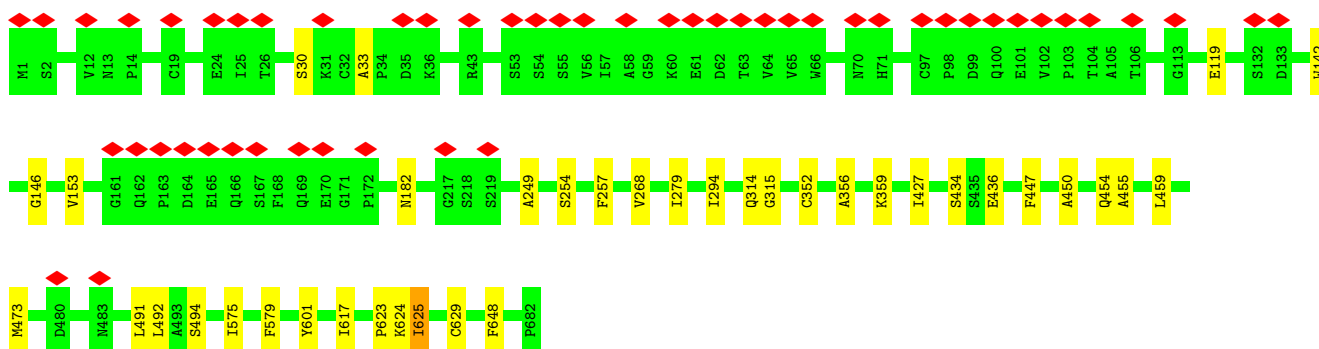
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain A: 91% 9%



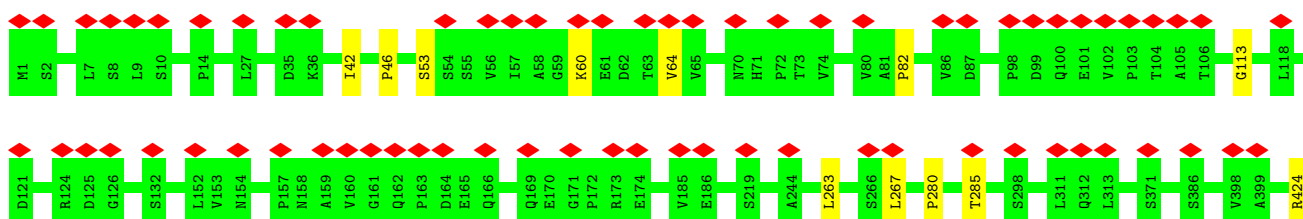
• Molecule 2: Inactive protein-arginine deiminase type-6

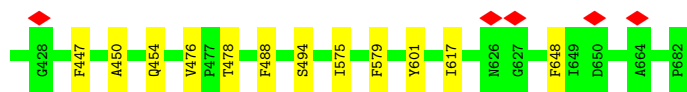
Chain B: 8% 94% 6%



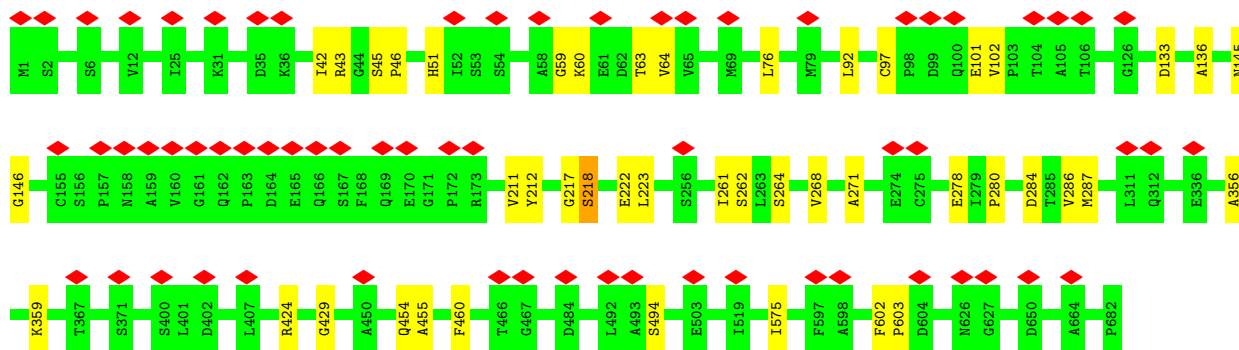
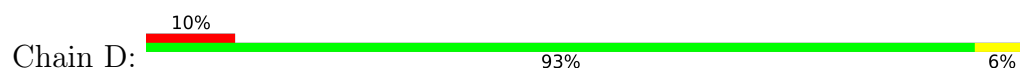
• Molecule 2: Inactive protein-arginine deiminase type-6

Chain C: 11% 96%

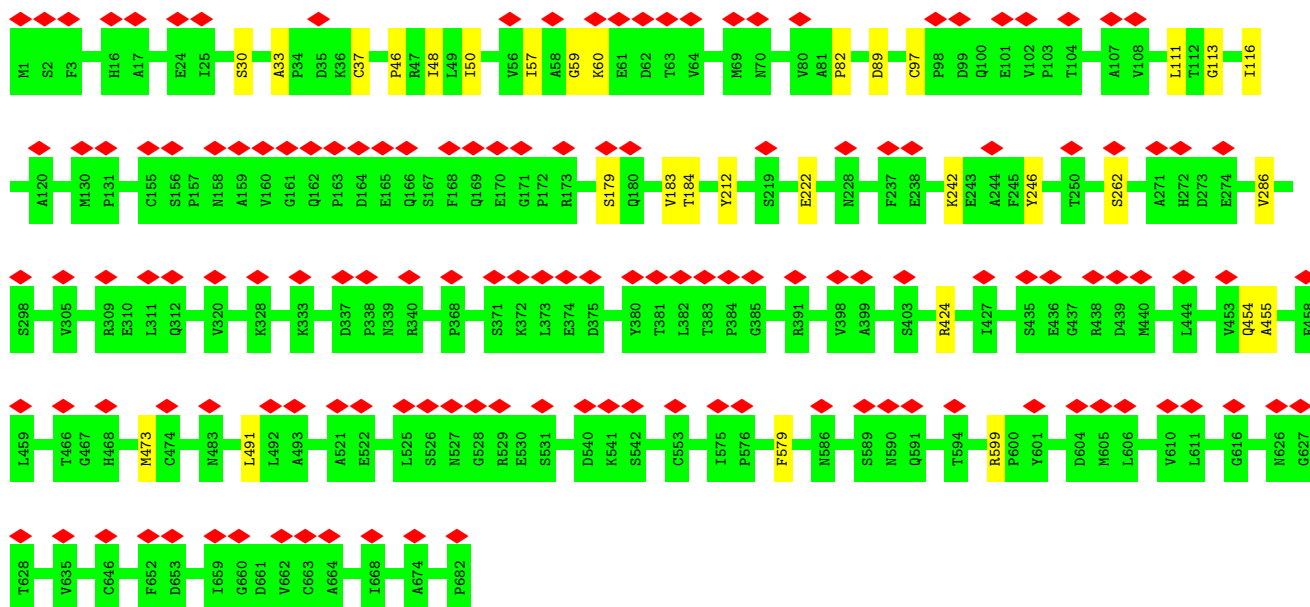




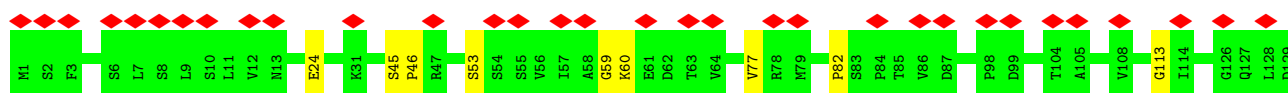
• Molecule 2: Inactive protein-arginine deiminase type-6

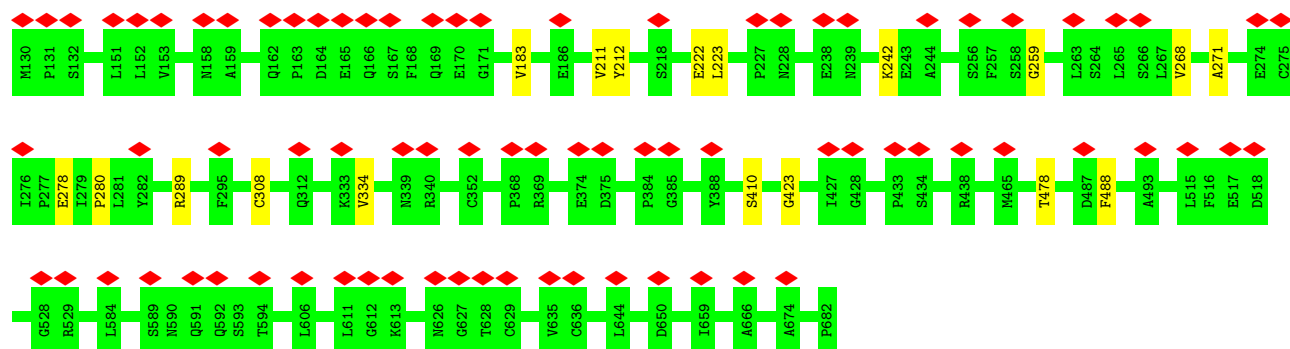


• Molecule 2: Inactive protein-arginine deiminase type-6

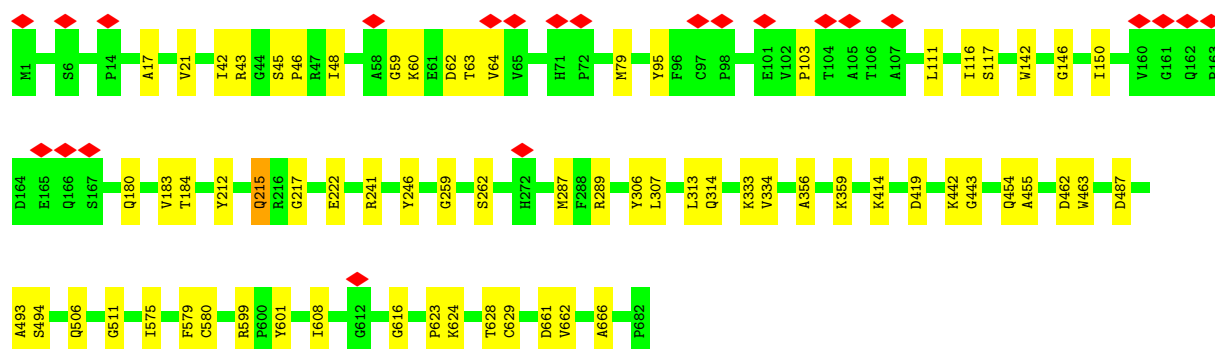


• Molecule 2: Inactive protein-arginine deiminase type-6

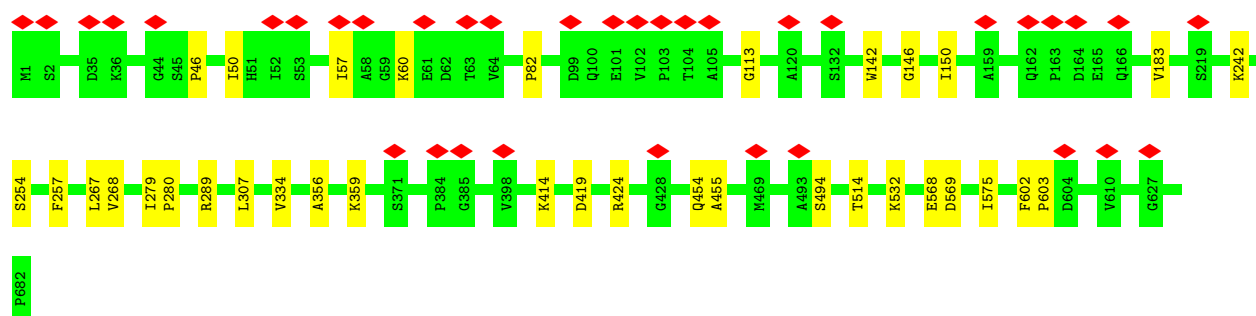




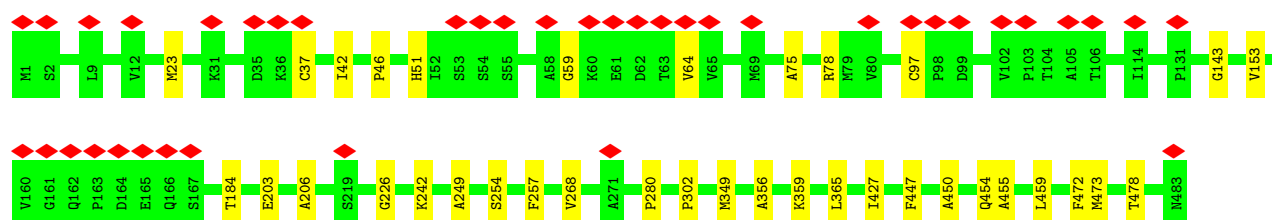
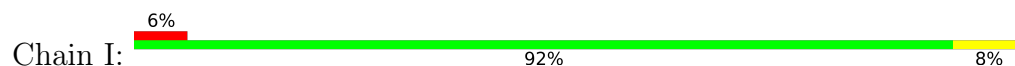
• Molecule 2: Inactive protein-arginine deiminase type-6

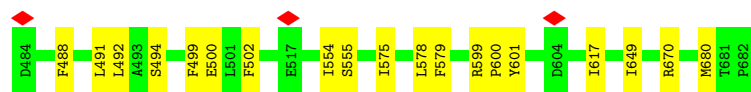


• Molecule 2: Inactive protein-arginine deiminase type-6

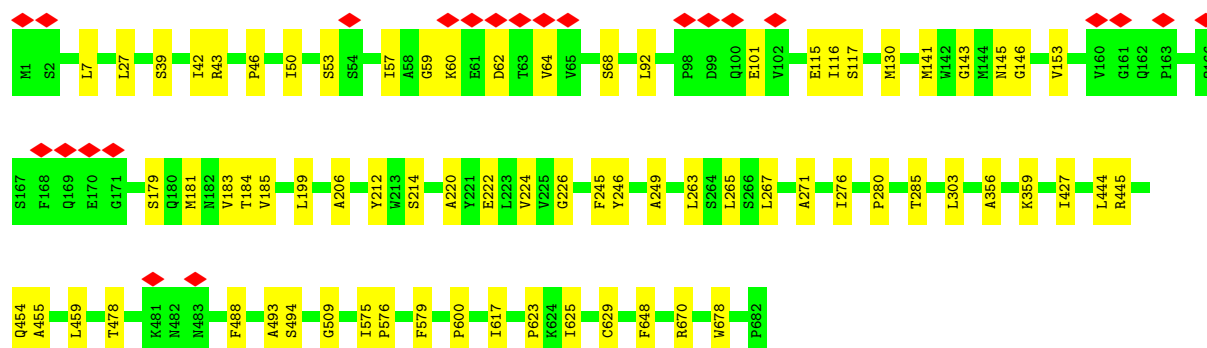
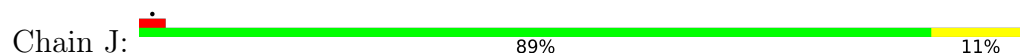


• Molecule 2: Inactive protein-arginine deiminase type-6

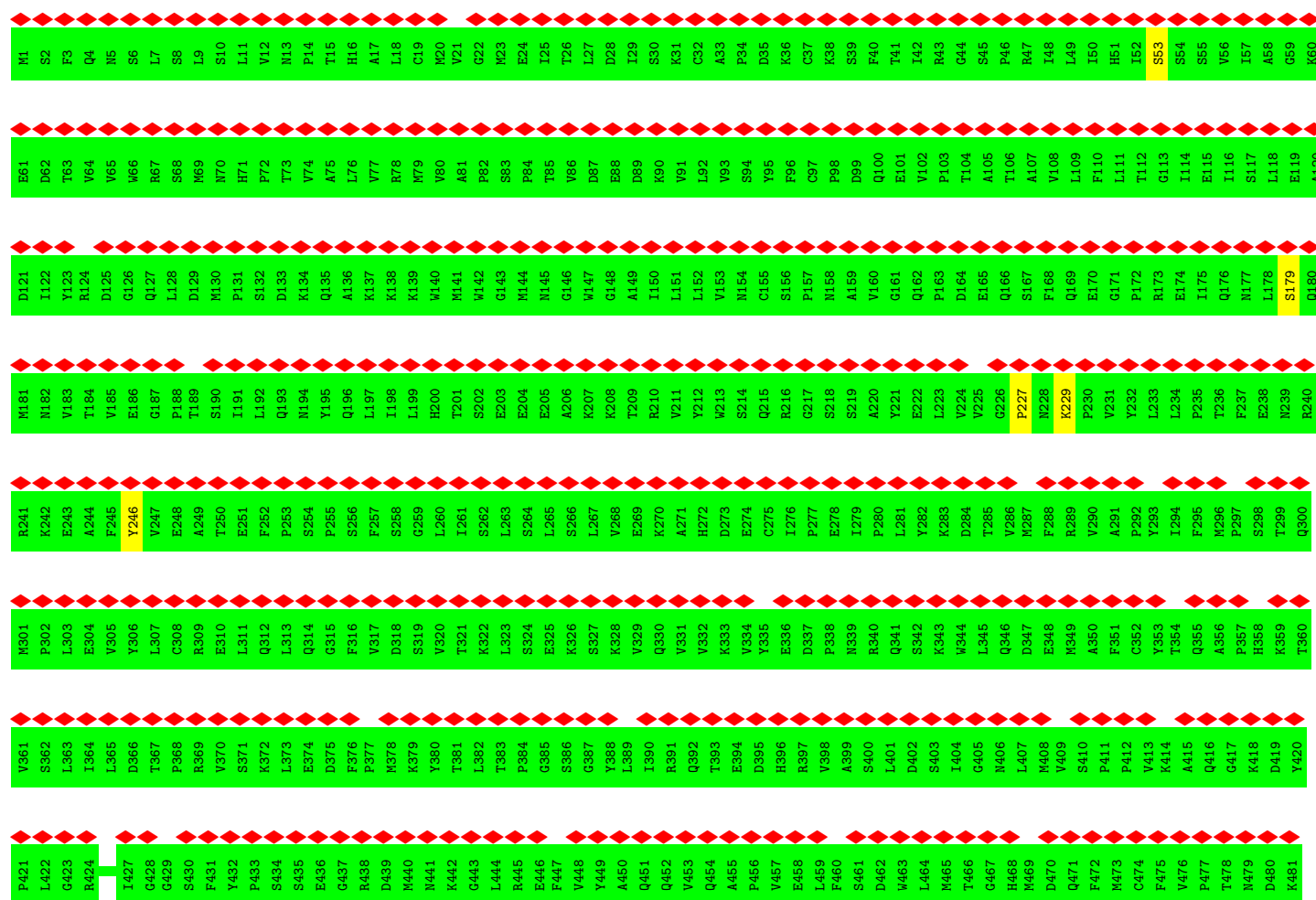


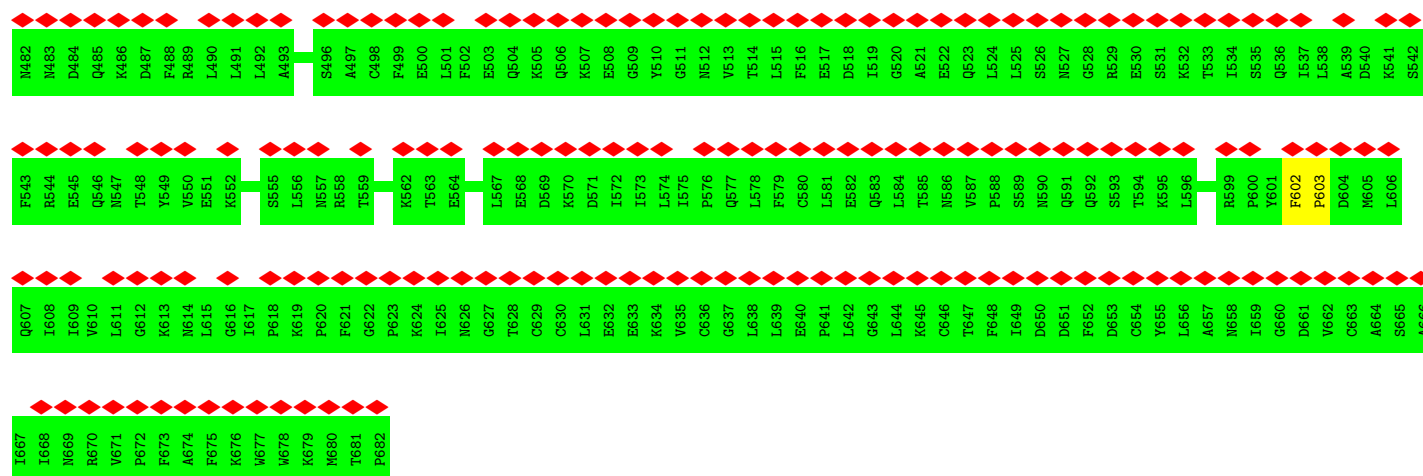


• Molecule 2: Inactive protein-arginine deiminase type-6

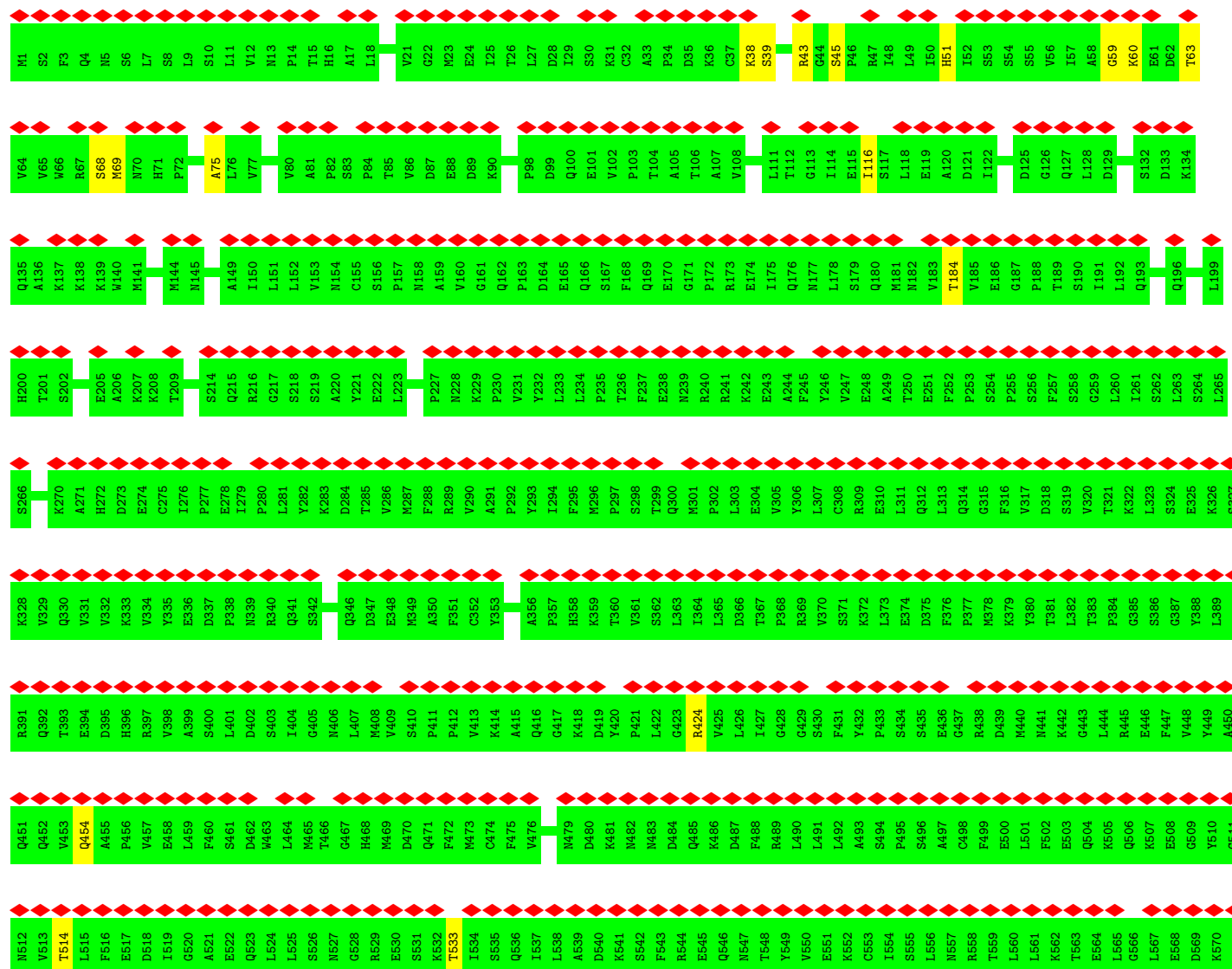
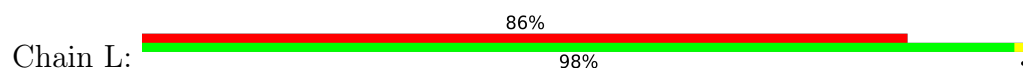


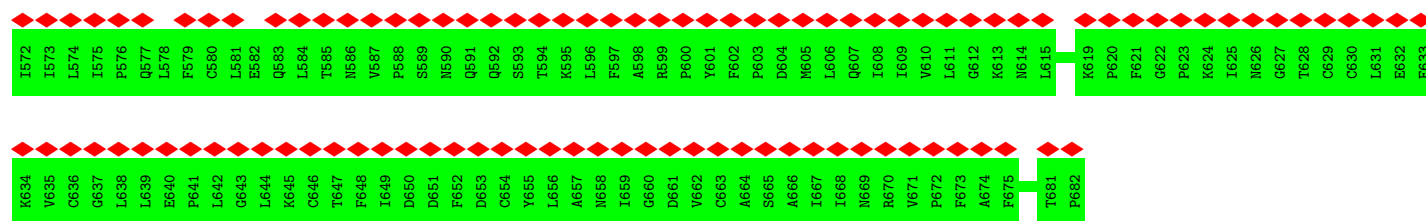
• Molecule 2: Inactive protein-arginine deiminase type-6



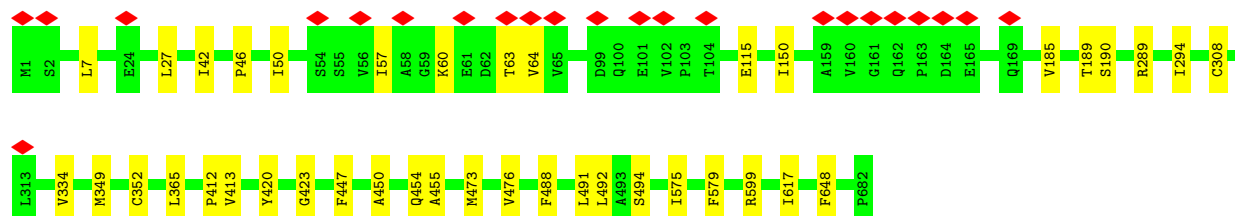


• Molecule 2: Inactive protein-arginine deiminase type-6

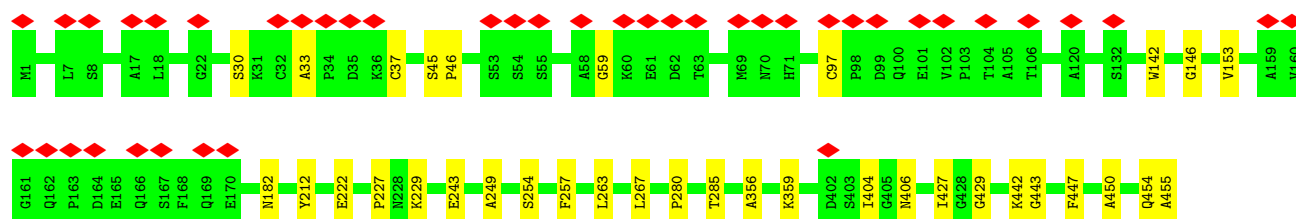




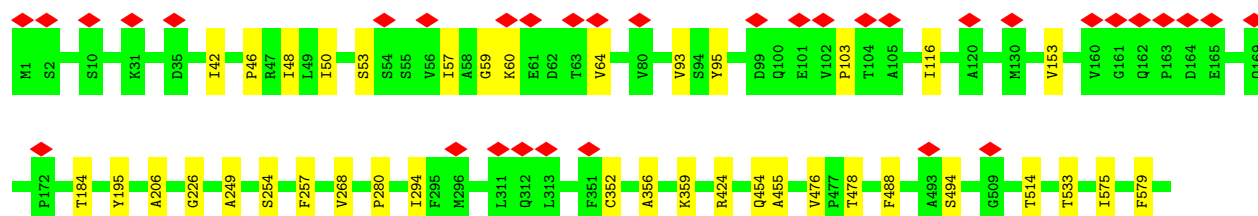
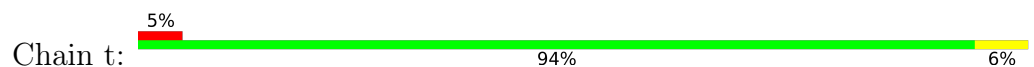
- Molecule 2: Inactive protein-arginine deiminase type-6



