Full wwPDB EM Validation Report (i)

Dec 18, 2024 – 08:40 pm GMT

PDB ID	:	9HCJ
EMDB ID	:	EMD-19137
Title	:	D. discoideum nuclear pore complex
Authors	:	Obarska-Kosinska, A.; Hoffmann, P.C.; Beck, M.
Deposited on	:	2024-11-10
Resolution	:	30.00 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 (i) 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 (i)) were used in the production of this report:

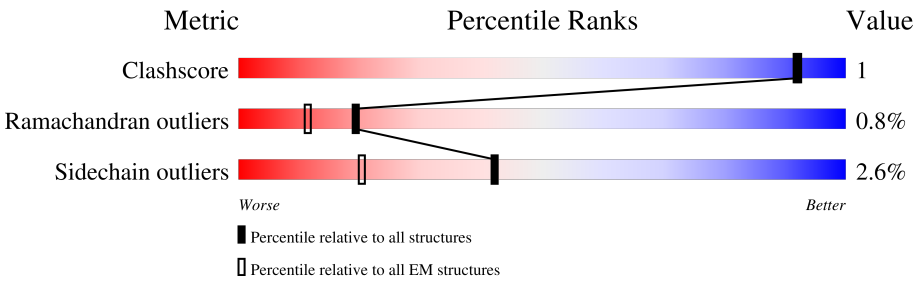
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 30.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	00	3566	7% 20% • 78%
1	01	3566	8% 20% • 78%
2	10	1916	30% 86% 6% 7%
2	11	1916	19% 86% 7% • 7%
2	12	1916	19% 86% 7% 7%
2	13	1916	20% 86% 7% 7%
2	14	1916	24% 86% 7% • 7%
2	15	1916	22% 85% 8% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	16	1916	18% 86% 7% 7%
2	17	1916	22% 87% 6% 7%
3	40	471	6% 94% 5%
3	41	471	13% 95% 5%
4	A0	979	18% 78% 18%
4	A1	979	13% 66% 5% 28%
4	A2	979	21% 67% 5% 28%
4	A3	979	8% 67% 5% 28%
4	A4	979	18% 67% 28%
4	A5	979	11% 73% 23%
5	B0	2174	30% 86% 5% 9%
5	B1	2174	26% 86% 5% 9%
6	C0	1916	20% 69% 27%
6	C1	1916	24% 65% 31%
6	C2	1916	24% 66% 31%
6	C3	1916	14% 69% 27%
7	D0	1575	20% 77% 19%
7	D1	1575	16% 78% 19%
7	D2	1575	19% 78% 19%
7	D3	1575	13% 77% 19%
8	E0	667	84% 11%
8	E1	667	84% 5% 11%
9	F0	95	53% 95% 5%
9	F1	95	61% 94% 6%
9	F2	95	33% 95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F3	95	20% 94% 6%
10	H0	440	10% 53% 44%
10	H1	440	20% 54% 44%
10	H2	440	24% 54% 44%
10	H3	440	12% 53% 44%
11	I0	581	12% 33% 66%
11	I1	581	8% 33% 66%
11	I2	581	10% 33% 66%
11	I3	581	10% 32% 66%
12	J0	709	9% 25% 73%
12	J1	709	9% 25% 73%
12	J2	709	7% 25% 74%
12	J3	709	8% 25% 74%
12	J4	709	10% 25% 74%
12	J5	709	6% 25% 74%
13	K0	1206	6% 55% 41%
13	K1	1206	12% 56% 41%
13	K2	1206	6% 56% 41%
13	K3	1206	56% 41%
14	L0	985	12% 75% 5% 19%
14	L1	985	75% 6% 19%
14	L2	985	5% 75% 5% 19%
14	L3	985	5% 76% 20%
15	M0	889	73% 23%
15	M1	889	72% 6% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	M2	889	13% 73% 23%
15	M3	889	7% 73% 5% 23%
16	N0	301	18% 97%
16	N1	301	18% 96%
16	N2	301	20% 97%
16	N3	301	20% 96%
17	O0	467	12% 62% 33%
17	O1	467	12% 60% 6% 33%
17	O2	467	6% 60% 6% 33%
17	O3	467	13% 60% 6% 33%
18	P0	890	19% 78% 6% 15%
18	P1	890	14% 78% 6% 15%
18	P2	890	18% 79% 6% 15%
18	P3	890	17% 79% 6% 15%
19	Q0	417	10% 83% 6% 11%
19	Q1	417	6% 82% 6% 11%
19	Q2	417	12% 85% 11%
19	Q3	417	13% 86% 11%
20	R0	1791	31% 93% 7%
20	R1	1791	18% 93% 7%
20	R2	1791	20% 93% 7%
20	R3	1791	24% 93% 7%
21	T0	2221	10% 44% 52%
21	T1	2221	8% 49% 47%
21	T2	2221	12% 49% 47%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	T3	2221	11% 48% 47%
22	U0	1164	98%
22	U1	1164	98%
22	U2	1164	98%
22	U3	1164	98%
23	V0	1704	14% 85%
23	V1	1704	6% 14% 85%
24	W0	961	33% 86% 7% 7%
24	W1	961	26% 87% 6% 7%
25	X0	405	14% 94% 5%
25	X1	405	17% 93% 7%
25	X2	405	12% 93% 6%
25	X3	405	18% 94% 5%

