Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:18 AM UTC

PDB ID	:	7VOP / pdb_00007vop
EMDB ID	:	EMD-32056
Title	:	Cryo-EM structure of Xenopus laevis nuclear pore complex cytoplasmic ring subunit
Authors	:	Tai, L.; Zhu, Y.; Sun, F.
Deposited on	:	2021-10-14
Resolution	:	8.70 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:

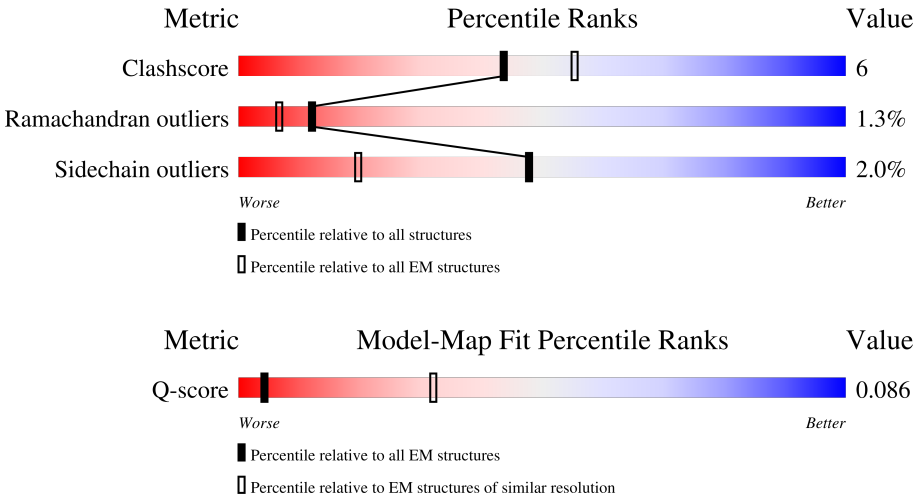
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	282 (8.20 - 9.20)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	653	10% 82% 18%
1	J	653	19% 79% 19%
2	B	375	21% 73% 26%
2	K	375	29% 75% 25%

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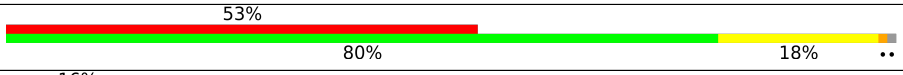
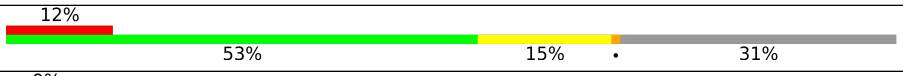
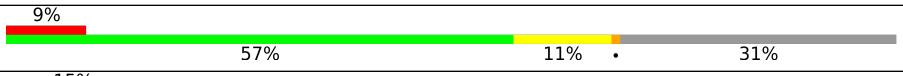
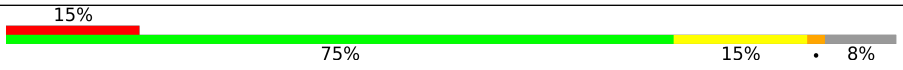
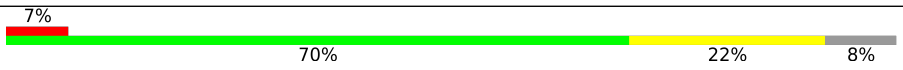
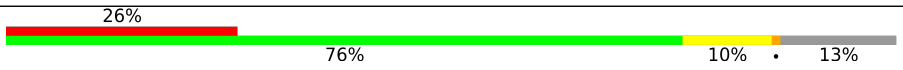
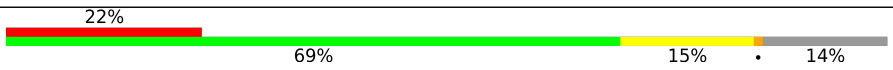
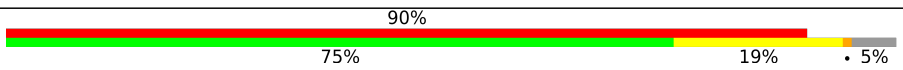
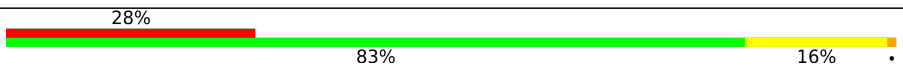
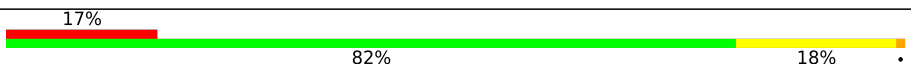
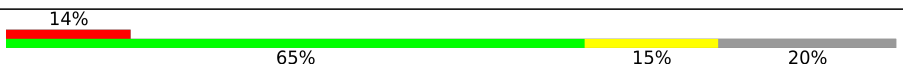
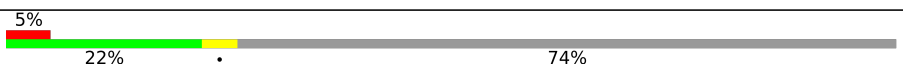
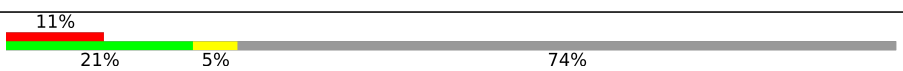
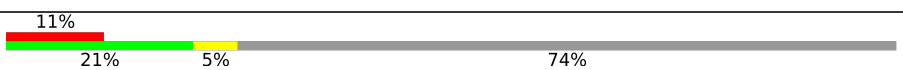
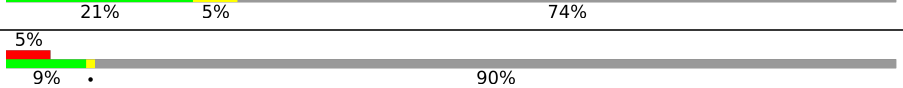
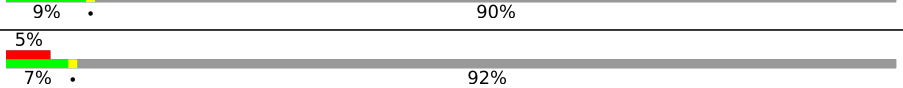
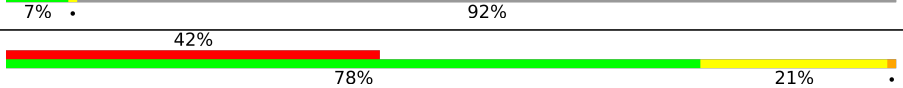
Mol	Chain	Length	Quality of chain
3	C	360	
3	L	360	
4	D	1414	
4	M	1414	
5	E	326	
5	N	326	
6	F	924	
6	O	924	
7	G	320	
7	P	320	
8	H	916	
8	Q	916	
9	I	1140	
9	R	1140	
10	S	2011	
10	T	2011	
11	U	820	
12	V	2931	
12	W	2931	
12	X	2931	
12	Y	2931	
12	Z	2931	
13	a	2037	
13	e	2037	
14	b	728	

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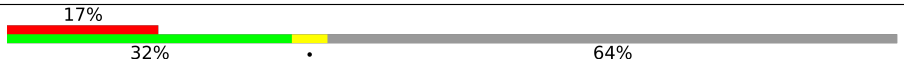
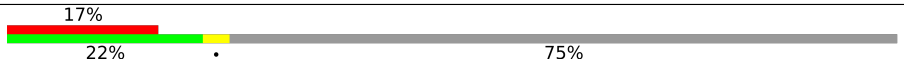
Mol	Chain	Length	Quality of chain
14	d	728	
15	c	547	
15	f	547	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 178773 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 Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	653	Total	C	N	O	S	0	0
			5268	3341	904	984	39		
1	J	653	Total	C	N	O	S	0	0
			5268	3341	904	984	39		

- Molecule 2 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	375	Total	C	N	O	S	0	0
			2927	1813	524	571	19		
2	K	375	Total	C	N	O	S	0	0
			2927	1813	524	571	19		

- Molecule 3 is a protein called Nucleoporin SEH1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	333	Total	C	N	O	S	0	0
			2607	1632	466	491	18		
3	L	325	Total	C	N	O	S	0	0
			2546	1592	455	482	17		

- Molecule 4 is a protein called Nucleoporin 160kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1394	Total	C	N	O	S	0	0
			11118	7052	1912	2086	68		
4	M	1394	Total	C	N	O	S	0	0
			11118	7052	1912	2086	68		

- Molecule 5 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	326	Total	C	N	O	S	0	0
			2573	1640	443	473	17		
5	N	326	Total	C	N	O	S	0	0
			2573	1640	443	473	17		

- Molecule 6 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	638	Total	C	N	O	S	0	0
			5177	3287	912	949	29		
6	O	637	Total	C	N	O	S	0	0
			5168	3282	911	946	29		

- Molecule 7 is a protein called GATOR complex protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	294	Total	C	N	O	S	0	0
			2300	1454	394	440	12		
7	P	294	Total	C	N	O	S	0	0
			2300	1454	394	440	12		

- Molecule 8 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	798	Total	C	N	O	S	0	0
			6494	4126	1096	1240	32		
8	Q	790	Total	C	N	O	S	0	0
			6430	4085	1087	1226	32		

- Molecule 9 is a protein called outer Nup133.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1076	Total	C	N	O	S	0	0
			8482	5362	1409	1661	50		
9	R	1082	Total	C	N	O	S	0	0
			8536	5397	1420	1669	50		

- Molecule 10 is a protein called MGC83295 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	2011	Total	C	N	O	S	0	0
			15974	10112	2785	2978	99		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	2011	Total	C	N	O	S	0	0
			15974	10112	2785	2978	99		

- Molecule 11 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	654	Total	C	N	O	S	0	0
			5260	3328	918	986	28		

- Molecule 12 is a protein called Nup358.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	772	Total	C	N	O	S	0	0
			6225	3966	1061	1166	32		
12	W	756	Total	C	N	O	S	0	0
			6100	3890	1040	1139	31		
12	X	767	Total	C	N	O	S	0	0
			6190	3944	1056	1158	32		
12	Y	761	Total	C	N	O	S	0	0
			6139	3912	1047	1149	31		
12	Z	758	Total	C	N	O	S	0	0
			6116	3898	1042	1145	31		

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	2480	GLY	-	insertion	UNP A0A1L8HGL2
V	2481	PHE	-	insertion	UNP A0A1L8HGL2
V	2482	ASN	-	insertion	UNP A0A1L8HGL2
V	2483	PHE	-	insertion	UNP A0A1L8HGL2
V	2484	SER	-	insertion	UNP A0A1L8HGL2
V	2485	LEU	-	insertion	UNP A0A1L8HGL2
V	2486	PHE	-	insertion	UNP A0A1L8HGL2
V	2487	LYS	-	insertion	UNP A0A1L8HGL2
V	2488	SER	-	insertion	UNP A0A1L8HGL2
V	2489	ASN	-	insertion	UNP A0A1L8HGL2
V	2490	PRO	-	insertion	UNP A0A1L8HGL2
V	2491	ARG	-	insertion	UNP A0A1L8HGL2
V	2492	ALA	-	insertion	UNP A0A1L8HGL2
V	2493	PHE	-	insertion	UNP A0A1L8HGL2
V	2494	TRP	-	insertion	UNP A0A1L8HGL2
V	2495	THR	-	insertion	UNP A0A1L8HGL2

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Chain	Residue	Modelled	Actual	Comment	Reference
V	2496	CYS	-	insertion	UNP A0A1L8HGL2
V	2497	THR	-	insertion	UNP A0A1L8HGL2
V	2498	SER	-	insertion	UNP A0A1L8HGL2
V	2499	SER	-	insertion	UNP A0A1L8HGL2
V	2500	SER	-	insertion	UNP A0A1L8HGL2
V	2501	LYS	-	insertion	UNP A0A1L8HGL2
V	2502	PRO	-	insertion	UNP A0A1L8HGL2
V	2503	GLU	-	insertion	UNP A0A1L8HGL2
V	2504	VAL	-	insertion	UNP A0A1L8HGL2
V	2505	GLU	-	insertion	UNP A0A1L8HGL2
W	2480	GLY	-	insertion	UNP A0A1L8HGL2
W	2481	PHE	-	insertion	UNP A0A1L8HGL2
W	2482	ASN	-	insertion	UNP A0A1L8HGL2
W	2483	PHE	-	insertion	UNP A0A1L8HGL2
W	2484	SER	-	insertion	UNP A0A1L8HGL2
W	2485	LEU	-	insertion	UNP A0A1L8HGL2
W	2486	PHE	-	insertion	UNP A0A1L8HGL2
W	2487	LYS	-	insertion	UNP A0A1L8HGL2
W	2488	SER	-	insertion	UNP A0A1L8HGL2
W	2489	ASN	-	insertion	UNP A0A1L8HGL2
W	2490	PRO	-	insertion	UNP A0A1L8HGL2
W	2491	ARG	-	insertion	UNP A0A1L8HGL2
W	2492	ALA	-	insertion	UNP A0A1L8HGL2
W	2493	PHE	-	insertion	UNP A0A1L8HGL2
W	2494	TRP	-	insertion	UNP A0A1L8HGL2
W	2495	THR	-	insertion	UNP A0A1L8HGL2
W	2496	CYS	-	insertion	UNP A0A1L8HGL2
W	2497	THR	-	insertion	UNP A0A1L8HGL2
W	2498	SER	-	insertion	UNP A0A1L8HGL2
W	2499	SER	-	insertion	UNP A0A1L8HGL2
W	2500	SER	-	insertion	UNP A0A1L8HGL2
W	2501	LYS	-	insertion	UNP A0A1L8HGL2
W	2502	PRO	-	insertion	UNP A0A1L8HGL2
W	2503	GLU	-	insertion	UNP A0A1L8HGL2
W	2504	VAL	-	insertion	UNP A0A1L8HGL2
W	2505	GLU	-	insertion	UNP A0A1L8HGL2
X	2480	GLY	-	insertion	UNP A0A1L8HGL2
X	2481	PHE	-	insertion	UNP A0A1L8HGL2
X	2482	ASN	-	insertion	UNP A0A1L8HGL2
X	2483	PHE	-	insertion	UNP A0A1L8HGL2
X	2484	SER	-	insertion	UNP A0A1L8HGL2
X	2485	LEU	-	insertion	UNP A0A1L8HGL2

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Chain	Residue	Modelled	Actual	Comment	Reference
X	2486	PHE	-	insertion	UNP A0A1L8HGL2
X	2487	LYS	-	insertion	UNP A0A1L8HGL2
X	2488	SER	-	insertion	UNP A0A1L8HGL2
X	2489	ASN	-	insertion	UNP A0A1L8HGL2
X	2490	PRO	-	insertion	UNP A0A1L8HGL2
X	2491	ARG	-	insertion	UNP A0A1L8HGL2
X	2492	ALA	-	insertion	UNP A0A1L8HGL2
X	2493	PHE	-	insertion	UNP A0A1L8HGL2
X	2494	TRP	-	insertion	UNP A0A1L8HGL2
X	2495	THR	-	insertion	UNP A0A1L8HGL2
X	2496	CYS	-	insertion	UNP A0A1L8HGL2
X	2497	THR	-	insertion	UNP A0A1L8HGL2
X	2498	SER	-	insertion	UNP A0A1L8HGL2
X	2499	SER	-	insertion	UNP A0A1L8HGL2
X	2500	SER	-	insertion	UNP A0A1L8HGL2
X	2501	LYS	-	insertion	UNP A0A1L8HGL2
X	2502	PRO	-	insertion	UNP A0A1L8HGL2
X	2503	GLU	-	insertion	UNP A0A1L8HGL2
X	2504	VAL	-	insertion	UNP A0A1L8HGL2
X	2505	GLU	-	insertion	UNP A0A1L8HGL2
Y	2480	GLY	-	insertion	UNP A0A1L8HGL2
Y	2481	PHE	-	insertion	UNP A0A1L8HGL2
Y	2482	ASN	-	insertion	UNP A0A1L8HGL2
Y	2483	PHE	-	insertion	UNP A0A1L8HGL2
Y	2484	SER	-	insertion	UNP A0A1L8HGL2
Y	2485	LEU	-	insertion	UNP A0A1L8HGL2
Y	2486	PHE	-	insertion	UNP A0A1L8HGL2
Y	2487	LYS	-	insertion	UNP A0A1L8HGL2
Y	2488	SER	-	insertion	UNP A0A1L8HGL2
Y	2489	ASN	-	insertion	UNP A0A1L8HGL2
Y	2490	PRO	-	insertion	UNP A0A1L8HGL2
Y	2491	ARG	-	insertion	UNP A0A1L8HGL2
Y	2492	ALA	-	insertion	UNP A0A1L8HGL2
Y	2493	PHE	-	insertion	UNP A0A1L8HGL2
Y	2494	TRP	-	insertion	UNP A0A1L8HGL2
Y	2495	THR	-	insertion	UNP A0A1L8HGL2
Y	2496	CYS	-	insertion	UNP A0A1L8HGL2
Y	2497	THR	-	insertion	UNP A0A1L8HGL2
Y	2498	SER	-	insertion	UNP A0A1L8HGL2
Y	2499	SER	-	insertion	UNP A0A1L8HGL2
Y	2500	SER	-	insertion	UNP A0A1L8HGL2
Y	2501	LYS	-	insertion	UNP A0A1L8HGL2

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	2502	PRO	-	insertion	UNP A0A1L8HGL2
Y	2503	GLU	-	insertion	UNP A0A1L8HGL2
Y	2504	VAL	-	insertion	UNP A0A1L8HGL2
Y	2505	GLU	-	insertion	UNP A0A1L8HGL2
Z	2480	GLY	-	insertion	UNP A0A1L8HGL2
Z	2481	PHE	-	insertion	UNP A0A1L8HGL2
Z	2482	ASN	-	insertion	UNP A0A1L8HGL2
Z	2483	PHE	-	insertion	UNP A0A1L8HGL2
Z	2484	SER	-	insertion	UNP A0A1L8HGL2
Z	2485	LEU	-	insertion	UNP A0A1L8HGL2
Z	2486	PHE	-	insertion	UNP A0A1L8HGL2
Z	2487	LYS	-	insertion	UNP A0A1L8HGL2
Z	2488	SER	-	insertion	UNP A0A1L8HGL2
Z	2489	ASN	-	insertion	UNP A0A1L8HGL2
Z	2490	PRO	-	insertion	UNP A0A1L8HGL2
Z	2491	ARG	-	insertion	UNP A0A1L8HGL2
Z	2492	ALA	-	insertion	UNP A0A1L8HGL2
Z	2493	PHE	-	insertion	UNP A0A1L8HGL2
Z	2494	TRP	-	insertion	UNP A0A1L8HGL2
Z	2495	THR	-	insertion	UNP A0A1L8HGL2
Z	2496	CYS	-	insertion	UNP A0A1L8HGL2
Z	2497	THR	-	insertion	UNP A0A1L8HGL2
Z	2498	SER	-	insertion	UNP A0A1L8HGL2
Z	2499	SER	-	insertion	UNP A0A1L8HGL2
Z	2500	SER	-	insertion	UNP A0A1L8HGL2
Z	2501	LYS	-	insertion	UNP A0A1L8HGL2
Z	2502	PRO	-	insertion	UNP A0A1L8HGL2
Z	2503	GLU	-	insertion	UNP A0A1L8HGL2
Z	2504	VAL	-	insertion	UNP A0A1L8HGL2
Z	2505	GLU	-	insertion	UNP A0A1L8HGL2

- Molecule 13 is a protein called Nucleoporin CAN.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	209	Total	C	N	O	S	0	0
			1738	1086	308	341	3		
13	e	155	Total	C	N	O	S	0	0
			1282	797	224	258	3		

- Molecule 14 is a protein called Nup88A protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	728	Total	C	N	O	S	0	0
			5787	3645	991	1119	32		
14	d	683	Total	C	N	O	S	0	0
			5414	3413	919	1051	31		

- Molecule 15 is a protein called IL4I1 protein.

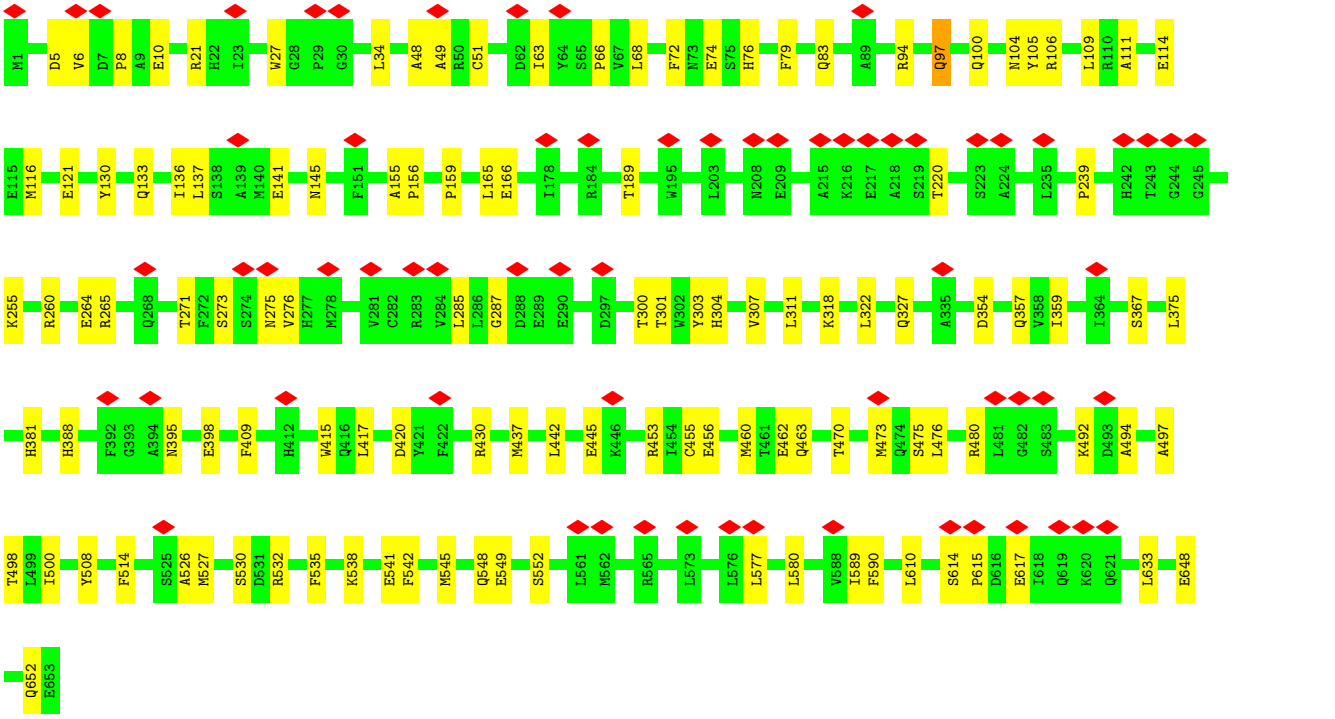
Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	198	Total	C	N	O	S	0	0
			1621	1001	286	327	7		
15	f	138	Total	C	N	O	S	0	0
			1141	708	197	232	4		

3 Residue-property plots (i)

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

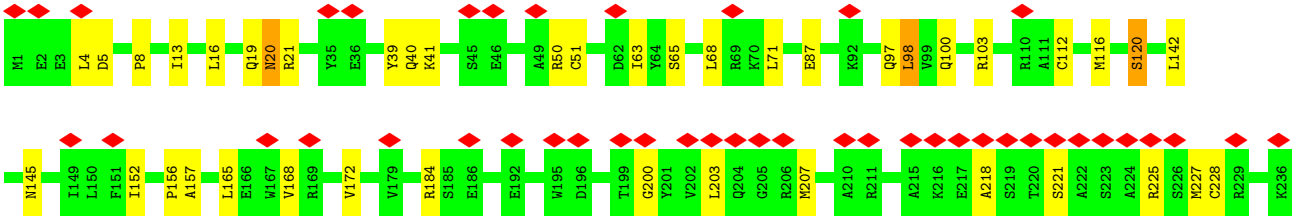
• Molecule 1: Nuclear pore complex protein Nup85

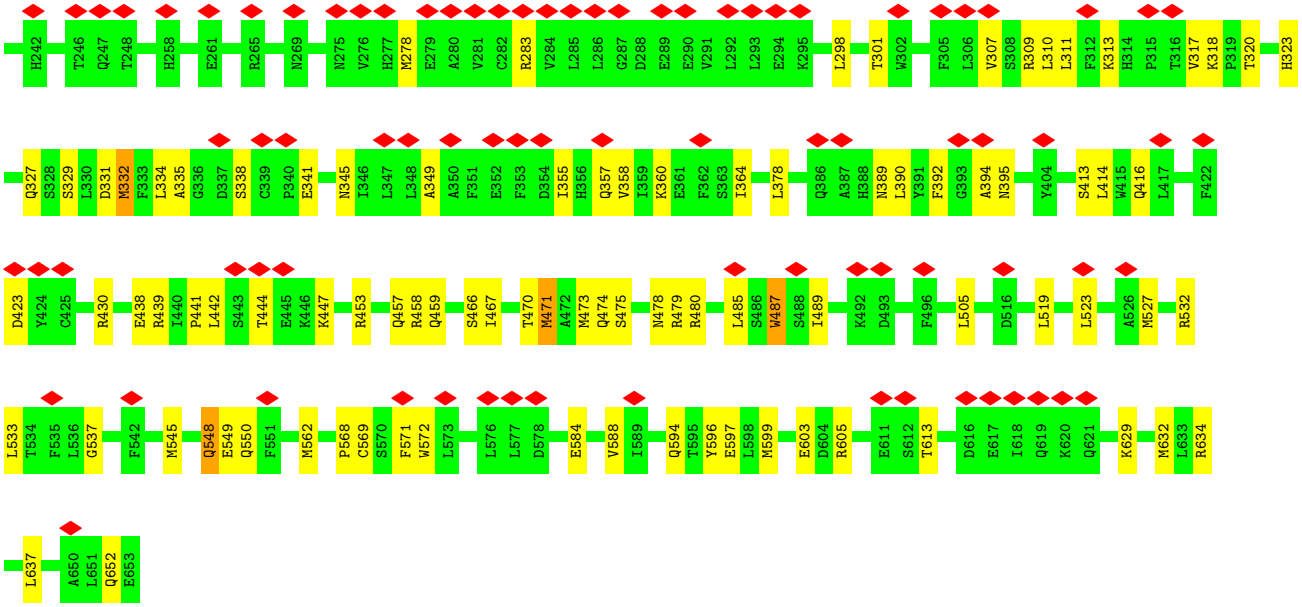
Chain A:



• Molecule 1: Nuclear pore complex protein Nup85

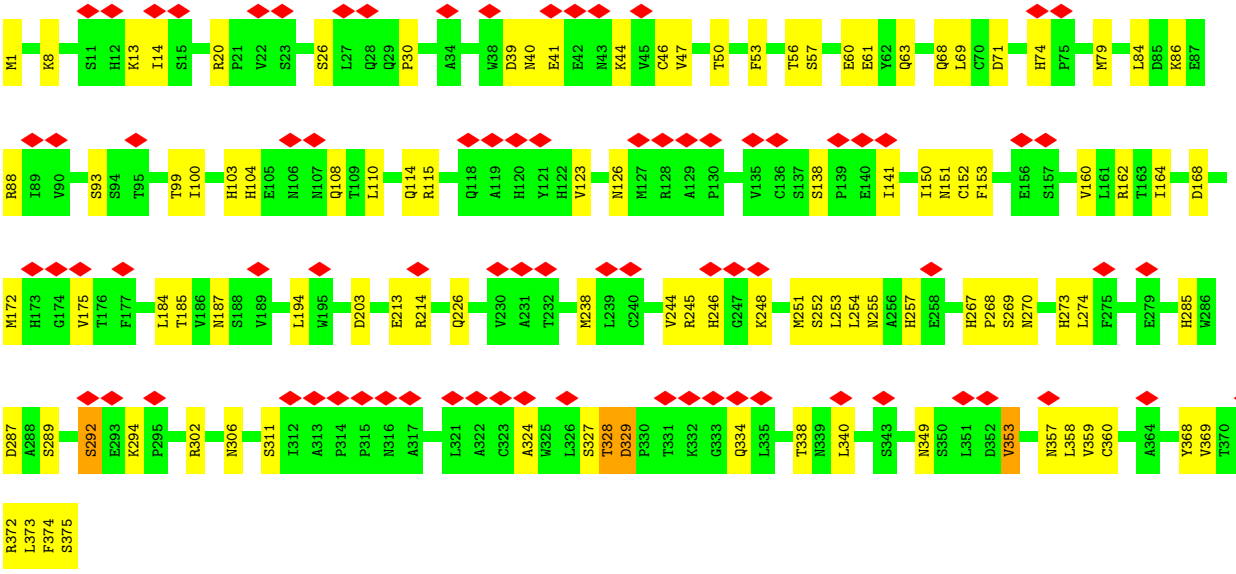
Chain J:





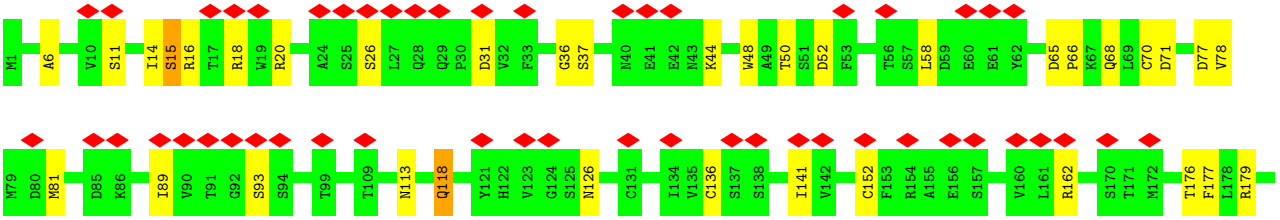
• Molecule 2: MGC154553 protein

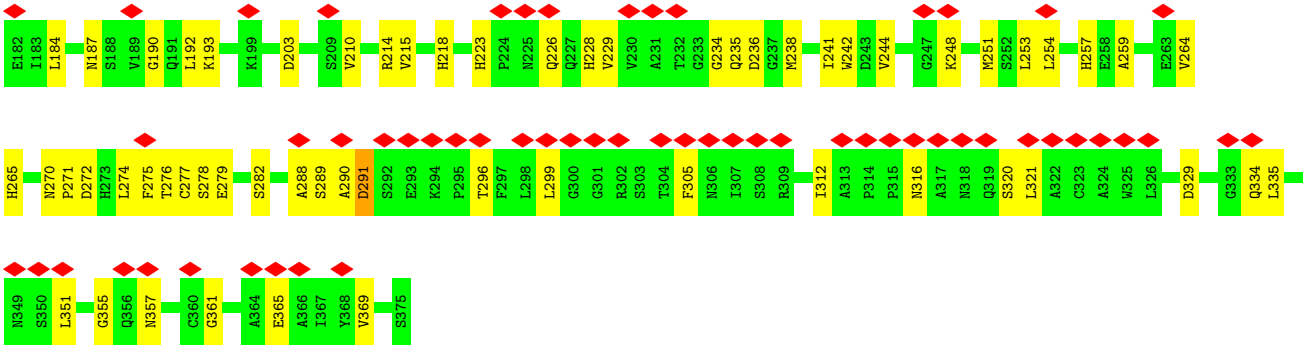
Chain B:



• Molecule 2: MGC154553 protein

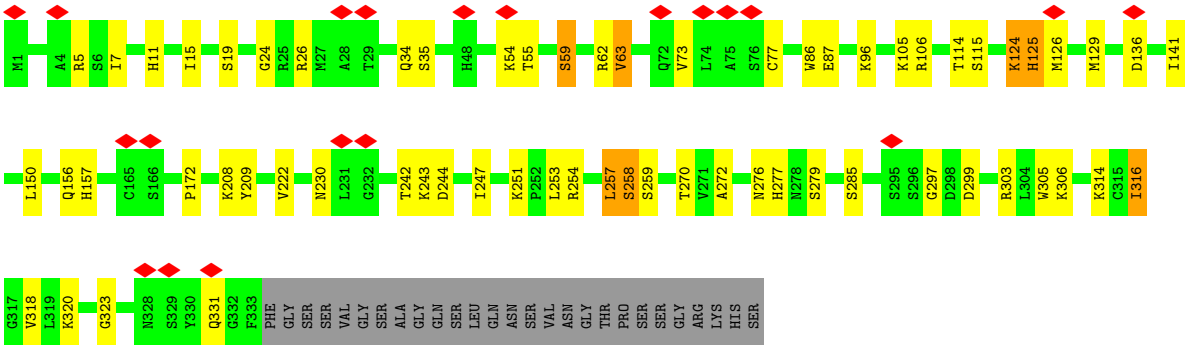
Chain K:





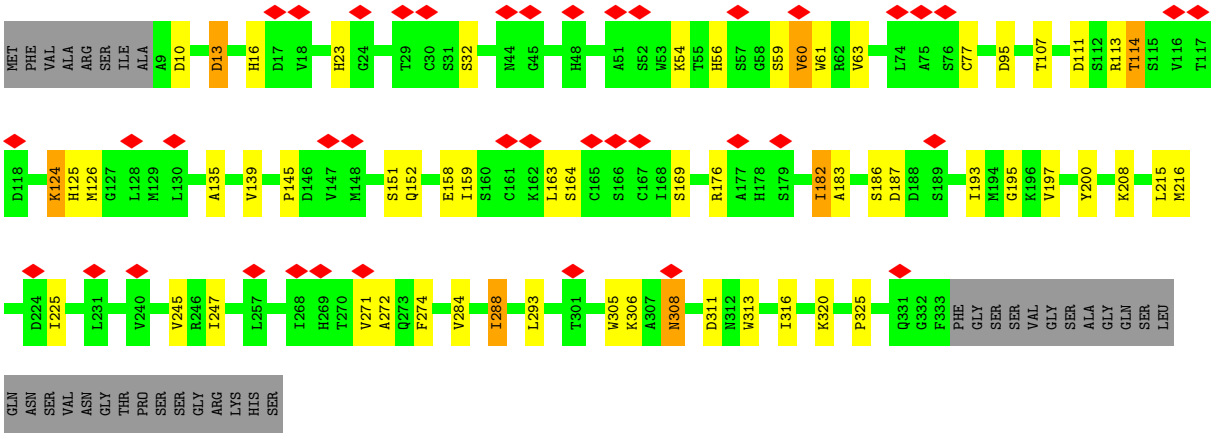
• Molecule 3: Nucleoporin SEH1-A

Chain C:



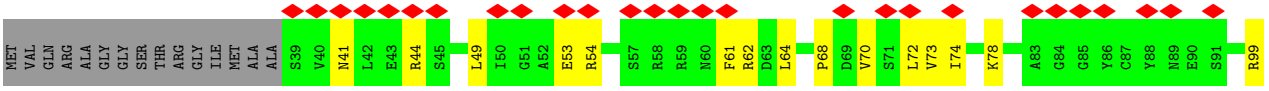
• Molecule 3: Nucleoporin SEH1-A

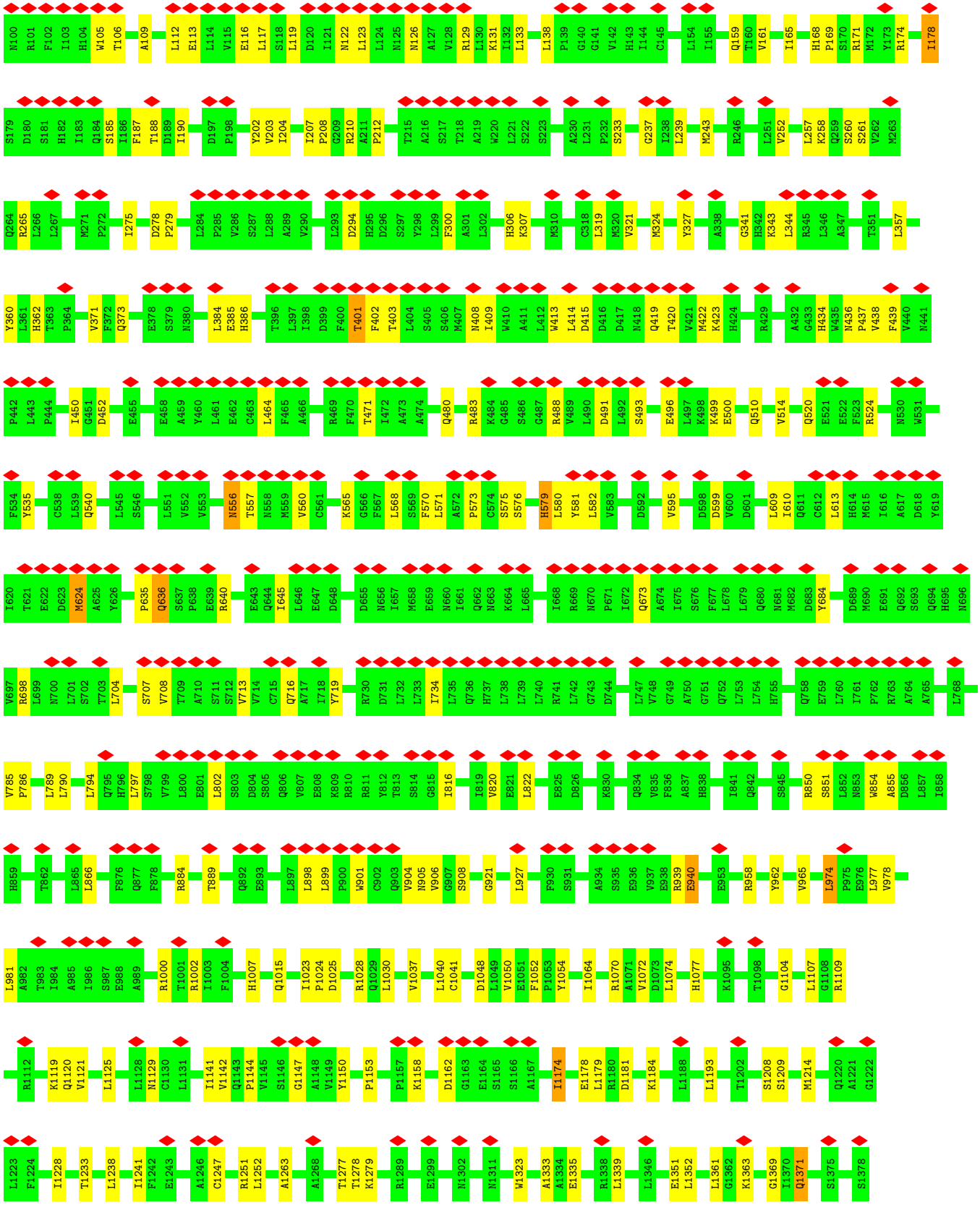
Chain L:



• Molecule 4: Nucleoporin 160kDa

Chain D:

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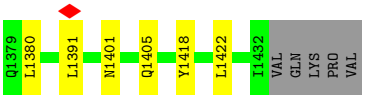
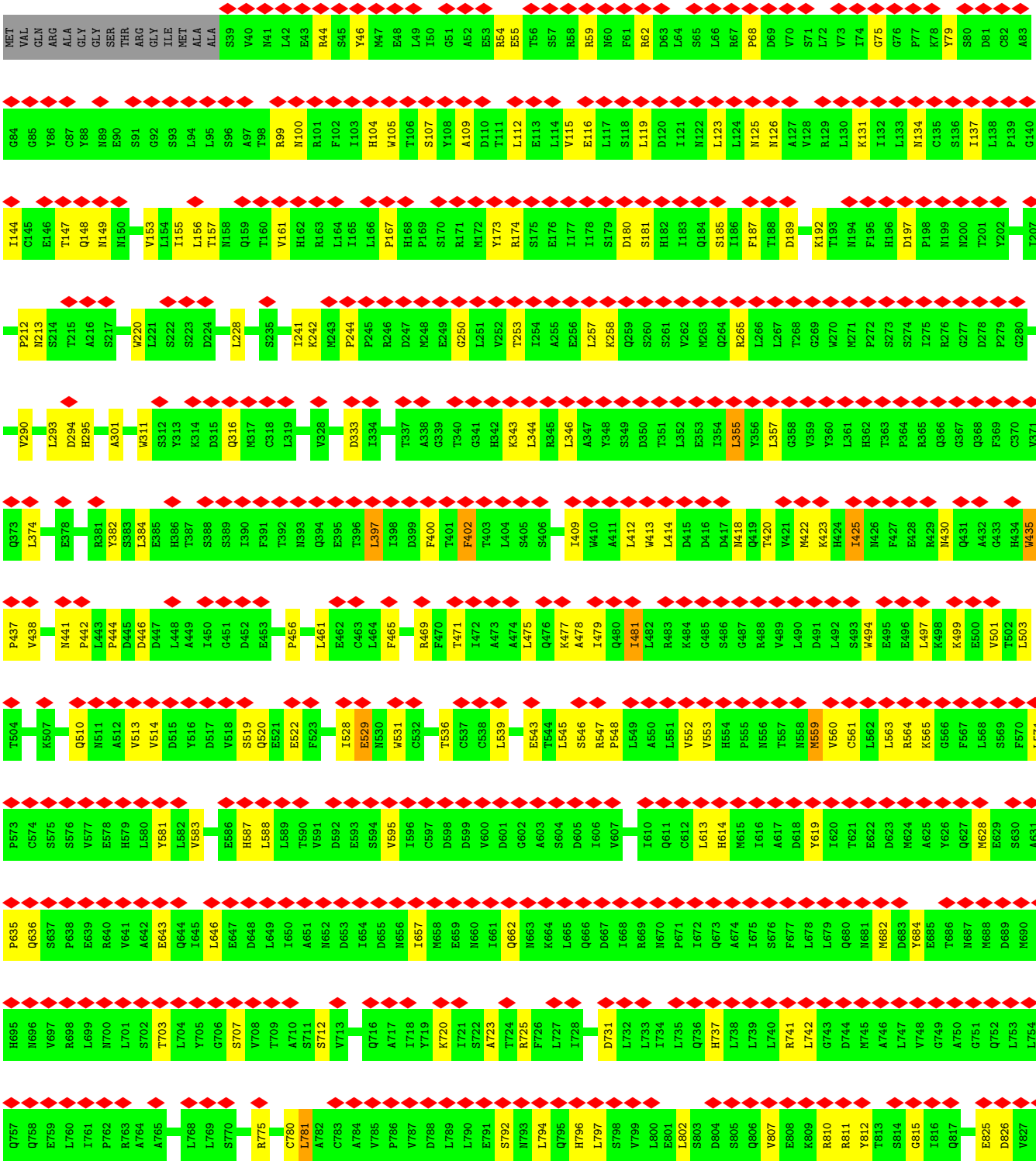
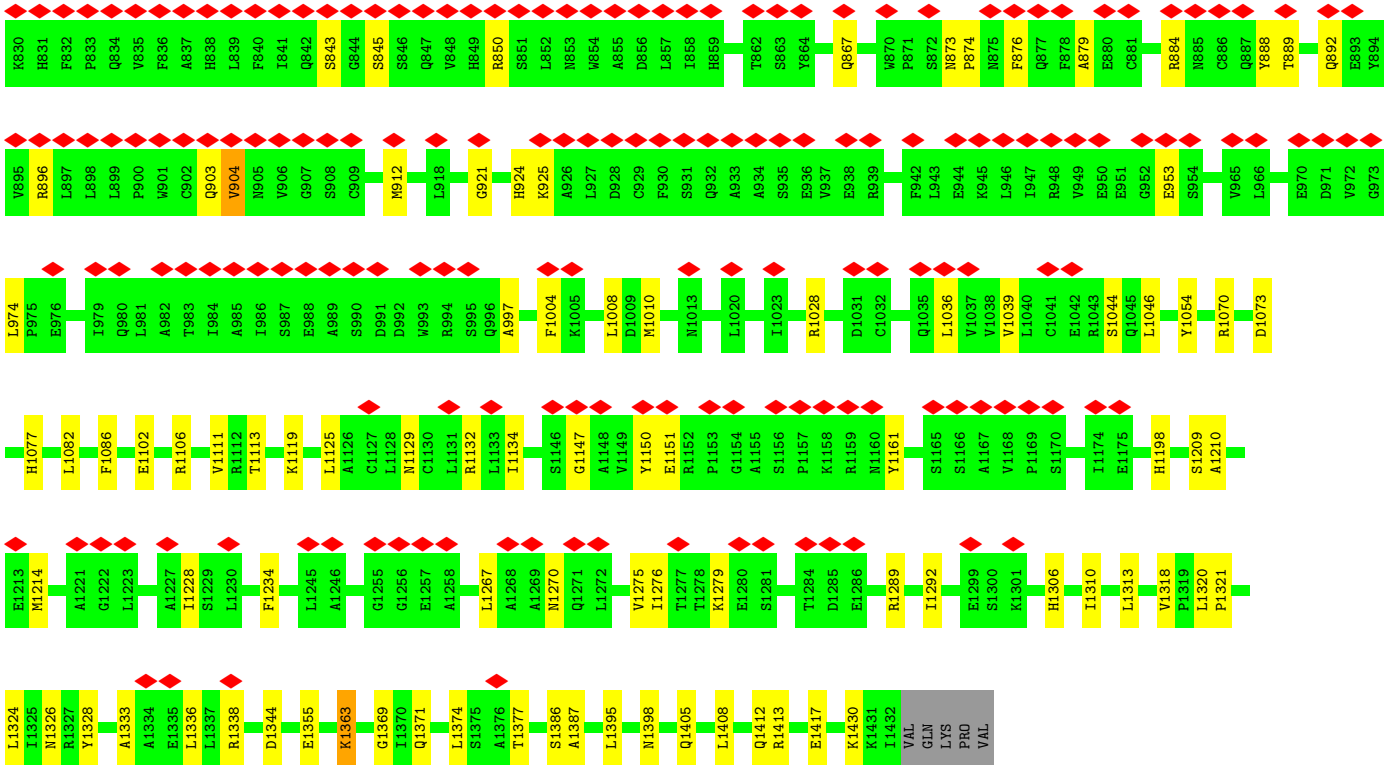
S179 D180 S181 H182 I183 Q184 S185 I186 F187 T188 D189 I190 D197 P198 Y202 V203 I204 I207 P208 G209 R210 A211 P212 T215 A216 S217 T218 A219 W220 L221 S222 S223 A230 L231 P232 S233 G237 I238 L239 M243 R246 L251 V252 L257 K258 Q259 S260 S261 V262 M263
Q264 R265 L266 L267 M271 P272 I275 D278 P279 L284 P285 V286 S287 L288 A289 V290 L293 D294 H295 D296 S297 Y298 L299 F300 A301 L302 H306 K307 M310 C318 L319 M320 V321 M324 Y327 A338 G341 H342 K343 L344 R345 L346 A347 T351 L357
Y360 L361 H362 T363 P364 V371 F372 Q373 E378 S379 N380 L384 E385 H386 T396 L397 I398 D399 F400 T401 F402 T403 L404 S405 S406 M407 N408 I409 W410 A411 L412 W413 L414 D415 D416 D417 N418 Q419 T420 V421 M422 K423 H424 R429 A432 G433 H434 W435 N436 P437 V438 F439 V440 N441
P442 L443 P444 I450 G451 D452 E455 E458 A459 Y460 L461 E462 C463 L464 F465 A466 R469 F470 T471 I472 A473 A474 Q480 R483 K484 G485 S486 G487 R488 V489 L490 D491 L492 S493 E496 L497 K498 K499 E500 Q510 V514 Q520 E521 E522 F523 R524 N530 W531
F534 Y535 C538 L539 Q540 L545 S546 L551 V552 V553 N556 T557 N558 M559 V560 C561 K565 G566 F567 L568 S569 F570 L571 A572 P573 C574 S575 S576 H579 L580 Y581 L582 V583 D592 V595 D598 D599 V600 D601 L609 I610 Q611 C612 L613 H614 M615 I616 A617 D618 Y619
I620 T621 E622 D623 M624 A625 Y626 P635 Q636 S637 P638 E639 R640 E643 G644 I645 L646 E647 D648 D655 N656 I657 M658 E659 N660 I661 Q662 N663 K664 L665 I668 R669 N670 P671 I672 Q673 A674 I675 S676 F677 L678 L679 Q680 N681 M682 D683 Y684 D689 M690 E691 Q692 S693 Q694 H695 N696
V697 R698 L699 N700 L701 S702 T703 L704 S707 V708 T709 A710 S711 S712 V713 V714 C715 Q716 A717 I718 Y719 R730 D731 L732 L733 I734 L735 Q736 H737 L738 L739 L740 R741 L742 G743 D744 L747 V748 G749 A750 G751 Q752 L753 L754 H755 Q758 E759 L760 I761 P762 R763 A764 A765 L768
V785 P786 L789 L790 L794 Q795 H796 L797 S798 V799 L800 E801 L802 S803 D804 S805 Q806 V807 E808 K809 R810 R811 Y812 T813 S814 G815 I816 I819 V820 E821 L822 E825 D826 K830 Q834 V835 F836 A837 H838 I841 Q842 S845 R850 S851 L852 N853 W854 A855 D856 L857 I858
H859 T862 L865 L866 F876 Q877 F878 R884 T889 Q892 E893 L897 L898 L899 P900 W901 C902 Q903 V904 N905 V906 G907 S908 G921 L927 F930 S931 A934 S935 E936 V937 E938 R939 E940 E953 R958 Y962 V965 L974 P975 E976 L977 V978
L981 A982 T983 I984 A985 I986 S987 E988 A989 R1000 T1001 R1002 I1003 F1004 H1007 Q1015 I1023 P1024 D1025 R1028 Q1029 L1030 V1037 L1040 C1041 D1048 L1049 V1050 E1051 F1052 P1053 Y1054 I1064 R1070 A1071 V1072 D1073 L1074 H1077 K1095 T1098 G1104 L1107 G1108 R1109
R1112 K1119 Q1120 V1121 L1125 L1128 N1129 C1130 L1131 I1141 V1142 Q1143 P1144 V1145 S1146 G1147 A1148 V1149 Y1150 P1153 P1157 K1158 D1162 G1163 E1164 S1165 S1166 A1167 I1174 E1178 L1179 R1180 D1181 K1184 L1188 L1193 T1202 S1208 S1209 M1214 Q1220 A1221 G1222
L1223 F1224 I1228 T1233 L1238 I1241 F1242 E1243 A1246 C1247 R1251 L1252 A1263 A1268 T1277 T1278 K1279 R1289 E1299 N1302 N1311 W1323 A1333 A1334 E1335 R1338 L1339 L1346 E1351 L1352 L1361 G1362 K1363 G1369 Y1370 Q1371 S1375 S1378



• Molecule 4: Nucleoporin 160kDa

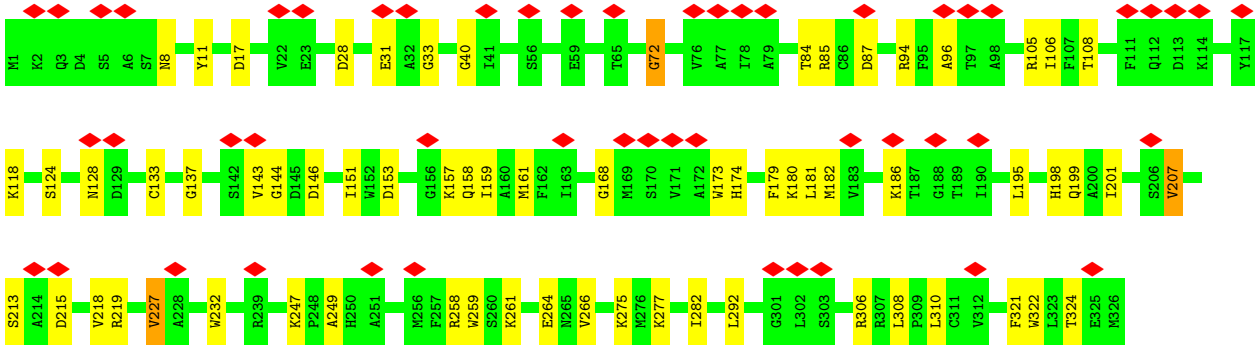
Chain M:





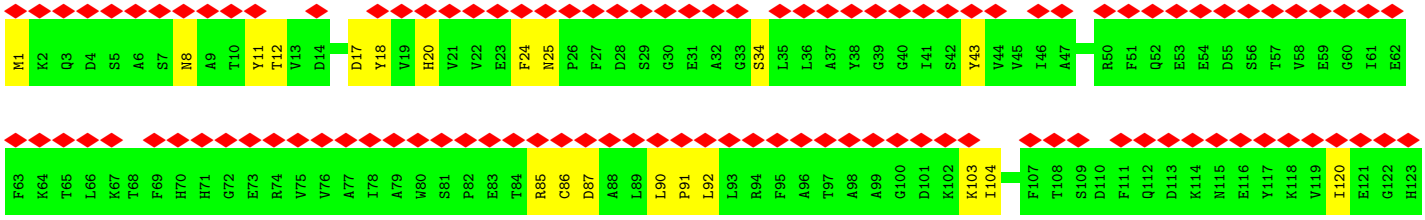
• Molecule 5: MGC83926 protein

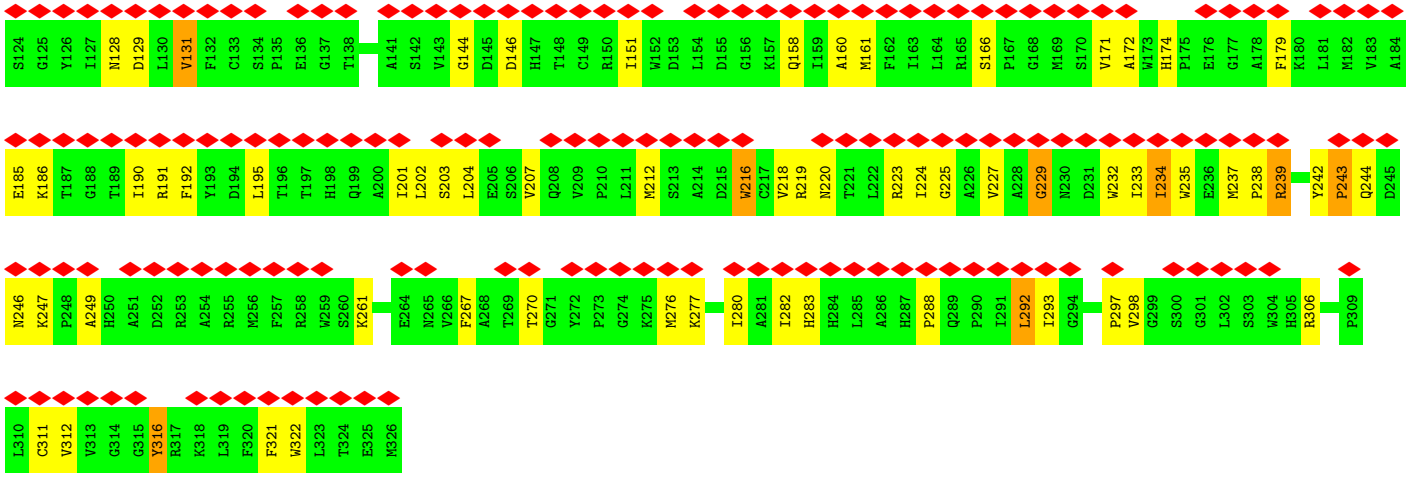
Chain E:



• Molecule 5: MGC83926 protein

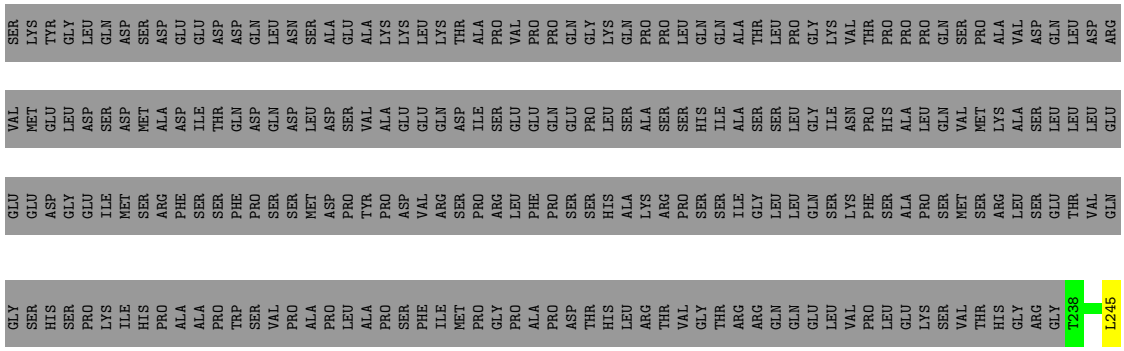
Chain N:

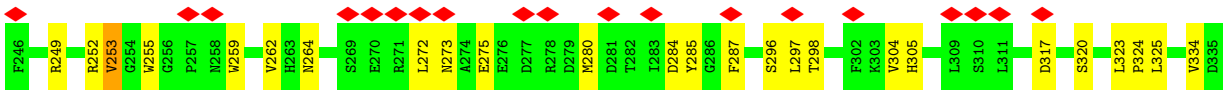


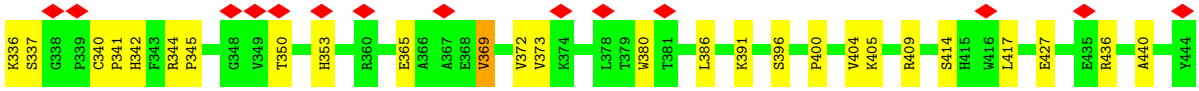


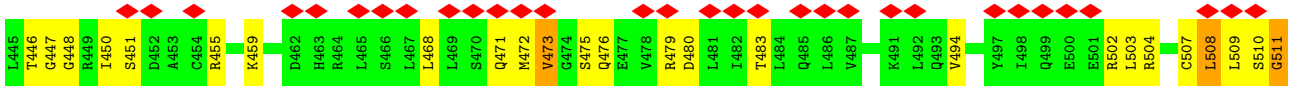
• Molecule 6: Nuclear pore complex protein Nup96

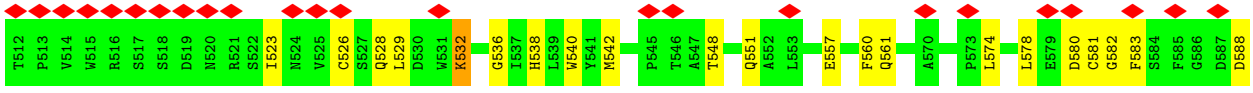
Chain F:

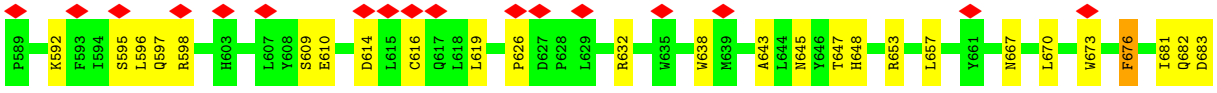




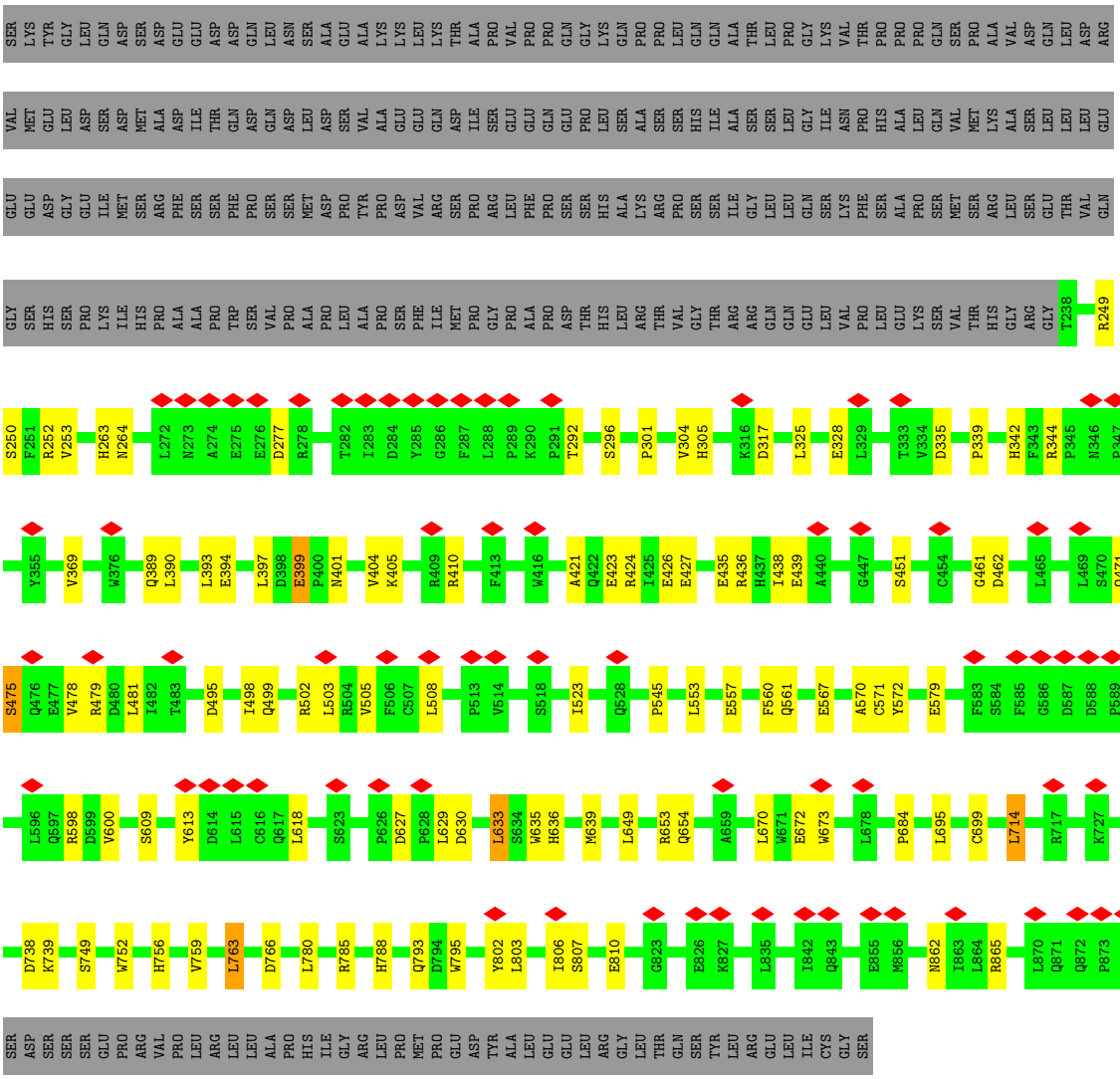




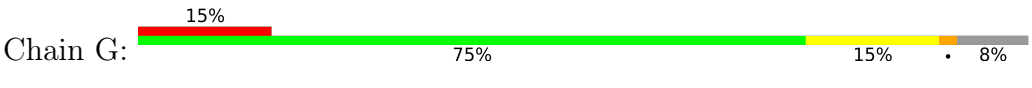


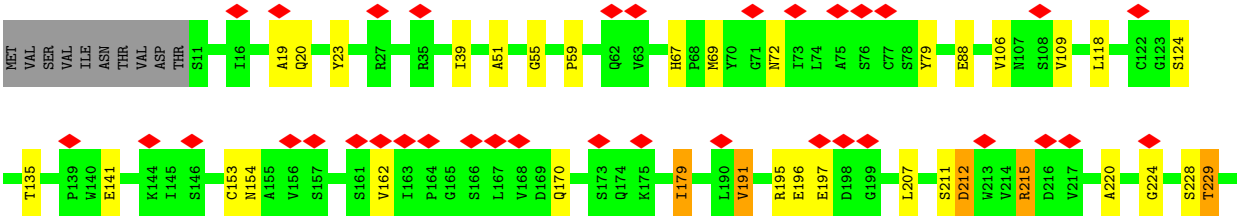


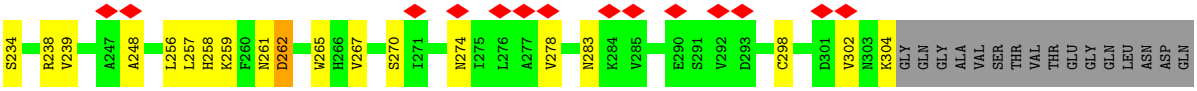
• Molecule 6: Nuclear pore complex protein Nup96