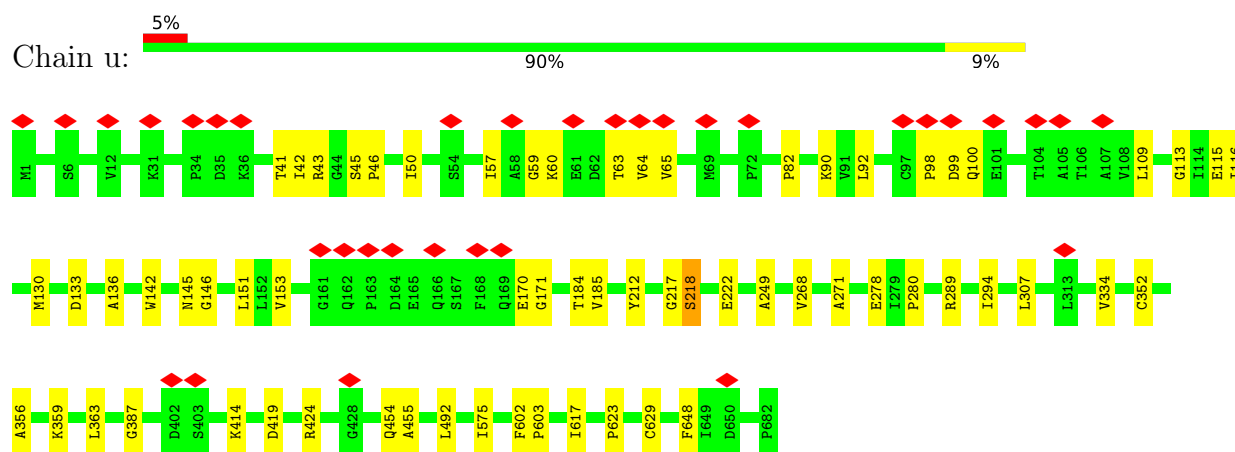
- Molecule 2: Inactive protein-arginine deiminase type-6



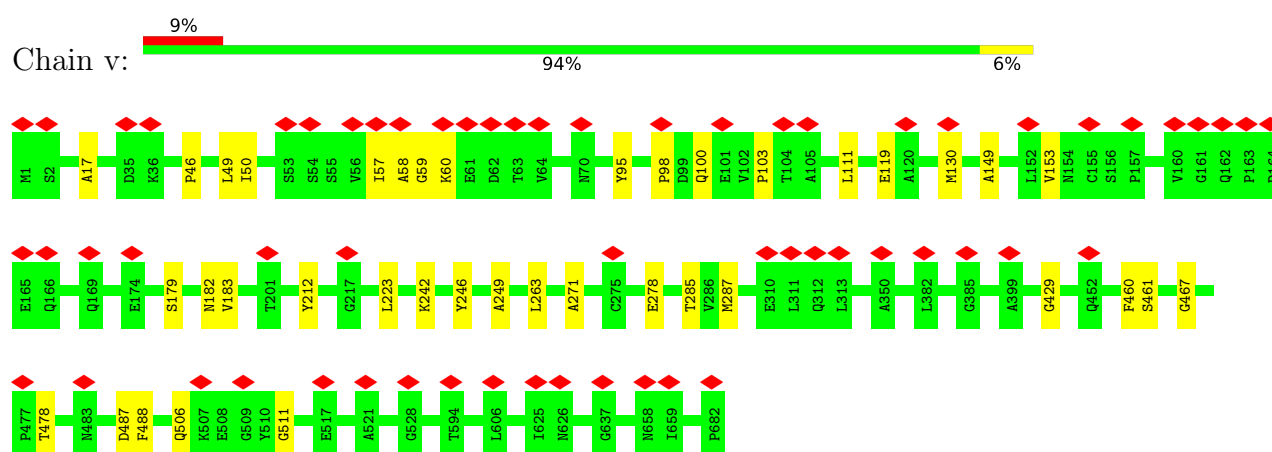
- Molecule 2: Inactive protein-arginine deiminase type-6



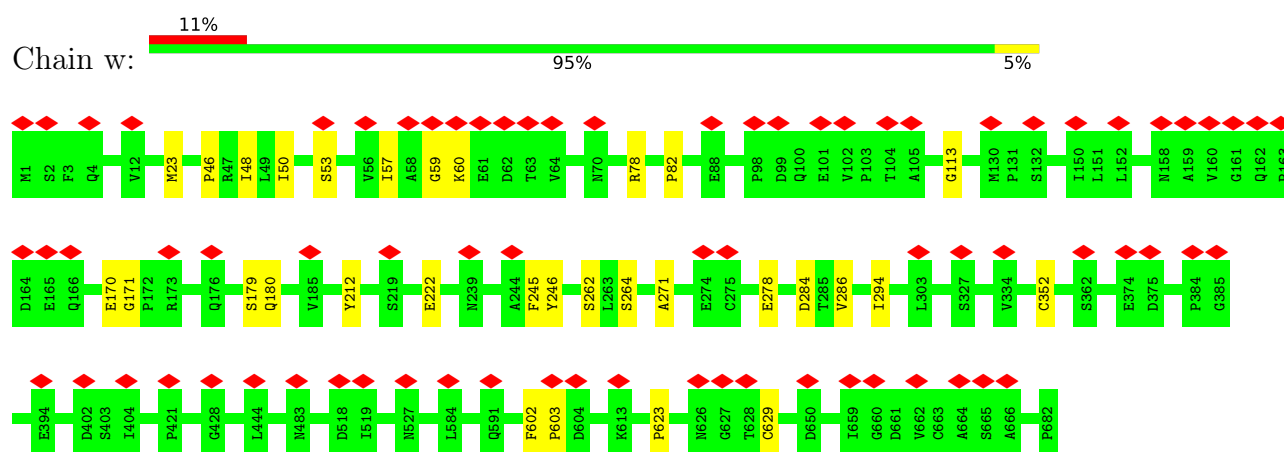
- Molecule 2: Inactive protein-arginine deiminase type-6



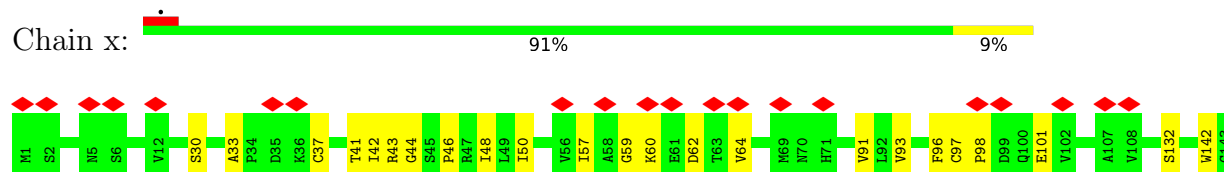
• Molecule 2: Inactive protein-arginine deiminase type-6

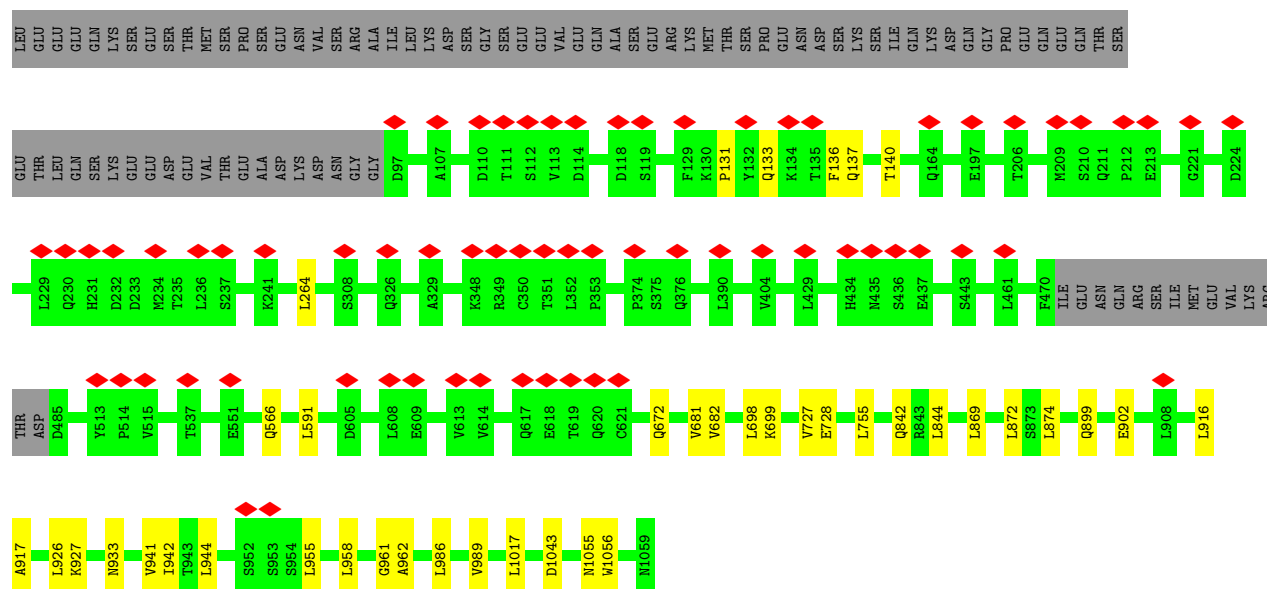


• Molecule 2: Inactive protein-arginine deiminase type-6

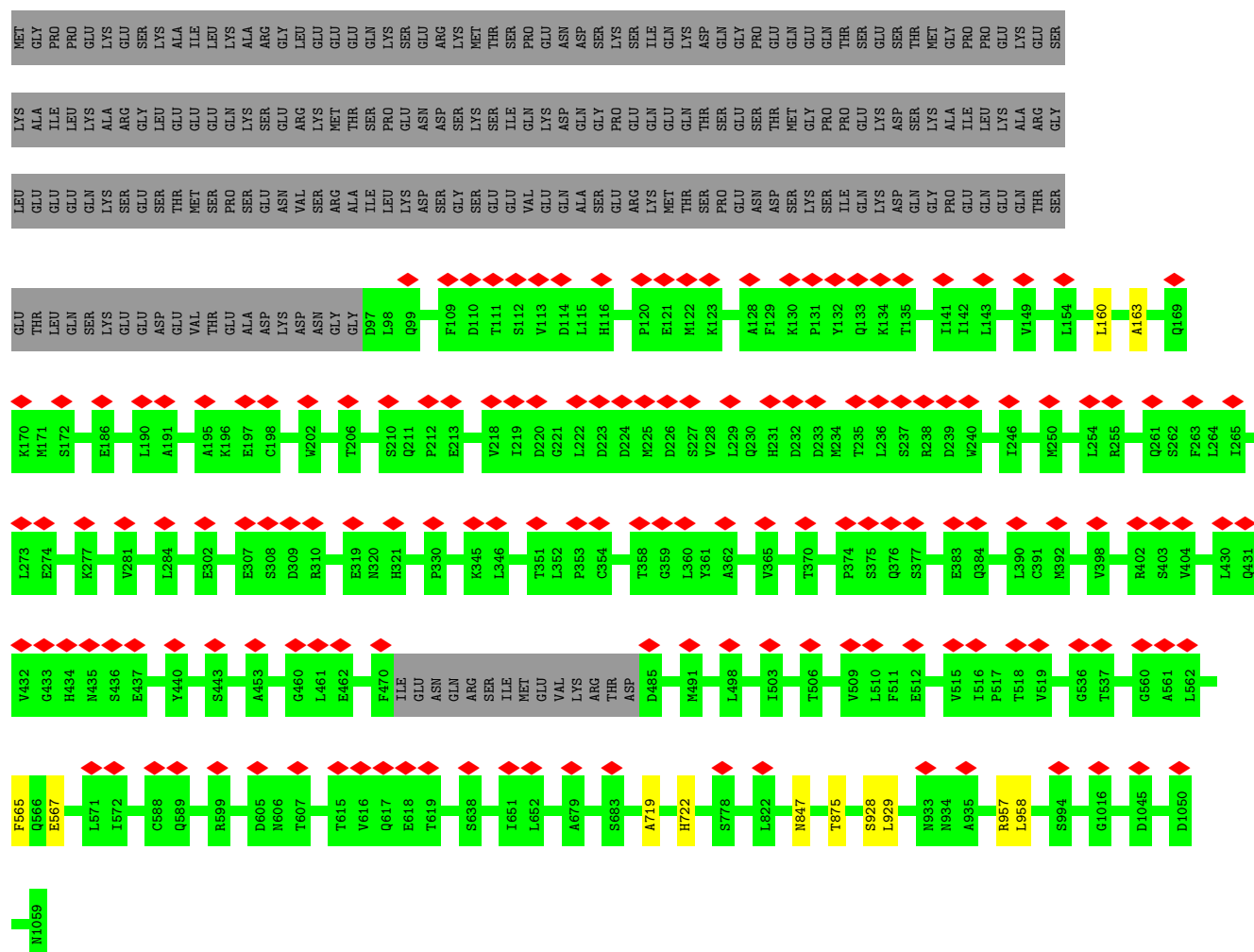
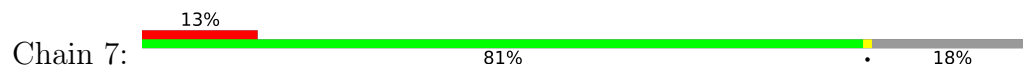


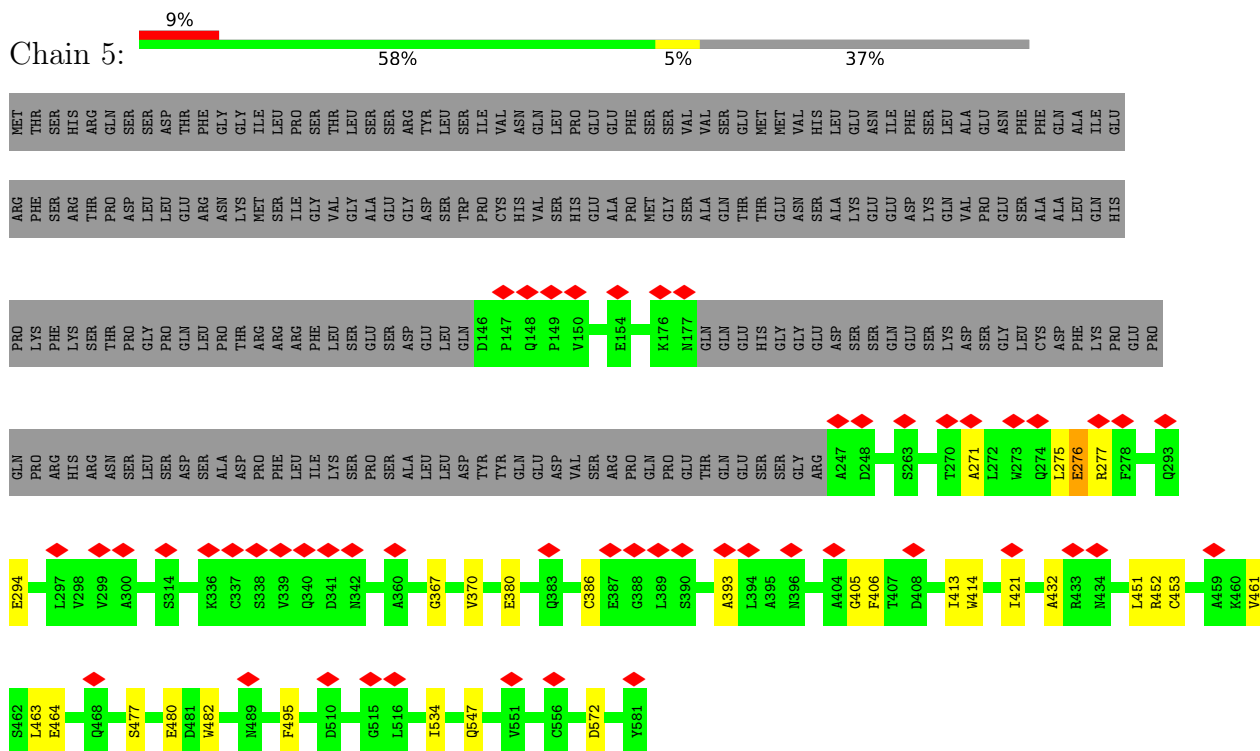
• Molecule 2: Inactive protein-arginine deiminase type-6



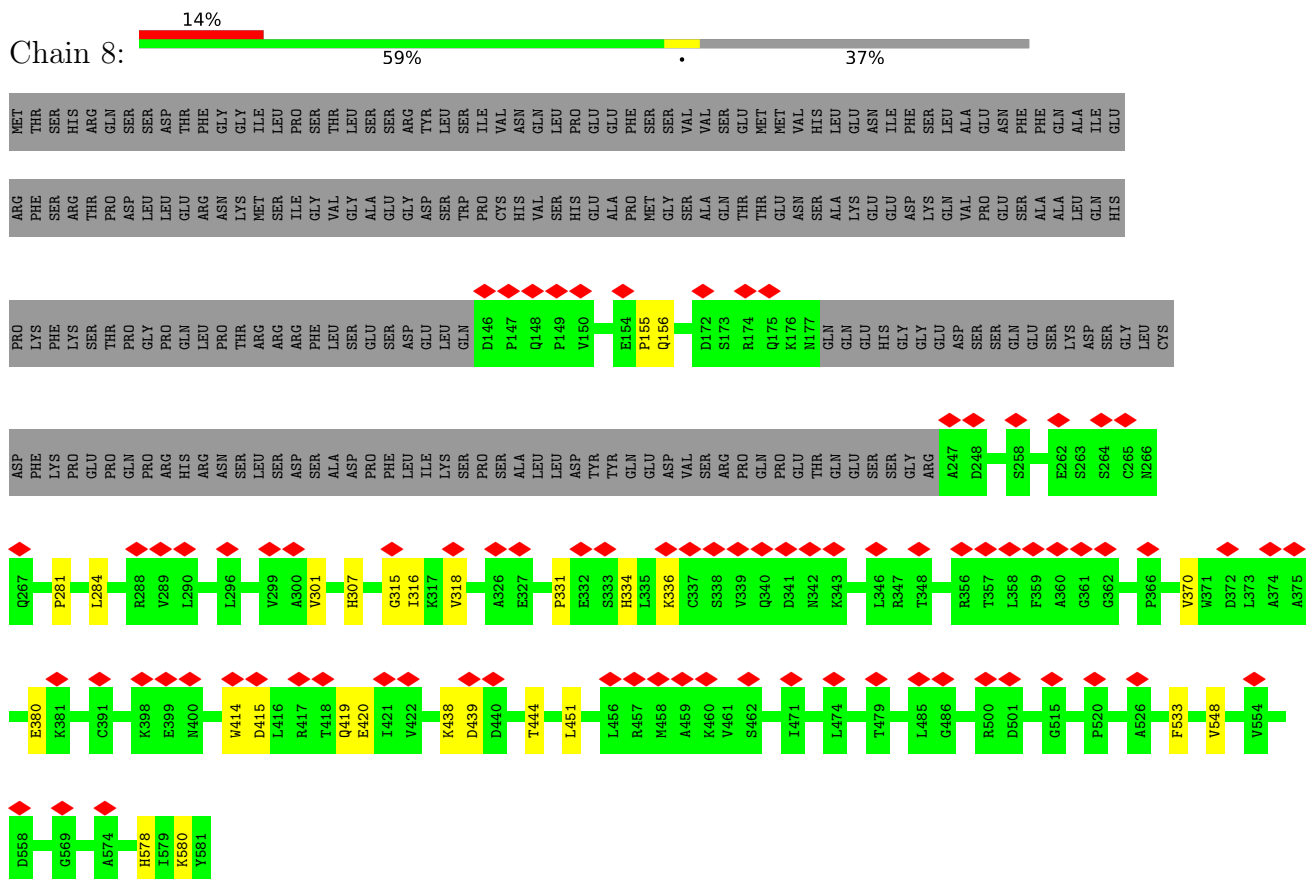


• Molecule 3: NACHT, LRR and PYD domains-containing protein 5

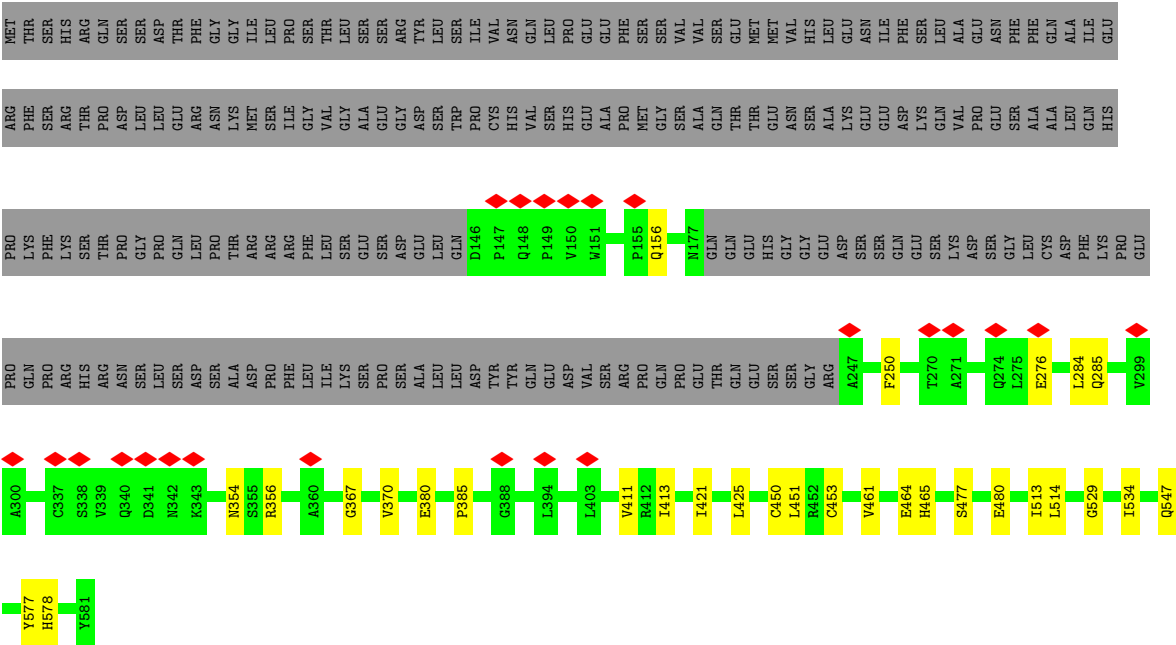




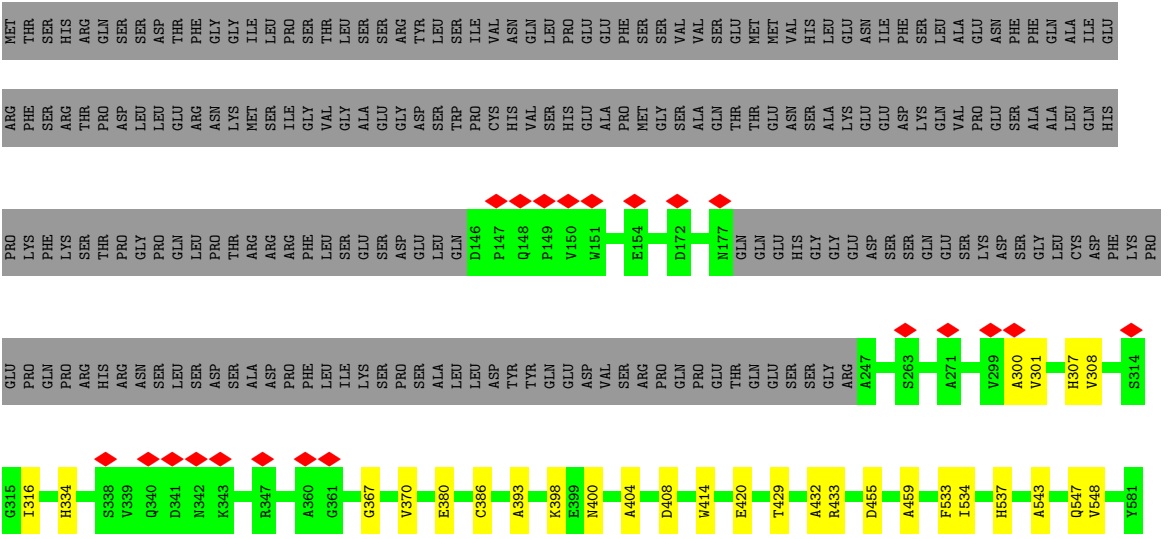
- Molecule 4: Transducin-like enhancer protein 6



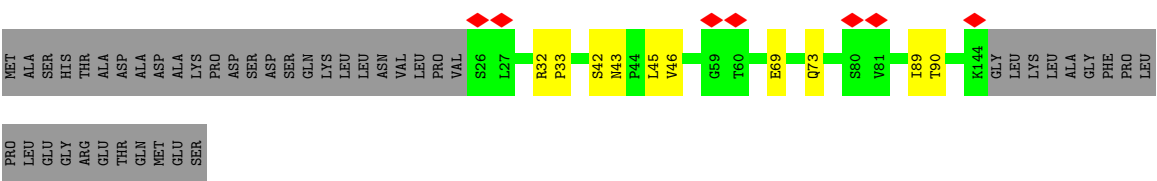
- Molecule 4: Transducin-like enhancer protein 6



• Molecule 4: Transducin-like enhancer protein 6

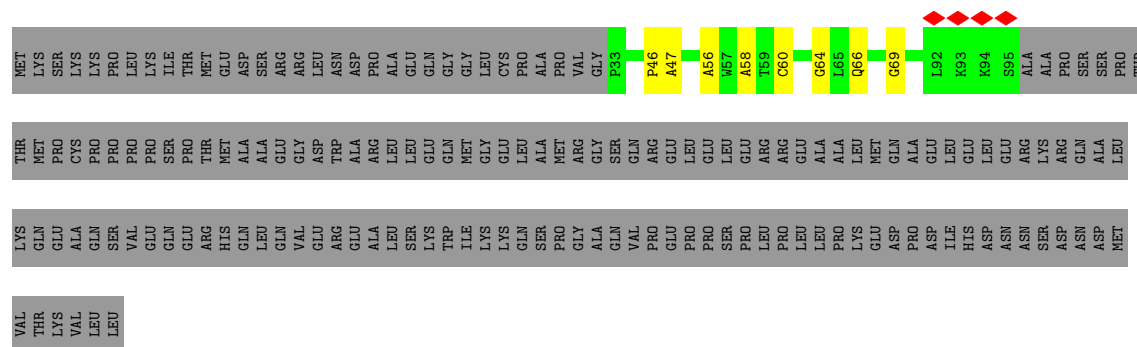


• Molecule 5: Oocyte-expressed protein homolog



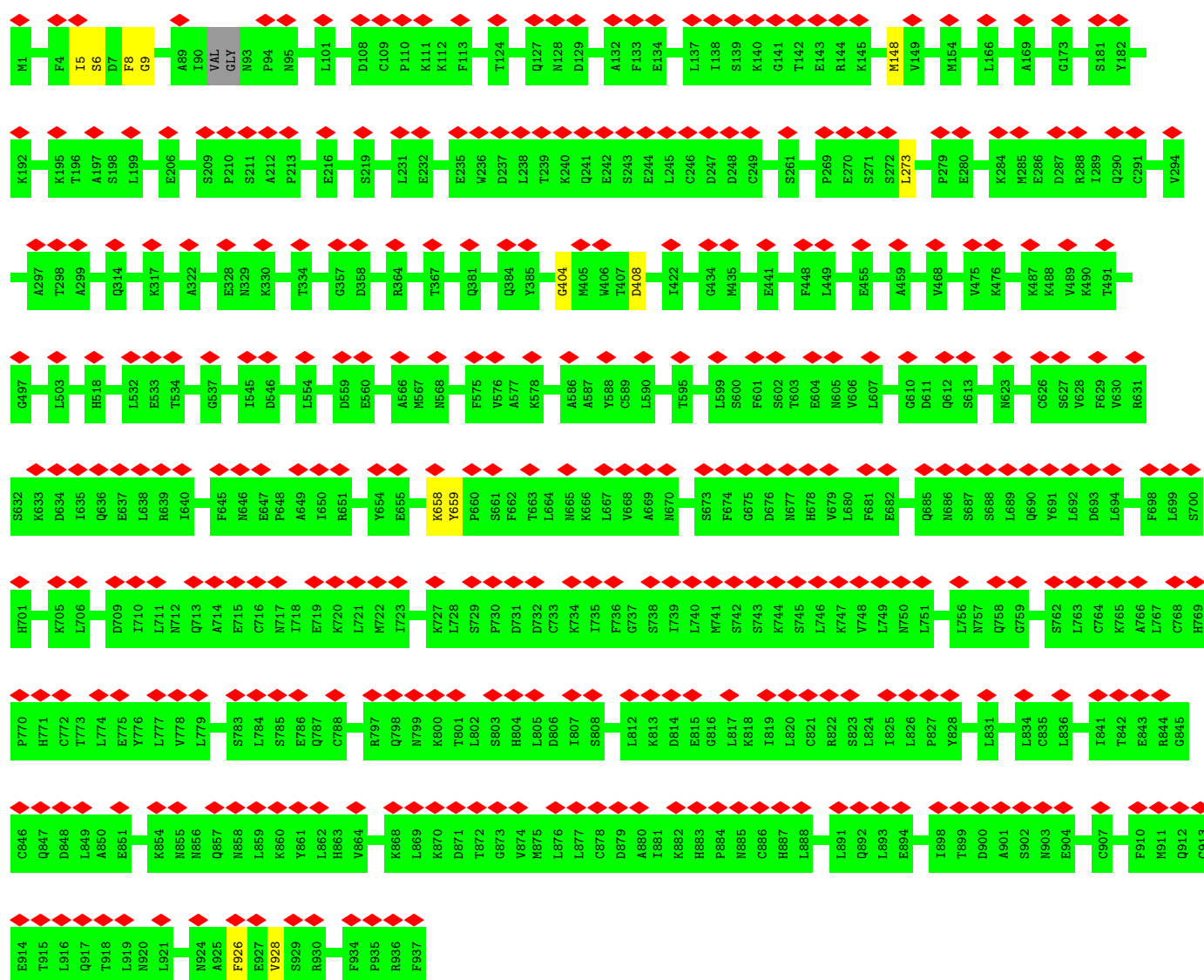
Chain 9:





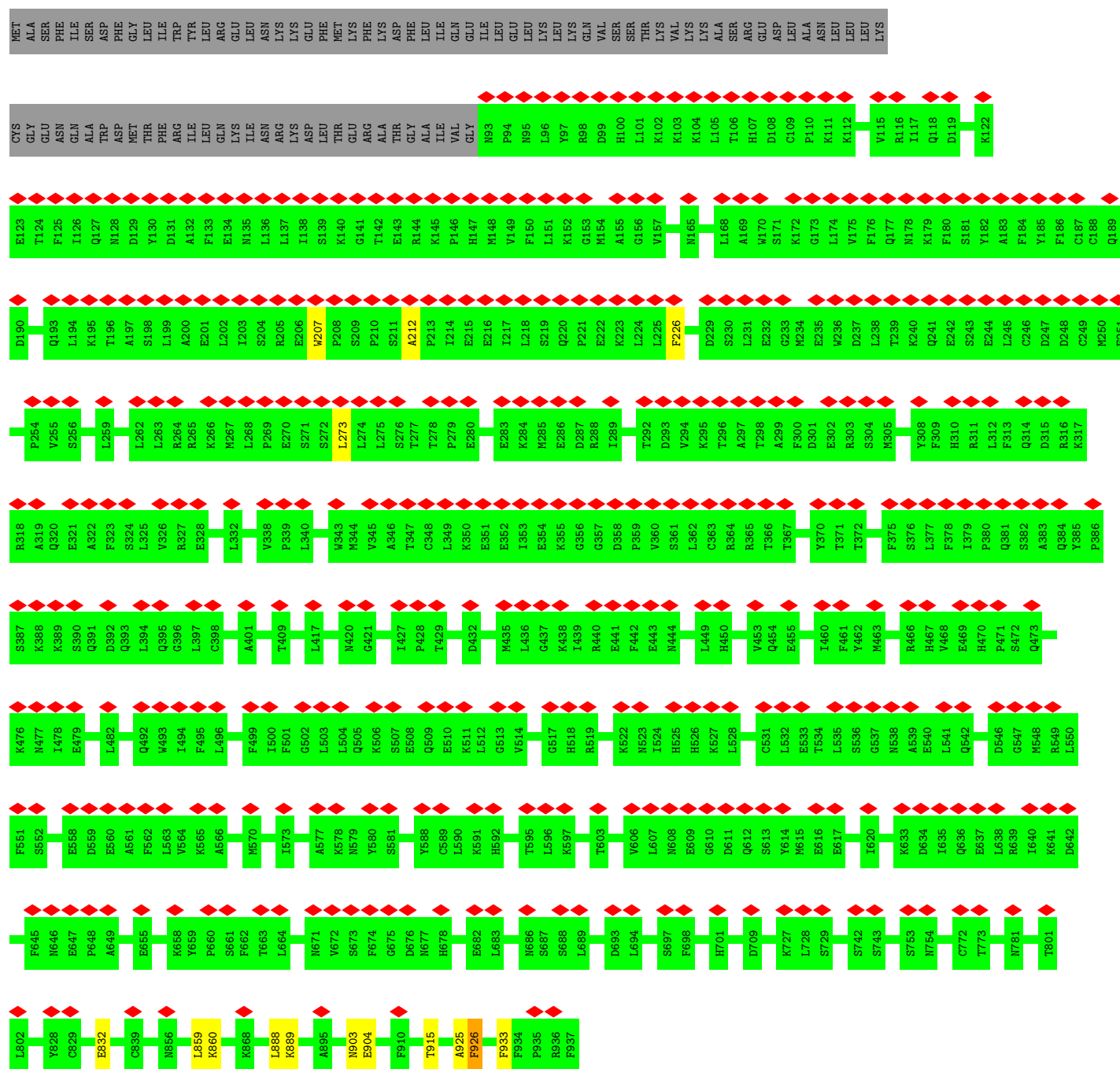
- Molecule 7: NLR family, pyrin domain containing 4F

Chain AE: 37% 99%

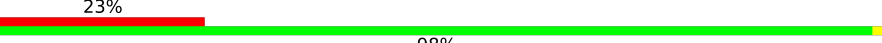


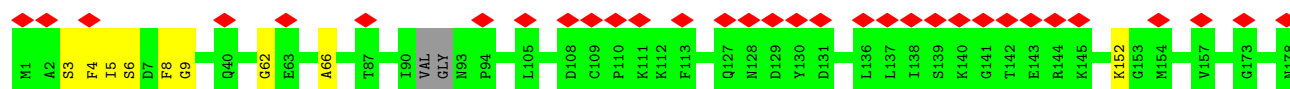
- Molecule 7: NLR family, pyrin domain containing 4F

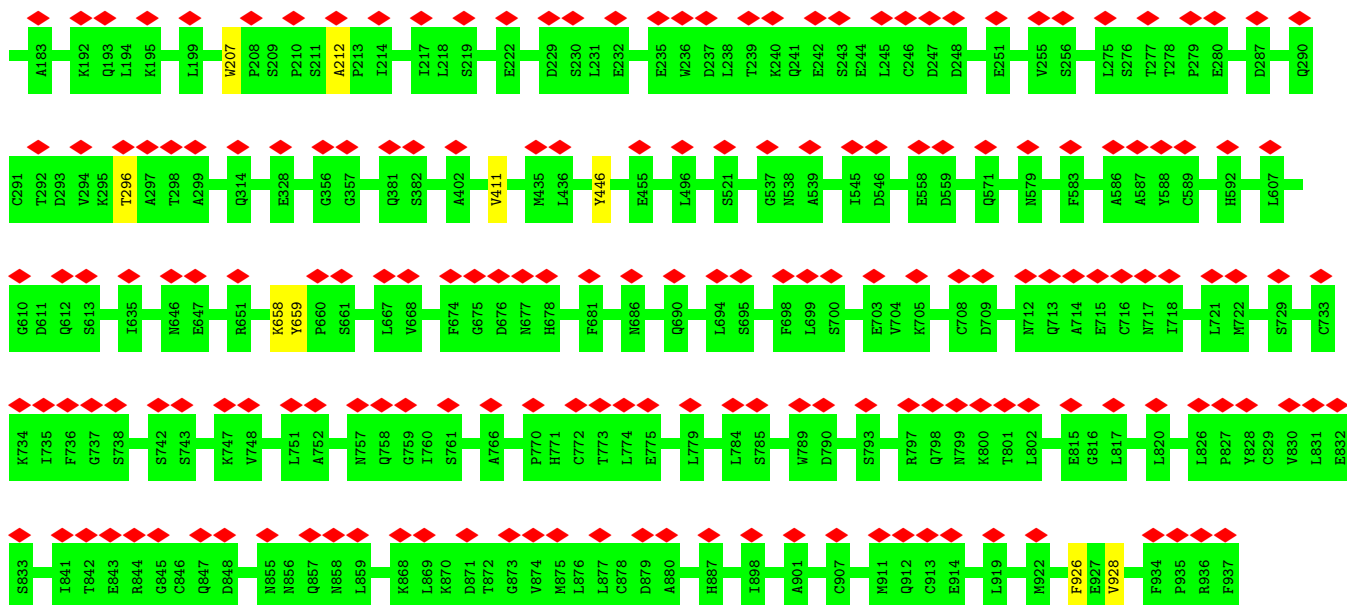
Chain AF: 



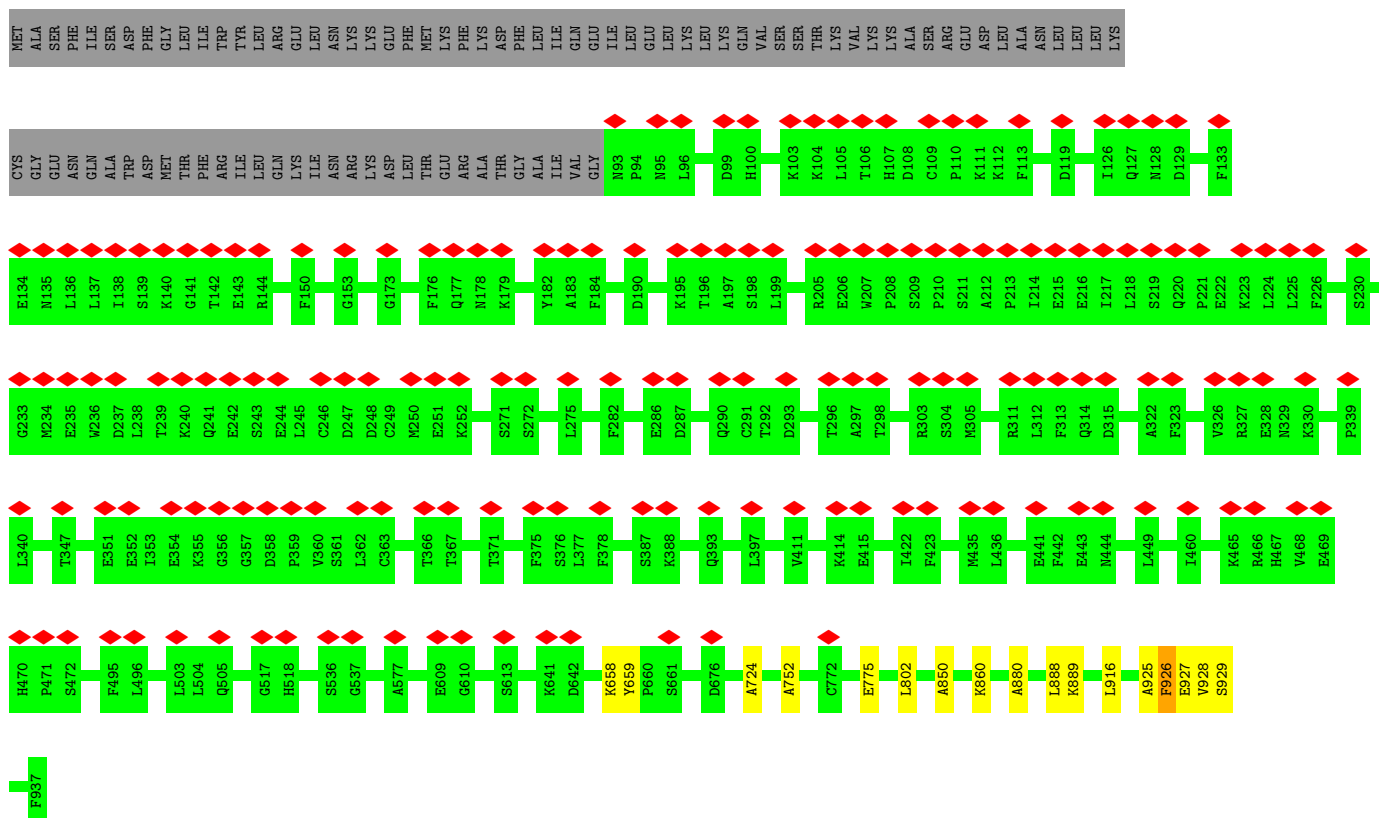
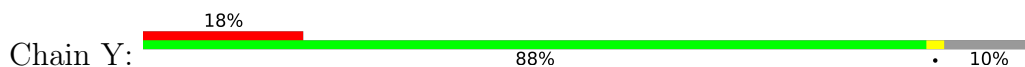
• Molecule 7: NLR family, pyrin domain containing 4F

Chain X: 



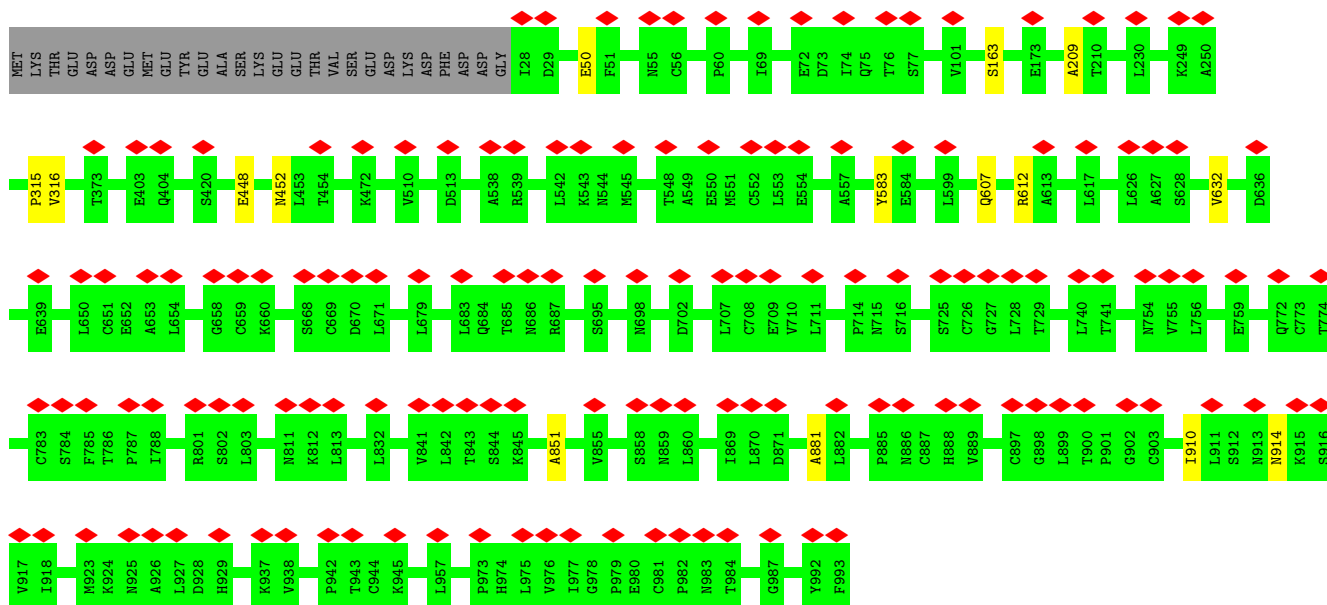


- Molecule 7: NLR family, pyrin domain containing 4F

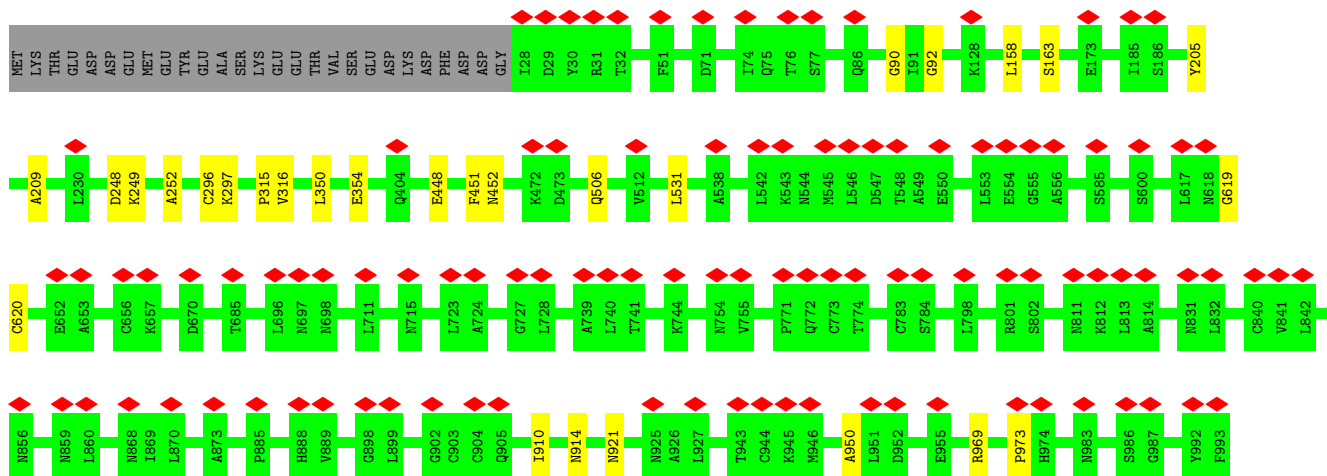
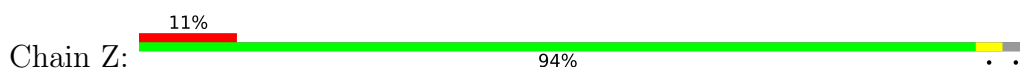


- Molecule 8: NACHT, LRR and PYD domains-containing protein 14

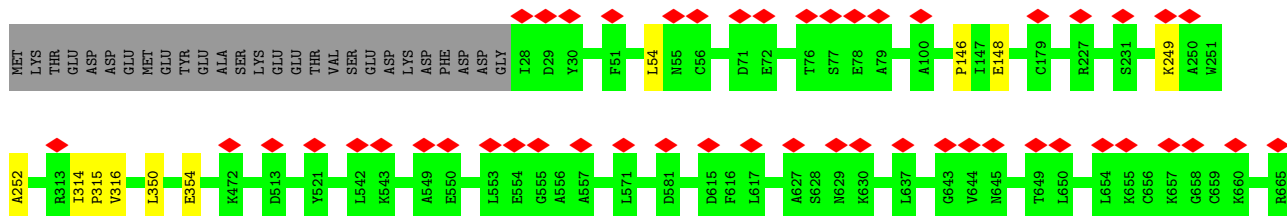


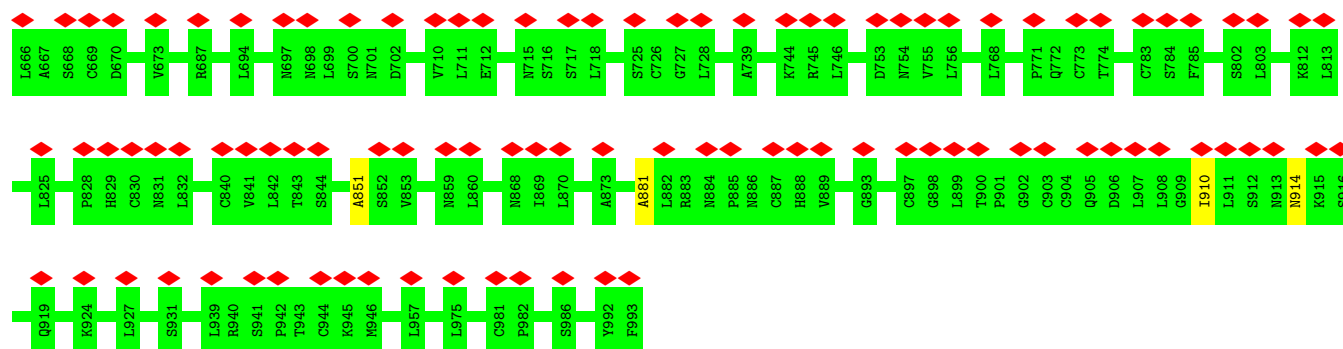


- Molecule 8: NACHT, LRR and PYD domains-containing protein 14

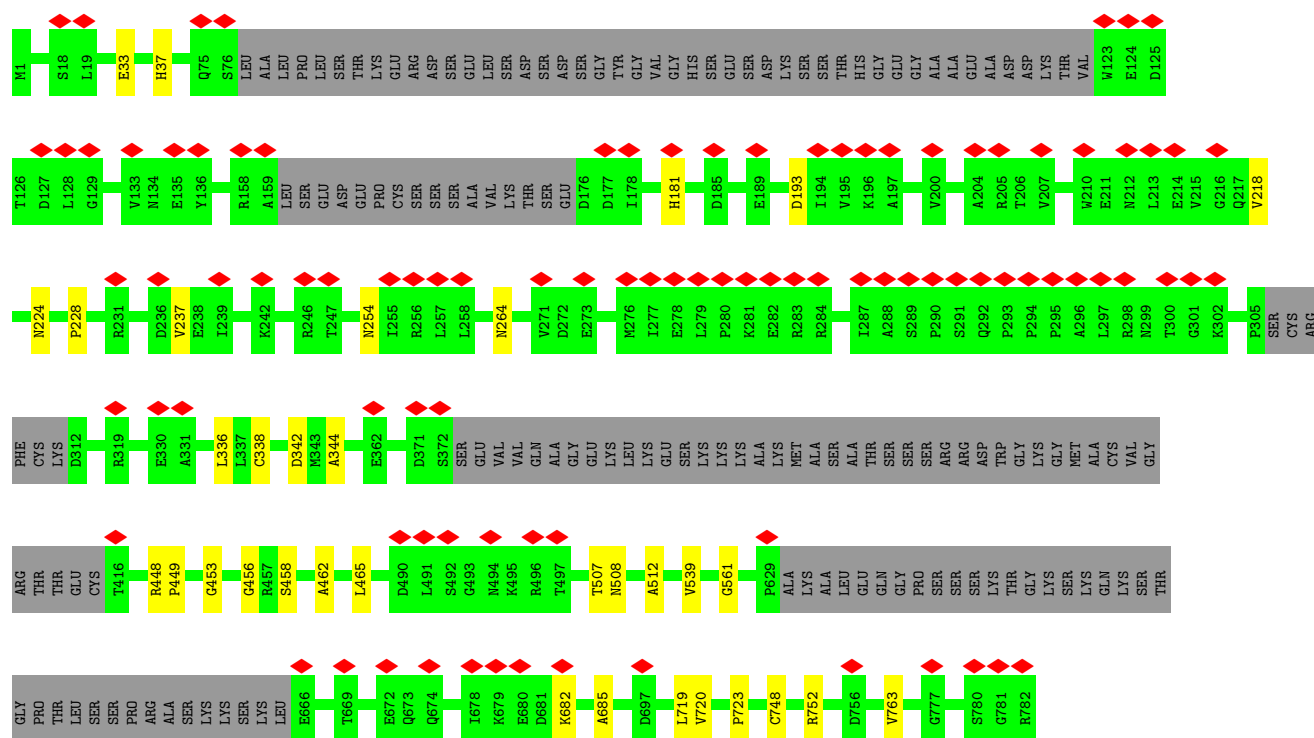
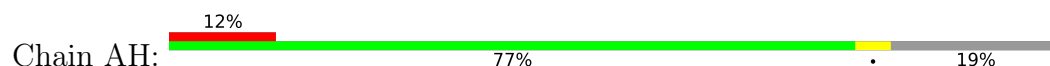


- Molecule 8: NACHT, LRR and PYD domains-containing protein 14

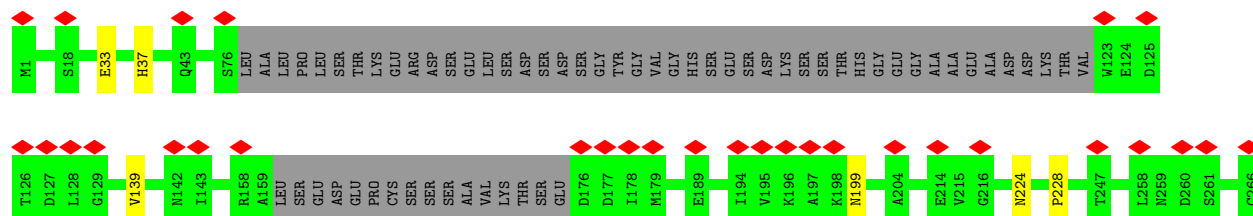


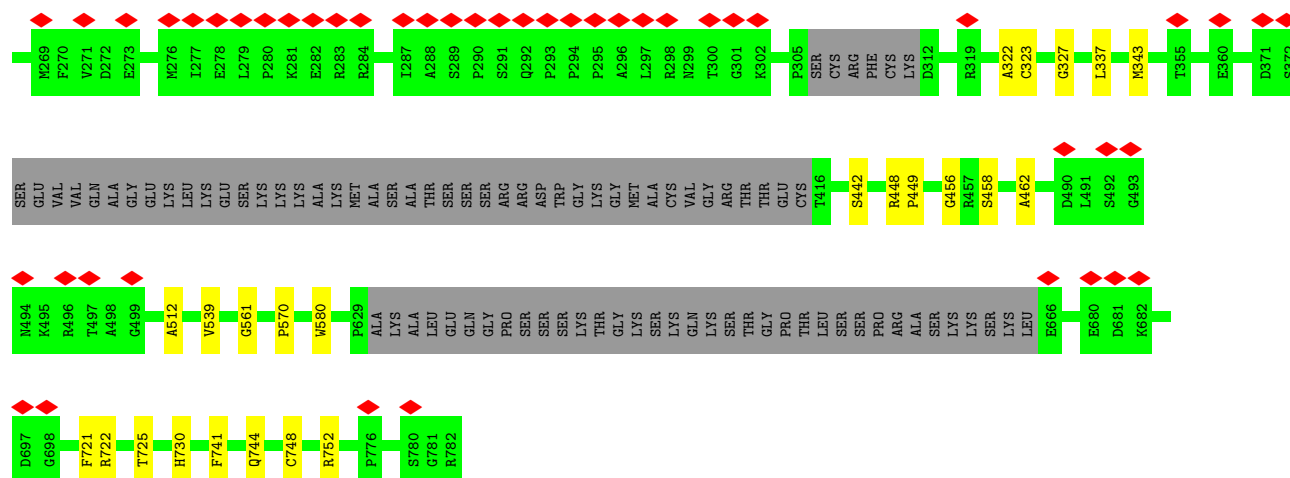


- Molecule 9: E3 ubiquitin-protein ligase UHRF1

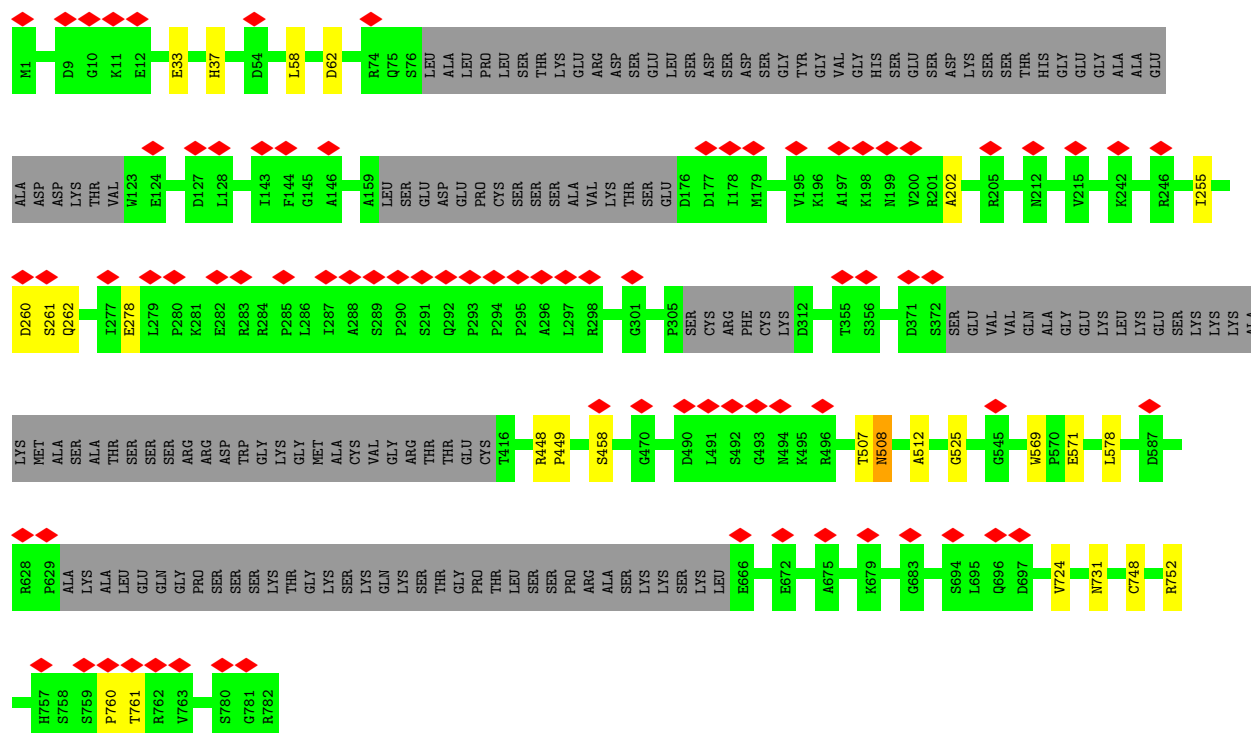


- Molecule 9: E3 ubiquitin-protein ligase UHRF1





• Molecule 9: E3 ubiquitin-protein ligase UHRF1



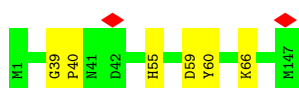
• Molecule 10: Ubiquitin-conjugating enzyme E2 D3



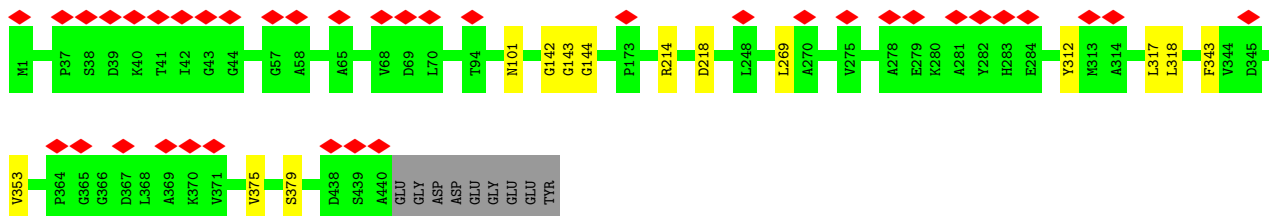
• Molecule 10: Ubiquitin-conjugating enzyme E2 D3



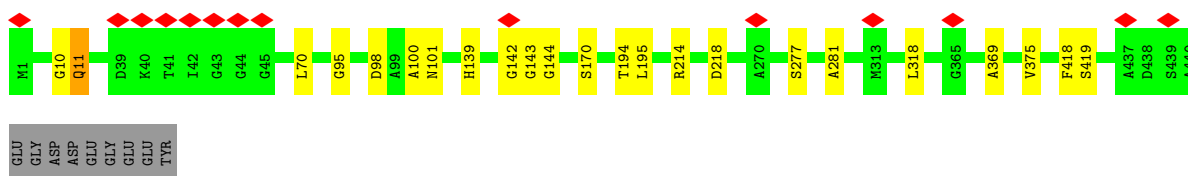
- Molecule 10: Ubiquitin-conjugating enzyme E2 D3