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 579851 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 RanBP2-type zinc finger.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	00	780	6455	4104	1065	1269	17	0	0
1	01	780	6455	4104	1065	1269	17	0	0

- Molecule 2 is a protein called Nucleoporin 210.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	10	1788	13985	8854	2349	2747	35	0	0
2	11	1788	13985	8854	2349	2747	35	0	0
2	12	1788	13985	8854	2349	2747	35	0	0
2	13	1788	13985	8854	2349	2747	35	0	0
2	14	1788	13985	8854	2349	2747	35	0	0
2	15	1788	13985	8854	2349	2747	35	0	0
2	16	1788	13985	8854	2349	2747	35	0	0
2	17	1788	13985	8854	2349	2747	35	0	0

- Molecule 3 is a protein called WD40 repeat-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	40	471	3808	2437	630	726	15	0	0
3	41	471	3808	2437	630	726	15	0	0

- Molecule 4 is a protein called Nuclear pore protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A0	801	6619	4185	1119	1295	20	0	0
4	A1	703	5782	3686	953	1126	17	0	0
4	A2	703	5782	3686	953	1126	17	0	0
4	A3	703	5782	3686	953	1126	17	0	0
4	A4	703	5782	3686	953	1126	17	0	0
4	A5	752	6200	3939	1040	1202	19	0	0

- Molecule 5 is a protein called Nup188.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B0	1987	16130	10274	2663	3147	46	0	0
5	B1	1987	16130	10274	2663	3147	46	0	0

- Molecule 6 is a protein called Nup205.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C0	1399	11337	7257	1859	2166	55	0	0
6	C1	1327	10779	6916	1760	2050	53	0	0
6	C2	1327	10779	6916	1760	2050	53	0	0
6	C3	1399	11337	7257	1859	2166	55	0	0

- Molecule 7 is a protein called Nucleoporin 155.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D0	1283	10402	6662	1707	2006	27	0	0
7	D1	1283	10402	6662	1707	2006	27	0	0
7	D2	1283	10402	6662	1707	2006	27	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D3	1283	10402	6662	1707	2006	27	0	0

- Molecule 8 is a protein called NDC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E0	595	4959	3273	784	885	17	0	0
			Total	C	N	O	S		
8	E1	595	4959	3273	784	885	17	0	0

- Molecule 9 is a protein called Nup35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F0	95	783	506	124	149	4	0	0
			Total	C	N	O	S		
9	F1	95	783	506	124	149	4	0	0
			Total	C	N	O	S		
9	F2	95	783	506	124	149	4	0	0
			Total	C	N	O	S		
9	F3	95	783	506	124	149	4	0	0

- Molecule 10 is a protein called Nuclear pore complex protein nup54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H0	245	2036	1295	343	388	10	0	0
			Total	C	N	O	S		
10	H1	245	2036	1295	343	388	10	0	0
			Total	C	N	O	S		
10	H2	245	2036	1295	343	388	10	0	0
			Total	C	N	O	S		
10	H3	245	2036	1295	343	388	10	0	0