• Molecule 7: GATOR complex protein SEC13

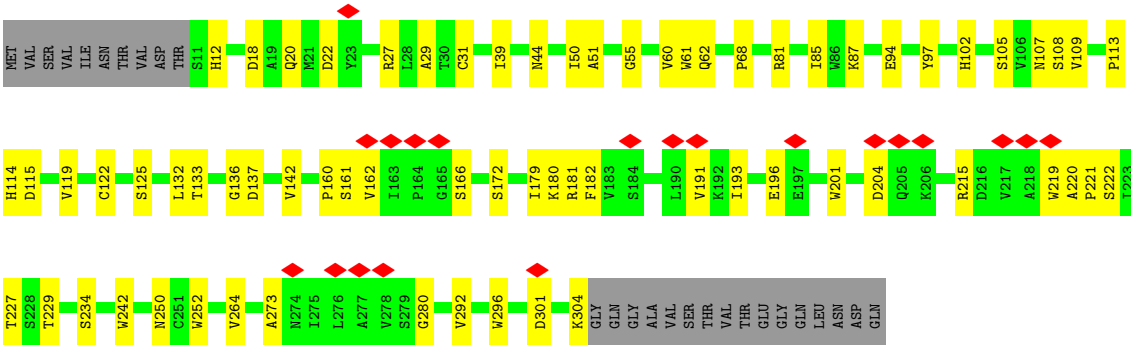






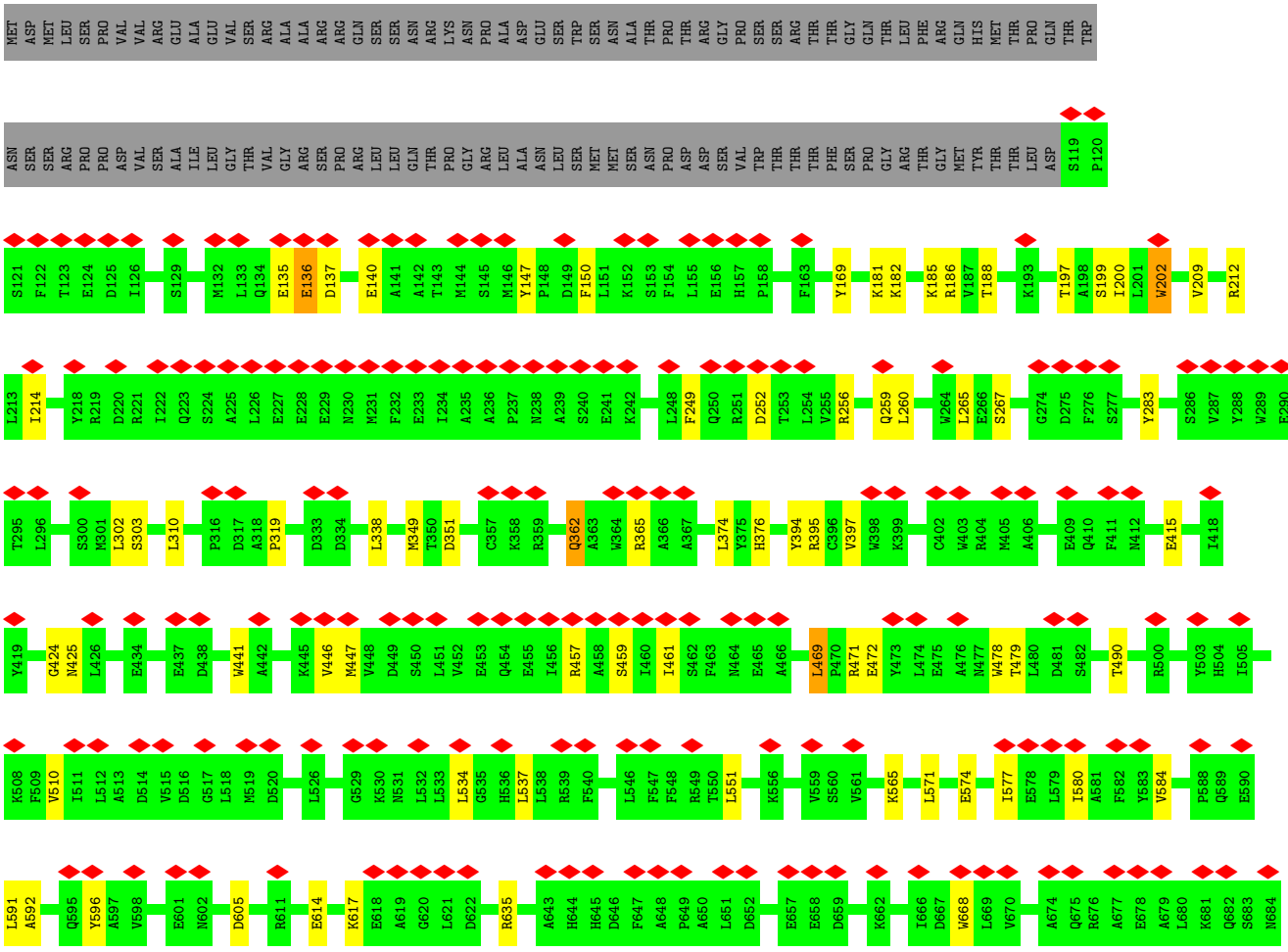
• Molecule 7: GATOR complex protein SEC13

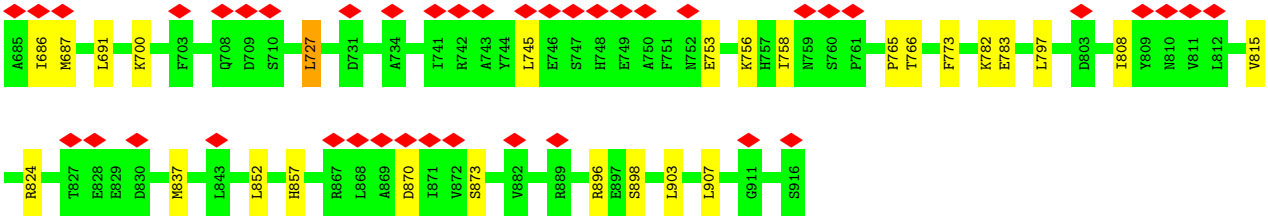
Chain P:



• Molecule 8: Nuclear pore complex protein

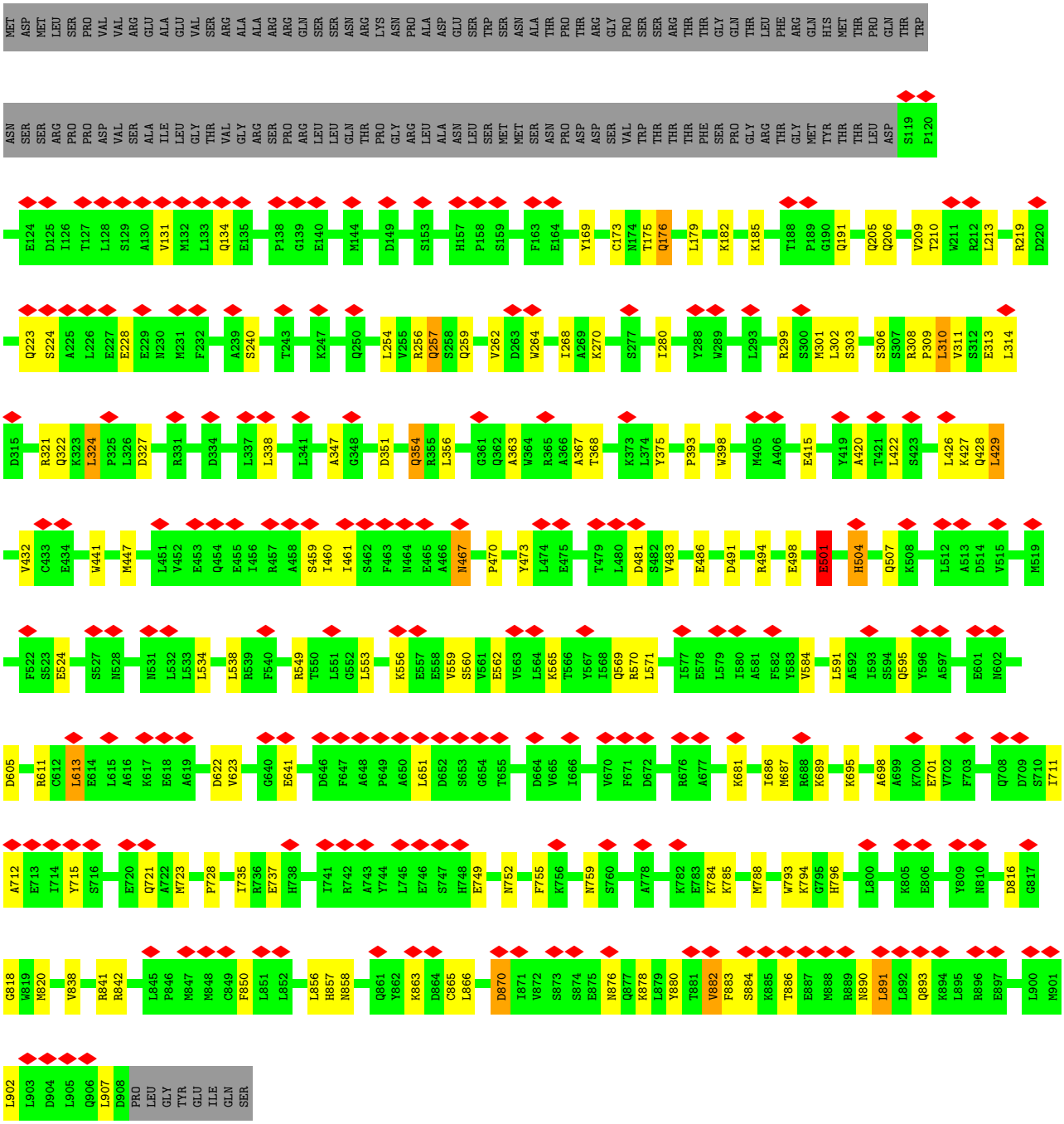
Chain H:





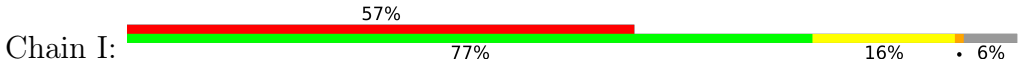
• Molecule 8: Nuclear pore complex protein

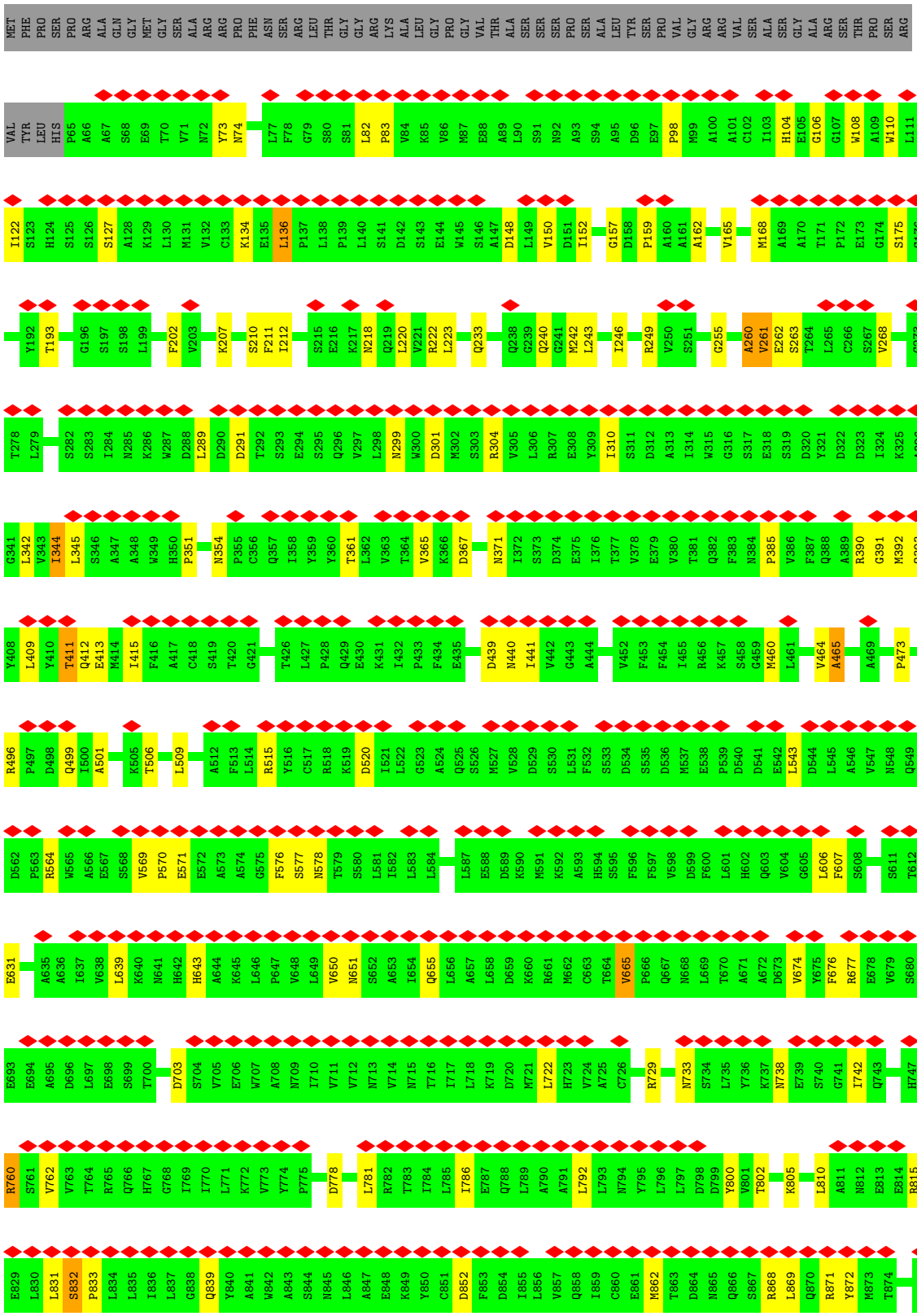
Chain Q:

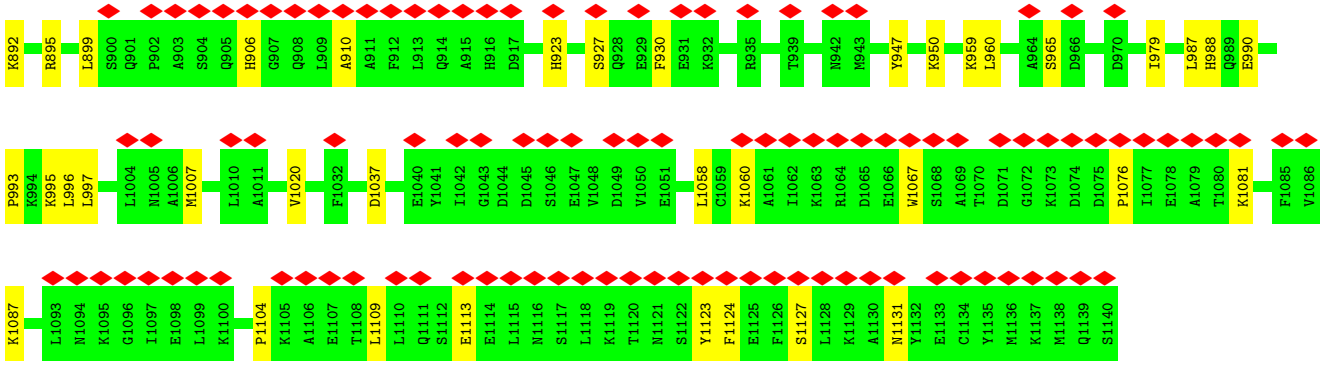


• Molecule 9: outer Nup133

Chain I:

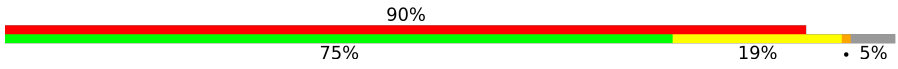


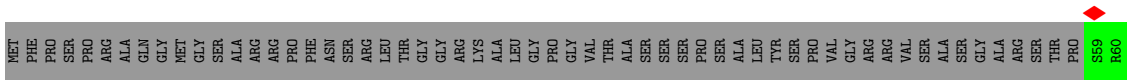


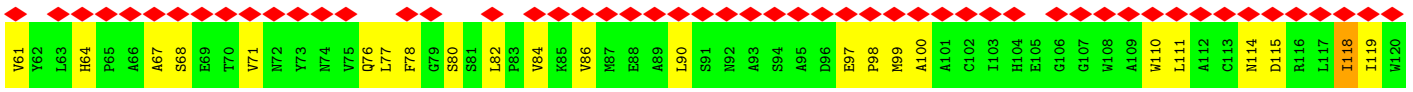


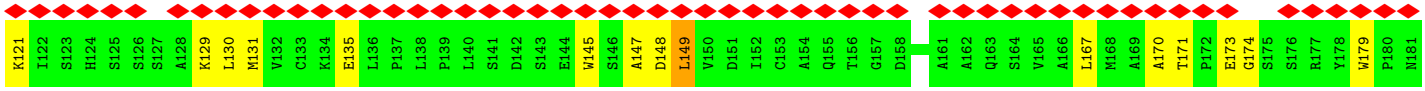
• Molecule 9: outer Nup133

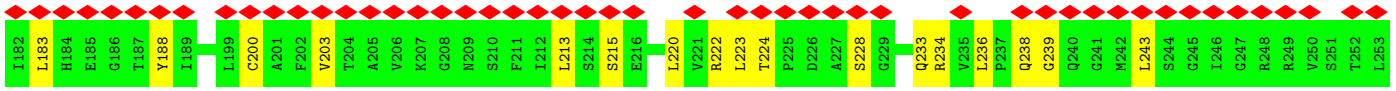
Chain R:

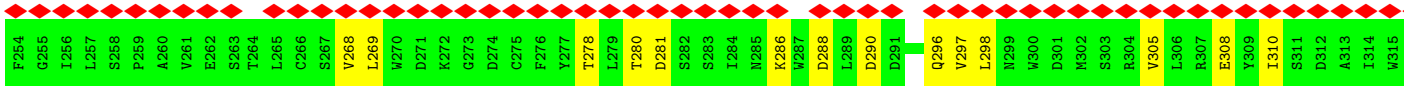


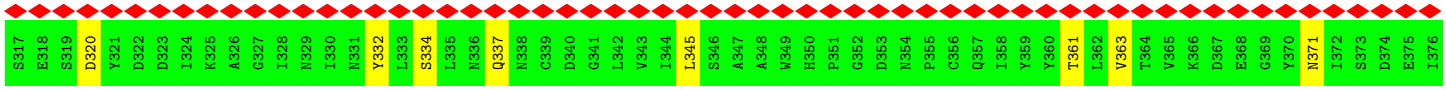


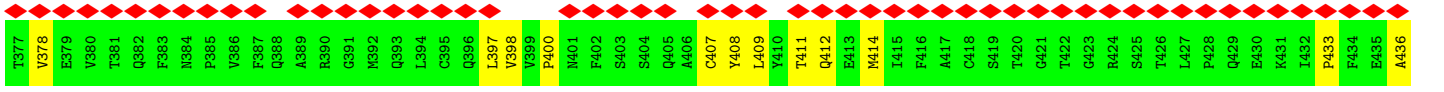


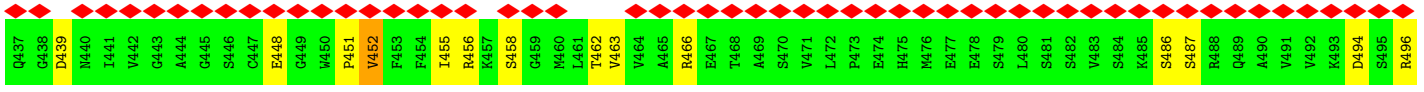


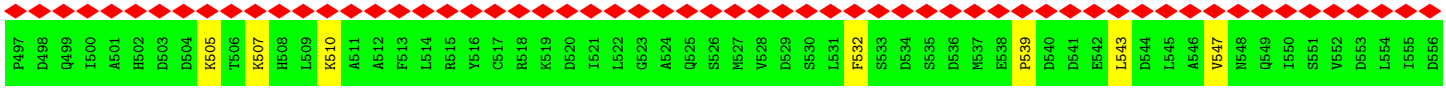


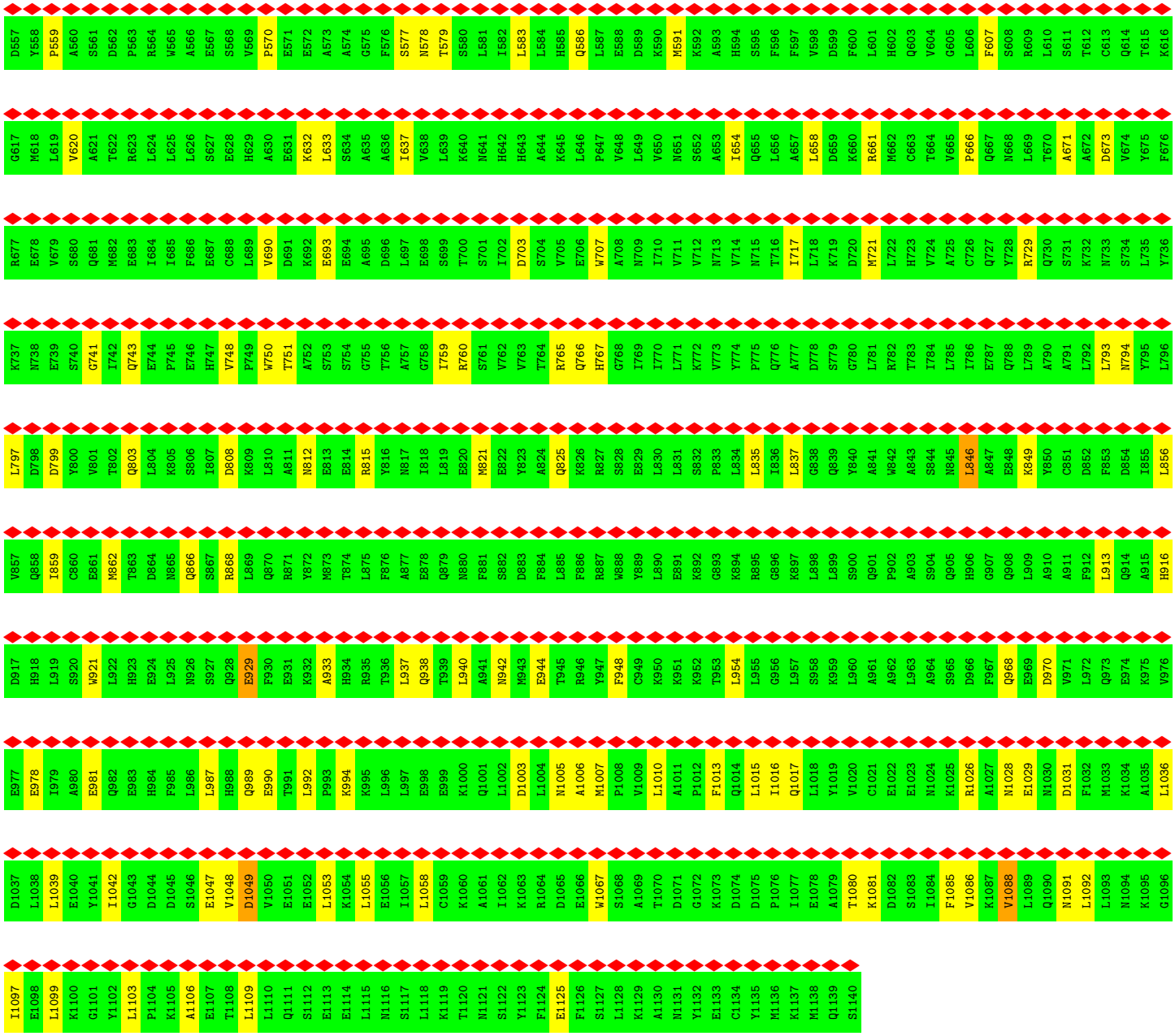






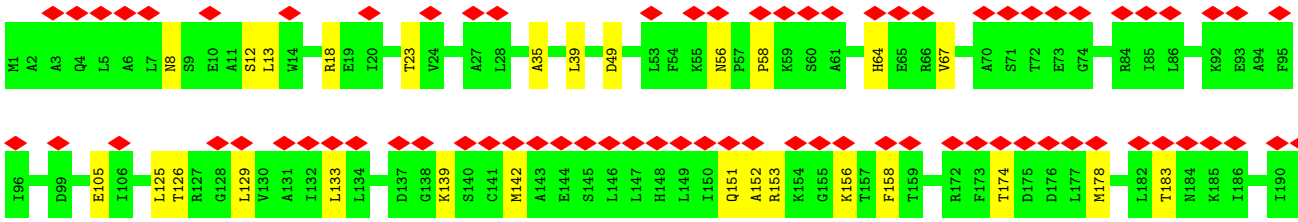


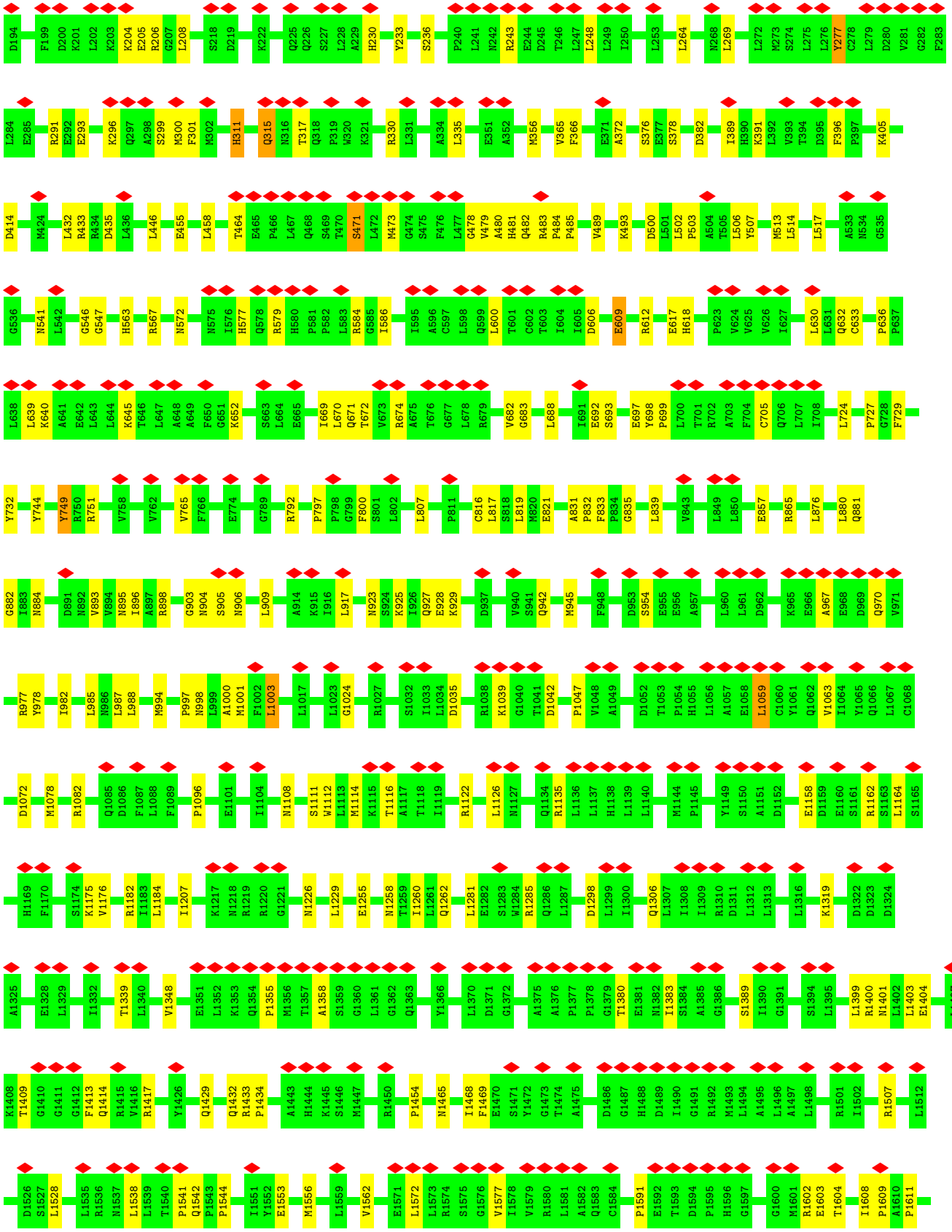




• Molecule 10: MGC83295 protein

Chain S:

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D414 M424 L432 R433 R434 D435 L436 L446 E455 L458 T464 E465 P466 L467 Q468 S469 T470 S471 L472 M473 G474 S475 F476 L477 G478 V479 A480 H481 Q482 R483 P484 P485 V489 K493 D500 L501 L502 P503 A504 T505 L506 Y507 M513 L514 L517 A533 N534 G535
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R977 Y978 I982 L985 N986 L987 L988 M994 P997 N998 L999 A1000 M1001 F1002 L1003 L1017 L1023 G1024 R1027 S1032 I1033 L1034 D1035 R1038 K1039 G1040 T1041 D1042 P1047 V1048 A1049 D1052 T1053 P1054 H1055 L1056 A1057 E1058 L1059 C1060 Y1061 Q1062 V1063 I1064 Y1065 Q1066 L1067 C1068
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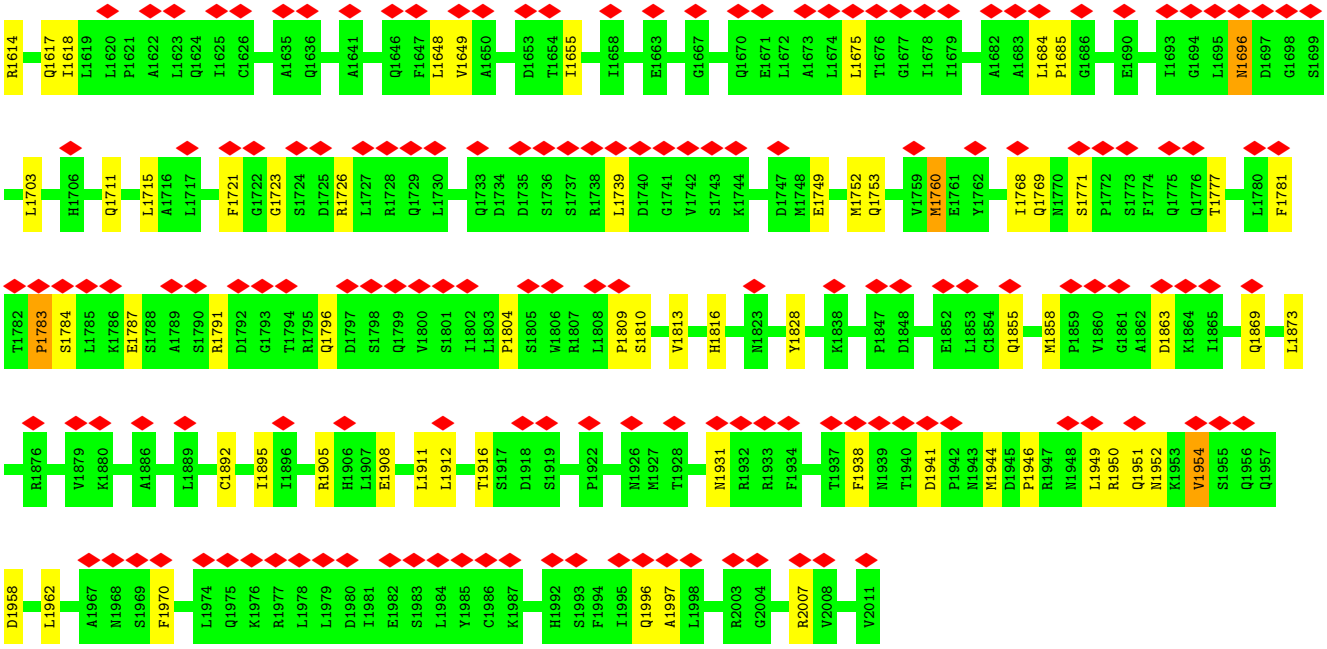
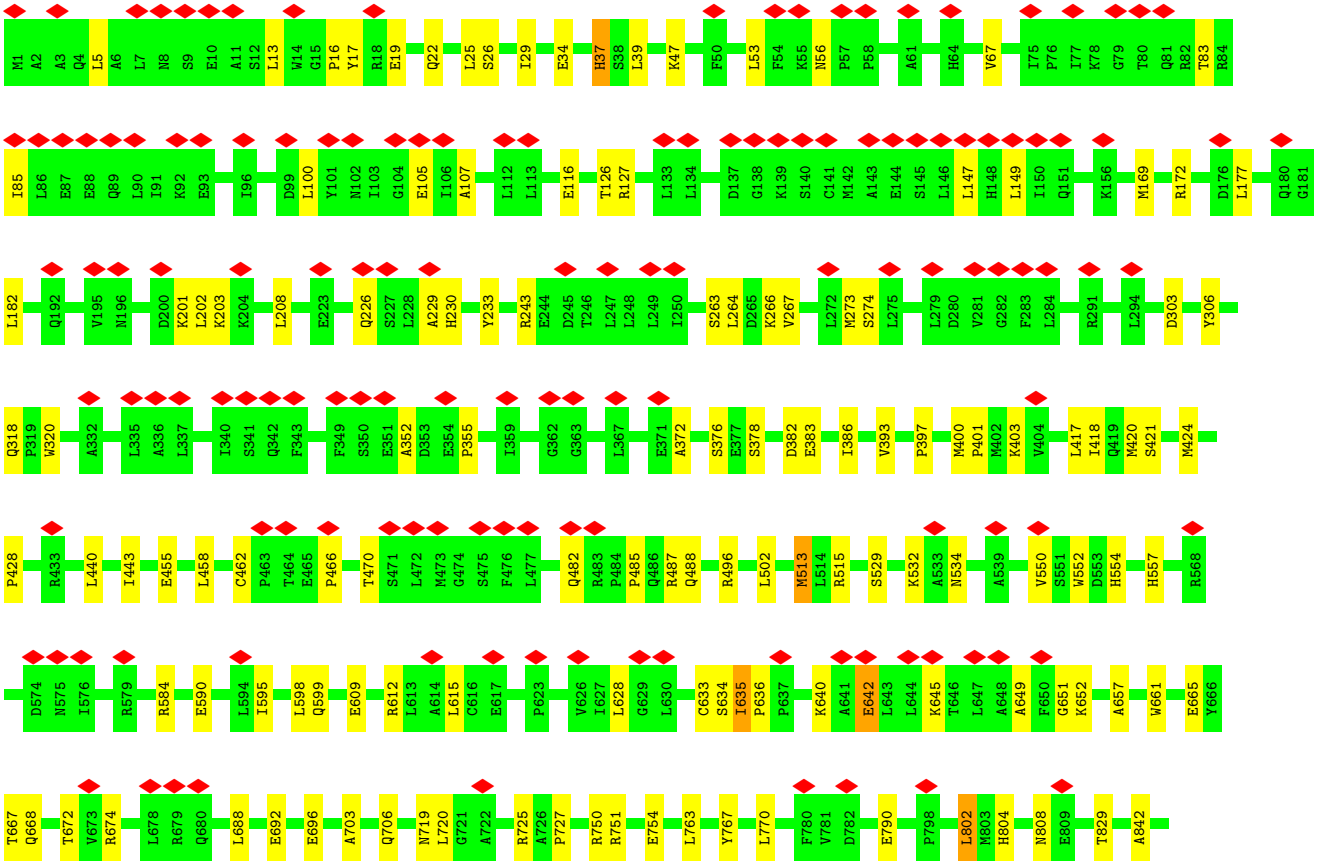
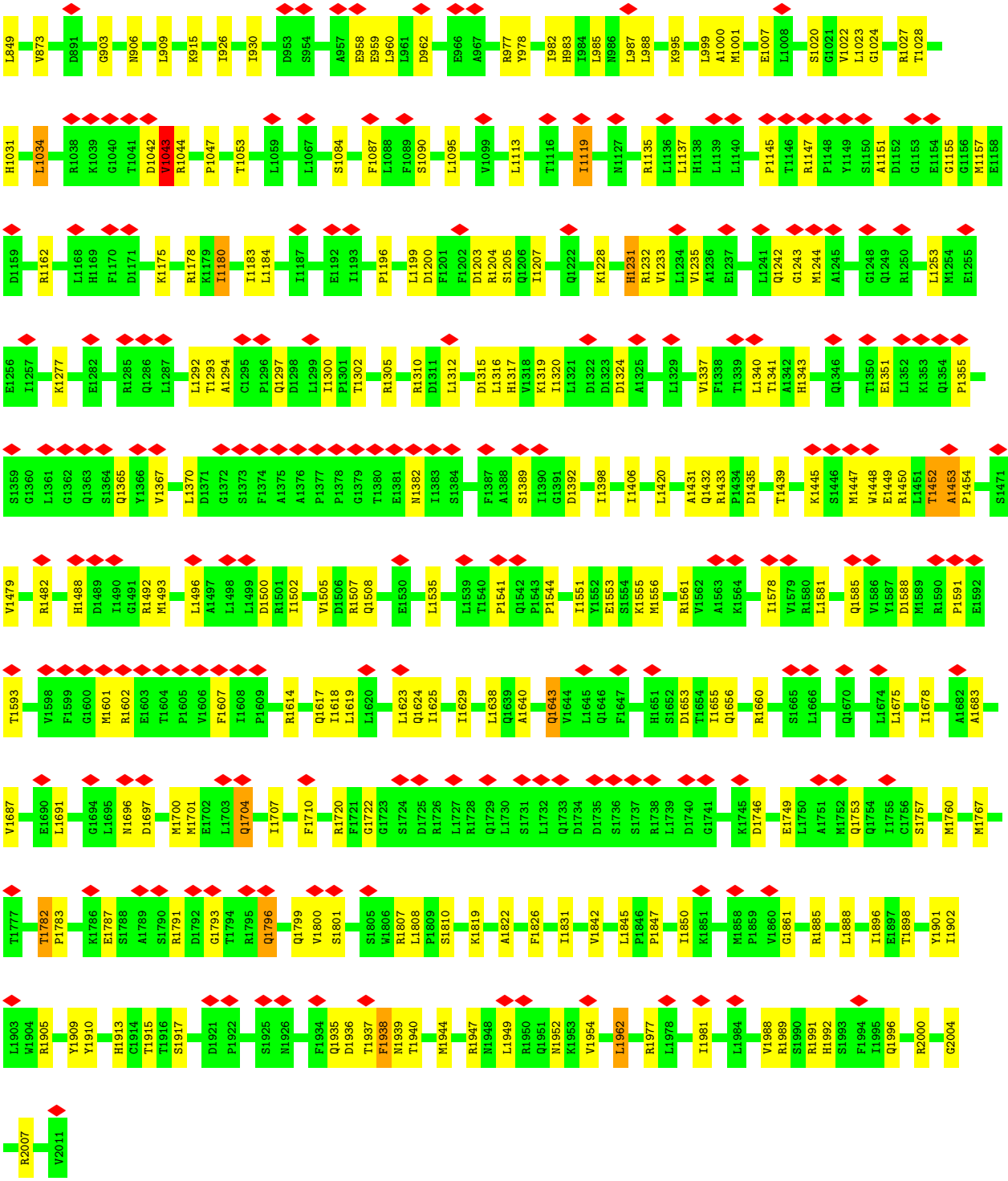
H1169 F1170 S1174 K1175 V1176 R1182 I1183 L1184 I1207 K1217 N1218 R1219 R1220 G1221 N1226 L1229 E1255 N1258 T1259 I1260 L1261 Q1262 L1281 E1282 S1283 W1284 R1285 Q1286 L1287 D1298 L1299 I1300 Q1306 L1307 I1308 I1309 R1310 D1311 L1312 L1313 L1316 K1319 D1322 D1323 D1324
A1325 E1328 L1329 I1332 T1339 L1340 V1348 E1351 L1352 K1353 Q1354 P1355 M1356 T1357 A1358 S1359 G1360 L1361 G1362 Q1363 Y1366 L1370 D1371 G1372 A1375 A1376 P1377 P1378 G1379 T1380 E1381 N1382 I1383 S1384 A1385 G1386 S1389 I1390 G1391 S1394 L1395 L1399 R1400 N1401 L1402 L1403 E1404 L1407
K1408 T1409 G1410 G1411 G1412 F1413 Q1414 R1415 V1416 R1417 Y1426 Q1429 Q1432 R1433 P1434 A1443 H1444 K1445 S1446 M1447 R1450 P1454 N1465 I1468 F1469 E1470 S1471 Y1472 G1473 T1474 A1475 D1486 G1487 H1488 D1489 I1490 G1491 R1492 M1493 L1494 A1495 L1496 A1497 L1498 R1501 I1502 R1507 L1512
D1526 S1527 L1528 L1535 R1536 N1537 L1538 L1539 T1540 P1541 Q1542 P1543 P1544 I1551 Y1552 E1553 M1556 L1559 V1562 E1571 L1572 L1573 R1574 S1575 G1576 V1577 I1578 V1579 R1580 L1581 A1582 Q1583 C1584 P1591 E1592 T1593 D1594 P1595 H1596 G1597 G1600 M1601 R1602 E1603 T1604 I1608 P1609 A1610 P1611



- Molecule 10: MGC83295 protein

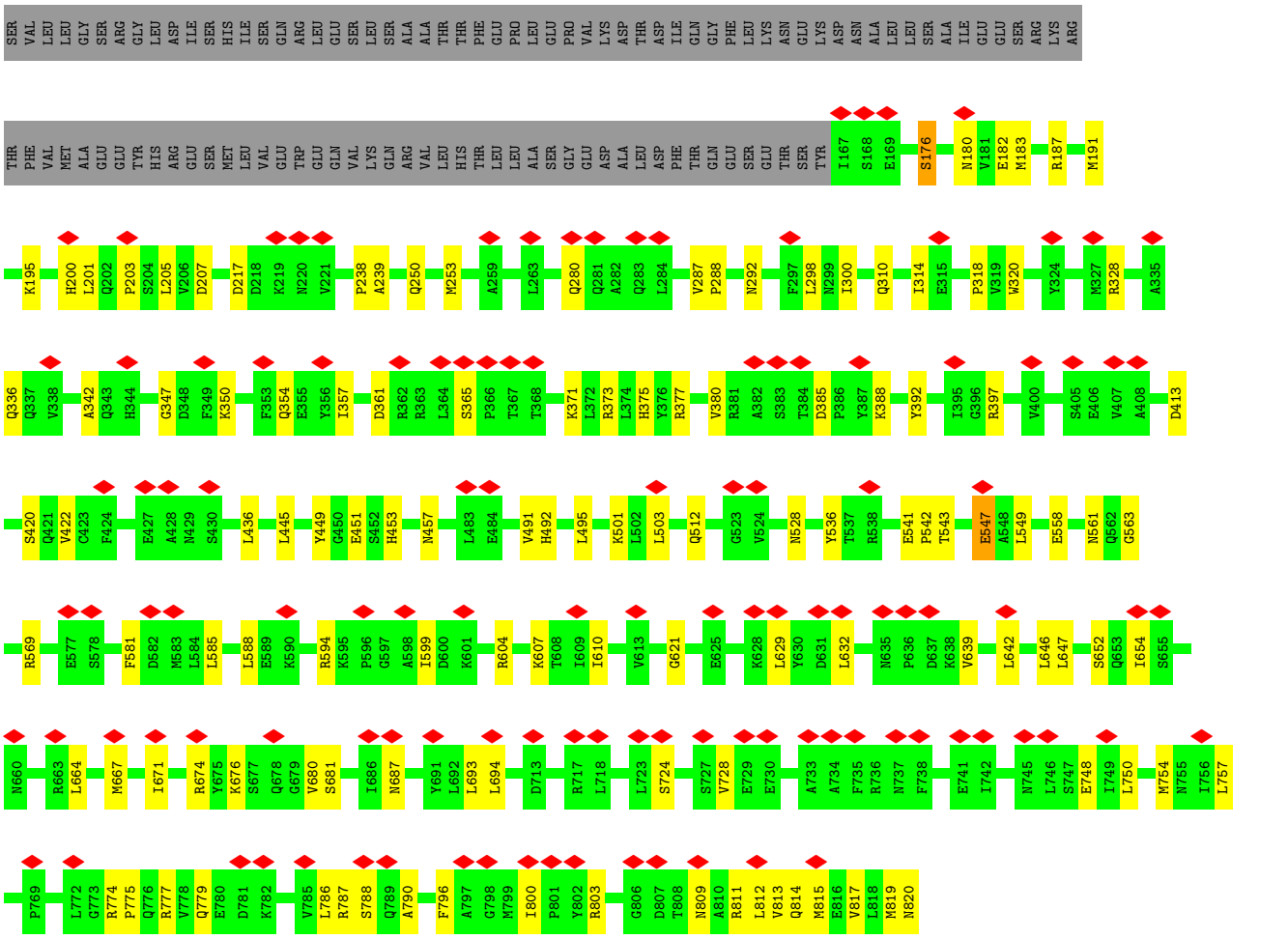
Chain T:





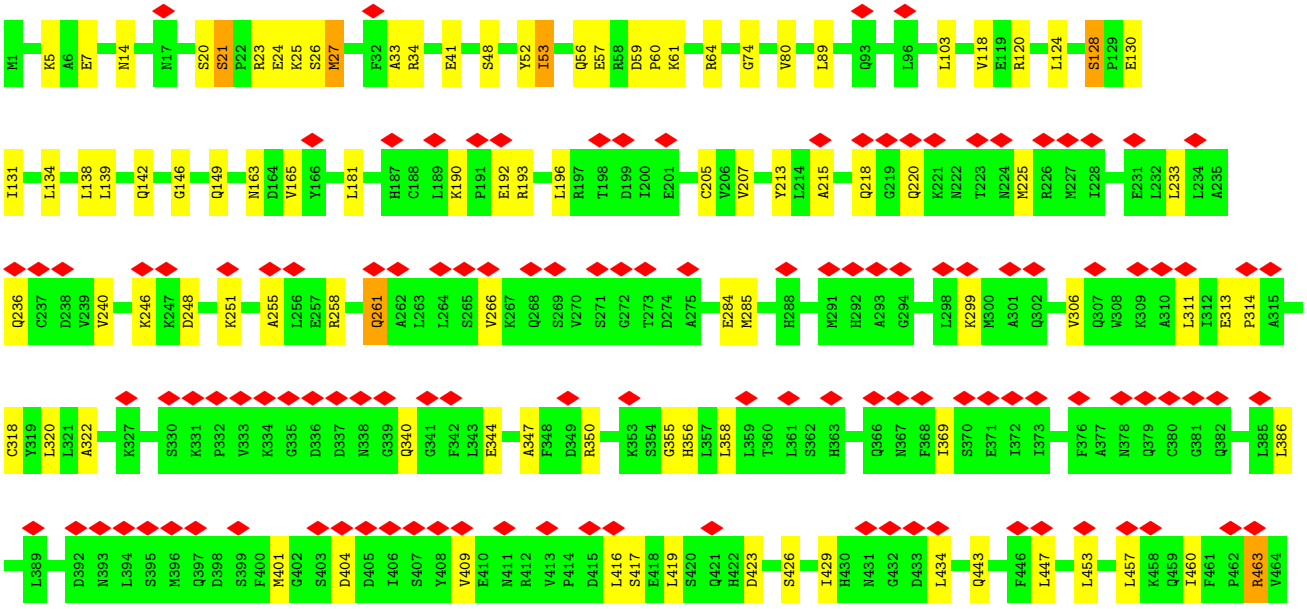
• Molecule 11: Nuclear pore complex protein Nup93

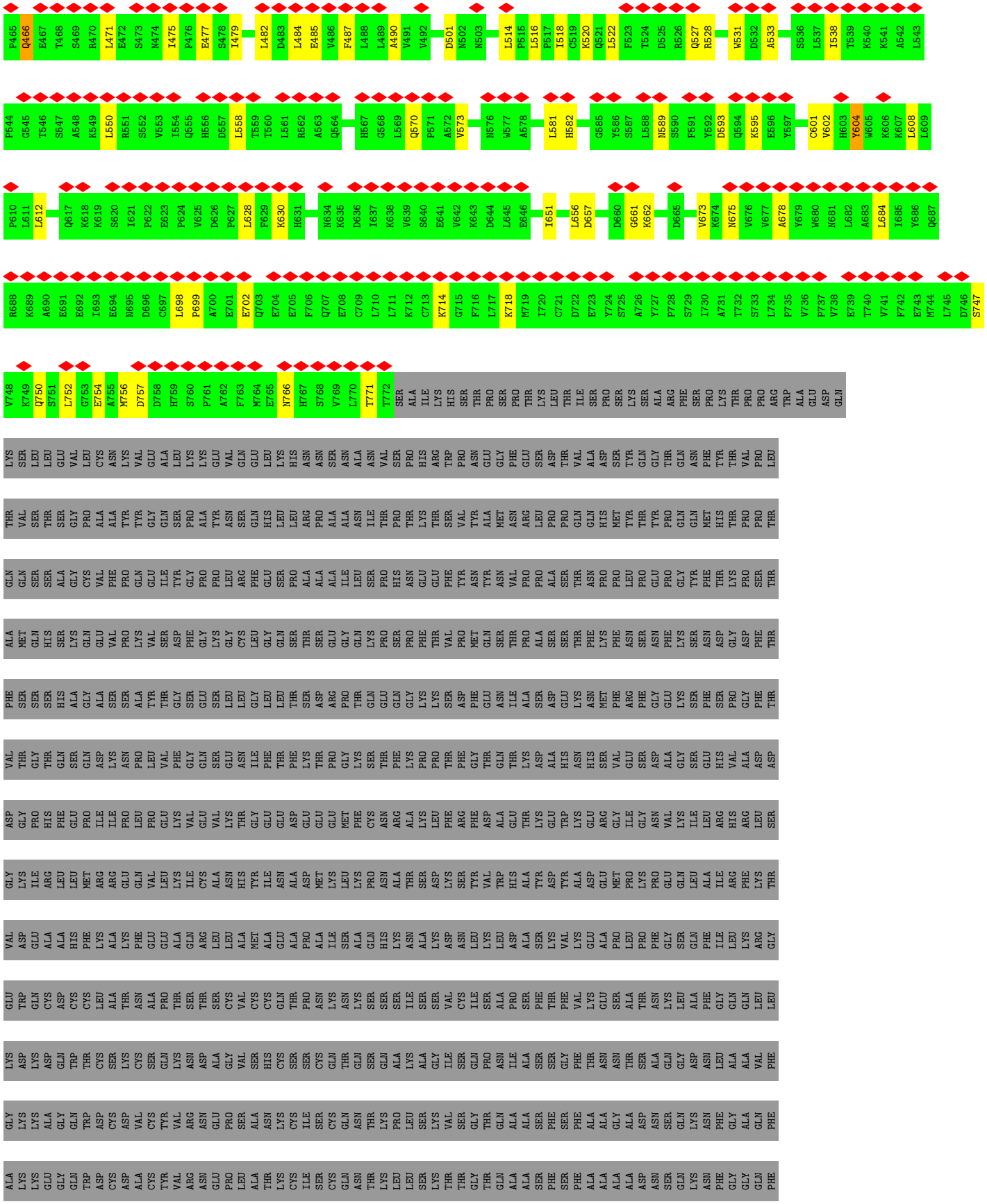
Chain U:



• Molecule 12: Nup358

Chain V:

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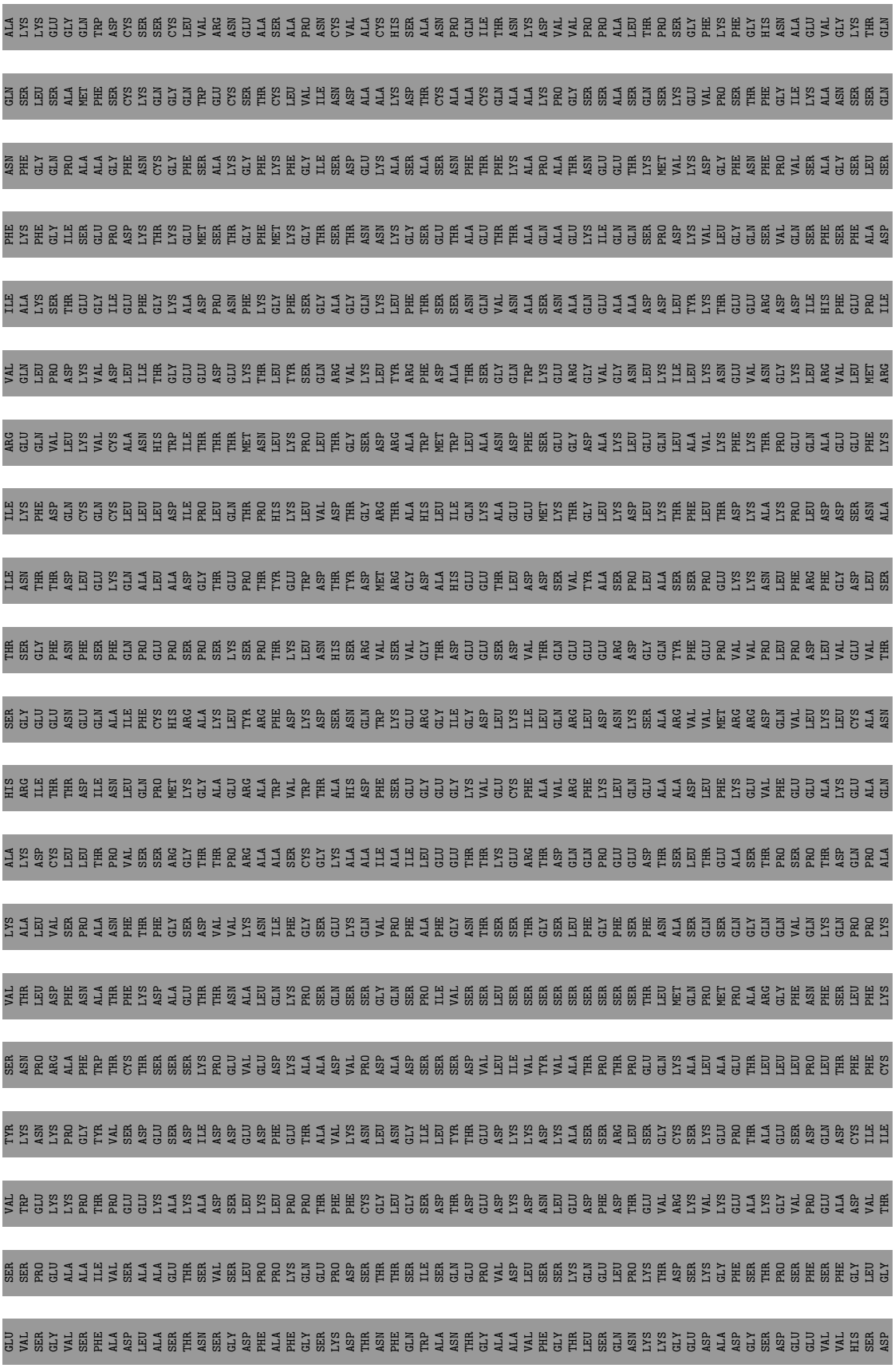
P544 G545 T546 S547 A548 K549 L550 R551 S552 V553 T554 Q555 H556 D557 L558 T559 T560 L561 R562 A563 Q564 H567 G568 L569 Q570 P571 A572 V573 N576 W577 A578 L581 H582 G585 Y586 S587 L588 N589 S590 F591 Y592 D593 Q594 K595 E596 Y597 C601 V602 H603 Y604 W605 K606 K607 L608 L609
P610 L611 L612 Q617 K618 K619 S620 I621 P622 E623 P624 V625 D626 P627 L628 F629 K630 H631 N634 K635 D636 I637 K638 V639 S640 E641 V642 K643 D644 L645 E646 I651 L656 D657 D660 G661 K662 D665 V673 K674 N675 V676 V677 A678 Y679 W680 N681 L682 A683 L684 I685 Y686 Q687
R688 K689 A690 E691 E692 I693 E694 N695 D696 C697 L698 P699 A700 E701 E702 Q703 E704 E705 F706 Q707 E708 C709 L710 L711 K712 C713 K714 G715 F716 L717 K718 M719 I720 C721 D722 E723 Y724 S725 A726 Y727 P728 S729 I730 A731 T732 S733 L734 P735 V736 P737 V738 E739 T740 V741 F742 E743 M744 L745 D746 S747
V748 K749 Q750 S751 L752 G753 E754 A755 M756 D757 D758 H759 S760 P761 A762 F763 M764 E765 N766 H767 S768 V769 L770 T771 T772 SER ALA ILE LYS HIS SER THR PRO SER PRO THR LYS LEU THR ILE SER PRO SER PRO LYS SER ALA ARG PHE SER PRO LYS THR PRO PRO ARG TRP ALA GLU ASP GLN
LYS SER LEU LEU GLU VAL LEU CYS ASN LYS VAL GLU ALA LEU LYS LYS GLU VAL GLN GLU LEU LYS HIS ASN ASN SER ASN ALA ASN VAL SER PRO HIS ARG TRP PRO ASN GLU GLY PHE GLU SER ASP THR VAL ALA ASP SER TYR GLN GLY THR GLN ASN PHE TYR THR VAL PRO LEU
THR VAL SER THR SER GLY PRO ALA ALA ALA TYR TYR GLY GLN SER PRO ALA TYR ASN SER GLN HIS LEU LEU ARG PRO ALA ALA ALA ASN ILE THR PRO THR LYS THR SER VAL TYR ALA MET ASN ARG LEU PRO PRO GLN GLN HIS MET TYR THR TYR PRO GLN GLN MET HIS THR PRO PRO THR
GLN GLN SER SER ALA GLY CYS VAL PHE PRO GLN GLU ILE TYR GLY PRO PRO LEU ARG PHE GLU SER PRO ALA ALA ALA ILE LEU SER PRO HIS ASN GLU GLU PHE TYR ASN TYR ASN VAL PRO PRO ALA SER SER THR ASN PRO PRO LEU PRO GLU PRO GLY TYR PHE THR LYS PRO SER THR
ALA MET GLN HIS SER LYS GLN GLU VAL PRO LYS VAL SER ASP PHE GLY LYS GLY CYS LEU GLY GLN SER THR SER GLU GLY GLN GLY LYS PRO SER PRO PHE THR VAL PRO MET GLN SER THR PRO ALA SER SER THR PHE LYS PHE ASN SER ASN PHE LYS SER ASN ASP GLY ASP PHE THR
PHE SER SER SER HIS ALA GLY ALA SER SER ALA TYR THR GLY SER GLU SER LEU LEU GLY GLY LEU LEU THR SER ASP ARG PRO THR GLN GLU GLN GLY GLY LYS LYS SER ASP PHE GLU ASN ILE ALA SER ASP GLU LYS ASN MET PHE ARG PHE GLY GLU LYS SER PHE SER PRO GLY PHE THR
VAL THR GLY THR GLN SER GLN ASP LYS ASN PRO LEU VAL PHE GLY GLN SER GLU VAL ASN ILE PHE THR PHE LYS THR PRO GLY LYS SER THR PHE LYS ASP ALA HIS ASN HIS SER VAL GLU SER ASP ALA GLY SER GLU HIS VAL ALA ASP ASP
ASP GLY PRO HIS PHE GLU PRO LEU PRO GLU LYS VAL GLU VAL LYS THR GLY GLU GLU ASP GLU GLU MET PHE CYS ASN ARG ALA LYS LEU PHE ARG PHE ASP ALA GLU THR LYS GLU TRP LYS GLU ARG GLY ILE GLY ASN VAL LYS ILE LEU ARG HIS ARG LEU SER
GLY LYS ILE ARG LEU LEU MET ARG GLU GLN VAL LEU LYS ILE CYS ALA ASN HIS TYR ILE ASN ALA ARG ASP MET LYS LEU LYS PRO ASN ALA THR SER ASP LYS SER TYR VAL TRP HIS ALA TYR ASP TYR ALA ASP GLU MET PRO LYS PRO ASN ALA GLU GLN LEU ALA ILE ARG PHE LYS THR
VAL ASP GLU ALA HIS PHE LYS ALA LYS PHE GLU GLU ALA GLN ARG LEU LEU ALA MET ALA GLU ALA PRO ALA ILE SER ALA GLN HIS LYS ASN LEU LYS LEU ASP ALA ALA SER LYS VAL LYS GLU ALA PRO LEU PRO PHE GLY SER GLN PHE ILE LEU LYS ARG GLY
GLU TRP GLN CYS ASP CYS CYS LEU ALA THR ASN ALA PRO THR CYS SER ILE SER CYS GLN THR PRO ASN LYS ASN LYS SER SER SER GLN ALA LYS ASN ILE SER THR SER ALA PRO SER PHE THR PHE VAL LYS GLU ALA SER ALA THR ASN LYS LEU GLU LEU ALA PHE GLY GLN GLN LEU LEU
LYS ASP LYS ASP GLN TRP THR CYS SER CYS SER CYS SER LYS SER CYS GLN THR GLN SER GLN ALA LYS SER ALA GLY ILE SER GLN PRO ASN ILE ALA SER SER GLY PHE THR ASN ASN THR SER ALA GLN GLY ASP ASN LEU ALA ALA VAL PHE
GLY LYS LYS ALA GLY GLN TRP ASP CYS ASP ALA CYS TYR VAL ARG ASN GLU PRO SER ALA ALA ASN LYS CYS ILE SER CYS GLN ASN THR LYS PRO LEU LEU SER LYS THR THR GLY THR GLN ALA ALA ALA SER PHE SER PHE ALA ALA ALA ALA ALA ASP ASN SER GLN LYS ASN PHE GLY GLN PHE
ALA LYS LYS GLU GLY GLN TRP ASP CYS ASP ALA CYS TYR VAL ARG ASN GLU PRO LEU ALA ALA THR LYS CYS ILE SER CYS GLN ASN THR LYS LEU LEU SER LYS THR THR GLY THR GLN ALA ALA ALA SER PHE SER PHE ALA ALA ALA ALA ALA ASP ASN SER GLN LYS ASN PHE GLY GLN PHE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GLN SER LEU SER ALA MET PHE SER CYS LYS GLN GLY GLN TRP GLU CYS SER THR CYS LEU VAL ILE SER ASN ASP ALA ALA LYS ASP THR CYS ALA ALA CYS GLN ALA ALA LYS PRO GLY SER SER ALA SER GLN SER LYS GLU VAL PRO SER THR PHE GLY ILE LYS ALA ASN SER SER GLN
ASN PHE GLY GLN PRO ALA ALA GLY PHE ASN CYS GLY PHE SER ALA LYS ALA SER ASN PHE THR PHE LYS ALA PRO ALA THR ASN GLU GLU THR LYS ILE GLU GLN LEU SER ASP GLY PHE LYS PHE GLY ILE SER ASP GLU LYS ALA SER ALA SER ASN PHE GLY GLN ASN ALA ASP GLY PHE ASN ASN LYS GLY SER GLU THR ASN GLU GLN GLN SER PRO ASP LYS VAL LEU GLY GLN SER PHE ASN PHE PRO VAL LYS ASP GLY PHE SER THR PHE GLY ILE LYS ALA ASN SER SER
PHE LYS PHE GLY ILE SER GLU PRO ASP LYS THR THR GLU MET SER THR GLY PHE MET LYS GLY THR SER THR ASN GLY GLU GLU THR LYS ILE GLN GLN LEU SER PRO ASP VAL GLN SER PHE SER LEU GLU
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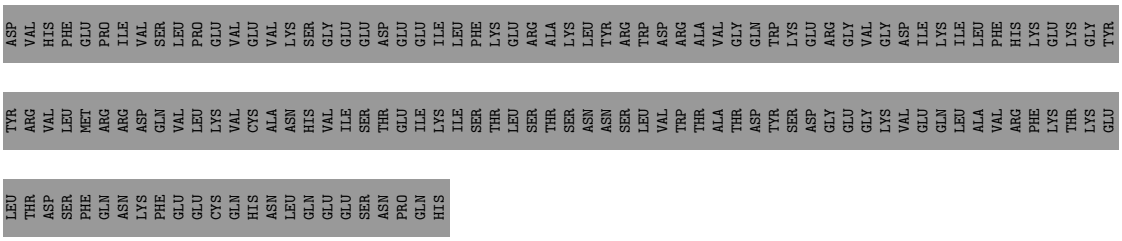
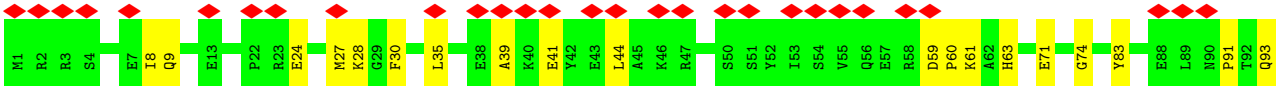
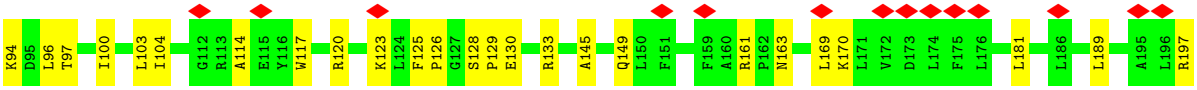
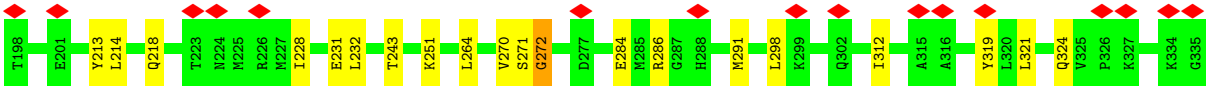