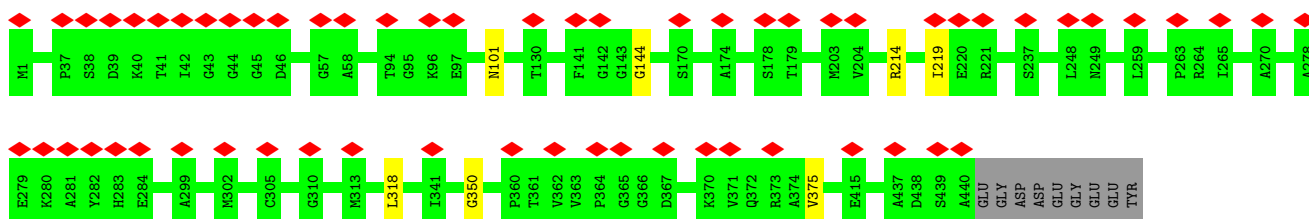
- Molecule 11: Tubulin alpha-1C chain



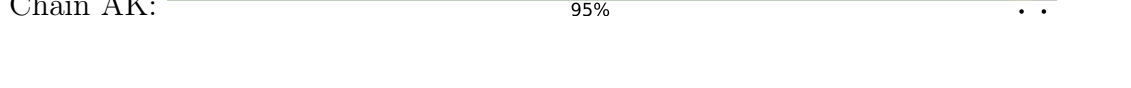
- Molecule 11: Tubulin alpha-1C chain

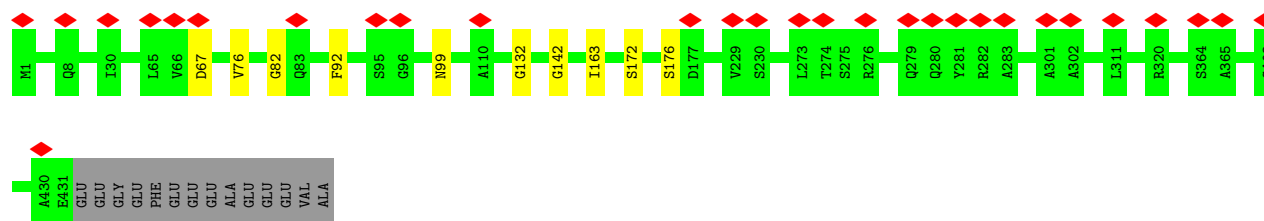


- Molecule 11: Tubulin alpha-1C chain

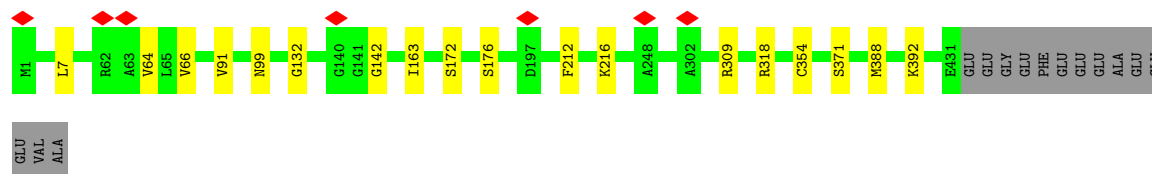


- Molecule 12: Tubulin beta-4B chain

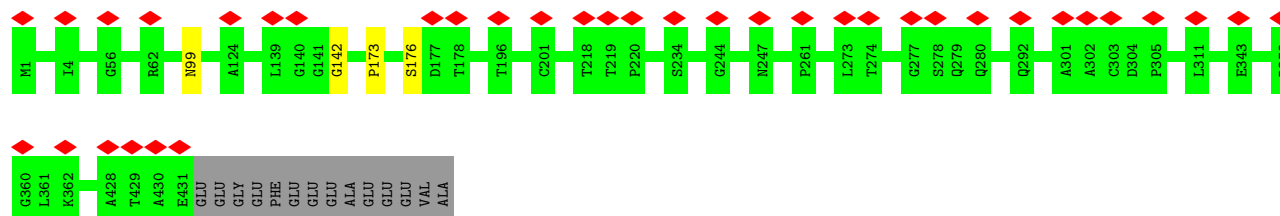




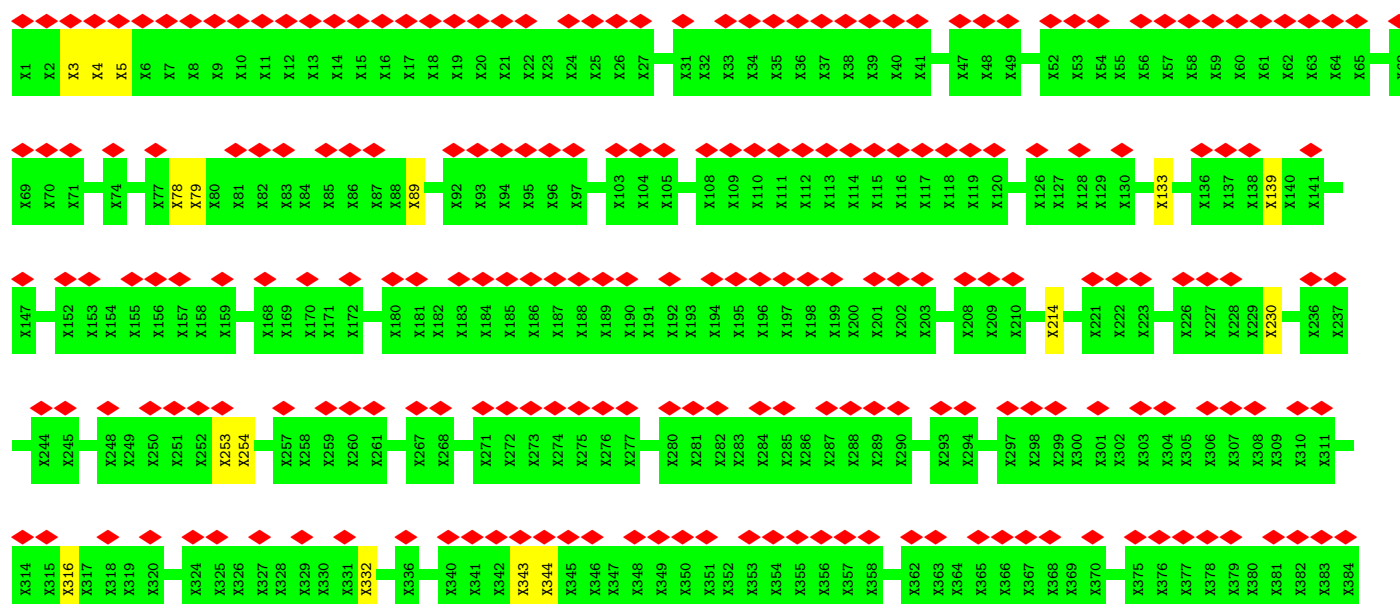
• Molecule 12: Tubulin beta-4B chain

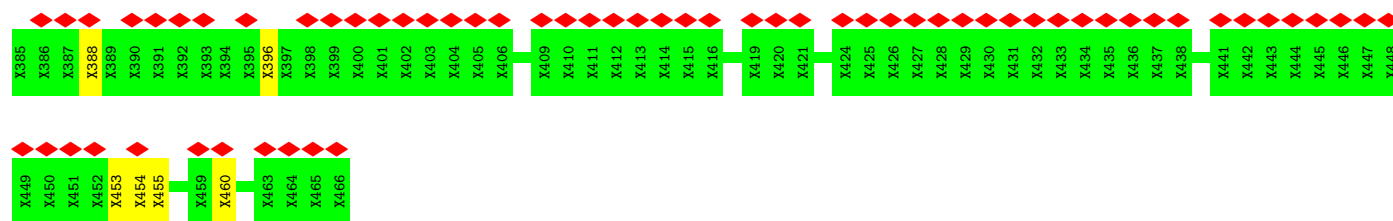


• Molecule 12: Tubulin beta-4B chain

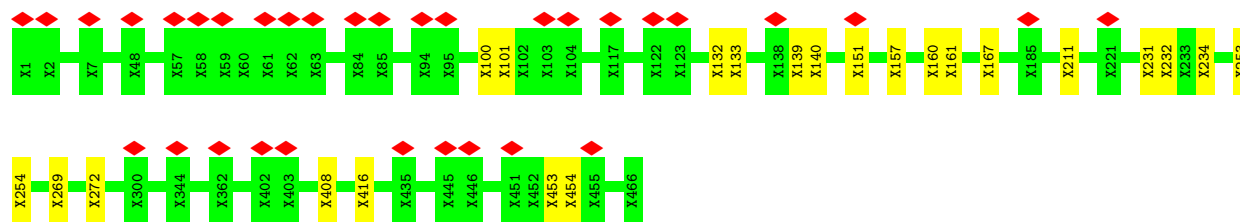


• Molecule 13: F-box/WD repeat-containing protein

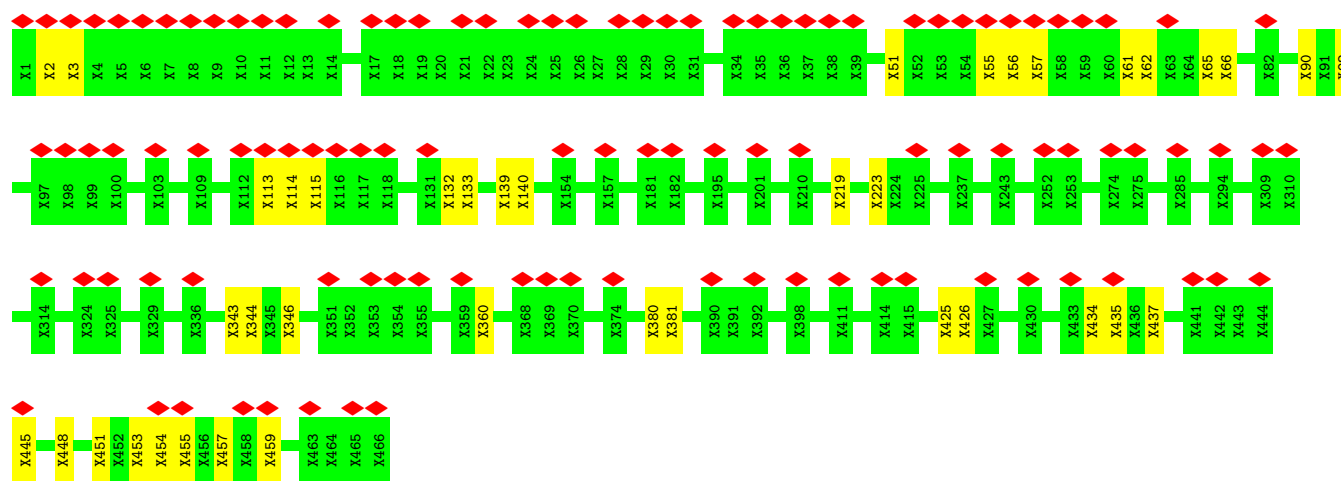
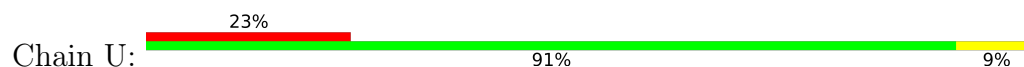




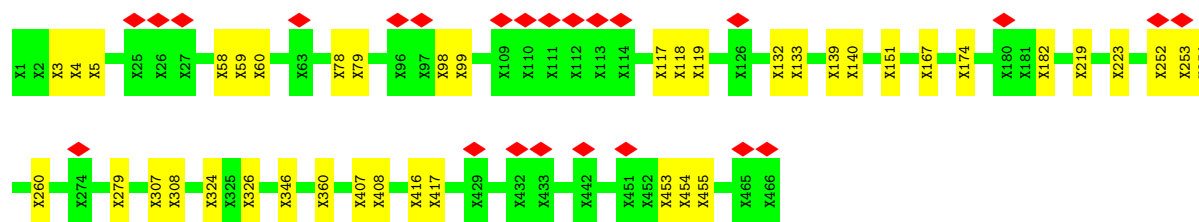
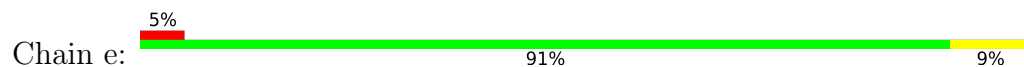
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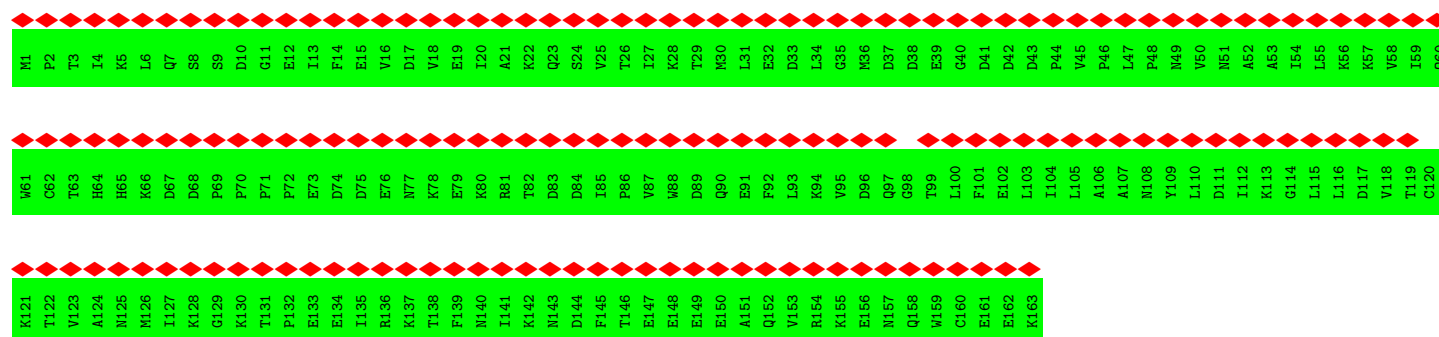
- Molecule 13: F-box/WD repeat-containing protein

Chain g:  90% 10%



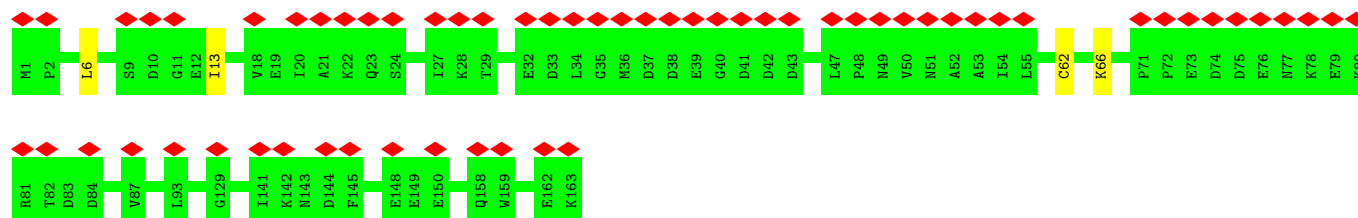
- Molecule 14: S-phase kinase-associated protein 1

Chain AM:  99% 100%



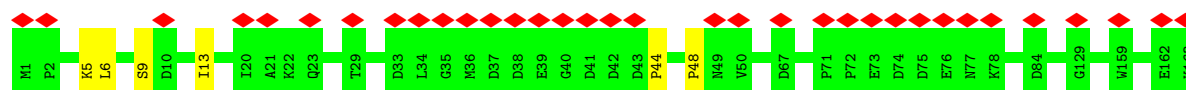
- Molecule 14: S-phase kinase-associated protein 1

Chain AO:  37% 98%



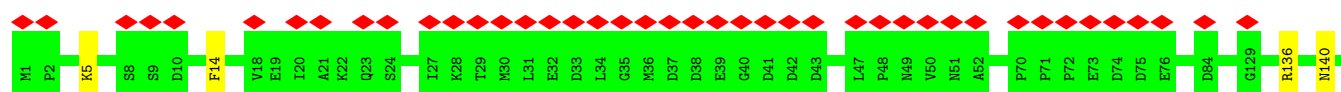
- Molecule 14: S-phase kinase-associated protein 1

Chain f:  21% 96%



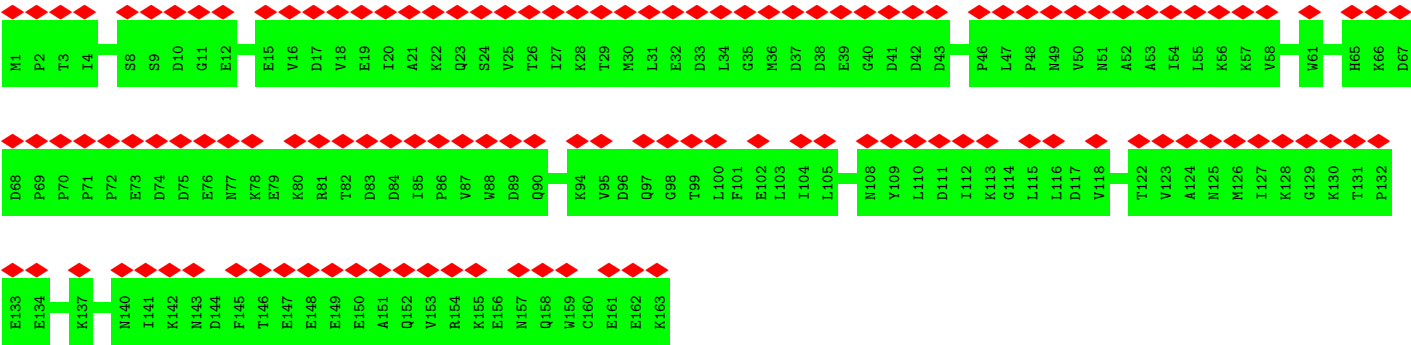
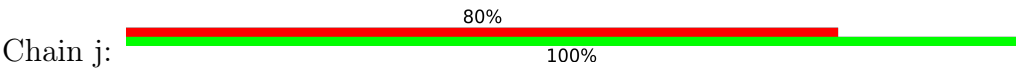
- Molecule 14: S-phase kinase-associated protein 1

Chain h:  27% 98%





• Molecule 14: S-phase kinase-associated protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	34451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	115	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.272	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	606.72, 606.72, 606.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.37, 2.37, 2.37	Depositor

5 Model quality

5.1 Standard geometry

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	0	0.28	0/672	0.41	0/935
1	S	0.31	0/672	0.45	0/935
2	1	0.28	0/3372	0.57	0/4697
2	2	0.14	0/3372	0.34	0/4697
2	3	0.14	0/3372	0.35	0/4697
2	A	0.34	0/3372	0.47	0/4697
2	B	0.33	0/3372	0.45	0/4697
2	C	0.24	0/3372	0.42	0/4697
2	D	0.24	0/3372	0.42	0/4697
2	E	0.21	0/3372	0.40	0/4697
2	F	0.20	0/3372	0.39	0/4697
2	G	0.36	0/3372	0.62	0/4697
2	H	0.28	0/3372	0.43	0/4697
2	I	0.31	0/3372	0.45	0/4697
2	J	0.34	0/3372	0.47	0/4697
2	K	0.14	0/3372	0.32	0/4697
2	L	0.15	0/3372	0.35	0/4697
2	m	0.33	0/3372	0.45	0/4697
2	s	0.33	0/3372	0.43	0/4697
2	t	0.29	0/3372	0.43	0/4697
2	u	0.34	0/3372	0.49	0/4697
2	v	0.23	0/3372	0.40	0/4697
2	w	0.23	0/3372	0.40	0/4697
2	x	0.35	0/3372	0.48	0/4697
2	y	0.29	0/3372	0.46	0/4697
2	z	0.23	0/3372	0.40	0/4697
3	4	0.29	0/4700	0.43	0/6551
3	7	0.24	0/4700	0.43	0/6551
3	M	0.36	1/4700 (0.0%)	0.49	0/6551
3	P	0.33	0/4700	0.47	0/6551
4	5	0.24	0/1810	0.42	0/2517
4	8	0.20	0/1810	0.43	0/2517
4	N	0.29	0/1810	0.46	0/2517
4	Q	0.27	0/1810	0.46	0/2517

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	6	0.32	0/591	0.45	0/824
5	9	0.21	0/441	0.44	0/614
5	O	0.35	0/591	0.44	0/824
5	R	0.32	0/441	0.58	0/614
6	AA	0.24	0/310	0.46	0/430
6	T	0.31	0/310	0.49	0/430
7	AE	0.19	0/4641	0.36	0/6475
7	AF	0.19	0/4195	0.39	0/5854
7	X	0.22	0/4641	0.39	0/6475
7	Y	0.22	0/4195	0.39	0/5854
8	AG	0.25	0/4793	0.42	0/6687
8	Z	0.26	0/4793	0.40	0/6687
8	n	0.23	0/4793	0.39	0/6687
9	AH	0.25	0/3125	0.40	0/4339
9	a	0.26	0/3125	0.42	0/4339
9	o	0.24	0/3125	0.40	0/4339
10	AI	0.37	0/728	0.49	0/1014
10	b	0.38	0/728	0.46	0/1014
10	p	0.35	0/728	0.45	0/1014
11	AJ	0.27	0/2166	0.39	0/3011
11	c	0.33	0/2166	0.44	0/3011
11	q	0.24	0/2166	0.36	0/3011
12	AK	0.30	0/2120	0.43	0/2946
12	d	0.38	0/2120	0.47	0/2946
12	r	0.26	0/2120	0.41	0/2946
14	AM	0.15	0/808	0.34	0/1126
14	AO	0.22	0/808	0.34	0/1126
14	f	0.27	0/808	0.38	0/1126
14	h	0.24	0/808	0.37	0/1126
14	j	0.18	0/808	0.33	0/1126
All	All	0.27	1/171504 (0.0%)	0.43	0/238885

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
2	1	0	2
2	G	0	1
2	J	0	1
7	AF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Z	0	1
8	n	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	876	MET	C-N	-6.18	1.23	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	129	ASP	Peptide
2	1	45	SER	Peptide
7	AF	933	PHE	Peptide
2	G	215	GLN	Peptide
2	J	509	GLY	Peptide
8	Z	248	ASP	Peptide
8	n	314	ILE	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	0	673	0	298	3	0
1	S	673	0	298	5	0
2	1	3373	0	1454	27	0
2	2	3373	0	1454	5	0
2	3	3373	0	1454	1	0
2	A	3373	0	1454	31	0
2	B	3373	0	1454	21	0
2	C	3373	0	1454	12	0
2	D	3373	0	1454	26	0
2	E	3373	0	1454	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3373	0	1454	14	0
2	G	3373	0	1454	41	0
2	H	3373	0	1454	18	0
2	I	3373	0	1454	30	0
2	J	3373	0	1454	41	0
2	K	3373	0	1454	3	0
2	L	3373	0	1454	10	0
2	m	3373	0	1454	21	0
2	s	3373	0	1454	31	0
2	t	3373	0	1454	25	0
2	u	3373	0	1454	37	0
2	v	3373	0	1454	24	0
2	w	3373	0	1454	16	0
2	x	3373	0	1454	40	0
2	y	3373	0	1454	27	0
2	z	3373	0	1454	12	0
3	4	4702	0	2048	21	0
3	7	4702	0	2048	6	0
3	M	4702	0	2048	33	0
3	P	4702	0	2048	18	0
4	5	1812	0	802	17	0
4	8	1812	0	802	13	0
4	N	1812	0	802	16	0
4	Q	1812	0	802	14	0
5	6	592	0	266	5	0
5	9	442	0	200	2	0
5	O	592	0	266	3	0
5	R	442	0	200	2	0
6	AA	311	0	140	2	0
6	T	311	0	140	4	0
7	AE	4643	0	2005	5	0
7	AF	4196	0	1802	7	0
7	X	4643	0	2005	8	0
7	Y	4196	0	1802	8	0
8	AG	4794	0	2077	8	0
8	Z	4794	0	2077	14	0
8	n	4794	0	2077	7	0
9	AH	3131	0	1365	18	0
9	a	3131	0	1365	17	0
9	o	3131	0	1365	13	0
10	AI	729	0	314	1	0
10	b	729	0	314	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	p	729	0	314	3	0
11	AJ	2167	0	1009	9	0
11	c	2167	0	1009	13	0
11	q	2167	0	1009	4	0
12	AK	2121	0	962	6	0
12	d	2121	0	962	9	0
12	r	2121	0	962	2	0
13	AL	2312	0	498	12	0
13	AN	2312	0	497	12	0
13	U	2312	0	505	22	0
13	e	2312	0	502	24	0
13	g	2312	0	505	25	0
14	AM	809	0	345	0	0
14	AO	809	0	345	2	0
14	f	809	0	345	3	0
14	h	809	0	345	2	0
14	j	809	0	345	0	0
All	All	183153	0	77131	947	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 4.