- Molecule 11 is a protein called Nup58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I0	197	1617	1031	271	310	5	0	0
			Total	C	N	O	S		
11	I1	197	1617	1031	271	310	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I2	197	1617	1031	271	310	5	0	0
11	I3	197	1617	1031	271	310	5	0	0

- Molecule 12 is a protein called Nuclear pore protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J0	189	1528	947	268	310	3	0	0
12	J1	189	1528	947	268	310	3	0	0
12	J2	184	1483	923	257	300	3	0	0
12	J3	184	1483	923	257	300	3	0	0
12	J4	184	1483	923	257	300	3	0	0
12	J5	184	1483	923	257	300	3	0	0

- Molecule 13 is a protein called Nucleoporin 133.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K0	717	5814	3721	962	1114	17	0	0
13	K1	717	5814	3721	962	1114	17	0	0
13	K2	717	5814	3721	962	1114	17	0	0
13	K3	717	5814	3721	962	1114	17	0	0

- Molecule 14 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L0	796	6582	4170	1113	1280	19	0	0
14	L1	796	6582	4170	1113	1280	19	0	0
14	L2	796	6582	4170	1113	1280	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L3	791	6547	4150	1108	1270	19	0	0

- Molecule 15 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M0	687	5650	3617	953	1071	9	0	0
15	M1	687	5650	3617	953	1071	9	0	0
15	M2	687	5650	3617	953	1071	9	0	0
15	M3	687	5650	3617	953	1071	9	0	0

- Molecule 16 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N0	301	2375	1512	408	447	8	0	0
16	N1	301	2375	1512	408	447	8	0	0
16	N2	301	2375	1512	408	447	8	0	0
16	N3	301	2375	1512	408	447	8	0	0

- Molecule 17 is a protein called Seh1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O0	311	2537	1599	437	485	16	0	0
17	O1	311	2537	1599	437	485	16	0	0
17	O2	311	2537	1599	437	485	16	0	0
17	O3	311	2537	1599	437	485	16	0	0

- Molecule 18 is a protein called Nuclear pore complex protein nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	P0	755	6121	3868	1034	1188	31	0	0
18	P1	755	6121	3868	1034	1188	31	0	0
18	P2	755	6121	3868	1034	1188	31	0	0
18	P3	755	6121	3868	1034	1188	31	0	0

- Molecule 19 is a protein called Nuclear pore complex protein nup43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q0	373	2962	1863	499	587	13	0	0
19	Q1	373	2962	1863	499	587	13	0	0
19	Q2	373	2962	1863	499	587	13	0	0
19	Q3	373	2962	1863	499	587	13	0	0

- Molecule 20 is a protein called Nup160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	R0	1790	14662	9233	2493	2889	47	0	0
20	R1	1790	14662	9233	2493	2889	47	0	0
20	R2	1790	14662	9233	2493	2889	47	0	0
20	R3	1790	14662	9233	2493	2889	47	0	0

- Molecule 21 is a protein called ELYS-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T0	1057	8600	5500	1420	1662	18	0	0
21	T1	1168	9517	6057	1583	1859	18	0	0
21	T2	1168	9517	6057	1583	1859	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T3	1168	9517	6057	1583	1859	18	0	0

- Molecule 22 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	U0	25	201	122	36	43	0	0
22	U1	25	201	122	36	43	0	0
22	U2	25	201	122	36	43	0	0
22	U3	25	201	122	36	43	0	0

- Molecule 23 is a protein called WD40-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V0	258	2120	1306	381	429	4	0	0
23	V1	258	2120	1306	381	429	4	0	0

- Molecule 24 is a protein called Nup88.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W0	890	7264	4570	1217	1458	19	0	0
24	W1	890	7264	4570	1217	1458	19	0	0

- Molecule 25 is a protein called Nup205.