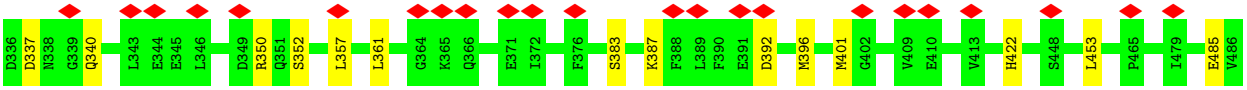
• Molecule 12: Nup358

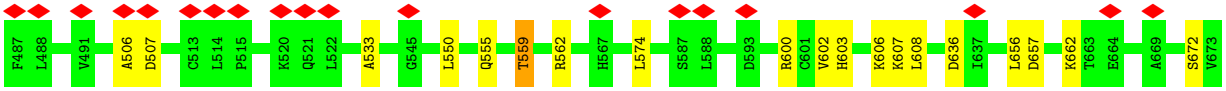
Chain W:

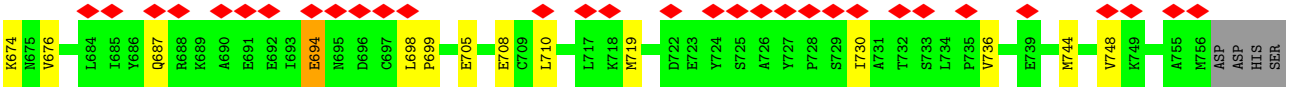


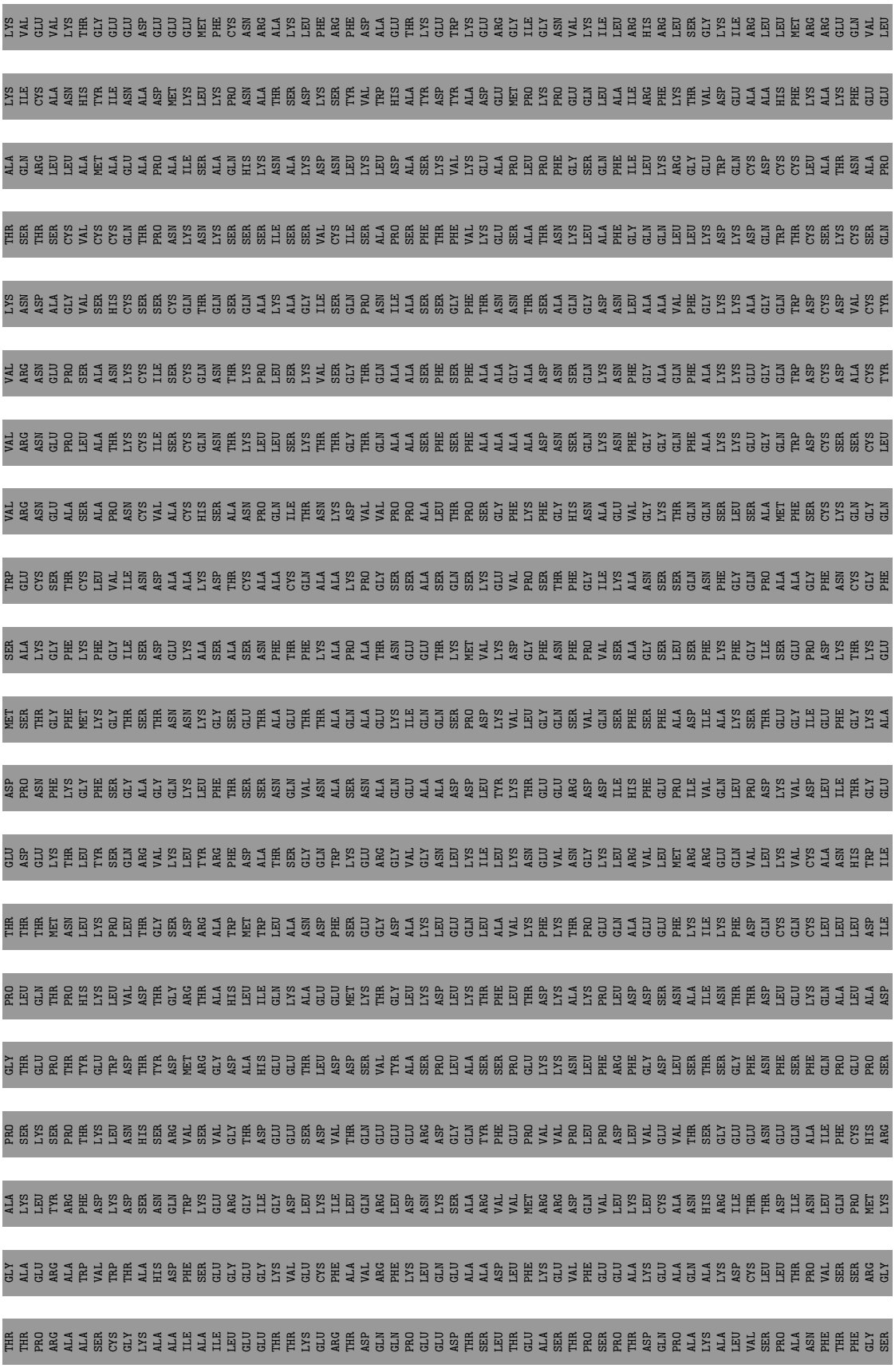








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LYS ILE CYS ALA ASN HIS TYR ILE ASN ALA ASP MET LYS LEU LYS PRO ASN ALA THR SER ASP LYS SER TYR VAL TRP HIS ALA TYR ASP TYR ALA ASP GLU MET PRO LYS PRO GLU GLN LEU ALA ILE ARG PHE LYS THR VAL ASP GLU GLN GLU
ALA GLN ARG LEU LEU ALA MET ALA GLU ALA PRO ALA ILE SER ALA GLN HIS LYS ASN ALA ALA LYS ASP ASN LEU LYS LEU ASP ALA ALA SER LYS VAL GLU TRP GLN CYS CYS ASP HIS PHE LYS ALA ALA THR ASN GLU PRO
THR SER THR SER CYS VAL CYS CYS GLN THR PRO ASN LYS ASN LYS SER SER SER ILE SER ALA PRO PHE THR PHE VAL LYS GLU SER ALA THR ASN LYS LEU ALA PHE GLY LEU LEU LYS ASP GLN TRP THR CYS SER THR ASP LYS ASP
LYS ASN ASP ALA GLY VAL SER HIS CYS SER SER CYS GLN THR GLN SER GLN ALA LYS ALA GLY ILE SER GLN PRO ASN ILE ALA ALA SER SER GLY ASP ASN LEU ALA ALA VAL PHE GLY LYS LYS ALA GLY GLN TRP ASP CYS ASP VAL CYS TYR
VAL ARG ASN GLU PRO SER ALA ASN LYS CYS ILE GLN SER ALA ALA LYS VAL SER GLY THR GLN ALA ALA SER PHE SER PHE ALA GLY GLN PHE ALA LYS LYS LYS ALA GLY GLN TRP ASP CYS ASP ALA CYS TYR
VAL ARG ASN GLU PRO LEU ALA THR LYS CYS ILE SER CYS GLN ASN THR LYS LEU LEU SER LYS THR THR GLY THR GLN ALA ALA SER PHE SER PHE ALA GLY GLN PHE ALA LYS LYS GLU GLY GLN TRP ASP CYS SER SER CYS LEU
VAL ARG ASN GLU ALA SER ALA PRO ASN CYS VAL ALA CYS HIS SER ALA ASN PRO GLN ILE THR ASN LYS ASP VAL PRO PRO ALA LEU THR PRO SER GLY PHE LYS PHE GLY HIS ASN ALA GLU VAL GLY LYS THR GLN GLN SER LEU SER ALA MET PHE SER CYS LYS GLN GLY GLN
TRP GLU CYS SER THR CYS LEU VAL ILE ASN ASP ALA ALA LYS ASP THR CYS ALA ALA CYS GLN ALA ALA LYS PRO GLY SER SER ALA SER GLN LYS ASN ALA ILE LYS ASN ASN PHE GLY PHE ASN SER GLN ASN PHE GLY GLY ASN CYS GLY PHE
SER ALA LYS GLY PHE LYS PHE GLY ILE SER ASP GLU LYS ALA SER ALA GLU SER ASN PHE THR PHE LYS ALA ALA PRO ALA THR ASN GLU GLU THR LYS MET VAL LYS ASP GLY PHE ASN PHE PRO VAL SER ALA GLY SER LEU SER PHE LYS PHE GLY ILE SER GLU PRO ASP LYS THR LYS GLU
MET SER THR GLY PHE MET LYS GLY THR SER THR ASN LYS ASN LYS GLY SER GLU THR ALA GLU THR THR ALA GLN ALA GLU LYS ILE GLN GLN SER PRO ASP LYS VAL LEU GLY GLN SER VAL GLN SER PHE SER PHE ALA ASP ILE ALA LYS SER LEU GLU GLY ILE GLU PHE GLY LYS ALA
ASP PRO ASN PHE LYS GLY PHE SER GLY ALA GLY GLN LYS LEU PHE THR SER ASN ALA GLN VAL ASN ALA SER ASN ALA GLN GLU ALA ALA SER ASP PHE ASP ASP ILE HIS PHE GLU PRO ILE VAL GLN LEU PRO ASP LYS LYS VAL ASP LEU ILE THR GLY GLU
GLU ASP GLU LYS THR LEU TYR SER GLN ARG VAL LYS LEU TYR ARG PHE ASP ALA THR SER GLY GLN TRP LYS GLU ARG GLY VAL GLY ASN LEU LYS ILE LEU LYS ASN GLU VAL ASN GLY LYS LEU ARG VAL LEU MET ARG GLU GLN VAL LEU LYS VAL CYS ALA ASN HIS ILE
THR THR THR MET ASN LEU LYS PRO LEU THR GLY SER ASP ARG ALA TRP MET TRP LEU ALA ASN ASP PHE SER GLU GLY ASP ALA LYS LEU GLU GLN LEU LEU ALA VAL LYS PHE LYS THR PRO GLU GLN ALA GLU GLU PHE LYS ILE LYS PHE ASP GLN CYS GLN CYS LEU LEU ASP ILE
PRO LEU GLN THR PRO HIS LYS LEU VAL ASP THR GLY ARG THR HIS LEU ILE GLN LYS ALA GLU MET LYS THR GLY LEU LYS ASP LEU LYS THR PHE LEU THR ASP LYS ALA LYS PRO LEU ASP SER ASN ALA ILE ASN THR THR ASP GLU LEU LYS GLN ALA LEU ASP
GLY THR GLU PRO THR TYR TRP ASP MET ARG GLY THR ASP ALA HIS GLU GLU THR LEU ASP ASP SER VAL TYR ALA SER PRO LEU ALA SER PRO GLU LYS ASN LEU PHE ARG PHE GLY ASP SER LEU SER THR SER GLY PHE ASN PHE SER PHE GLN PHE ASP
PRO SER LYS PRO LEU ASN SER ARG ASP VAL THR GLN GLU GLU GLU ARG ASP GLY GLN TYR PHE GLU PRO VAL THR PRO ASP LEU VAL GLU VAL THR SER GLY GLU GLU GLN ALA CYS PHE ALA ILE
ALA LYS LEU TYR ARG PHE ASP LYS ASN SER ILE LEU GLN ARG LEU ASP ASN LYS SER ALA ARG VAL VAL MET ARG ARG ASP GLN VAL LEU LYS LEU CYS ALA ASN HIS ARG ILE THR THR ASP ILE ASN LEU GLN PRO ILE LEU
GLY ALA GLU ARG ALA TRP VAL TRP THR ASP GLN ARG LEU PHE LYS LEU GLN GLU ALA ALA ASP PHE GLU LYS VAL GLU VAL PHE GLU GLU ALA LYS ASP ALA GLN ALA ALA LYS ASP CYS ILE SER ASP PRO ASP SER
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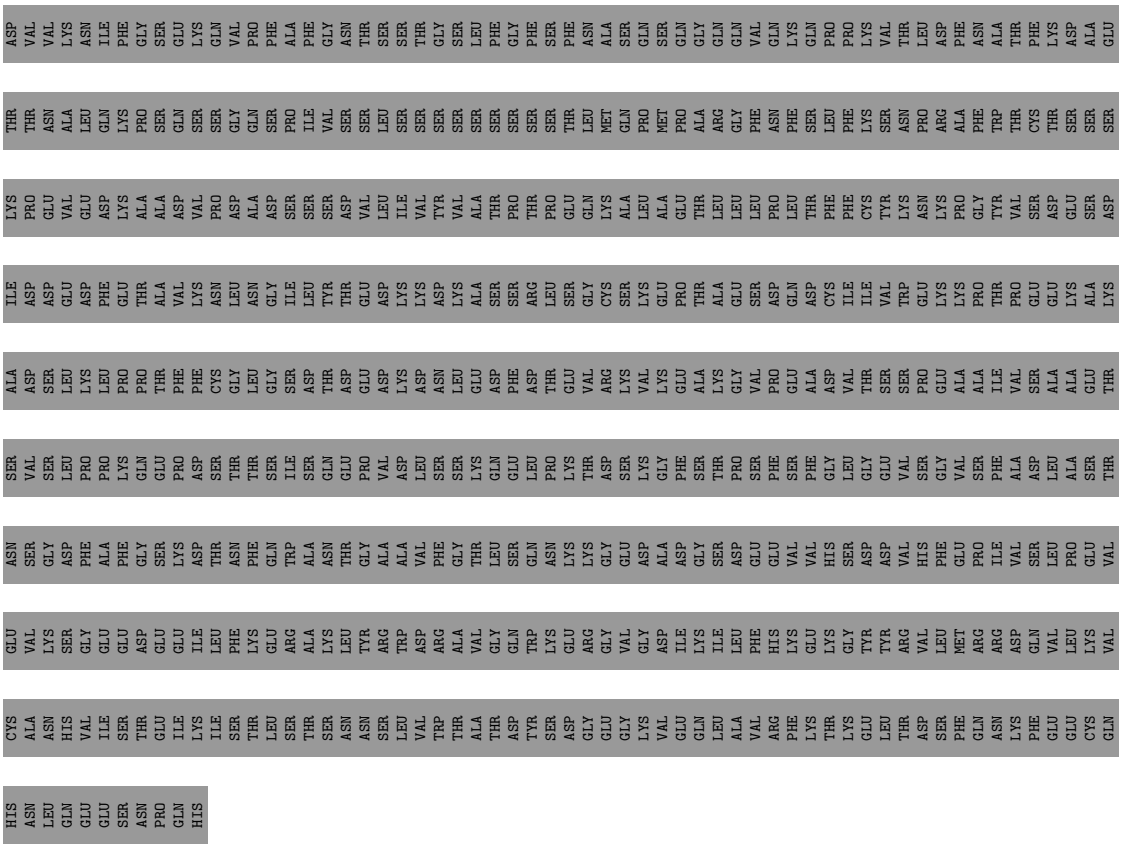
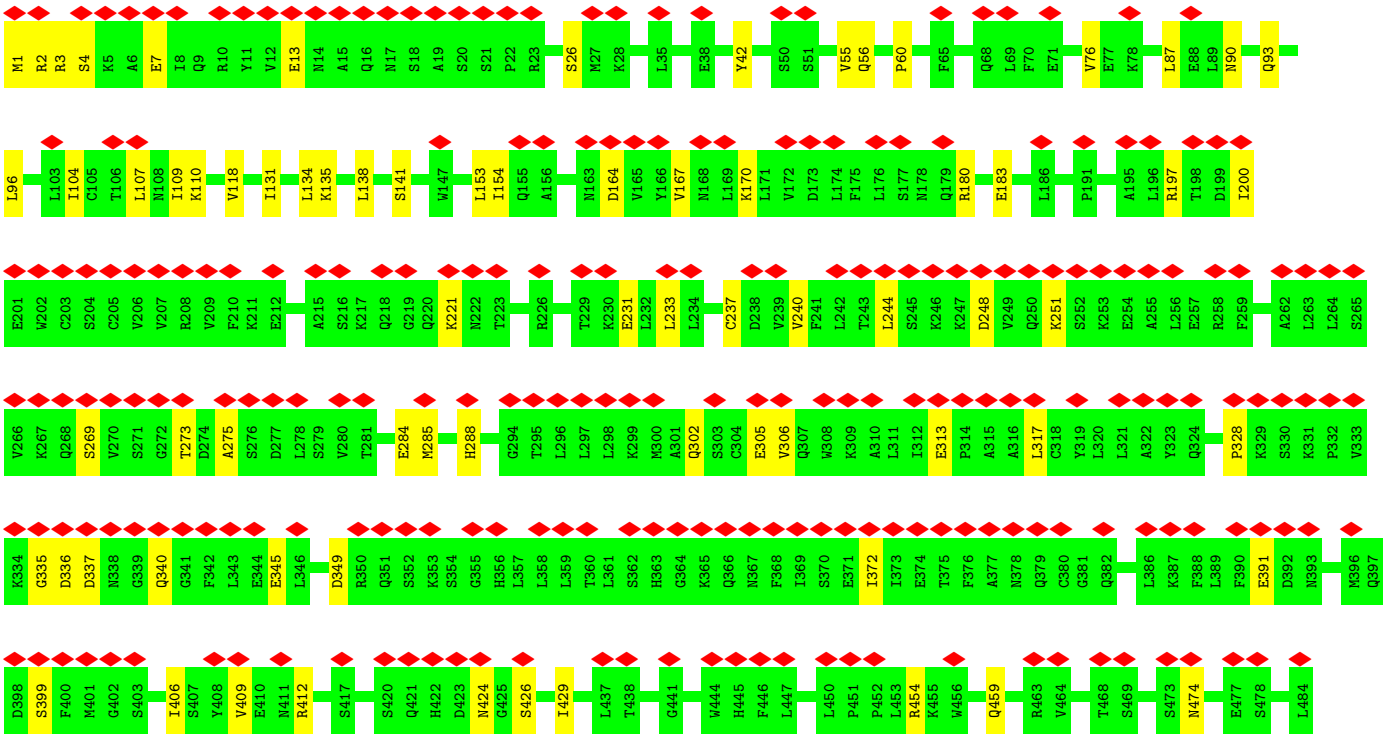
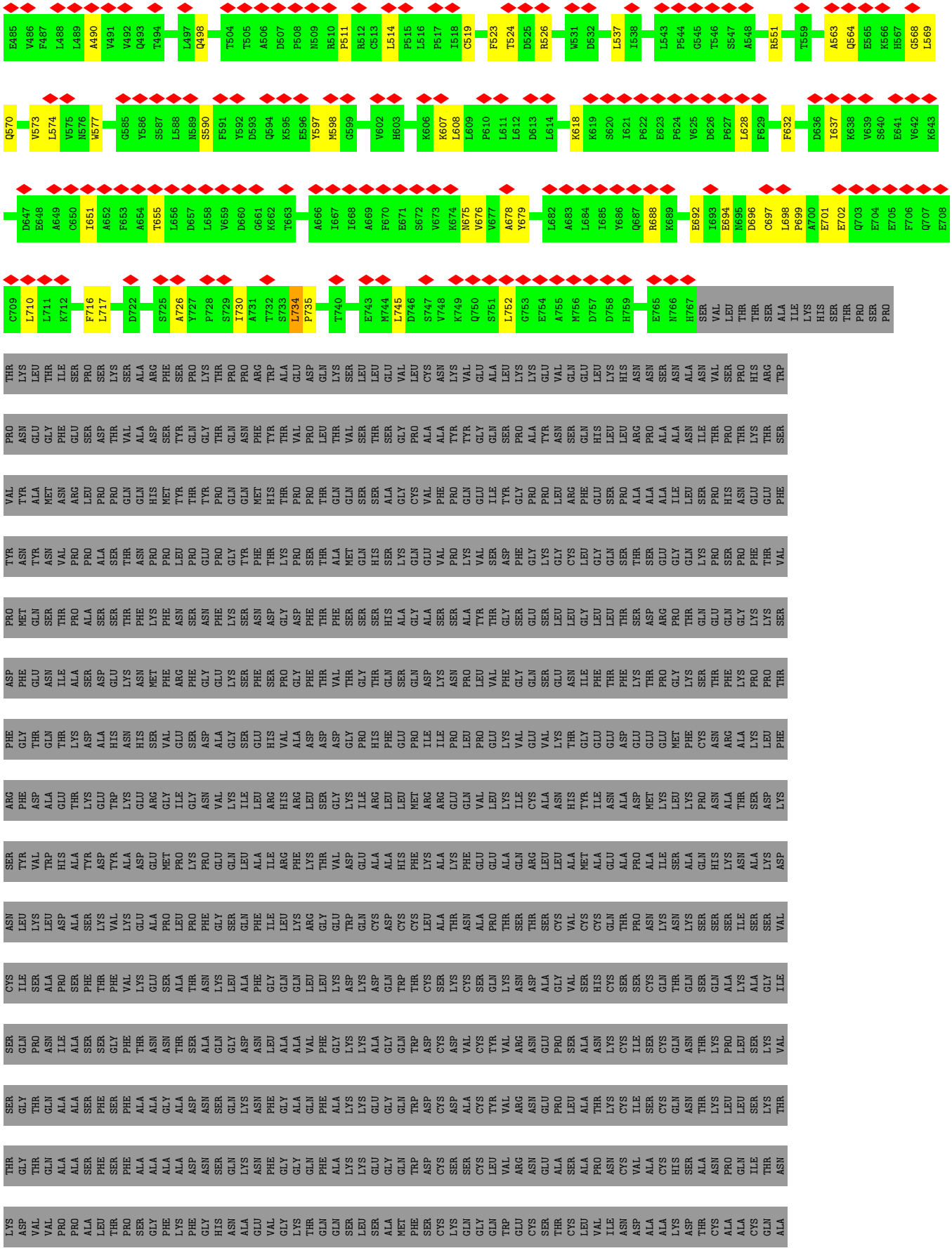


- Molecule 12: Nup358

Chain X:

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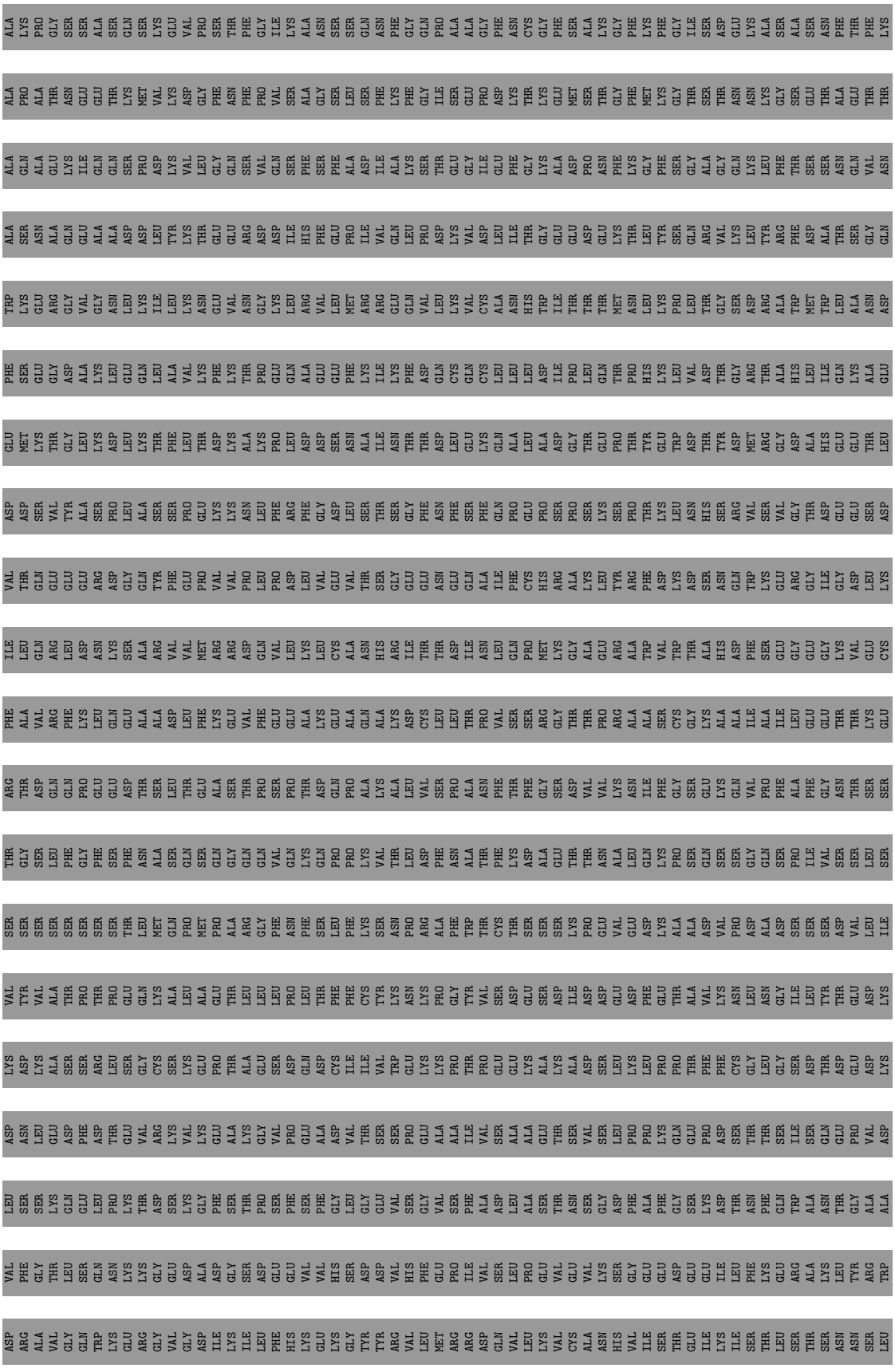
Q570 V573 L574 V575 N576 W577 G585 Y586 S587 L588 N589 S590 F591 Y592 D593 Q594 K595 E596 Y597 N598 Q599 V602 H603 K606 K607 L608 L609 P610 L611 L612 D613 L614 K618 K619 S620 I621 P622 E623 P624 V625 D626 P627 L628 F629 F632 D636 I637 K638 V639 S640 E641 V642 K643
D647 E648 A649 C650 I651 A652 F653 A654 T655 L656 D657 L658 V659 D660 G661 K662 T663 A666 I667 I668 A669 F670 E671 S672 V673 K674 N675 V676 V677 A678 Y679 L682 A683 L684 I685 Y686 Q687 R688 K689 E692 I693 E694 N695 D696 C697 L698 P699 A700 E701 E702 Q703 E704 E705 F706 Q707 E708
C709 L710 L711 K712 F716 L717 D722 S725 A726 Y727 P728 S729 I730 A731 T732 S733 L734 P735 T740 E743 M744 L745 D746 S747 V748 K749 Q750 S751 L752 G753 E754 A755 M756 D757 D758 H759 E765 N766 H767
THR LYS LEU THR ILE SER PRO SER LYS SER ALA ARG PHE SER PRO LYS THR PRO PRO ARG TRP ALA GLU ASP GLN LYS SER LEU LEU LEU GLU VAL LEU CYS ASN LYS VAL GLU ALA LEU LYS LYS GLU VAL GLN GLU LEU LYS HIS ASN ASN SER ASN ALA ASN VAL SER PRO HIS ARG TRP
PRO ASN GLU GLY PHE GLU SER ASP THR VAL ALA ASP SER TYR GLN GLY THR GLN ASN PHE TYR THR VAL PRO LEU THR VAL SER THR SER GLY PRO ALA ALA TYR TYR GLY GLN SER PRO ALA TYR ASN SER GLN HIS LEU LEU LEU ARG PRO ALA ALA ASN ILE THR PRO THR LYS THR SER
VAL TYR ALA MET ASN ARG LEU PRO PRO GLN GLN HIS MET TYR THR TYR PRO GLN GLN MET HIS THR PRO PRO THR GLN GLN SER SER ALA GLY CYS VAL PHE PRO PRO GLN GLU ILE TYR GLY PRO PRO LEU ARG PHE GLU SER PRO ALA ALA ALA ILE LEU SER PRO HIS ASN GLU GLU PHE
TYR ASN TYR ASN VAL PRO PRO ALA SER THR ASN PRO PRO LEU PRO GLU PRO GLY TYR PHE THR LYS PRO SER THR ALA MET GLN HIS SER LYS GLN GLU VAL PRO LYS VAL SER ASP PHE GLY LYS GLY CYS LEU GLY GLN SER THR SER GLU GLY GLN LYS PRO HIS ASN GLU GLU PHE
PRO MET GLN SER THR PRO ALA SER SER THR PHE LYS PHE ASN SER ASN PHE LYS SER ASN ASP GLY ASP PHE THR PHE SER SER SER HIS ALA GLY ALA SER SER ALA TYR THR GLY SER GLU SER LEU LEU GLY LEU LEU THR SER ASP ARG PRO THR GLN GLU GLN GLY LYS LYS SER
ASP PHE GLU ASN ILE ALA SER ASP GLU LYS SER ARG PHE SER PRO GLY PHE THR VAL THR GLY THR THR GLN SER GLN ASP LYS ASN PRO LEU VAL PHE GLY GLN SER GLU ASN ILE PHE THR PHE LYS THR PRO GLY LYS PHE SER PRO PRO THR
PHE GLY THR GLN THR LYS ASP ALA HIS ASN HIS SER VAL GLU SER ASP ALA GLY SER GLU HIS VAL ALA ASP ASP ASP GLY PRO HIS PHE GLU PRO ILE ILE PRO LEU PRO GLU LYS VAL GLU VAL LYS THR GLY GLU GLU ASP GLU GLU GLU MET PHE CYS ASN ARG ALA LYS LEU PHE
ARG PHE ASP ALA GLU THR LYS GLU ARG GLY ILE GLY ASN VAL LYS ILE LEU ARG HIS ARG LEU SER GLY LYS ILE ARG LEU LEU MET ARG ARG GLU GLN GLN VAL LEU LYS ILE CYS ALA ASN HIS TYR ILE ASN ALA ASP MET LYS LEU LYS PRO ASN ALA THR SER ASP LYS
SER TYR VAL TRP HIS ALA TYR ASP TYR ALA ASP GLU MET PRO LYS PRO GLU GLN LEU ALA ILE ARG PHE LYS THR VAL ASP GLU ALA ALA HIS PHE LYS ALA LYS PHE GLU GLU ALA GLN ARG LEU LEU ALA MET ALA GLU GLU ALA PRO ALA ILE SER ALA GLN HIS LYS ASN ALA LYS ASP
ASN LEU LYS LEU ASP ALA SER LYS VAL LYS GLU ALA GLN LEU PRO PHE GLY SER GLN PHE ILE LEU LYS ARG GLY GLU TRP GLN CYS CYS ASP CYS CYS LEU ALA THR ASN ALA PRO THR SER THR SER CYS VAL CYS CYS GLN THR PRO ASN LYS ASN LYS SER SER SER LYS ILE SER SER VAL
CYS ILE SER ALA PRO PHE THR PHE VAL LYS GLU SER ALA THR ASN LYS LEU ALA PHE GLY GLN GLN LEU LEU LYS ASP LYS ASP GLN TRP THR CYS SER LYS LYS CYS SER GLN LYS ASN ASP ALA GLY VAL SER HIS CYS SER SER CYS GLN THR GLN SER GLN ALA LYS ALA GLY SER
SER GLN PRO ASN ILE ALA SER PHE THR ASN ASN GLY ASP ASN LEU ALA VAL PHE GLY PHE LYS GLY GLU GLY TRP ASP CYS ASP VAL CYS TYR VAL ARG ASN GLU PRO SER ALA ASN LYS CYS ILE SER CYS GLN ASN THR LYS PRO LEU SER LYS VAL
SER GLY THR GLN ALA ALA ALA GLY ALA SER PHE SER PHE ALA LYS LYS GLU GLY GLN TRP ASP CYS ASP ALA CYS TYR VAL ARG ASN GLU PRO LEU ALA THR LYS CYS ILE SER CYS GLN ASN THR LYS LEU LEU LEU SER LYS THR
THR GLY THR GLN ALA ALA ALA SER PHE SER PHE ALA LYS LYS GLU GLY GLN TRP ASP CYS SER SER CYS LEU VAL ARG ASN GLU ALA SER ALA PRO ASN CYS VAL ALA CYS HIS SER ALA ASN PRO GLN ILE THR ASN
LYS ASP VAL VAL PRO PRO SER GLY PHE LYS PHE PHE GLY HIS ASN ALA GLU VAL GLY LYS THR GLN GLN SER LEU SER ALA MET PHE SER CYS LYS GLN GLY GLN TRP GLU CYS GLY SER THR CYS LEU VAL ILE ASN ASP ALA ALA CYS HIS ASP ALA ASP THR CYS ALA LEU ALA ASP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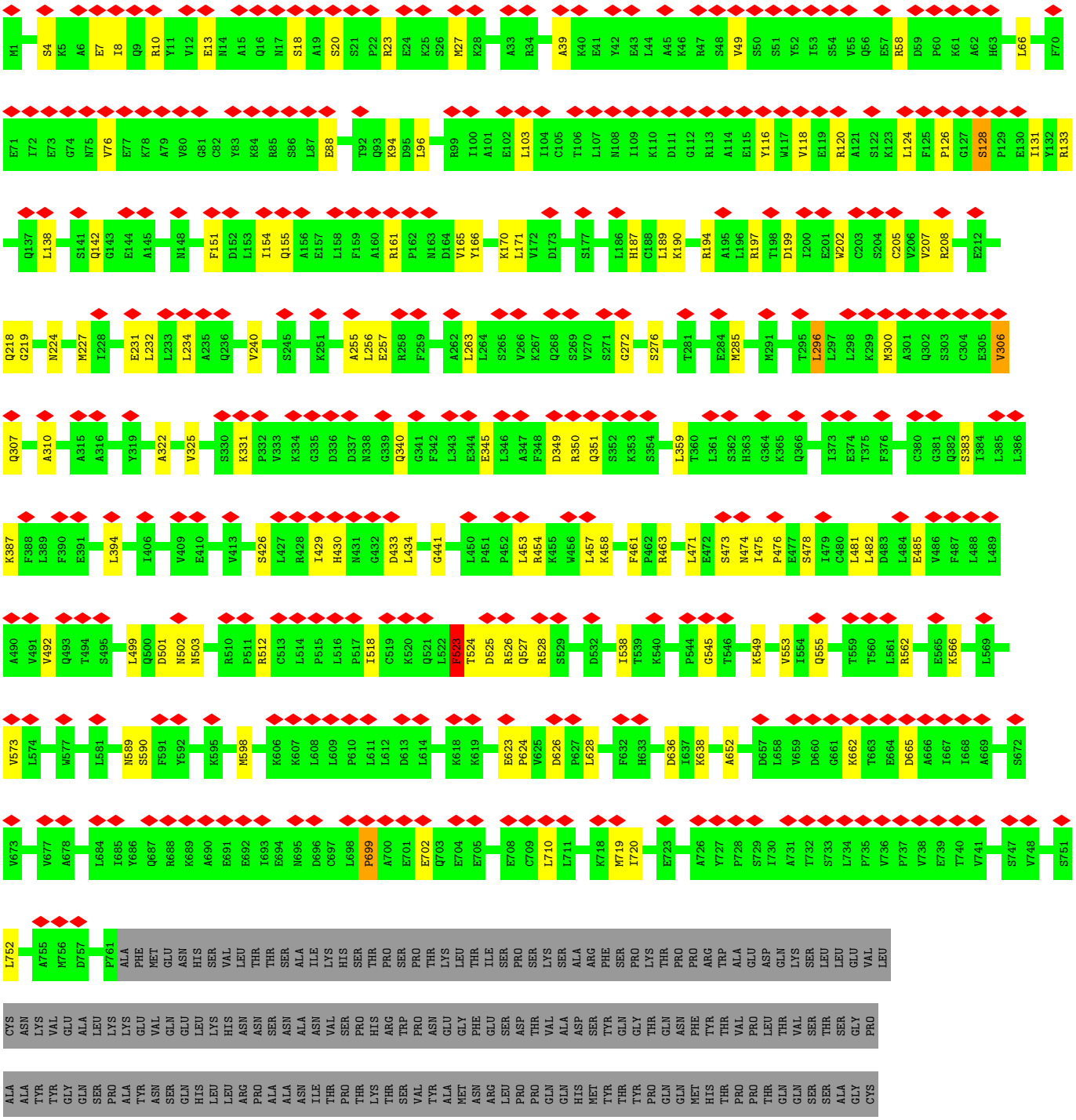
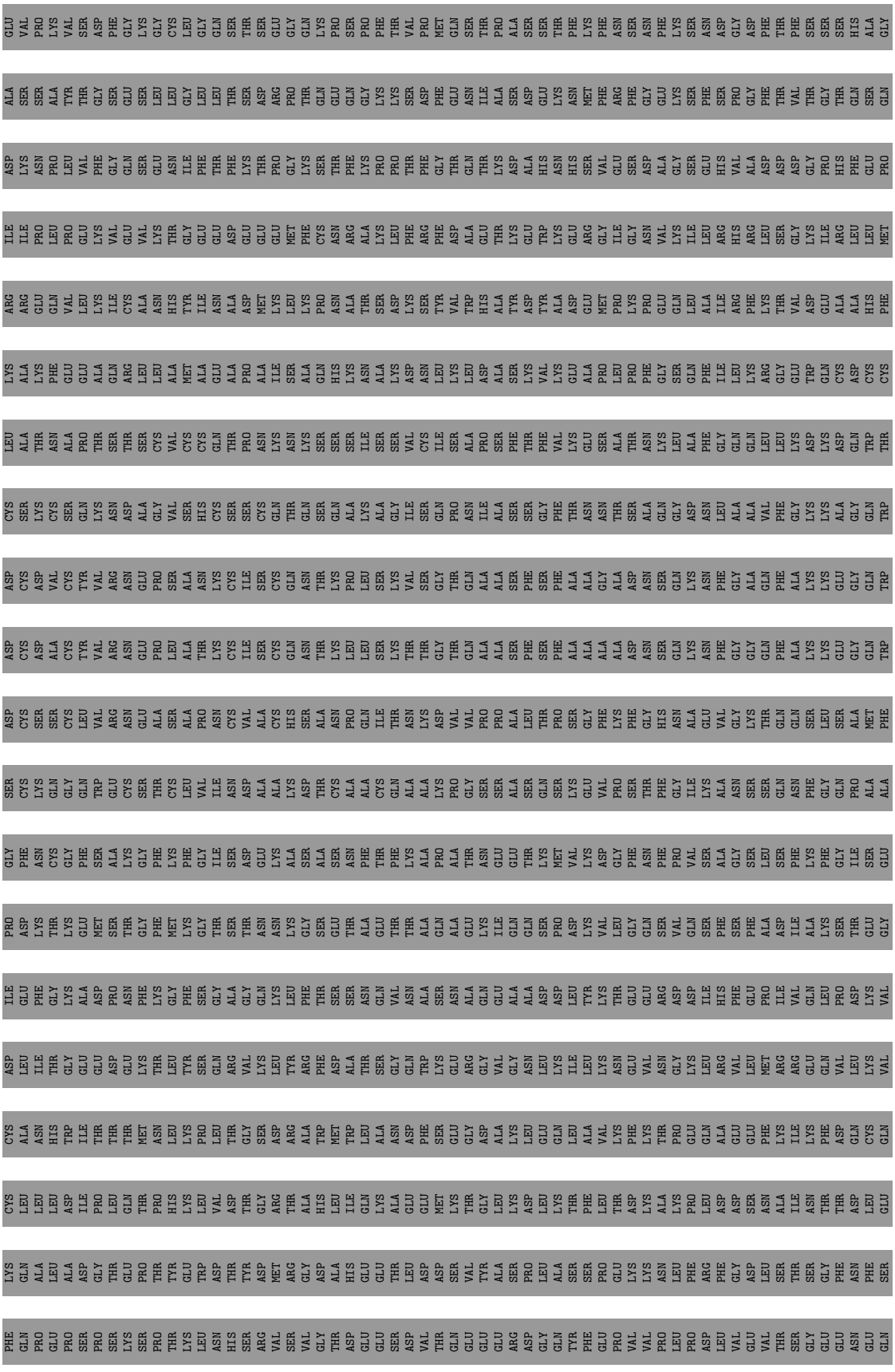
ALA PRO ALA THR ASN GLU GLU THR LYS MET VAL LYS ASP GLY PHE ASN PHE PRO VAL SER ALA GLY SER LEU SER PHE LYS PHE GLY ILE SER GLU PRO ASP LYS THR LYS GLU MET SER THR GLY PHE MET LYS GLY THR SER THR GLY ALA GLY GLN LYS LEU PHE THR SER GLU THR ALA GLU THR THR
ALA GLN ALA GLU LYS ILE GLN GLN SER PRO ASP LYS VAL LEU GLY GLN SER VAL GLN SER PHE SER PHE ALA ASP ILE ALA LYS SER GLU PHE GLU PHE GLY LYS ALA ASP PRO ASN PHE LYS GLY PHE SER GLY ALA GLY GLN LYS LEU PHE THR SER SER GLU THR ASN GLN VAL ASN
ALA SER ASN ALA GLN GLU ALA ALA ASP ASP LEU TYR LYS THR GLU GLU ARG ASP ASP ILE HIS PHE GLU PRO ILE VAL GLN LEU PRO ASP LYS VAL ASP LEU ILE THR GLY GLU GLU ASP PRO ASN LYS THR LYS GLU TYR SER GLN ARG VAL LYS LEU TYR ARG PHE ASP ALA THR SER GLY
TRP LYS GLU ARG GLY VAL GLY ASN LEU LYS ILE LEU LYS ASN GLU VAL ASN GLY LYS LEU ARG VAL LEU MET ARG ARG GLU GLN VAL LEU LYS VAL CYS ALA ASN HIS TRP ILE THR THR THR MET ASN LEU LYS PRO LEU VAL THR GLY SER ASP ARG ALA ALA TRP MET TRP LEU ALA ASN ASP
PHE SER GLU GLY ASP ALA LYS LEU GLN LYS LEU GLU GLU PHE LYS ILE LEU GLN ALA GLU GLU PHE LYS THR PRO GLU GLN LEU ASP ILE PRO LEU GLN THR PRO HIS LYS LEU GLU PRO THR ASP GLY ARG THR ALA HIS LEU ILE GLN LYS ALA GLU
GLU MET LYS THR GLY LEU LYS ASP LEU LYS THR PHE LEU THR ASP LYS ALA LYS PRO LEU ASP ASP SER ASN ALA ILE ASN THR THR ASP LEU GLU LYS GLN ALA LEU ALA ASP GLY THR GLU PRO THR TYR GLU TRP ASP THR TYR ASP MET ARG ALA GLY ASP ALA HIS GLU GLU THR LEU
ASP ASP SER VAL TYR ALA SER PRO LEU ALA SER SER PRO GLU LYS LYS ASN LEU PHE ARG PHE GLY ASP LEU SER THR SER GLY PHE ASN PHE SER GLN PRO GLU PRO HIS SER ARG VAL SER VAL GLY THR ASP ASP SER
VAL THR GLN GLU GLU GLU ARG ASP GLY GLN TYR PHE GLU PRO VAL VAL PRO LEU PRO ASP LEU VAL GLU VAL THR SER GLY GLU GLN ALA ILE PHE CYS HIS ARG ALA LYS LEU TYR ARG PHE ASP LYS ASP SER ASN GLN TRP LYS GLU ARG GLY ILE GLY ASP LEU LYS
ILE LEU GLN ARG LEU ASP ASN LYS SER ALA ARG VAL VAL MET ARG ARG ASP GLN LEU LEU LYS LEU CYS ALA ASN HIS ARG ILE THR THR ASP ILE ASN LEU GLN PRO MET LYS GLY ALA GLU ARG ALA TRP VAL TRP THR ALA HIS ASP PHE SER GLU GLY GLU GLY LYS VAL GLU CYS
PHE ALA VAL ARG PHE LYS LEU GLN GLU ALA ASP LEU PHE LYS GLU VAL PHE GLU GLU ALA LYS GLU ALA GLN ALA LYS ASP CYS LEU LEU LEU THR THR PRO ARG ALA ALA SER CYS GLY LYS ALA ILE ALA ILE LEU GLU GLU GLU THR THR LYS GLU
ARG THR ASP GLN GLN PRO GLU GLU GLN ASP THR SER GLN GLY GLN THR PRO GLN ALA LYS ALA LEU GLN LYS ALA ASP VAL VAL LYS ASN ILE PHE GLY SER GLU LYS GLN VAL PRO PHE ALA PHE GLY ASN THR SER SER
THR GLY SER LEU PHE GLY PHE SER SER PHE ASN ALA GLN GLN VAL PRO PRO LYS VAL THR LEU ASP PHE ASN ALA THR PHE LYS ASP ALA GLU THR THR ASN ALA LEU GLN LYS PRO SER GLN SER SER GLY ILE VAL SER LEU SER
SER SER SER SER SER SER SER THR LEU MET GLN PRO MET PRO ALA ARG GLY PHE ASN PHE SER LEU PHE LYS SER ASN PRO ARG ALA PHE TRP THR THR CYS THR SER SER SER ASP LYS PRO GLU VAL GLU ASP LYS ALA ASP VAL PRO ASP ALA ASP SER SER SER ASP VAL LEU ILE
VAL TYR VAL ALA THR PRO THR PRO GLU GLN LYS ALA LEU LEU LEU PRO LEU THR PHE PHE CYS TYR LYS ASN LYS PRO GLY TYR VAL SER ASP PHE GLU THR ALA VAL LYS ASN LEU GLN ASN GLY ILE SER GLU LEU ASP PHE GLU THR ALA ASP
LYS ASP LYS ALA SER GLY CYS SER LYS GLU PRO THR ALA GLU LEU SER GLY LYS ALA ASP SER ILE CYS ILE ILE VAL TRP GLU LYS LYS PRO THR PRO GLY LEU LYS LEU PRO PRO THR PHE PHE CYS SER GLY LEU GLY SER ASP THR ASP ASP LYS
ASP ASN LEU GLU ASP PHE VAL ARG LYS VAL LYS GLU ALA ALA ILE VAL SER ALA ALA GLU THR SER VAL SER LEU PRO PRO LYS GLN GLU PRO ASP SER THR THR SER ILE SER GLN GLU GLN ASP
LEU SER SER LYS GLN GLU PRO THR SER GLY LEU GLY VAL SER PHE ALA GLY GLU VAL GLY PHE ALA PHE GLY SER LYS ASP THR ASN THR SER GLY ILE PHE GLN TRP ALA ASN THR ASP ALA ALA
VAL PHE GLY THR LEU SER HIS PHE GLU PRO ILE VAL GLU VAL HIS VAL ASP ASP VAL GLU GLY VAL GLU GLU ILE LEU PHE LYS GLU ARG ALA LYS LEU TYR ARG TRP
ASP ARG ALA VAL GLY GLN TRP LYS GLU GLY VAL ASP ILE LYS ILE LEU PHE HIS LYS GLU LYS GLY TYR TYR ARG VAL LEU MET ARG ARG ASP GLN VAL LEU LYS VAL CYS ALA ASN HIS VAL ILE SER THR GLU ILE LYS ILE LEU SER THR SER ASN ASN SER LEU

• Molecule 12: Nup358

Chain Y:

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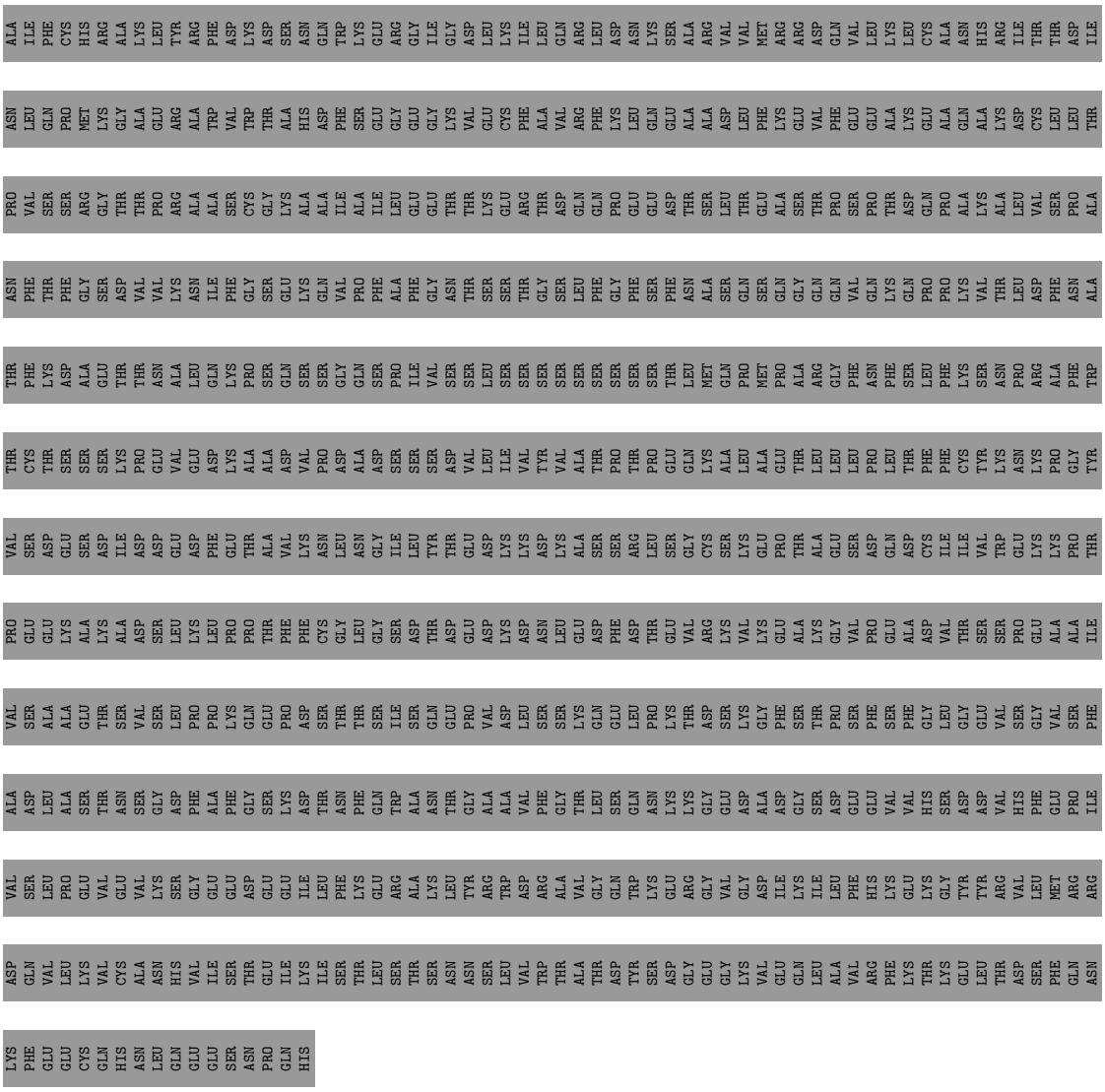
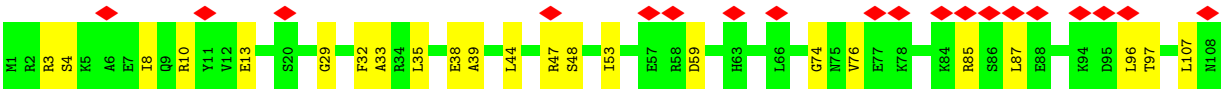
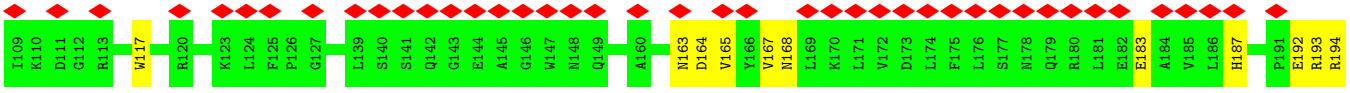
ALA SER SER ALA TYR THR GLY SER GLU LEU LEU GLY LEU LEU THR SER ASP ARG PRO THR GLN GLU GLN GLY LYS LYS SER ASP PHE GLU ASN ASN ILE ALA SER ASP GLU LYS ASN MET PHE ARG PHE GLY GLU LYS SER PHE SER PRO GLY PHE THR VAL ASP PHE GLN
ASP LYS ASN PRO LEU VAL PHE GLY GLN SER GLU ASN ILE PHE THR PHE LYS THR PHE LYS PRO PRO GLY THR GLN THR LYS ASP ALA HIS ASN HIS SER VAL GLU SER ASP ALA GLY SER GLU HIS ARG LEU ASP ASP GLY LYS ILE ARG LEU GLU PRO
ILE ILE PRO LEU PRO GLU LYS VAL GLU VAL LYS THR GLY GLU GLU ASP GLU GLU MET PHE CYS ASN ARG ALA LYS LEU PHE ARG PHE ASP ALA GLU THR LYS GLU TRP LYS GLU ARG GLY ILE GLY ASN VAL LYS ILE LEU ARG HIS ARG LEU SER GLY LYS ILE ARG LEU LEU MET
ARG ARG GLU GLN VAL LEU LYS ILE CYS ALA ASN ASN ALA THR SER ASP LYS SER TYR VAL TRP HIS ALA TYR ASP TYR ALA ASP GLU MET PRO LYS PRO GLU GLN LEU ALA ILE ARG PHE LYS THR VAL ASP GLU GLY CYS ALA ALA HIS PHE
LYS ALA LYS PHE GLU GLU ALA GLN ARG LEU ALA LEU LEU ALA MET ALA GLU ALA PRO ALA ILE SER ALA GLN HIS LYS ASN ALA LYS ASP ALA LEU LYS LEU LEU ARG LEU GLU LEU SER ASP ASP PRO LEU PRO PHE GLY SER GLN LEU ALA PHE ILE LEU ARG GLY GLU TRP GLN CYS ASP CYS CYS
LEU ALA THR ASN ALA PRO THR SER THR SER CYS VAL CYS CYS GLN THR PRO ASN LYS ASN LYS SER SER SER ILE SER SER ALA PRO SER PHE THR PHE VAL LYS GLU SER ALA THR ASN SER ALA GLN GLY ASP ASN LEU ALA PHE GLY GLN GLN LEU LEU LYS ASP LYS ASP GLN TRP THR
CYS SER LYS CYS SER GLN LYS ASN ASP ALA GLY VAL SER HIS CYS SER SER CYS GLN THR GLN SER GLN ALA LYS ALA GLY ILE SER GLN PRO ASN ILE ALA SER SER GLY PHE THR ASN ASN THR SER ALA GLN GLY ASP ASN LEU ALA ALA VAL PHE GLY LYS LYS ASP GLN TRP
ASP CYS ASP VAL CYS TYR VAL ARG ASN GLU PRO SER ALA ASN LYS CYS ILE SER CYS GLN ASN THR LYS PRO LEU SER LYS VAL SER GLY THR GLN ALA ALA ALA SER SER PHE SER PHE ALA ALA GLY ASP ASN SER GLN LYS ASN PHE GLY ALA GLN PHE ALA LYS LYS GLU GLY GLN TRP
ASP CYS ASP ALA CYS TYR VAL ARG ASN GLU PRO LEU ALA THR LYS CYS ILE SER CYS GLN ASN THR LYS LEU LEU SER LYS THR THR GLY THR GLN ALA ALA ALA SER PHE SER PHE ALA ALA GLY ALA ASP ASN SER GLN LYS ASN PHE GLY GLY GLN PHE ALA LYS LYS GLU GLY GLN TRP
ASP CYS SER SER CYS LEU VAL ARG ASN GLU ALA SER ALA PRO ASN CYS VAL ALA CYS HIS SER ALA ASN SER ASN PRO GLN ILE THR ASN LYS ASP VAL VAL PRO PRO ALA LEU LEU THR PRO SER GLY PHE LYS PHE GLY HIS ASN ALA GLU VAL GLY LYS THR GLN GLN SER LEU SER ALA MET PHE
SER CYS LYS GLN GLY GLN ILE VAL ILE ASN ASP ALA LYS ASP THR CYS ALA ALA CYS GLN ALA ALA LYS PRO GLY SER SER ALA GLU LEU THR PHE GLY ILE LYS ALA ASN SER GLN ASN PHE GLY GLN PRO ALA ALA
GLY PHE ASN CYS GLY PHE SER ALA LYS GLY PHE LYS ALA SER ALA SER ASN PHE THR PHE LYS ALA PRO ALA THR ASN GLU GLU LYS ILE GLU GLU THR LYS MET VAL LYS ASP GLY PHE ASN PHE PRO VAL SER ALA GLY SER LEU SER ALA GLU
PRO ASP LYS THR LYS GLU THR GLY PHE MET LYS GLY THR SER THR ASN ASN LYS ALA GLU THR THR ALA GLN ALA GLU LYS ILE GLN GLN SER PRO ASP LYS VAL LEU GLY GLN SER VAL GLN SER PHE SER PHE ALA ASP ILE ALA LYS SER GLU GLY
ILE GLU PHE GLY LYS ALA ASP PRO ASN PHE LYS GLY PHE SER GLY PHE THR SER GLN ASN VAL ASN ALA SER ASN ALA GLN ALA GLU ASP LEU TYR LYS THR GLU GLU ARG ASP ASP ILE HIS PHE GLU PRO ILE VAL GLN LEU ASP LYS
ASP LEU ILE THR LEU TYR LYS ARG VAL LYS LEU TYR ARG PHE ASP ALA THR SER GLY GLN TRP LYS GLU ARG GLY VAL GLY ASN LEU LYS ILE LEU LYS ASN GLU VAL ASN GLY LYS LEU ARG VAL LEU MET ARG ARG GLU GLN VAL LEU
CYS ALA ASN HIS TRP ILE THR THR MET THR LEU ALA THR SER GLU GLY GLY SER ASP ARG ALA ALA TRP MET TRP LEU ALA ASN ASP PHE SER GLU GLY ASP ALA LYS LEU GLU GLN LYS PHE LYS THR ASP PRO GLU GLN ALA GLU GLU PHE LYS ILE LYS PHE ASP GLN CYS GLN
CYS LEU LEU LEU ASP ILE PRO LEU GLN LYS ILE LEU GLN LYS ALA GLU GLU MET LYS THR GLY LEU LYS ASP LEU LYS LYS THR PHE LEU THR ASP LYS LYS ALA PRO LEU ASP ASP SER ASN ALA ILE ASN THR THR ASP GLU
LYS GLN ALA LEU ASP THR TYR GLY ARG THR ALA HIS LEU LEU ILE GLN LYS ALA GLU GLU THR GLY ALA ASP SER VAL TYR ALA ALA SER SER PRO GLU LYS LYS ASN SER ASP PHE GLU ASP ASP ASP PHE ASP ASN PHE SER
PHE GLN GLN PRO GLU GLU THR GLN GLU GLU ARG ASP GLY GLU GLN GLU ASP ASP ASP