All (947) 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)
4:5:393:ALA:HB2	4:5:432:ALA:O	1.81	0.80
2:x:271:ALA:HB2	2:x:278:GLU:N	2.03	0.74
9:a:458:SER:HA	9:a:512:ALA:HB2	1.74	0.70
3:M:566:GLN:HA	3:M:591:LEU:HA	1.75	0.69
2:u:271:ALA:HB2	2:u:278:GLU:N	2.09	0.67
8:Z:249:LYS:HA	8:Z:252:ALA:HB3	1.77	0.67
2:B:153:VAL:HA	2:B:249:ALA:HB3	1.77	0.64
4:5:393:ALA:HB3	4:5:405:GLY:HA3	1.80	0.64
2:x:46:PRO:HA	2:x:60:LYS:HA	1.82	0.62
13:e:346:UNK:HA	13:e:360:UNK:C	2.30	0.61
2:E:46:PRO:HA	2:E:60:LYS:HA	1.81	0.61
3:4:566:GLN:HA	3:4:591:LEU:HA	1.82	0.61
4:Q:534:ILE:O	4:Q:547:GLN:HA	2.02	0.59
2:u:116:ILE:HA	2:u:184:THR:O	2.02	0.59
2:w:46:PRO:HA	2:w:60:LYS:HA	1.85	0.59
2:y:494:SER:N	2:y:575:ILE:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:46:PRO:HA	2:H:60:LYS:HA	1.85	0.59
11:c:281:ALA:HB2	11:c:369:ALA:HB1	1.85	0.58
2:y:46:PRO:HA	2:y:60:LYS:HA	1.84	0.58
2:t:268:VAL:HA	2:t:280:PRO:HA	1.83	0.58
2:D:42:ILE:O	2:D:64:VAL:HA	2.04	0.58
2:G:306:TYR:O	2:G:666:ALA:HB1	2.02	0.58
13:g:231:UNK:O	13:g:232:UNK:C	2.51	0.58
3:M:728:GLU:HA	3:M:755:LEU:HA	1.84	0.58
2:G:414:LYS:HA	2:G:419:ASP:HA	1.84	0.58
4:5:393:ALA:HB3	4:5:405:GLY:CA	2.33	0.58
2:B:356:ALA:HB3	2:B:359:LYS:O	2.04	0.58
2:G:307:LEU:O	2:G:333:LYS:HA	2.05	0.57
2:u:46:PRO:HA	2:u:60:LYS:O	2.04	0.57
2:G:494:SER:N	2:G:575:ILE:O	2.37	0.57
9:AH:456:GLY:HA3	9:AH:462:ALA:HA	1.87	0.57
2:C:46:PRO:HA	2:C:60:LYS:HA	1.87	0.57
11:c:101:ASN:HA	11:c:144:GLY:HA3	1.88	0.56
9:AH:682:LYS:HA	9:AH:685:ALA:HB2	1.88	0.56
2:J:617:ILE:O	2:J:648:PHE:HA	2.06	0.56
2:t:46:PRO:HA	2:t:60:LYS:HA	1.87	0.56
2:J:153:VAL:HA	2:J:249:ALA:HB3	1.88	0.56
2:I:494:SER:N	2:I:575:ILE:O	2.39	0.55
13:AN:231:UNK:O	13:AN:232:UNK:C	2.55	0.55
8:Z:921:ASN:HA	8:Z:950:ALA:HB3	1.88	0.55
13:AN:132:UNK:O	13:AN:140:UNK:HA	2.06	0.55
2:J:212:TYR:HA	2:J:222:GLU:O	2.07	0.55
2:J:46:PRO:O	2:J:60:LYS:N	2.39	0.55
3:M:144:HIS:HA	3:M:268:THR:O	2.07	0.55
9:a:442:SER:HA	9:a:448:ARG:HA	1.89	0.55
13:U:425:UNK:O	13:U:426:UNK:C	2.55	0.55
2:s:429:GLY:O	2:s:460:PHE:HA	2.06	0.55
4:5:370:VAL:O	4:5:380:GLU:HA	2.06	0.54
2:x:427:ILE:O	2:x:459:LEU:N	2.40	0.54
13:U:51:UNK:HA	13:U:57:UNK:CB	2.37	0.54
2:u:133:ASP:O	2:u:136:ALA:HB3	2.07	0.54
2:y:183:VAL:O	2:y:242:LYS:HA	2.08	0.54
9:AH:539:VAL:N	9:AH:561:GLY:HA3	2.23	0.54
3:4:899:GLN:HA	3:4:926:LEU:HA	1.89	0.54
2:x:492:LEU:O	2:x:575:ILE:N	2.40	0.54
3:M:657:MET:O	3:M:658:LYS:C	2.51	0.54
11:c:318:LEU:O	11:c:375:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AK:67:ASP:O	12:AK:92:PHE:HA	2.07	0.53
8:Z:448:GLU:O	8:Z:452:ASN:N	2.41	0.53
3:4:140:THR:HA	3:4:264:LEU:O	2.09	0.53
3:M:899:GLN:HA	3:M:926:LEU:HA	1.89	0.53
11:c:214:ARG:O	11:c:218:ASP:HA	2.09	0.53
2:x:493:ALA:HA	2:x:575:ILE:O	2.08	0.53
2:A:427:ILE:O	2:A:459:LEU:N	2.42	0.53
5:O:69:GLU:O	5:O:73:GLN:N	2.41	0.53
9:a:224:ASN:O	9:a:228:PRO:HA	2.09	0.53
4:5:477:SER:O	4:5:480:GLU:O	2.26	0.52
2:G:45:SER:O	2:G:59:GLY:O	2.27	0.52
4:N:451:LEU:O	4:N:464:GLU:HA	2.09	0.52
2:I:447:PHE:O	2:I:450:ALA:HB3	2.09	0.52
2:t:424:ARG:HA	2:t:454:GLN:O	2.09	0.52
11:AJ:101:ASN:HA	11:AJ:144:GLY:CA	2.40	0.52
2:G:215:GLN:O	2:G:217:GLY:N	2.43	0.52
13:AL:316:UNK:HA	13:AL:332:UNK:O	2.09	0.52
2:I:554:ILE:O	2:I:555:SER:C	2.53	0.52
9:a:33:GLU:O	9:a:37:HIS:HA	2.09	0.52
13:g:157:UNK:O	13:g:161:UNK:N	2.42	0.52
8:n:249:LYS:HA	8:n:252:ALA:HB3	1.91	0.52
9:o:33:GLU:O	9:o:37:HIS:HA	2.09	0.52
2:u:617:ILE:O	2:u:648:PHE:HA	2.09	0.52
3:4:958:LEU:O	3:4:986:LEU:HA	2.09	0.52
13:AN:453:UNK:O	13:AN:454:UNK:C	2.58	0.52
13:U:219:UNK:O	13:U:223:UNK:HA	2.10	0.52
2:u:41:THR:HA	2:u:65:VAL:O	2.10	0.52
2:v:46:PRO:HA	2:v:60:LYS:HA	1.92	0.52
13:U:2:UNK:O	13:U:3:UNK:C	2.58	0.52
2:1:46:PRO:HA	2:1:60:LYS:C	2.35	0.52
2:G:262:SER:HA	2:G:287:MET:HA	1.91	0.52
3:M:870:THR:HA	3:M:898:LEU:HA	1.92	0.52
1:S:3:SER:N	1:S:77:VAL:O	2.43	0.52
2:I:37:CYS:HA	2:I:97:CYS:HA	1.92	0.51
2:y:429:GLY:O	2:y:460:PHE:HA	2.10	0.51
2:B:454:GLN:O	2:B:455:ALA:C	2.53	0.51
2:I:302:PRO:HA	2:I:670:ARG:HA	1.93	0.51
2:J:427:ILE:O	2:J:459:LEU:N	2.43	0.51
3:M:672:GLN:HA	3:M:698:LEU:HA	1.93	0.51
8:Z:315:PRO:O	8:Z:316:VAL:C	2.53	0.51
2:B:579:PHE:HA	2:B:601:TYR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:VAL:O	2:C:488:PHE:HA	2.10	0.51
2:A:181:MET:N	2:A:245:PHE:O	2.43	0.51
2:J:46:PRO:HA	2:J:60:LYS:HA	1.91	0.51
9:o:202:ALA:HB3	9:o:278:GLU:CB	2.40	0.51
2:1:180:GLN:HA	2:1:246:TYR:HA	1.92	0.51
2:J:206:ALA:HB1	2:J:226:GLY:O	2.09	0.51
2:z:268:VAL:HA	2:z:280:PRO:HA	1.92	0.51
2:D:271:ALA:HB2	2:D:278:GLU:N	2.26	0.51
2:s:356:ALA:HB3	2:s:359:LYS:O	2.10	0.51
2:s:579:PHE:HA	2:s:601:TYR:H	1.75	0.51
2:E:46:PRO:O	2:E:60:LYS:N	2.44	0.51
7:Y:850:ALA:HB1	7:Y:880:ALA:HB2	1.91	0.51
2:u:98:PRO:O	2:u:100:GLN:N	2.44	0.51
2:A:254:SER:O	2:A:257:PHE:O	2.28	0.51
7:AE:8:PHE:O	7:AE:9:GLY:C	2.53	0.50
2:t:478:THR:H	2:t:488:PHE:HA	1.75	0.50
2:B:494:SER:N	2:B:575:ILE:O	2.44	0.50
2:L:39:SER:HA	2:L:68:SER:HA	1.92	0.50
4:Q:316:ILE:O	4:Q:334:HIS:HA	2.10	0.50
4:5:453:CYS:O	4:5:461:VAL:HA	2.11	0.50
9:AH:453:GLY:O	9:AH:465:LEU:HA	2.11	0.50
2:C:617:ILE:O	2:C:648:PHE:HA	2.12	0.50
2:I:51:HIS:O	2:I:75:ALA:HA	2.11	0.50
13:U:343:UNK:O	13:U:344:UNK:C	2.59	0.50
2:s:626:ASN:C	2:s:628:THR:H	2.19	0.50
2:B:427:ILE:O	2:B:459:LEU:N	2.45	0.50
2:D:43:ARG:HA	2:D:63:THR:O	2.12	0.50
2:E:454:GLN:O	2:E:455:ALA:C	2.55	0.50
2:u:212:TYR:HA	2:u:222:GLU:O	2.12	0.50
13:U:346:UNK:HA	13:U:360:UNK:O	2.11	0.50
13:g:132:UNK:O	13:g:140:UNK:HA	2.11	0.50
3:4:927:LYS:HA	3:4:955:LEU:HA	1.92	0.50
2:J:62:ASP:O	2:x:132:SER:HA	2.11	0.50
2:J:153:VAL:HA	2:J:249:ALA:O	2.12	0.50
2:E:116:ILE:HA	2:E:184:THR:O	2.12	0.50
2:F:268:VAL:HA	2:F:280:PRO:HA	1.94	0.50
2:w:50:ILE:N	2:w:57:ILE:O	2.45	0.50
13:U:90:UNK:HA	13:U:459:UNK:O	2.11	0.50
2:u:115:GLU:O	2:u:185:VAL:HA	2.11	0.50
2:v:153:VAL:HA	2:v:249:ALA:HB3	1.94	0.50
9:a:322:ALA:HB1	9:a:327:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:132:GLY:HA3	12:d:163:ILE:O	2.12	0.50
2:m:476:VAL:O	2:m:488:PHE:HA	2.12	0.50
2:C:579:PHE:HA	2:C:601:TYR:H	1.77	0.49
2:u:356:ALA:HB3	2:u:359:LYS:O	2.12	0.49
14:AO:6:LEU:O	14:AO:13:ILE:HA	2.12	0.49
3:M:966:THR:HA	3:M:992:ASP:O	2.12	0.49
2:1:47:ARG:N	2:1:60:LYS:HA	2.27	0.49
2:t:153:VAL:HA	2:t:249:ALA:O	2.12	0.49
2:y:492:LEU:O	2:y:575:ILE:N	2.45	0.49
13:AL:3:UNK:O	13:AL:4:UNK:C	2.59	0.49
2:D:262:SER:HA	2:D:286:VAL:O	2.13	0.49
4:8:155:PRO:O	4:8:156:GLN:C	2.55	0.49
2:x:153:VAL:HA	2:x:249:ALA:HB3	1.93	0.49
2:z:494:SER:N	2:z:575:ILE:O	2.45	0.49
2:C:447:PHE:O	2:C:450:ALA:HB3	2.13	0.49
13:g:407:UNK:HA	13:g:417:UNK:O	2.13	0.49
2:w:262:SER:HA	2:w:286:VAL:O	2.12	0.49
2:1:261:ILE:O	2:1:288:PHE:N	2.46	0.49
2:D:46:PRO:HA	2:D:60:LYS:O	2.13	0.49
2:I:42:ILE:O	2:I:64:VAL:HA	2.13	0.49
2:x:307:LEU:O	2:x:334:VAL:N	2.46	0.49
9:AH:465:LEU:O	9:AH:539:VAL:HA	2.13	0.49
13:AL:253:UNK:O	13:AL:254:UNK:C	2.61	0.49
3:P:1055:ASN:O	3:P:1056:TRP:C	2.56	0.49
13:g:367:UNK:O	13:g:374:UNK:HA	2.13	0.49
8:n:350:LEU:O	8:n:354:GLU:N	2.46	0.49
2:v:429:GLY:O	2:v:460:PHE:HA	2.13	0.49
2:A:506:GLN:HA	2:A:511:GLY:H	1.78	0.49
12:AK:132:GLY:HA3	12:AK:163:ILE:O	2.12	0.49
4:N:450:CYS:HA	4:N:465:HIS:O	2.13	0.49
2:z:302:PRO:HA	2:z:670:ARG:HA	1.95	0.49
2:1:97:CYS:O	2:1:101:GLU:HA	2.14	0.48
2:F:46:PRO:HA	2:F:60:LYS:HA	1.94	0.48
2:y:442:LYS:O	2:y:443:GLY:C	2.55	0.48
2:1:44:GLY:O	2:1:62:ASP:HA	2.13	0.48
4:8:316:ILE:O	4:8:334:HIS:HA	2.13	0.48
2:C:478:THR:H	2:C:488:PHE:HA	1.78	0.48
2:H:150:ILE:HA	2:H:289:ARG:O	2.13	0.48
2:J:130:MET:O	2:x:62:ASP:O	2.32	0.48
12:d:66:VAL:HA	12:d:91:VAL:O	2.13	0.48
2:s:263:LEU:O	2:s:285:THR:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:179:SER:O	2:y:246:TYR:HA	2.13	0.48
2:2:617:ILE:O	2:2:648:PHE:HA	2.13	0.48
2:A:442:LYS:O	2:A:443:GLY:C	2.54	0.48
2:A:494:SER:N	2:A:575:ILE:O	2.46	0.48
2:A:579:PHE:HA	2:A:601:TYR:N	2.29	0.48
4:Q:432:ALA:O	4:Q:433:ARG:C	2.56	0.48
11:c:281:ALA:HB2	11:c:369:ALA:CB	2.43	0.48
2:G:46:PRO:HA	2:G:60:LYS:O	2.12	0.48
2:z:212:TYR:HA	2:z:222:GLU:O	2.14	0.48
7:X:5:ILE:O	7:X:6:SER:C	2.55	0.48
2:x:181:MET:O	2:x:245:PHE:N	2.46	0.48
2:A:49:LEU:HA	2:A:58:ALA:HA	1.96	0.48
2:A:212:TYR:HA	2:A:222:GLU:O	2.13	0.48
2:I:427:ILE:O	2:I:459:LEU:N	2.46	0.48
2:J:179:SER:O	2:J:246:TYR:HA	2.13	0.48
3:P:1015:ILE:O	3:P:1042:ILE:HA	2.13	0.48
2:m:46:PRO:C	2:m:60:LYS:HA	2.38	0.48
2:G:356:ALA:HB3	2:G:359:LYS:O	2.12	0.48
12:d:309:ARG:O	12:d:371:SER:HA	2.14	0.48
4:5:451:LEU:O	4:5:464:GLU:HA	2.13	0.48
5:6:45:LEU:O	5:6:90:THR:HA	2.13	0.48
2:A:349:MET:HA	2:A:365:LEU:O	2.14	0.48
13:AL:343:UNK:O	13:AL:344:UNK:C	2.61	0.48
4:N:367:GLY:HA3	4:N:385:PRO:HA	1.95	0.48
9:a:721:PHE:O	9:a:722:ARG:C	2.57	0.48
13:g:166:UNK:HA	13:g:171:UNK:O	2.14	0.48
2:B:314:GLN:O	2:B:315:GLY:C	2.57	0.48
2:J:579:PHE:HA	2:J:600:PRO:HA	1.95	0.48
2:t:617:ILE:O	2:t:648:PHE:HA	2.14	0.48
3:M:958:LEU:O	3:M:986:LEU:HA	2.14	0.48
4:N:370:VAL:O	4:N:380:GLU:HA	2.14	0.48
9:a:539:VAL:N	9:a:561:GLY:HA3	2.29	0.48
12:d:172:SER:O	12:d:176:SER:N	2.47	0.48
2:y:182:ASN:HA	2:y:243:GLU:O	2.14	0.48
11:AJ:318:LEU:O	11:AJ:375:VAL:HA	2.13	0.47
2:H:356:ALA:HB3	2:H:359:LYS:O	2.13	0.47
9:a:748:CYS:O	9:a:752:ARG:HA	2.14	0.47
13:e:133:UNK:HA	13:e:139:UNK:O	2.14	0.47
2:x:153:VAL:HA	2:x:249:ALA:O	2.14	0.47
2:x:306:TYR:O	2:x:666:ALA:HB1	2.14	0.47
2:y:116:ILE:HA	2:y:184:THR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AJ:214:ARG:O	11:AJ:218:ASP:HA	2.14	0.47
3:P:874:LEU:O	3:P:903:LEU:HA	2.14	0.47
12:d:7:LEU:HA	12:d:64:VAL:O	2.13	0.47
13:e:59:UNK:O	13:e:60:UNK:C	2.62	0.47
2:m:42:ILE:O	2:m:64:VAL:HA	2.13	0.47
4:5:452:ARG:HA	4:5:463:LEU:O	2.13	0.47
7:X:207:TRP:CB	7:X:212:ALA:HB2	2.44	0.47
2:m:617:ILE:O	2:m:648:PHE:HA	2.14	0.47
2:v:153:VAL:HA	2:v:249:ALA:O	2.14	0.47
1:0:3:SER:N	1:0:77:VAL:O	2.47	0.47
3:4:874:LEU:O	3:4:902:GLU:O	2.33	0.47
2:A:42:ILE:O	2:A:64:VAL:HA	2.13	0.47
8:AG:315:PRO:O	8:AG:316:VAL:C	2.56	0.47
2:J:7:LEU:O	2:J:27:LEU:HA	2.14	0.47
12:d:99:ASN:HA	12:d:142:GLY:HA3	1.96	0.47
2:w:82:PRO:HA	2:w:113:GLY:C	2.39	0.47
2:C:42:ILE:O	2:C:64:VAL:HA	2.14	0.47
2:D:424:ARG:HA	2:D:454:GLN:O	2.14	0.47
11:c:10:GLY:O	11:c:11:GLN:C	2.58	0.47
2:u:45:SER:N	2:u:59:GLY:O	2.47	0.47
2:x:46:PRO:HA	2:x:59:GLY:O	2.14	0.47
2:x:46:PRO:O	2:x:60:LYS:N	2.48	0.47
4:8:284:LEU:HA	4:8:578:HIS:O	2.15	0.47
2:B:492:LEU:O	2:B:575:ILE:N	2.47	0.47
2:J:115:GLU:O	2:J:185:VAL:HA	2.14	0.47
3:P:958:LEU:O	3:P:986:LEU:HA	2.15	0.47
4:Q:414:TRP:HA	4:Q:420:GLU:O	2.15	0.47
13:U:133:UNK:HA	13:U:139:UNK:O	2.14	0.47
2:z:429:GLY:N	2:z:459:LEU:O	2.47	0.47
9:AH:33:GLU:O	9:AH:37:HIS:HA	2.15	0.47
13:AN:133:UNK:HA	13:AN:139:UNK:O	2.15	0.47
2:B:624:LYS:O	2:B:625:ILE:C	2.57	0.47
2:H:183:VAL:O	2:H:242:LYS:HA	2.14	0.47
2:H:424:ARG:HA	2:H:454:GLN:O	2.14	0.47
2:J:181:MET:O	2:J:245:PHE:N	2.48	0.47
8:AG:448:GLU:O	8:AG:452:ASN:N	2.48	0.47
9:AH:336:LEU:O	9:AH:344:ALA:HA	2.15	0.47
2:G:17:ALA:O	2:G:111:LEU:HA	2.15	0.47
2:H:454:GLN:O	2:H:455:ALA:C	2.58	0.47
3:M:699:LYS:HA	3:M:727:VAL:HA	1.96	0.47
4:N:477:SER:O	4:N:480:GLU:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:191:ALA:H	3:P:241:LYS:HA	1.79	0.47
13:e:453:UNK:O	13:e:454:UNK:C	2.61	0.47
13:g:248:UNK:O	13:g:261:UNK:HA	2.15	0.47
2:t:454:GLN:O	2:t:455:ALA:C	2.56	0.47
2:u:363:LEU:HA	2:u:387:GLY:O	2.15	0.47
2:w:46:PRO:O	2:w:60:LYS:N	2.47	0.47
12:AK:99:ASN:HA	12:AK:142:GLY:N	2.30	0.47
2:F:45:SER:O	2:F:59:GLY:HA3	2.14	0.47
2:G:150:ILE:HA	2:G:289:ARG:O	2.13	0.47
2:G:454:GLN:O	2:G:455:ALA:C	2.56	0.47
2:I:472:PHE:O	2:I:492:LEU:HA	2.14	0.47
13:U:132:UNK:O	13:U:140:UNK:HA	2.15	0.47
13:g:453:UNK:O	13:g:454:UNK:C	2.60	0.47
2:J:143:GLY:HA2	2:J:678:TRP:O	2.13	0.47
2:L:45:SER:O	2:L:59:GLY:O	2.32	0.47
13:e:408:UNK:O	13:e:416:UNK:HA	2.15	0.47
2:t:356:ALA:HB3	2:t:359:LYS:O	2.14	0.47
2:x:271:ALA:HB2	2:x:278:GLU:H	1.78	0.47
2:G:307:LEU:O	2:G:333:LYS:CA	2.63	0.46
8:Z:296:CYS:O	8:Z:297:LYS:C	2.58	0.46
2:u:170:GLU:O	2:u:171:GLY:C	2.58	0.46
3:7:929:LEU:O	3:7:958:LEU:HA	2.15	0.46
1:S:73:ILE:HA	1:S:87:TRP:O	2.15	0.46
2:G:212:TYR:HA	2:G:222:GLU:O	2.15	0.46
2:I:478:THR:H	2:I:488:PHE:HA	1.80	0.46
2:I:617:ILE:O	2:I:649:ILE:N	2.48	0.46
8:Z:90:GLY:C	8:Z:92:GLY:H	2.23	0.46
13:e:151:UNK:HA	13:e:167:UNK:HA	1.97	0.46
13:e:174:UNK:O	13:e:182:UNK:HA	2.15	0.46
13:g:346:UNK:HA	13:g:360:UNK:O	2.16	0.46
2:s:212:TYR:HA	2:s:222:GLU:O	2.15	0.46
2:1:477:PRO:HA	2:1:488:PHE:HA	1.97	0.46
2:A:493:ALA:HA	2:A:575:ILE:O	2.16	0.46
2:B:617:ILE:O	2:B:648:PHE:HA	2.15	0.46
3:M:508:GLU:O	3:M:512:GLU:N	2.49	0.46
2:t:494:SER:N	2:t:575:ILE:O	2.48	0.46
2:t:514:THR:HA	2:t:533:THR:HA	1.97	0.46
2:v:46:PRO:O	2:v:60:LYS:N	2.49	0.46
2:z:349:MET:HA	2:z:365:LEU:O	2.16	0.46
2:D:217:GLY:O	2:D:218:SER:O	2.34	0.46
2:E:424:ARG:HA	2:E:454:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:TRP:O	2:H:146:GLY:HA3	2.16	0.46
13:U:453:UNK:C	13:U:455:UNK:N	2.74	0.46
2:t:95:TYR:O	2:t:103:PRO:HA	2.16	0.46
2:v:478:THR:H	2:v:488:PHE:HA	1.81	0.46
2:A:116:ILE:HA	2:A:184:THR:O	2.15	0.46
2:D:97:CYS:O	2:D:101:GLU:HA	2.16	0.46
2:D:454:GLN:O	2:D:455:ALA:C	2.57	0.46
2:J:493:ALA:HA	2:J:575:ILE:O	2.16	0.46
13:U:114:UNK:O	13:U:115:UNK:C	2.63	0.46
13:U:448:UNK:O	13:U:455:UNK:HA	2.16	0.46
13:e:407:UNK:HA	13:e:417:UNK:O	2.16	0.46
2:m:454:GLN:O	2:m:455:ALA:C	2.58	0.46
2:u:268:VAL:HA	2:u:280:PRO:HA	1.97	0.46
4:8:281:PRO:HA	4:8:580:LYS:O	2.16	0.46
2:A:271:ALA:HB2	2:A:278:GLU:N	2.30	0.46
6:AA:59:THR:HA	6:AA:65:LEU:O	2.15	0.46
10:AI:39:GLY:HA3	10:AI:45:TYR:O	2.16	0.46
13:AL:388:UNK:HA	13:AL:396:UNK:O	2.16	0.46
2:B:119:GLU:N	2:B:182:ASN:O	2.49	0.46
2:G:493:ALA:HA	2:G:575:ILE:O	2.16	0.46
3:P:681:VAL:O	3:P:682:VAL:C	2.59	0.46
9:a:323:CYS:O	9:a:327:GLY:HA2	2.15	0.46
2:m:115:GLU:O	2:m:185:VAL:HA	2.16	0.46
11:q:101:ASN:HA	11:q:144:GLY:HA3	1.96	0.46
2:s:493:ALA:HA	2:s:575:ILE:O	2.16	0.46
2:t:42:ILE:HA	2:t:93:VAL:HA	1.97	0.46
2:v:17:ALA:O	2:v:111:LEU:HA	2.15	0.46
3:4:672:GLN:HA	3:4:698:LEU:HA	1.96	0.46
13:AL:4:UNK:O	13:AL:5:UNK:C	2.64	0.46
2:F:211:VAL:O	2:F:223:LEU:HA	2.16	0.46
2:J:50:ILE:N	2:J:57:ILE:O	2.49	0.46
8:Z:619:GLY:O	8:Z:620:CYS:C	2.58	0.46
2:s:617:ILE:O	2:s:648:PHE:HA	2.16	0.46
2:u:45:SER:O	2:u:60:LYS:HA	2.16	0.46
2:v:506:GLN:HA	2:v:511:GLY:CA	2.46	0.46
13:AN:253:UNK:O	13:AN:254:UNK:C	2.64	0.45
2:C:494:SER:N	2:C:575:ILE:O	2.49	0.45
2:G:623:PRO:O	2:G:629:CYS:HA	2.16	0.45
2:I:499:PHE:O	2:I:500:GLU:C	2.59	0.45
3:M:874:LEU:O	3:M:902:GLU:O	2.34	0.45
5:O:32:ARG:O	5:O:33:PRO:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:212:PHE:O	12:d:216:LYS:HA	2.16	0.45
13:e:219:UNK:O	13:e:223:UNK:HA	2.16	0.45
13:g:253:UNK:O	13:g:254:UNK:C	2.63	0.45
2:B:268:VAL:HA	2:B:279:ILE:O	2.17	0.45
2:D:45:SER:N	2:D:59:GLY:O	2.50	0.45
2:G:180:GLN:HA	2:G:246:TYR:HA	1.99	0.45
2:I:454:GLN:O	2:I:455:ALA:C	2.60	0.45
4:N:453:CYS:O	4:N:461:VAL:HA	2.15	0.45
13:U:453:UNK:O	13:U:454:UNK:C	2.65	0.45
8:n:315:PRO:O	8:n:316:VAL:C	2.59	0.45
9:AH:723:PRO:O	9:AH:763:VAL:HA	2.16	0.45
13:AL:214:UNK:HA	13:AL:230:UNK:HA	1.97	0.45
2:I:268:VAL:HA	2:I:280:PRO:HA	1.98	0.45
2:J:43:ARG:HA	2:J:64:VAL:HA	1.99	0.45
3:M:322:GLN:O	3:M:323:LEU:C	2.59	0.45
3:P:760:LEU:O	3:P:788:ILE:O	2.35	0.45
1:S:42:LYS:O	1:S:87:TRP:HA	2.16	0.45
7:X:152:LYS:H	7:X:296:THR:HA	1.82	0.45
2:u:294:ILE:O	2:u:352:CYS:HA	2.16	0.45
3:4:699:LYS:HA	3:4:727:VAL:HA	1.97	0.45
2:G:307:LEU:O	2:G:334:VAL:N	2.50	0.45
4:N:534:ILE:O	4:N:547:GLN:HA	2.17	0.45
4:Q:301:VAL:O	4:Q:307:HIS:O	2.35	0.45
13:U:55:UNK:O	13:U:56:UNK:C	2.65	0.45
2:x:48:ILE:O	2:x:59:GLY:N	2.49	0.45
2:A:473:MET:HA	2:A:491:LEU:O	2.16	0.45
2:D:429:GLY:O	2:D:460:PHE:HA	2.17	0.45
13:g:170:UNK:O	13:g:187:UNK:HA	2.17	0.45
9:o:255:ILE:O	9:o:262:GLN:HA	2.17	0.45
9:o:724:VAL:O	9:o:731:ASN:HA	2.16	0.45
12:r:99:ASN:HA	12:r:142:GLY:N	2.31	0.45
2:u:492:LEU:O	2:u:575:ILE:N	2.50	0.45
2:w:180:GLN:HA	2:w:245:PHE:O	2.15	0.45
2:x:356:ALA:HB3	2:x:359:LYS:O	2.16	0.45
2:1:617:ILE:O	2:1:648:PHE:HA	2.17	0.45
7:AF:925:ALA:O	7:AF:926:PHE:O	2.34	0.45
11:AJ:101:ASN:HA	11:AJ:144:GLY:HA3	1.97	0.45
13:AN:157:UNK:O	13:AN:161:UNK:N	2.49	0.45
2:I:492:LEU:O	2:I:575:ILE:N	2.49	0.45
4:N:413:ILE:O	4:N:421:ILE:HA	2.16	0.45
5:6:32:ARG:O	5:6:33:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:847:ASN:C	3:7:875:THR:O	2.59	0.45
13:AN:211:UNK:C	13:AN:234:UNK:O	2.65	0.45
2:D:45:SER:O	2:D:60:LYS:HA	2.17	0.45
3:P:785:GLN:HA	3:P:812:LEU:HA	1.98	0.45
2:v:263:LEU:O	2:v:285:THR:HA	2.17	0.45
2:1:42:ILE:O	2:1:64:VAL:HA	2.17	0.45
2:A:623:PRO:O	2:A:629:CYS:HA	2.17	0.45
2:B:473:MET:HA	2:B:491:LEU:O	2.16	0.45
4:Q:367:GLY:HA2	4:Q:386:CYS:N	2.32	0.45
13:e:3:UNK:O	13:e:4:UNK:C	2.64	0.45
2:s:37:CYS:HA	2:s:97:CYS:HA	1.98	0.45
2:1:43:ARG:HA	2:1:63:THR:O	2.17	0.45
2:B:579:PHE:HA	2:B:601:TYR:N	2.31	0.45
2:G:624:LYS:HA	2:G:628:THR:C	2.41	0.45
11:c:98:ASP:C	11:c:100:ALA:H	2.25	0.45
13:e:58:UNK:O	13:e:59:UNK:C	2.65	0.45
2:m:494:SER:N	2:m:575:ILE:O	2.50	0.45
2:w:23:MET:O	2:w:78:ARG:HA	2.17	0.45
2:w:48:ILE:O	2:w:59:GLY:N	2.50	0.45
2:y:153:VAL:HA	2:y:249:ALA:HB3	1.99	0.45
2:y:427:ILE:O	2:y:459:LEU:N	2.50	0.45
3:7:565:PHE:C	3:7:567:GLU:H	2.24	0.45
2:E:48:ILE:O	2:E:59:GLY:N	2.50	0.45
2:F:308:CYS:HA	2:F:334:VAL:O	2.17	0.45
2:I:579:PHE:HA	2:I:601:TYR:H	1.82	0.45
2:J:214:SER:HA	2:J:220:ALA:O	2.17	0.45
3:M:681:VAL:O	3:M:682:VAL:C	2.60	0.45
2:s:30:SER:HA	2:s:33:ALA:HB3	1.99	0.45
2:1:46:PRO:HA	2:1:60:LYS:HA	1.99	0.44
13:AL:453:UNK:O	13:AL:454:UNK:C	2.65	0.44
2:E:262:SER:HA	2:E:286:VAL:O	2.17	0.44
2:G:313:LEU:O	2:G:314:GLN:C	2.60	0.44
2:I:23:MET:O	2:I:78:ARG:HA	2.16	0.44
10:b:39:GLY:C	10:b:46:GLN:HA	2.42	0.44
13:g:260:UNK:HA	13:g:279:UNK:O	2.17	0.44
2:t:116:ILE:HA	2:t:184:THR:O	2.18	0.44
2:z:39:SER:HA	2:z:68:SER:HA	1.98	0.44
2:1:49:LEU:HA	2:1:58:ALA:HA	1.99	0.44
4:8:444:THR:O	4:8:451:LEU:HA	2.18	0.44
2:G:116:ILE:HA	2:G:184:THR:O	2.18	0.44
9:a:456:GLY:CA	9:a:462:ALA:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:4:UNK:O	13:e:5:UNK:C	2.64	0.44
13:g:320:UNK:HA	13:g:328:UNK:O	2.17	0.44
2:m:7:LEU:O	2:m:27:LEU:HA	2.17	0.44
2:t:294:ILE:O	2:t:352:CYS:HA	2.17	0.44
2:x:41:THR:O	2:x:93:VAL:HA	2.17	0.44
2:y:617:ILE:O	2:y:648:PHE:HA	2.17	0.44
5:9:94:GLN:O	5:9:95:PRO:C	2.59	0.44
2:B:142:TRP:O	2:B:146:GLY:HA3	2.16	0.44
2:F:212:TYR:HA	2:F:222:GLU:O	2.17	0.44
2:J:39:SER:HA	2:J:68:SER:HA	1.98	0.44
4:N:514:LEU:H	4:N:529:GLY:HA2	1.81	0.44
13:U:434:UNK:O	13:U:435:UNK:C	2.65	0.44
8:Z:158:LEU:HA	8:Z:205:TYR:O	2.18	0.44
14:f:6:LEU:O	14:f:13:ILE:HA	2.17	0.44
2:s:142:TRP:O	2:s:146:GLY:HA3	2.17	0.44
2:s:454:GLN:O	2:s:455:ALA:C	2.61	0.44
2:y:7:LEU:O	2:y:27:LEU:HA	2.17	0.44
2:2:424:ARG:HA	2:2:454:GLN:O	2.17	0.44
2:D:264:SER:HA	2:D:284:ASP:O	2.18	0.44
2:E:37:CYS:HA	2:E:97:CYS:HA	2.00	0.44
2:G:661:ASP:O	2:G:662:VAL:C	2.61	0.44
9:a:725:THR:HA	9:a:730:HIS:O	2.18	0.44
13:e:132:UNK:O	13:e:140:UNK:HA	2.18	0.44
13:g:94:UNK:HA	13:g:456:UNK:HA	1.98	0.44
9:o:58:LEU:O	9:o:62:ASP:N	2.50	0.44
2:s:267:LEU:O	2:s:280:PRO:HA	2.17	0.44
2:x:267:LEU:O	2:x:280:PRO:HA	2.18	0.44
9:AH:224:ASN:O	9:AH:228:PRO:HA	2.18	0.44
2:D:602:PHE:O	2:D:603:PRO:C	2.60	0.44
2:J:623:PRO:O	2:J:629:CYS:HA	2.17	0.44
2:L:116:ILE:HA	2:L:184:THR:O	2.18	0.44
3:M:281:VAL:O	3:M:282:SER:C	2.60	0.44
3:M:847:ASN:C	3:M:849:CYS:H	2.26	0.44
3:P:566:GLN:HA	3:P:591:LEU:HA	2.00	0.44
9:o:748:CYS:O	9:o:752:ARG:HA	2.18	0.44
2:s:579:PHE:HA	2:s:601:TYR:N	2.33	0.44
2:u:43:ARG:N	2:u:92:LEU:O	2.51	0.44
2:w:212:TYR:HA	2:w:222:GLU:O	2.17	0.44
3:4:917:ALA:HB2	3:4:944:LEU:HA	1.98	0.44
5:6:69:GLU:O	5:6:73:GLN:N	2.51	0.44
2:A:261:ILE:O	2:A:288:PHE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:605:MET:O	2:A:607:GLN:N	2.50	0.44
9:AH:338:CYS:O	9:AH:342:ASP:HA	2.17	0.44
2:I:206:ALA:HB1	2:I:226:GLY:O	2.18	0.44
3:M:397:GLY:O	3:M:401:MET:N	2.51	0.44
13:e:98:UNK:O	13:e:99:UNK:C	2.66	0.44
13:g:265:UNK:C	13:g:267:UNK:N	2.81	0.44
2:m:349:MET:HA	2:m:365:LEU:O	2.18	0.44
2:t:476:VAL:O	2:t:488:PHE:HA	2.17	0.44
2:u:82:PRO:HA	2:u:113:GLY:C	2.43	0.44
2:v:130:MET:O	2:y:61:GLU:O	2.35	0.44
2:z:579:PHE:HA	2:z:599:ARG:O	2.17	0.44
4:5:413:ILE:O	4:5:421:ILE:HA	2.17	0.44
4:8:415:ASP:O	4:8:419:GLN:N	2.51	0.44
7:AE:404:GLY:O	7:AE:408:ASP:N	2.50	0.44
2:G:579:PHE:HA	2:G:601:TYR:H	1.83	0.44
3:M:1017:LEU:N	3:M:1043:ASP:O	2.51	0.44
7:X:411:VAL:HA	7:X:446:TYR:O	2.17	0.44
14:f:9:SER:HA	14:f:48:PRO:HA	1.99	0.44
14:h:136:ARG:O	14:h:140:ASN:N	2.51	0.44
2:u:42:ILE:O	2:u:64:VAL:HA	2.17	0.44
2:v:183:VAL:O	2:v:242:LYS:HA	2.17	0.44
2:1:48:ILE:H	2:1:60:LYS:CA	2.31	0.44
2:1:49:LEU:N	2:1:78:ARG:O	2.51	0.44
13:AN:100:UNK:O	13:AN:101:UNK:C	2.66	0.44
2:D:268:VAL:HA	2:D:280:PRO:HA	2.00	0.44
2:I:578:LEU:O	2:I:600:PRO:HA	2.18	0.44
2:J:42:ILE:HA	2:J:92:LEU:O	2.17	0.44
3:M:429:LEU:HA	3:M:442:PHE:HA	1.99	0.44
3:M:984:ASN:HA	3:M:1012:LEU:HA	1.99	0.44
4:N:284:LEU:HA	4:N:578:HIS:O	2.18	0.44
13:U:55:UNK:HA	13:U:113:UNK:HA	2.00	0.44
13:g:408:UNK:O	13:g:416:UNK:HA	2.17	0.44
2:s:46:PRO:HA	2:s:59:GLY:C	2.42	0.44
2:u:43:ARG:HA	2:u:63:THR:O	2.17	0.44
2:u:90:LYS:HA	2:u:109:LEU:O	2.17	0.44
2:v:212:TYR:HA	2:v:223:LEU:HA	2.00	0.44
2:1:311:LEU:O	2:1:312:GLN:C	2.61	0.44
2:F:259:GLY:O	2:F:289:ARG:HA	2.18	0.44
7:X:658:LYS:O	7:X:659:TYR:C	2.61	0.44
2:s:254:SER:O	2:s:257:PHE:O	2.35	0.44
2:x:50:ILE:N	2:x:57:ILE:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:17:ALA:O	2:y:111:LEU:HA	2.18	0.44
2:y:24:GLU:HA	2:y:77:VAL:O	2.18	0.44
2:z:170:GLU:O	2:z:171:GLY:C	2.61	0.44
7:AF:207:TRP:CB	7:AF:212:ALA:HB2	2.48	0.43
9:AH:254:ASN:HA	9:AH:264:ASN:HA	2.00	0.43
2:B:30:SER:HA	2:B:33:ALA:HB3	1.99	0.43
2:E:82:PRO:HA	2:E:113:GLY:HA3	1.99	0.43
2:E:183:VAL:O	2:E:242:LYS:HA	2.18	0.43
2:F:271:ALA:HB2	2:F:278:GLU:N	2.33	0.43
3:M:1017:LEU:O	3:M:1043:ASP:O	2.36	0.43
14:h:5:LYS:HA	14:h:14:PHE:O	2.18	0.43
2:u:602:PHE:O	2:u:603:PRO:C	2.61	0.43
2:y:454:GLN:O	2:y:455:ALA:C	2.61	0.43
4:5:406:PHE:O	4:5:432:ALA:HB3	2.18	0.43
2:D:101:GLU:O	2:D:102:VAL:C	2.60	0.43
4:Q:300:ALA:O	4:Q:308:VAL:HA	2.18	0.43
13:e:118:UNK:O	13:e:119:UNK:C	2.66	0.43
9:o:525:GLY:HA3	9:o:569:TRP:HA	2.00	0.43
2:t:254:SER:O	2:t:257:PHE:O	2.36	0.43
2:u:307:LEU:O	2:u:334:VAL:N	2.51	0.43
2:w:170:GLU:O	2:w:171:GLY:C	2.61	0.43
2:2:602:PHE:O	2:2:603:PRO:C	2.61	0.43
3:4:1055:ASN:O	3:4:1056:TRP:C	2.61	0.43
4:8:301:VAL:O	4:8:307:HIS:O	2.36	0.43
2:E:46:PRO:HA	2:E:59:GLY:O	2.18	0.43
2:I:473:MET:HA	2:I:491:LEU:O	2.18	0.43
2:K:179:SER:O	2:K:246:TYR:HA	2.18	0.43
6:T:60:CYS:O	6:T:64:GLY:HA2	2.19	0.43
13:g:59:UNK:O	13:g:60:UNK:C	2.66	0.43
2:s:153:VAL:HA	2:s:249:ALA:O	2.18	0.43
2:y:602:PHE:O	2:y:603:PRO:C	2.60	0.43
3:4:842:GLN:HA	3:4:869:LEU:HA	2.00	0.43
3:7:719:ALA:O	3:7:722:HIS:CB	2.66	0.43
2:A:617:ILE:O	2:A:649:ILE:N	2.50	0.43
2:I:153:VAL:HA	2:I:249:ALA:O	2.18	0.43
9:o:507:THR:O	9:o:508:ASN:C	2.62	0.43
2:s:182:ASN:HA	2:s:243:GLU:O	2.18	0.43
2:t:42:ILE:O	2:t:64:VAL:HA	2.18	0.43
2:v:49:LEU:HA	2:v:58:ALA:HA	2.00	0.43
2:x:424:ARG:HA	2:x:454:GLN:O	2.18	0.43
2:z:427:ILE:O	2:z:459:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:181:HIS:HA	9:AH:193:ASP:O	2.17	0.43
2:D:145:ASN:O	2:D:146:GLY:C	2.60	0.43
2:G:493:ALA:C	2:G:575:ILE:O	2.62	0.43
2:H:602:PHE:O	2:H:603:PRO:C	2.62	0.43
2:J:478:THR:H	2:J:488:PHE:HA	1.84	0.43
13:U:380:UNK:O	13:U:381:UNK:C	2.66	0.43
9:o:760:PRO:O	9:o:761:THR:C	2.61	0.43
2:s:492:LEU:O	2:s:575:ILE:N	2.51	0.43
2:y:46:PRO:HA	2:y:59:GLY:O	2.18	0.43
4:5:367:GLY:HA2	4:5:386:CYS:H	1.83	0.43
7:AE:5:ILE:O	7:AE:6:SER:C	2.60	0.43
2:G:21:VAL:HA	2:G:79:MET:O	2.19	0.43
2:H:494:SER:N	2:H:575:ILE:O	2.51	0.43
2:I:499:PHE:O	2:I:502:PHE:N	2.52	0.43
5:R:94:GLN:O	5:R:95:PRO:C	2.61	0.43
8:Z:163:SER:HA	8:Z:209:ALA:O	2.18	0.43
13:g:368:UNK:HA	13:g:373:UNK:O	2.19	0.43
2:1:580:CYS:N	2:1:599:ARG:O	2.52	0.43
4:5:271:ALA:HB3	4:5:276:GLU:HA	2.00	0.43
8:AG:583:TYR:HA	8:AG:612:ARG:O	2.18	0.43
2:D:356:ALA:HB3	2:D:359:LYS:O	2.19	0.43
2:J:116:ILE:HA	2:J:184:THR:O	2.17	0.43
2:J:117:SER:O	2:J:183:VAL:HA	2.18	0.43
4:N:354:ASN:C	4:N:356:ARG:H	2.26	0.43
7:Y:775:GLU:HA	7:Y:802:LEU:HA	1.99	0.43
2:s:153:VAL:HA	2:s:249:ALA:HB3	2.00	0.43
2:y:254:SER:O	2:y:257:PHE:O	2.36	0.43
4:5:414:TRP:HA	4:5:421:ILE:HA	2.01	0.43
12:AK:99:ASN:HA	12:AK:142:GLY:HA3	2.01	0.43
12:AK:172:SER:O	12:AK:176:SER:N	2.51	0.43
2:G:43:ARG:HA	2:G:63:THR:O	2.19	0.43
2:H:254:SER:O	2:H:257:PHE:O	2.36	0.43
2:I:349:MET:HA	2:I:365:LEU:O	2.19	0.43
2:J:356:ALA:HB3	2:J:359:LYS:O	2.19	0.43
2:J:494:SER:N	2:J:575:ILE:O	2.52	0.43
2:m:50:ILE:N	2:m:57:ILE:O	2.52	0.43
10:p:59:ASP:O	10:p:60:TYR:C	2.61	0.43
12:r:173:PRO:HA	12:r:176:SER:CB	2.48	0.43
2:s:447:PHE:O	2:s:450:ALA:HB3	2.17	0.43
2:y:476:VAL:O	2:y:488:PHE:HA	2.19	0.43
1:0:42:LYS:O	1:0:87:TRP:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:933:ASN:HA	3:4:962:ALA:O	2.19	0.43
2:A:454:GLN:O	2:A:455:ALA:C	2.61	0.43
2:G:579:PHE:HA	2:G:601:TYR:N	2.33	0.43
2:J:46:PRO:HA	2:J:59:GLY:O	2.19	0.43
3:M:133:GLN:O	3:M:136:PHE:O	2.37	0.43
5:O:93:GLY:O	5:O:94:GLN:C	2.59	0.43
3:P:144:HIS:O	3:P:287:LEU:HA	2.18	0.43
9:a:570:PRO:HA	9:a:580:TRP:HA	2.01	0.43
11:c:418:PHE:O	11:c:419:SER:C	2.62	0.43
13:g:265:UNK:O	13:g:266:UNK:C	2.67	0.43
13:g:454:UNK:O	13:g:455:UNK:C	2.67	0.43
2:m:294:ILE:O	2:m:352:CYS:HA	2.19	0.43
2:w:264:SER:HA	2:w:284:ASP:O	2.19	0.43
7:AF:889:LYS:HA	7:AF:915:THR:O	2.19	0.43
9:AH:748:CYS:O	9:AH:752:ARG:HA	2.19	0.43
12:AK:76:VAL:O	12:AK:82:GLY:HA3	2.18	0.43
2:D:212:TYR:HA	2:D:222:GLU:O	2.19	0.43
3:M:1023:TYR:O	3:M:1024:ALA:C	2.62	0.43
13:e:346:UNK:HA	13:e:360:UNK:O	2.19	0.43
2:t:195:TYR:HA	2:t:268:VAL:O	2.19	0.43
2:u:153:VAL:HA	2:u:249:ALA:HB3	2.01	0.43
2:1:45:SER:O	2:1:59:GLY:O	2.36	0.42
2:1:115:GLU:O	2:1:185:VAL:HA	2.19	0.42
2:2:370:VAL:O	2:2:371:SER:C	2.61	0.42
2:K:602:PHE:O	2:K:603:PRO:C	2.60	0.42
8:Z:506:GLN:HA	8:Z:531:LEU:HA	2.01	0.42
11:c:194:THR:O	11:c:195:LEU:C	2.62	0.42
13:e:252:UNK:C	13:e:254:UNK:N	2.81	0.42
8:n:910:ILE:O	8:n:914:ASN:N	2.52	0.42
9:o:571:GLU:O	9:o:578:LEU:HA	2.18	0.42
2:x:206:ALA:HB1	2:x:226:GLY:O	2.19	0.42
2:1:494:SER:O	2:1:576:PRO:HA	2.19	0.42
7:AE:658:LYS:O	7:AE:659:TYR:C	2.62	0.42
8:AG:607:GLN:HA	8:AG:632:VAL:HA	2.00	0.42
9:AH:458:SER:HA	9:AH:512:ALA:HB2	2.01	0.42
2:J:303:LEU:N	2:J:670:ARG:HA	2.34	0.42
4:Q:533:PHE:HA	4:Q:548:VAL:O	2.19	0.42
7:X:8:PHE:O	7:X:9:GLY:C	2.61	0.42
2:m:579:PHE:HA	2:m:599:ARG:O	2.19	0.42
8:n:851:ALA:HA	8:n:881:ALA:HB2	2.01	0.42
11:q:318:LEU:O	11:q:375:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:227:PRO:C	2:s:229:LYS:H	2.25	0.42
2:t:206:ALA:HB1	2:t:226:GLY:O	2.19	0.42
2:x:454:GLN:O	2:x:455:ALA:C	2.62	0.42
2:B:254:SER:O	2:B:257:PHE:O	2.37	0.42
2:G:45:SER:HA	2:G:62:ASP:HA	2.01	0.42
2:G:608:ILE:HA	2:G:616:GLY:O	2.19	0.42
2:J:267:LEU:O	2:J:280:PRO:HA	2.19	0.42
2:J:494:SER:O	2:J:576:PRO:HA	2.19	0.42
4:N:285:GLN:O	4:N:577:TYR:HA	2.19	0.42
9:o:260:ASP:O	9:o:261:SER:C	2.62	0.42
9:o:458:SER:HA	9:o:512:ALA:HB2	2.01	0.42
2:y:119:GLU:N	2:y:182:ASN:O	2.52	0.42
13:AL:133:UNK:HA	13:AL:139:UNK:O	2.20	0.42
13:AN:408:UNK:O	13:AN:416:UNK:HA	2.19	0.42
2:J:141:MET:O	2:J:146:GLY:O	2.38	0.42
2:L:39:SER:HA	2:L:69:MET:H	1.83	0.42
2:L:424:ARG:HA	2:L:454:GLN:O	2.20	0.42
8:Z:451:PHE:O	8:Z:452:ASN:C	2.63	0.42
12:d:318:ARG:HA	12:d:354:CYS:O	2.19	0.42
2:s:442:LYS:O	2:s:443:GLY:C	2.62	0.42
2:u:424:ARG:HA	2:u:454:GLN:O	2.18	0.42
2:x:42:ILE:O	2:x:64:VAL:HA	2.20	0.42
2:1:262:SER:HA	2:1:286:VAL:O	2.19	0.42
2:A:476:VAL:O	2:A:488:PHE:HA	2.19	0.42
2:B:447:PHE:O	2:B:450:ALA:HB3	2.20	0.42
2:C:267:LEU:O	2:C:280:PRO:HA	2.19	0.42
2:F:82:PRO:HA	2:F:113:GLY:C	2.45	0.42
2:L:38:LYS:O	2:L:69:MET:N	2.52	0.42
2:L:51:HIS:O	2:L:75:ALA:HA	2.19	0.42
3:M:240:TRP:C	3:M:242:ASP:H	2.27	0.42
3:P:1016:GLY:HA2	3:P:1043:ASP:O	2.19	0.42
7:Y:927:GLU:C	7:Y:929:SER:H	2.27	0.42
10:b:39:GLY:HA3	10:b:45:TYR:O	2.19	0.42
13:g:388:UNK:HA	13:g:396:UNK:O	2.18	0.42
2:m:63:THR:HA	2:u:130:MET:O	2.20	0.42
2:u:151:LEU:N	2:u:289:ARG:O	2.52	0.42
2:w:271:ALA:HB2	2:w:278:GLU:N	2.35	0.42
2:w:602:PHE:O	2:w:603:PRO:C	2.63	0.42
2:1:447:PHE:O	2:1:450:ALA:HB3	2.20	0.42
4:5:534:ILE:O	4:5:547:GLN:HA	2.20	0.42
7:AF:226:PHE:O	7:AF:273:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:448:ARG:O	9:AH:449:PRO:C	2.61	0.42
13:AL:89:UNK:O	13:AL:460:UNK:HA	2.19	0.42
2:C:263:LEU:O	2:C:285:THR:HA	2.20	0.42
2:G:306:TYR:O	2:G:666:ALA:CB	2.67	0.42
2:I:579:PHE:HA	2:I:599:ARG:O	2.20	0.42
2:J:444:LEU:O	2:J:445:ARG:C	2.62	0.42
3:M:431:GLN:HA	3:M:439:CYS:O	2.20	0.42
4:N:354:ASN:C	4:N:356:ARG:N	2.77	0.42
2:x:617:ILE:O	2:x:648:PHE:HA	2.19	0.42
4:5:482:TRP:HA	4:5:495:PHE:O	2.19	0.42
8:AG:851:ALA:HB1	8:AG:881:ALA:HB2	2.02	0.42
11:AJ:312:TYR:H	11:AJ:343:PHE:HA	1.84	0.42
2:G:95:TYR:O	2:G:103:PRO:HA	2.20	0.42
3:P:189:SER:HA	3:P:243:GLU:HA	2.02	0.42
3:P:281:VAL:O	3:P:282:SER:C	2.62	0.42
9:a:139:VAL:HA	9:a:199:ASN:O	2.20	0.42
12:d:388:MET:O	12:d:392:LYS:N	2.53	0.42
14:f:5:LYS:O	14:f:44:PRO:HA	2.20	0.42
11:q:214:ARG:HA	11:q:219:ILE:O	2.20	0.42
4:8:318:VAL:O	4:8:331:PRO:CB	2.67	0.42
2:F:46:PRO:HA	2:F:59:GLY:C	2.45	0.42
2:G:142:TRP:O	2:G:146:GLY:HA3	2.20	0.42
2:G:184:THR:HA	2:G:241:ARG:O	2.19	0.42
3:M:787:LEU:O	3:M:815:LEU:HA	2.20	0.42
4:N:513:ILE:HA	4:N:529:GLY:HA2	2.00	0.42
4:Q:537:HIS:HA	4:Q:543:ALA:O	2.19	0.42
7:Y:658:LYS:O	7:Y:659:TYR:C	2.63	0.42
13:e:253:UNK:O	13:e:254:UNK:C	2.65	0.42
13:e:260:UNK:HA	13:e:279:UNK:O	2.20	0.42
2:x:43:ARG:O	2:x:91:VAL:HA	2.20	0.42
4:8:414:TRP:HA	4:8:420:GLU:O	2.19	0.42
2:A:356:ALA:HB3	2:A:359:LYS:O	2.20	0.42
8:AG:163:SER:HA	8:AG:209:ALA:O	2.20	0.42
2:E:212:TYR:HA	2:E:222:GLU:O	2.20	0.42
2:J:263:LEU:O	2:J:285:THR:HA	2.19	0.42
8:Z:910:ILE:O	8:Z:914:ASN:N	2.53	0.42
9:a:741:PHE:C	9:a:744:GLN:H	2.27	0.42
13:e:307:UNK:O	13:e:308:UNK:C	2.67	0.42
2:s:45:SER:O	2:s:59:GLY:HA3	2.19	0.42
2:v:461:SER:O	2:v:467:GLY:HA2	2.20	0.42
2:x:97:CYS:O	2:x:98:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:170:GLU:O	2:x:171:GLY:C	2.62	0.42
2:x:212:TYR:HA	2:x:223:LEU:HA	2.01	0.42
2:z:6:SER:HA	2:z:26:THR:O	2.20	0.42
2:z:478:THR:H	2:z:488:PHE:HA	1.83	0.42
3:4:844:LEU:O	3:4:872:LEU:HA	2.19	0.42
11:AJ:317:LEU:O	11:AJ:353:VAL:HA	2.19	0.42
2:B:623:PRO:O	2:B:629:CYS:HA	2.20	0.42
2:C:424:ARG:HA	2:C:454:GLN:O	2.20	0.42
2:E:46:PRO:O	2:E:59:GLY:C	2.63	0.42
2:F:478:THR:H	2:F:488:PHE:HA	1.85	0.42
3:M:570:LEU:O	3:M:596:VAL:HA	2.20	0.42
3:M:929:LEU:O	3:M:958:LEU:HA	2.19	0.42
11:c:70:LEU:O	11:c:95:GLY:C	2.63	0.42
2:u:50:ILE:O	2:u:57:ILE:O	2.38	0.42
2:x:44:GLY:O	2:x:62:ASP:HA	2.19	0.42
2:A:311:LEU:O	2:A:312:GLN:C	2.63	0.41
8:AG:910:ILE:O	8:AG:914:ASN:N	2.53	0.41
4:Q:370:VAL:O	4:Q:380:GLU:HA	2.20	0.41
7:X:3:SER:O	7:X:4:PHE:C	2.63	0.41
13:e:454:UNK:O	13:e:455:UNK:C	2.68	0.41
2:v:98:PRO:C	2:v:100:GLN:H	2.28	0.41
13:AL:454:UNK:O	13:AL:455:UNK:C	2.69	0.41
2:D:51:HIS:O	2:D:76:LEU:N	2.53	0.41
2:E:50:ILE:N	2:E:57:ILE:O	2.53	0.41
2:G:48:ILE:O	2:G:60:LYS:N	2.53	0.41
2:J:271:ALA:HB1	2:J:276:ILE:O	2.20	0.41
5:R:98:GLN:O	5:R:102:LYS:N	2.53	0.41
2:m:492:LEU:O	2:m:575:ILE:N	2.53	0.41
2:t:579:PHE:HA	2:t:601:TYR:H	1.85	0.41
2:v:478:THR:O	2:v:487:ASP:O	2.38	0.41
2:w:179:SER:O	2:w:246:TYR:HA	2.20	0.41
2:w:294:ILE:O	2:w:352:CYS:HA	2.20	0.41
2:x:142:TRP:O	2:x:146:GLY:HA3	2.19	0.41
2:x:579:PHE:HA	2:x:601:TYR:H	1.85	0.41
2:y:90:LYS:HA	2:y:109:LEU:O	2.20	0.41
2:1:93:VAL:O	2:1:106:THR:HA	2.20	0.41
2:1:562:LYS:O	2:1:566:GLY:N	2.54	0.41
2:2:179:SER:O	2:2:246:TYR:HA	2.20	0.41
3:4:728:GLU:HA	3:4:755:LEU:HA	2.03	0.41
13:AN:151:UNK:HA	13:AN:167:UNK:HA	2.02	0.41
14:AO:62:CYS:O	14:AO:66:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:VAL:O	2:F:242:LYS:HA	2.20	0.41
2:J:222:GLU:O	2:J:224:VAL:N	2.53	0.41
3:M:885:LYS:O	3:M:886:LEU:C	2.63	0.41
3:P:1055:ASN:O	3:P:1058:LYS:N	2.54	0.41
2:m:412:PRO:HA	2:m:423:GLY:N	2.35	0.41
10:p:39:GLY:O	10:p:40:PRO:C	2.62	0.41
2:s:579:PHE:HA	2:s:600:PRO:HA	2.02	0.41
2:y:212:TYR:HA	2:y:222:GLU:O	2.20	0.41
6:AA:43:HIS:N	6:AA:59:THR:O	2.53	0.41
7:AE:148:MET:HA	7:AE:273:LEU:O	2.20	0.41
7:AF:832:GLU:HA	7:AF:859:LEU:HA	2.01	0.41
9:AH:719:LEU:O	9:AH:720:VAL:C	2.63	0.41
2:E:473:MET:HA	2:E:491:LEU:O	2.20	0.41
2:G:42:ILE:O	2:G:64:VAL:HA	2.21	0.41
2:G:259:GLY:O	2:G:289:ARG:HA	2.21	0.41
7:Y:925:ALA:O	7:Y:926:PHE:O	2.38	0.41
2:m:150:ILE:HA	2:m:289:ARG:O	2.20	0.41
2:m:473:MET:HA	2:m:491:LEU:O	2.20	0.41
2:t:50:ILE:N	2:t:57:ILE:O	2.53	0.41
2:x:37:CYS:HA	2:x:96:PHE:O	2.20	0.41
2:x:579:PHE:HA	2:x:600:PRO:HA	2.02	0.41
3:4:681:VAL:O	3:4:682:VAL:C	2.62	0.41
4:8:438:LYS:O	4:8:439:ASP:C	2.64	0.41
2:A:343:LYS:O	2:A:344:TRP:C	2.62	0.41
2:B:294:ILE:O	2:B:352:CYS:HA	2.19	0.41
2:D:211:VAL:O	2:D:223:LEU:HA	2.20	0.41
2:E:30:SER:HA	2:E:33:ALA:HB3	2.01	0.41
2:E:579:PHE:HA	2:E:599:ARG:O	2.21	0.41
2:I:356:ALA:HB3	2:I:359:LYS:O	2.21	0.41
2:J:454:GLN:O	2:J:455:ALA:C	2.62	0.41
4:N:411:VAL:N	4:N:425:LEU:O	2.53	0.41
13:U:437:UNK:CB	13:U:445:UNK:O	2.69	0.41
13:g:232:UNK:O	13:g:233:UNK:C	2.69	0.41
2:t:46:PRO:HA	2:t:59:GLY:C	2.46	0.41
2:x:494:SER:N	2:x:575:ILE:O	2.53	0.41
1:0:73:ILE:HA	1:0:87:TRP:O	2.21	0.41
2:A:179:SER:O	2:A:246:TYR:HA	2.20	0.41
13:AL:78:UNK:O	13:AL:79:UNK:C	2.68	0.41
2:D:217:GLY:O	2:D:218:SER:C	2.64	0.41
2:H:268:VAL:HA	2:H:279:ILE:O	2.20	0.41
2:L:514:THR:HA	2:L:533:THR:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:56:ALA:O	6:T:69:GLY:N	2.53	0.41
13:U:92:UNK:HA	13:U:457:UNK:O	2.21	0.41
13:e:117:UNK:O	13:e:118:UNK:C	2.69	0.41
13:g:341:UNK:O	13:g:342:UNK:C	2.68	0.41
9:o:448:ARG:O	9:o:449:PRO:C	2.64	0.41
4:8:533:PHE:HA	4:8:548:VAL:O	2.19	0.41
5:9:44:PRO:O	5:9:91:ILE:O	2.39	0.41
2:A:681:THR:O	2:A:682:PRO:C	2.64	0.41
2:D:43:ARG:N	2:D:92:LEU:O	2.54	0.41
3:P:189:SER:HA	3:P:242:ASP:O	2.21	0.41
2:m:413:VAL:O	2:m:420:TYR:N	2.54	0.41
2:s:404:ILE:C	2:s:406:ASN:H	2.27	0.41
2:t:579:PHE:HA	2:t:599:ARG:O	2.20	0.41
2:v:179:SER:O	2:v:246:TYR:HA	2.19	0.41
2:A:45:SER:O	2:A:59:GLY:O	2.38	0.41
2:G:462:ASP:O	2:G:463:TRP:C	2.64	0.41
2:H:514:THR:HA	2:H:532:LYS:O	2.19	0.41
2:I:254:SER:O	2:I:257:PHE:O	2.38	0.41
6:T:46:PRO:O	6:T:47:ALA:C	2.63	0.41
7:X:62:GLY:O	7:X:66:ALA:HB2	2.21	0.41
7:Y:724:ALA:HB1	7:Y:752:ALA:O	2.21	0.41
7:Y:860:LYS:HA	7:Y:888:LEU:HA	2.03	0.41
8:Z:969:ARG:O	8:Z:973:PRO:N	2.54	0.41
10:b:36:THR:HA	10:b:50:PHE:O	2.21	0.41
13:e:78:UNK:O	13:e:79:UNK:C	2.68	0.41
2:m:447:PHE:O	2:m:450:ALA:HB3	2.21	0.41
2:u:623:PRO:O	2:u:629:CYS:HA	2.20	0.41
2:v:46:PRO:HA	2:v:59:GLY:C	2.45	0.41
2:v:119:GLU:N	2:v:182:ASN:O	2.53	0.41
2:y:307:LEU:O	2:y:334:VAL:N	2.53	0.41
2:1:212:TYR:HA	2:1:222:GLU:O	2.20	0.41
2:1:626:ASN:C	2:1:628:THR:N	2.78	0.41
2:3:24:GLU:HA	2:3:77:VAL:O	2.20	0.41
3:4:1017:LEU:O	3:4:1043:ASP:O	2.38	0.41
5:6:42:SER:O	5:6:43:ASN:C	2.63	0.41
5:6:46:VAL:HA	5:6:89:ILE:O	2.20	0.41
2:A:262:SER:HA	2:A:287:MET:HA	2.03	0.41
2:A:624:LYS:O	2:A:625:ILE:C	2.63	0.41
7:AF:903:ASN:O	7:AF:904:GLU:C	2.62	0.41
11:AJ:142:GLY:O	11:AJ:143:GLY:C	2.64	0.41
13:AN:269:UNK:O	13:AN:272:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:PRO:HA	2:C:113:GLY:C	2.46	0.41
2:D:494:SER:N	2:D:575:ILE:O	2.54	0.41
2:E:179:SER:O	2:E:246:TYR:HA	2.20	0.41
2:G:117:SER:O	2:G:183:VAL:HA	2.21	0.41
2:H:50:ILE:N	2:H:57:ILE:O	2.54	0.41
2:I:143:GLY:HA2	2:I:680:MET:C	2.46	0.41
2:I:184:THR:HA	2:I:242:LYS:HA	2.03	0.41
2:L:43:ARG:HA	2:L:63:THR:O	2.20	0.41
2:L:45:SER:O	2:L:60:LYS:HA	2.21	0.41
3:M:649:ASP:O	3:M:650:SER:C	2.63	0.41
3:M:782:CYS:O	3:M:783:LEU:C	2.63	0.41
4:N:156:GLN:O	4:N:250:PHE:CB	2.69	0.41
3:P:619:THR:O	3:P:620:GLN:C	2.63	0.41
6:T:58:ALA:O	6:T:66:GLN:HA	2.20	0.41
13:U:61:UNK:O	13:U:62:UNK:C	2.68	0.41
13:U:451:UNK:C	13:U:453:UNK:N	2.83	0.41
13:g:218:UNK:HA	13:g:224:UNK:O	2.21	0.41
2:s:478:THR:H	2:s:488:PHE:HA	1.85	0.41
2:t:48:ILE:O	2:t:59:GLY:N	2.53	0.41
2:v:149:ALA:HB3	2:v:287:MET:O	2.21	0.41
2:y:206:ALA:HB1	2:y:226:GLY:O	2.20	0.41
3:4:961:GLY:CA	3:4:989:VAL:O	2.68	0.41
4:8:370:VAL:O	4:8:380:GLU:HA	2.21	0.41
7:AF:860:LYS:HA	7:AF:888:LEU:HA	2.02	0.41
8:AG:50:GLU:CB	11:AJ:353:VAL:H	2.35	0.41
3:M:813:THR:HA	3:M:841:LEU:HA	2.03	0.41
4:Q:398:LYS:C	4:Q:400:ASN:H	2.29	0.41
1:S:8:GLN:H	1:S:59:GLY:HA3	1.86	0.41
7:Y:889:LYS:HA	7:Y:916:LEU:HA	2.03	0.41
10:b:31:PHE:O	10:b:55:HIS:HA	2.21	0.41
8:n:54:LEU:HA	11:q:350:GLY:CA	2.51	0.41
2:t:623:PRO:O	2:t:629:CYS:HA	2.20	0.41
2:v:50:ILE:N	2:v:57:ILE:O	2.53	0.41
2:v:95:TYR:O	2:v:103:PRO:HA	2.21	0.41
2:x:48:ILE:H	2:x:59:GLY:HA3	1.86	0.41
3:7:160:LEU:O	3:7:163:ALA:HB3	2.21	0.40
9:AH:507:THR:O	9:AH:508:ASN:C	2.64	0.40
2:B:434:SER:C	2:B:436:GLU:H	2.29	0.40
2:D:261:ILE:O	2:D:287:MET:HA	2.21	0.40
2:H:307:LEU:O	2:H:334:VAL:N	2.54	0.40
2:H:568:GLU:O	2:H:569:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:307:GLU:C	3:M:309:ASP:H	2.28	0.40
8:Z:350:LEU:O	8:Z:354:GLU:N	2.54	0.40
9:a:337:LEU:HA	9:a:343:MET:O	2.21	0.40
9:a:448:ARG:O	9:a:449:PRO:C	2.62	0.40
11:c:142:GLY:O	11:c:143:GLY:C	2.64	0.40
13:e:324:UNK:C	13:e:326:UNK:N	2.83	0.40
2:m:189:THR:O	2:m:190:SER:C	2.64	0.40
8:n:146:PRO:O	8:n:148:GLU:N	2.55	0.40
2:u:217:GLY:O	2:u:218:SER:C	2.64	0.40
2:v:46:PRO:O	2:v:59:GLY:C	2.64	0.40
2:x:30:SER:HA	2:x:33:ALA:HB3	2.02	0.40
2:y:165:GLU:O	2:y:169:GLN:N	2.54	0.40
2:1:71:HIS:O	2:1:73:THR:N	2.55	0.40
2:1:661:ASP:O	2:1:662:VAL:C	2.63	0.40
3:4:941:VAL:O	3:4:942:ILE:C	2.64	0.40
4:5:275:LEU:O	4:5:277:ARG:N	2.54	0.40
4:5:294:GLU:O	4:5:572:ASP:HA	2.21	0.40
2:A:268:VAL:HA	2:A:280:PRO:HA	2.03	0.40
2:A:514:THR:HA	2:A:532:LYS:O	2.21	0.40
11:AJ:269:LEU:N	11:AJ:379:SER:O	2.55	0.40
2:G:442:LYS:O	2:G:443:GLY:C	2.62	0.40
2:H:267:LEU:O	2:H:280:PRO:HA	2.22	0.40
2:I:46:PRO:HA	2:I:59:GLY:HA3	2.03	0.40
2:I:203:GLU:O	2:I:206:ALA:HB3	2.21	0.40
2:K:227:PRO:C	2:K:229:LYS:H	2.29	0.40
3:P:982:HIS:O	3:P:983:LEU:C	2.64	0.40
2:m:308:CYS:HA	2:m:334:VAL:O	2.22	0.40
2:s:568:GLU:O	2:s:569:ASP:C	2.64	0.40
2:s:579:PHE:HA	2:s:599:ARG:O	2.21	0.40
2:u:217:GLY:O	2:u:218:SER:O	2.39	0.40
2:u:414:LYS:HA	2:u:419:ASP:HA	2.02	0.40
2:u:454:GLN:O	2:u:455:ALA:C	2.64	0.40
2:v:271:ALA:HB2	2:v:278:GLU:N	2.36	0.40
3:4:916:LEU:O	3:4:917:ALA:C	2.63	0.40
4:8:315:GLY:HA2	4:8:336:LYS:HA	2.02	0.40
2:E:89:ASP:O	2:E:111:LEU:N	2.53	0.40
2:F:24:GLU:HA	2:F:77:VAL:O	2.21	0.40
2:G:506:GLN:HA	2:G:511:GLY:H	1.87	0.40
2:J:145:ASN:H	2:x:101:GLU:CB	2.33	0.40
4:Q:408:ASP:O	4:Q:429:THR:HA	2.21	0.40
9:a:456:GLY:HA3	9:a:462:ALA:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:26:VAL:O	10:b:27:GLY:C	2.64	0.40
2:s:427:ILE:O	2:s:458:GLU:HA	2.22	0.40
2:s:494:SER:N	2:s:575:ILE:O	2.54	0.40
3:4:133:GLN:O	3:4:136:PHE:O	2.40	0.40
3:7:928:SER:HA	3:7:957:ARG:O	2.22	0.40
13:AN:160:UNK:O	13:AN:161:UNK:C	2.69	0.40
2:D:133:ASP:O	2:D:136:ALA:HB3	2.21	0.40
2:G:580:CYS:N	2:G:599:ARG:O	2.55	0.40
2:H:414:LYS:HA	2:H:419:ASP:HA	2.02	0.40
2:J:199:LEU:HA	2:J:265:LEU:HA	2.03	0.40
3:P:728:GLU:HA	3:P:755:LEU:HA	2.02	0.40
4:Q:455:ASP:O	4:Q:459:ALA:HA	2.20	0.40
13:U:65:UNK:O	13:U:66:UNK:C	2.68	0.40
13:g:160:UNK:C	13:g:162:UNK:N	2.81	0.40
10:p:55:HIS:O	10:p:66:LYS:N	2.55	0.40
2:u:142:TRP:O	2:u:146:GLY:HA2	2.22	0.40
2:w:623:PRO:O	2:w:629:CYS:HA	2.22	0.40
3:4:131:PRO:HA	3:4:137:GLN:HA	2.04	0.40
9:AH:218:VAL:HA	9:AH:237:VAL:O	2.20	0.40
2:F:410:SER:O	2:F:423:GLY:HA3	2.22	0.40
2:H:82:PRO:HA	2:H:113:GLY:C	2.47	0.40
2:J:101:GLU:C	2:x:144:MET:HA	2.46	0.40
4:Q:393:ALA:O	4:Q:404:ALA:HB1	2.22	0.40
1:S:16:LYS:O	1:S:17:GLN:C	2.63	0.40
11:c:139:HIS:O	11:c:170:SER:HA	2.21	0.40
11:c:277:SER:O	11:c:369:ALA:HB2	2.20	0.40
2:u:59:GLY:O	2:u:60:LYS:C	2.64	0.40
2:u:145:ASN:O	2:u:146:GLY:C	2.62	0.40
2:x:363:LEU:HA	2:x:387:GLY:O	2.22	0.40