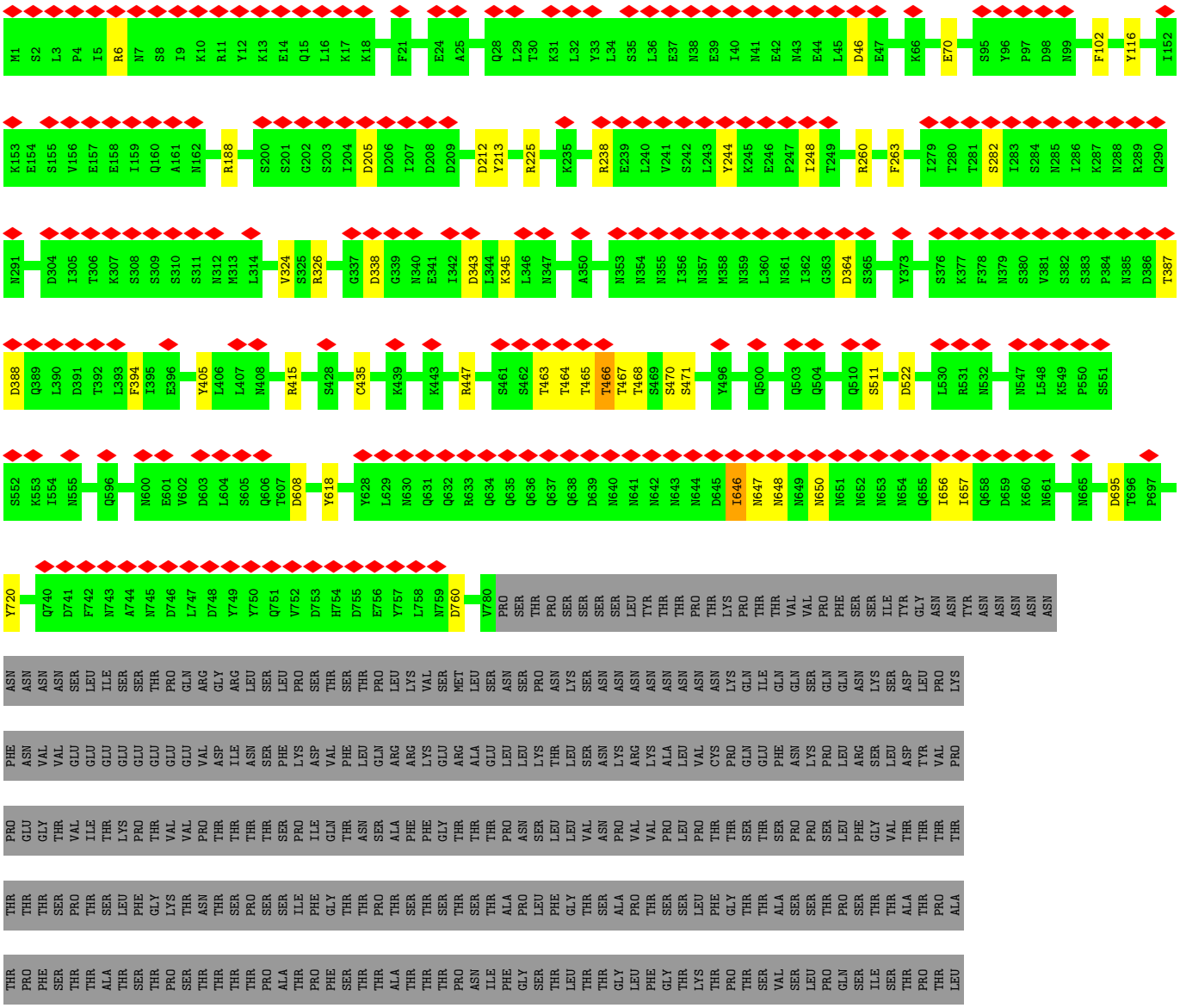
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X0	405	3312	2101	554	646	11	0	0
25	X1	405	3312	2101	554	646	11	0	0
25	X2	405	3312	2101	554	646	11	0	0
25	X3	405	3312	2101	554	646	11	0	0

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: RanBP2-type zinc finger

Chain 00:



| | | |

| | | |

GLN ASN GLN THR ILE GLU LYS GLU ASN GLU GLU ILE SER GLU LEU LYS ASP ILE GLN GLU ASN ASN GLU ASN ASN GLU GLU SER SER THR SER SER ASP GLY GLU GLU SER LYS SER ILE LYS ASP VAL ASP THR SER TYR ASP ASP VAL ASP