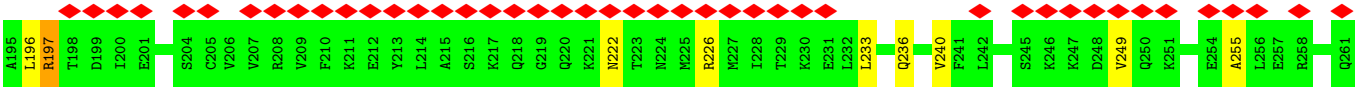


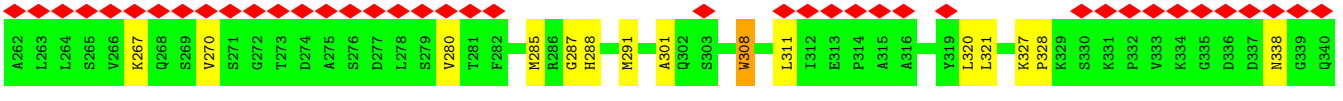
• Molecule 12: Nup358

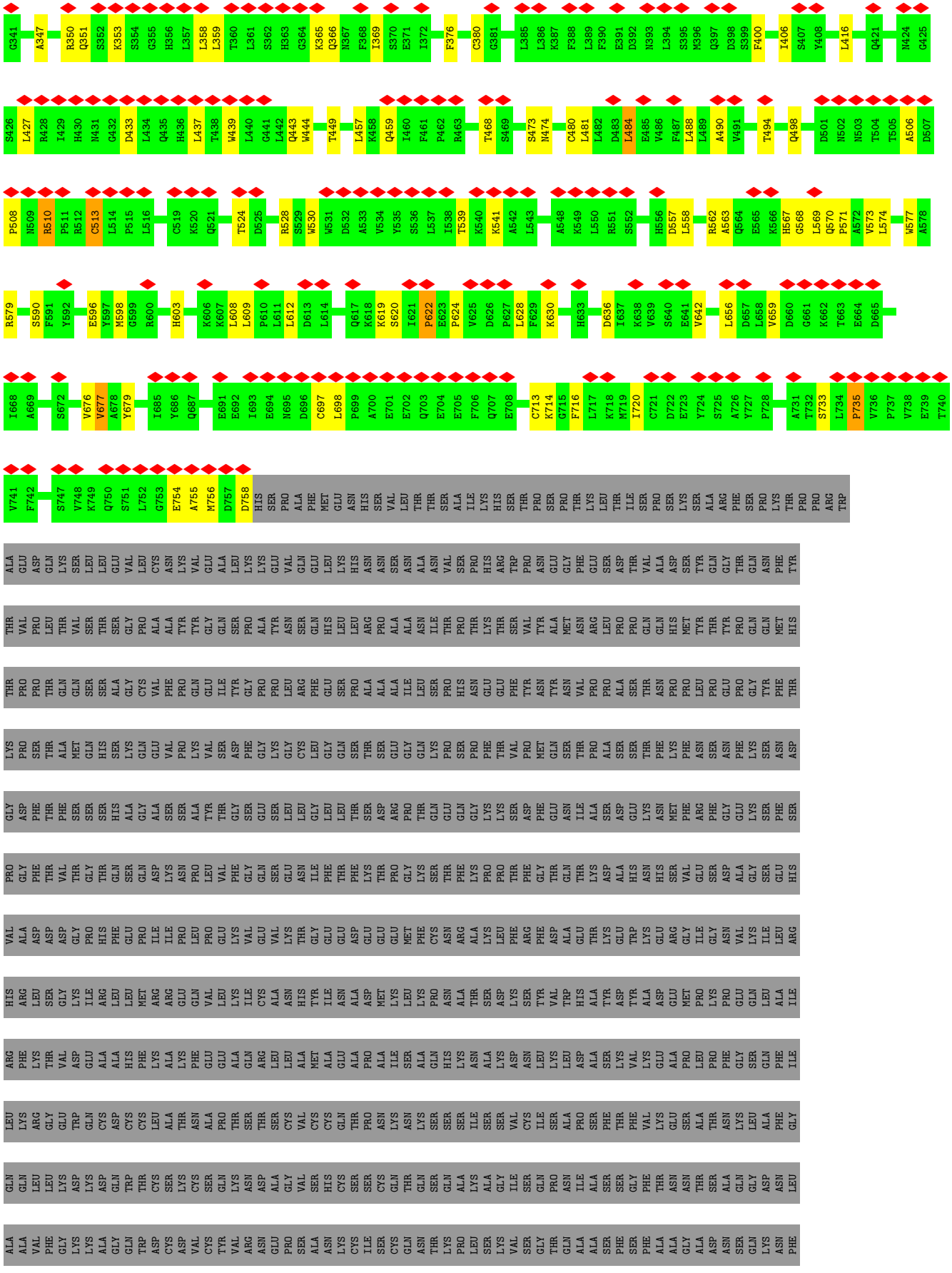
Chain Z:







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S426 L427 R428 I429 H430 N431 G432 D433 L434 Q435 H436 L437 T438 W439 L440 G441 L442 Q443 W444 T449 L457 K458 Q459 I460 F461 P462 R463 T468 S469 S473 N474 C480 L481 L482 D483 L484 E485 V486 F487 L488 L489 A490 V491 T494 Q498 D501 N502 N503 T504 T505 A506 D507
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V741 F742 S747 V748 K749 Q750 S751 L752 G753 E754 A755 M756 D757 D758 HIS SER PRO ALA PHE MET GLU ASN HIS SER VAL LEU THR THR SER ALA ILE LYS HIS SER THR PRO SER PRO THR LYS LEU THR ILE SER PRO SER LYS SER ALA ARG PHE SER PRO LYS THR PRO PRO ARG TRP
ALA GLU ASP GLN LYS SER LEU LEU GLU VAL LEU CYS ASN LYS VAL GLU ALA LEU LYS LYS GLU VAL GLN GLU LEU LYS HIS ASN ASN SER ASN ALA ASN VAL SER PRO HIS ARG TRP PRO ASN GLU GLY PHE GLU SER ASP THR VAL ALA ASP SER TYR GLN GLY THR GLN ASN PHE TYR
THR VAL PRO LEU THR VAL SER THR SER GLY PRO ALA ALA TYR TYR GLY GLN SER PRO ALA TYR ASN SER GLN HIS LEU LEU LEU ARG PRO ALA ALA ASN ILE THR PRO THR LYS THR SER VAL TYR ALA MET ASN ARG LEU PRO PRO GLN GLN HIS MET TYR THR TYR PRO GLN GLN MET HIS
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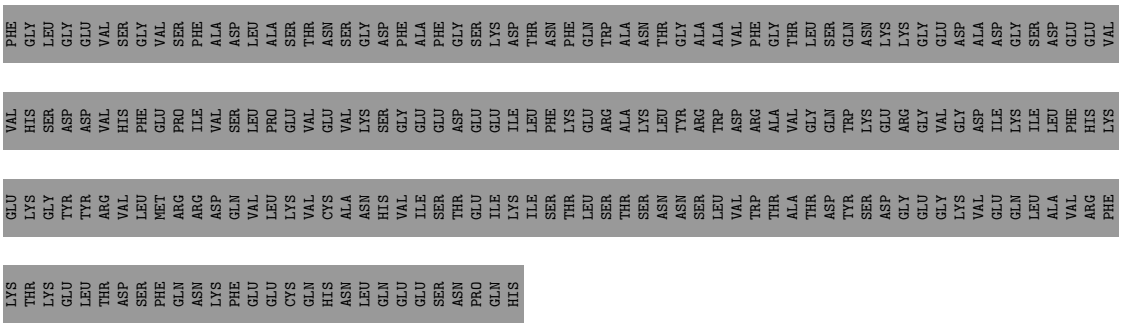
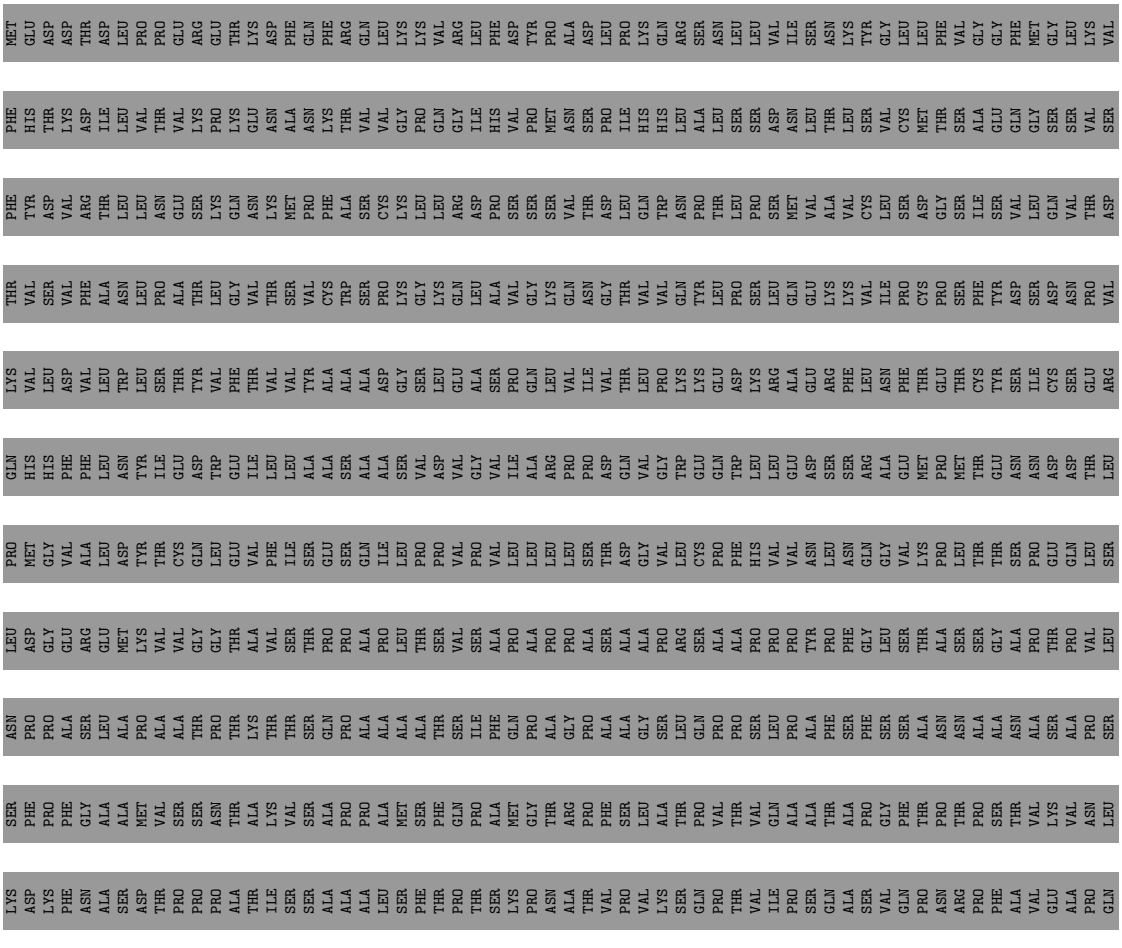
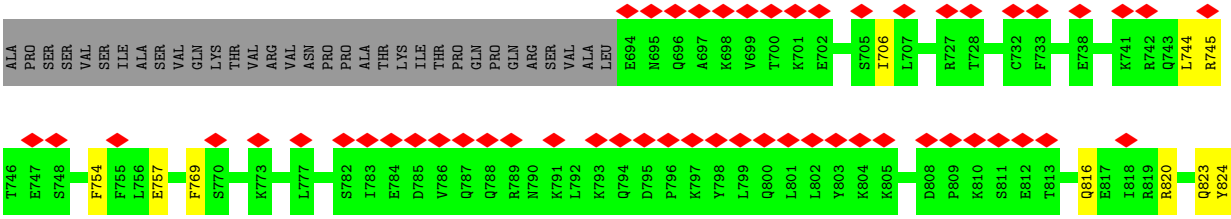
LYS PRO SER THR ALA MET GLN HIS SER LYS GLN GLU VAL PRO LYS VAL SER ASP PHE GLY LYS GLY CYS LEU GLY GLN SER THR SER GLU GLU VAL LEU GLY LEU LEU THR SER ASP GLU LYS LYS SER ASP PHE GLU ASN ILE ALA SER ASP GLU LYS ASN ASP
GLY ASP PHE THR PHE SER SER SER HIS ALA GLY GLN ALA SER SER GLU SER LEU LEU LEU GLY LEU LEU THR SER ASP ARG PRO THR GLN GLU GLN GLY LYS LYS SER ASP PHE GLU ASN ILE ALA SER ASP GLU LYS ASN MET PHE ARG PHE GLY GLU LYS SER PHE SER
PRO GLY PHE THR VAL THR GLY PRO HIS PHE GLU PRO ILE ILE PRO LEU PRO GLU VAL PHE GLY GLN SER GLU ASN ILE PHE THR PHE LYS THR PRO GLY LYS SER THR PHE LYS PRO PRO THR PHE GLY THR GLN THR PHE LYS ASP ALA HIS ASN HIS SER VAL GLU SER ASP ALA GLU
VAL ALA ASP ASP ASP GLY PRO HIS PHE GLU PRO ILE ILE PRO LEU PRO GLU VAL LYS VAL GLU VAL LYS THR GLY GLU GLU ASP GLU GLU GLU MET PHE CYS ASN ARG ALA LYS LEU PHE ARG PHE ASP ALA ILE GLU THR LYS GLU TRP LYS GLU ARG ASP PHE ASP ILE GLU
HIS ARG LEU SER GLY LYS ILE ARG LEU LEU MET ARG ARG GLU GLN VAL LEU LYS ILE CYS ALA ASN HIS TYR ILE ASN ALA ASP MET LYS LEU LYS PRO ASN ARG ALA THR SER ASP LYS SER TYR VAL TRP HIS ALA TYR ASP TYR ALA ASP GLU MET PRO LYS PRO GLU GLN LEU ALA ILE
ARG PHE LYS THR VAL ASP GLU ALA HIS PHE LYS ALA LYS PHE GLU GLU ALA GLN ARG LEU LEU ALA MET ALA GLU ALA ASP PRO ALA ILE SER ALA GLN HIS LYS ASN ALA LYS ASP ASN LEU LYS LEU ASP ALA PRO THR SER LYS VAL LYS GLU ALA PRO LEU PHE GLY SER GLN LEU ILE PHE
LEU LYS ARG GLY GLU TRP GLN CYS CYS ASP CYS CYS LEU ALA THR ASN ALA PRO CYS VAL CYS CYS GLN THR PRO ASN LYS ASN LYS SER SER ILE SER THR CYS VAL CYS ILE SER ALA PRO SER PHE THR PHE VAL LYS GLU ALA SER THR ASN ASN PHE GLY
GLN GLN LEU LEU LYS ASP LYS GLN SER GLN LYS ASN ASP ALA GLY VAL SER HIS CYS SER SER CYS GLN THR GLN SER GLN ALA LYS ALA GLY ILE SER GLN PRO ASN ILE ALA SER SER GLY PHE THR ASN ASN THR SER ALA GLN ASN LEU
ALA ALA VAL PHE GLY LYS LYS ALA GLY GLN TRP ASP CYS ASP VAL CYS TYR VAL ARG ASN GLU PRO SER ALA ASN LYS CYS ILE SER CYS GLN ASN THR LYS PRO LEU SER LYS VAL SER GLY THR GLN ALA ALA SER PHE SER PHE ALA ALA GLY ALA ASP ASN SER GLN LYS ASN PHE
WORLDWIDE PDB PROTEIN DATA BANK

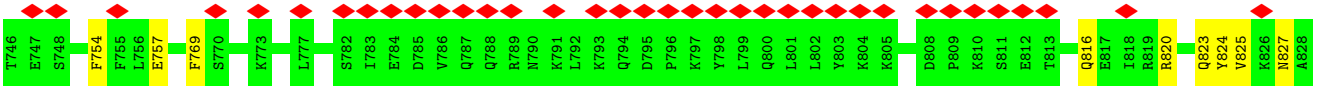


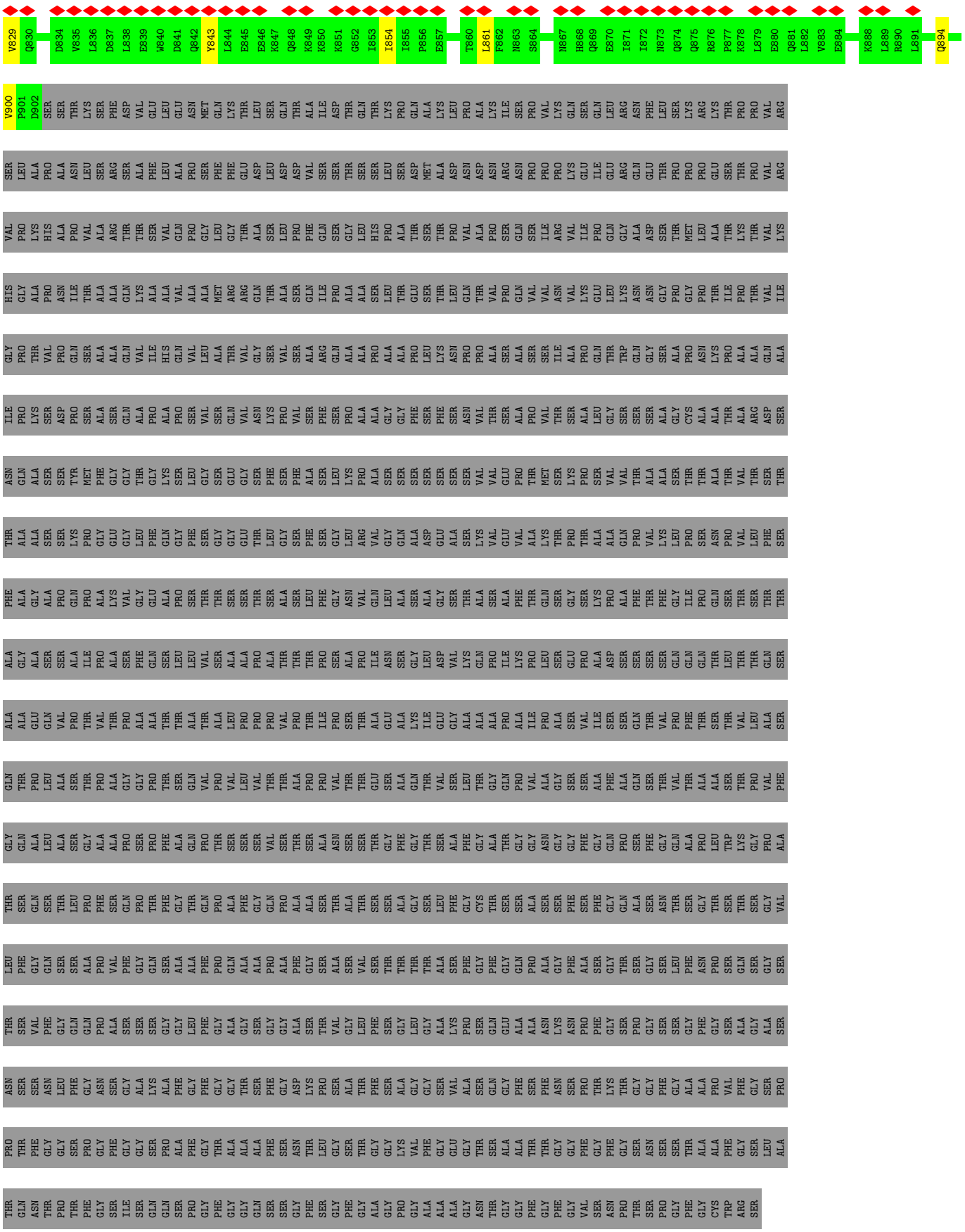
- Molecule 13: Nucleoporin CAN

Chain a: 5% 9% 90%





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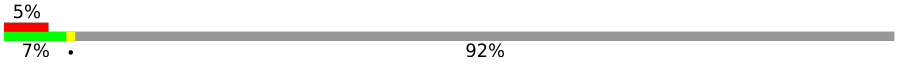
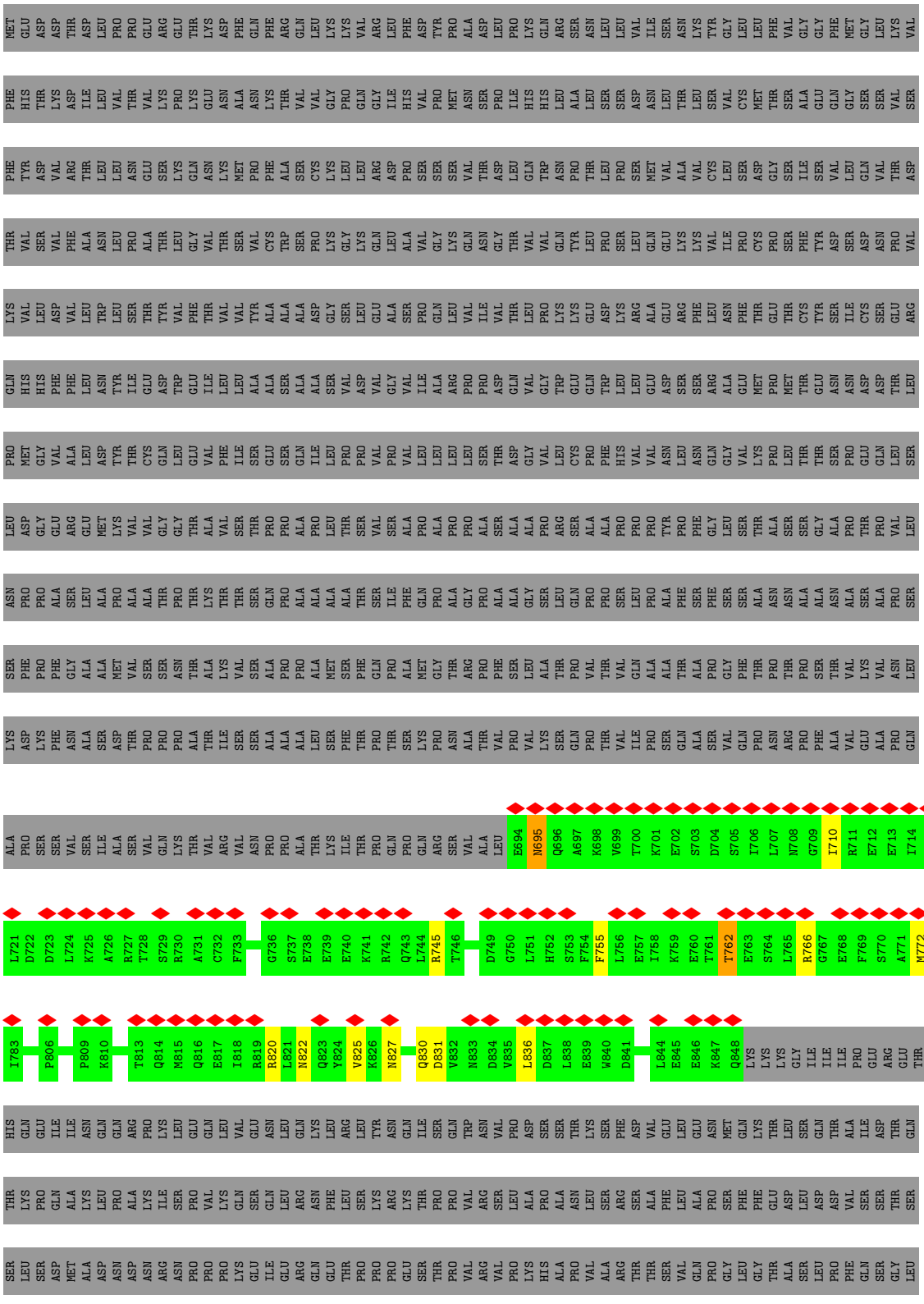
V900 P901 D902

• Molecule 13: Nucleoporin CAN

Chain e:





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SER LEU THR GLU SER THR LEU GLN THR VAL PRO GLN VAL VAL ASN VAL LYS GLU LEU LYS ASN ASN GLY PRO GLY PRO THR ILE PRO THR VAL ILE GLY PRO THR VAL PRO GLN SER ALA ALA GLN VAL ILE HIS GLN VAL LEU ALA THR VAL GLY SER VAL SER ALA GLN VAL SER ALA ARG GLN ALA ALA

PRO ALA ALA PRO LEU LYS ASN PRO PRO ALA SER ALA SER SER ILE ALA PRO GLN THR TRP GLN GLY SER ALA PRO ASN LYS PRO ALA ALA ALA GLN ILE ALA PRO LYS SER ASP PRO SER ALA ALA SER GLN ALA PRO SER LEU ALA PRO PHE SER PRO ALA

ALA GLY GLY PHE SER PHE SER ASN VAL THR SER ALA PRO VAL THR SER ALA LEU GLY SER SER SER SER ALA GLY CYS ALA ALA THR ALA ARG ASP SER ASN GLN LEU GLY GLY THR GLY LYS SER LEU GLY SER PHE SER PHE SER ALA SER GLY GLU GLY

ALA SER SER SER SER SER SER VAL VAL GLU PRO THR MET SER LYS PRO SER VAL VAL THR ALA ALA ALA SER THR THR ALA ALA THR VAL THR SER THR THR THR ALA ALA SER SER LYS PRO GLY GLU GLY LEU PHE GLN GLY PHE SER GLY GLY GLU THR LEU GLY PHE SER GLY LEU ARG

VAL GLY GLN ALA ASP GLU ALA SER LYS VAL GLU VAL ALA LYS THR PRO THR ALA ALA GLN PRO VAL LYS LEU PRO SER ASN PRO VAL LEU PHE SER PHE ALA GLY ALA PRO GLN PRO ALA LYS VAL GLY GLU ALA PRO SER THR THR SER ALA SER THR SER ALA LEU PRO GLY GLU

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ILE ASN SER GLY LEU ASP VAL LYS GLN PRO ILE LYS PRO LEU SER GLU PRO ALA ASP SER SER SER GLN GLN GLN THR LEU THR THR GLN SER ALA ALA GLU GLN VAL PRO THR ALA ALA THR ALA ALA THR ALA LEU PRO PRO PRO VAL PRO THR THR PRO ILE PRO SER THR

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THR GLY PHE GLY THR SER ALA PHE GLY ALA THR GLY GLY ASN GLY GLY PHE GLY GLN PRO SER PHE GLY GLN ALA THR LEU PRO PHE SER GLN PRO VAL PRO ALA PHE GLY GLN PRO ALA ALA SER THR ALA THR

SER SER ALA GLY SER LEU PHE GLY CYS THR SER SER SER ALA SER GLY PHE GLY GLN ALA SER GLY VAL LEU PHE GLY GLN SER ALA ALA PHE PRO GLN ALA ALA PRO ALA PHE GLY GLN SER THR SER THR THR SER GLY VAL LEU PHE GLY GLN SER SER ALA PRO VAL PHE GLY GLN SER SER GLY GLY LEU PHE GLY ALA GLY SER GLY GLY ALA GLY

SER THR THR THR ALA SER PHE GLY PHE GLY GLN PRO ALA GLY PHE ALA SER GLY THR SER GLY SER GLN SER GLY SER THR SER VAL PHE GLY GLN GLN PRO ALA ALA SER SER SER GLY GLY LEU PHE GLY ALA ALA PRO ALA PHE GLY GLY GLY ALA SER THR VAL GLY LEU

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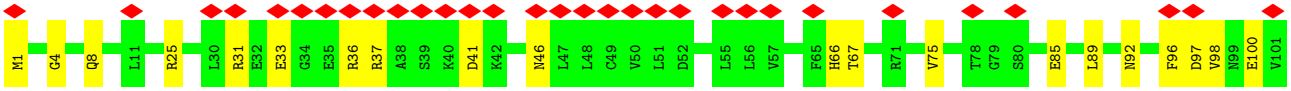
PHE SER ALA GLY GLY SER GLN GLY PHE SER PHE ASN SER PRO THR LYS THR GLY GLY PHE GLY SER PRO PRO THR PHE GLY GLY SER PRO GLY PHE GLY GLY SER PRO ALA PHE GLY THR ALA GLY SER ASN THR LEU GLY SER THR

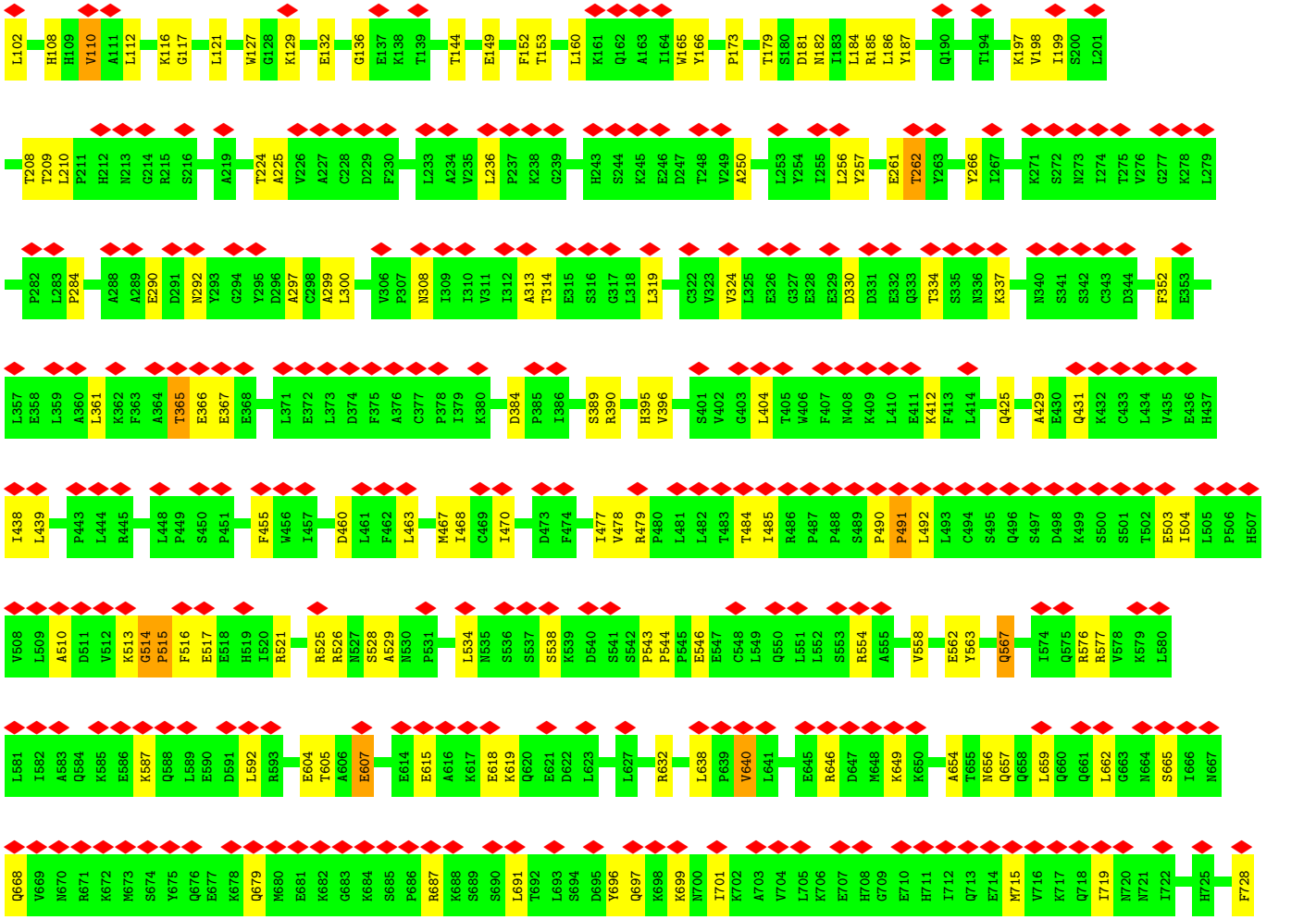
GLY GLY LYS VAL PHE GLY GLU GLY THR THR SER ALA ALA GLY PHE GLY SER ASN SER SER THR ALA ALA PHE GLY SER LEU ALA THR GLN GLY ASN THR PRO THR PHE GLY SER ILE SER GLN GLN SER PRO GLY PHE GLY GLY GLN SER SER GLY PHE SER GLY PHE GLY

ALA GLY PRO GLY ALA ALA GLY ASN THR GLY GLY PHE GLY PHE GLY VAL SER ASN PRO THR SER PRO GLY PHE GLY CYS TRP ARG SER

- Molecule 14: Nup88A protein

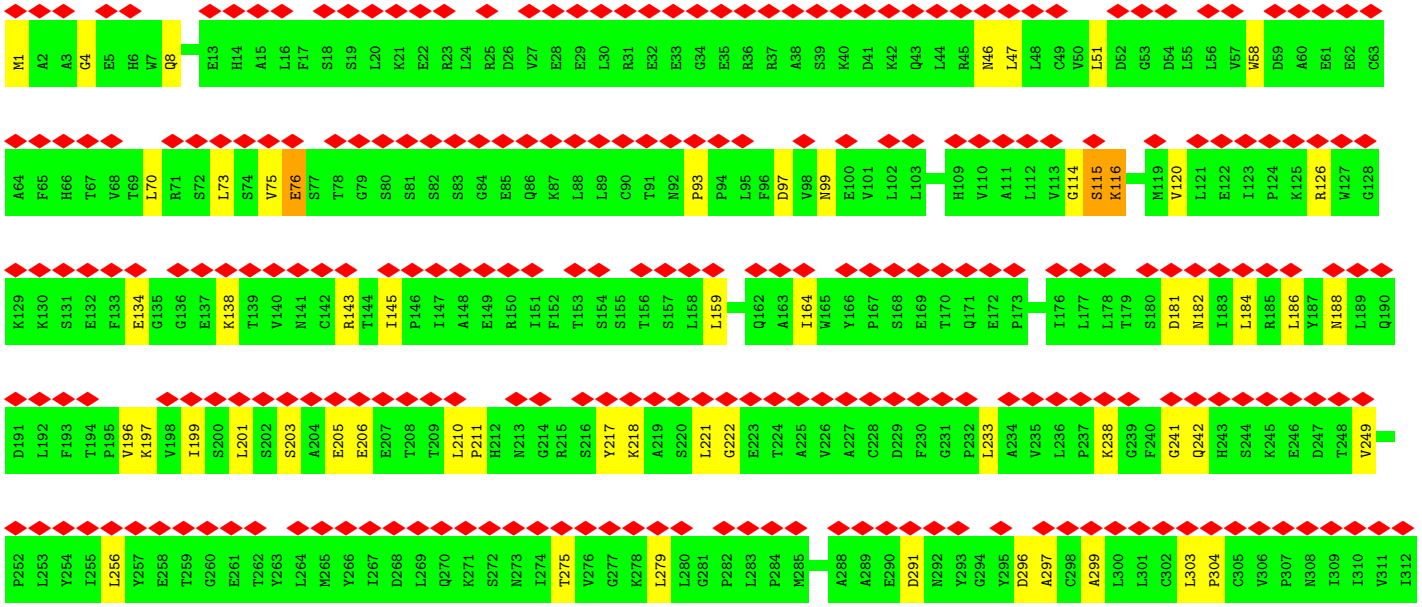
Chain b:

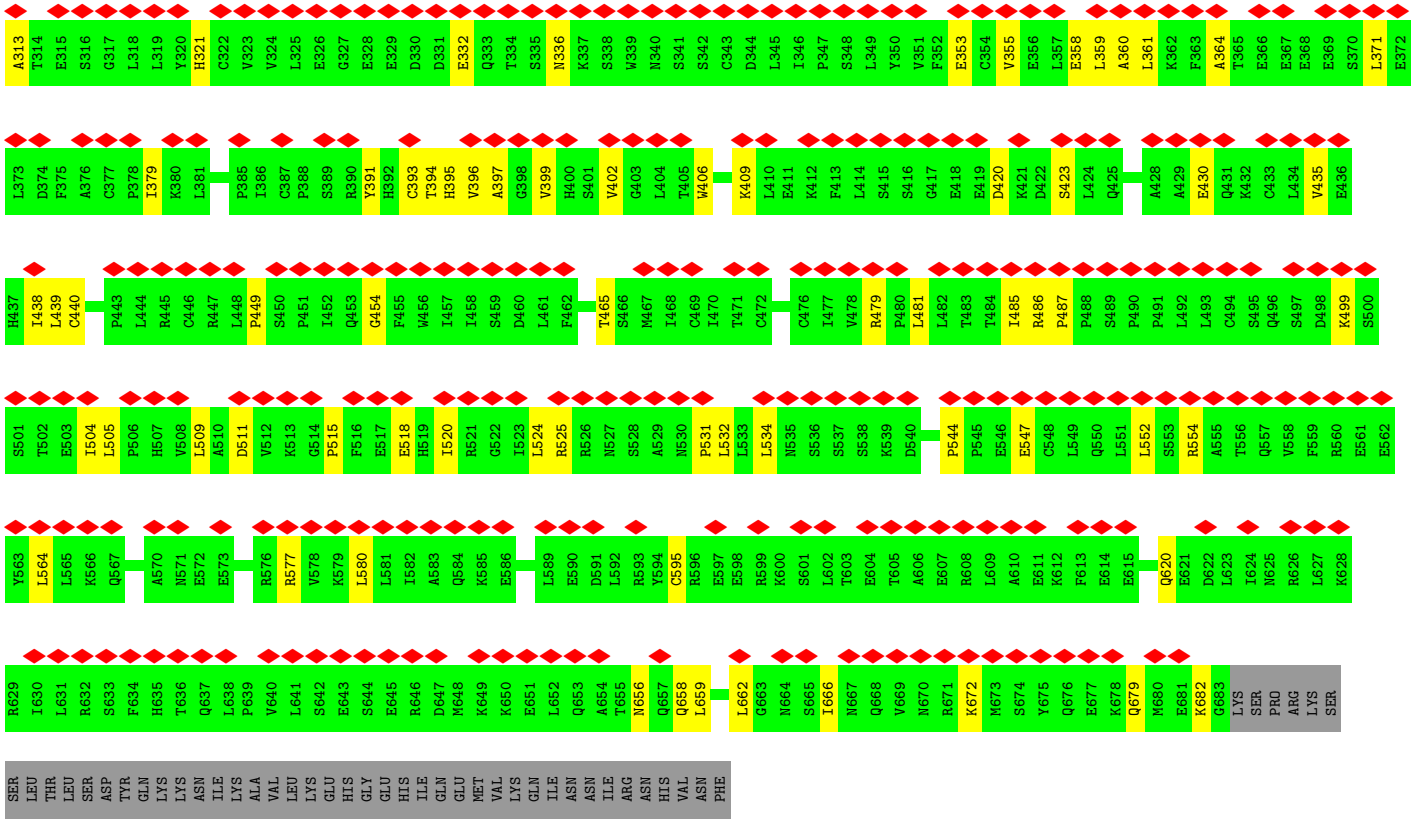




• Molecule 14: Nup88A protein

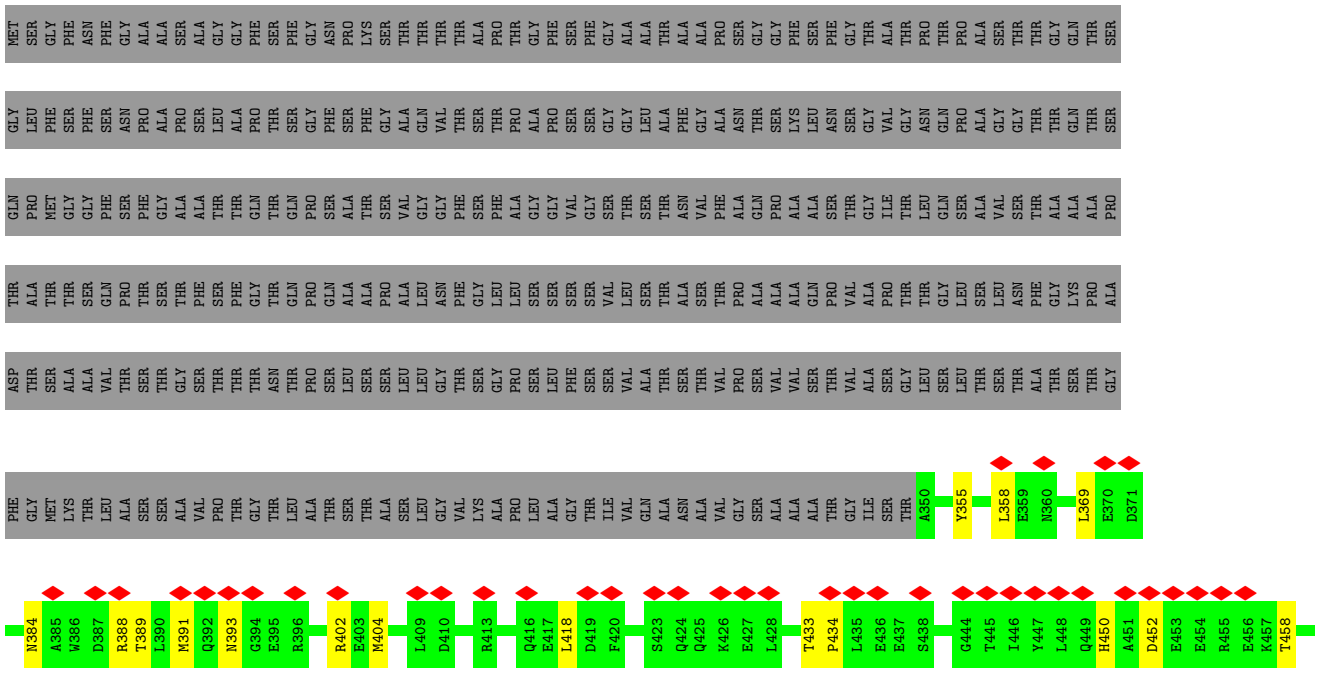
Chain d:

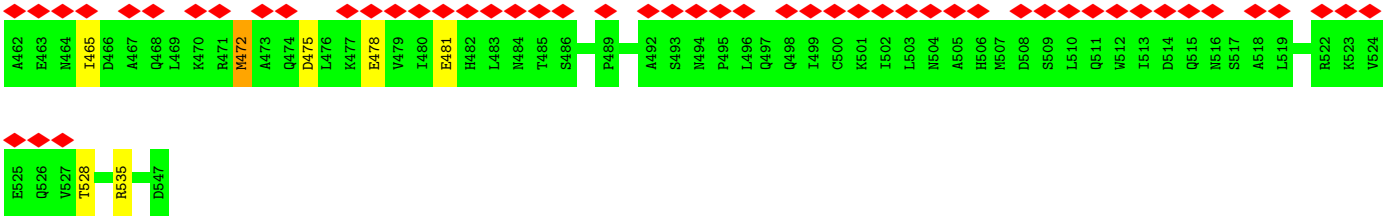




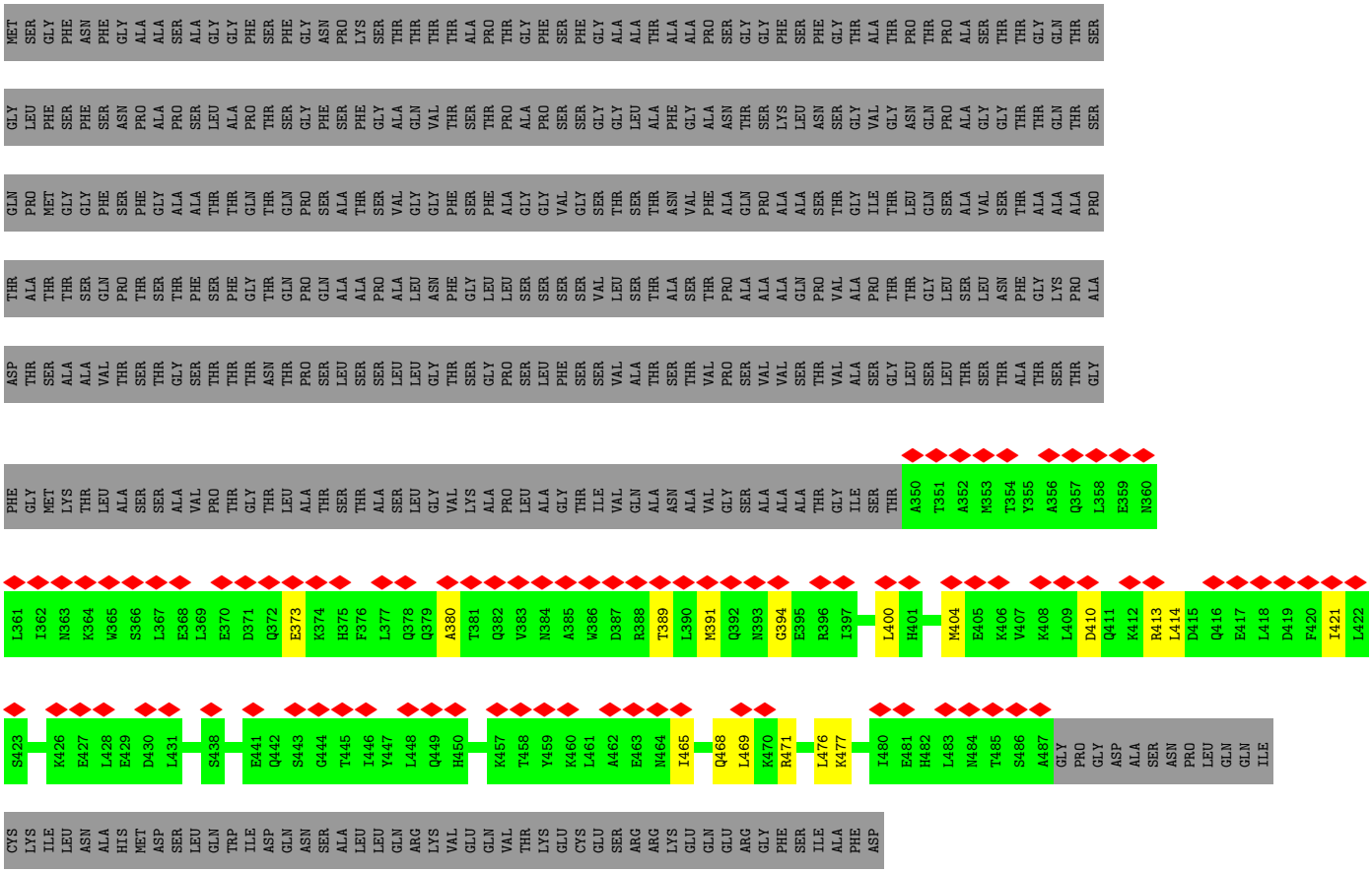
• Molecule 15: IL4I1 protein

Chain c:





• Molecule 15: IL4I1 protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.582	Depositor
Minimum map value	-2.369	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.112	Depositor
Recommended contour level	0.505	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.24, 2.24, 2.24	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	A	0.08	0/5377	0.23	0/7265
1	J	0.91	7/5377 (0.1%)	0.26	1/7265 (0.0%)
2	B	0.09	0/2996	0.26	0/4074
2	K	0.08	0/2996	0.22	0/4074
3	C	0.08	0/2674	0.21	0/3628
3	L	0.09	0/2612	0.23	0/3545
4	D	0.08	0/11349	0.22	1/15414 (0.0%)
4	M	0.08	0/11349	0.20	0/15414
5	E	0.08	0/2643	0.23	0/3587
5	N	0.08	0/2643	0.25	0/3587
6	F	0.09	0/5308	0.23	0/7201
6	O	0.08	0/5299	0.20	0/7189
7	G	0.08	0/2367	0.22	0/3231
7	P	0.08	0/2367	0.25	0/3231
8	H	0.08	0/6628	0.20	0/8968
8	Q	0.09	0/6562	0.23	0/8879
9	I	0.08	0/8647	0.22	0/11720
9	R	0.08	0/8703	0.21	0/11797
10	S	0.08	0/16272	0.21	0/22021
10	T	0.08	0/16272	0.21	0/22021
11	U	0.09	0/5360	0.23	0/7239
12	V	0.07	0/6356	0.19	0/8594
12	W	0.07	0/6227	0.18	0/8417
12	X	0.07	0/6321	0.18	0/8545
12	Y	0.08	0/6268	0.18	0/8474
12	Z	0.82	8/6243 (0.1%)	0.34	4/8439 (0.0%)
13	a	0.07	0/1762	0.16	0/2365
13	e	0.08	0/1298	0.16	0/1738
14	b	0.09	0/5896	0.21	0/7976
14	d	0.08	0/5517	0.22	0/7471
15	c	0.08	0/1641	0.15	0/2206
15	f	0.08	0/1154	0.15	0/1553
All	All	0.23	15/182484 (0.0%)	0.22	6/247128 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	471	MET	SD-CE	53.19	3.12	1.79
12	Z	308	TRP	CE3-CZ3	34.69	2.42	1.38
12	Z	308	TRP	CE2-CZ2	26.61	1.95	1.39
12	Z	308	TRP	CZ3-CH2	24.37	2.01	1.40
1	J	487	TRP	CE3-CZ3	21.94	2.04	1.38
12	Z	510	ARG	CD-NE	20.69	1.75	1.46
12	Z	308	TRP	CZ2-CH2	19.40	1.74	1.37
12	Z	308	TRP	CD2-CE2	19.09	1.73	1.41
12	Z	308	TRP	CD2-CE3	17.63	1.68	1.40
1	J	487	TRP	CE2-CZ2	17.56	1.76	1.39
1	J	487	TRP	CZ3-CH2	16.21	1.80	1.40
12	Z	510	ARG	NE-CZ	14.14	1.48	1.33
1	J	487	TRP	CD2-CE2	13.66	1.64	1.41
1	J	487	TRP	CZ2-CH2	13.19	1.62	1.37
1	J	487	TRP	CD2-CE3	12.43	1.60	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	510	ARG	CD-NE-CZ	21.63	154.69	124.40
1	J	471	MET	CG-SD-CE	12.01	127.33	100.90
12	Z	308	TRP	CE3-CZ3-CH2	-7.41	111.47	121.10
12	Z	510	ARG	CG-CD-NE	6.40	126.08	112.00
4	D	514	VAL	N-CA-C	-5.08	108.89	113.71
12	Z	510	ARG	NE-CZ-NH1	5.03	126.53	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5268	0	5226	68	0
1	J	5268	0	5226	104	0
2	B	2927	0	2800	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	2927	0	2800	49	0
3	C	2607	0	2513	40	0
3	L	2546	0	2444	34	0
4	D	11118	0	11035	144	0
4	M	11118	0	11035	168	0
5	E	2573	0	2503	36	0
5	N	2573	0	2503	53	0
6	F	5177	0	5086	82	0
6	O	5168	0	5080	66	0
7	G	2300	0	2180	32	0
7	P	2300	0	2180	38	0
8	H	6494	0	6413	54	0
8	Q	6430	0	6353	87	0
9	I	8482	0	8354	111	0
9	R	8536	0	8407	118	0
10	S	15974	0	16156	181	0
10	T	15974	0	16156	213	0
11	U	5260	0	5256	79	0
12	V	6225	0	6236	88	0
12	W	6100	0	6128	59	0
12	X	6190	0	6197	69	0
12	Y	6139	0	6155	85	0
12	Z	6116	0	6136	118	0
13	a	1738	0	1741	14	0
13	e	1282	0	1269	16	0
14	b	5787	0	5811	103	0
14	d	5414	0	5424	79	0
15	c	1621	0	1597	20	0
15	f	1141	0	1127	16	0
All	All	178773	0	177527	2285	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 6.