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	0	134/440 (30%)	125 (93%)	9 (7%)	0	100	100
1	S	134/440 (30%)	123 (92%)	11 (8%)	0	100	100
2	1	680/682 (100%)	607 (89%)	72 (11%)	1 (0%)	48	83
2	2	680/682 (100%)	650 (96%)	30 (4%)	0	100	100
2	3	680/682 (100%)	650 (96%)	30 (4%)	0	100	100
2	A	680/682 (100%)	608 (89%)	71 (10%)	1 (0%)	48	83
2	B	680/682 (100%)	618 (91%)	61 (9%)	1 (0%)	48	83
2	C	680/682 (100%)	630 (93%)	49 (7%)	1 (0%)	48	83
2	D	680/682 (100%)	627 (92%)	52 (8%)	1 (0%)	48	83
2	E	680/682 (100%)	635 (93%)	45 (7%)	0	100	100
2	F	680/682 (100%)	631 (93%)	48 (7%)	1 (0%)	48	83
2	G	680/682 (100%)	601 (88%)	78 (12%)	1 (0%)	48	83
2	H	680/682 (100%)	624 (92%)	56 (8%)	0	100	100
2	I	680/682 (100%)	611 (90%)	69 (10%)	0	100	100
2	J	680/682 (100%)	604 (89%)	74 (11%)	2 (0%)	36	72
2	K	680/682 (100%)	648 (95%)	31 (5%)	1 (0%)	48	83
2	L	680/682 (100%)	652 (96%)	28 (4%)	0	100	100
2	m	680/682 (100%)	613 (90%)	67 (10%)	0	100	100
2	s	680/682 (100%)	621 (91%)	59 (9%)	0	100	100
2	t	680/682 (100%)	624 (92%)	55 (8%)	1 (0%)	48	83
2	u	680/682 (100%)	605 (89%)	73 (11%)	2 (0%)	36	72
2	v	680/682 (100%)	624 (92%)	56 (8%)	0	100	100
2	w	680/682 (100%)	629 (92%)	50 (7%)	1 (0%)	48	83
2	x	680/682 (100%)	610 (90%)	70 (10%)	0	100	100
2	y	680/682 (100%)	608 (89%)	71 (10%)	1 (0%)	48	83
2	z	680/682 (100%)	637 (94%)	43 (6%)	0	100	100
3	4	945/1163 (81%)	861 (91%)	84 (9%)	0	100	100
3	7	945/1163 (81%)	871 (92%)	74 (8%)	0	100	100
3	M	945/1163 (81%)	847 (90%)	98 (10%)	0	100	100
3	P	945/1163 (81%)	839 (89%)	106 (11%)	0	100	100
4	5	363/581 (62%)	325 (90%)	37 (10%)	1 (0%)	36	72
4	8	363/581 (62%)	317 (87%)	46 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	363/581 (62%)	318 (88%)	44 (12%)	1 (0%)	36	72
4	Q	363/581 (62%)	311 (86%)	52 (14%)	0	100	100
5	6	117/164 (71%)	111 (95%)	6 (5%)	0	100	100
5	9	87/164 (53%)	80 (92%)	7 (8%)	0	100	100
5	O	117/164 (71%)	110 (94%)	7 (6%)	0	100	100
5	R	87/164 (53%)	74 (85%)	13 (15%)	0	100	100
6	AA	61/228 (27%)	56 (92%)	5 (8%)	0	100	100
6	T	61/228 (27%)	53 (87%)	8 (13%)	0	100	100
7	AE	931/937 (99%)	871 (94%)	58 (6%)	2 (0%)	43	78
7	AF	843/937 (90%)	788 (94%)	54 (6%)	1 (0%)	48	83
7	X	931/937 (99%)	873 (94%)	56 (6%)	2 (0%)	43	78
7	Y	843/937 (90%)	792 (94%)	49 (6%)	2 (0%)	43	78
8	AG	964/993 (97%)	892 (92%)	72 (8%)	0	100	100
8	Z	964/993 (97%)	904 (94%)	60 (6%)	0	100	100
8	n	964/993 (97%)	886 (92%)	78 (8%)	0	100	100
9	AH	623/782 (80%)	565 (91%)	58 (9%)	0	100	100
9	a	623/782 (80%)	573 (92%)	50 (8%)	0	100	100
9	o	623/782 (80%)	563 (90%)	59 (10%)	1 (0%)	43	78
10	AI	145/147 (99%)	132 (91%)	13 (9%)	0	100	100
10	b	145/147 (99%)	133 (92%)	12 (8%)	0	100	100
10	p	145/147 (99%)	133 (92%)	12 (8%)	0	100	100
11	AJ	438/449 (98%)	412 (94%)	26 (6%)	0	100	100
11	c	438/449 (98%)	404 (92%)	33 (8%)	1 (0%)	43	78
11	q	438/449 (98%)	414 (94%)	24 (6%)	0	100	100
12	AK	429/445 (96%)	398 (93%)	31 (7%)	0	100	100
12	d	429/445 (96%)	400 (93%)	29 (7%)	0	100	100
12	r	429/445 (96%)	416 (97%)	13 (3%)	0	100	100
14	AM	161/163 (99%)	156 (97%)	5 (3%)	0	100	100
14	AO	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
14	f	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
14	h	161/163 (99%)	152 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	j	161/163 (99%)	150 (93%)	11 (7%)	0	100	100
All	All	34500/38347 (90%)	31701 (92%)	2773 (8%)	26 (0%)	49	83