- Molecule 1: RanBP2-type zinc finger

Chain 01: 8% 20% 78%

M1 S2 L3 P4 I5 R6 N7 S8 I9 K10 R11 Y12 K13 E14 Q15 L16 K17 K18 P19 L20 F21 K22 N23 E24 A25 L26 Y27 Q28 L29 T30 K31 L32 Y33 L34 S35 L36 E37 N38 E39 I40 N41 E42 N43 E44 L45 D46 E47 C48 K49 D50 Y51 F52 V60 L61 Q65 K66 E67 L68

K69 E70 I71 D74 F75 Q76 T77 I78 T79 K80 Q81 Y82 F102 I112 Y116 D145 N146 V147 A148 I149 K150 A151 I152 K153 E154 S155 V156 E157 E158 I159 Q160 A161 N162 T163 Y172 R188 H192 G202 S203 I204 D205 D206 I207 D208 D209 I210 G211 D212 Y213 Y214

N217 R225 K228 K231 K232 K235 K236 I237 R238 E239 L240 V241 S242 L243 Y244 K245 E246 P247 I248 R260 F263 Y273 I276 S277 N278 I279 T280 T281 S282 I283 S284 N285 I286 K287 N288 R289 Q290 N291 P292 K295 I305 T306 K307 S308 V324 S325 R326 I335

I336 G337 D338 G339 N340 E341 I342 D343 L344 K345 L346 N347 F348 Y349 A350 S351 L352 N353 N354 N355 I356 N357 M358 N359 L360 N361 I362 G363 D364 S365 G366 M367 Y373 L374 V375 S376 K377 F378 N379 S380 V381 S382 S383 P384 N385 D386 T387 D388 Q389 L390 L393 F394 Y405 R415 C435

R447 S460 S461 S462 T463 T464 T465 T466 T467 T468 S469 S470 S471 Q506 Q507 Q508 Q509 Q510 S511 Y512 Q513 D522 L530 R531 N532 S533 L534 P535 W536 K537 N540 S541 Y544 K549 P550 S551 S552 K553 I554 N555 S556 T557 E558 I559 F560 S561 I562 T563 T564 Q596 H597

Y598 Q599 N600 E601 V602 D603 L604 S605 D608 Y618 Y628 Q631 Q632 R633 Q634 Q635 Q636 Q637 Q638 D639 N640 N641 N642 N643 N644 D645 I646 N647 N648 N649 N650 N651 N652 N653 N654 Q655 I656 I657 P697 I698 Y720 T721 R722 F742 N743 A744 N745 D746 L747 D748 Y749 Y750 Q751

V752 D753 H754 D755 E756 Y757 L758 N759 D760 I761 D762 K770 N776 D779 V780 PRO SER THR PRO SER SER SER LEU TYR THR THR PRO THR LYS PRO THR THR VAL VAL PRO PHE SER SER ILE TYR GLY ASN ASN TYR ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN SER LEU ILE

SER SER THR PRO GLN ARG GLY ARG LEU SER LEU PRO SER THR SER THR PRO LEU LYS VAL SER MET LEU SER ASN SER PRO ASN LYS SER ASN ASN ASN ASN ASN ASN ASN LYS GLN ILE GLN GLN SER GLN GLN ASN LYS SER ASP LEU PRO LYS PHE ASN VAL VAL GLU GLU GLU