All (2285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:487:TRP:CZ2	1:J:487:TRP:CE2	1.76	1.70
1:J:487:TRP:CH2	1:J:487:TRP:CZ3	1.81	1.63
12:Z:308:TRP:CZ2	12:Z:308:TRP:CE2	1.95	1.51
12:Z:510:ARG:CD	12:Z:510:ARG:NE	1.75	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:308:TRP:CZ3	12:Z:510:ARG:NE	1.73	1.47
12:Z:308:TRP:CZ3	12:Z:308:TRP:CH2	2.01	1.46
1:J:487:TRP:CZ3	1:J:487:TRP:CE3	2.04	1.43
12:Z:308:TRP:CE3	12:Z:510:ARG:NE	1.83	1.43
12:Z:308:TRP:CH2	12:Z:510:ARG:NE	1.96	1.34
1:J:471:MET:SD	1:J:487:TRP:CZ3	2.28	1.27
12:Z:308:TRP:CE2	12:Z:510:ARG:NE	2.07	1.23
1:J:471:MET:SD	1:J:487:TRP:CE3	2.30	1.23
12:Z:308:TRP:CD2	12:Z:510:ARG:NE	2.05	1.22
1:J:471:MET:SD	1:J:487:TRP:CE2	2.33	1.22
12:Z:308:TRP:CZ2	12:Z:510:ARG:NE	2.08	1.22
1:J:471:MET:SD	1:J:487:TRP:CD2	2.37	1.18
1:J:471:MET:SD	1:J:487:TRP:CH2	2.37	1.18
1:J:471:MET:SD	1:J:487:TRP:CZ2	2.38	1.17
12:Z:308:TRP:CE2	12:Z:510:ARG:CD	2.26	1.16
1:J:471:MET:CE	1:J:487:TRP:CD2	2.30	1.13
1:J:471:MET:CE	1:J:487:TRP:CE2	2.30	1.13
1:J:471:MET:CE	1:J:487:TRP:CE3	2.31	1.11
1:J:471:MET:CE	1:J:487:TRP:CZ3	2.34	1.09
12:Z:308:TRP:CE2	12:Z:510:ARG:CZ	2.38	1.06
12:Z:308:TRP:CZ3	12:Z:308:TRP:CE3	2.42	1.06
12:Z:308:TRP:CD2	12:Z:510:ARG:CD	2.41	1.03
1:J:471:MET:CE	1:J:487:TRP:CZ2	2.42	1.02
1:J:471:MET:CE	1:J:487:TRP:CH2	2.44	1.01
12:Z:308:TRP:CE2	12:Z:510:ARG:NH1	2.28	1.01
12:Z:308:TRP:CD2	12:Z:510:ARG:CZ	2.43	1.01
12:Z:308:TRP:CZ2	12:Z:510:ARG:CD	2.45	0.99
12:Z:308:TRP:CD2	12:Z:510:ARG:HD2	1.99	0.97
12:Z:308:TRP:CE3	12:Z:510:ARG:CZ	2.47	0.97
12:Z:308:TRP:CZ2	12:Z:510:ARG:HD3	2.00	0.97
12:Z:308:TRP:CE2	12:Z:510:ARG:HD3	1.96	0.96
12:Z:308:TRP:CZ2	12:Z:510:ARG:CZ	2.49	0.95
12:Z:308:TRP:CE3	12:Z:510:ARG:CD	2.51	0.93
1:J:471:MET:HE2	1:J:487:TRP:CE3	2.06	0.91
1:J:471:MET:HE3	1:J:487:TRP:CE2	2.06	0.87
12:Z:308:TRP:CZ3	12:Z:510:ARG:CZ	2.56	0.87
12:Z:308:TRP:CH2	12:Z:510:ARG:CZ	2.59	0.85
9:I:74:ASN:HB2	9:I:464:VAL:O	1.76	0.85
7:P:39:ILE:HB	7:P:51:ALA:HB3	1.62	0.82
12:Z:308:TRP:CH2	12:Z:510:ARG:CD	2.64	0.81
12:Z:308:TRP:CZ3	12:Z:510:ARG:CD	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:397:LEU:HD11	4:M:400:PHE:HB3	1.66	0.78
10:T:1909:TYR:O	10:T:1913:HIS:HB2	1.83	0.77
12:V:756:MET:HE1	12:X:42:TYR:H	1.51	0.76
1:J:471:MET:HE1	1:J:487:TRP:CH2	2.22	0.75
6:O:695:LEU:O	6:O:699:CYS:HB2	1.88	0.74
1:J:471:MET:HE1	1:J:487:TRP:CZ3	2.22	0.74
14:b:186:LEU:HB2	14:b:197:LYS:HB3	1.70	0.74
1:A:455:CYS:SG	1:A:463:GLN:NE2	2.61	0.73
12:V:747:SER:HB3	12:X:3:ARG:HB2	1.70	0.73
1:J:471:MET:HE2	1:J:487:TRP:CD2	2.23	0.72
1:J:227:MET:HG2	1:J:278:MET:HG3	1.70	0.72
12:V:53:ILE:HG23	12:V:57:GLU:HG2	1.72	0.72
12:X:4:SER:H	12:X:7:GLU:HB2	1.56	0.71
12:Z:308:TRP:CZ2	12:Z:510:ARG:NH1	2.59	0.71
5:N:232:TRP:HD1	5:N:249:ALA:HB2	1.55	0.71
3:L:247:ILE:HB	3:L:272:ALA:HB3	1.73	0.70
10:S:125:LEU:HD22	10:S:208:LEU:HB2	1.74	0.69
6:O:389:GLN:HE21	6:O:393:LEU:HB2	1.58	0.69
12:W:602:VAL:HG21	12:W:656:LEU:HD22	1.75	0.69
5:N:11:TYR:HB2	5:N:321:PHE:HB2	1.75	0.69
6:O:759:VAL:HA	6:O:763:LEU:HB2	1.76	0.68
14:d:299:ALA:HB3	14:d:313:ALA:HB3	1.75	0.68
9:I:993:PRO:HG2	9:I:996:LEU:HB3	1.74	0.68
12:V:33:ALA:HB2	12:V:48:SER:HB2	1.74	0.68
10:T:633:CYS:SG	10:T:634:SER:N	2.65	0.68
14:d:186:LEU:HB3	14:d:197:LYS:HB3	1.74	0.68
9:R:90:LEU:HD13	9:R:456:ARG:HG3	1.76	0.68
3:C:247:ILE:HB	3:C:272:ALA:HB3	1.75	0.67
6:F:683:ASP:HB3	6:F:687:ARG:HB2	1.75	0.67
10:S:697:GLU:HG3	10:S:699:PRO:HD3	1.77	0.67
12:Z:308:TRP:CE3	12:Z:510:ARG:HD2	2.26	0.67
5:E:232:TRP:HD1	5:E:249:ALA:HB2	1.58	0.67
12:Y:257:GLU:HG2	12:Y:394:LEU:HD11	1.75	0.67
14:b:132:GLU:HB2	14:b:136:GLY:HA2	1.76	0.67
12:Y:199:ASP:HB3	12:Y:202:TRP:HB3	1.77	0.66
14:b:468:ILE:HG12	14:b:478:VAL:HG13	1.77	0.66
9:R:729:ARG:HH22	9:R:803:GLN:HB2	1.59	0.66
4:M:520:GLN:HB2	5:N:201:ILE:HG13	1.77	0.66
1:A:51:CYS:SG	3:C:5:ARG:NH1	2.68	0.66
6:F:557:GLU:O	6:F:561:GLN:HB2	1.95	0.66
4:M:116:GLU:O	4:M:126:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASP:HB3	1:A:357:GLN:HB2	1.77	0.66
12:Z:76:VAL:HG21	12:Z:107:LEU:HD13	1.77	0.66
2:B:175:VAL:HG12	2:B:185:THR:HG22	1.77	0.66
5:N:212:MET:HE3	5:N:229:GLY:H	1.62	0.66
1:J:453:ARG:HD3	2:K:271:PRO:HD2	1.77	0.65
11:U:790:ALA:HB2	11:U:819:MET:HB2	1.77	0.65
12:Z:481:LEU:HA	12:Z:484:LEU:HD12	1.78	0.65
7:G:298:CYS:SG	12:Y:23:ARG:NH2	2.69	0.65
1:J:471:MET:HE3	1:J:487:TRP:CZ2	2.30	0.65
2:K:215:VAL:HG11	2:K:236:ASP:HB2	1.77	0.65
6:F:714:LEU:HD23	6:F:718:LEU:HD12	1.78	0.65
14:b:513:LYS:O	15:c:388:ARG:NH2	2.29	0.65
9:R:167:LEU:HB2	9:R:179:TRP:HB2	1.78	0.65
12:W:129:PRO:HB3	12:W:170:LYS:HG3	1.79	0.65
10:S:1768:ILE:HA	10:S:1771:SER:HB2	1.78	0.65
12:X:164:ASP:HB3	12:X:167:VAL:HB	1.79	0.65
8:H:773:PHE:HB2	1:J:527:MET:HE1	1.79	0.65
1:J:471:MET:CG	1:J:487:TRP:CD2	2.79	0.65
1:J:334:LEU:HA	1:J:338:SER:HB2	1.77	0.65
4:M:510:GLN:HE21	5:N:239:ARG:HB3	1.61	0.65
10:T:1302:THR:HB	10:T:1351:GLU:HG2	1.79	0.65
14:d:666:ILE:HG12	15:f:476:LEU:HD21	1.79	0.65
4:M:418:ASN:ND2	4:M:543:GLU:OE1	2.30	0.64
12:X:563:ALA:HB1	12:X:607:LYS:HD2	1.79	0.64
12:X:679:TYR:HB3	12:X:716:PHE:HB3	1.79	0.64
1:A:494:ALA:O	1:A:532:ARG:NH2	2.29	0.64
10:S:606:ASP:OD2	10:S:645:LYS:NZ	2.30	0.64
10:S:1760:MET:HE1	10:S:1895:ILE:HG23	1.80	0.64
4:D:78:LYS:H	9:I:390:ARG:HH22	1.45	0.64
6:O:478:VAL:HG13	8:Q:367:ALA:HB1	1.79	0.64
12:W:8:ILE:HD11	12:W:35:LEU:HD22	1.80	0.64
8:H:310:LEU:HD12	8:H:319:PRO:HG2	1.79	0.64
4:M:46:TYR:HB2	4:M:438:VAL:HG22	1.79	0.64
10:T:1028:THR:H	10:T:1031:HIS:HB2	1.61	0.64
2:B:41:GLU:H	2:B:44:LYS:HZ1	1.45	0.64
6:O:389:GLN:HE22	6:O:394:GLU:HG3	1.62	0.64
12:V:26:SER:HB3	12:V:52:TYR:HD1	1.63	0.64
12:Y:207:VAL:HG22	12:Y:232:LEU:HG	1.78	0.64
2:B:88:ARG:HH11	3:C:96:LYS:HE3	1.63	0.64
4:M:258:LYS:HD2	4:M:265:ARG:HD3	1.79	0.64
10:T:513:MET:N	10:T:513:MET:SD	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:306:LYS:HB2	3:C:316:ILE:HD12	1.79	0.64
1:A:359:ILE:HD11	1:A:375:LEU:HD11	1.80	0.64
4:M:156:LEU:HG	4:M:161:VAL:HG12	1.79	0.64
12:Z:350:ARG:HH21	12:Z:351:GLN:HE22	1.45	0.64
10:T:719:ASN:HA	10:T:727:PRO:HG3	1.78	0.63
5:E:219:ARG:HB2	5:E:264:GLU:HB3	1.79	0.63
9:I:210:SER:HB2	9:I:222:ARG:HH12	1.63	0.63
9:R:794:ASN:HA	9:R:846:LEU:HD21	1.80	0.63
9:I:997:LEU:HD22	9:I:1007:MET:HE1	1.79	0.63
6:O:600:VAL:HG11	6:O:633:LEU:HD11	1.80	0.63
12:V:657:ASP:HB3	12:V:662:LYS:HB2	1.81	0.63
12:Z:480:CYS:SG	12:Z:481:LEU:N	2.72	0.63
8:H:447:MET:HG2	8:H:478:TRP:HB3	1.81	0.63
4:M:147:THR:O	4:M:149:ASN:N	2.30	0.63
9:R:451:PRO:HG2	9:R:463:VAL:HG23	1.80	0.63
1:A:116:MET:SD	1:A:133:GLN:NE2	2.69	0.63
8:H:903:LEU:HD11	9:I:895:ARG:HE	1.64	0.63
10:S:1648:LEU:HD23	10:S:1655:ILE:HD13	1.80	0.63
9:R:397:LEU:HD13	9:R:409:LEU:HG	1.81	0.62
1:J:471:MET:HG3	1:J:487:TRP:CD2	2.34	0.62
5:N:224:ILE:HD13	5:N:237:MET:HB3	1.80	0.62
10:T:532:LYS:HA	10:T:552:TRP:HE1	1.64	0.62
4:D:1104:GLY:O	4:D:1120:GLN:NE2	2.33	0.62
2:K:152:CYS:HB2	2:K:162:ARG:HB3	1.81	0.62
10:S:269:LEU:HD23	10:S:378:SER:HB3	1.82	0.62
8:H:584:VAL:HG13	8:H:592:ALA:HB1	1.81	0.62
8:Q:870:ASP:OD1	8:Q:870:ASP:N	2.32	0.62
3:L:16:HIS:HE1	3:L:59:SER:HB3	1.64	0.62
9:R:239:GLY:HA2	9:R:296:GLN:HE22	1.64	0.62
14:b:514:GLY:O	15:c:384:ASN:ND2	2.33	0.62
9:R:1047:GLU:HG2	9:R:1048:VAL:HG23	1.79	0.62
6:F:528:GLN:HE21	12:Y:10:ARG:HH22	1.47	0.62
10:T:1095:LEU:HG	10:T:1113:LEU:HD23	1.82	0.62
12:Z:679:TYR:HB3	12:Z:716:PHE:HB3	1.82	0.61
1:A:66:PRO:O	2:B:245:ARG:NH2	2.33	0.61
1:A:530:SER:OG	1:A:532:ARG:NH1	2.33	0.61
2:B:150:ILE:HB	2:B:164:ILE:HB	1.81	0.61
8:H:338:LEU:HD13	8:H:415:GLU:HB2	1.81	0.61
9:I:162:ALA:HB1	9:I:181:ASN:HD21	1.65	0.61
3:C:35:SER:HB3	3:C:54:LYS:HD3	1.83	0.61
4:M:355:LEU:HB3	4:M:374:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:928:GLU:HG3	10:S:997:PRO:HD2	1.82	0.61
10:T:1447:MET:SD	10:T:1450:ARG:NH1	2.74	0.61
2:K:20:ARG:HH12	2:K:89:ILE:HD13	1.66	0.61
6:O:292:THR:HB	10:T:674:ARG:HB2	1.82	0.61
9:R:559:PRO:O	9:R:586:GLN:NE2	2.33	0.61
11:U:288:PRO:HD2	12:Y:120:ARG:HH21	1.65	0.61
14:b:102:LEU:HB3	14:b:165:TRP:HE1	1.65	0.61
14:b:290:GLU:HG3	14:b:292:ASN:H	1.65	0.61
2:K:264:VAL:HG22	2:K:276:THR:HG23	1.83	0.61
9:R:455:ILE:HB	9:R:458:SER:HB2	1.82	0.61
10:T:418:ILE:HG23	10:T:428:PRO:HB3	1.81	0.61
1:J:444:THR:H	1:J:447:LYS:HE2	1.64	0.61
4:M:123:LEU:HB3	4:M:185:SER:HB2	1.82	0.61
4:M:423:LYS:HD3	4:M:435:TRP:HB3	1.82	0.61
8:Q:850:PHE:HB3	8:Q:891:LEU:HD22	1.83	0.61
9:R:937:LEU:HD22	9:R:954:LEU:HD22	1.82	0.61
10:T:393:VAL:HG21	10:T:443:ILE:HD13	1.82	0.61
4:D:794:LEU:HB2	4:D:884:ARG:HE	1.66	0.61
11:U:314:ILE:HD11	11:U:342:ALA:HB2	1.81	0.61
14:d:479:ARG:HH11	14:d:532:LEU:HD12	1.65	0.61
4:D:560:VAL:HB	4:D:571:LEU:HB2	1.82	0.61
6:F:249:ARG:HD3	6:F:252:ARG:HG2	1.83	0.61
6:O:389:GLN:HG2	6:O:393:LEU:HD12	1.83	0.61
10:S:1400:ARG:HH12	10:S:1468:ILE:HG21	1.65	0.61
10:S:1541:PRO:HG2	10:S:1603:GLU:HB2	1.83	0.61
9:R:591:MET:HE1	9:R:637:ILE:HB	1.83	0.60
9:I:827:ARG:HH21	5:N:1:MET:H2	1.47	0.60
2:K:296:THR:HG21	2:K:305:PHE:HB3	1.84	0.60
4:M:59:ARG:HD3	4:M:125:ASN:H	1.65	0.60
4:M:503:LEU:HD22	5:N:242:TYR:HA	1.81	0.60
4:M:1398:ASN:HD21	10:T:790:GLU:HG3	1.67	0.60
9:R:334:SER:HB2	9:R:345:LEU:HB3	1.84	0.60
9:R:1036:LEU:HA	9:R:1039:LEU:HD12	1.83	0.60
10:T:466:PRO:HG2	10:T:529:SER:HB3	1.83	0.60
1:A:273:SER:HB2	13:a:745:ARG:HH22	1.67	0.60
6:F:532:LYS:NZ	6:F:580:ASP:OD1	2.33	0.60
1:J:523:LEU:HD12	2:K:58:LEU:HD22	1.84	0.60
7:G:220:ALA:HB2	7:G:229:THR:HG22	1.84	0.60
4:M:1113:THR:HB	10:T:470:THR:HG21	1.83	0.60
10:S:1399:LEU:HD13	10:S:1465:ASN:HD21	1.66	0.60
12:Y:322:ALA:O	12:Y:351:GLN:NE2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:570:GLN:NE2	12:Z:636:ASP:OD1	2.35	0.60
7:P:166:SER:HA	7:P:226:PRO:HG2	1.83	0.60
10:S:1111:SER:HA	10:S:1114:MET:HE2	1.84	0.60
10:T:1938:PHE:HB2	10:T:1947:ARG:HG2	1.84	0.60
7:G:215:ARG:H	7:G:234:SER:HA	1.67	0.60
1:J:50:ARG:NH2	1:J:51:CYS:SG	2.74	0.60
4:M:104:HIS:HB2	4:M:563:LEU:HD21	1.84	0.60
14:b:184:LEU:HB2	14:b:199:ILE:HB	1.82	0.60
9:I:117:LEU:HB3	9:I:136:LEU:HB2	1.84	0.60
9:I:823:TYR:CZ	9:I:827:ARG:HD2	2.37	0.60
1:J:389:ASN:HA	1:J:394:ALA:HA	1.82	0.60
10:T:1316:LEU:HD22	10:T:1340:LEU:HD22	1.84	0.60
9:I:1058:LEU:HD22	9:I:1104:PRO:HD2	1.83	0.60
12:V:23:ARG:HH12	12:V:56:GLN:HB3	1.67	0.60
12:Z:443:GLN:NE2	12:Z:513:CYS:SG	2.75	0.60
4:M:536:THR:HG21	9:R:80:SER:HA	1.84	0.59
4:M:1073:ASP:HB3	4:M:1151:GLU:HA	1.84	0.59
9:R:397:LEU:HD11	9:R:407:CYS:HB3	1.83	0.59
8:H:857:HIS:HE1	8:H:898:SER:HB3	1.67	0.59
1:J:65:SER:HB3	1:J:68:LEU:HB2	1.83	0.59
3:L:16:HIS:ND1	3:L:60:VAL:O	2.33	0.59
12:V:466:GLN:NE2	12:V:593:ASP:OD1	2.35	0.59
12:W:214:LEU:O	12:W:218:GLN:NE2	2.35	0.59
10:S:985:LEU:HD23	10:S:988:LEU:HD21	1.83	0.59
10:T:25:LEU:O	10:T:29:ILE:HB	2.02	0.59
11:U:501:LYS:NZ	12:Y:474:ASN:OD1	2.35	0.59
10:T:47:LYS:HD2	10:T:172:ARG:HD3	1.85	0.59
12:X:180:ARG:HD2	12:X:183:GLU:HG3	1.84	0.59
12:Y:457:LEU:HB3	12:Y:481:LEU:HD22	1.84	0.59
6:F:336:LYS:HG3	6:F:719:CYS:HB3	1.84	0.59
12:Y:76:VAL:HG12	12:Y:103:LEU:HD22	1.84	0.59
14:d:395:HIS:HD2	14:d:397:ALA:HB3	1.67	0.59
4:M:1070:ARG:NH2	4:M:1102:GLU:OE2	2.35	0.59
12:Z:308:TRP:CZ3	12:Z:510:ARG:NH2	2.69	0.59
6:O:471:GLN:NE2	8:Q:368:THR:O	2.35	0.59
10:S:563:HIS:HB2	10:S:630:LEU:HD21	1.84	0.59
11:U:288:PRO:HB3	12:Y:124:LEU:HD11	1.85	0.59
4:D:116:GLU:O	4:D:126:ASN:ND2	2.35	0.59
8:Q:301:MET:HG3	8:Q:302:LEU:HG	1.85	0.59
12:X:302:GLN:NE2	12:X:511:PRO:O	2.36	0.59
3:C:62:ARG:HB2	3:C:77:CYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:LYS:HB2	9:I:354:ASN:HB3	1.84	0.59
1:J:423:ASP:OD1	1:J:430:ARG:NH2	2.35	0.59
10:T:767:TYR:HA	10:T:849:LEU:HD21	1.83	0.59
1:A:133:GLN:HA	1:A:136:ILE:HG12	1.84	0.59
4:D:889:THR:HG23	5:E:186:LYS:HG3	1.85	0.59
6:F:538:HIS:HA	6:F:542:MET:HG3	1.84	0.59
5:N:270:THR:HG22	5:N:280:ILE:HG22	1.83	0.59
6:O:735:ARG:NH1	7:P:68:PRO:O	2.35	0.59
14:b:182:ASN:HB2	14:b:224:THR:HG22	1.85	0.59
9:R:100:ALA:HB3	9:R:147:ALA:H	1.68	0.58
12:X:313:GLU:HB3	12:X:372:ILE:HD11	1.85	0.58
14:b:256:LEU:HB2	14:b:300:LEU:HD13	1.85	0.58
4:M:539:LEU:HD21	9:R:130:LEU:HD12	1.86	0.58
4:M:1161:TYR:HB2	10:T:482:GLN:HB2	1.85	0.58
6:O:503:LEU:HD23	6:O:523:ILE:HG13	1.86	0.58
9:R:539:PRO:HA	9:R:543:LEU:HD22	1.85	0.58
5:E:282:ILE:HB	5:E:292:LEU:HB3	1.85	0.58
1:J:474:GLN:OE1	1:J:478:ASN:ND2	2.36	0.58
4:M:137:ILE:HG12	4:M:155:ILE:HD11	1.84	0.58
8:Q:420:ALA:HB1	8:Q:429:LEU:HG	1.84	0.58
11:U:757:LEU:HB3	11:U:819:MET:HE3	1.84	0.58
12:V:215:ALA:O	12:V:218:GLN:NE2	2.36	0.58
12:Z:563:ALA:HB1	12:Z:608:LEU:HD13	1.84	0.58
9:I:1076:PRO:HB3	9:I:1123:TYR:HB3	1.85	0.58
12:V:356:HIS:HA	12:V:443:GLN:HE22	1.69	0.58
12:X:699:PRO:HD2	12:X:702:GLU:HB2	1.85	0.58
14:b:236:LEU:HD12	14:b:250:ALA:HB3	1.85	0.58
10:T:1433:ARG:HH21	10:T:1445:LYS:HD2	1.68	0.58
12:V:487:PHE:HE1	12:V:527:GLN:HE21	1.50	0.58
9:I:832:SER:H	9:I:833:PRO:HD2	1.67	0.58
4:M:633:CYS:SG	4:M:896:ARG:NH1	2.76	0.58
9:R:729:ARG:NH2	9:R:799:ASP:O	2.36	0.58
11:U:422:VAL:HG13	11:U:436:LEU:H	1.69	0.58
1:A:94:ARG:NH2	1:A:381:HIS:O	2.37	0.58
6:F:337:SER:HB2	6:F:342:HIS:HB2	1.84	0.58
4:M:285:PRO:HB3	4:M:301:ALA:HB1	1.86	0.58
7:P:162:VAL:O	7:P:181:ARG:NH2	2.37	0.58
7:P:242:TRP:HB3	7:P:252:TRP:HB3	1.85	0.58
10:T:1439:THR:HB	10:T:1624:GLN:HG2	1.86	0.58
14:b:8:GLN:HB3	14:b:478:VAL:HB	1.85	0.58
14:d:515:PRO:HG2	14:d:518:GLU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:CYS:HB2	2:B:162:ARG:HB3	1.84	0.58
2:K:6:ALA:HB3	2:K:369:VAL:HB	1.85	0.58
6:O:399:GLU:O	6:O:405:LYS:NZ	2.36	0.58
3:C:34:GLN:HE22	3:C:59:SER:H	1.52	0.58
6:F:830:THR:HA	6:F:833:MET:HE2	1.85	0.58
9:I:729:ARG:HH21	9:I:733:ASN:HA	1.68	0.58
8:Q:299:ARG:HE	8:Q:306:SER:HB2	1.68	0.58
12:Y:4:SER:H	12:Y:7:GLU:HB2	1.69	0.58
9:R:1099:LEU:HA	9:R:1103:LEU:HB2	1.85	0.58
12:Z:164:ASP:HB3	12:Z:167:VAL:HB	1.84	0.58
11:U:581:PHE:HB2	11:U:585:LEU:HB2	1.85	0.57
2:B:53:PHE:HB2	2:B:57:SER:HB3	1.84	0.57
10:S:636:PRO:HD2	10:S:639:LEU:HD12	1.85	0.57
10:T:1701:MET:SD	10:T:1704:GLN:NE2	2.77	0.57
14:b:225:ALA:HA	14:b:257:TYR:HA	1.85	0.57
14:b:659:LEU:HD12	15:c:472:MET:HE3	1.86	0.57
5:E:72:GLY:H	5:E:105:ARG:HH12	1.51	0.57
9:I:218:ASN:ND2	9:I:263:SER:O	2.31	0.57
1:J:562:MET:SD	1:J:605:ARG:NE	2.76	0.57
9:R:286:LYS:NZ	9:R:288:ASP:OD1	2.37	0.57
10:S:389:ILE:HD12	10:S:446:LEU:HD21	1.86	0.57
4:M:553:VAL:HG22	4:M:560:VAL:HG13	1.84	0.57
4:M:1008:LEU:HD13	4:M:1039:VAL:HG21	1.86	0.57
9:R:436:ALA:HB3	9:R:439:ASP:HB2	1.86	0.57
9:R:751:THR:O	9:R:760:ARG:NH1	2.37	0.57
10:T:17:TYR:OH	10:T:56:ASN:ND2	2.37	0.57
11:U:610:ILE:HG23	11:U:629:LEU:HG	1.87	0.57
12:Z:308:TRP:CD1	12:Z:308:TRP:H	2.21	0.57
14:b:438:ILE:O	14:b:479:ARG:NH2	2.37	0.57
4:M:1313:LEU:HG	4:M:1318:VAL:HG13	1.86	0.57
7:P:280:GLY:O	7:P:304:LYS:NZ	2.37	0.57
12:Y:205:CYS:SG	12:Y:208:ARG:NH2	2.78	0.57
12:Y:699:PRO:HD2	12:Y:702:GLU:HB2	1.87	0.57
14:b:526:ARG:NH2	14:b:562:GLU:O	2.34	0.57
4:D:1000:ARG:HD3	4:D:1023:ILE:HG12	1.86	0.57
14:b:33:GLU:HA	14:b:36:ARG:HD2	1.86	0.57
6:F:504:ARG:NH1	6:F:507:CYS:SG	2.78	0.57
4:M:62:ARG:HH21	4:M:187:PHE:HB3	1.68	0.57
5:N:225:GLY:HA3	5:N:234:ILE:HD13	1.87	0.57
10:T:674:ARG:HH22	10:T:720:LEU:HD22	1.70	0.57
10:T:1310:ARG:NH1	10:T:1389:SER:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:292:ASN:ND2	12:Y:116:TYR:OH	2.37	0.57
12:Y:598:MET:HE1	12:Y:652:ALA:HB1	1.85	0.57
1:A:109:LEU:HD23	1:A:141:GLU:HG2	1.87	0.57
8:H:181:LYS:O	8:H:185:LYS:HB3	2.05	0.57
9:I:506:THR:HG23	9:I:550:ILE:HG13	1.85	0.57
1:J:349:ALA:HB1	1:J:357:GLN:HE22	1.69	0.57
10:S:1358:ALA:HA	10:S:1869:GLN:HE22	1.70	0.57
10:T:202:LEU:HB3	10:T:208:LEU:HD11	1.87	0.57
13:e:762:THR:O	13:e:766:ARG:HD3	2.04	0.57
2:B:238:MET:HG3	2:B:255:ASN:HA	1.87	0.57
2:K:118:GLN:HB3	2:K:126:ASN:H	1.68	0.57
12:W:27:MET:HG3	12:W:28:LYS:HG2	1.87	0.57
2:B:251:MET:SD	2:B:252:SER:OG	2.61	0.57
6:O:553:LEU:HD21	6:O:609:SER:HB3	1.87	0.57
13:a:706:ILE:HD13	14:b:546:GLU:HG3	1.87	0.57
14:d:509:LEU:H	15:f:391:MET:HE1	1.69	0.57
8:Q:890:ASN:HB3	11:U:814:GLN:HG2	1.86	0.56
12:W:123:LYS:O	12:W:161:ARG:NH1	2.38	0.56
12:W:562:ARG:HA	12:W:600:ARG:HH22	1.70	0.56
13:a:816:GLN:OE1	13:a:820:ARG:NH1	2.38	0.56
4:D:119:LEU:HD23	4:D:713:VAL:HG21	1.87	0.56
9:I:246:ILE:H	9:I:249:ARG:HH12	1.54	0.56
1:J:335:ALA:HA	15:c:450:HIS:HB2	1.87	0.56
2:K:277:CYS:HB3	2:K:351:LEU:HD22	1.86	0.56
5:N:128:ASN:H	5:N:144:GLY:HA2	1.69	0.56
10:T:1783:PRO:HA	10:T:1962:LEU:HD13	1.87	0.56
12:V:322:ALA:O	12:V:350:ARG:NH1	2.34	0.56
12:W:181:LEU:HD21	12:W:213:TYR:HA	1.87	0.56
3:C:156:GLN:HA	4:D:1323:TRP:HB3	1.87	0.56
6:F:436:ARG:HG3	6:F:440:ALA:HB2	1.85	0.56
6:F:616:CYS:SG	6:F:653:ARG:NH2	2.78	0.56
7:G:59:PRO:HD2	7:G:79:TYR:HB3	1.87	0.56
9:I:607:PHE:HE2	9:I:738:ASN:HB2	1.69	0.56
1:J:218:ALA:O	1:J:225:ARG:NH1	2.38	0.56
1:J:453:ARG:NH2	1:J:457:GLN:OE1	2.37	0.56
1:J:548:GLN:HE21	1:J:550:GLN:HB2	1.70	0.56
2:K:223:HIS:HB2	2:K:229:VAL:HB	1.86	0.56
4:M:144:ILE:HG12	4:M:153:VAL:HG22	1.88	0.56
4:M:147:THR:C	4:M:149:ASN:H	2.13	0.56
9:R:86:VAL:HG22	9:R:118:ILE:HD12	1.86	0.56
11:U:750:LEU:HD13	11:U:812:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:501:ASP:OD2	12:V:630:LYS:NZ	2.38	0.56
12:W:91:PRO:O	12:W:120:ARG:NH2	2.38	0.56
14:b:367:GLU:OE2	14:b:554:ARG:NH2	2.39	0.56
14:b:715:MET:HE3	14:b:719:ILE:HG12	1.88	0.56
2:B:203:ASP:N	2:B:203:ASP:OD1	2.38	0.56
7:G:195:ARG:NH1	7:G:196:GLU:O	2.39	0.56
4:M:547:ARG:NH1	9:R:135:GLU:OE1	2.38	0.56
4:M:583:VAL:HG13	4:M:587:HIS:HB3	1.87	0.56
4:M:826:ASP:OD2	4:M:884:ARG:NH2	2.39	0.56
6:F:510:SER:OG	6:F:511:GLY:N	2.39	0.56
2:K:226:GLN:OE1	2:K:228:HIS:NE2	2.38	0.56
9:R:236:LEU:O	9:R:238:GLN:NE2	2.38	0.56
9:R:767:HIS:HE1	9:R:793:LEU:HD12	1.71	0.56
10:S:139:LYS:HD3	10:S:142:MET:HE2	1.88	0.56
10:S:1791:ARG:NH1	10:S:1813:VAL:O	2.39	0.56
11:U:680:VAL:HG13	12:Z:620:SER:HB2	1.88	0.56
2:B:311:SER:HB2	2:B:375:SER:H	1.70	0.56
4:D:483:ARG:NH2	4:D:500:GLU:OE1	2.38	0.56
4:D:1121:VAL:HG21	4:D:1193:LEU:HD13	1.88	0.56
10:T:243:ARG:NH1	10:T:303:ASP:OD2	2.38	0.56
10:T:263:SER:HB3	10:T:376:SER:HB2	1.88	0.56
14:d:394:THR:HG23	14:d:399:VAL:HG22	1.87	0.56
14:d:486:ARG:O	14:d:499:LYS:NZ	2.38	0.56
14:d:552:LEU:HD23	13:e:710:ILE:HD12	1.87	0.56
1:A:155:ALA:HB1	1:A:159:PRO:HB2	1.88	0.56
7:G:153:CYS:SG	7:G:154:ASN:N	2.77	0.56
6:O:739:LYS:NZ	6:O:766:ASP:OD2	2.38	0.56
12:V:651:ILE:HG13	12:V:675:ASN:HB2	1.87	0.56
12:W:453:LEU:HB3	12:W:485:GLU:HG2	1.87	0.56
12:Z:192:GLU:OE2	12:Z:193:ARG:NH1	2.39	0.56
4:D:1380:LEU:HA	4:D:1422:LEU:HD21	1.87	0.56
9:I:823:TYR:OH	9:I:827:ARG:NH1	2.39	0.56
10:S:821:GLU:OE1	10:S:895:ASN:ND2	2.36	0.56
11:U:594:ARG:HD2	11:U:607:LYS:HE2	1.86	0.56
7:G:67:HIS:HD2	7:G:69:MET:HB2	1.71	0.56
9:I:577:SER:OG	9:I:578:ASN:N	2.38	0.56
3:L:169:SER:HB2	3:L:183:ALA:HB3	1.87	0.56
5:N:282:ILE:HB	5:N:292:LEU:HB2	1.87	0.56
6:O:249:ARG:HH11	6:O:250:SER:H	1.54	0.56
10:S:204:LYS:HG3	10:S:205:GLU:HG3	1.86	0.56
11:U:676:LYS:NZ	11:U:687:ASN:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:495:SER:HB2	9:I:501:ALA:HB1	1.88	0.56
9:I:947:TYR:HB3	9:I:950:LYS:HB2	1.87	0.56
10:T:1917:SER:HB2	10:T:1954:VAL:HG12	1.88	0.56
13:a:894:GLN:NE2	13:a:900:VAL:O	2.39	0.56
14:b:587:LYS:NZ	14:d:138:LYS:O	2.39	0.56
1:A:304:HIS:HA	1:A:307:VAL:HG22	1.88	0.55
2:B:353:VAL:HG22	2:B:358:LEU:HD13	1.87	0.55
7:P:264:VAL:HA	7:P:280:GLY:HA3	1.87	0.55
11:U:238:PRO:HG2	12:Y:474:ASN:HD21	1.71	0.55
12:V:482:LEU:HD21	12:V:581:LEU:HD11	1.88	0.55
4:D:1142:VAL:HB	4:D:1174:ILE:HD11	1.89	0.55
5:N:243:PRO:HB3	5:N:246:ASN:HB2	1.89	0.55
7:P:180:LYS:HB2	7:P:196:GLU:HG2	1.88	0.55
10:S:1696:ASN:OD1	10:S:1696:ASN:N	2.39	0.55
11:U:182:GLU:OE1	11:U:492:HIS:NE2	2.36	0.55
4:D:1107:LEU:HD22	4:D:1119:LYS:HD3	1.88	0.55
6:F:645:ASN:HB3	11:U:176:SER:HA	1.87	0.55
6:F:653:ARG:NH2	11:U:217:ASP:OD2	2.39	0.55
10:S:1753:GLN:NE2	10:S:1892:CYS:SG	2.80	0.55
10:T:958:GLU:HA	10:T:962:ASP:HB2	1.88	0.55
10:T:1655:ILE:HG23	10:T:1675:LEU:HD21	1.88	0.55
12:X:93:GLN:HB3	12:X:96:LEU:HB2	1.88	0.55
12:Y:527:GLN:NE2	12:Y:628:LEU:O	2.39	0.55
2:B:13:LYS:O	2:B:40:ASN:ND2	2.39	0.55
7:G:212:ASP:N	7:G:212:ASP:OD1	2.40	0.55
10:T:642:GLU:HA	10:T:645:LYS:HE2	1.88	0.55
11:U:647:LEU:HD11	11:U:693:LEU:HD13	1.87	0.55
2:B:46:CYS:HB3	2:B:68:GLN:HE22	1.71	0.55
1:J:360:LYS:HZ2	1:J:364:ILE:HD11	1.71	0.55
4:M:867:GLN:O	4:M:873:ASN:ND2	2.40	0.55
6:O:421:ALA:HA	6:O:424:ARG:HE	1.72	0.55
10:T:383:GLU:HA	10:T:386:ILE:HD12	1.89	0.55
10:T:515:ARG:HD3	10:T:599:GLN:HB3	1.89	0.55
10:T:554:HIS:O	10:T:557:HIS:ND1	2.40	0.55
12:V:306:VAL:HB	12:V:311:LEU:HD11	1.89	0.55
12:Y:126:PRO:HB2	12:Y:161:ARG:HH12	1.70	0.55
4:D:105:TRP:HB2	4:D:112:LEU:HD11	1.89	0.55
6:F:341:PRO:O	6:F:687:ARG:NH2	2.39	0.55
2:K:289:SER:O	2:K:291:ASP:N	2.39	0.55
8:Q:856:LEU:HD22	8:Q:865:CYS:HB2	1.89	0.55
10:S:925:LYS:HD2	10:S:994:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:684:LEU:HD22	12:X:2:ARG:HH21	1.72	0.55
12:X:730:ILE:O	12:X:734:LEU:HB2	2.05	0.55
5:N:220:ASN:HD22	5:N:223:ARG:HH21	1.53	0.55
1:A:614:SER:HB2	1:A:617:GLU:HB2	1.89	0.55
9:I:392:MET:HE1	9:I:395:CYS:HB3	1.89	0.55
9:R:111:LEU:HD23	9:R:118:ILE:HD11	1.89	0.55
10:S:1715:LEU:HD22	10:S:1809:PRO:HG2	1.87	0.55
10:T:22:GLN:NE2	10:T:959:GLU:OE1	2.40	0.55
11:U:195:LYS:HE2	11:U:200:HIS:HB3	1.88	0.55
12:Z:53:ILE:HG21	12:Z:85:ARG:HH22	1.72	0.55
14:b:429:ALA:HB2	14:d:211:PRO:HB3	1.89	0.55
14:d:524:LEU:HD13	15:f:373:GLU:HG2	1.88	0.55
4:D:965:VAL:HG12	4:D:981:LEU:HD21	1.89	0.55
9:R:411:THR:OG1	9:R:412:GLN:N	2.33	0.55
10:T:628:LEU:HD11	10:T:667:THR:HG21	1.89	0.55
12:V:248:ASP:HB3	12:V:251:LYS:HB2	1.89	0.55
14:b:468:ILE:HG23	14:b:478:VAL:HG22	1.88	0.55
3:L:306:LYS:HG2	3:L:316:ILE:HG21	1.89	0.54
4:M:44:ARG:NH2	4:M:595:VAL:O	2.39	0.54
9:R:994:LYS:HE3	9:R:1005:ASN:HD21	1.72	0.54
11:U:361:ASP:OD1	11:U:361:ASP:N	2.40	0.54
12:Y:501:ASP:O	12:Y:503:ASN:N	2.38	0.54
14:d:544:PRO:HG2	14:d:547:GLU:HB2	1.89	0.54
1:A:94:ARG:HH22	1:A:381:HIS:HB3	1.73	0.54
6:F:796:GLU:HA	6:F:800:LYS:HD3	1.87	0.54
8:H:150:PHE:O	8:H:169:TYR:OH	2.24	0.54
9:I:1058:LEU:HD23	9:I:1109:LEU:HD21	1.88	0.54
9:R:703:ASP:H	9:R:707:TRP:HZ3	1.55	0.54
12:W:197:ARG:HH22	12:W:231:GLU:HB3	1.73	0.54
14:d:51:LEU:HD23	14:d:126:ARG:HE	1.72	0.54
4:M:75:GLY:O	4:M:213:ASN:ND2	2.40	0.54
7:P:31:CYS:HB2	7:P:60:VAL:HB	1.89	0.54
8:Q:538:LEU:HD12	8:Q:570:ARG:HG3	1.88	0.54
9:R:693:GLU:OE2	9:R:766:GLN:NE2	2.41	0.54
10:T:804:HIS:O	10:T:808:ASN:ND2	2.41	0.54
14:b:110:VAL:HG13	14:b:121:LEU:HB3	1.89	0.54
1:A:300:THR:OG1	1:A:301:THR:N	2.39	0.54
4:D:540:GLN:HG3	9:I:439:ASP:HA	1.88	0.54
6:F:476:GLN:HG2	6:F:479:ARG:HB3	1.88	0.54
9:I:869:LEU:HD11	9:I:885:LEU:HD21	1.90	0.54
5:N:166:SER:HB3	5:N:185:GLU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:557:GLU:O	6:O:561:GLN:HB2	2.07	0.54
8:Q:470:PRO:HD2	8:Q:473:TYR:HD2	1.73	0.54
10:S:299:SER:O	10:S:301:PHE:N	2.41	0.54
10:S:473:MET:SD	10:S:483:ARG:NH2	2.81	0.54
12:V:347:ALA:HB1	12:V:350:ARG:HH21	1.72	0.54
12:V:582:HIS:NE2	12:V:601:CYS:SG	2.74	0.54
3:C:106:ARG:HG2	3:C:150:LEU:HB2	1.89	0.54
4:D:73:VAL:HG21	9:I:260:ALA:HB2	1.89	0.54
6:F:548:THR:HG23	6:F:551:GLN:H	1.72	0.54
1:J:97:GLN:HG2	2:K:320:SER:HB3	1.90	0.54
3:L:176:ARG:HH22	10:T:1233:VAL:HG22	1.71	0.54
9:R:286:LYS:HB3	9:R:298:LEU:HB3	1.88	0.54
9:R:414:MET:HG3	9:R:433:PRO:HA	1.88	0.54
10:S:1184:LEU:HD13	10:S:1319:LYS:HG2	1.89	0.54
10:T:1500:ASP:OD1	10:T:1561:ARG:NE	2.39	0.54
10:T:1767:MET:SD	10:T:1905:ARG:NH1	2.81	0.54
11:U:280:GLN:HG2	12:Y:88:GLU:HG3	1.89	0.54
12:X:284:GLU:HG3	12:X:328:PRO:HG3	1.89	0.54
12:Z:183:GLU:O	12:Z:187:HIS:ND1	2.41	0.54
12:Z:194:ARG:NH2	12:Z:338:ASN:OD1	2.41	0.54
12:Z:624:PRO:HB3	12:Z:630:LYS:HD3	1.89	0.54
4:D:1107:LEU:HD13	4:D:1119:LYS:HB3	1.90	0.54
6:O:325:LEU:HB3	6:O:673:TRP:HD1	1.73	0.54
10:S:671:GLN:HB2	10:S:732:TYR:HD1	1.71	0.54
10:T:635:ILE:HG22	10:T:640:LYS:HG3	1.90	0.54
12:Y:545:GLY:O	12:Y:549:LYS:NZ	2.37	0.54
4:M:1338:ARG:HH12	4:M:1387:ALA:HB2	1.73	0.54
7:P:20:GLN:HG2	7:P:29:ALA:HB3	1.90	0.54
7:P:62:GLN:HE21	7:P:108:SER:HB2	1.72	0.54
7:G:72:ASN:HB3	7:G:88:GLU:HB3	1.89	0.54
9:I:515:ARG:HB3	9:I:520:ASP:HB2	1.89	0.54
2:K:184:LEU:HD11	2:K:192:LEU:HD23	1.88	0.54
4:M:442:PRO:HD3	4:M:720:LYS:HE3	1.89	0.54
4:M:684:TYR:HB3	4:M:867:GLN:HG3	1.89	0.54
5:N:34:SER:HA	5:N:306:ARG:HH12	1.73	0.54
10:T:1935:GLN:OE1	13:e:827:ASN:ND2	2.40	0.54
12:X:197:ARG:NH1	12:X:231:GLU:OE1	2.41	0.54
14:d:182:ASN:HD22	14:d:206:GLU:HG3	1.73	0.54
1:A:79:PHE:O	1:A:83:GLN:NE2	2.40	0.54
4:M:810:ARG:NH2	4:M:825:GLU:OE1	2.40	0.54
12:V:608:LEU:HG	12:V:612:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:47:LEU:HB3	14:d:58:TRP:HB3	1.90	0.54
2:B:100:ILE:HB	2:B:114:GLN:HG2	1.90	0.54
2:B:328:THR:HG22	2:B:329:ASP:H	1.73	0.54
6:F:414:SER:HB3	6:F:540:TRP:HE1	1.73	0.54
9:I:722:LEU:HD12	9:I:792:LEU:HD11	1.89	0.54
5:N:277:LYS:HD2	5:N:297:PRO:HA	1.90	0.54
8:Q:794:LYS:NZ	8:Q:858:ASN:O	2.37	0.54
9:R:110:TRP:HB3	9:R:119:ILE:HG13	1.90	0.54
10:S:514:LEU:HD23	10:S:600:LEU:HD21	1.90	0.54
10:T:661:TRP:NE1	10:T:665:GLU:OE2	2.41	0.54
10:T:1488:HIS:O	10:T:1492:ARG:NH1	2.41	0.54
3:C:242:THR:OG1	3:C:243:LYS:N	2.38	0.53
5:N:129:ASP:HB3	5:N:171:VAL:HG12	1.90	0.53
10:S:1184:LEU:HB3	10:S:1319:LYS:HE2	1.90	0.53
10:T:1687:VAL:HG13	10:T:1691:LEU:HD21	1.91	0.53
10:T:1722:GLY:HA3	10:T:1791:ARG:HH22	1.72	0.53
11:U:812:LEU:HD23	11:U:815:MET:HE2	1.90	0.53
1:A:72:PHE:O	1:A:76:HIS:ND1	2.41	0.53
2:B:53:PHE:O	2:B:357:ASN:ND2	2.41	0.53
4:D:786:PRO:HD2	4:D:789:LEU:HD12	1.90	0.53
6:F:528:GLN:HE21	12:Y:10:ARG:NH2	2.06	0.53
2:K:113:ASN:ND2	3:L:95:ASP:OD2	2.41	0.53
8:Q:311:VAL:HA	8:Q:322:GLN:HE22	1.73	0.53
8:Q:712:ALA:HA	8:Q:715:TYR:CE2	2.43	0.53
10:S:264:LEU:HD22	10:S:372:ALA:HB1	1.91	0.53
14:b:96:PHE:HB2	14:b:116:LYS:HB2	1.90	0.53
2:B:372:ARG:NH2	2:B:374:PHE:O	2.41	0.53
9:I:211:PHE:H	9:I:223:LEU:HB3	1.71	0.53
4:M:107:SER:HB2	4:M:112:LEU:HD13	1.90	0.53
4:M:581:TYR:O	4:M:614:HIS:NE2	2.41	0.53
6:O:684:PRO:HG3	7:P:172:SER:H	1.74	0.53
10:S:489:VAL:HG12	10:S:493:LYS:HE2	1.91	0.53
11:U:512:GLN:O	11:U:528:ASN:ND2	2.39	0.53
12:Y:430:HIS:NE2	12:Y:433:ASP:OD2	2.41	0.53
3:L:158:GLU:OE2	4:M:1326:ASN:ND2	2.41	0.53
3:L:182:ILE:HG23	3:L:200:TYR:HB2	1.90	0.53
8:Q:759:ASN:OD1	11:U:803:ARG:NH2	2.41	0.53
10:S:1908:GLU:O	10:S:1912:LEU:HB2	2.07	0.53
12:X:60:PRO:HG2	12:X:90:ASN:HD21	1.74	0.53
1:A:5:ASP:HB2	3:C:314:LYS:HB3	1.91	0.53
9:I:334:SER:HB2	9:I:345:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:565:LYS:O	8:Q:569:GLN:NE2	2.41	0.53
10:S:688:LEU:HA	10:S:692:GLU:HB2	1.90	0.53
10:S:1035:ASP:OD2	10:S:1039:LYS:NZ	2.41	0.53
12:Y:133:ARG:HH12	12:Y:166:TYR:HB3	1.72	0.53
8:H:252:ASP:O	8:H:256:ARG:NH1	2.41	0.53
9:I:631:GLU:OE2	9:I:729:ARG:NH1	2.42	0.53
1:J:471:MET:HG3	1:J:487:TRP:CG	2.43	0.53
4:M:1276:ILE:HB	10:T:1244:MET:HG3	1.89	0.53
6:O:560:PHE:HB3	6:O:570:ALA:HB3	1.89	0.53
10:T:1292:LEU:HB2	10:T:1343:HIS:HE1	1.74	0.53
12:W:93:GLN:HB3	12:W:96:LEU:HB2	1.90	0.53
12:Z:754:GLU:O	12:Z:756:MET:N	2.41	0.53
14:d:181:ASP:OD1	14:d:181:ASP:N	2.38	0.53
3:C:114:THR:OG1	3:C:115:SER:N	2.42	0.53
4:D:401:THR:OG1	4:D:402:PHE:N	2.41	0.53
4:D:414:LEU:HD12	4:D:420:THR:HB	1.91	0.53
9:I:643:HIS:HB2	9:I:650:VAL:HG11	1.91	0.53
4:M:546:SER:OG	4:M:564:ARG:NH1	2.42	0.53
5:N:151:ILE:HB	5:N:160:ALA:HB3	1.91	0.53
9:R:658:LEU:HA	9:R:661:ARG:HG2	1.91	0.53
10:S:985:LEU:HD22	10:S:1063:VAL:HG21	1.91	0.53
10:S:1931:ASN:HB3	10:S:1950:ARG:HB3	1.91	0.53
12:X:474:ASN:OD1	12:X:564:GLN:NE2	2.41	0.53
12:X:702:GLU:OE1	12:Y:454:ARG:NH2	2.42	0.53
4:M:811:ARG:HH21	4:M:829:ARG:HE	1.55	0.53
7:P:119:VAL:HG22	7:P:133:THR:HG23	1.90	0.53
7:P:215:ARG:H	7:P:234:SER:HA	1.72	0.53
12:V:233:LEU:HD13	12:V:285:MET:HG3	1.91	0.53
12:W:694:GLU:HA	12:W:698:LEU:HD21	1.91	0.53
4:M:422:MET:HB3	4:M:438:VAL:HB	1.91	0.53
10:T:1915:THR:HA	10:T:1952:ASN:HD22	1.74	0.53
12:V:118:VAL:HG21	12:V:138:LEU:HD11	1.91	0.53
12:X:514:LEU:HB2	12:X:519:CYS:HB2	1.90	0.53
12:Z:444:TRP:CD1	12:Z:449:THR:HG23	2.44	0.53
14:b:66:HIS:HE1	14:b:85:GLU:HB3	1.74	0.53
14:d:114:GLY:O	14:d:116:LYS:N	2.40	0.53
14:d:233:LEU:HD22	14:d:249:VAL:HB	1.90	0.53
6:F:317:ASP:OD1	6:F:320:SER:OG	2.22	0.53
9:R:989:GLN:HB2	9:R:1015:LEU:HD11	1.89	0.53
12:X:574:LEU:HB3	12:X:608:LEU:HD22	1.91	0.53
12:Z:240:VAL:HG22	12:Z:255:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:656:ASN:HB2	15:f:465:ILE:HD11	1.89	0.53
1:J:599:MET:HB2	1:J:637:LEU:HD21	1.90	0.52
7:P:18:ASP:N	7:P:18:ASP:OD1	2.40	0.52
10:S:1726:ARG:NH2	10:S:1796:GLN:O	2.41	0.52
10:T:1910:TYR:O	10:T:1915:THR:OG1	2.26	0.52
12:Z:267:LYS:HD3	12:Z:400:PHE:HB2	1.91	0.52
14:b:390:ARG:HD2	14:b:485:ILE:HG22	1.91	0.52
14:d:296:ASP:N	14:d:296:ASP:OD1	2.42	0.52
9:I:106:GLY:O	9:I:121:LYS:NZ	2.38	0.52
3:L:245:VAL:HB	3:L:274:PHE:O	2.09	0.52
10:T:958:GLU:O	10:T:960:LEU:N	2.42	0.52
4:D:415:ASP:OD2	4:D:419:GLN:NE2	2.42	0.52
8:H:727:LEU:O	8:H:824:ARG:NH1	2.43	0.52
1:J:475:SER:HB3	1:J:480:ARG:HB2	1.91	0.52
6:O:498:ILE:HG12	8:Q:314:LEU:H	1.73	0.52
6:O:780:LEU:HD21	6:O:802:TYR:HB3	1.91	0.52
8:Q:549:ARG:NH2	8:Q:560:SER:OG	2.42	0.52
10:S:1787:GLU:HB3	10:S:1813:VAL:HG23	1.91	0.52
2:B:360:CYS:HB3	2:B:368:TYR:HB3	1.91	0.52
6:F:455:ARG:HE	6:F:459:LYS:HG2	1.74	0.52
9:I:499:GLN:NE2	4:M:180:ASP:OD2	2.42	0.52
3:L:163:LEU:HB2	3:L:186:SER:HB3	1.90	0.52
6:O:462:ASP:OD1	8:Q:321:ARG:NH1	2.43	0.52
10:T:1896:ILE:HD13	10:T:1981:ILE:HD13	1.90	0.52
12:V:5:LYS:NZ	12:V:41:GLU:OE2	2.41	0.52
12:X:55:VAL:HG12	12:X:56:GLN:HG2	1.92	0.52
12:Y:128:SER:HB2	12:Y:131:ILE:HG22	1.91	0.52
14:d:205:GLU:HA	14:d:221:LEU:HD13	1.91	0.52
4:D:408:ASN:OD1	4:D:408:ASN:N	2.43	0.52
8:H:425:ASN:HA	8:H:472:GLU:HG3	1.92	0.52
10:S:1938:PHE:HB2	10:S:1951:GLN:HB3	1.92	0.52
10:T:400:MET:HB3	10:T:403:LYS:HB2	1.91	0.52
12:Z:679:TYR:HB2	12:Z:720:ILE:HD11	1.92	0.52
14:b:352:PHE:HE1	14:b:431:GLN:HG2	1.74	0.52
1:A:497:ALA:HB3	1:A:532:ARG:HH22	1.74	0.52
7:P:87:LYS:NZ	7:P:94:GLU:OE2	2.36	0.52
8:Q:591:LEU:O	8:Q:595:GLN:NE2	2.42	0.52
10:S:1941:ASP:N	10:S:1941:ASP:OD1	2.43	0.52
12:W:383:SER:OG	12:W:396:MET:SD	2.65	0.52
12:X:651:ILE:HG12	12:X:678:ALA:HB2	1.92	0.52
4:D:974:LEU:HD23	4:D:977:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:259:TRP:HZ3	6:F:667:ASN:HD21	1.58	0.52
6:F:273:ASN:ND2	6:F:275:GLU:OE1	2.43	0.52
7:G:39:ILE:HB	7:G:51:ALA:HB3	1.91	0.52
7:G:212:ASP:OD2	7:G:238:ARG:NH1	2.43	0.52
4:M:1338:ARG:NH2	4:M:1386:SER:OG	2.42	0.52
8:Q:447:MET:HE1	8:Q:483:VAL:HG22	1.91	0.52
9:R:970:ASP:N	9:R:970:ASP:OD1	2.42	0.52
10:T:1842:VAL:HA	10:T:1845:LEU:HG	1.91	0.52
12:Z:301:ALA:HB2	12:Z:311:LEU:HD12	1.92	0.52
14:b:166:TYR:HB3	14:b:173:PRO:HA	1.91	0.52
14:b:179:THR:OG1	14:b:181:ASP:OD1	2.26	0.52
2:B:254:LEU:HD22	2:B:289:SER:HA	1.91	0.52
3:C:276:ASN:HB2	3:C:303:ARG:HH22	1.75	0.52
6:F:386:LEU:HD23	6:F:409:ARG:HH21	1.75	0.52
8:H:249:PHE:HE1	8:H:259:GLN:HG2	1.75	0.52
2:K:259:ALA:HB1	2:K:279:GLU:HG2	1.91	0.52
7:P:193:ILE:HG23	7:P:204:ASP:HB2	1.91	0.52
10:S:584:ARG:NH1	10:S:586:ILE:O	2.43	0.52
10:T:1697:ASP:O	10:T:1701:MET:N	2.42	0.52
10:T:1937:THR:OG1	13:e:831:ASP:OD2	2.28	0.52
12:Y:454:ARG:HH11	12:Y:458:LYS:HD2	1.74	0.52
14:b:460:ASP:HB2	14:b:463:LEU:HB2	1.91	0.52
4:D:161:VAL:HG23	4:D:204:ILE:HG12	1.92	0.52
8:H:766:THR:HB	8:H:782:LYS:HD2	1.90	0.52
2:K:265:HIS:ND1	2:K:351:LEU:O	2.42	0.52
4:M:1102:GLU:HG2	4:M:1106:ARG:HE	1.75	0.52
8:Q:749:GLU:HA	8:Q:752:ASN:ND2	2.25	0.52
9:R:1055:LEU:HD23	9:R:1109:LEU:HD23	1.91	0.52
10:S:455:GLU:HB3	10:S:458:LEU:HB3	1.91	0.52
10:S:1528:LEU:HD11	10:S:1577:VAL:HG13	1.90	0.52
13:a:861:LEU:HD13	14:b:701:ILE:HD13	1.92	0.52
14:b:117:GLY:HA3	14:b:149:GLU:HA	1.92	0.52
15:c:402:ARG:NH1	14:d:134:GLU:OE2	2.43	0.52
3:C:277:HIS:HE1	3:C:297:GLY:HA3	1.75	0.52
4:D:113:GLU:HG3	4:D:129:ARG:HG2	1.92	0.52
9:R:507:LYS:HA	9:R:510:LYS:HE3	1.92	0.52
9:R:1067:TRP:HE1	9:R:1080:THR:HG22	1.75	0.52
10:S:1403:LEU:HD13	10:S:1469:PHE:HE1	1.75	0.52
12:Y:197:ARG:HH22	12:Y:231:GLU:HB3	1.74	0.52
4:D:1184:LYS:NZ	4:D:1233:THR:O	2.43	0.51
9:I:760:ARG:HH21	9:I:800:TYR:HE1	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:113:ARG:HH12	4:M:1363:LYS:HB3	1.74	0.51
10:T:1184:LEU:HB3	10:T:1319:LYS:HE2	1.91	0.51
11:U:809:ASN:O	11:U:813:VAL:HG23	2.10	0.51
12:X:598:MET:HG3	12:X:655:THR:HG21	1.91	0.51
4:D:1401:ASN:O	4:D:1405:GLN:NE2	2.43	0.51
6:F:255:TRP:O	7:G:20:GLN:NE2	2.44	0.51
6:F:340:CYS:SG	6:F:687:ARG:NH2	2.83	0.51
1:J:634:ARG:HH12	4:M:1132:ARG:HD3	1.75	0.51
4:M:258:LYS:O	4:M:311:TRP:NE1	2.40	0.51
4:M:499:LYS:O	4:M:503:LEU:HG	2.11	0.51
10:T:635:ILE:HG13	10:T:636:PRO:HD2	1.92	0.51
10:T:1535:LEU:HD22	10:T:1618:ILE:HD12	1.93	0.51
10:T:1541:PRO:HG3	10:T:1607:PHE:HA	1.92	0.51
4:D:210:ARG:HA	4:D:233:SER:HA	1.91	0.51
8:Q:210:THR:HG22	8:Q:507:GLN:HE21	1.75	0.51
14:d:1:MET:HG2	14:d:4:GLY:H	1.75	0.51
7:G:298:CYS:HB3	12:Y:27:MET:HE3	1.92	0.51
8:H:212:ARG:NH2	8:H:267:SER:OG	2.44	0.51
9:I:331:ASN:OD1	9:I:390:ARG:NH2	2.44	0.51
1:J:355:ILE:HA	1:J:358:VAL:HG22	1.92	0.51
4:M:446:ASP:HB3	9:R:129:LYS:HD3	1.91	0.51
4:M:1289:ARG:HE	4:M:1292:ILE:HD12	1.74	0.51
10:T:1178:ARG:NH2	10:T:1315:ASP:OD2	2.43	0.51
10:T:1819:LYS:HE3	10:T:1977:ARG:HH22	1.75	0.51
14:b:181:ASP:OD1	14:b:181:ASP:N	2.42	0.51
14:b:576:ARG:HG2	14:d:93:PRO:HG2	1.92	0.51
4:M:244:PRO:HG2	4:M:250:GLY:H	1.76	0.51
4:M:780:CYS:SG	4:M:781:LEU:N	2.84	0.51
10:S:513:MET:HE3	10:S:517:LEU:HD11	1.92	0.51
14:b:528:SER:OG	14:b:529:ALA:N	2.44	0.51
14:d:620:GLN:HE21	13:e:772:MET:HG3	1.75	0.51
6:O:598:ARG:NH2	6:O:613:TYR:OH	2.43	0.51
9:R:987:LEU:HA	9:R:990:GLU:HB3	1.92	0.51
12:Z:193:ARG:O	12:Z:197:ARG:HG2	2.10	0.51
1:A:100:GLN:NE2	1:A:104:ASN:OD1	2.41	0.51
4:D:133:LEU:HD22	9:I:351:PRO:HB2	1.93	0.51
4:D:233:SER:HB2	4:D:239:LEU:HB2	1.92	0.51
4:M:412:LEU:HD13	4:M:422:MET:HG2	1.93	0.51
4:M:545:LEU:HA	4:M:565:LYS:HB3	1.91	0.51
10:S:967:ALA:HB1	10:S:970:GLN:HB2	1.92	0.51
10:T:177:LEU:HD13	10:T:182:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:1204:ARG:NH1	10:T:1205:SER:OG	2.44	0.51
12:V:142:GLN:HB2	12:V:146:GLY:HA3	1.92	0.51
12:W:533:ALA:HB2	12:W:550:LEU:HD22	1.91	0.51
12:X:131:ILE:HD13	12:X:134:LEU:HD21	1.93	0.51
12:Z:165:VAL:HG22	12:Z:196:LEU:HD22	1.92	0.51
8:H:182:LYS:HA	8:H:185:LYS:HD3	1.92	0.51
1:J:320:THR:O	1:J:323:HIS:NE2	2.43	0.51
4:M:402:PHE:HB3	4:M:409:ILE:HG12	1.92	0.51
10:T:462:CYS:HA	10:T:488:GLN:HB3	1.92	0.51
10:T:1452:THR:HG22	10:T:1453:ALA:H	1.76	0.51
11:U:558:GLU:OE2	11:U:561:ASN:ND2	2.42	0.51
12:X:26:SER:HB3	12:X:55:VAL:HG21	1.93	0.51
14:b:116:LYS:HD2	14:b:153:THR:HA	1.92	0.51
2:K:14:ILE:HG21	2:K:361:GLY:HA3	1.93	0.51
4:M:220:TRP:CE2	4:M:290:VAL:HG21	2.46	0.51
7:P:62:GLN:NE2	7:P:109:VAL:O	2.41	0.51
8:Q:219:ARG:NH2	8:Q:223:GLN:OE1	2.44	0.51
10:S:1787:GLU:HB2	10:S:1810:SER:HB2	1.92	0.51
14:d:182:ASN:HB3	14:d:201:LEU:HD12	1.93	0.51
14:d:210:LEU:HD13	14:d:217:TYR:HB2	1.93	0.51
3:C:257:LEU:O	3:C:259:SER:N	2.44	0.51
5:E:213:SER:H	5:E:227:VAL:HG23	1.76	0.51
5:E:215:ASP:OD2	5:E:258:ARG:NH1	2.44	0.51
4:M:879:ALA:HB1	4:M:912:MET:HG2	1.92	0.51
4:M:1046:LEU:HD22	4:M:1082:LEU:HD11	1.93	0.51
8:Q:793:TRP:HD1	8:Q:796:HIS:CE1	2.29	0.51
9:R:591:MET:HE2	9:R:633:LEU:HB3	1.92	0.51
12:V:60:PRO:HG3	12:V:89:LEU:HB3	1.92	0.51
12:V:386:LEU:HB2	12:V:401:MET:HB2	1.93	0.51
4:D:327:TYR:HB3	4:D:386:HIS:HB2	1.93	0.50
8:H:700:LYS:HD2	8:H:745:LEU:HD13	1.93	0.50
6:O:335:ASP:HB2	6:O:342:HIS:HB3	1.92	0.50
9:R:743:GLN:H	9:R:808:ASP:HB2	1.75	0.50
10:T:1034:LEU:HD12	10:T:1087:PHE:HZ	1.76	0.50
11:U:549:LEU:HD22	11:U:599:ILE:HD13	1.93	0.50
4:D:49:LEU:HD22	4:D:716:GLN:HB3	1.93	0.50
9:I:703:ASP:HB3	4:M:1150:TYR:HE2	1.77	0.50
1:J:100:GLN:NE2	2:K:321:LEU:O	2.43	0.50
9:R:310:ILE:HG23	9:R:361:THR:HG21	1.93	0.50
10:S:502:LEU:HD13	10:S:547:GLY:HA2	1.93	0.50
10:T:1300:ILE:HG13	10:T:1305:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:1683:ALA:HB1	10:T:1707:ILE:HG12	1.93	0.50
12:X:391:GLU:OE1	12:X:399:SER:OG	2.29	0.50
12:Z:288:HIS:HA	12:Z:291:MET:HE3	1.93	0.50
14:d:4:GLY:O	14:d:8:GLN:NE2	2.44	0.50
14:d:396:VAL:HB	14:d:449:PRO:HB2	1.93	0.50
14:d:679:GLN:OE1	14:d:682:LYS:NZ	2.41	0.50
4:D:1369:GLY:O	4:D:1371:GLN:NE2	2.45	0.50
8:H:374:LEU:HD21	8:H:376:HIS:HB3	1.92	0.50
9:I:134:LYS:NZ	9:I:185:GLU:OE1	2.44	0.50
1:J:413:SER:OG	2:K:179:ARG:NH2	2.44	0.50
9:R:297:VAL:HG12	9:R:371:ASN:HD21	1.77	0.50
12:W:93:GLN:HG3	12:W:96:LEU:H	1.77	0.50
12:Y:636:ASP:O	12:Y:638:LYS:NZ	2.44	0.50
5:E:33:GLY:O	5:E:306:ARG:NH2	2.44	0.50
1:J:309:ARG:HB3	1:J:313:LYS:HE2	1.93	0.50
4:M:465:PHE:HB3	4:M:781:LEU:HD21	1.92	0.50
4:M:662:GLN:HG2	4:M:742:LEU:HD22	1.92	0.50
7:P:301:ASP:N	7:P:301:ASP:OD1	2.44	0.50
10:T:1447:MET:O	10:T:1449:GLU:N	2.44	0.50
12:Y:8:ILE:HG21	12:Y:39:ALA:HB2	1.94	0.50
1:A:552:SER:HA	1:A:589:ILE:HG21	1.93	0.50
4:D:343:LYS:HG3	4:D:360:TYR:HD2	1.77	0.50
5:E:259:TRP:HE1	5:E:264:GLU:HA	1.77	0.50
6:F:681:ILE:O	6:F:687:ARG:NH1	2.44	0.50
1:J:168:VAL:HG21	1:J:307:VAL:HG21	1.93	0.50
4:M:99:ARG:HB2	4:M:174:ARG:HH22	1.76	0.50
4:M:444:PRO:HA	4:M:469:ARG:HE	1.76	0.50
4:M:1209:SER:OG	4:M:1210:ALA:N	2.44	0.50
8:Q:134:GLN:HE21	11:U:512:GLN:HE21	1.58	0.50
9:R:223:LEU:HD22	9:R:233:GLN:HG3	1.92	0.50
9:R:821:MET:SD	9:R:825:GLN:NE2	2.85	0.50
10:T:1493:MET:HB2	10:T:1551:ILE:HG12	1.94	0.50
10:T:1541:PRO:HD3	10:T:1607:PHE:HD1	1.76	0.50
10:T:1623:LEU:HG	10:T:1678:ILE:HD12	1.93	0.50
11:U:445:LEU:HA	11:U:449:TYR:HB2	1.92	0.50
11:U:543:THR:OG1	11:U:547:GLU:OE2	2.29	0.50
12:Z:163:ASN:HA	12:Z:196:LEU:HD21	1.94	0.50
4:D:1158:LYS:HB3	10:S:291:ARG:HH21	1.76	0.50
6:F:837:LYS:HE2	12:V:89:LEU:HD23	1.94	0.50
4:M:682:MET:SD	4:M:725:ARG:NH2	2.73	0.50
5:N:158:GLN:HG3	5:N:161:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:494:ARG:HE	8:Q:498:GLU:HG3	1.76	0.50
9:R:607:PHE:HD2	9:R:741:GLY:HA3	1.77	0.50
10:S:1135:ARG:HH22	10:S:1164:LEU:HD23	1.76	0.50
10:T:1180:ILE:HD12	10:T:1312:LEU:HD11	1.94	0.50
10:T:1228:LYS:O	10:T:1231:HIS:ND1	2.41	0.50
12:W:126:PRO:HG2	12:W:163:ASN:HB3	1.94	0.50
12:Y:187:HIS:O	12:Y:190:LYS:NZ	2.37	0.50
1:A:49:ALA:HB3	3:C:7:ILE:HD12	1.94	0.50
3:C:73:VAL:HG12	3:C:87:GLU:HG3	1.93	0.50
5:E:94:ARG:HH22	5:E:137:GLY:HA3	1.76	0.50
6:F:476:GLN:HB3	6:F:480:ASP:HB2	1.94	0.50
6:F:673:TRP:HA	6:F:676:PHE:HD1	1.75	0.50
9:I:987:LEU:HA	9:I:990:GLU:HB2	1.94	0.50
10:T:1787:GLU:OE2	10:T:1807:ARG:NH2	2.40	0.50
12:X:118:VAL:HG21	12:X:138:LEU:HD22	1.93	0.50
12:Z:676:VAL:HG12	12:Z:720:ILE:HG12	1.94	0.50
9:R:496:ARG:HH11	9:R:507:LYS:HB3	1.77	0.50
10:S:479:VAL:HG23	10:S:483:ARG:HB2	1.94	0.50
10:S:503:PRO:HG2	10:S:506:LEU:HD12	1.93	0.50
10:S:609:GLU:HA	10:S:612:ARG:HD2	1.93	0.50
10:S:1176:VAL:HG11	10:S:1182:ARG:HD3	1.92	0.50
10:T:440:LEU:HB3	10:T:513:MET:HG2	1.93	0.50
10:T:1614:ARG:NH1	10:T:1617:GLN:OE1	2.45	0.50
10:T:1989:ARG:HB2	10:T:1991:ARG:HH11	1.76	0.50
11:U:397:ARG:NH1	11:U:420:SER:O	2.45	0.50
12:Z:457:LEU:HB3	12:Z:481:LEU:HD22	1.94	0.50
6:F:417:LEU:HD13	6:F:536:GLY:HA2	1.94	0.50
1:J:439:ARG:HH12	3:L:288:ILE:HG23	1.76	0.50
1:J:603:GLU:OE2	4:M:1129:ASN:ND2	2.44	0.50
6:O:495:ASP:OD1	6:O:495:ASP:N	2.45	0.50
8:Q:711:ILE:HG21	8:Q:735:ILE:HA	1.94	0.50
9:R:743:GLN:HB2	9:R:808:ASP:H	1.77	0.50
12:V:457:LEU:HD23	12:V:460:ILE:HD11	1.93	0.50
12:W:243:THR:HG22	12:W:251:LYS:HD3	1.94	0.50
14:b:284:PRO:HB3	14:b:334:THR:HA	1.93	0.50
14:b:330:ASP:OD2	14:b:425:GLN:NE2	2.45	0.50
14:d:379:ILE:HG23	14:d:395:HIS:HD1	1.77	0.50
13:e:755:PHE:HD2	15:f:400:LEU:HD22	1.76	0.50
4:D:645:ILE:HG22	4:D:734:ILE:HD11	1.94	0.49
5:E:158:GLN:HE22	5:E:161:MET:HE3	1.76	0.49
7:G:267:VAL:HG22	7:G:278:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:GLU:HA	10:T:1454:PRO:HD3	1.93	0.49
9:I:342:LEU:H	9:I:365:VAL:HB	1.77	0.49
9:I:674:VAL:HA	9:I:677:ARG:HH11	1.77	0.49
1:J:310:LEU:HD22	1:J:317:VAL:HG11	1.94	0.49
10:T:496:ARG:NH2	10:T:534:ASN:OD1	2.40	0.49
10:T:1593:THR:HA	10:T:1653:ASP:HB3	1.94	0.49
1:A:165:LEU:HD21	1:A:311:LEU:HD21	1.95	0.49
2:B:268:PRO:O	2:B:270:ASN:N	2.45	0.49
2:B:292:SER:OG	2:B:324:ALA:O	2.24	0.49
2:B:327:SER:O	2:B:327:SER:OG	2.26	0.49
3:C:244:ASP:OD1	3:C:244:ASP:N	2.46	0.49
3:C:258:SER:OG	3:C:259:SER:N	2.45	0.49
4:D:306:HIS:HB3	4:D:324:MET:HB2	1.94	0.49
9:I:651:ASN:O	9:I:655:GLN:NE2	2.45	0.49
5:N:237:MET:HE3	5:N:238:PRO:HB3	1.94	0.49
9:R:812:ASN:OD1	9:R:815:ARG:NH2	2.45	0.49
10:S:1380:THR:HB	10:S:1433:ARG:HE	1.77	0.49
10:T:1553:GLU:HA	10:T:1556:MET:HE2	1.94	0.49
11:U:371:LYS:O	11:U:375:HIS:ND1	2.44	0.49
12:Y:475:ILE:HG23	12:Y:478:SER:H	1.77	0.49
12:Z:570:GLN:HB2	12:Z:573:VAL:HG23	1.94	0.49
14:b:92:ASN:ND2	14:b:144:THR:O	2.45	0.49
14:b:563:TYR:HD2	15:c:369:LEU:HD13	1.77	0.49
14:b:656:ASN:HB2	15:c:465:ILE:HD11	1.93	0.49
5:E:94:ARG:HB2	5:E:108:THR:HG23	1.93	0.49
10:S:579:ARG:HD3	10:S:683:GLY:HA2	1.93	0.49
12:Y:151:PHE:O	12:Y:155:GLN:NE2	2.43	0.49
15:c:389:THR:O	15:c:393:ASN:ND2	2.45	0.49
1:A:189:THR:HG1	1:A:220:THR:HG1	1.57	0.49
7:G:179:ILE:HG22	7:G:196:GLU:HB3	1.94	0.49
8:H:457:ARG:HH11	8:H:461:ILE:HG13	1.77	0.49
1:J:98:LEU:HG	1:J:378:LEU:HD22	1.94	0.49
3:L:139:VAL:HG22	3:L:159:ILE:HB	1.94	0.49
4:M:635:PRO:HG3	5:N:146:ASP:HB2	1.94	0.49
10:T:1782:THR:OG1	10:T:1810:SER:OG	2.30	0.49
10:T:1842:VAL:HG23	10:T:1845:LEU:HD12	1.93	0.49
12:V:355:GLY:HA3	12:V:419:LEU:HD21	1.94	0.49
12:W:291:MET:HG3	12:W:350:ARG:HG3	1.95	0.49
12:W:657:ASP:HB3	12:W:662:LYS:HG3	1.94	0.49
12:X:490:ALA:HB2	12:X:577:TRP:CD1	2.47	0.49
14:d:291:ASP:OD1	14:d:291:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:N	2:B:39:ASP:OD1	2.46	0.49
4:D:62:ARG:HD2	4:D:190:ILE:HG13	1.92	0.49
4:D:99:ARG:HH22	4:D:704:LEU:HD21	1.78	0.49
5:E:179:PHE:HB3	5:E:195:LEU:HB2	1.94	0.49
1:J:459:GLN:HB3	10:T:1203:ASP:HB3	1.95	0.49
4:M:1004:PHE:HZ	4:M:1036:LEU:HB2	1.77	0.49
10:S:1306:GLN:HG3	10:S:1389:SER:HB2	1.93	0.49
14:b:25:ARG:NH2	14:b:538:SER:OG	2.46	0.49
8:H:469:LEU:O	8:H:471:ARG:NH1	2.45	0.49
9:I:110:TRP:CD1	9:I:119:ILE:HG23	2.48	0.49
7:P:220:ALA:HB3	7:P:229:THR:HG23	1.94	0.49
10:S:609:GLU:OE1	10:S:612:ARG:NH1	2.46	0.49
10:S:1355:PRO:HG3	10:S:1873:LEU:HD11	1.93	0.49
10:T:770:LEU:HD21	10:T:802:LEU:HD22	1.93	0.49
12:V:128:SER:HB2	12:V:131:ILE:HB	1.95	0.49
12:Z:187:HIS:O	12:Z:193:ARG:NE	2.42	0.49
14:d:332:GLU:O	14:d:336:ASN:ND2	2.45	0.49
4:D:904:VAL:HG12	4:D:905:ASN:H	1.76	0.49
9:I:83:PRO:HA	9:I:127:SER:HA	1.95	0.49
9:I:275:CYS:SG	9:I:371:ASN:ND2	2.86	0.49
9:I:815:ARG:HH12	9:I:819:LEU:HD13	1.77	0.49
1:J:471:MET:CG	1:J:487:TRP:CE2	2.96	0.49
9:R:859:ILE:HA	9:R:862:MET:HG2	1.94	0.49
9:R:921:TRP:CD1	9:R:921:TRP:H	2.30	0.49
10:S:688:LEU:O	10:S:693:SER:OG	2.26	0.49
10:S:1096:PRO:HG3	10:S:1182:ARG:HG2	1.95	0.49
10:T:116:GLU:HG3	10:T:127:ARG:HE	1.78	0.49
12:V:698:LEU:HD22	12:V:702:GLU:HB3	1.95	0.49
12:W:337:ASP:HA	12:W:340:GLN:HB2	1.94	0.49
1:A:480:ARG:HH11	2:B:86:LYS:HZ3	1.60	0.49
2:B:287:ASP:OD2	2:B:338:THR:OG1	2.30	0.49
2:K:77:ASP:HB2	2:K:93:SER:HB3	1.95	0.49
8:Q:262:VAL:HG22	8:Q:441:TRP:HD1	1.77	0.49
10:T:26:SER:OG	10:T:959:GLU:OE2	2.31	0.49
10:T:226:GLN:HE21	10:T:230:HIS:CD2	2.31	0.49
14:d:203:SER:OG	14:d:279:LEU:O	2.31	0.49
14:d:364:ALA:HB2	14:d:554:ARG:HB2	1.94	0.49
4:D:1030:LEU:HG	4:D:1064:ILE:HD11	1.95	0.49
6:O:475:SER:O	6:O:479:ARG:NH1	2.45	0.49
10:S:692:GLU:HB3	10:S:698:TYR:HD1	1.78	0.49
10:T:978:TYR:CZ	10:T:982:ILE:HD11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:1297:GLN:OE1	10:T:1305:ARG:NH1	2.45	0.49
10:T:1502:ILE:HA	10:T:1505:VAL:HG22	1.95	0.49
12:W:60:PRO:HA	12:W:63:HIS:HD2	1.78	0.49
12:Y:471:LEU:HB2	12:Y:562:ARG:HD3	1.94	0.49
14:b:514:GLY:O	15:c:388:ARG:NH2	2.45	0.49
1:A:498:THR:OG1	1:A:532:ARG:NH2	2.46	0.49
2:B:74:HIS:HE2	2:B:93:SER:HG	1.61	0.49
2:K:52:ASP:OD1	2:K:357:ASN:ND2	2.46	0.49
6:O:394:GLU:O	12:V:14:ASN:ND2	2.46	0.49
8:Q:556:LYS:HB2	8:Q:559:VAL:HG22	1.95	0.49
9:R:835:LEU:HD13	9:R:862:MET:HE1	1.94	0.49
12:Y:154:ILE:HG21	12:Y:171:LEU:HD22	1.95	0.49
4:D:904:VAL:HG13	4:D:939:ARG:HE	1.78	0.48
4:M:105:TRP:HB2	4:M:112:LEU:HD11	1.94	0.48
4:M:167:PRO:HG3	4:M:192:LYS:HD2	1.95	0.48
4:M:374:LEU:HD22	4:M:382:TYR:HB3	1.94	0.48
4:M:413:TRP:HZ3	4:M:423:LYS:HD2	1.78	0.48
10:S:632:GLN:HE22	10:S:669:ILE:HG13	1.78	0.48
10:T:169:MET:SD	10:T:172:ARG:NH2	2.78	0.48
12:V:340:GLN:HE21	12:V:344:GLU:HG3	1.78	0.48
12:X:221:LYS:NZ	12:X:269:SER:O	2.42	0.48
12:Y:434:LEU:HD23	12:Y:528:ARG:HD3	1.95	0.48
13:a:824:TYR:HA	13:a:827:ASN:HD21	1.78	0.48
14:b:256:LEU:HD21	14:b:297:ALA:HB1	1.95	0.48
3:C:125:HIS:O	4:D:1279:LYS:NZ	2.47	0.48
6:F:468:LEU:O	6:F:475:SER:OG	2.31	0.48
8:H:136:GLU:HG3	10:T:1454:PRO:HD2	1.95	0.48
9:I:1081:LYS:O	9:I:1087:LYS:NZ	2.45	0.48
9:I:1127:SER:O	9:I:1131:ASN:ND2	2.46	0.48
1:J:39:TYR:O	1:J:41:LYS:N	2.46	0.48
2:K:215:VAL:HG22	2:K:238:MET:HB2	1.94	0.48
5:N:267:PHE:CE2	5:N:283:HIS:HB2	2.48	0.48
2:B:71:ASP:OD1	2:B:71:ASP:N	2.42	0.48
4:D:402:PHE:HB3	4:D:409:ILE:HG23	1.94	0.48
1:J:596:TYR:O	1:J:599:MET:HG3	2.14	0.48
5:N:85:ARG:HB2	5:N:92:LEU:HB2	1.95	0.48
10:S:507:TYR:HB2	10:S:546:GLY:HA2	1.94	0.48
10:S:954:SER:O	10:S:977:ARG:NE	2.46	0.48
10:S:1429:GLN:HE22	10:S:1434:PRO:HD3	1.78	0.48
10:T:229:ALA:HB2	10:T:267:VAL:HG13	1.95	0.48
12:X:337:ASP:HA	12:X:340:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:590:SER:O	12:X:688:ARG:NH1	2.42	0.48
6:O:571:CYS:SG	6:O:572:TYR:N	2.86	0.48
10:T:421:SER:HA	10:T:424:MET:HE2	1.96	0.48
10:T:1095:LEU:HD22	10:T:1183:ILE:HD11	1.95	0.48
12:Z:490:ALA:HB2	12:Z:577:TRP:HZ2	1.77	0.48
5:E:173:TRP:HZ3	5:E:179:PHE:HA	1.77	0.48
9:R:938:GLN:NE2	9:R:942:ASN:OD1	2.47	0.48
10:T:1581:LEU:HD11	10:T:1625:ILE:HD11	1.96	0.48
10:T:1753:GLN:HG3	10:T:1888:LEU:HD23	1.96	0.48
11:U:239:ALA:HA	12:Y:475:ILE:HD12	1.94	0.48
11:U:652:SER:HA	11:U:748:GLU:HG2	1.96	0.48
12:W:24:GLU:HA	12:W:27:MET:HG2	1.94	0.48
12:Z:347:ALA:O	12:Z:351:GLN:NE2	2.46	0.48
12:Z:568:GLY:HA3	12:Z:628:LEU:HD12	1.94	0.48
14:b:1:MET:HG2	14:b:4:GLY:H	1.77	0.48
4:D:161:VAL:HB	4:D:202:TYR:HB3	1.95	0.48
5:E:106:ILE:HG23	5:E:118:LYS:HB2	1.94	0.48
6:F:811:MET:HB3	6:F:828:LEU:HD13	1.96	0.48
4:M:357:LEU:HD12	4:M:384:LEU:HD21	1.94	0.48
7:P:179:ILE:HG13	7:P:181:ARG:HH11	1.77	0.48
8:Q:459:SER:OG	12:V:34:ARG:NH2	2.47	0.48
10:S:1723:GLY:HA2	10:S:1816:HIS:HE1	1.79	0.48
10:T:67:VAL:HG21	10:T:105:GLU:HB3	1.95	0.48
10:T:1585:GLN:NE2	10:T:1588:ASP:OD2	2.46	0.48
11:U:788:SER:HB2	12:Z:506:ALA:HB2	1.96	0.48
12:V:520:LYS:O	12:V:528:ARG:NH1	2.46	0.48
12:Z:697:CYS:SG	12:Z:698:LEU:N	2.87	0.48
5:N:104:ILE:HB	5:N:120:ILE:HB	1.96	0.48
8:Q:749:GLU:HA	8:Q:752:ASN:HD21	1.79	0.48
10:S:174:THR:HG22	10:S:178:MET:HE2	1.95	0.48
10:S:670:LEU:HG	10:S:672:THR:H	1.76	0.48
10:T:100:LEU:HD13	10:T:201:LYS:HE2	1.94	0.48
12:X:692:GLU:HB3	12:Y:590:SER:HA	1.96	0.48
12:Y:499:LEU:HD11	12:Y:512:ARG:HB3	1.94	0.48
12:Z:233:LEU:HB3	12:Z:285:MET:HG3	1.95	0.48
12:Z:353:LYS:HA	12:Z:439:TRP:HH2	1.78	0.48
1:A:648:GLU:O	1:A:652:GLN:NE2	2.46	0.48
4:D:210:ARG:HB2	9:I:261:VAL:HG12	1.95	0.48
6:F:264:ASN:HD22	6:F:304:VAL:HG22	1.78	0.48
6:F:738:ASP:OD1	6:F:738:ASP:N	2.42	0.48
6:O:317:ASP:OD1	6:O:317:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:410:ARG:NH1	6:O:545:PRO:O	2.46	0.48
8:Q:420:ALA:HA	8:Q:428:GLN:HE22	1.79	0.48
12:V:356:HIS:HE1	12:V:419:LEU:HB3	1.79	0.48
12:Y:473:SER:HA	12:Y:555:GLN:HE22	1.78	0.48
12:Z:474:ASN:OD1	12:Z:603:HIS:NE2	2.42	0.48
6:F:450:ILE:HG13	6:F:451:SER:H	1.79	0.48
1:J:157:ALA:HB2	1:J:318:LYS:HD3	1.96	0.48
2:K:37:SER:HB2	2:K:44:LYS:H	1.77	0.48
4:M:514:VAL:HG21	9:R:68:SER:HB2	1.95	0.48
5:N:8:ASN:OD1	5:N:322:TRP:NE1	2.47	0.48
5:N:218:VAL:HG11	5:N:261:LYS:HD3	1.95	0.48
10:T:147:LEU:HD13	10:T:230:HIS:HB3	1.95	0.48
10:T:1001:MET:HB3	10:T:1007:GLU:HA	1.96	0.48
10:T:1940:THR:OG1	13:e:820:ARG:NH2	2.47	0.48
12:X:135:LYS:HD3	12:X:153:LEU:HD21	1.96	0.48
12:Y:194:ARG:HH12	12:Y:234:LEU:HD13	1.78	0.48
14:b:297:ALA:HA	14:b:314:THR:HA	1.96	0.48
4:M:414:LEU:HD22	9:R:183:LEU:HG	1.96	0.48
6:O:752:TRP:HB3	6:O:756:HIS:CE1	2.49	0.48
8:Q:299:ARG:HH21	8:Q:306:SER:H	1.62	0.48
10:S:8:ASN:HD21	10:S:49:ASP:HB3	1.79	0.48
10:S:1783:PRO:HB2	10:S:1958:ASP:HB3	1.94	0.48
4:D:403:THR:OG1	4:D:408:ASN:OD1	2.31	0.47
4:D:439:PHE:HB2	4:D:582:LEU:HD11	1.96	0.47
9:I:831:LEU:HD22	5:N:1:MET:HB3	1.96	0.47
3:L:61:TRP:N	3:L:77:CYS:O	2.39	0.47
6:O:435:GLU:HG2	6:O:436:ARG:HD3	1.96	0.47
10:T:1760:MET:HB2	10:T:1898:THR:HG21	1.95	0.47
12:V:207:VAL:HG11	12:V:258:ARG:HH21	1.79	0.47
12:V:240:VAL:HG22	12:V:255:ALA:HB1	1.96	0.47
12:W:705:GLU:O	12:W:708:GLU:HG3	2.14	0.47
12:Z:287:GLY:HA3	12:Z:350:ARG:HH11	1.77	0.47
14:b:649:LYS:HD3	15:c:458:THR:HG23	1.95	0.47
14:d:511:ASP:N	14:d:511:ASP:OD1	2.47	0.47
13:e:745:ARG:HH21	15:f:389:THR:HA	1.78	0.47
1:A:94:ARG:HH11	1:A:97:GLN:HE21	1.61	0.47
2:B:245:ARG:HH11	2:B:246:HIS:HB2	1.79	0.47
4:D:797:LEU:HD22	4:D:884:ARG:HA	1.96	0.47
6:F:588:ASP:OD1	6:F:588:ASP:N	2.44	0.47
8:H:765:PRO:HB3	8:H:783:GLU:HG2	1.95	0.47
4:M:479:ILE:HD11	4:M:501:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:268:VAL:HG12	9:R:278:THR:HG22	1.96	0.47
12:V:190:LYS:HG3	12:V:193:ARG:HH21	1.78	0.47
12:V:533:ALA:HB1	12:V:550:LEU:HB3	1.95	0.47
14:b:615:GLU:O	14:b:618:GLU:HG3	2.14	0.47
9:I:397:LEU:HD12	9:I:409:LEU:HD13	1.95	0.47
9:I:569:VAL:HG12	9:I:571:GLU:HG3	1.94	0.47
9:I:1067:TRP:HE1	9:I:1124:PHE:HB2	1.79	0.47
1:J:116:MET:O	1:J:120:SER:OG	2.32	0.47
2:K:270:ASN:O	2:K:272:ASP:N	2.46	0.47
6:O:785:ARG:HB2	6:O:788:HIS:CD2	2.49	0.47
10:S:671:GLN:HB3	10:S:674:ARG:HH21	1.78	0.47
10:S:1175:LYS:NZ	10:S:1176:VAL:O	2.47	0.47
10:T:672:THR:OG1	10:T:725:ARG:NH2	2.48	0.47
10:T:1656:GLN:OE1	10:T:1660:ARG:NH1	2.47	0.47
11:U:298:LEU:HD21	11:U:318:PRO:HG2	1.95	0.47
12:V:514:LEU:HB2	12:V:522:LEU:HD11	1.95	0.47
1:A:367:SER:HB2	3:C:331:GLN:HB3	1.96	0.47
2:B:245:ARG:NH1	2:B:246:HIS:HB2	2.29	0.47
6:F:344:ARG:NH2	6:F:682:GLN:OE1	2.47	0.47
8:H:534:LEU:H	8:H:537:LEU:HD12	1.79	0.47
6:O:653:ARG:HE	6:O:653:ARG:HB3	1.47	0.47
10:S:1454:PRO:HD3	10:S:1507:ARG:HH12	1.79	0.47
10:T:1591:PRO:HA	10:T:1602:ARG:HG2	1.95	0.47
14:b:490:PRO:O	14:b:492:LEU:N	2.46	0.47
14:d:577:ARG:HD3	14:d:580:LEU:HD12	1.96	0.47
14:d:672:LYS:HB2	13:e:836:LEU:HD13	1.95	0.47
4:D:275:ILE:HG13	4:D:278:ASP:H	1.79	0.47
7:G:270:SER:HB2	7:G:274:ASN:H	1.80	0.47
1:J:341:GLU:O	1:J:345:ASN:ND2	2.42	0.47
5:N:191:ARG:HA	5:N:203:SER:HA	1.96	0.47
8:Q:280:ILE:HG21	8:Q:356:LEU:HD12	1.96	0.47
10:S:1258:ASN:O	10:S:1262:GLN:NE2	2.48	0.47
12:Y:118:VAL:HG21	12:Y:138:LEU:HD22	1.96	0.47
12:Z:714:LYS:NZ	12:Z:758:ASP:OD2	2.43	0.47
1:A:239:PRO:HG3	1:A:255:LYS:HB3	1.97	0.47
4:D:1209:SER:OG	4:D:1214:MET:SD	2.63	0.47
6:F:592:LYS:NZ	6:F:597:GLN:O	2.38	0.47
1:J:505:LEU:HD23	1:J:532:ARG:HH11	1.79	0.47
4:M:845:SER:HB3	4:M:850:ARG:HB2	1.97	0.47
4:M:892:GLN:HG2	5:N:186:LYS:HE3	1.96	0.47
10:S:330:ARG:HE	10:S:356:MET:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:336:GLN:HE22	11:U:354:GLN:HG3	1.78	0.47
12:Z:677:VAL:HG22	12:Z:735:PRO:HD3	1.96	0.47
1:A:409:PHE:HD1	1:A:415:TRP:HB2	1.80	0.47
1:A:445:GLU:HB3	2:B:26:SER:HB3	1.96	0.47
2:B:153:PHE:HE1	2:B:160:VAL:HA	1.79	0.47
4:D:520:GLN:HB3	5:E:201:ILE:HD13	1.96	0.47
4:D:573:PRO:HD2	4:D:854:TRP:HB2	1.96	0.47
6:F:472:MET:HG2	6:F:473:VAL:HG23	1.96	0.47
6:F:479:ARG:HG3	6:F:509:LEU:HD13	1.95	0.47
6:F:697:ARG:HH21	7:G:23:TYR:HB3	1.80	0.47
7:G:135:THR:OG1	7:G:141:GLU:OE1	2.27	0.47
9:I:74:ASN:HD22	9:I:465:ALA:HA	1.79	0.47
9:I:988:HIS:HE1	9:I:1037:ASP:HB2	1.80	0.47
1:J:505:LEU:HD22	1:J:571:PHE:CE1	2.49	0.47
1:J:603:GLU:HB3	4:M:1125:LEU:HD22	1.96	0.47
1:J:652:GLN:HG3	4:M:1044:SER:HB3	1.97	0.47
2:K:176:THR:OG1	2:K:177:PHE:N	2.47	0.47
4:M:99:ARG:NH2	4:M:703:THR:O	2.47	0.47
5:N:179:PHE:HD1	5:N:195:LEU:HB2	1.80	0.47
5:N:227:VAL:HG12	5:N:232:TRP:HB3	1.96	0.47
6:O:292:THR:OG1	10:T:674:ARG:NH2	2.47	0.47
6:O:793:GLN:C	6:O:795:TRP:H	2.23	0.47
7:P:250:ASN:N	7:P:250:ASN:OD1	2.46	0.47
9:R:940:LEU:O	9:R:944:GLU:HB2	2.15	0.47
10:S:672:THR:HG23	10:S:729:PHE:HA	1.97	0.47
12:V:423:ASP:HA	12:V:426:SER:HB3	1.96	0.47
12:Y:476:PRO:HG3	12:Y:538:ILE:HG13	1.97	0.47
12:Z:376:PHE:HB3	12:Z:380:CYS:HB3	1.96	0.47
14:b:308:ASN:HB2	14:b:324:VAL:HB	1.97	0.47
1:A:189:THR:OG1	1:A:220:THR:OG1	2.27	0.47
2:B:253:LEU:H	2:B:328:THR:HA	1.80	0.47
4:D:68:PRO:HG2	4:D:72:LEU:HD21	1.97	0.47
9:I:340:ASP:O	9:I:367:ASP:N	2.48	0.47
8:Q:695:LYS:HD2	8:Q:695:LYS:HA	1.74	0.47
12:Y:94:LYS:HB3	12:Y:124:LEU:HD13	1.96	0.47
4:D:123:LEU:HB3	4:D:185:SER:HB3	1.97	0.47
6:F:855:GLU:O	6:F:858:LYS:HG3	2.14	0.47
4:M:444:PRO:HB2	4:M:539:LEU:HD12	1.96	0.47
9:R:632:LYS:HZ1	9:R:750:TRP:CD1	2.32	0.47
10:T:1435:ASP:HB2	10:T:1561:ARG:HH22	1.80	0.47
14:b:691:LEU:HD13	14:b:697:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:452:ASP:O	4:D:524:ARG:NH1	2.45	0.47
9:I:73:TYR:HB3	9:I:465:ALA:HB2	1.96	0.47
9:I:175:SER:HA	9:I:233:GLN:HG3	1.96	0.47
4:M:181:SER:OG	4:M:829:ARG:NH2	2.47	0.47
4:M:425:ILE:HD12	4:M:425:ILE:HA	1.80	0.47
6:O:756:HIS:CE1	6:O:788:HIS:HB3	2.50	0.47
9:R:222:ARG:HB3	9:R:234:ARG:HG3	1.97	0.47
10:S:942:GLN:O	10:S:945:MET:HG3	2.15	0.47