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AF	926	PHE
2	D	218	SER
7	Y	928	VAL
11	c	11	GLN
2	u	99	ASP
2	u	218	SER
2	B	625	ILE
4	5	276	GLU
2	A	53	SER
2	J	53	SER
2	J	625	ILE
9	o	508	ASN
2	y	53	SER
2	C	53	SER
2	K	53	SER
4	N	276	GLU
7	X	926	PHE
2	t	53	SER
2	w	53	SER
7	AE	926	PHE
2	F	53	SER
2	G	487	ASP
2	1	99	ASP
7	Y	926	PHE
7	X	928	VAL
7	AE	928	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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.

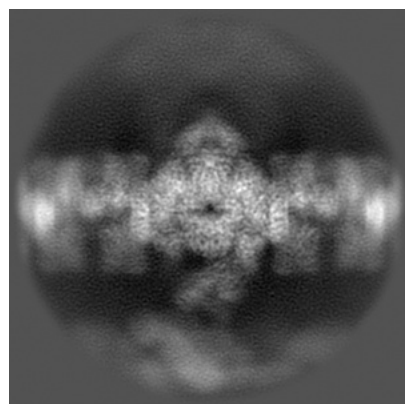
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55604. These allow visual inspection of the internal detail of the map and identification of artifacts.

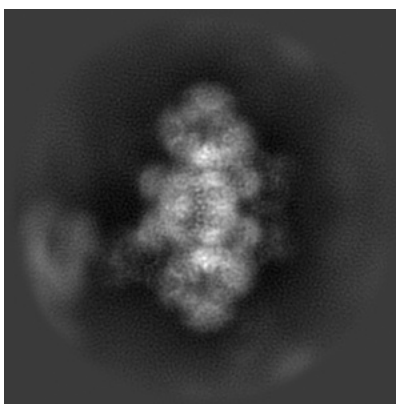
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

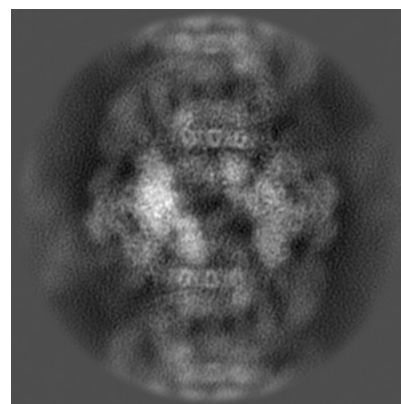
6.1.1 Primary map



X

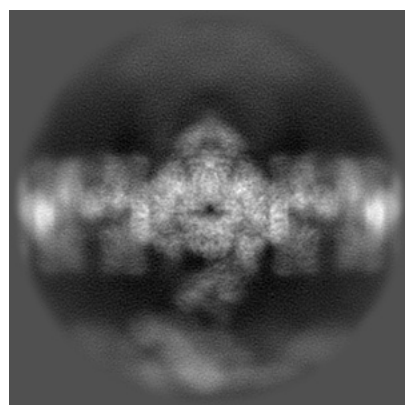


Y

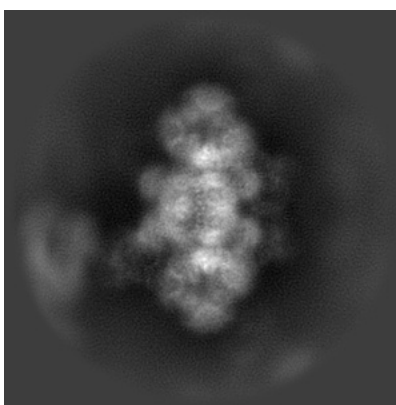


Z

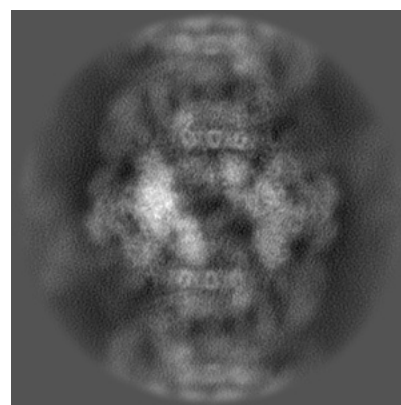
6.1.2 Raw map



X



Y

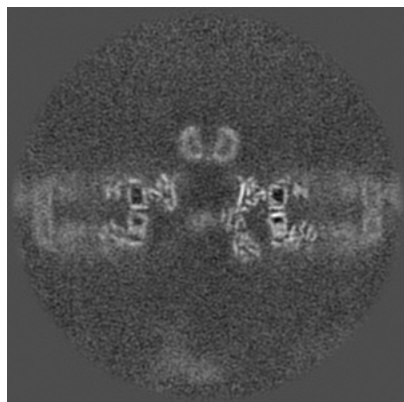


Z

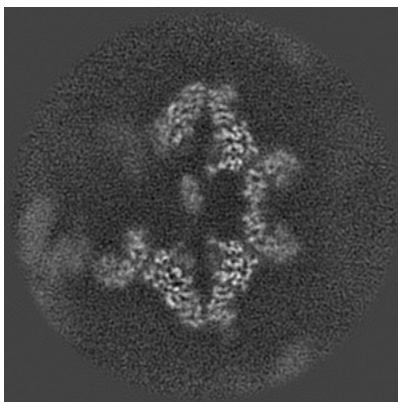
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

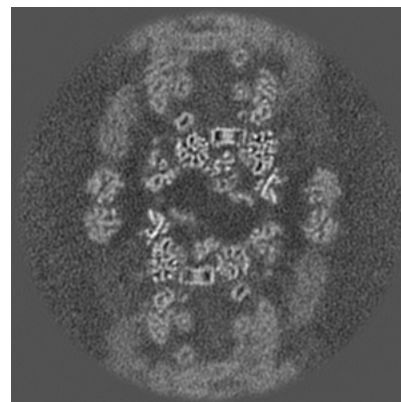
6.2.1 Primary map



X Index: 128

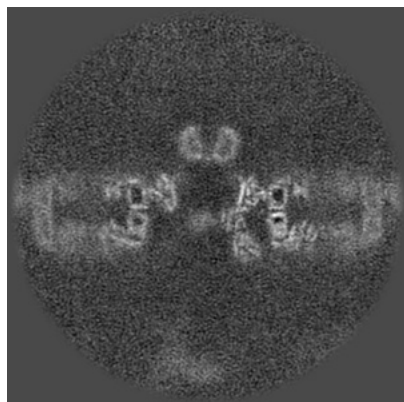


Y Index: 128

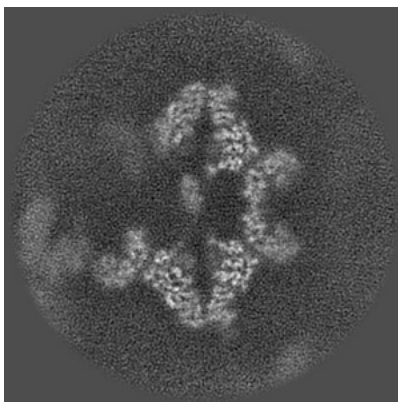


Z Index: 128

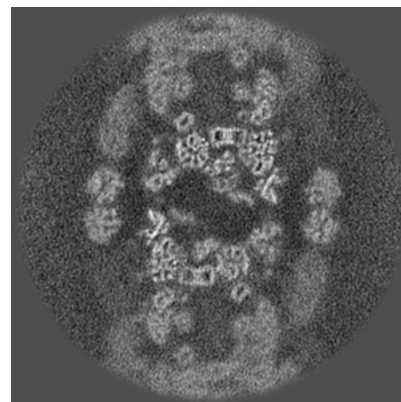
6.2.2 Raw map



X Index: 128



Y Index: 128

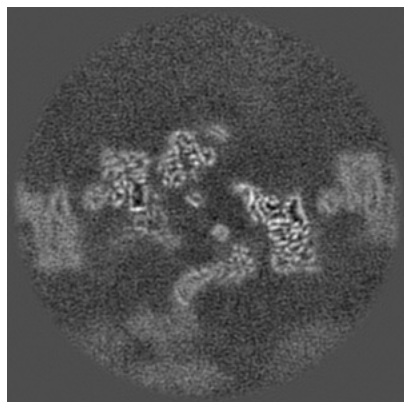


Z Index: 128

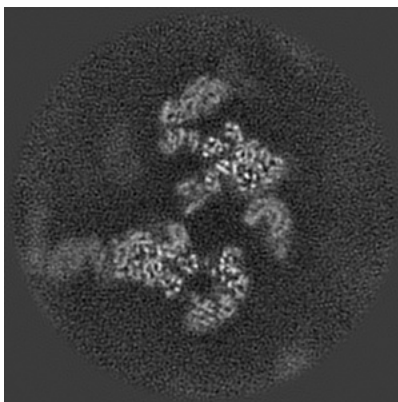
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

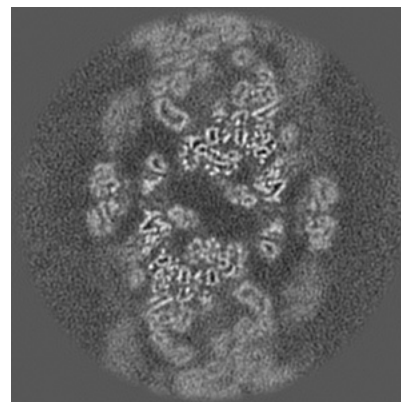
6.3.1 Primary map



X Index: 111

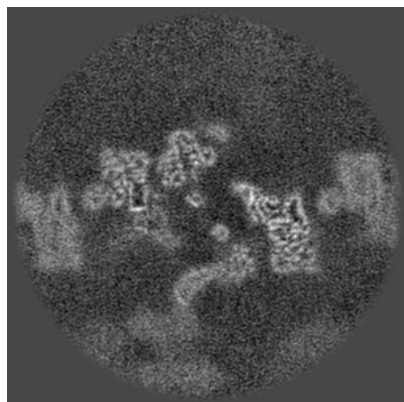


Y Index: 137

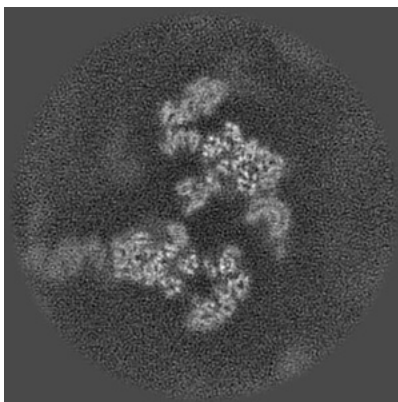


Z Index: 133

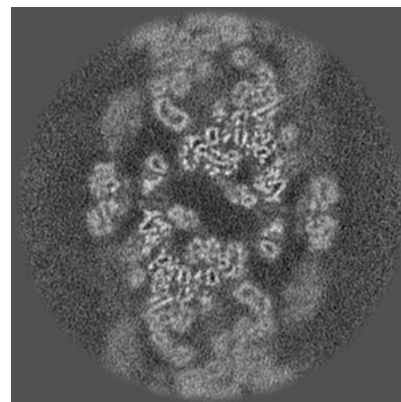
6.3.2 Raw map



X Index: 111



Y Index: 138

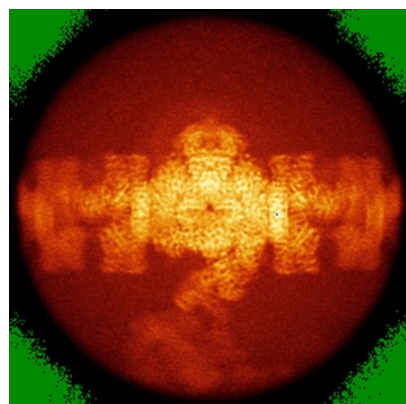


Z Index: 133

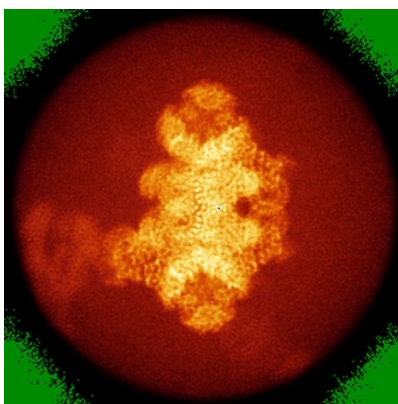
The images above show the largest variance slices of the map in three orthogonal directions.

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

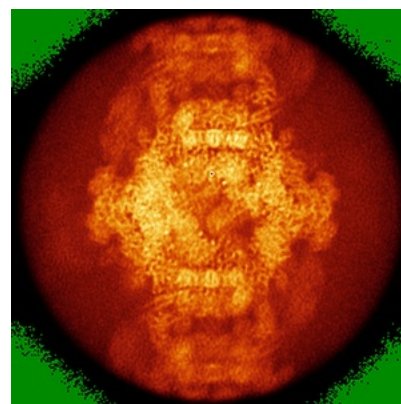
6.4.1 Primary map



X

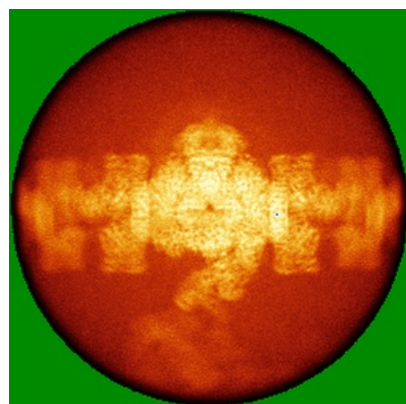


Y

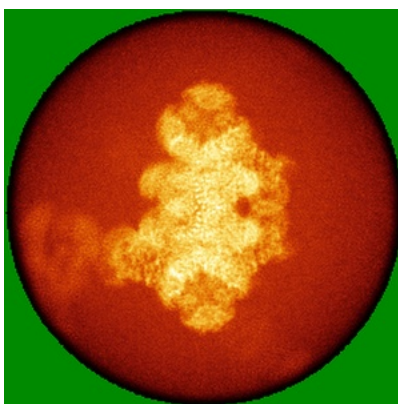


Z

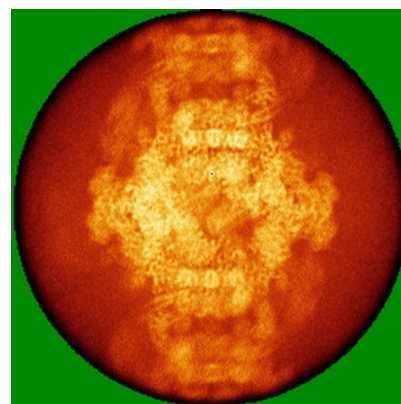
6.4.2 Raw map



X



Y

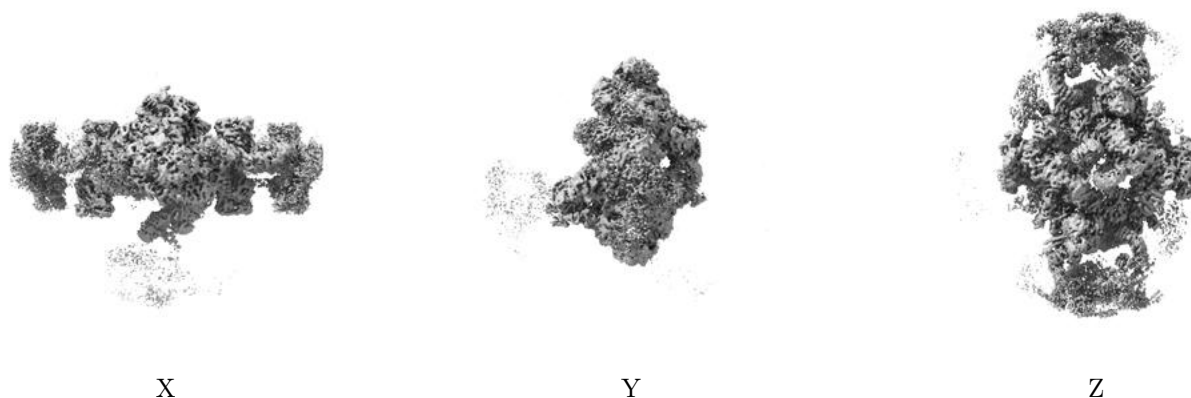


Z

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.