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

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

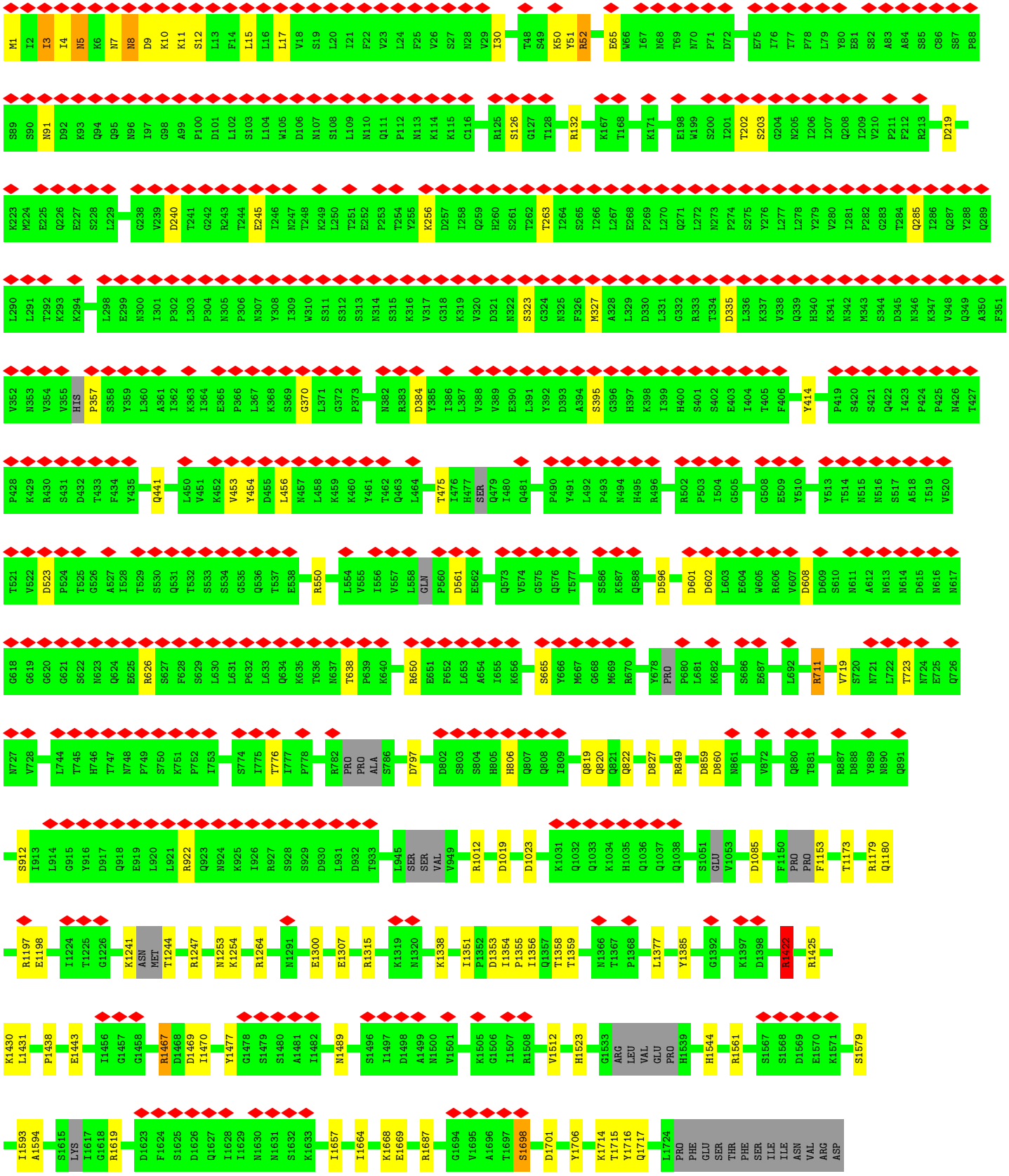
LEU PHE GLY LYS THR ASN THR SER PRO SER SER ILE PHE GLY THR THR PRO THR SER THR SER THR SER THR ALA PRO LEU PHE GLY THR SER ALA PRO THR SER SER SER LEU PHE GLY THR THR THR SER ALA SER SER THR PRO PRO SER THR THR ALA THR PRO PHE SER THR THR ALA