10:T:1601:MET:HG3	15:c:528:THR:HG21	1.97	0.47
10:T:1831:ILE:HD13	10:T:1885:ARG:HH21	1.80	0.47
12:W:286:ARG:NH2	12:W:401:MET:SD	2.88	0.47
12:Y:296:LEU:HD23	12:Y:300:MET:HE2	1.96	0.47
14:b:491:PRO:HB3	14:b:510:ALA:H	1.80	0.47
14:d:97:ASP:OD2	14:d:115:SER:OG	2.32	0.47
2:B:20:ARG:HB2	2:B:30:PRO:HG2	1.97	0.46
3:C:55:THR:HG23	3:C:86:TRP:HE1	1.80	0.46
4:D:719:TYR:HB2	4:D:820:VAL:HG21	1.97	0.46
4:D:1228:ILE:HG13	4:D:1241:ILE:HG21	1.97	0.46
8:H:753:GLU:O	8:H:756:LYS:HG3	2.15	0.46
1:J:438:GLU:OE2	1:J:466:SER:OG	2.30	0.46
4:M:1395:LEU:HD22	4:M:1408:LEU:HG	1.96	0.46
6:O:481:LEU:HD11	8:Q:363:ALA:HB1	1.96	0.46
9:R:115:ASP:OD1	9:R:115:ASP:N	2.47	0.46
9:R:363:VAL:HG22	9:R:378:VAL:HG22	1.97	0.46
9:R:948:PHE:HZ	9:R:990:GLU:HB2	1.80	0.46
9:R:992:LEU:O	9:R:994:LYS:NZ	2.37	0.46
10:S:335:LEU:HD11	10:S:396:PHE:HD1	1.80	0.46
11:U:724:SER:O	11:U:728:VAL:HG23	2.15	0.46
12:V:27:MET:HE2	12:V:27:MET:HB3	1.71	0.46
15:c:475:ASP:O	15:c:478:GLU:HG3	2.15	0.46
14:d:359:LEU:C	14:d:361:LEU:H	2.23	0.46
2:B:168:ASP:OD1	2:B:168:ASP:N	2.46	0.46
8:H:362:GLN:OE1	8:H:365:ARG:NH2	2.45	0.46
8:H:896:ARG:NH2	9:I:899:LEU:O	2.47	0.46
4:M:346:LEU:HB2	4:M:355:LEU:HD21	1.97	0.46
7:P:220:ALA:HB1	7:P:273:ALA:HB1	1.96	0.46
9:R:82:LEU:HD12	9:R:86:VAL:HB	1.96	0.46
9:R:97:GLU:HB2	9:R:99:MET:HE2	1.97	0.46
9:R:1026:ARG:O	9:R:1028:ASN:ND2	2.48	0.46
10:T:1370:LEU:HD23	10:T:1392:ASP:HB3	1.96	0.46
10:T:1757:SER:HA	10:T:1760:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:1782:THR:HG1	10:T:1810:SER:HG	1.61	0.46
11:U:310:GLN:HB2	11:U:320:TRP:HZ2	1.81	0.46
11:U:664:LEU:O	11:U:667:MET:HG3	2.15	0.46
12:V:220:GLN:HA	12:V:225:MET:HG3	1.96	0.46
12:V:358:LEU:HG	12:V:369:ILE:HG12	1.97	0.46
12:Z:571:PRO:HA	12:Z:574:LEU:HD12	1.96	0.46
13:a:823:GLN:O	13:a:827:ASN:ND2	2.48	0.46
14:d:481:LEU:HD12	14:d:485:ILE:HD11	1.97	0.46
14:d:659:LEU:HD13	15:f:469:LEU:HG	1.97	0.46
4:D:237:GLY:HA2	4:D:257:LEU:O	2.15	0.46
9:I:289:LEU:HG	9:I:291:ASP:H	1.80	0.46
2:K:218:HIS:HB2	2:K:234:GLY:HA2	1.98	0.46
2:K:254:LEU:HD23	2:K:335:LEU:HD13	1.97	0.46
5:N:247:LYS:HD2	5:N:288:PRO:HA	1.96	0.46
6:O:649:LEU:O	6:O:654:GLN:NE2	2.48	0.46
8:Q:878:LYS:HZ3	8:Q:882:VAL:H	1.63	0.46
10:S:153:ARG:NH1	10:S:174:THR:OG1	2.41	0.46
10:S:705:CYS:HB3	10:S:765:VAL:HG11	1.96	0.46
10:T:34:GLU:HA	10:T:37:HIS:HD2	1.80	0.46
12:W:83:TYR:HB3	12:W:100:ILE:HG12	1.98	0.46
12:X:424:ASN:HB3	12:X:459:GLN:HG3	1.98	0.46
2:B:14:ILE:O	2:B:349:ASN:ND2	2.49	0.46
9:I:543:LEU:HD11	9:I:606:LEU:HD13	1.97	0.46
1:J:165:LEU:HD11	1:J:311:LEU:HD13	1.96	0.46
3:L:145:PRO:HD2	3:L:152:GLN:HG2	1.97	0.46
10:S:1355:PRO:HB3	10:S:1873:LEU:HD21	1.98	0.46
10:T:1822:ALA:HB1	10:T:1977:ARG:HD2	1.97	0.46
11:U:787:ARG:HD3	11:U:820:ASN:HA	1.97	0.46
12:V:416:LEU:HD11	12:V:447:LEU:HD12	1.97	0.46
12:X:569:LEU:HB3	12:X:570:GLN:H	1.52	0.46
12:Y:471:LEU:HD12	12:Y:562:ARG:HB3	1.96	0.46
4:D:422:MET:HG3	4:D:438:VAL:HB	1.97	0.46
7:G:191:VAL:HG12	7:G:207:LEU:HB3	1.98	0.46
7:G:211:SER:HB2	11:U:300:ILE:HG23	1.97	0.46
8:H:181:LYS:HD3	8:H:181:LYS:HA	1.73	0.46
4:M:1267:LEU:HA	4:M:1270:ASN:HD22	1.81	0.46
9:R:578:ASN:N	9:R:673:ASP:OD2	2.47	0.46
10:S:405:LYS:HD3	10:S:405:LYS:HA	1.73	0.46
12:V:482:LEU:HD11	12:V:581:LEU:HG	1.96	0.46
12:W:676:VAL:HG11	12:W:730:ILE:HG23	1.98	0.46
12:W:687:GLN:NE2	12:W:744:MET:SD	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:383:SER:OG	12:Y:387:LYS:NZ	2.46	0.46
14:b:455:PHE:HE1	14:b:467:MET:HE2	1.80	0.46
14:b:577:ARG:HH11	14:d:143:ARG:HH22	1.62	0.46
1:A:508:TYR:HB2	1:A:514:PHE:HD1	1.81	0.46
4:D:635:PRO:HG2	5:E:124:SER:HB2	1.97	0.46
4:D:1162:ASP:HA	10:S:479:VAL:HG21	1.97	0.46
9:I:819:LEU:O	9:I:822:GLU:HG3	2.16	0.46
5:N:242:TYR:O	5:N:244:GLN:N	2.48	0.46
7:P:22:ASP:HB2	7:P:27:ARG:HB3	1.97	0.46
10:S:264:LEU:HB3	10:S:376:SER:HB2	1.98	0.46
10:T:906:ASN:HB3	10:T:909:LEU:HD12	1.97	0.46
10:T:1231:HIS:CE1	10:T:1232:ARG:HG2	2.50	0.46
12:V:163:ASN:HA	12:V:196:LEU:HD21	1.98	0.46
12:V:718:LYS:HD3	12:V:718:LYS:HA	1.75	0.46
12:X:454:ARG:NH2	12:X:597:TYR:OH	2.48	0.46
12:Y:263:LEU:HD13	12:Y:285:MET:HB3	1.98	0.46
12:Z:437:LEU:HD13	12:Z:488:LEU:HD11	1.98	0.46
14:d:662:LEU:HD13	13:e:825:VAL:HG12	1.98	0.46
13:e:695:ASN:N	13:e:695:ASN:OD1	2.47	0.46
4:D:1181:ASP:N	4:D:1181:ASP:OD1	2.46	0.46
1:J:594:GLN:O	1:J:597:GLU:HG3	2.16	0.46
4:M:119:LEU:HD22	4:M:559:MET:HE2	1.97	0.46
8:Q:173:CYS:HA	8:Q:176:GLN:CD	2.41	0.46
9:R:794:ASN:OD1	9:R:849:LYS:NZ	2.47	0.46
10:S:12:SER:OG	10:S:13:LEU:N	2.46	0.46
10:S:906:ASN:HD21	10:S:909:LEU:HD12	1.80	0.46
10:S:1602:ARG:HH11	10:S:1611:PRO:HB2	1.81	0.46
10:T:1317:HIS:HA	10:T:1320:ILE:HG12	1.98	0.46
11:U:777:ARG:H	11:U:777:ARG:HG2	1.61	0.46
14:d:206:GLU:HA	14:d:218:LYS:HE2	1.98	0.46
13:e:766:ARG:HH21	15:f:410:ASP:HB3	1.81	0.46
3:C:141:ILE:HB	3:C:157:HIS:HB2	1.98	0.46
4:D:499:LYS:HA	5:E:207:VAL:HG11	1.98	0.46
8:H:394:TYR:HB2	8:H:397:VAL:HB	1.98	0.46
8:H:457:ARG:HD3	8:H:461:ILE:HD11	1.97	0.46
9:I:122:ILE:HG12	9:I:460:MET:HE3	1.98	0.46
9:I:220:LEU:HB2	9:I:240:GLN:HG3	1.98	0.46
8:Q:175:THR:O	8:Q:179:LEU:HG	2.16	0.46
8:Q:467:ASN:OD1	8:Q:467:ASN:N	2.42	0.46
10:S:617:GLU:O	10:S:618:HIS:ND1	2.49	0.46
10:T:266:LYS:HG3	10:T:378:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:145:ALA:O	12:W:149:GLN:NE2	2.49	0.46
13:a:843:TYR:CZ	14:b:679:GLN:HB3	2.51	0.46
2:B:69:LEU:HD13	2:B:108:GLN:HB3	1.96	0.46
6:F:596:LEU:O	6:F:598:ARG:NH1	2.49	0.46
6:F:731:VAL:HG22	7:G:69:MET:HE3	1.98	0.46
4:M:397:LEU:HA	4:M:413:TRP:HD1	1.80	0.46
9:R:1106:ALA:HA	9:R:1109:LEU:HD12	1.98	0.46
10:T:554:HIS:HA	10:T:557:HIS:HD1	1.81	0.46
10:T:1944:MET:HE3	10:T:1944:MET:HB3	1.77	0.46
11:U:813:VAL:O	11:U:817:VAL:HG23	2.15	0.46
12:X:701:GLU:OE1	12:Y:463:ARG:NH2	2.49	0.46
12:Y:240:VAL:HG22	12:Y:255:ALA:HB1	1.98	0.46
12:Z:468:THR:OG1	12:Z:596:GLU:OE1	2.33	0.46
14:d:440:CYS:HB2	14:d:531:PRO:HB2	1.97	0.46
1:A:130:TYR:O	1:A:133:GLN:HG3	2.16	0.46
1:A:395:ASN:HB3	1:A:398:GLU:HB2	1.98	0.46
3:C:222:VAL:HA	3:C:242:THR:HG22	1.98	0.46
6:F:753:ASN:HD21	8:Q:491:ASP:HB2	1.81	0.46
9:I:242:MET:HB3	9:I:263:SER:HB3	1.97	0.46
4:M:119:LEU:O	4:M:707:SER:OG	2.32	0.46
4:M:423:LYS:HG2	4:M:437:PRO:HA	1.98	0.46
6:O:325:LEU:HB3	6:O:673:TRP:CD1	2.51	0.46
7:P:85:ILE:HB	7:P:97:TYR:HB3	1.97	0.46
10:T:1938:PHE:HZ	15:f:477:LYS:HA	1.81	0.46
12:V:190:LYS:HB2	12:V:193:ARG:HE	1.81	0.46
12:V:581:LEU:HD13	12:V:604:TYR:HE2	1.81	0.46
12:Z:598:MET:HE1	12:Z:659:VAL:HG21	1.98	0.46
1:A:265:ARG:HB3	14:b:504:ILE:HG13	1.97	0.45
9:I:665:VAL:HG23	9:I:674:VAL:HG21	1.97	0.45
2:K:210:VAL:HG11	2:K:253:LEU:HD13	1.98	0.45
8:Q:863:LYS:HA	8:Q:863:LYS:HD3	1.73	0.45
9:R:452:VAL:HA	9:R:462:THR:HA	1.97	0.45
10:S:133:LEU:HD11	10:S:208:LEU:HD13	1.98	0.45
10:T:202:LEU:HD22	10:T:208:LEU:HD21	1.98	0.45
12:W:710:LEU:HD22	12:W:748:VAL:HG22	1.98	0.45
12:X:526:ARG:HH21	12:X:628:LEU:HD22	1.82	0.45
13:a:744:LEU:HD22	14:b:592:LEU:HD12	1.98	0.45
14:b:567:GLN:HE22	15:c:369:LEU:HD23	1.80	0.45
14:d:402:VAL:HG13	14:d:435:VAL:HG22	1.98	0.45
4:D:243:MET:HG3	4:D:252:VAL:HG12	1.98	0.45
8:H:214:ILE:HD11	8:H:510:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:778:ASP:H	9:I:781:LEU:HD12	1.81	0.45
4:M:1374:LEU:O	4:M:1377:THR:OG1	2.34	0.45
7:P:222:SER:HA	7:P:273:ALA:HB3	1.97	0.45
9:R:486:SER:HA	9:R:487:SER:HA	1.58	0.45
10:S:414:ASP:HB2	10:S:432:LEU:HB2	1.99	0.45
10:T:1145:PRO:O	10:T:1147:ARG:NH1	2.48	0.45
12:W:574:LEU:HB3	12:W:608:LEU:HD11	1.97	0.45
12:W:603:HIS:HA	12:W:606:LYS:HD3	1.98	0.45
12:Z:619:LYS:HB3	12:Z:620:SER:H	1.59	0.45
14:b:236:LEU:HD13	14:b:266:TYR:HD1	1.80	0.45
14:b:389:SER:HB2	14:b:404:LEU:HB2	1.98	0.45
4:D:464:LEU:HD21	4:D:535:TYR:HD1	1.80	0.45
8:H:565:LYS:HD3	8:H:591:LEU:HD22	1.97	0.45
8:H:758:ILE:HG22	8:H:797:LEU:HD11	1.99	0.45
9:I:310:ILE:HG12	9:I:361:THR:HG21	1.98	0.45
1:J:19:GLN:O	1:J:21:ARG:NH1	2.50	0.45
1:J:329:SER:HA	1:J:332:MET:SD	2.56	0.45
1:J:442:LEU:HD13	1:J:467:ILE:HG12	1.97	0.45
2:K:136:CYS:HB3	2:K:141:ILE:HG12	1.98	0.45
2:K:187:ASN:HD21	2:K:193:LYS:HE3	1.80	0.45
4:M:1279:LYS:HG3	10:T:1242:GLN:HE22	1.81	0.45
8:Q:299:ARG:NH1	8:Q:303:SER:O	2.50	0.45
8:Q:322:GLN:HG3	8:Q:324:LEU:HB2	1.97	0.45
10:S:567:ARG:NH1	10:S:633:CYS:SG	2.90	0.45
10:T:243:ARG:HD2	10:T:306:TYR:HB2	1.97	0.45
10:T:651:GLY:O	10:T:657:ALA:HB2	2.16	0.45
10:T:665:GLU:O	10:T:725:ARG:NH1	2.49	0.45
10:T:1151:ALA:HB3	10:T:1162:ARG:HD2	1.98	0.45
10:T:2004:GLY:HA2	10:T:2007:ARG:HE	1.81	0.45
12:X:104:ILE:HG12	12:X:109:ILE:HB	1.97	0.45
12:Z:8:ILE:HG13	12:Z:39:ALA:HB2	1.98	0.45
12:Z:87:LEU:HB2	12:Z:96:LEU:HD23	1.99	0.45
12:Z:569:LEU:HB3	12:Z:570:GLN:H	1.58	0.45
1:A:111:ALA:O	1:A:114:GLU:HG3	2.17	0.45
2:B:103:HIS:HB2	2:B:110:LEU:HA	1.98	0.45
2:B:151:ASN:HB3	2:B:153:PHE:CZ	2.52	0.45
3:C:320:LYS:HE3	3:C:323:GLY:H	1.82	0.45
4:D:1072:VAL:HG11	4:D:1153:PRO:HD3	1.97	0.45
4:D:1120:GLN:HG3	10:S:471:SER:HA	1.97	0.45
7:G:106:VAL:HA	7:G:124:SER:HB3	1.97	0.45
9:I:393:GLN:HA	9:I:396:GLN:HE21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:569:VAL:O	9:I:571:GLU:N	2.50	0.45
2:K:179:ARG:HA	2:K:179:ARG:HD2	1.69	0.45
3:L:107:THR:HB	3:L:151:SER:HA	1.99	0.45
4:M:1408:LEU:O	4:M:1412:GLN:NE2	2.50	0.45
5:N:311:CYS:SG	5:N:312:VAL:N	2.90	0.45
8:Q:460:ILE:HG22	8:Q:461:ILE:HG12	1.97	0.45
9:R:224:THR:OG1	9:R:234:ARG:NH2	2.49	0.45
10:S:881:GLN:HB3	10:S:929:LYS:HG2	1.97	0.45
10:S:1649:VAL:HG21	10:S:1703:LEU:HD23	1.99	0.45
10:S:1911:LEU:HD23	10:S:1911:LEU:HA	1.86	0.45
10:T:1027:ARG:HE	10:T:1031:HIS:HB3	1.82	0.45
12:Z:427:LEU:HB3	12:Z:459:GLN:HE22	1.82	0.45
14:b:640:VAL:N	15:c:452:ASP:OD1	2.47	0.45
3:C:172:PRO:O	3:C:230:ASN:ND2	2.49	0.45
9:I:104:HIS:HD2	9:I:152:ILE:HD12	1.82	0.45
9:I:335:LEU:HD13	9:I:344:ILE:HG12	1.97	0.45
9:I:786:ILE:HG21	9:I:839:GLN:HG3	1.97	0.45
8:Q:398:TRP:HH2	8:Q:422:LEU:HD13	1.82	0.45
10:S:1432:GLN:O	10:S:1433:ARG:NH1	2.47	0.45
11:U:451:GLU:O	11:U:453:HIS:ND1	2.48	0.45
11:U:787:ARG:NE	11:U:820:ASN:OXT	2.49	0.45
12:V:61:LYS:HD2	12:V:64:ARG:HE	1.80	0.45
12:W:123:LYS:HD3	12:W:123:LYS:HA	1.77	0.45
12:W:284:GLU:HA	12:W:350:ARG:HH12	1.81	0.45
12:Z:76:VAL:HG11	12:Z:107:LEU:HB2	1.98	0.45
13:a:861:LEU:HD22	14:b:701:ILE:HG21	1.99	0.45
14:b:665:SER:O	14:b:668:GLN:HG3	2.17	0.45
1:J:423:ASP:HA	1:J:430:ARG:HH22	1.81	0.45
4:M:444:PRO:HG3	4:M:469:ARG:HB2	1.99	0.45
5:N:87:ASP:OD1	5:N:87:ASP:N	2.48	0.45
8:Q:893:GLN:HB3	11:U:817:VAL:HG12	1.99	0.45
11:U:385:ASP:HB3	11:U:388:LYS:HB3	1.98	0.45
12:V:463:ARG:NH2	12:V:477:GLU:O	2.49	0.45
12:V:463:ARG:HH12	12:V:538:ILE:HG12	1.81	0.45
12:X:697:CYS:SG	12:X:698:LEU:N	2.89	0.45
14:d:241:GLY:H	14:d:275:THR:HB	1.81	0.45
14:d:256:LEU:HD21	14:d:297:ALA:HB1	1.99	0.45
1:A:8:PRO:HB3	3:C:318:VAL:HB	1.99	0.45
3:C:24:GLY:O	3:C:26:ARG:N	2.43	0.45
4:D:1361:LEU:HD21	4:D:1418:TYR:HB2	1.99	0.45
6:F:400:PRO:O	6:F:405:LYS:NZ	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:557:GLU:HA	6:F:560:PHE:CE1	2.52	0.45
8:H:265:LEU:HD13	8:H:441:TRP:HB2	1.98	0.45
3:L:54:LYS:NZ	3:L:56:HIS:O	2.42	0.45
8:Q:426:LEU:HA	8:Q:429:LEU:HB2	1.99	0.45
8:Q:784:LYS:HD2	8:Q:788:MET:HE3	1.99	0.45
10:S:584:ARG:HG2	10:S:586:ILE:H	1.82	0.45
10:S:880:LEU:HA	10:S:884:ASN:HD21	1.82	0.45
10:S:927:GLN:HB3	10:S:998:ASN:HA	1.99	0.45
10:S:1538:LEU:HB3	10:S:1618:ILE:HD11	1.98	0.45
12:W:607:LYS:HA	12:W:607:LYS:HD3	1.74	0.45
12:X:110:LYS:NZ	12:X:141:SER:O	2.38	0.45
12:X:154:ILE:HD11	12:X:167:VAL:HG13	1.98	0.45
13:a:854:ILE:HD13	14:b:687:ARG:HG3	1.98	0.45
4:D:117:LEU:HD22	4:D:568:LEU:HD13	1.99	0.45
1:J:485:LEU:HD11	1:J:533:LEU:HD11	1.98	0.45
4:M:494:TRP:HE1	4:M:781:LEU:HG	1.82	0.45
4:M:1134:ILE:HD12	4:M:1134:ILE:HA	1.90	0.45
11:U:373:ARG:HH11	11:U:377:ARG:HH12	1.65	0.45
11:U:754:MET:SD	11:U:811:ARG:HB3	2.57	0.45
12:X:676:VAL:HG21	12:X:730:ILE:HG23	1.98	0.45
14:d:658:GLN:OE1	13:e:822:ASN:ND2	2.50	0.45
15:f:414:LEU:HD23	15:f:414:LEU:HA	1.77	0.45
3:C:129:MET:SD	3:C:156:GLN:NE2	2.90	0.45
3:C:208:LYS:HB3	3:C:209:TYR:H	1.60	0.45
5:E:128:ASN:H	5:E:144:GLY:HA2	1.81	0.45
5:E:218:VAL:HG21	5:E:261:LYS:HA	1.98	0.45
6:F:369:VAL:HG23	6:F:373:VAL:HB	1.99	0.45
6:F:614:ASP:OD1	11:U:187:ARG:NH1	2.47	0.45
1:J:98:LEU:HD21	1:J:378:LEU:HD13	1.99	0.45
1:J:519:LEU:HD22	1:J:537:GLY:HA3	1.98	0.45
4:M:792:SER:O	4:M:796:HIS:ND1	2.46	0.45
4:M:1106:ARG:NH1	4:M:1147:GLY:O	2.46	0.45
7:P:105:SER:O	7:P:125:SER:OG	2.31	0.45
9:R:220:LEU:HB3	9:R:236:LEU:HD13	1.99	0.45
10:S:484:PRO:HA	10:S:485:PRO:HD3	1.91	0.45
10:S:724:LEU:HD23	10:S:792:ARG:HH12	1.82	0.45
10:T:16:PRO:O	10:T:19:GLU:HG3	2.17	0.45
12:V:589:ASN:HB2	12:X:2:ARG:HG2	1.99	0.45
14:d:218:LYS:NZ	14:d:222:GLY:O	2.48	0.45
5:E:232:TRP:CZ2	5:E:247:LYS:HB2	2.52	0.45
4:M:441:ASN:N	4:M:441:ASN:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1320:LEU:HD23	4:M:1320:LEU:H	1.82	0.45
9:R:978:GLU:O	9:R:981:GLU:HG3	2.17	0.45
9:R:1003:ASP:HB3	9:R:1006:ALA:HB3	1.99	0.45
9:R:1081:LYS:HD3	9:R:1086:VAL:HG11	1.98	0.45
10:S:1685:PRO:HD2	10:S:1769:GLN:HG3	1.98	0.45
10:T:1119:ILE:HD12	10:T:1119:ILE:HA	1.87	0.45
11:U:492:HIS:O	11:U:495:LEU:HG	2.17	0.45
11:U:588:LEU:HD21	11:U:632:LEU:HB2	1.98	0.45
12:V:80:VAL:HG12	12:V:103:LEU:HD13	1.98	0.45
12:Z:539:THR:OG1	12:Z:541:LYS:NZ	2.44	0.45
14:b:632:ARG:HA	14:b:632:ARG:HD3	1.80	0.45
14:d:358:GLU:HB2	14:d:371:LEU:HD22	1.99	0.45
6:F:249:ARG:HG3	7:G:265:TRP:CE2	2.51	0.44
4:M:1363:LYS:HA	4:M:1363:LYS:HD3	1.81	0.44
5:N:218:VAL:HG23	5:N:219:ARG:HG2	1.99	0.44
6:O:567:GLU:HG2	12:W:91:PRO:HG2	1.98	0.44
10:S:18:ARG:HD3	10:S:18:ARG:HA	1.85	0.44
10:S:697:GLU:OE1	10:S:751:ARG:NH1	2.50	0.44
10:S:1226:ASN:HB3	10:S:1229:LEU:HB3	1.99	0.44
10:S:1401:ASN:O	10:S:1404:GLU:HG2	2.16	0.44
10:S:1739:LEU:HD21	10:S:1855:GLN:HB3	1.99	0.44
12:V:570:GLN:HB2	12:V:573:VAL:HG23	1.99	0.44
12:W:387:LYS:HD2	12:W:392:ASP:HA	1.97	0.44
12:Z:301:ALA:C	12:Z:510:ARG:HH12	2.25	0.44
14:d:70:LEU:HA	14:d:73:LEU:HD12	1.99	0.44
4:D:636:GLN:HG2	4:D:640:ARG:HG2	1.99	0.44
5:E:174:HIS:HB3	5:E:180:LYS:HB2	1.99	0.44
5:E:198:HIS:O	5:E:199:GLN:NE2	2.50	0.44
4:M:583:VAL:HG12	4:M:588:LEU:HG	1.98	0.44
4:M:924:HIS:CD2	4:M:925:LYS:HG3	2.52	0.44
8:Q:256:ARG:O	8:Q:259:GLN:HG3	2.17	0.44
9:R:717:ILE:O	9:R:721:MET:HG2	2.17	0.44
9:R:856:LEU:HD23	9:R:859:ILE:HD11	1.98	0.44
9:R:1016:ILE:HG21	9:R:1053:LEU:HD22	1.99	0.44
10:T:233:TYR:HA	10:T:274:SER:HB2	1.98	0.44
4:D:307:LYS:HD2	4:D:321:VAL:HG12	1.99	0.44
4:D:1025:ASP:OD1	4:D:1025:ASP:N	2.49	0.44
5:E:266:VAL:HG21	5:E:324:THR:HG21	2.00	0.44
8:H:424:GLY:HA2	8:H:446:VAL:HG22	1.99	0.44
9:I:802:THR:HG23	9:I:805:LYS:HE3	1.98	0.44
4:M:257:LEU:HD22	4:M:316:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:81:ARG:HB3	7:P:102:HIS:HB2	1.98	0.44
9:R:64:HIS:HB3	9:R:67:ALA:HB3	1.98	0.44
9:R:76:GLN:HE21	9:R:466:ARG:HH22	1.65	0.44
10:T:1292:LEU:HG	10:T:1293:THR:HG23	1.98	0.44
10:T:1619:LEU:HG	10:T:1623:LEU:HD13	2.00	0.44
12:Y:307:GLN:HG3	12:Y:310:ALA:H	1.83	0.44
12:Z:33:ALA:HB2	12:Z:48:SER:HB2	1.98	0.44
14:b:31:ARG:HD3	14:b:31:ARG:HA	1.78	0.44
1:A:430:ARG:HH21	1:A:460:MET:HB3	1.81	0.44
1:J:489:ILE:HD11	2:K:26:SER:HB2	1.98	0.44
2:K:50:THR:HG22	2:K:66:PRO:HG3	1.99	0.44
4:M:420:THR:HG21	4:M:548:PRO:HG3	1.99	0.44
6:O:423:GLU:O	6:O:426:GLU:HG3	2.16	0.44
8:Q:876:ASN:OD1	8:Q:876:ASN:N	2.51	0.44
9:R:78:PHE:HZ	9:R:448:GLU:HB2	1.83	0.44
10:S:23:THR:HG21	10:S:39:LEU:HD22	1.98	0.44
10:S:391:LYS:HA	10:S:391:LYS:HD2	1.71	0.44
10:T:1406:ILE:HG12	10:T:1420:LEU:HD13	1.98	0.44
10:T:1783:PRO:HD3	10:T:1952:ASN:HA	1.99	0.44
11:U:187:ARG:HG2	11:U:191:MET:HE1	1.99	0.44
12:X:1:MET:HE2	12:X:3:ARG:HG3	1.99	0.44
12:Y:197:ARG:HG2	12:Y:202:TRP:HE1	1.82	0.44
12:Y:224:ASN:O	12:Y:227:MET:HG3	2.17	0.44
12:Y:349:ASP:HA	12:Y:426:SER:HB2	2.00	0.44
12:Y:662:LYS:HB3	12:Y:665:ASP:HB2	2.00	0.44
12:Z:3:ARG:HB2	12:Z:4:SER:H	1.59	0.44
12:Z:308:TRP:CZ3	12:Z:510:ARG:CG	3.00	0.44
14:b:299:ALA:HB3	14:b:313:ALA:HB3	1.98	0.44
1:A:260:ARG:NH1	1:A:285:LEU:O	2.51	0.44
4:D:556:ASN:ND2	4:D:851:SER:OG	2.41	0.44
4:D:898:LEU:HD12	4:D:901:TRP:HE1	1.81	0.44
4:D:1007:HIS:CE1	4:D:1015:GLN:HB3	2.53	0.44
5:E:143:VAL:HB	5:E:168:GLY:HA3	1.99	0.44
8:H:140:GLU:HG2	8:H:200:ILE:HG13	2.00	0.44
4:M:634:HIS:HD1	4:M:636:GLN:HG3	1.83	0.44
10:S:151:GLN:HE22	10:S:158:PHE:HB3	1.83	0.44
10:S:230:HIS:HA	10:S:233:TYR:HB3	1.99	0.44
10:T:485:PRO:HB2	10:T:488:GLN:HG2	1.98	0.44
11:U:336:GLN:HG2	11:U:357:ILE:HG21	1.99	0.44
12:V:602:VAL:HG21	12:V:656:LEU:HD22	1.99	0.44
12:W:100:ILE:HG21	12:W:117:TRP:HD1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:439:LEU:HD11	14:b:534:LEU:HB2	1.99	0.44
14:b:543:PRO:HA	14:b:544:PRO:HD3	1.91	0.44
14:d:358:GLU:OE2	14:d:554:ARG:NH2	2.51	0.44
1:A:610:LEU:HD23	1:A:615:PRO:HD3	2.00	0.44
2:B:244:VAL:HG22	2:B:248:LYS:HA	2.00	0.44
2:B:273:HIS:CE1	2:B:374:PHE:HB2	2.52	0.44
4:D:434:HIS:NE2	4:D:436:ASN:OD1	2.51	0.44
4:D:609:LEU:O	4:D:613:LEU:HG	2.16	0.44
6:F:647:THR:HB	6:F:648:HIS:H	1.66	0.44
9:I:509:LEU:HB3	9:I:550:ILE:HD11	1.98	0.44
1:J:458:ARG:NH2	10:T:1205:SER:OG	2.50	0.44
6:O:301:PRO:HB2	7:P:12:HIS:HB3	1.99	0.44
6:O:389:GLN:NE2	6:O:390:LEU:O	2.51	0.44
8:Q:270:LYS:HA	8:Q:347:ALA:HB1	1.99	0.44
10:T:203:LYS:HD3	10:T:203:LYS:HA	1.83	0.44
12:X:170:LYS:HA	12:X:170:LYS:HD2	1.80	0.44
12:X:569:LEU:HD12	12:X:573:VAL:HG21	2.00	0.44
12:Z:222:ASN:O	12:Z:226:ARG:HG2	2.18	0.44
14:b:619:LYS:HD3	14:b:619:LYS:HA	1.83	0.44
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.90	0.44
4:D:624:MET:HG3	4:D:645:ILE:HG23	1.99	0.44
4:D:898:LEU:HD12	4:D:901:TRP:NE1	2.33	0.44
4:D:1247:CYS:SG	4:D:1251:ARG:NH2	2.88	0.44
5:E:11:TYR:HB2	5:E:321:PHE:HB2	2.00	0.44
5:E:153:ASP:OD2	5:E:157:LYS:NZ	2.49	0.44
6:F:400:PRO:HB2	6:F:404:VAL:HB	2.00	0.44
4:M:478:ALA:HA	4:M:481:ILE:HG22	2.00	0.44
4:M:794:LEU:HD13	4:M:807:VAL:HG13	1.99	0.44
6:O:636:HIS:HA	6:O:639:MET:HG2	2.00	0.44
9:R:171:THR:O	9:R:173:GLU:N	2.49	0.44
10:S:1553:GLU:O	10:S:1556:MET:HG3	2.17	0.44
10:T:397:PRO:HG2	10:T:487:ARG:HH22	1.83	0.44
10:T:1199:LEU:HB2	10:T:1207:ILE:HG12	1.99	0.44
10:T:1200:ASP:N	10:T:1200:ASP:OD1	2.50	0.44
12:Z:8:ILE:HG23	12:Z:35:LEU:HB3	1.99	0.44
12:Z:97:THR:HB	12:Z:117:TRP:HB3	2.00	0.44
12:Z:321:LEU:HD21	12:Z:406:ILE:HG12	2.00	0.44
14:b:696:TYR:O	14:b:699:LYS:HG3	2.17	0.44
14:d:353:GLU:OE2	14:d:406:TRP:NE1	2.48	0.44
1:A:271:THR:OG1	14:b:503:GLU:OE2	2.29	0.44
3:C:253:LEU:HG	3:C:254:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:299:ASP:OD1	3:C:299:ASP:N	2.51	0.44
8:H:551:LEU:HD23	8:H:551:LEU:HA	1.85	0.44
9:I:1123:TYR:HD1	9:R:577:SER:HB3	1.82	0.44
4:M:1413:ARG:NH2	4:M:1417:GLU:OE2	2.50	0.44
5:N:18:TYR:CE2	5:N:20:HIS:HB3	2.53	0.44
8:Q:213:LEU:HB2	8:Q:264:TRP:CZ2	2.52	0.44
8:Q:491:ASP:N	8:Q:491:ASP:OD1	2.49	0.44
8:Q:622:ASP:OD1	8:Q:622:ASP:N	2.47	0.44
10:T:1317:HIS:HD2	10:T:1320:ILE:HD11	1.83	0.44
11:U:207:ASP:OD2	12:Y:549:LYS:NZ	2.44	0.44
12:X:87:LEU:HD13	12:X:96:LEU:HD23	1.98	0.44
12:Z:29:GLY:HA2	12:Z:32:PHE:HB2	1.99	0.44
12:Z:233:LEU:HD22	12:Z:285:MET:HG3	2.00	0.44
9:I:862:MET:SD	9:I:892:LYS:NZ	2.91	0.44
6:O:862:ASN:O	6:O:865:ARG:HG3	2.17	0.44
10:S:1414:GLN:O	10:S:1417:ARG:HG3	2.17	0.44
10:S:1721:PHE:HA	10:S:1726:ARG:HG3	1.99	0.44
10:S:1777:THR:HG23	10:S:1905:ARG:HH21	1.82	0.44
11:U:775:PRO:O	11:U:779:GLN:HG2	2.18	0.44
12:V:320:LEU:HD21	12:V:409:VAL:HG11	1.99	0.44
14:d:99:ASN:HB2	14:d:114:GLY:HA2	2.00	0.44
14:d:487:PRO:HA	14:d:525:ARG:HH22	1.83	0.44
4:D:1252:LEU:HD21	4:D:1263:ALA:HB3	1.99	0.43
9:I:753:SER:O	9:I:760:ARG:NH2	2.51	0.43
9:I:1020:VAL:HG22	9:I:1060:LYS:HG3	2.00	0.43
1:J:416:GLN:OE1	2:K:226:GLN:NE2	2.51	0.43
9:R:110:TRP:CD1	9:R:147:ALA:HB1	2.53	0.43
10:S:64:HIS:NE2	10:S:105:GLU:OE2	2.51	0.43
11:U:328:ARG:HE	11:U:413:ASP:HA	1.83	0.43
12:V:651:ILE:HG23	12:V:678:ALA:HB2	2.00	0.43
1:A:21:ARG:HH12	1:A:48:ALA:HB2	1.83	0.43
1:A:577:LEU:HD12	1:A:633:LEU:HD11	2.00	0.43
2:B:184:LEU:HD12	2:B:194:LEU:HB2	2.00	0.43
4:D:53:GLU:OE1	4:D:471:THR:OG1	2.30	0.43
5:E:8:ASN:O	5:E:322:TRP:NE1	2.35	0.43
5:E:146:ASP:N	5:E:146:ASP:OD1	2.51	0.43
4:M:79:TYR:OH	4:M:212:PRO:O	2.36	0.43
4:M:797:LEU:HD22	4:M:802:LEU:HD12	2.00	0.43
6:O:397:LEU:HD23	12:V:7:GLU:HG3	2.00	0.43
10:S:126:THR:HG23	10:S:129:LEU:H	1.83	0.43
10:S:1614:ARG:O	10:S:1617:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:1863:ASP:OD1	10:S:1863:ASP:N	2.49	0.43
10:T:915:LYS:HG2	10:T:983:HIS:CE1	2.53	0.43
10:T:1020:SER:HA	10:T:1031:HIS:CE1	2.53	0.43
12:V:233:LEU:HB3	12:V:285:MET:HG3	1.99	0.43
12:V:417:SER:HB3	12:X:13:GLU:HG3	2.00	0.43
12:V:757:ASP:OD1	12:V:757:ASP:N	2.51	0.43
12:W:41:GLU:HG2	12:W:44:LEU:HD12	1.99	0.43
12:X:337:ASP:N	12:X:337:ASP:OD1	2.50	0.43
14:b:98:VAL:HG13	14:b:112:LEU:HB3	2.00	0.43
15:c:404:MET:HE2	15:c:404:MET:HB2	1.86	0.43
1:A:437:MET:HE3	1:A:463:GLN:HG3	2.00	0.43
3:C:251:LYS:HE3	3:C:251:LYS:HB3	1.90	0.43
4:D:599:ASP:HB2	4:D:673:GLN:HG3	1.99	0.43
4:D:1048:ASP:HB3	4:D:1052:PHE:HE1	1.83	0.43
8:H:873:SER:HB3	9:I:960:LEU:HB2	2.01	0.43
5:N:86:CYS:HA	5:N:91:PRO:HB3	2.00	0.43
7:P:137:ASP:N	7:P:137:ASP:OD1	2.51	0.43
8:Q:562:GLU:HA	8:Q:565:LYS:HG2	2.00	0.43
9:R:148:ASP:O	9:R:203:VAL:N	2.50	0.43
10:S:1035:ASP:O	10:S:1039:LYS:HG2	2.18	0.43
10:S:1784:SER:H	10:S:1962:LEU:HB2	1.83	0.43
10:T:417:LEU:O	10:T:420:MET:HG3	2.18	0.43
10:T:584:ARG:HD3	10:T:590:GLU:HB3	2.00	0.43
10:T:649:ALA:HA	10:T:652:LYS:HG3	1.99	0.43
10:T:688:LEU:HA	10:T:692:GLU:HB2	2.00	0.43
11:U:796:PHE:O	11:U:800:ILE:HG12	2.18	0.43
12:V:258:ARG:HA	12:V:261:GLN:CD	2.44	0.43
14:b:33:GLU:OE2	14:b:37:ARG:NH2	2.51	0.43
14:b:361:LEU:HD23	14:b:558:VAL:HG11	1.99	0.43
14:d:355:VAL:HG11	14:d:435:VAL:HG21	2.00	0.43
2:B:115:ARG:HH21	6:O:277:ASP:HB3	1.81	0.43
4:D:116:GLU:HB3	4:D:126:ASN:HB2	1.99	0.43
4:D:850:ARG:HH22	4:D:854:TRP:CG	2.36	0.43
4:D:977:LEU:HA	4:D:977:LEU:HD23	1.83	0.43
6:F:626:PRO:HB2	12:Y:20:SER:HB2	2.01	0.43
1:J:470:THR:O	1:J:473:MET:HG2	2.19	0.43
5:N:131:VAL:HG11	5:N:172:ALA:HA	2.01	0.43
9:R:220:LEU:HB2	9:R:236:LEU:HB2	2.00	0.43
10:S:277:TYR:HD1	10:S:277:TYR:HA	1.73	0.43
10:S:500:ASP:O	10:S:541:ASN:ND2	2.41	0.43
10:S:1122:ARG:HE	10:S:1126:LEU:HG	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:104:ILE:HG13	12:W:114:ALA:HB2	2.00	0.43
12:W:130:GLU:O	12:W:133:ARG:HG3	2.18	0.43
12:X:248:ASP:HB2	12:X:251:LYS:HB2	2.00	0.43
13:a:769:PHE:CZ	15:c:418:LEU:HD22	2.54	0.43
14:b:365:THR:HB	14:b:366:GLU:H	1.70	0.43
14:b:654:ALA:O	14:b:657:GLN:HG3	2.18	0.43
6:F:391:LYS:HD3	6:F:391:LYS:HA	1.83	0.43
8:H:283:TYR:O	10:T:2000:ARG:NH1	2.52	0.43
2:K:278:SER:HB3	2:K:282:SER:HB2	2.01	0.43
4:M:100:ASN:HB3	4:M:119:LEU:HB2	2.01	0.43
10:S:129:LEU:HD22	10:S:208:LEU:HB3	1.99	0.43
10:T:1365:GLN:HG3	10:T:1367:VAL:H	1.83	0.43
10:T:1720:ARG:HG2	10:T:1801:SER:HB3	1.99	0.43
12:V:299:LYS:HB2	12:V:518:ILE:HG21	2.01	0.43
12:X:523:PHE:HB2	12:X:524:THR:H	1.61	0.43
12:Z:10:ARG:O	12:Z:13:GLU:HG3	2.19	0.43
14:b:116:LYS:HA	14:b:152:PHE:HB3	1.99	0.43
9:I:639:LEU:HD23	9:I:676:PHE:HE1	1.82	0.43
9:I:906:HIS:CG	9:I:927:SER:HG	2.37	0.43
1:J:545:MET:HE3	1:J:545:MET:HB3	1.68	0.43
3:L:208:LYS:HA	3:L:208:LYS:HD3	1.84	0.43
4:M:126:ASN:HA	4:M:187:PHE:HD2	1.82	0.43
4:M:131:LYS:HE3	4:M:131:LYS:HB3	1.78	0.43
4:M:189:ASP:OD1	4:M:189:ASP:N	2.49	0.43
4:M:888:TYR:O	4:M:892:GLN:NE2	2.51	0.43
5:N:297:PRO:HB3	5:N:316:TYR:CZ	2.53	0.43
8:Q:838:VAL:O	8:Q:841:ARG:HG2	2.19	0.43
8:Q:880:TYR:HA	8:Q:883:PHE:HD2	1.84	0.43
10:S:906:ASN:ND2	10:S:909:LEU:HD12	2.33	0.43
10:S:1108:ASN:HB3	10:S:1112:TRP:CZ3	2.54	0.43
10:T:264:LEU:HG	10:T:372:ALA:HB1	2.00	0.43
10:T:1317:HIS:HE1	10:T:1398:ILE:HG23	1.84	0.43
1:A:475:SER:HB3	1:A:480:ARG:HB2	2.00	0.43
2:B:172:MET:HA	2:B:187:ASN:HA	2.01	0.43
2:B:285:HIS:HB3	2:B:338:THR:HB	2.00	0.43
2:B:306:ASN:OD1	2:B:306:ASN:N	2.51	0.43
2:B:359:VAL:HG12	2:B:369:VAL:HG12	2.01	0.43
4:D:480:GLN:OE1	4:D:488:ARG:NH2	2.52	0.43
7:G:283:ASN:HA	7:G:304:LYS:HB2	2.01	0.43
9:I:868:ARG:O	9:I:871:ARG:HG3	2.18	0.43
2:K:71:ASP:OD1	2:K:71:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:275:PHE:HB3	2:K:351:LEU:HD11	2.00	0.43
8:Q:681:LYS:HD2	8:Q:681:LYS:HA	1.83	0.43
10:T:1796:GLN:HG2	10:T:1801:SER:HB2	2.00	0.43
12:W:555:GLN:O	12:W:559:THR:OG1	2.34	0.43
12:Z:598:MET:HE2	12:Z:598:MET:HB3	1.77	0.43
14:b:261:GLU:OE2	14:b:337:LYS:NZ	2.43	0.43
2:B:47:VAL:H	2:B:68:GLN:HE22	1.65	0.43
3:C:96:LYS:HA	3:C:96:LYS:HD3	1.78	0.43
3:C:136:ASP:N	3:C:136:ASP:OD1	2.52	0.43
4:D:49:LEU:HB2	4:D:570:PHE:HB3	2.00	0.43
4:D:575:SER:HA	4:D:855:ALA:HB1	2.00	0.43
6:F:752:TRP:HB3	6:F:792:ILE:HD13	2.00	0.43
9:I:193:THR:HA	9:I:233:GLN:HB2	2.01	0.43
1:J:599:MET:HB3	1:J:637:LEU:HD11	2.01	0.43
8:Q:785:LYS:HA	8:Q:785:LYS:HD3	1.81	0.43
9:R:200:CYS:HA	9:R:215:SER:HA	2.01	0.43
10:S:67:VAL:HG21	10:S:105:GLU:HB3	2.00	0.43
10:S:831:ALA:O	10:S:833:PHE:N	2.51	0.43
10:T:1507:ARG:HG3	10:T:1508:GLN:HG2	2.00	0.43
11:U:380:VAL:HG11	11:U:392:TYR:HD2	1.84	0.43
12:V:714:LYS:HE3	12:V:752:LEU:HD22	2.01	0.43
12:Z:528:ARG:HD3	12:Z:528:ARG:HA	1.84	0.43
12:Z:563:ALA:HA	12:Z:567:HIS:CE1	2.54	0.43
14:b:395:HIS:CD2	14:b:396:VAL:H	2.36	0.43
1:A:141:GLU:O	1:A:145:ASN:ND2	2.52	0.43
2:B:214:ARG:HA	2:B:214:ARG:HD3	1.81	0.43
1:J:569:CYS:HA	1:J:572:TRP:HB2	2.00	0.43
3:L:124:LYS:HG3	10:T:1244:MET:HE2	2.01	0.43
4:M:333:ASP:HA	9:R:228:SER:HB2	2.01	0.43
4:M:461:LEU:HG	4:M:531:TRP:HE1	1.83	0.43
4:M:477:LYS:HD3	9:R:84:VAL:HG21	2.01	0.43
4:M:529:GLU:HG3	9:R:77:LEU:HB3	2.00	0.43
10:S:903:GLY:O	10:S:905:SER:N	2.52	0.43
10:T:455:GLU:HB3	10:T:458:LEU:HG	2.01	0.43
10:T:763:LEU:HD12	10:T:842:ALA:HB1	2.01	0.43
10:T:1042:ASP:HB3	10:T:1090:SER:HB3	2.01	0.43
10:T:1235:VAL:HG22	10:T:1253:LEU:HD21	2.00	0.43
12:Z:598:MET:HG3	12:Z:656:LEU:HD13	2.01	0.43
14:d:75:VAL:HG12	14:d:76:GLU:OE1	2.19	0.43
14:d:188:ASN:HB2	14:d:196:VAL:HG21	1.99	0.43
1:A:27:TRP:HE1	3:C:285:SER:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1277:THR:OG1	4:D:1278:THR:N	2.52	0.43
5:E:17:ASP:HB2	5:E:40:GLY:HA3	2.01	0.43
5:E:28:ASP:HB3	5:E:85:ARG:HH22	1.84	0.43
6:F:262:VAL:HG11	7:G:19:ALA:HB3	2.01	0.43
6:F:574:LEU:HD22	6:F:583:PHE:H	1.83	0.43
8:H:302:LEU:HB3	8:H:303:SER:H	1.54	0.43
4:M:147:THR:C	4:M:149:ASN:N	2.77	0.43
6:O:249:ARG:HH11	6:O:250:SER:N	2.17	0.43
8:Q:481:ASP:OD1	8:Q:481:ASP:N	2.52	0.43
9:R:121:LYS:HB3	9:R:131:MET:HB3	2.00	0.43
9:R:494:ASP:HB3	9:R:496:ARG:HH21	1.84	0.43
9:R:1092:LEU:HD22	9:R:1097:ILE:HG21	2.01	0.43
12:V:453:LEU:HD21	12:V:485:GLU:HG2	2.01	0.43
12:Y:525:ASP:OD1	12:Y:525:ASP:N	2.52	0.43
12:Z:308:TRP:CD1	12:Z:508:PRO:HB2	2.54	0.43
1:A:535:PHE:O	1:A:538:LYS:HG2	2.19	0.42
2:B:8:LYS:HG2	2:B:63:GLN:HB3	2.00	0.42
4:D:1380:LEU:HD13	6:F:245:LEU:HD21	2.01	0.42
6:F:609:SER:OG	6:F:610:GLU:N	2.52	0.42
8:H:186:ARG:HD2	8:H:186:ARG:HA	1.83	0.42
1:J:327:GLN:HB3	14:b:646:ARG:NE	2.33	0.42
2:K:36:GLY:HA3	2:K:78:VAL:HG11	2.01	0.42
5:N:232:TRP:CD1	5:N:249:ALA:HB2	2.45	0.42
7:P:219:TRP:HD1	7:P:220:ALA:H	1.66	0.42
9:R:320:ASP:OD1	9:R:320:ASP:N	2.49	0.42
9:R:929:GLU:HB3	9:R:933:ALA:HB2	2.01	0.42
10:S:1158:GLU:HB2	10:S:1162:ARG:HH21	1.84	0.42
10:S:1348:VAL:HG11	10:S:1383:ILE:HG23	2.01	0.42
10:T:703:ALA:O	10:T:706:GLN:HG3	2.19	0.42
10:T:995:LYS:HA	10:T:995:LYS:HD3	1.89	0.42
11:U:671:ILE:O	11:U:674:ARG:HG2	2.19	0.42
12:V:20:SER:HA	12:V:25:LYS:HE2	2.00	0.42
12:W:319:TYR:CZ	12:W:357:LEU:HD13	2.54	0.42
12:X:349:ASP:OD1	12:X:426:SER:OG	2.29	0.42
12:X:694:GLU:HA	12:X:698:LEU:HD21	2.01	0.42
12:Y:350:ARG:HE	12:Y:351:GLN:HE21	1.66	0.42
12:Z:490:ALA:HB2	12:Z:577:TRP:CZ2	2.54	0.42
15:f:413:ARG:HA	15:f:413:ARG:HD2	1.89	0.42
4:D:899:LEU:HD11	4:D:906:VAL:HG13	2.01	0.42
4:D:1041:CYS:SG	4:D:1077:HIS:NE2	2.91	0.42
4:D:1141:ILE:HD12	4:D:1141:ILE:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:262:ASP:OD1	7:G:262:ASP:N	2.50	0.42
9:I:564:ARG:HD2	9:I:564:ARG:HA	1.77	0.42
3:L:164:SER:OG	3:L:187:ASP:O	2.37	0.42
9:R:452:VAL:HG22	9:R:462:THR:HB	2.01	0.42
9:R:913:LEU:HD22	9:R:916:HIS:HB2	2.01	0.42
10:T:751:ARG:HB3	10:T:754:GLU:HG3	2.00	0.42
10:T:1555:LYS:HA	10:T:1555:LYS:HD2	1.81	0.42
10:T:1936:ASP:OD2	10:T:1947:ARG:NH2	2.52	0.42
12:X:537:LEU:HD11	12:X:551:ARG:HG3	2.01	0.42
12:Z:327:LYS:HA	12:Z:327:LYS:HD2	1.87	0.42
14:b:515:PRO:HB2	14:b:516:PHE:H	1.60	0.42
1:A:420:ASP:N	1:A:420:ASP:OD1	2.49	0.42
2:B:213:GLU:O	2:B:214:ARG:NH1	2.53	0.42
4:D:168:HIS:CG	4:D:169:PRO:HD2	2.55	0.42
6:F:581:CYS:HB3	12:Y:18:SER:HA	2.01	0.42
6:F:739:LYS:O	6:F:742:GLU:HG2	2.18	0.42
7:G:118:LEU:HD23	7:G:118:LEU:HA	1.85	0.42
9:I:212:ILE:HG12	9:I:222:ARG:HD2	2.01	0.42
1:J:441:PRO:HB3	3:L:23:HIS:HB3	2.01	0.42
4:M:344:LEU:HD21	4:M:357:LEU:HD22	2.01	0.42
4:M:560:VAL:HB	4:M:571:LEU:HB2	2.02	0.42
5:N:17:ASP:HB2	5:N:43:TYR:HE1	1.84	0.42
6:O:401:ASN:HB2	6:O:404:VAL:HB	2.00	0.42
8:Q:351:ASP:HA	8:Q:354:GLN:NE2	2.34	0.42
9:R:1013:PHE:O	9:R:1017:GLN:NE2	2.51	0.42
10:S:1749:GLU:OE1	10:S:1828:TYR:OH	2.37	0.42
10:T:1337:VAL:O	10:T:1341:THR:OG1	2.33	0.42
10:T:1638:LEU:HD22	10:T:1691:LEU:HD22	2.01	0.42
11:U:541:GLU:O	11:U:543:THR:N	2.52	0.42
12:V:236:GLN:O	12:V:240:VAL:HG23	2.19	0.42
12:W:270:VAL:O	12:W:272:GLY:N	2.52	0.42
12:W:312:ILE:HD12	12:W:361:LEU:HD22	2.02	0.42
12:X:717:LEU:HD13	12:X:745:LEU:HA	1.99	0.42
4:D:41:ASN:HB2	4:D:595:VAL:HG21	1.99	0.42
4:D:1109:ARG:HD2	10:S:483:ARG:HH12	1.85	0.42
5:E:151:ILE:HB	5:E:159:ILE:HB	2.01	0.42
8:H:349:MET:HE3	8:H:351:ASP:HB3	2.01	0.42
9:I:243:LEU:HB3	9:I:262:GLU:HA	2.02	0.42
1:J:13:ILE:HG13	1:J:16:LEU:H	1.85	0.42
1:J:479:ARG:O	1:J:480:ARG:NE	2.49	0.42
3:L:311:ASP:N	3:L:311:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:613:LEU:HD22	4:M:731:ASP:HB3	2.01	0.42
8:Q:206:GLN:O	8:Q:209:VAL:HG12	2.20	0.42
10:S:293:GLU:HA	10:S:296:LYS:HE3	2.00	0.42
10:S:929:LYS:HE2	10:S:929:LYS:HB2	1.84	0.42
10:S:1562:VAL:HG12	10:S:1572:LEU:HD11	2.00	0.42
10:T:1137:LEU:HD13	10:T:1305:ARG:HH22	1.84	0.42
10:T:1382:ASN:OD1	10:T:1382:ASN:N	2.52	0.42
10:T:1935:GLN:HG3	13:e:830:GLN:HB3	2.00	0.42
12:V:181:LEU:HB3	12:V:213:TYR:HD1	1.85	0.42
12:V:718:LYS:HZ2	12:V:766:ASN:H	1.67	0.42
12:X:76:VAL:HB	12:X:107:LEU:HD21	2.00	0.42
12:Y:453:LEU:HB2	12:Y:485:GLU:HG2	2.02	0.42
12:Z:280:VAL:HG13	12:Z:328:PRO:HB3	2.01	0.42
14:d:205:GLU:HG2	14:d:221:LEU:HD22	2.01	0.42
2:B:84:LEU:HD13	2:B:141:ILE:HG13	2.01	0.42
4:D:908:SER:HB3	4:D:940:GLU:HB2	2.00	0.42
6:F:323:LEU:HB3	6:F:324:PRO:HD3	2.01	0.42
7:G:239:VAL:HG12	7:G:259:LYS:HD3	2.01	0.42
9:I:742:ILE:HA	9:I:810:LEU:HD11	2.01	0.42
1:J:221:SER:O	1:J:225:ARG:NH1	2.53	0.42
2:K:18:ARG:NH1	2:K:81:MET:O	2.53	0.42
3:L:195:GLY:HA3	3:L:216:MET:HE2	2.02	0.42
4:M:54:ARG:HG2	4:M:712:SER:HB2	2.00	0.42
4:M:475:LEU:HD13	4:M:497:LEU:HD21	2.00	0.42
9:R:505:LYS:HD2	9:R:505:LYS:HA	1.70	0.42
9:R:1029:GLU:HG2	9:R:1088:VAL:HG23	2.01	0.42
9:R:1029:GLU:OE2	9:R:1091:ASN:ND2	2.46	0.42
10:S:311:HIS:CG	10:S:315:GLN:HE22	2.37	0.42
11:U:320:TRP:CG	11:U:388:LYS:HB2	2.54	0.42
12:Z:494:THR:HG22	12:Z:498:GLN:HE21	1.83	0.42
13:a:754:PHE:O	13:a:757:GLU:HG3	2.18	0.42
14:d:439:LEU:HB2	14:d:479:ARG:HH12	1.84	0.42
2:B:257:HIS:O	2:B:334:GLN:NE2	2.50	0.42
4:D:237:GLY:HA3	4:D:258:LYS:HG2	2.02	0.42
4:D:258:LYS:HB3	4:D:279:PRO:HG2	2.02	0.42
4:D:300:PHE:HB3	4:D:344:LEU:HD21	2.02	0.42
4:D:576:SER:O	4:D:579:HIS:ND1	2.49	0.42
4:D:1208:SER:HB3	10:S:464:THR:HG22	2.02	0.42
6:F:578:LEU:HD11	6:F:626:PRO:HG3	2.01	0.42
1:J:200:GLY:HA3	1:J:298:LEU:HD11	2.00	0.42
1:J:629:LYS:O	1:J:632:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:643:GLU:OE1	4:M:741:ARG:NH2	2.53	0.42
6:O:752:TRP:O	6:O:756:HIS:ND1	2.52	0.42
7:P:109:VAL:HG12	7:P:122:CYS:HA	2.00	0.42
8:Q:270:LYS:HE2	8:Q:270:LYS:HB3	1.91	0.42
8:Q:737:GLU:HG2	8:Q:820:MET:HG3	2.00	0.42
10:S:243:ARG:H	10:S:243:ARG:HG2	1.69	0.42
10:S:744:TYR:O	10:S:749:TYR:OH	2.32	0.42
10:T:930:ILE:HG23	10:T:999:LEU:HD21	2.01	0.42
11:U:328:ARG:HA	11:U:328:ARG:HD2	1.85	0.42
12:W:636:ASP:OD1	12:W:636:ASP:N	2.50	0.42
12:X:651:ILE:HD11	12:X:675:ASN:HB3	2.02	0.42
14:d:520:ILE:HD12	15:f:380:ALA:HB2	2.01	0.42
14:d:595:CYS:HA	15:f:404:MET:HE1	2.01	0.42
1:A:318:LYS:O	1:A:322:LEU:N	2.43	0.42
4:D:207:ILE:HA	4:D:208:PRO:HA	1.85	0.42
4:D:1125:LEU:HG	4:D:1129:ASN:HD21	1.84	0.42
6:F:345:PRO:HB2	6:F:643:ALA:HB2	2.01	0.42
9:I:136:LEU:HD13	9:I:136:LEU:HA	1.94	0.42
9:I:220:LEU:H	9:I:240:GLN:HG2	1.84	0.42
2:K:48:TRP:CE2	2:K:68:GLN:HB2	2.54	0.42
4:M:646:LEU:HD22	4:M:737:HIS:HB3	2.02	0.42
4:M:889:THR:HA	5:N:186:LYS:HD3	2.01	0.42
10:S:1916:THR:HG22	10:S:1954:VAL:HG13	2.01	0.42
10:T:598:LEU:HD12	10:T:598:LEU:HA	1.87	0.42
10:T:1902:ILE:O	10:T:1905:ARG:HG2	2.20	0.42
12:V:750:GLN:HA	12:V:771:THR:HG21	2.02	0.42
12:X:305:GLU:HB3	12:X:306:VAL:H	1.63	0.42
12:Y:345:GLU:HB3	12:Y:429:ILE:HG21	2.01	0.42
12:Z:433:ASP:OD1	12:Z:528:ARG:NH1	2.52	0.42
14:b:1:MET:SD	14:b:1:MET:N	2.79	0.42
14:b:129:LYS:HE2	14:b:129:LYS:HB2	1.79	0.42
15:c:433:THR:OG1	15:c:434:PRO:HD3	2.20	0.42
14:d:120:VAL:HG23	14:d:145:ILE:HB	2.01	0.42
14:d:509:LEU:HD13	15:f:394:GLY:HA3	2.00	0.42
1:A:94:ARG:HD2	1:A:97:GLN:NE2	2.35	0.42
4:D:450:ILE:HD12	4:D:450:ILE:HA	1.90	0.42
4:D:575:SER:OG	4:D:576:SER:N	2.53	0.42
4:D:1028:ARG:HD2	4:D:1028:ARG:HA	1.85	0.42
6:F:396:SER:HA	12:Z:10:ARG:HE	1.84	0.42
8:H:249:PHE:CE1	8:H:259:GLN:HG2	2.54	0.42
6:O:502:ARG:HA	6:O:505:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:807:SER:O	6:O:810:GLU:HG3	2.20	0.42
8:Q:182:LYS:HA	8:Q:185:LYS:HG2	2.02	0.42
8:Q:641:GLU:H	8:Q:689:LYS:HD2	1.84	0.42
8:Q:686:ILE:HG13	8:Q:687:MET:HE2	2.01	0.42
10:S:151:GLN:O	10:S:153:ARG:N	2.52	0.42
10:S:797:PRO:HG2	10:S:800:PHE:HB3	2.00	0.42
10:S:896:ILE:HD13	10:S:896:ILE:HA	1.89	0.42
10:T:1656:GLN:HG2	10:T:1710:PHE:HE1	1.85	0.42
11:U:563:GLY:O	11:U:569:ARG:NH2	2.53	0.42
12:W:97:THR:HG22	12:W:117:TRP:HB3	2.01	0.42
12:W:189:LEU:HD11	12:W:228:ILE:HD11	2.02	0.42
12:X:233:LEU:HB3	12:X:285:MET:HE3	2.01	0.42
12:X:240:VAL:HG13	12:X:244:LEU:HD12	2.02	0.42
12:Z:308:TRP:CE3	12:Z:510:ARG:NH2	2.87	0.42
12:Z:359:LEU:HD12	12:Z:359:LEU:HA	1.92	0.42
14:b:208:THR:HG23	14:b:209:THR:HG23	2.01	0.42
14:b:262:THR:O	14:b:262:THR:OG1	2.35	0.42
14:b:384:ASP:OD2	14:b:390:ARG:NE	2.53	0.42
14:b:477:ILE:HG21	14:b:534:LEU:HD21	2.02	0.42
14:b:604:GLU:HA	14:b:607:GLU:CD	2.44	0.42
13:e:772:MET:HE3	15:f:421:ILE:HD13	2.02	0.42
15:f:468:GLN:O	15:f:471:ARG:HG3	2.19	0.42
4:D:260:SER:H	4:D:265:ARG:HE	1.66	0.42
4:D:341:GLY:HA3	4:D:362:HIS:HB3	2.02	0.42
4:D:579:HIS:CE1	4:D:580:LEU:HG	2.54	0.42
9:I:411:THR:O	9:I:413:GLU:N	2.53	0.42
9:I:906:HIS:ND1	9:I:927:SER:OG	2.53	0.42
1:J:98:LEU:HD22	1:J:152:ILE:HG21	2.02	0.42
3:L:114:THR:HB	3:L:135:ALA:HB3	2.01	0.42
5:N:232:TRP:CZ2	5:N:247:LYS:HB2	2.54	0.42
6:O:499:GLN:H	8:Q:313:GLU:HG3	1.85	0.42
8:Q:613:LEU:HD13	8:Q:623:VAL:HG11	2.02	0.42
10:S:1042:ASP:OD1	10:S:1042:ASP:N	2.52	0.42
10:T:1043:VAL:HB	10:T:1044:ARG:H	1.67	0.42
10:T:1479:VAL:HG22	10:T:1482:ARG:HH21	1.84	0.42
10:T:1640:ALA:HA	10:T:1643:GLN:NE2	2.35	0.42
11:U:347:GLY:O	11:U:350:LYS:NZ	2.51	0.42
12:V:61:LYS:O	12:V:64:ARG:HG2	2.20	0.42
12:Z:558:LEU:HG	12:Z:562:ARG:HG2	2.01	0.42
12:Z:562:ARG:HD3	12:Z:562:ARG:HA	1.74	0.42
14:b:160:LEU:HA	14:b:179:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASP:HB3	1:A:6:VAL:H	1.55	0.42
4:D:61:PHE:CD1	4:D:129:ARG:HG3	2.54	0.42
4:D:169:PRO:HD3	4:D:174:ARG:HB3	2.02	0.42
6:F:800:LYS:HB3	6:F:838:TRP:HZ3	1.85	0.42
3:L:320:LYS:HD3	3:L:320:LYS:HA	1.93	0.42
4:M:126:ASN:N	4:M:126:ASN:OD1	2.53	0.42
7:P:160:PRO:HG3	7:P:221:PRO:HA	2.01	0.42
10:S:865:ARG:HA	10:S:865:ARG:HD3	1.84	0.42
10:S:1655:ILE:HG23	10:S:1675:LEU:HD13	2.02	0.42
10:S:1970:PHE:O	10:S:2007:ARG:NH2	2.52	0.42
12:V:139:LEU:HD13	12:V:149:GLN:HG3	2.02	0.42
12:X:237:CYS:SG	12:X:288:HIS:ND1	2.93	0.42
12:Z:44:LEU:O	12:Z:47:ARG:HG3	2.20	0.42
12:Z:530:TRP:CD1	12:Z:557:ASP:HB2	2.55	0.42
13:a:829:VAL:HG11	14:b:662:LEU:HD22	2.02	0.42
13:e:762:THR:HG23	13:e:766:ARG:CZ	2.50	0.42
2:B:1:MET:HA	2:B:373:LEU:HA	2.00	0.41
6:F:684:PRO:HD2	7:G:170:GLN:NE2	2.35	0.41
8:H:808:ILE:HG21	8:H:852:LEU:HD13	2.02	0.41
9:I:910:ALA:HB2	9:I:923:HIS:HE1	1.84	0.41
9:I:959:LYS:HA	9:I:979:ILE:HD13	2.02	0.41
4:M:539:LEU:O	4:M:543:GLU:HG2	2.20	0.41
4:M:903:GLN:HG2	4:M:904:VAL:HG23	2.02	0.41
9:R:149:LEU:HD12	9:R:170:ALA:HB3	2.02	0.41
9:R:1007:MET:HE1	9:R:1010:LEU:HD11	2.02	0.41
10:S:572:ASN:OD1	10:S:577:HIS:NE2	2.45	0.41
10:T:668:GLN:OE1	10:T:725:ARG:NH2	2.52	0.41
10:T:1697:ASP:HA	10:T:1700:MET:HB2	2.02	0.41
12:V:434:LEU:HB2	12:V:531:TRP:CG	2.55	0.41
12:Y:133:ARG:HH22	12:Y:166:TYR:HB3	1.85	0.41
12:Y:256:LEU:HD22	12:Y:296:LEU:HD13	2.02	0.41
12:Y:457:LEU:O	12:Y:461:PHE:HB2	2.20	0.41
14:b:517:GLU:H	14:b:517:GLU:HG3	1.66	0.41
14:d:439:LEU:HD11	14:d:534:LEU:HD13	2.02	0.41
14:d:465:THR:OG1	14:d:481:LEU:O	2.32	0.41
1:A:492:LYS:HE2	1:A:527:MET:HE1	2.01	0.41
2:B:285:HIS:HB2	2:B:340:LEU:HD11	2.01	0.41
4:D:49:LEU:HD12	4:D:570:PHE:HD2	1.86	0.41
4:D:491:ASP:N	4:D:491:ASP:OD1	2.53	0.41
4:D:540:GLN:OE1	9:I:440:ASN:ND2	2.53	0.41
4:D:978:VAL:HG12	4:D:1002:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:137:ASP:HB2	8:H:140:GLU:HG3	2.02	0.41
8:H:700:LYS:HD3	8:H:700:LYS:HA	1.92	0.41
9:I:177:ARG:HA	9:I:177:ARG:HD3	1.87	0.41
1:J:20:ASN:HD22	1:J:21:ARG:H	1.69	0.41
2:K:214:ARG:HA	2:K:238:MET:HE2	2.01	0.41
4:M:228:LEU:HD22	4:M:242:LYS:HG2	2.01	0.41
4:M:1054:TYR:HB2	4:M:1086:PHE:HZ	1.86	0.41
5:N:131:VAL:HG22	5:N:171:VAL:HG13	2.01	0.41
6:O:349:VAL:HG13	6:O:352:ILE:HD12	2.02	0.41
8:Q:755:PHE:CD2	11:U:809:ASN:HB3	2.55	0.41
10:S:917:LEU:HB3	10:S:987:LEU:HD13	2.02	0.41
10:T:906:ASN:HD22	10:T:909:LEU:HD12	1.85	0.41
10:T:1746:ASP:O	10:T:1749:GLU:HG2	2.19	0.41
12:V:192:GLU:OE2	12:V:193:ARG:NH1	2.54	0.41
12:V:558:LEU:HD12	12:V:558:LEU:HA	1.89	0.41
12:W:298:LEU:HD12	12:W:298:LEU:HA	1.88	0.41
12:W:352:SER:HB2	12:W:422:HIS:HB3	2.01	0.41
12:W:507:ASP:OD1	12:W:507:ASP:N	2.53	0.41
12:Z:567:HIS:HB2	12:Z:622:PRO:HB3	2.02	0.41
12:Z:609:LEU:HD23	12:Z:612:LEU:HD12	2.02	0.41
1:A:303:TYR:O	1:A:307:VAL:HG13	2.20	0.41
2:B:126:ASN:N	2:B:126:ASN:OD1	2.53	0.41
4:D:1278:THR:HG23	4:D:1279:LYS:HG2	2.03	0.41
5:E:87:ASP:OD1	5:E:87:ASP:N	2.53	0.41
6:F:592:LYS:HE3	6:F:592:LYS:HB3	1.89	0.41
1:J:8:PRO:HB2	3:L:325:PRO:HB3	2.01	0.41
1:J:218:ALA:HB1	1:J:225:ARG:HA	2.02	0.41
3:L:163:LEU:HD11	3:L:193:ILE:HG21	2.02	0.41
4:M:116:GLU:OE2	4:M:185:SER:OG	2.37	0.41
10:T:1135:ARG:HB2	10:T:1157:MET:H	1.84	0.41
10:T:1614:ARG:HA	10:T:1614:ARG:HD3	1.89	0.41
11:U:604:ARG:HD2	12:Y:566:LYS:HE2	2.02	0.41
12:V:479:ILE:HG12	12:V:484:LEU:HG	2.03	0.41
12:V:595:LYS:HA	12:V:595:LYS:HD2	1.89	0.41
12:Y:441:GLY:HA3	12:Y:492:VAL:HG21	2.01	0.41
12:Y:710:LEU:HB3	12:Y:752:LEU:HG	2.02	0.41
1:A:453:ARG:O	1:A:456:GLU:HG3	2.21	0.41
4:D:1040:LEU:HD23	4:D:1040:LEU:HA	1.87	0.41
6:F:324:PRO:HG2	6:F:632:ARG:HD2	2.03	0.41
3:L:10:ASP:OD1	3:L:10:ASP:N	2.53	0.41
4:M:343:LYS:HG3	4:M:397:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:456:PRO:HG2	4:M:528:ILE:HB	2.01	0.41
4:M:843:SER:O	4:M:850:ARG:NH1	2.53	0.41
4:M:997:ALA:HB1	4:M:1028:ARG:HG3	2.02	0.41
4:M:1321:PRO:HD2	4:M:1324:LEU:HD13	2.02	0.41
7:P:160:PRO:O	7:P:181:ARG:NH2	2.52	0.41
8:Q:651:LEU:HD12	11:U:654:ILE:HD11	2.03	0.41
9:R:98:PRO:O	9:R:145:TRP:NE1	2.54	0.41
10:T:1847:PRO:HA	10:T:1850:ILE:HG12	2.02	0.41
10:T:1938:PHE:HD1	10:T:1938:PHE:HA	1.77	0.41
11:U:250:GLN:O	11:U:253:MET:HG3	2.21	0.41
12:V:246:LYS:O	12:V:299:LYS:NZ	2.48	0.41
12:X:498:GLN:HG2	12:X:632:PHE:HE1	1.84	0.41
12:X:710:LEU:HD13	12:X:752:LEU:HG	2.02	0.41
12:Z:579:ARG:NH2	12:Z:733:SER:OG	2.54	0.41
14:b:46:ASN:H	14:b:100:GLU:HG2	1.85	0.41
14:b:185:ARG:HB3	14:b:187:TYR:HE1	1.85	0.41
2:B:287:ASP:O	2:B:294:LYS:NZ	2.39	0.41
8:H:249:PHE:CZ	8:H:256:ARG:HG3	2.55	0.41
4:M:123:LEU:HB2	4:M:126:ASN:ND2	2.35	0.41
5:N:174:HIS:HA	5:N:216:TRP:HZ2	1.86	0.41
6:O:252:ARG:NH1	6:O:253:VAL:O	2.54	0.41
6:O:803:LEU:HA	6:O:806:ILE:HG12	2.01	0.41
10:S:998:ASN:HD21	10:S:1001:MET:HE2	1.84	0.41
10:S:1711:GLN:HE22	10:S:1946:PRO:HB3	1.84	0.41
12:X:317:LEU:HD22	12:X:409:VAL:HG11	2.01	0.41
12:X:696:ASP:OD1	12:Y:589:ASN:ND2	2.53	0.41
12:Y:49:VAL:HG11	12:Y:66:LEU:HD13	2.02	0.41
12:Y:306:VAL:HB	12:Y:307:GLN:H	1.68	0.41
12:Y:359:LEU:HD23	12:Y:359:LEU:HA	1.92	0.41
12:Z:358:LEU:HD11	12:Z:365:LYS:HE2	2.03	0.41
14:b:412:LYS:HD3	14:b:412:LYS:HA	1.81	0.41
14:b:563:TYR:HB3	15:c:369:LEU:HD22	2.02	0.41
1:A:470:THR:O	1:A:473:MET:HG3	2.21	0.41
6:F:253:VAL:HG12	6:F:264:ASN:H	1.85	0.41
6:F:350:THR:O	6:F:353:HIS:NE2	2.53	0.41
1:J:207:MET:H	1:J:207:MET:HG3	1.62	0.41
4:M:242:LYS:HB2	4:M:253:THR:OG1	2.20	0.41
5:N:216:TRP:HB2	5:N:224:ILE:HG13	2.03	0.41
8:Q:264:TRP:CZ2	8:Q:268:ILE:HD11	2.56	0.41
10:S:898:ARG:HD2	10:S:898:ARG:HA	1.81	0.41
10:S:1781:PHE:O	10:S:1952:ASN:ND2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:609:GLU:OE1	10:T:612:ARG:NH1	2.54	0.41
10:T:1023:LEU:HD12	10:T:1023:LEU:HA	1.93	0.41
11:U:180:ASN:HA	11:U:183:MET:HE3	2.02	0.41
12:W:94:LYS:NZ	12:W:125:PHE:O	2.41	0.41
12:W:103:LEU:HD23	12:W:103:LEU:HA	1.87	0.41
12:W:672:SER:O	12:W:674:LYS:NZ	2.43	0.41
4:D:44:ARG:HH22	4:D:403:THR:HG21	1.86	0.41
4:D:373:GLN:HG3	4:D:385:GLU:HB3	2.02	0.41
4:D:797:LEU:HG	4:D:802:LEU:HD12	2.03	0.41
6:F:574:LEU:HB3	6:F:582:GLY:HA3	2.02	0.41
4:M:293:LEU:O	4:M:295:HIS:N	2.53	0.41
5:N:192:PHE:CD1	5:N:202:LEU:HB3	2.56	0.41
7:P:196:GLU:HB3	7:P:201:TRP:CD2	2.55	0.41
8:Q:842:ARG:HG2	8:Q:883:PHE:HE1	1.86	0.41
10:S:480:ALA:O	10:S:482:GLN:N	2.54	0.41
10:S:1059:LEU:HD23	10:S:1059:LEU:HA	1.77	0.41
10:T:1578:ILE:HD11	10:T:1629:ILE:HD11	2.02	0.41
12:X:618:LYS:HE3	12:X:618:LYS:HB3	1.83	0.41
14:d:46:ASN:HA	14:d:454:GLY:HA2	2.02	0.41
1:A:63:ILE:HD12	1:A:63:ILE:HA	1.90	0.41
1:A:535:PHE:HA	1:A:538:LYS:HD3	2.02	0.41
4:D:684:TYR:HB3	4:D:866:LEU:HD22	2.03	0.41
4:D:790:LEU:HD23	4:D:790:LEU:HA	1.95	0.41
4:D:1339:LEU:HD23	4:D:1339:LEU:HA	1.97	0.41
5:E:133:CYS:HB3	5:E:181:LEU:HD13	2.03	0.41
6:F:280:MET:HG2	6:F:305:HIS:HD2	1.86	0.41
8:H:571:LEU:HA	8:H:574:GLU:HG2	2.02	0.41
9:I:392:MET:O	9:I:396:GLN:NE2	2.53	0.41
9:I:415:ILE:HD11	9:I:441:ILE:HG12	2.03	0.41
1:J:548:GLN:NE2	1:J:550:GLN:HB2	2.35	0.41
2:K:274:LEU:HD13	2:K:334:GLN:NE2	2.36	0.41
4:M:55:GLU:HA	4:M:815:GLY:H	1.84	0.41
4:M:137:ILE:HA	4:M:157:THR:HG22	2.02	0.41
5:N:24:PHE:HB3	5:N:25:ASN:H	1.75	0.41
7:P:132:LEU:HD12	7:P:142:VAL:HG22	2.03	0.41
8:Q:902:LEU:HD13	8:Q:907:LEU:HD23	2.02	0.41
10:T:318:GLN:O	10:T:320:TRP:N	2.54	0.41
10:T:403:LYS:HD3	10:T:403:LYS:HA	1.91	0.41
11:U:491:VAL:HG11	11:U:536:TYR:CZ	2.56	0.41
12:W:100:ILE:HG21	12:W:117:TRP:CD1	2.56	0.41
12:Y:523:PHE:HB2	12:Y:524:THR:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:526:ARG:H	12:Y:526:ARG:HG2	1.72	0.41
14:d:47:LEU:HD22	14:d:58:TRP:HD1	1.84	0.41
14:d:238:LYS:HA	14:d:242:GLN:HE21	1.85	0.41
14:d:360:ALA:H	14:d:397:ALA:HB1	1.85	0.41
14:d:402:VAL:HG22	14:d:435:VAL:HG13	2.02	0.41
1:A:388:HIS:HB3	14:b:127:TRP:HZ3	1.86	0.41
1:A:542:PHE:HA	1:A:545:MET:HB2	2.02	0.41
2:B:162:ARG:HA	2:B:162:ARG:HD2	1.94	0.41
3:C:124:LYS:O	3:C:126:MET:N	2.54	0.41
4:D:413:TRP:HZ3	4:D:423:LYS:HB2	1.85	0.41
4:D:1070:ARG:NE	4:D:1147:GLY:O	2.48	0.41
4:D:1352:LEU:HD23	4:D:1352:LEU:HA	1.94	0.41
7:G:261:ASN:HB2	12:Y:58:ARG:HH11	1.86	0.41
9:I:301:ASP:HB3	9:I:304:ARG:HG2	2.01	0.41
9:I:495:SER:O	9:I:496:ARG:NE	2.54	0.41
9:I:852:ASP:OD1	9:I:852:ASP:N	2.54	0.41
9:I:930:PHE:HB3	9:I:965:SER:HA	2.03	0.41
1:J:4:LEU:HB3	1:J:5:ASP:H	1.68	0.41
1:J:71:LEU:HG	1:J:112:CYS:HB2	2.03	0.41
2:K:70:CYS:SG	2:K:71:ASP:N	2.94	0.41
2:K:242:TRP:HZ2	2:K:251:MET:HB2	1.86	0.41
4:M:619:TYR:HB2	4:M:657:ILE:HD13	2.03	0.41
4:M:1328:TYR:HD2	4:M:1336:LEU:HG	1.85	0.41
5:N:261:LYS:HB2	5:N:306:ARG:HA	2.01	0.41
6:O:670:LEU:HD12	6:O:673:TRP:HB2	2.03	0.41
6:O:672:GLU:HG2	6:O:714:LEU:HB2	2.03	0.41
7:P:115:ASP:HB3	7:P:161:SER:HB3	2.02	0.41
7:P:166:SER:HB2	7:P:227:THR:HA	2.03	0.41
8:Q:427:LYS:HA	8:Q:427:LYS:HD2	1.84	0.41
8:Q:501:GLU:OE2	8:Q:504:HIS:ND1	2.51	0.41
10:S:23:THR:HG23	10:S:35:ALA:HB1	2.03	0.41
10:S:183:THR:HB	10:S:248:LEU:HD11	2.03	0.41
10:S:807:LEU:HD23	10:S:876:LEU:HB2	2.03	0.41
10:S:1298:ASP:OD1	10:S:1298:ASP:N	2.41	0.41
10:S:1572:LEU:HD22	10:S:1577:VAL:HG21	2.02	0.41
10:S:1996:GLN:HG2	10:S:1997:ALA:N	2.35	0.41
10:T:13:LEU:HG	10:T:107:ALA:HB1	2.03	0.41
10:T:696:GLU:HB2	10:T:750:ARG:HE	1.85	0.41
10:T:930:ILE:HG21	10:T:999:LEU:HD11	2.03	0.41
10:T:1799:GLN:HB3	10:T:1800:VAL:H	1.56	0.41
11:U:287:VAL:HB	11:U:292:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:130:GLU:O	12:V:134:LEU:HG	2.21	0.41
12:V:313:GLU:HB2	12:V:314:PRO:HD3	2.03	0.41
12:W:71:GLU:HG3	12:W:103:LEU:HD21	2.02	0.41
12:Y:331:LYS:HD2	12:Y:340:GLN:HG2	2.03	0.41
12:Y:720:ILE:HD13	12:Y:720:ILE:HA	1.90	0.41
12:Z:267:LYS:HA	12:Z:270:VAL:HB	2.03	0.41
1:A:94:ARG:HA	1:A:97:GLN:NE2	2.35	0.41
3:C:11:HIS:CD2	3:C:15:ILE:HD13	2.55	0.41
4:D:54:ARG:HH12	4:D:816:ILE:HB	1.86	0.41
4:D:159:GLN:NE2	4:D:204:ILE:O	2.54	0.41
4:D:1178:GLU:HB3	4:D:1179:LEU:H	1.60	0.41
8:H:199:SER:HA	8:H:202:TRP:HD1	1.85	0.41
1:J:349:ALA:HB1	1:J:357:GLN:NE2	2.34	0.41
3:L:13:ASP:HB2	3:L:32:SER:HB2	2.03	0.41
3:L:124:LYS:O	3:L:126:MET:N	2.54	0.41
3:L:197:VAL:HB	3:L:215:LEU:HB2	2.03	0.41
4:M:510:GLN:HA	4:M:513:VAL:HG12	2.03	0.41
4:M:723:ALA:HA	4:M:775:ARG:HG3	2.03	0.41
4:M:1004:PHE:CZ	4:M:1036:LEU:HB2	2.56	0.41
4:M:1369:GLY:O	4:M:1371:GLN:NE2	2.54	0.41
6:O:344:ARG:HA	6:O:344:ARG:HD3	1.89	0.41
8:Q:695:LYS:HG3	8:Q:698:ALA:HB3	2.03	0.41
9:R:269:LEU:HD21	9:R:337:GLN:HB2	2.03	0.41
10:S:816:CYS:O	10:S:819:LEU:HG	2.21	0.41
10:T:988:LEU:HD23	10:T:1000:ALA:HA	2.02	0.41
11:U:639:VAL:O	11:U:642:LEU:HG	2.21	0.41
12:V:120:ARG:HE	12:V:124:LEU:HG	1.86	0.41
12:W:9:GLN:HG3	12:W:39:ALA:HB1	2.03	0.41
12:W:321:LEU:O	12:W:324:GLN:HG3	2.21	0.41
12:Y:307:GLN:HB3	12:Y:310:ALA:HB3	2.03	0.41
12:Z:320:LEU:HD21	12:Z:369:ILE:HG23	2.03	0.41
15:c:535:ARG:HA	15:c:535:ARG:HD2	1.94	0.41
2:B:20:ARG:HH21	2:B:30:PRO:HB3	1.86	0.40
3:C:19:SER:HB2	3:C:63:VAL:HG13	2.02	0.40
4:D:1125:LEU:O	4:D:1129:ASN:ND2	2.54	0.40
6:F:673:TRP:HA	6:F:676:PHE:CD1	2.55	0.40
8:H:283:TYR:HE1	10:T:1996:GLN:HB3	1.86	0.40
9:I:690:VAL:HG21	9:I:762:VAL:HG13	2.03	0.40
9:I:872:TYR:HD1	9:I:872:TYR:HA	1.76	0.40
2:K:329:ASP:OD1	2:K:329:ASP:N	2.51	0.40
4:M:1046:LEU:HD11	4:M:1077:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:253:VAL:HA	6:O:264:ASN:HB3	2.03	0.40
8:Q:254:LEU:HA	8:Q:257:GLN:NE2	2.35	0.40
8:Q:501:GLU:H	8:Q:501:GLU:HG2	1.61	0.40
9:R:654:ILE:HG22	9:R:671:ALA:HB1	2.03	0.40
10:S:579:ARG:HH21	10:S:640:LYS:HD3	1.86	0.40
10:S:1000:ALA:O	10:S:1003:LEU:HD23	2.20	0.40
10:T:1175:LYS:HA	10:T:1178:ARG:HD3	2.02	0.40
12:W:30:PHE:CZ	12:W:61:LYS:HB3	2.56	0.40
12:Y:170:LYS:HD3	12:Y:170:LYS:HA	1.88	0.40
14:b:41:ASP:HA	14:b:396:VAL:HG11	2.02	0.40
14:d:409:LYS:HE3	14:d:423:SER:HB3	2.03	0.40
1:A:106:ARG:HH22	1:A:141:GLU:HG2	1.85	0.40
3:C:303:ARG:HE	3:C:305:TRP:HZ2	1.68	0.40
4:D:122:ASN:HB2	4:D:707:SER:HB3	2.03	0.40
4:D:138:LEU:HD22	4:D:212:PRO:HG2	2.03	0.40
6:F:538:HIS:O	6:F:542:MET:HB2	2.21	0.40
7:G:257:LEU:HB3	7:G:258:HIS:H	1.65	0.40
8:H:614:GLU:HA	8:H:617:LYS:HG2	2.03	0.40
9:I:995:LYS:HD2	9:I:995:LYS:HA	1.91	0.40
1:J:218:ALA:HB2	1:J:228:CYS:HB2	2.03	0.40
4:M:519:SER:HB2	4:M:522:GLU:HG3	2.03	0.40
4:M:1306:HIS:CE1	4:M:1310:ILE:HD13	2.57	0.40
4:M:1430:LYS:HA	4:M:1430:LYS:HD3	1.91	0.40
5:N:190:ILE:HB	5:N:204:LEU:HB3	2.03	0.40
6:O:263:HIS:ND1	6:O:305:HIS:O	2.54	0.40
8:Q:375:TYR:HE2	8:Q:393:PRO:HD3	1.86	0.40
8:Q:611:ARG:HA	8:Q:611:ARG:HD2	1.87	0.40
10:S:857:GLU:OE2	10:S:923:ASN:ND2	2.54	0.40
10:S:1684:LEU:HB3	10:S:1769:GLN:HE21	1.86	0.40
10:T:985:LEU:HA	10:T:988:LEU:HD12	2.03	0.40
11:U:201:LEU:HB3	12:Y:553:VAL:HG22	2.03	0.40
11:U:786:LEU:HB3	11:U:819:MET:HB3	2.02	0.40
12:X:345:GLU:HG3	12:X:429:ILE:HG21	2.03	0.40
2:B:79:MET:HE3	2:B:79:MET:HB3	1.96	0.40
4:D:357:LEU:HD13	4:D:384:LEU:HD22	2.04	0.40
4:D:423:LYS:HG2	4:D:437:PRO:HA	2.02	0.40
4:D:493:SER:HB3	4:D:496:GLU:HB2	2.03	0.40
4:D:581:TYR:HA	4:D:610:ILE:HG23	2.02	0.40
4:D:958:ARG:NH2	4:D:962:TYR:OH	2.54	0.40
6:F:296:SER:O	6:F:298:THR:N	2.55	0.40
8:H:577:ILE:O	8:H:580:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:635:ARG:HH21	8:H:686:ILE:HG21	1.86	0.40
9:I:157:GLY:H	9:I:207:LYS:HA	1.87	0.40
3:L:187:ASP:N	3:L:187:ASP:OD1	2.53	0.40
4:M:241:ILE:HD13	4:M:241:ILE:HA	1.92	0.40
4:M:1344:ASP:OD1	6:O:296:SER:OG	2.26	0.40
5:N:103:LYS:HD3	5:N:103:LYS:HA	1.92	0.40
6:O:627:ASP:HB3	6:O:629:LEU:HD13	2.04	0.40
9:R:280:THR:OG1	9:R:281:ASP:N	2.54	0.40
9:R:579:THR:H	9:R:583:LEU:HD12	1.86	0.40
10:S:311:HIS:CD2	10:S:315:GLN:HE22	2.39	0.40
10:S:982:ILE:HD13	10:S:1059:LEU:HD12	2.03	0.40
10:S:1072:ASP:OD1	10:S:1072:ASP:N	2.41	0.40
10:S:1281:LEU:O	10:S:1285:ARG:HG2	2.21	0.40
10:S:1752:MET:HE3	10:S:1752:MET:HB3	1.80	0.40
10:T:39:LEU:HD21	10:T:149:LEU:HD21	2.03	0.40
10:T:1277:LYS:NZ	10:T:1324:ASP:O	2.43	0.40
10:T:1885:ARG:HD3	10:T:1885:ARG:HA	1.93	0.40
11:U:457:ASN:OD1	11:U:457:ASN:N	2.53	0.40
12:V:490:ALA:HB1	12:V:628:LEU:HD13	2.03	0.40
12:Y:623:GLU:HA	12:Y:624:PRO:HD3	1.98	0.40
12:Z:563:ALA:HA	12:Z:567:HIS:HE1	1.86	0.40
14:b:97:ASP:OD1	14:b:97:ASP:N	2.38	0.40
14:b:638:LEU:HD23	14:b:638:LEU:HA	1.95	0.40
14:b:728:PHE:HD1	14:b:728:PHE:HA	1.78	0.40
1:A:476:LEU:HD13	1:A:500:ILE:HG22	2.03	0.40
2:B:267:HIS:HB3	2:B:273:HIS:HB2	2.04	0.40
5:E:308:LEU:O	5:E:310:LEU:N	2.54	0.40
8:H:395:ARG:H	8:H:395:ARG:HG2	1.72	0.40
9:I:104:HIS:HB2	9:I:108:TRP:HB2	2.02	0.40
1:J:103:ARG:NH2	1:J:145:ASN:OD1	2.54	0.40
1:J:168:VAL:O	1:J:172:VAL:HB	2.20	0.40
2:K:11:SER:HA	2:K:365:GLU:HB3	2.02	0.40
4:M:104:HIS:NE2	4:M:115:VAL:HB	2.37	0.40
4:M:552:VAL:HB	4:M:561:CYS:HB2	2.04	0.40
8:Q:224:SER:O	8:Q:228:GLU:HG2	2.20	0.40
8:Q:721:GLN:HE21	8:Q:723:MET:HB3	1.85	0.40
9:R:1039:LEU:HA	9:R:1042:ILE:HD12	2.03	0.40
9:R:1058:LEU:HD13	9:R:1085:PHE:HE1	1.87	0.40
10:S:366:PHE:HE2	10:S:435:ASP:HB3	1.86	0.40
10:S:1804:PRO:HA	10:S:1944:MET:HE1	2.02	0.40
10:S:1949:LEU:HB2	10:S:1950:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:352:ALA:C	10:T:355:PRO:HD2	2.46	0.40
12:V:233:LEU:HD11	12:V:266:VAL:HG21	2.02	0.40
12:Y:566:LYS:HD3	12:Y:566:LYS:HA	1.87	0.40
12:Z:236:GLN:O	12:Z:240:VAL:HG23	2.22	0.40
14:d:184:LEU:HB2	14:d:199:ILE:HB	2.04	0.40
2:B:13:LYS:HE2	2:B:13:LYS:HB2	1.95	0.40
5:E:96:ALA:HA	5:E:106:ILE:HA	2.03	0.40
6:F:325:LEU:HB3	6:F:673:TRP:CD1	2.56	0.40
6:F:686:VAL:HG22	7:G:162:VAL:HB	2.04	0.40
9:I:148:ASP:HB2	9:I:202:PHE:HD1	1.86	0.40
1:J:184:ARG:HD3	1:J:184:ARG:HA	1.92	0.40
2:K:15:SER:OG	2:K:16:ARG:N	2.50	0.40
3:L:305:TRP:HB3	3:L:313:TRP:HB3	2.03	0.40
4:M:1119:LYS:HA	4:M:1119:LYS:HD2	1.87	0.40
6:O:389:GLN:NE2	6:O:394:GLU:HG3	2.34	0.40
8:Q:210:THR:HG22	8:Q:507:GLN:HG2	2.03	0.40
8:Q:308:ARG:O	8:Q:310:LEU:N	2.54	0.40
9:R:200:CYS:HB3	9:R:213:LEU:HD11	2.04	0.40
9:R:398:VAL:HG12	9:R:408:TYR:HB2	2.04	0.40
10:S:1078:MET:SD	10:S:1082:ARG:NH2	2.94	0.40
12:V:21:SER:HB3	12:V:24:GLU:HB2	2.04	0.40
12:X:734:LEU:HD23	12:X:735:PRO:HD2	2.03	0.40
12:Y:189:LEU:HD23	12:Y:189:LEU:HA	1.91	0.40
14:b:543:PRO:HB3	15:c:355:TYR:CE2	2.57	0.40
14:d:303:LEU:HA	14:d:304:PRO:HD3	1.96	0.40
14:d:321:HIS:NE2	14:d:391:TYR:OH	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	651/653 (100%)	584 (90%)	60 (9%)	7 (1%)	11	46
1	J	651/653 (100%)	590 (91%)	53 (8%)	8 (1%)	10	44
2	B	373/375 (100%)	300 (80%)	64 (17%)	9 (2%)	4	27
2	K	373/375 (100%)	306 (82%)	53 (14%)	14 (4%)	2	19
3	C	331/360 (92%)	286 (86%)	40 (12%)	5 (2%)	8	40
3	L	323/360 (90%)	268 (83%)	49 (15%)	6 (2%)	6	32
4	D	1392/1414 (98%)	1227 (88%)	144 (10%)	21 (2%)	8	40
4	M	1392/1414 (98%)	1254 (90%)	125 (9%)	13 (1%)	14	51
5	E	324/326 (99%)	275 (85%)	46 (14%)	3 (1%)	14	51
5	N	324/326 (99%)	273 (84%)	45 (14%)	6 (2%)	6	32
6	F	636/924 (69%)	530 (83%)	91 (14%)	15 (2%)	4	27
6	O	635/924 (69%)	560 (88%)	68 (11%)	7 (1%)	11	46
7	G	292/320 (91%)	251 (86%)	35 (12%)	6 (2%)	5	30
7	P	292/320 (91%)	235 (80%)	50 (17%)	7 (2%)	4	27
8	H	796/916 (87%)	736 (92%)	53 (7%)	7 (1%)	14	51
8	Q	788/916 (86%)	704 (89%)	75 (10%)	9 (1%)	11	46
9	I	1074/1140 (94%)	926 (86%)	131 (12%)	17 (2%)	7	38
9	R	1080/1140 (95%)	957 (89%)	113 (10%)	10 (1%)	14	51
10	S	2009/2011 (100%)	1790 (89%)	193 (10%)	26 (1%)	9	42
10	T	2009/2011 (100%)	1815 (90%)	171 (8%)	23 (1%)	11	46
11	U	652/820 (80%)	593 (91%)	51 (8%)	8 (1%)	10	44
12	V	770/2931 (26%)	702 (91%)	59 (8%)	9 (1%)	10	44
12	W	754/2931 (26%)	690 (92%)	57 (8%)	7 (1%)	14	51
12	X	765/2931 (26%)	698 (91%)	62 (8%)	5 (1%)	18	56
12	Y	759/2931 (26%)	699 (92%)	49 (6%)	11 (1%)	9	40
12	Z	756/2931 (26%)	688 (91%)	58 (8%)	10 (1%)	9	42
13	a	207/2037 (10%)	202 (98%)	5 (2%)	0	100	100
13	e	153/2037 (8%)	149 (97%)	3 (2%)	1 (1%)	18	56
14	b	726/728 (100%)	653 (90%)	65 (9%)	8 (1%)	11	46
14	d	681/728 (94%)	609 (89%)	65 (10%)	7 (1%)	12	49
15	c	196/547 (36%)	192 (98%)	4 (2%)	0	100	100
15	f	136/547 (25%)	136 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	22300/38977 (57%)	19878 (89%)	2137 (10%)	285 (1%)	12 42