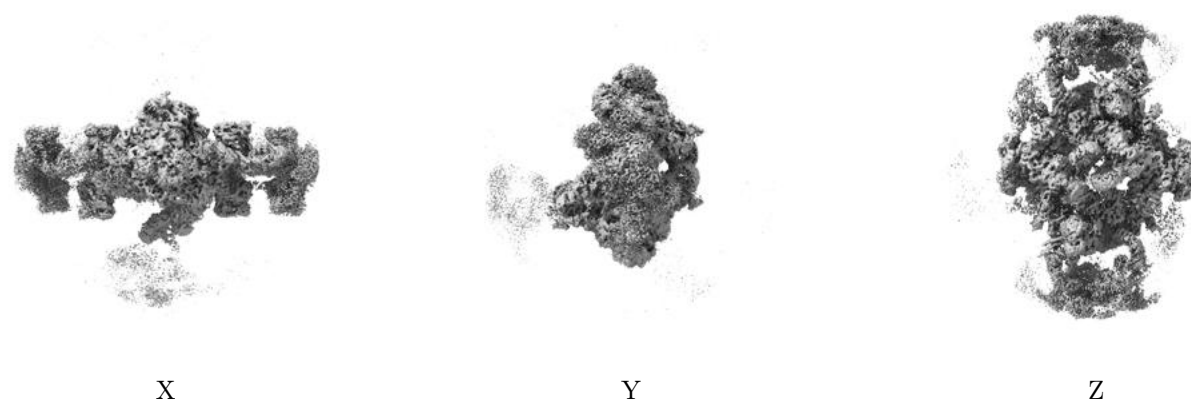
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

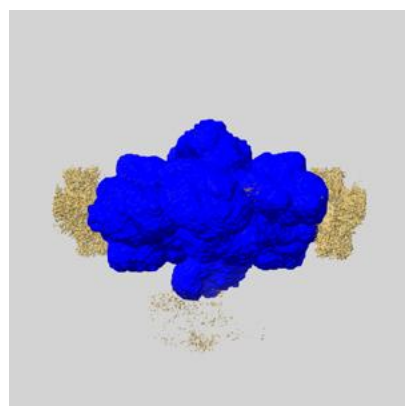
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

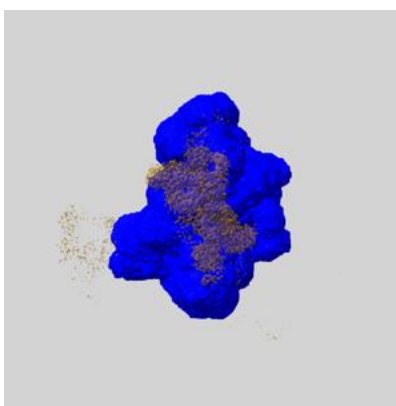
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

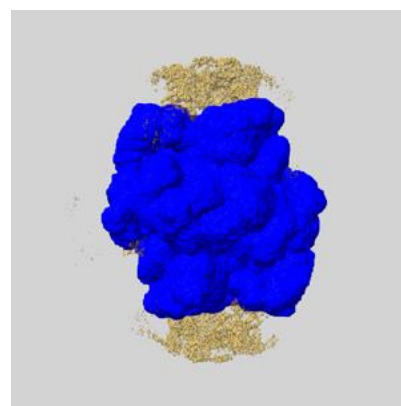
6.6.1 emd_55604_msk_1.map [i](#)



X



Y

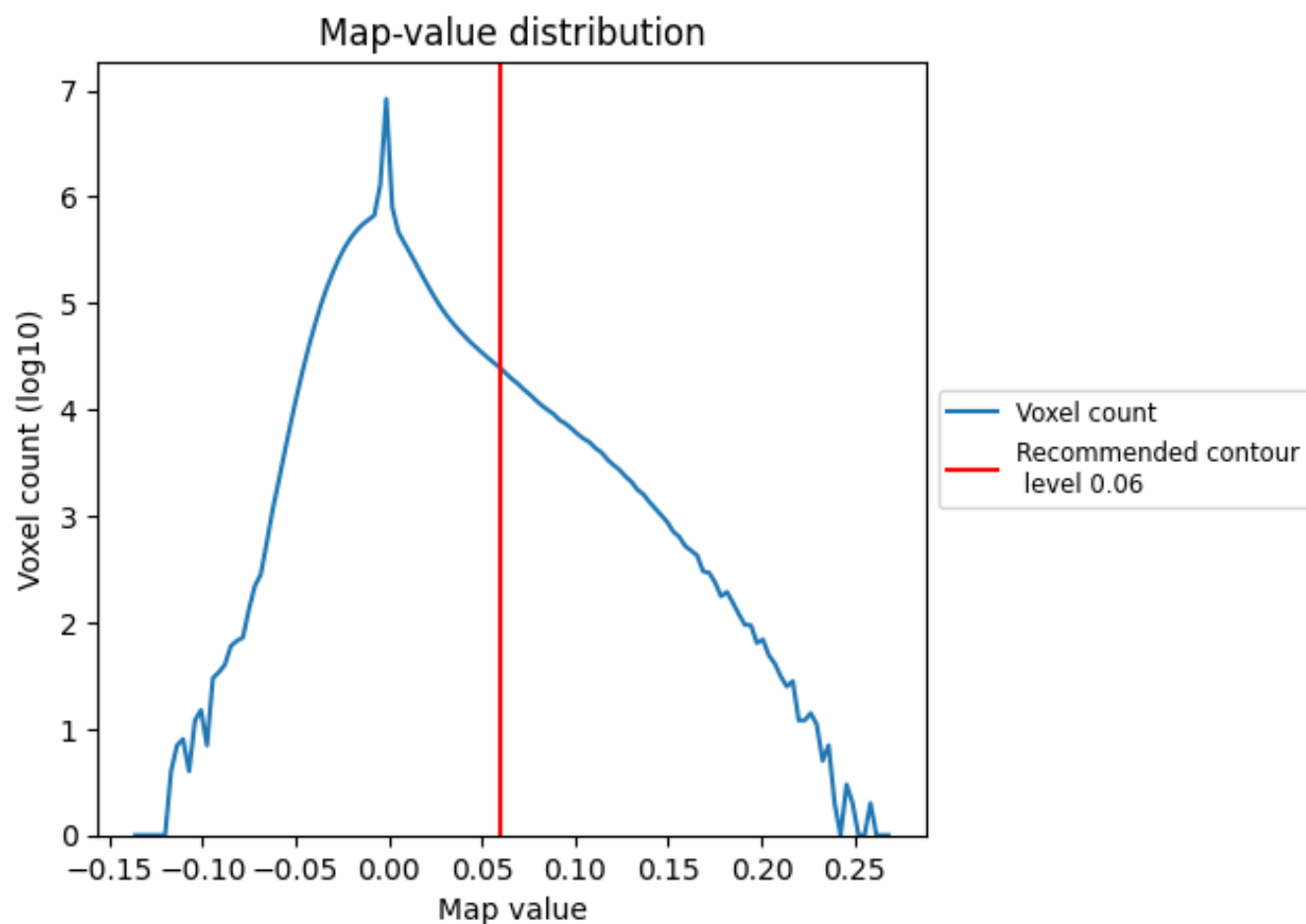


Z

7 Map analysis [i](#)

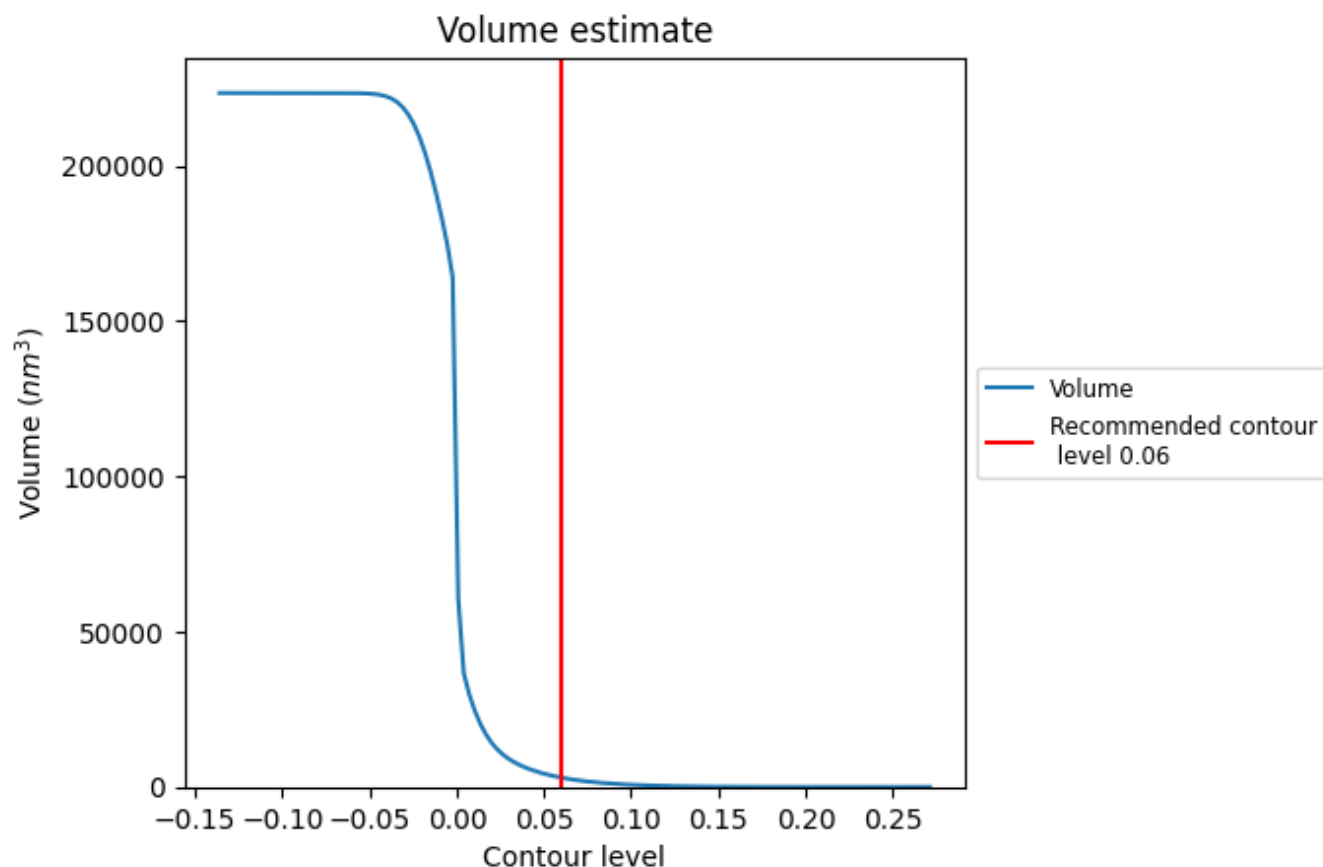
This section contains the results of statistical analysis of the map.

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.

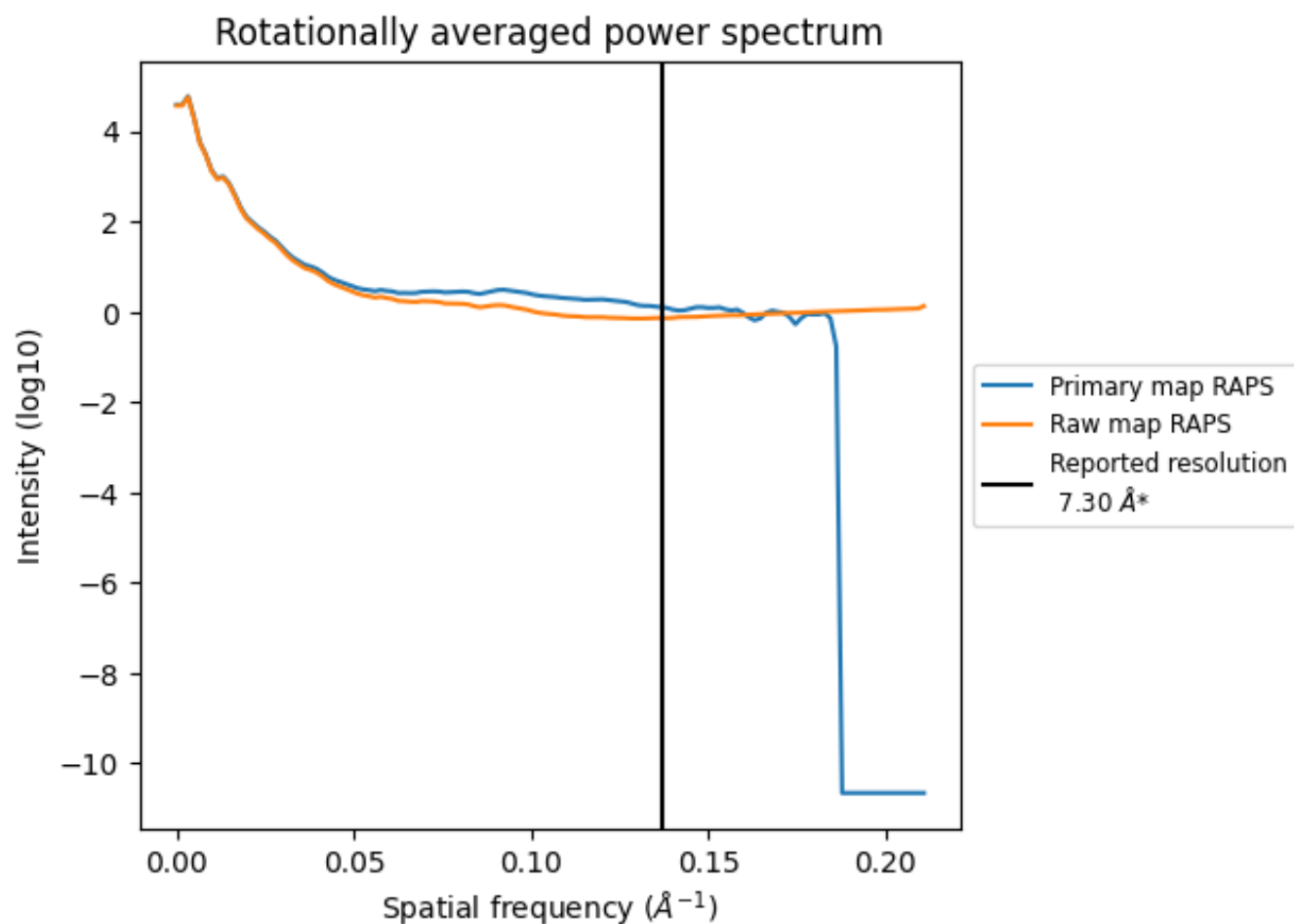
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3001 nm³; this corresponds to an approximate mass of 2711 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 ⓘ

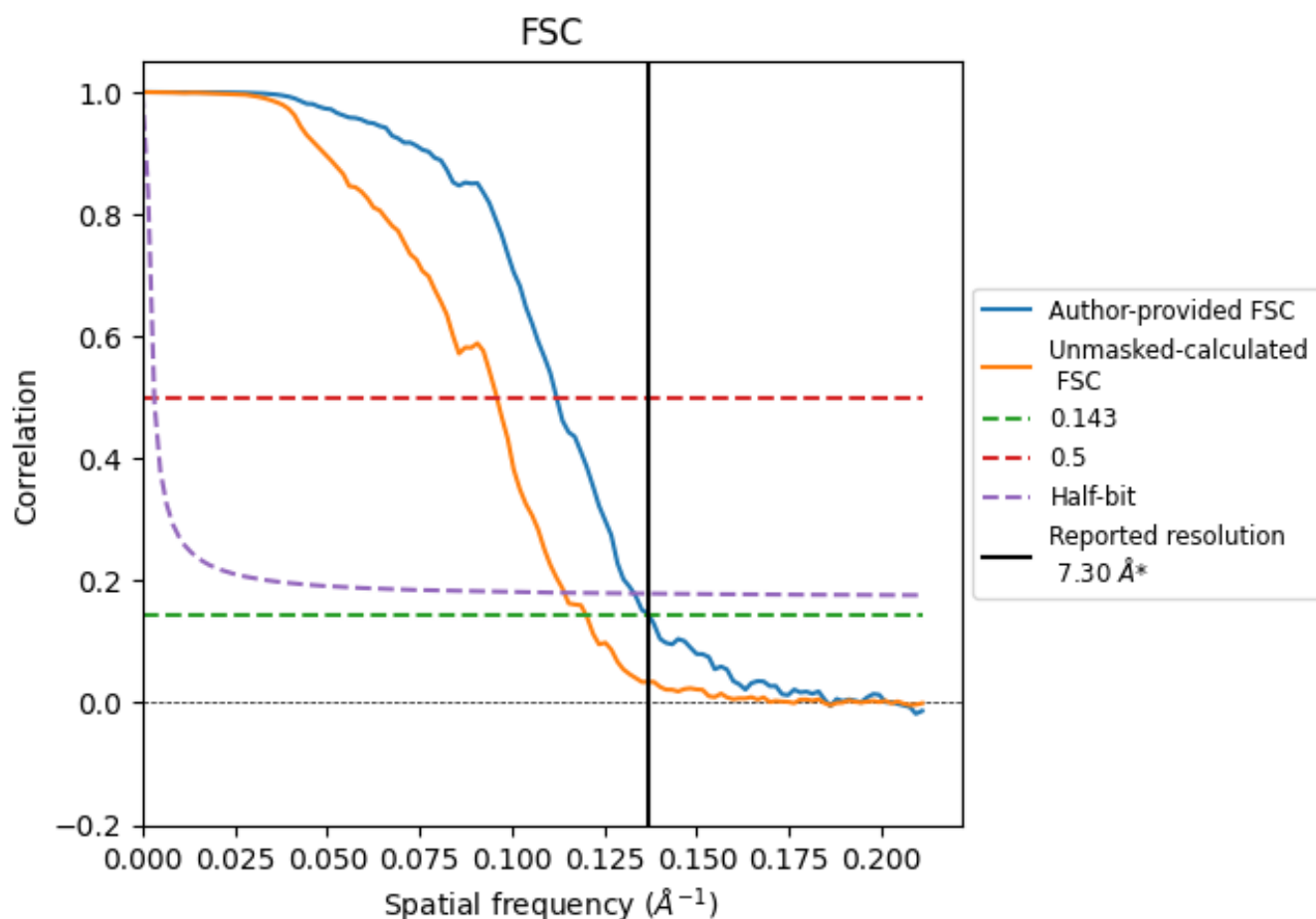


*Reported resolution corresponds to spatial frequency of 0.137 Å⁻¹

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 0.137 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

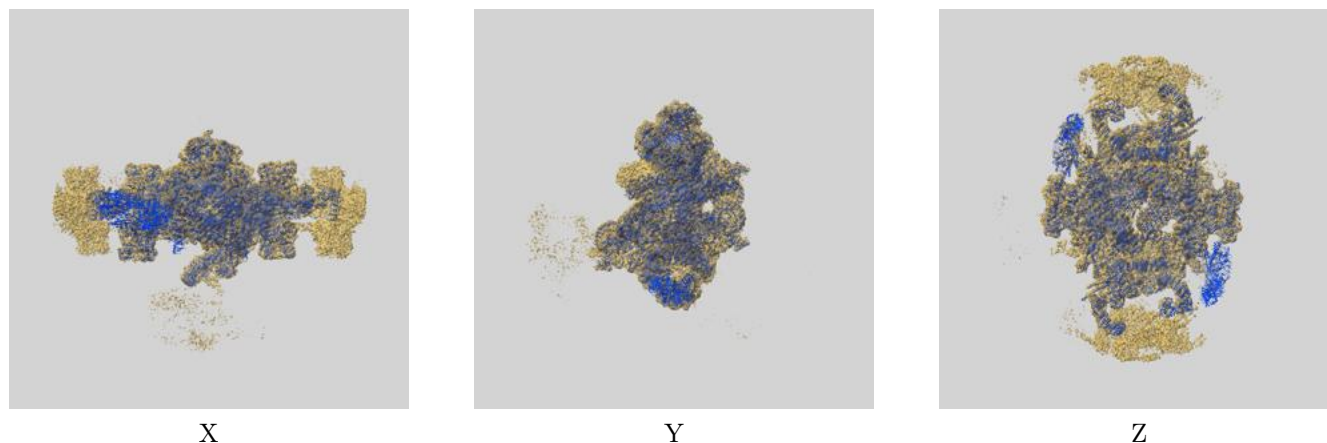
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	7.29	8.92	7.51
Unmasked-calculated*	8.33	10.43	8.76

*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 8.33 differs from the reported value 7.3 by more than 10 %

9 Map-model fit [i](#)

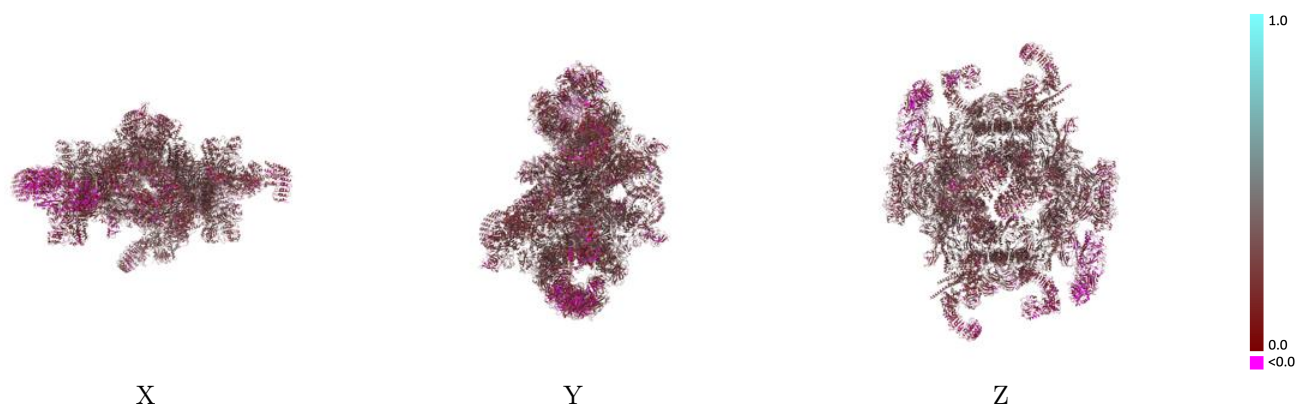
This section contains information regarding the fit between EMDB map EMD-55604 and PDB model 9T64. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



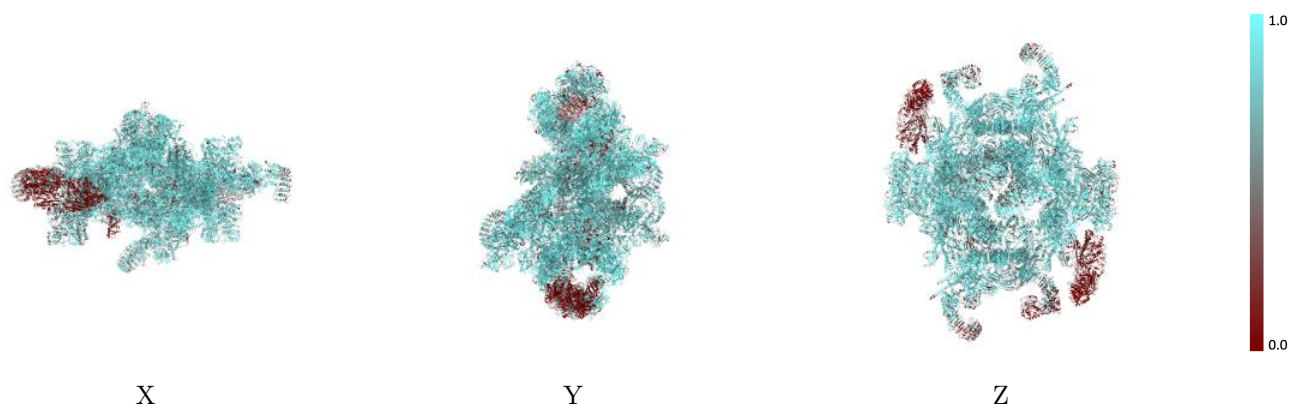
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



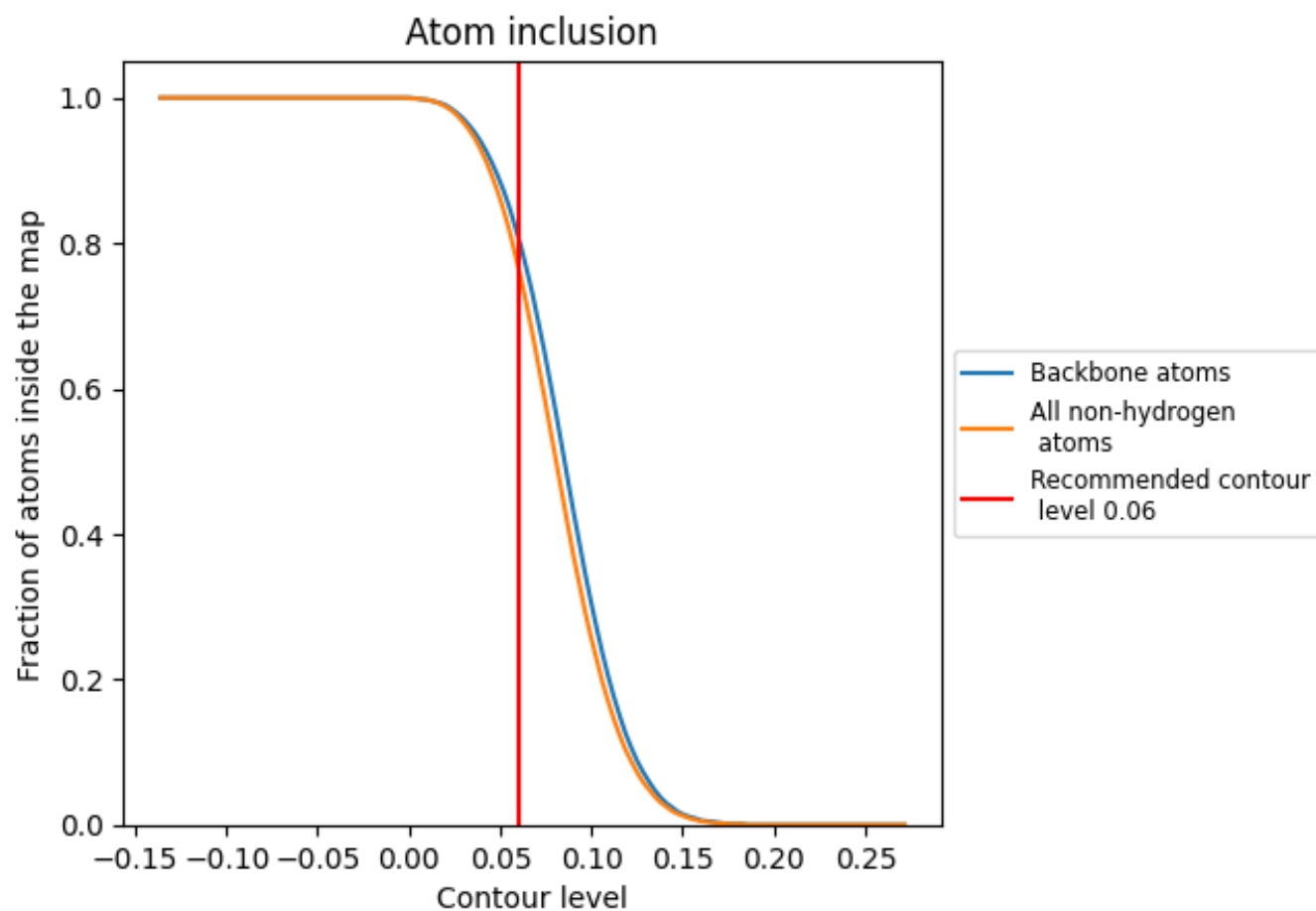
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.2450
0	 0.8600	 0.2670
1	 0.8710	 0.2780
2	 0.0190	 0.0740
3	 0.0290	 0.0720
4	 0.8750	 0.2660
5	 0.8210	 0.2440
6	 0.8850	 0.2750
7	 0.7810	 0.2270
8	 0.7260	 0.2030
9	 0.6900	 0.2070
A	 0.9150	 0.3010
AA	 0.7490	 0.2070
AE	 0.6060	 0.1800
AF	 0.4950	 0.1510
AG	 0.8020	 0.2370
AH	 0.8060	 0.2500
AI	 0.9450	 0.2970
AJ	 0.8620	 0.2640
AK	 0.8680	 0.2610
AL	 0.4060	 0.2200
AM	 0.0250	 0.1130
AN	 0.8680	 0.2560
AO	 0.6000	 0.2380
B	 0.8850	 0.2950
C	 0.8380	 0.2460
D	 0.8420	 0.2560
E	 0.7420	 0.2060
F	 0.7770	 0.2180
G	 0.9190	 0.3020
H	 0.9010	 0.2820
I	 0.8960	 0.2900
J	 0.9190	 0.3060
K	 0.0870	 0.1030
L	 0.1520	 0.1330



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Chain	Atom inclusion	Q-score
M	 0.9160	 0.2880
N	 0.8810	 0.2640
O	 0.8870	 0.2900
P	 0.9150	 0.2740
Q	 0.8850	 0.2710
R	 0.8510	 0.2740
S	 0.8780	 0.2700
T	 0.8940	 0.2670
U	 0.6940	 0.2680
X	 0.7230	 0.2080
Y	 0.7590	 0.2220
Z	 0.8410	 0.2480
a	 0.8430	 0.2530
b	 0.9490	 0.2970
c	 0.9090	 0.2830
d	 0.9400	 0.2930
e	 0.8900	 0.2910
f	 0.7610	 0.2610
g	 0.9430	 0.3080
h	 0.6860	 0.2270
j	 0.2460	 0.2030
m	 0.9250	 0.3020
n	 0.7970	 0.2330
o	 0.8340	 0.2560
p	 0.9410	 0.2930
q	 0.8000	 0.2490
r	 0.8340	 0.2730
s	 0.8960	 0.2990
t	 0.9050	 0.2740
u	 0.9080	 0.2960
v	 0.8490	 0.2470
w	 0.8450	 0.2380
x	 0.9140	 0.3000
y	 0.9140	 0.2910
z	 0.7980	 0.2470