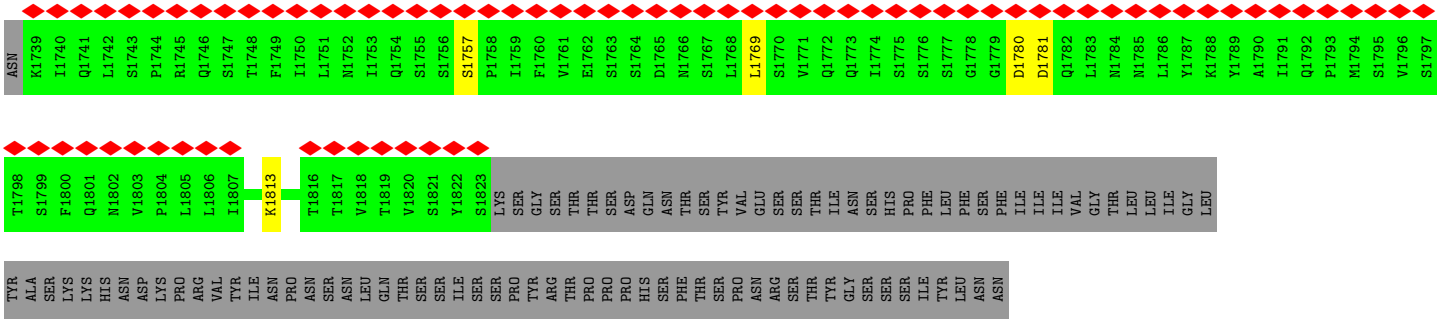
THR SER THR PRO SER THR THR THR PRO PRO ALA THR PRO PHE SER THR THR THR ALA THR THR PRO ASN ILE PHE GLY SER THR LEU THR THR GLY LEU PHE GLY THR LYS THR PRO THR SER VAL SER LEU PRO GLN SER ILE SER THR THR LEU ALA ASP LYS THR ILE LYS THR