All (285) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	178	ILE
4	D	565	LYS
9	R	837	LEU
11	U	203	PRO
12	W	271	SER
12	Z	197	ARG
14	b	515	PRO
2	B	61	GLU
2	B	302	ARG
3	C	124	LYS
3	C	125	HIS
4	D	109	ALA
4	D	187	PHE
4	D	1363	LYS
6	F	297	LEU
6	F	508	LEU
6	F	684	PRO
9	I	159	PRO
9	I	385	PRO
9	I	400	PRO
9	I	473	PRO
1	J	588	VAL
2	K	235	GLN
2	K	299	LEU
2	K	355	GLY
3	L	124	LYS
3	L	125	HIS
4	M	68	PRO
4	M	109	ALA
4	M	148	GLN
4	M	294	ASP
4	M	874	PRO
4	M	1363	LYS
5	N	229	GLY
7	P	107	ASN
9	R	114	ASN
9	R	400	PRO

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Mol	Chain	Res	Type
10	S	609	GLU
10	T	401	PRO
10	T	903	GLY
10	T	1047	PRO
10	T	1084	SER
10	T	1355	PRO
12	W	699	PRO
12	X	726	ALA
12	Y	142	GLN
12	Y	218	GLN
12	Z	735	PRO
14	b	640	VAL
1	A	590	PHE
2	B	56	THR
2	B	60	GLU
2	B	269	SER
2	B	292	SER
3	C	258	SER
3	C	279	SER
4	D	261	SER
4	D	319	LEU
4	D	557	THR
4	D	636	GLN
5	E	275	LYS
5	E	277	LYS
6	F	448	GLY
6	F	523	ILE
6	F	526	CYS
7	G	248	ALA
8	H	136	GLU
9	I	751	THR
9	I	832	SER
1	J	40	GLN
1	J	156	PRO
2	K	248	LYS
3	L	13	ASP
3	L	288	ILE
4	M	953	GLU
5	N	239	ARG
8	Q	818	GLY
9	R	290	ASP
9	R	1049	ASP

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Mol	Chain	Res	Type
10	S	156	LYS
10	S	382	ASP
10	S	481	HIS
10	S	904	ASN
10	S	1542	GLN
10	T	1024	GLY
10	T	1196	PRO
10	T	1448	TRP
10	T	1544	PRO
10	T	1988	VAL
10	T	1992	HIS
11	U	542	PRO
11	U	621	GLY
12	V	74	GLY
12	V	661	GLY
12	W	506	ALA
12	X	568	GLY
12	Y	523	PHE
12	Y	626	ASP
12	Z	74	GLY
12	Z	473	SER
12	Z	755	ALA
14	b	491	PRO
14	b	525	ARG
14	d	115	SER
14	d	116	LYS
14	d	430	GLU
1	A	10	GLU
2	B	226	GLN
4	D	556	ASN
4	D	940	GLU
4	D	1371	GLN
6	F	284	ASP
6	F	285	TYR
6	F	595	SER
6	F	837	LYS
7	G	212	ASP
8	H	362	GLN
9	I	114	ASN
9	I	255	GLY
9	I	465	ALA
1	J	392	PHE

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Mol	Chain	Res	Type
1	J	395	ASN
2	K	15	SER
2	K	203	ASP
2	K	257	HIS
2	K	290	ALA
2	K	316	ASN
3	L	111	ASP
5	N	276	MET
6	O	369	VAL
6	O	475	SER
6	O	738	ASP
7	P	44	ASN
7	P	55	GLY
7	P	61	TRP
8	Q	240	SER
8	Q	309	PRO
8	Q	327	ASP
8	Q	501	GLU
8	Q	605	ASP
8	Q	884	SER
9	R	174	GLY
9	R	968	GLN
10	S	300	MET
10	S	317	THR
10	S	433	ARG
10	S	471	SER
10	S	478	GLY
10	S	835	GLY
10	T	53	LEU
10	T	382	ASP
10	T	1043	VAL
10	T	1243	GLY
10	T	1431	ALA
10	T	1696	ASN
11	U	176	SER
11	U	365	SER
11	U	503	LEU
12	V	59	ASP
12	V	128	SER
12	V	404	ASP
12	Y	128	SER
12	Y	502	ASN

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Mol	Chain	Res	Type
12	Y	699	PRO
12	Z	59	ASP
12	Z	590	SER
14	d	76	GLU
14	d	420	ASP
1	A	156	PRO
1	A	275	ASN
1	A	549	GLU
2	B	138	SER
2	B	329	ASP
4	D	294	ASP
4	D	1144	PRO
4	D	1333	ALA
6	F	287	PHE
6	F	511	GLY
8	H	188	THR
8	H	727	LEU
9	I	82	LEU
9	I	260	ALA
9	I	328	ILE
9	I	391	GLY
9	I	412	GLN
9	I	570	PRO
9	I	576	PHE
1	J	414	LEU
1	J	549	GLU
2	K	312	ILE
3	L	308	ASN
4	M	134	ASN
4	M	197	ASP
4	M	435	TRP
4	M	1333	ALA
5	N	316	TYR
6	O	339	PRO
6	O	630	ASP
7	P	113	PRO
7	P	114	HIS
7	P	136	GLY
8	Q	728	PRO
8	Q	816	ASP
10	S	152	ALA
10	S	206	ARG

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Mol	Chain	Res	Type
10	S	1413	PHE
10	S	1544	PRO
10	S	1783	PRO
10	T	1294	ALA
10	T	1453	ALA
10	T	1939	ASN
11	U	681	SER
12	V	21	SER
12	V	466	GLN
12	W	59	ASP
12	Y	276	SER
12	Z	366	GLN
12	Z	513	CYS
14	b	108	HIS
14	d	438	ILE
14	d	504	ILE
1	A	526	ALA
3	C	59	SER
4	D	171	ARG
4	D	1024	PRO
5	E	72	GLY
6	F	619	LEU
7	G	215	ARG
7	G	262	ASP
8	H	147	TYR
8	H	459	SER
8	H	605	ASP
1	J	568	PRO
2	K	31	ASP
2	K	288	ALA
5	N	90	LEU
5	N	243	PRO
6	O	451	SER
10	S	58	PRO
10	S	832	PRO
10	S	1609	PRO
12	V	699	PRO
12	W	272	GLY
12	X	275	ALA
12	Y	306	VAL
14	b	210	LEU
13	e	695	ASN

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Mol	Chain	Res	Type
4	D	74	ILE
6	F	447	GLY
6	F	473	VAL
2	K	65	ASP
2	K	190	GLY
6	O	461	GLY
9	R	666	PRO
10	S	1024	GLY
10	T	1155	GLY
10	T	1861	GLY
12	W	128	SER
12	Y	219	GLY
12	Y	272	GLY
12	Z	622	PRO
1	A	287	GLY
4	D	921	GLY
4	M	974	LEU
10	S	727	PRO
11	U	774	ARG
12	X	335	GLY
12	X	637	ILE
14	b	514	GLY
4	D	974	LEU
9	I	98	PRO
4	M	921	GLY
9	R	61	VAL
10	S	1047	PRO
10	S	1591	PRO
12	V	429	ILE
14	b	75	VAL
7	G	55	GLY
7	G	224	GLY
9	R	570	PRO
10	S	682	VAL
10	S	882	GLY
10	T	1793	GLY
12	W	74	GLY
4	D	70	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/580 (100%)	564 (97%)	16 (3%)	38	60
1	J	580/580 (100%)	565 (97%)	15 (3%)	40	62
2	B	329/329 (100%)	322 (98%)	7 (2%)	47	65
2	K	329/329 (100%)	325 (99%)	4 (1%)	63	75
3	C	288/309 (93%)	283 (98%)	5 (2%)	53	69
3	L	282/309 (91%)	273 (97%)	9 (3%)	34	56
4	D	1230/1244 (99%)	1204 (98%)	26 (2%)	47	65
4	M	1230/1244 (99%)	1206 (98%)	24 (2%)	48	66
5	E	275/275 (100%)	270 (98%)	5 (2%)	51	68
5	N	275/275 (100%)	265 (96%)	10 (4%)	31	52
6	F	564/816 (69%)	542 (96%)	22 (4%)	28	49
6	O	563/816 (69%)	547 (97%)	16 (3%)	38	60
7	G	250/272 (92%)	242 (97%)	8 (3%)	34	56
7	P	250/272 (92%)	245 (98%)	5 (2%)	48	66
8	H	712/816 (87%)	697 (98%)	15 (2%)	47	65
8	Q	705/816 (86%)	675 (96%)	30 (4%)	26	47
9	I	944/993 (95%)	929 (98%)	15 (2%)	55	70
9	R	950/993 (96%)	925 (97%)	25 (3%)	40	62
10	S	1779/1779 (100%)	1753 (98%)	26 (2%)	57	72
10	T	1779/1779 (100%)	1740 (98%)	39 (2%)	45	64
11	U	577/721 (80%)	573 (99%)	4 (1%)	76	81
12	V	692/2545 (27%)	678 (98%)	14 (2%)	48	66
12	W	677/2545 (27%)	670 (99%)	7 (1%)	68	78
12	X	687/2545 (27%)	681 (99%)	6 (1%)	70	79
12	Y	682/2545 (27%)	672 (98%)	10 (2%)	57	72
12	Z	679/2545 (27%)	670 (99%)	9 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	a	195/1634 (12%)	194 (100%)	1 (0%)	81 83
13	e	143/1634 (9%)	141 (99%)	2 (1%)	59 72
14	b	660/660 (100%)	647 (98%)	13 (2%)	48 66
14	d	617/660 (94%)	612 (99%)	5 (1%)	73 80
15	c	179/429 (42%)	175 (98%)	4 (2%)	45 64
15	f	126/429 (29%)	126 (100%)	0	100 100
All	All	19808/33718 (59%)	19411 (98%)	397 (2%)	48 66

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	68	LEU
1	A	74	GLU
1	A	97	GLN
1	A	105	TYR
1	A	121	GLU
1	A	137	LEU
1	A	166	GLU
1	A	264	GLU
1	A	276	VAL
1	A	327	GLN
1	A	417	LEU
1	A	462	GLU
1	A	541	GLU
1	A	548	GLN
1	A	580	LEU
2	B	50	THR
2	B	99	THR
2	B	104	HIS
2	B	123	VAL
2	B	274	LEU
2	B	328	THR
2	B	353	VAL
3	C	63	VAL
3	C	105	LYS
3	C	257	LEU
3	C	270	THR
3	C	316	ILE
4	D	64	LEU

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Mol	Chain	Res	Type
4	D	106	THR
4	D	165	ILE
4	D	178	ILE
4	D	188	THR
4	D	203	VAL
4	D	371	VAL
4	D	401	THR
4	D	510	GLN
4	D	579	HIS
4	D	624	MET
4	D	698	ARG
4	D	708	VAL
4	D	785	VAL
4	D	822	LEU
4	D	927	LEU
4	D	1037	VAL
4	D	1050	VAL
4	D	1054	TYR
4	D	1074	LEU
4	D	1150	TYR
4	D	1174	ILE
4	D	1238	LEU
4	D	1335	GLU
4	D	1351	GLU
4	D	1391	LEU
5	E	31	GLU
5	E	84	THR
5	E	182	MET
5	E	207	VAL
5	E	227	VAL
6	F	253	VAL
6	F	272	LEU
6	F	334	VAL
6	F	365	GLU
6	F	369	VAL
6	F	372	VAL
6	F	380	TRP
6	F	427	GLU
6	F	446	THR
6	F	471	GLN
6	F	483	THR
6	F	494	VAL

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Mol	Chain	Res	Type
6	F	502	ARG
6	F	503	LEU
6	F	508	LEU
6	F	529	LEU
6	F	532	LYS
6	F	638	TRP
6	F	657	LEU
6	F	670	LEU
6	F	676	PHE
6	F	750	HIS
7	G	109	VAL
7	G	179	ILE
7	G	191	VAL
7	G	197	GLU
7	G	228	SER
7	G	229	THR
7	G	256	LEU
7	G	302	VAL
8	H	197	THR
8	H	202	TRP
8	H	209	VAL
8	H	260	LEU
8	H	469	LEU
8	H	479	THR
8	H	490	THR
8	H	596	TYR
8	H	668	TRP
8	H	687	MET
8	H	691	LEU
8	H	815	VAL
8	H	837	MET
8	H	870	ASP
8	H	907	LEU
9	I	136	LEU
9	I	150	VAL
9	I	165	VAL
9	I	168	MET
9	I	261	VAL
9	I	268	VAL
9	I	275	CYS
9	I	299	ASN
9	I	344	ILE

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Mol	Chain	Res	Type
9	I	411	THR
9	I	665	VAL
9	I	684	ILE
9	I	760	ARG
9	I	887	ARG
9	I	1113	GLU
1	J	20	ASN
1	J	63	ILE
1	J	87	GLU
1	J	98	LEU
1	J	120	SER
1	J	142	LEU
1	J	203	LEU
1	J	283	ARG
1	J	301	THR
1	J	331	ASP
1	J	332	MET
1	J	390	LEU
1	J	548	GLN
1	J	584	GLU
1	J	613	THR
2	K	118	GLN
2	K	241	ILE
2	K	244	VAL
2	K	291	ASP
3	L	60	VAL
3	L	63	VAL
3	L	114	THR
3	L	182	ILE
3	L	225	ILE
3	L	271	VAL
3	L	284	VAL
3	L	293	LEU
3	L	308	ASN
4	M	173	TYR
4	M	355	LEU
4	M	397	LEU
4	M	402	PHE
4	M	425	ILE
4	M	430	ASN
4	M	471	THR
4	M	481	ILE

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Mol	Chain	Res	Type
4	M	529	GLU
4	M	559	MET
4	M	628	MET
4	M	781	LEU
4	M	812	TYR
4	M	876	PHE
4	M	904	VAL
4	M	1010	MET
4	M	1111	VAL
4	M	1198	HIS
4	M	1214	MET
4	M	1228	ILE
4	M	1234	PHE
4	M	1275	VAL
4	M	1355	GLU
4	M	1405	GLN
5	N	12	THR
5	N	131	VAL
5	N	207	VAL
5	N	216	TRP
5	N	233	ILE
5	N	234	ILE
5	N	235	TRP
5	N	292	LEU
5	N	293	ILE
5	N	298	VAL
6	O	304	VAL
6	O	328	GLU
6	O	349	VAL
6	O	399	GLU
6	O	427	GLU
6	O	438	ILE
6	O	439	GLU
6	O	472	MET
6	O	508	LEU
6	O	579	GLU
6	O	618	LEU
6	O	633	LEU
6	O	635	TRP
6	O	714	LEU
6	O	749	SER
6	O	763	LEU

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Mol	Chain	Res	Type
7	P	50	ILE
7	P	182	PHE
7	P	191	VAL
7	P	292	VAL
7	P	296	TRP
8	Q	131	VAL
8	Q	169	TYR
8	Q	176	GLN
8	Q	191	GLN
8	Q	205	GLN
8	Q	257	GLN
8	Q	310	LEU
8	Q	324	LEU
8	Q	338	LEU
8	Q	354	GLN
8	Q	415	GLU
8	Q	429	LEU
8	Q	432	VAL
8	Q	467	ASN
8	Q	486	GLU
8	Q	501	GLU
8	Q	504	HIS
8	Q	524	GLU
8	Q	534	LEU
8	Q	553	LEU
8	Q	571	LEU
8	Q	584	VAL
8	Q	613	LEU
8	Q	701	GLU
8	Q	857	HIS
8	Q	866	LEU
8	Q	870	ASP
8	Q	882	VAL
8	Q	886	THR
8	Q	891	LEU
9	R	71	VAL
9	R	118	ILE
9	R	149	LEU
9	R	188	TYR
9	R	243	LEU
9	R	305	VAL
9	R	308	GLU

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Mol	Chain	Res	Type
9	R	332	TYR
9	R	452	VAL
9	R	532	PHE
9	R	547	VAL
9	R	620	VAL
9	R	690	VAL
9	R	748	VAL
9	R	759	ILE
9	R	765	ARG
9	R	797	LEU
9	R	846	LEU
9	R	866	GLN
9	R	868	ARG
9	R	929	GLU
9	R	1031	ASP
9	R	1049	ASP
9	R	1088	VAL
9	R	1125	GLU
10	S	56	ASN
10	S	236	SER
10	S	277	TYR
10	S	311	HIS
10	S	315	GLN
10	S	365	VAL
10	S	652	LYS
10	S	749	TYR
10	S	817	LEU
10	S	839	LEU
10	S	893	VAL
10	S	978	TYR
10	S	1003	LEU
10	S	1059	LEU
10	S	1116	THR
10	S	1207	ILE
10	S	1255	GLU
10	S	1260	ILE
10	S	1339	THR
10	S	1409	THR
10	S	1604	THR
10	S	1608	ILE
10	S	1696	ASN
10	S	1760	MET

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Mol	Chain	Res	Type
10	S	1858	MET
10	S	1954	VAL
10	T	5	LEU
10	T	37	HIS
10	T	83	THR
10	T	85	ILE
10	T	126	THR
10	T	273	MET
10	T	502	LEU
10	T	513	MET
10	T	550	VAL
10	T	595	ILE
10	T	615	LEU
10	T	635	ILE
10	T	642	GLU
10	T	802	LEU
10	T	829	THR
10	T	873	VAL
10	T	926	ILE
10	T	977	ARG
10	T	987	LEU
10	T	1022	VAL
10	T	1034	LEU
10	T	1043	VAL
10	T	1053	THR
10	T	1119	ILE
10	T	1180	ILE
10	T	1231	HIS
10	T	1432	GLN
10	T	1452	THR
10	T	1496	LEU
10	T	1643	GLN
10	T	1704	GLN
10	T	1782	THR
10	T	1796	GLN
10	T	1808	LEU
10	T	1826	PHE
10	T	1901	TYR
10	T	1938	PHE
10	T	1949	LEU
10	T	1962	LEU
11	U	205	LEU

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Mol	Chain	Res	Type
11	U	547	GLU
11	U	646	LEU
11	U	694	LEU
12	V	27	MET
12	V	53	ILE
12	V	165	VAL
12	V	205	CYS
12	V	261	GLN
12	V	284	GLU
12	V	318	CYS
12	V	463	ARG
12	V	471	LEU
12	V	475	ILE
12	V	516	LEU
12	V	604	TYR
12	V	673	VAL
12	V	754	GLU
12	W	169	LEU
12	W	232	LEU
12	W	264	LEU
12	W	559	THR
12	W	694	GLU
12	W	719	MET
12	W	736	VAL
12	X	200	ILE
12	X	273	THR
12	X	336	ASP
12	X	406	ILE
12	X	412	ARG
12	X	734	LEU
12	Y	13	GLU
12	Y	96	LEU
12	Y	165	VAL
12	Y	296	LEU
12	Y	325	VAL
12	Y	482	LEU
12	Y	518	ILE
12	Y	523	PHE
12	Y	573	VAL
12	Y	719	MET
12	Z	38	GLU
12	Z	168	ASN

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Mol	Chain	Res	Type
12	Z	249	VAL
12	Z	416	LEU
12	Z	484	LEU
12	Z	524	THR
12	Z	642	VAL
12	Z	677	VAL
12	Z	713	CYS
13	a	825	VAL
14	b	67	THR
14	b	89	LEU
14	b	110	VAL
14	b	198	VAL
14	b	262	THR
14	b	319	LEU
14	b	365	THR
14	b	470	ILE
14	b	484	THR
14	b	521	ARG
14	b	567	GLN
14	b	605	THR
14	b	607	GLU
15	c	358	LEU
15	c	391	MET
15	c	472	MET
15	c	481	GLU
14	d	159	LEU
14	d	164	ILE
14	d	393	CYS
14	d	505	LEU
14	d	564	LEU
13	e	762	THR
13	e	778	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (533) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	128	GLN
1	A	171	HIS
1	A	177	ASN
1	A	180	GLN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	257	GLN
1	A	356	HIS
1	A	386	GLN
1	A	389	ASN
1	A	478	ASN
1	A	550	GLN
1	A	621	GLN
2	B	29	GLN
2	B	43	ASN
2	B	68	GLN
2	B	82	GLN
2	B	108	GLN
2	B	173	HIS
2	B	187	ASN
2	B	226	GLN
2	B	267	HIS
2	B	273	HIS
3	C	16	HIS
3	C	34	GLN
3	C	72	GLN
3	C	324	ASN
4	D	159	GLN
4	D	306	HIS
4	D	366	GLN
4	D	368	GLN
4	D	394	GLN
4	D	419	GLN
4	D	424	HIS
4	D	457	GLN
4	D	476	GLN
4	D	511	ASN
4	D	530	ASN
4	D	556	ASN
4	D	558	ASN
4	D	614	HIS
4	D	644	GLN
4	D	662	GLN
4	D	681	ASN
4	D	696	ASN
4	D	793	ASN
4	D	847	GLN
4	D	873	ASN

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Mol	Chain	Res	Type
4	D	887	GLN
4	D	963	ASN
4	D	996	GLN
4	D	1022	GLN
4	D	1056	ASN
4	D	1087	HIS
4	D	1092	ASN
4	D	1122	ASN
4	D	1129	ASN
4	D	1220	GLN
4	D	1260	GLN
4	D	1311	ASN
4	D	1322	ASN
4	D	1379	GLN
4	D	1400	ASN
4	D	1402	GLN
5	E	115	ASN
5	E	158	GLN
5	E	199	GLN
5	E	244	GLN
5	E	250	HIS
5	E	263	ASN
5	E	265	ASN
5	E	283	HIS
5	E	289	GLN
6	F	258	ASN
6	F	406	ASN
6	F	458	GLN
6	F	528	GLN
6	F	612	GLN
6	F	654	GLN
6	F	685	HIS
6	F	750	HIS
6	F	756	HIS
6	F	813	ASN
6	F	843	GLN
7	G	67	HIS
7	G	154	ASN
8	H	134	GLN
8	H	157	HIS
8	H	205	GLN
8	H	206	GLN

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Mol	Chain	Res	Type
8	H	230	ASN
8	H	354	GLN
8	H	454	GLN
8	H	507	GLN
8	H	586	HIS
8	H	608	GLN
8	H	633	ASN
8	H	675	GLN
8	H	684	ASN
8	H	708	GLN
8	H	738	HIS
8	H	763	GLN
8	H	857	HIS
8	H	877	GLN
9	I	72	ASN
9	I	74	ASN
9	I	114	ASN
9	I	181	ASN
9	I	219	GLN
9	I	329	ASN
9	I	350	HIS
9	I	371	ASN
9	I	382	GLN
9	I	440	ASN
9	I	548	ASN
9	I	549	GLN
9	I	586	GLN
9	I	602	HIS
9	I	603	GLN
9	I	651	ASN
9	I	655	GLN
9	I	668	ASN
9	I	713	ASN
9	I	738	ASN
9	I	743	GLN
9	I	803	GLN
9	I	825	GLN
9	I	839	GLN
9	I	870	GLN
9	I	901	GLN
9	I	1001	GLN
9	I	1090	GLN

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Mol	Chain	Res	Type
9	I	1121	ASN
1	J	18	GLN
1	J	20	ASN
1	J	97	GLN
1	J	177	ASN
1	J	269	ASN
1	J	386	GLN
1	J	427	ASN
1	J	459	GLN
1	J	463	GLN
1	J	474	GLN
1	J	478	ASN
1	J	522	ASN
1	J	548	GLN
1	J	621	GLN
1	J	627	ASN
2	K	40	ASN
2	K	68	GLN
2	K	113	ASN
2	K	151	ASN
2	K	200	GLN
2	K	223	HIS
3	L	67	HIS
3	L	72	GLN
3	L	100	GLN
3	L	149	ASN
3	L	157	HIS
3	L	178	HIS
3	L	192	ASN
3	L	205	ASN
3	L	230	ASN
3	L	269	HIS
3	L	280	GLN
4	M	100	ASN
4	M	149	ASN
4	M	150	ASN
4	M	184	GLN
4	M	194	ASN
4	M	264	GLN
4	M	291	HIS
4	M	306	HIS
4	M	418	ASN

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Mol	Chain	Res	Type
4	M	434	HIS
4	M	436	ASN
4	M	510	GLN
4	M	527	ASN
4	M	530	ASN
4	M	579	HIS
4	M	587	HIS
4	M	636	GLN
4	M	692	GLN
4	M	875	ASN
4	M	892	GLN
4	M	924	HIS
4	M	960	GLN
4	M	1013	ASN
4	M	1022	GLN
4	M	1077	HIS
4	M	1087	HIS
4	M	1122	ASN
4	M	1143	GLN
4	M	1270	ASN
4	M	1306	HIS
4	M	1307	HIS
4	M	1371	GLN
4	M	1379	GLN
4	M	1398	ASN
4	M	1402	GLN
4	M	1412	GLN
5	N	3	GLN
5	N	20	HIS
5	N	198	HIS
5	N	244	GLN
6	O	389	GLN
6	O	401	ASN
6	O	406	ASN
6	O	415	HIS
6	O	490	ASN
6	O	493	GLN
6	O	524	ASN
6	O	612	GLN
6	O	642	GLN
6	O	645	ASN
6	O	685	HIS

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Mol	Chain	Res	Type
6	O	716	GLN
6	O	726	HIS
6	O	754	GLN
6	O	762	HIS
6	O	788	HIS
6	O	791	HIS
6	O	813	ASN
6	O	871	GLN
7	P	72	ASN
7	P	107	ASN
7	P	114	HIS
7	P	205	GLN
8	Q	134	GLN
8	Q	157	HIS
8	Q	238	ASN
8	Q	250	GLN
8	Q	322	GLN
8	Q	376	HIS
8	Q	412	ASN
8	Q	425	ASN
8	Q	428	GLN
8	Q	528	ASN
8	Q	536	HIS
8	Q	543	HIS
8	Q	569	GLN
8	Q	645	HIS
8	Q	684	ASN
8	Q	721	GLN
8	Q	836	GLN
8	Q	861	GLN
9	R	76	GLN
9	R	114	ASN
9	R	155	GLN
9	R	285	ASN
9	R	296	GLN
9	R	336	ASN
9	R	382	GLN
9	R	499	GLN
9	R	508	HIS
9	R	525	GLN
9	R	548	ASN
9	R	586	GLN

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Mol	Chain	Res	Type
9	R	641	ASN
9	R	655	GLN
9	R	709	ASN
9	R	727	GLN
9	R	767	HIS
9	R	803	GLN
9	R	825	GLN
9	R	845	ASN
9	R	908	GLN
9	R	928	GLN
9	R	938	GLN
9	R	942	ASN
9	R	1001	GLN
9	R	1005	ASN
9	R	1014	GLN
9	R	1017	GLN
9	R	1028	ASN
9	R	1094	ASN
9	R	1116	ASN
10	S	22	GLN
10	S	56	ASN
10	S	81	GLN
10	S	225	GLN
10	S	226	GLN
10	S	315	GLN
10	S	316	ASN
10	S	318	GLN
10	S	342	GLN
10	S	409	ASN
10	S	468	GLN
10	S	543	GLN
10	S	580	HIS
10	S	783	GLN
10	S	838	HIS
10	S	851	ASN
10	S	858	ASN
10	S	878	GLN
10	S	884	ASN
10	S	1109	GLN
10	S	1198	GLN
10	S	1262	GLN
10	S	1268	ASN

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Mol	Chain	Res	Type
10	S	1286	GLN
10	S	1317	HIS
10	S	1327	GLN
10	S	1346	GLN
10	S	1368	GLN
10	S	1401	ASN
10	S	1432	GLN
10	S	1488	HIS
10	S	1508	GLN
10	S	1624	GLN
10	S	1662	GLN
10	S	1704	GLN
10	S	1753	GLN
10	S	1754	GLN
10	S	1758	ASN
10	S	1764	GLN
10	S	1775	GLN
10	S	1820	GLN
10	S	1832	HIS
10	S	1834	GLN
10	S	1841	ASN
10	S	1869	GLN
10	S	1883	ASN
10	S	1926	ASN
10	S	1951	GLN
10	S	1975	GLN
10	T	22	GLN
10	T	32	GLN
10	T	37	HIS
10	T	56	ASN
10	T	68	GLN
10	T	89	GLN
10	T	119	GLN
10	T	162	HIS
10	T	180	GLN
10	T	226	GLN
10	T	297	GLN
10	T	315	GLN
10	T	318	GLN
10	T	406	GLN
10	T	419	GLN
10	T	482	GLN

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Mol	Chain	Res	Type
10	T	488	GLN
10	T	522	GLN
10	T	599	GLN
10	T	662	GLN
10	T	680	GLN
10	T	689	ASN
10	T	719	ASN
10	T	734	GLN
10	T	776	GLN
10	T	808	ASN
10	T	881	GLN
10	T	906	ASN
10	T	973	GLN
10	T	983	HIS
10	T	998	ASN
10	T	1031	HIS
10	T	1091	GLN
10	T	1127	ASN
10	T	1134	GLN
10	T	1213	ASN
10	T	1222	GLN
10	T	1242	GLN
10	T	1314	GLN
10	T	1317	HIS
10	T	1368	GLN
10	T	1401	ASN
10	T	1414	GLN
10	T	1432	GLN
10	T	1567	GLN
10	T	1585	GLN
10	T	1646	GLN
10	T	1689	ASN
10	T	1719	ASN
10	T	1753	GLN
10	T	1764	GLN
10	T	1769	GLN
10	T	1776	GLN
10	T	1841	ASN
10	T	1869	GLN
10	T	1920	GLN
10	T	1948	ASN
10	T	1952	ASN

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Mol	Chain	Res	Type
10	T	1968	ASN
11	U	193	ASN
11	U	200	HIS
11	U	202	GLN
11	U	250	GLN
11	U	280	GLN
11	U	292	ASN
11	U	340	ASN
11	U	421	GLN
11	U	459	GLN
11	U	489	HIS
11	U	522	GLN
11	U	635	ASN
11	U	725	GLN
11	U	755	ASN
11	U	760	GLN
11	U	789	GLN
12	V	137	GLN
12	V	142	GLN
12	V	155	GLN
12	V	163	ASN
12	V	340	GLN
12	V	366	GLN
12	V	421	GLN
12	V	435	GLN
12	V	436	HIS
12	V	443	GLN
12	V	509	ASN
12	V	527	GLN
12	V	675	ASN
12	V	750	GLN
12	W	108	ASN
12	W	148	ASN
12	W	149	GLN
12	W	168	ASN
12	W	218	GLN
12	W	268	GLN
12	W	307	GLN
12	W	363	HIS
12	W	382	GLN
12	W	393	ASN
12	W	422	HIS

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Mol	Chain	Res	Type
12	W	431	ASN
12	W	564	GLN
12	W	695	ASN
12	W	750	GLN
12	X	16	GLN
12	X	63	HIS
12	X	90	ASN
12	X	148	ASN
12	X	302	GLN
12	X	324	GLN
12	X	363	HIS
12	X	366	GLN
12	X	459	GLN
12	X	500	GLN
12	X	509	ASN
12	X	603	HIS
12	X	675	ASN
12	X	750	GLN
12	X	766	ASN
12	Y	14	ASN
12	Y	108	ASN
12	Y	137	GLN
12	Y	163	ASN
12	Y	222	ASN
12	Y	393	ASN
12	Y	422	HIS
12	Y	424	ASN
12	Y	431	ASN
12	Y	445	HIS
12	Y	466	GLN
12	Y	493	GLN
12	Y	498	GLN
12	Y	555	GLN
12	Y	556	HIS
12	Y	570	GLN
12	Y	675	ASN
12	Y	681	ASN
12	Y	750	GLN
12	Z	16	GLN
12	Z	75	ASN
12	Z	108	ASN
12	Z	137	GLN

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Mol	Chain	Res	Type
12	Z	178	ASN
12	Z	250	GLN
12	Z	261	GLN
12	Z	351	GLN
12	Z	356	HIS
12	Z	367	ASN
12	Z	382	GLN
12	Z	424	ASN
12	Z	435	GLN
12	Z	443	GLN
12	Z	459	GLN
12	Z	498	GLN
12	Z	521	GLN
12	Z	556	HIS
12	Z	564	GLN
12	Z	567	HIS
12	Z	582	HIS
13	a	718	GLN
13	a	790	ASN
13	a	863	ASN
13	a	867	ASN
13	a	894	GLN
14	b	8	GLN
14	b	66	HIS
14	b	109	HIS
14	b	141	ASN
14	b	182	ASN
14	b	188	ASN
14	b	308	ASN
14	b	408	ASN
14	b	550	GLN
14	b	557	GLN
14	b	567	GLN
14	b	584	GLN
14	b	620	GLN
14	b	661	GLN
14	b	697	GLN
15	c	360	ASN
15	c	384	ASN
15	c	425	GLN
15	c	494	ASN
15	c	504	ASN

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Mol	Chain	Res	Type
15	c	516	ASN
15	c	521	GLN
15	c	526	GLN
14	d	174	HIS
14	d	182	ASN
14	d	242	GLN
14	d	243	HIS
14	d	270	GLN
14	d	530	ASN
14	d	575	GLN
14	d	584	GLN
14	d	588	GLN
14	d	620	GLN
14	d	656	ASN
14	d	664	ASN
14	d	667	ASN
13	e	743	GLN
13	e	787	GLN
13	e	822	ASN
13	e	842	GLN
13	e	848	GLN
15	f	363	ASN
15	f	424	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

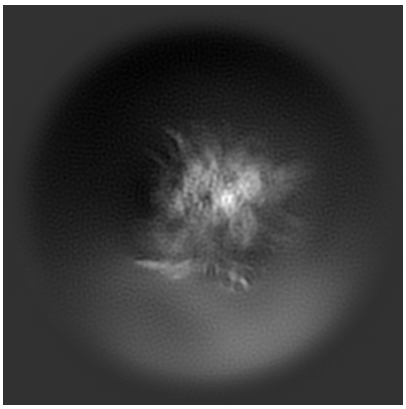
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32056. These allow visual inspection of the internal detail of the map and identification of artifacts.

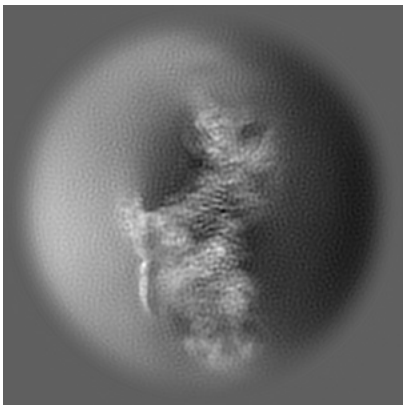
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

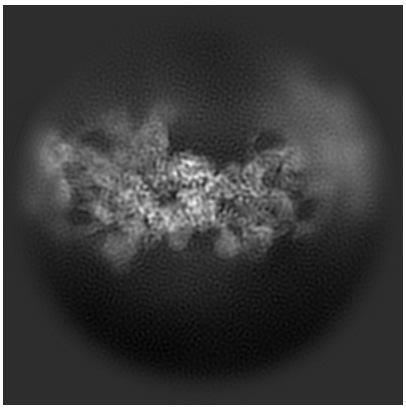
6.1.1 Primary map



X

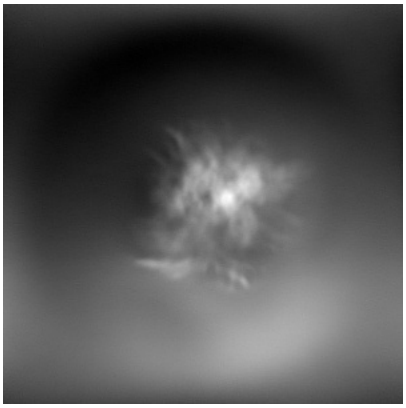


Y

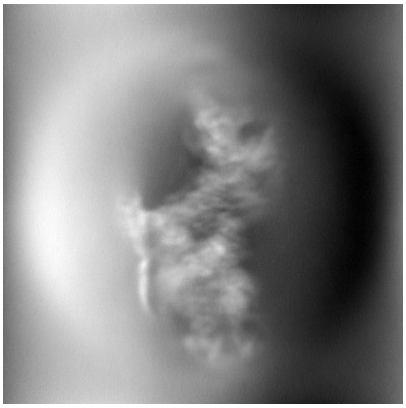


Z

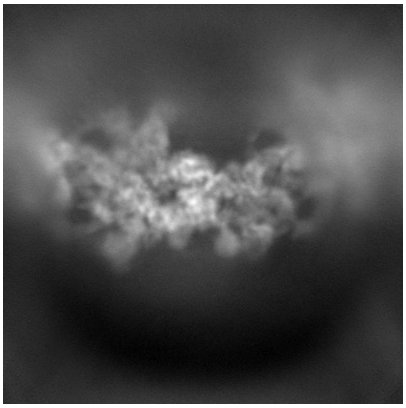
6.1.2 Raw map



X



Y

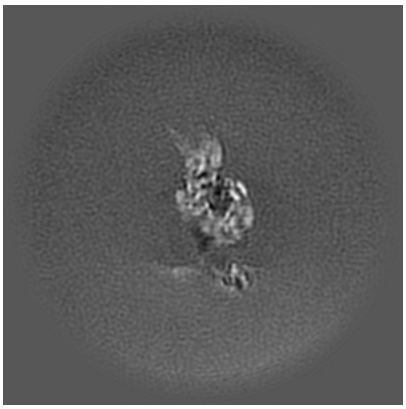


Z

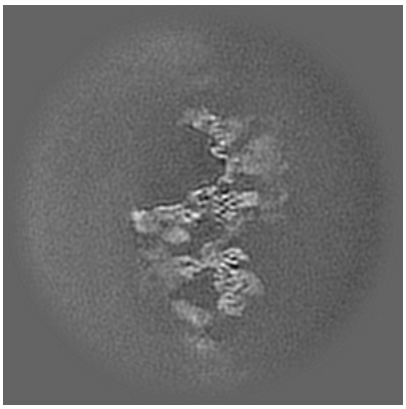
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

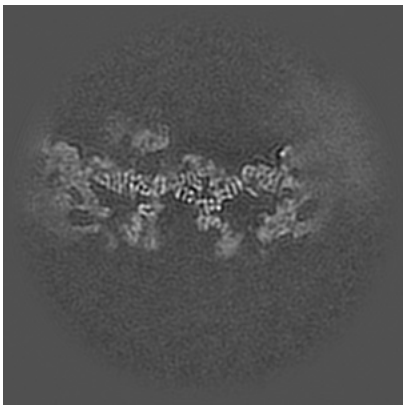
6.2.1 Primary map



X Index: 160

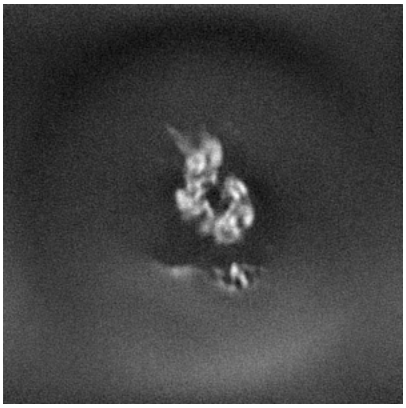


Y Index: 160

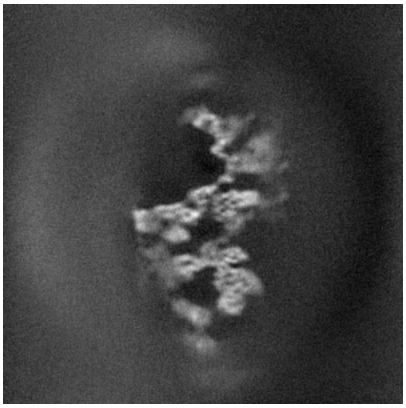


Z Index: 160

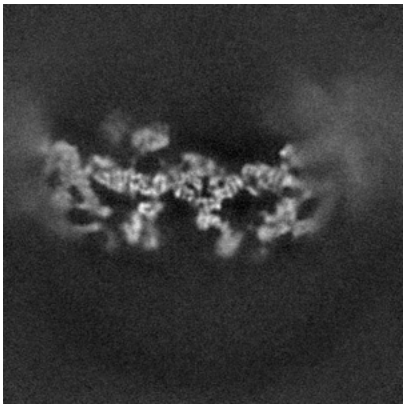
6.2.2 Raw map



X Index: 160



Y Index: 160

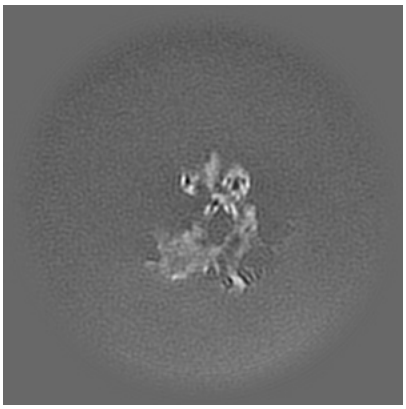


Z Index: 160

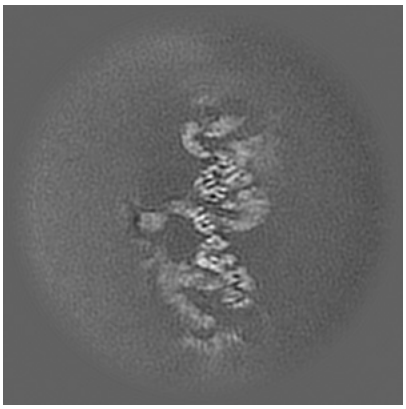
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

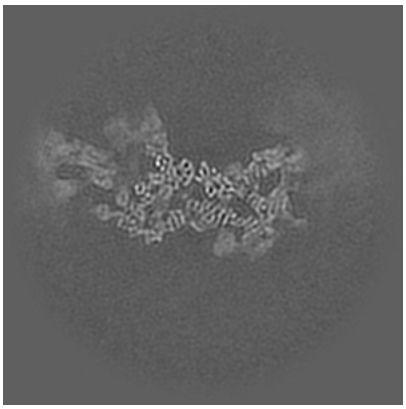
6.3.1 Primary map



X Index: 143

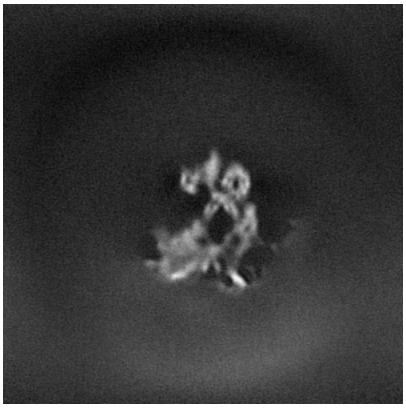


Y Index: 169

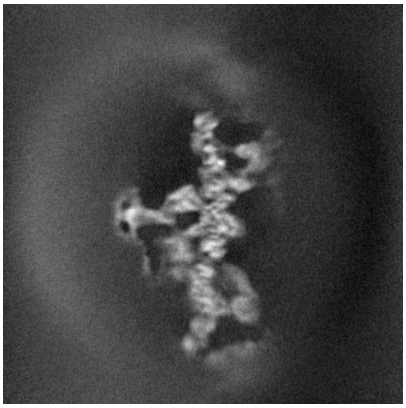


Z Index: 171

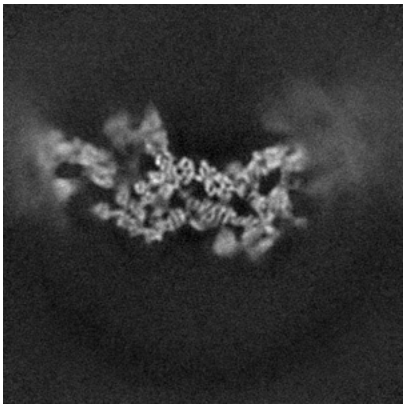
6.3.2 Raw map



X Index: 143



Y Index: 182

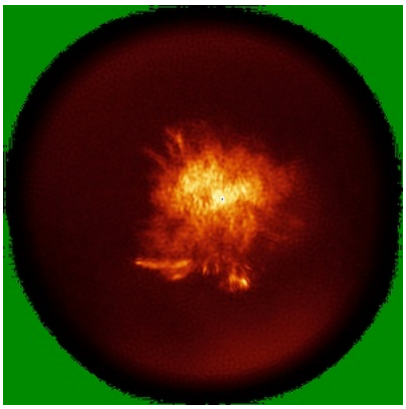


Z Index: 171

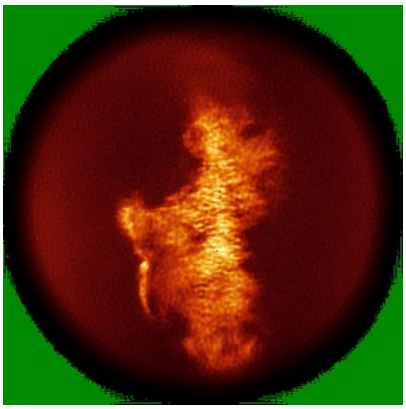
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

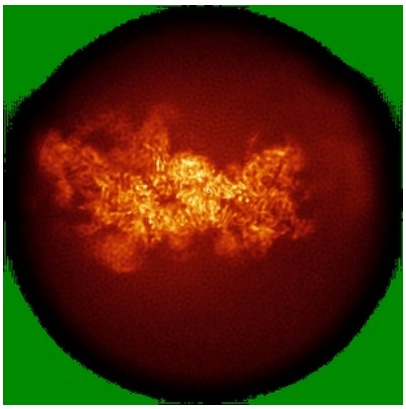
6.4.1 Primary map



X

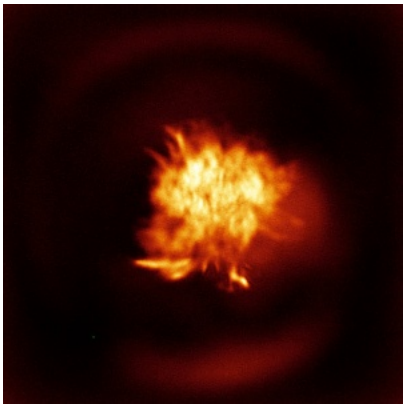


Y

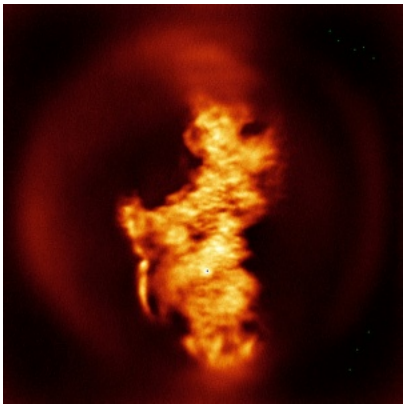


Z

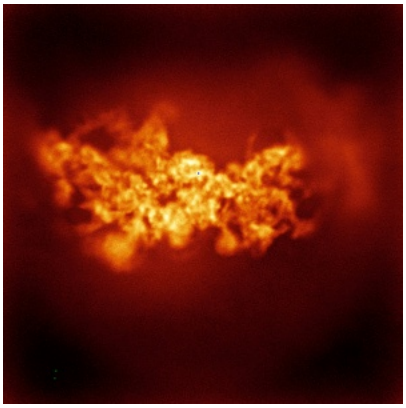
6.4.2 Raw map



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

X

Y

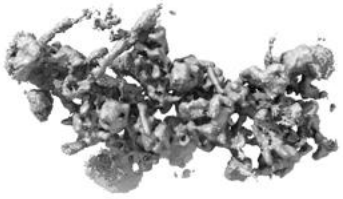
Z

The images above show the 3D surface view of the map at the recommended contour level 0.505. 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

X

Y



Z

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.

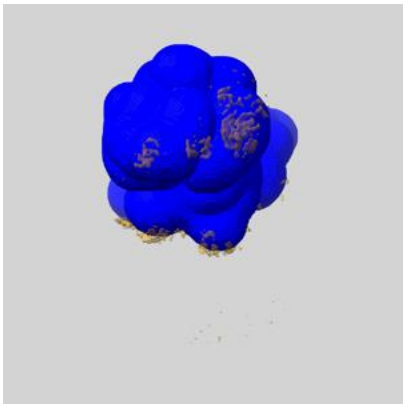
6.6 Mask visualisation

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

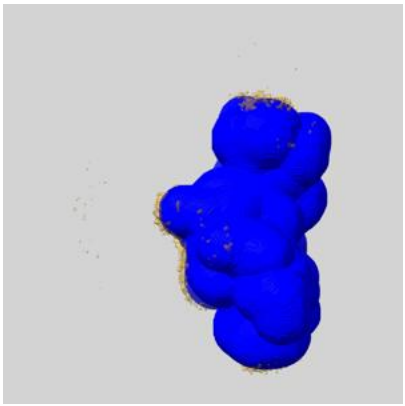
A mask typically either:

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

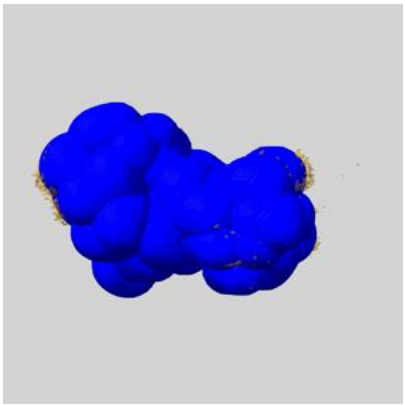
6.6.1 emd_32056_msk_1.map



X



Y

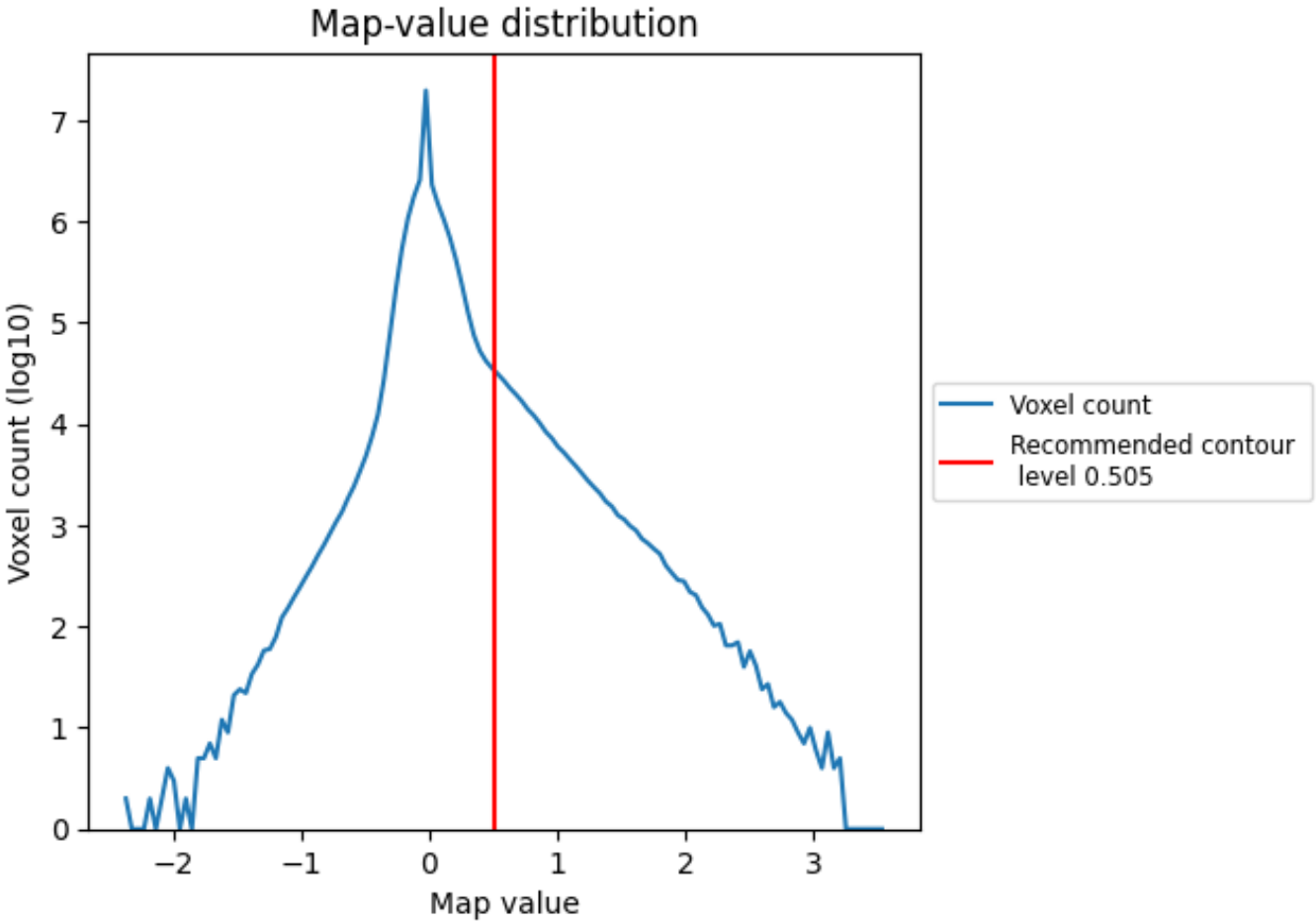


Z

7 Map analysis

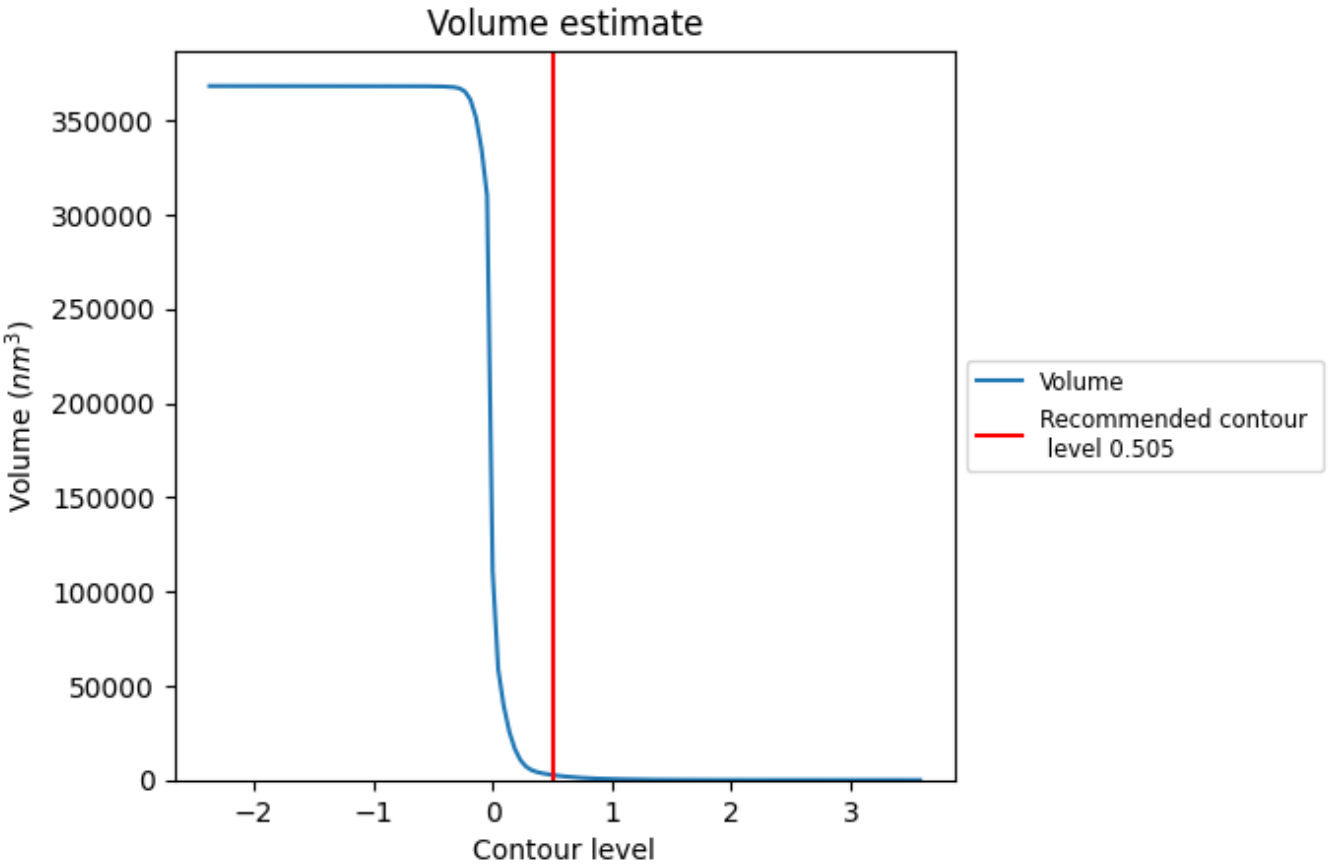
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

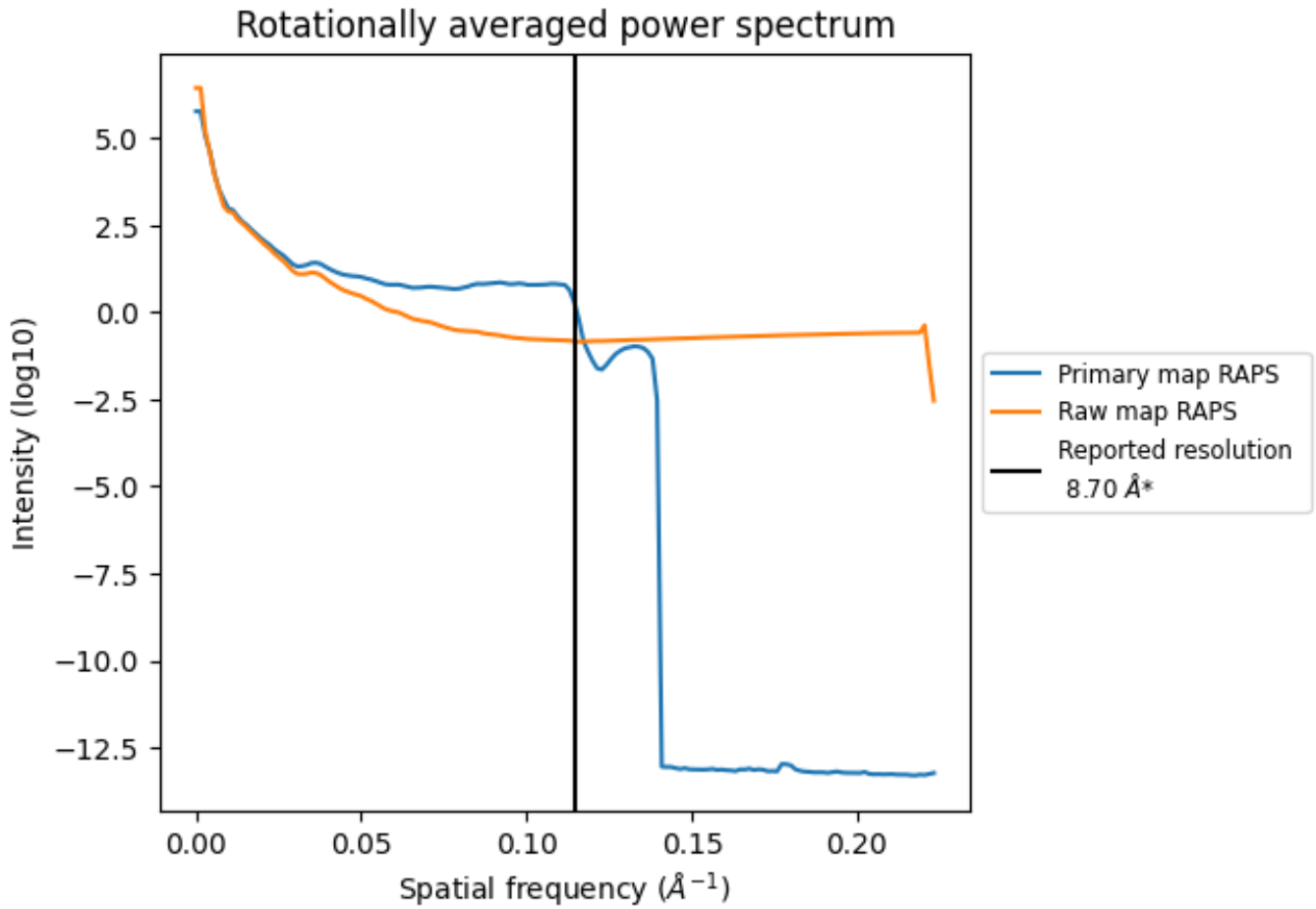
7.2 Volume estimate



The volume at the recommended contour level is 2642 nm^3; this corresponds to an approximate mass of 2387 kDa.

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

7.3 Rotationally averaged power spectrum (i)

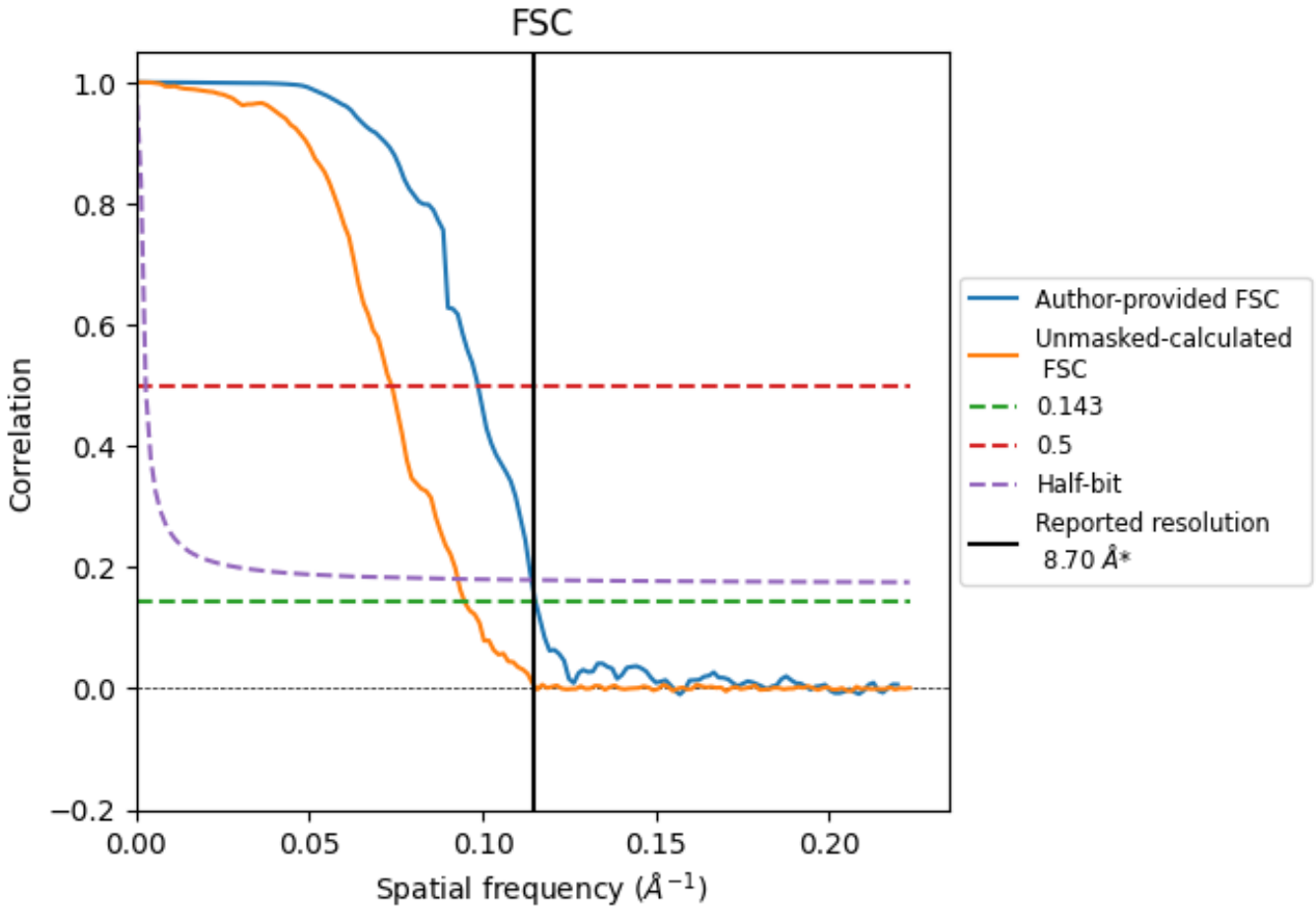


*Reported resolution corresponds to spatial frequency of 0.115 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.115 Å^{-1}

8.2 Resolution estimates (i)

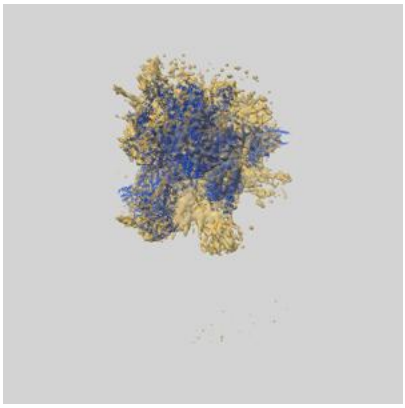
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.68	10.14	8.76
Unmasked-calculated*	10.56	13.55	10.78

*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 10.56 differs from the reported value 8.7 by more than 10 %

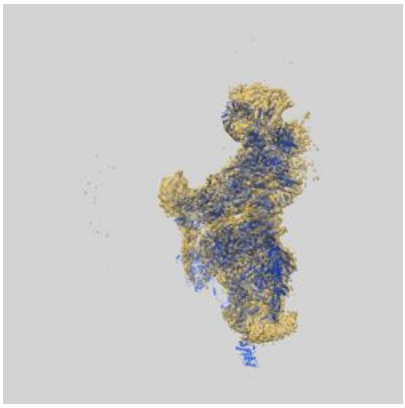
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32056 and PDB model 7VOP. Per-residue inclusion information can be found in section 3 on page 12.

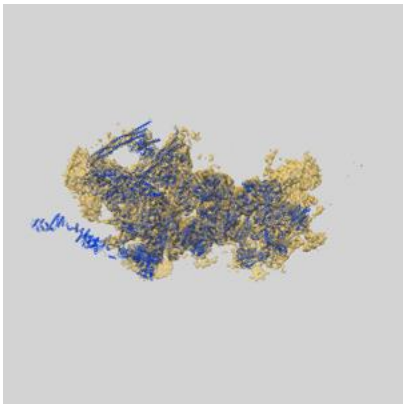
9.1 Map-model overlay



X



Y



Z

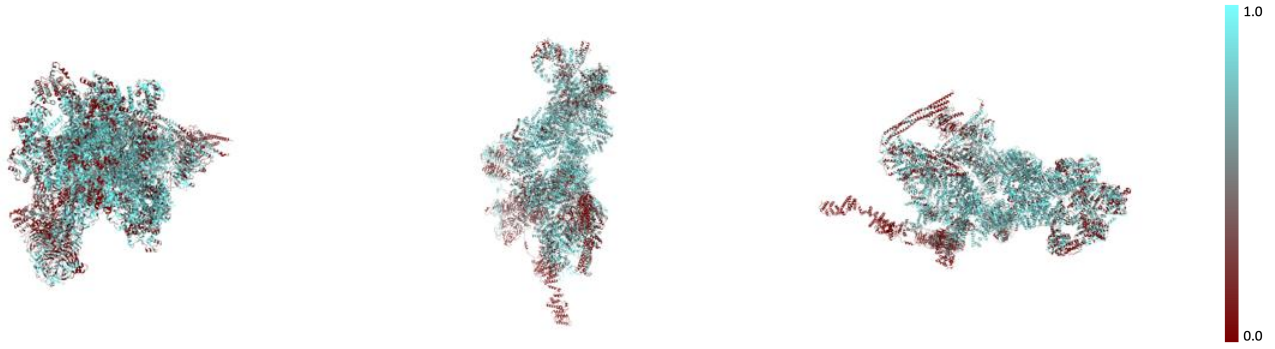
The images above show the 3D surface view of the map at the recommended contour level 0.505 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

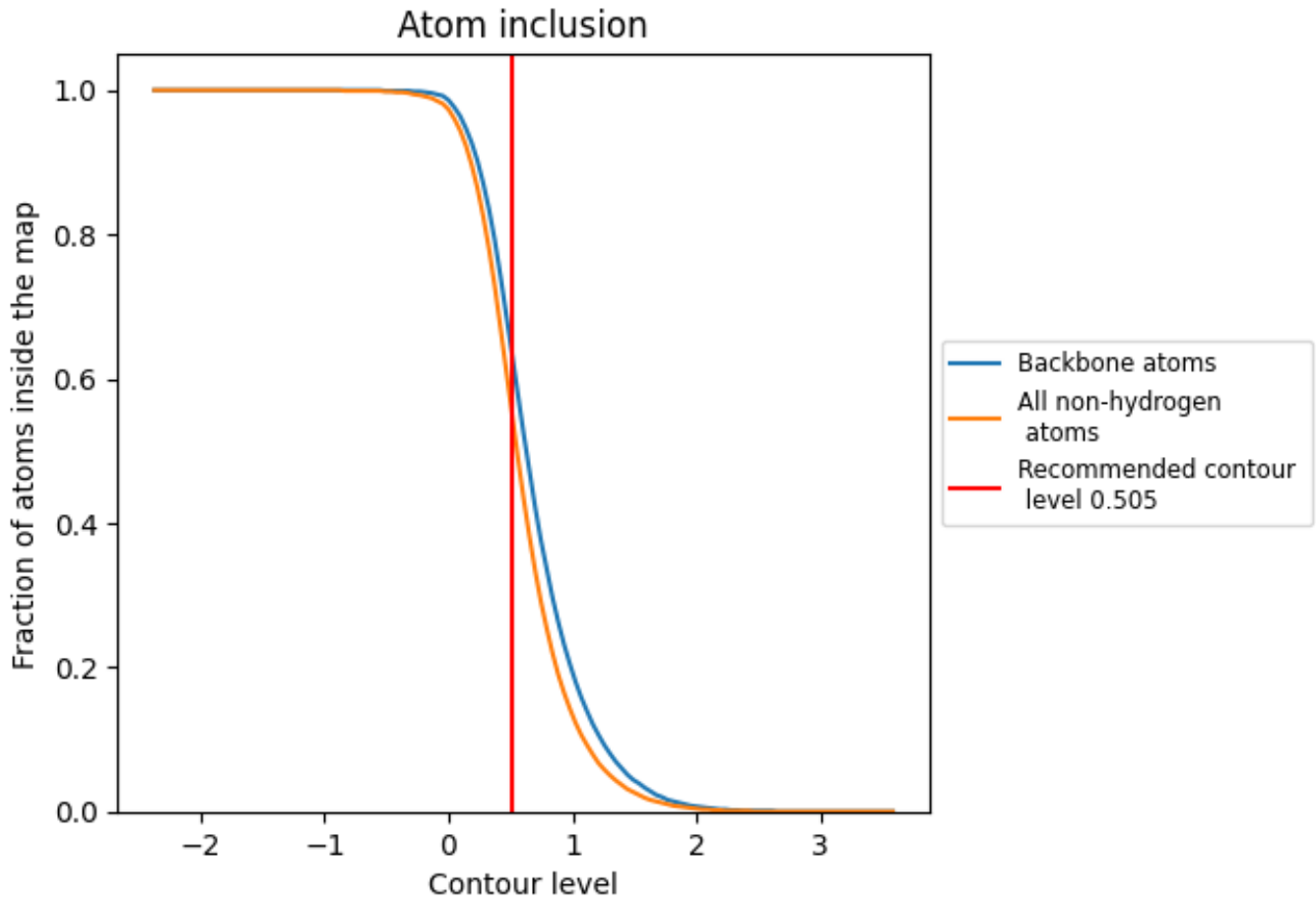
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.505).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 56% 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 (0.505) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5610	0.0860
A	0.7260	0.1500
B	0.6850	0.0950
C	0.8050	0.1310
D	0.6360	0.0820
E	0.7930	0.0860
F	0.7050	0.1140
G	0.7030	0.1080
H	0.6260	0.0910
I	0.3520	0.0610
J	0.6650	0.1240
K	0.6430	0.0790
L	0.7590	0.1190
M	0.4190	0.0550
N	0.1560	0.0390
O	0.7360	0.1380
P	0.8080	0.1180
Q	0.6300	0.1170
R	0.0450	0.0030
S	0.6450	0.1010
T	0.7120	0.1190
U	0.7090	0.1000
V	0.5220	0.0830
W	0.7180	0.1070
X	0.4620	0.0360
Y	0.5210	0.0410
Z	0.5150	0.0490
a	0.4520	0.1090
b	0.4980	0.0840
c	0.4480	0.1040
d	0.2060	0.0500
e	0.3420	0.0740
f	0.3160	0.0280