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

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

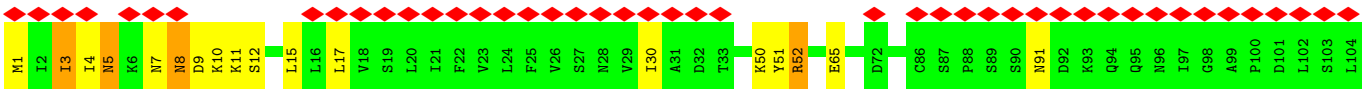
| | | |

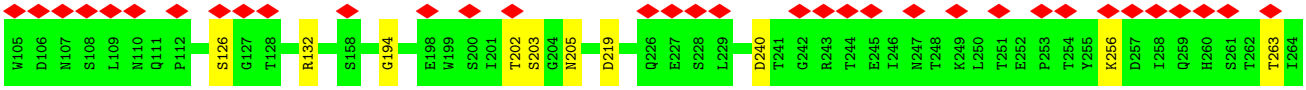

M1 I2 I3 I4 N5 K6 N7 N8 D9 K10 K11 S12 L13 F14 L15 L16 L17 V18 S19 L20 I21 F22 V23 L24 F25 V26 S27 N28 V29 I30 T48 S49 K50 Y51 R52 E65 W66 I67 N68 T69 N70 P71 D72 E75 I76 T77 P78 L79 Y80 E81 S82 A83 A84 S85 C86 S87 P88
S89 S90 N91 D92 K93 Q94 Q95 N96 I97 G98 A99 P100 D101 L102 S103 L104 W105 D106 N107 S108 L109 N110 Q111 P112 N113 K114 K115 C116 R125 S126 G127 T128 R132 K167 T168 K171 E198 W199 S200 I201 T202 S203 G204 N205 I206 I207 Q208 I209 V210 P211 F212 R213 D219
K223 M224 E225 Q226 E227 S228 L229 G238 V239 D240 T241 G242 R243 T244 E245 I246 N247 T248 K249 L250 T251 E252 P253 T254 Y255 K256 D257 I258 Q259 H260 S261 T262 T263 I264 S265 I266 L267 E268 P269 L270 Q271 L272 N273 P274 S275 Y276 L277 L278 Y279 V280 I281 P282 G283 T284 Q285 I286 Q287 Y288 Q289
L290 L291 T292 K293 K294 L298 E299 N300 I301 P302 L303 P304 N305 P306 N307 Y308 I309 W310 S311 S312 S313 N314 S315 K316 V317 G318 K319 V320 D321 N322 S323 G324 N325 F326 M327 A328 L329 D330 L331 G332 R333 T334 D335 L336 K337 V338 Q339 H340 K341 N342 M343 S344 D345 N346 K347 V348 Q349 A350 F351
V352 N353 V354 V355 HIS P357 S358 Y359 L360 A361 I362 K363 I364 E365 P366 L367 K368 S369 G370 L371 G372 P373 N382 R383 D384 Y385 I386 L387 V388 V389 E390 L391 Y392 D393 A394 S395 G396 H397 K398 I399 H400 S401 S402 E403 I404 T405 F406 Y414 P419 S420 S421 Q422 I423 P424 P425 N426 T427
P428 K429 R430 S431 D432 T433 F434 Y435 Q441 L450 V451 K452 V453 Y454 D455 L456 N457 L458 K459 K460 Y461 T462 Q463 L464 T475 I476 H477 SER Q479 I480 Q481 P490 Y491 L492 P493 N494 H495 R496 R502 P503 I504 G505 G508 E509 Y510 Y513 T514 N515 N516 S517 A518 I519 V520
T521 V522 D523 P524 T525 G526 A527 I528 T529 S530 Q531 T532 S533 S534 G535 Q536 T537 E538 R550 L554 V555 I556 V557 L558 GLN P560 D561 E562 Q573 V574 G575 Q576 T577 S586 K587 Q588 D596 D601 D602 L603 E604 W605 R606 V607 D608 D609 S610 N611 A612 N613 M614 D615 N616 N617
G618 G619 G620 G621 S622 N623 Q624 E625 R626 S627 F628 S629 L630 L631 P632 L633 Q634 K635 T636 N637 T638 P639 K640 R650 E651 F652 L653 A654 I655 K656 S665 Y666 M667 G668 M669 R670 Y678 PRO P680 L681 K682 S686 E687 L692 R711 V719 S720 N721 L722 T723 N724 E725 Q726
N727 V728 L744 T745 H746 T747 N748 P749 S750 K751 P752 I753 S774 I775 T776 I777 P778 R782 PRO PRO ALA S786 D797 D802 S803 S804 H805 H806 Q807 Q808 I809 Q819 Q820 Q821 Q822 D827 R849 D859 D860 N861 V872 Q880 T881 R887 D888 Y889 N890 Q891
S912 I913 L914 G915 Y916 D917 Q918 E919 L920 L921 R922 Q923 N924 K925 I926 R927 S928 S929 D930 L931 D932 T933 L945 SER SER VAL V949 R1012 D1019 D1023 K1031 Q1032 Q1033 K1034 H1035 Q1036 Q1037 Q1038 S1051 GLU V1053 D1085 F1150 PRO PRO F1153 T1173 R1179 Q1180
R1197 E1198 I1224 T1225 G1226 K1241 ASN MET T1244 R1247 N1253 K1254 R1264 N1291 E1300 E1307 R1315 K1319 N1320 K1338 I1351 P1352 D1353 I1354 P1355 I1356 Q1357 T1358 T1359 N1366 T1367 P1368 L1377 Y1385 G1392 K1397 D1398 R1422 R1425
K1430 L1431 P1438 E1443 T1456 G1457 G1458 R1467 D1468 D1469 T1470 Y1477 G1478 S1479 S1480 A1481 I1482 N1489 S1496 I1497 D1498 A1499 N1500 V1501 K1505 G1506 I1507 R1508 V1512 H1523 G1533 ARG LEU VAL GLU PRO H1539 H1544 R1561 S1567 S1568 D1569 E1570 K1571 S1579
I1593 A1594 S1615 LYS I1617 G1618 R1619 D1623 F1624 S1625 D1626 Q1627 I1628 I1629 N1630 N1631 S1632 K1633 I1657 I1664 K1668 E1669 R1687 G1694 V1695 A1696 T1697 S1698 D1701 Y1706 K1714 T1715 Y1716 Q1717 L1724 PRO PHE GLU SER THR PHE SER ILE ILE ASN VAL ARG ASP

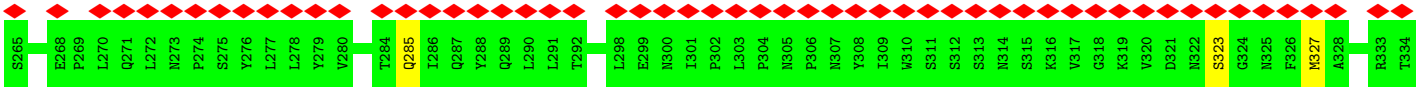


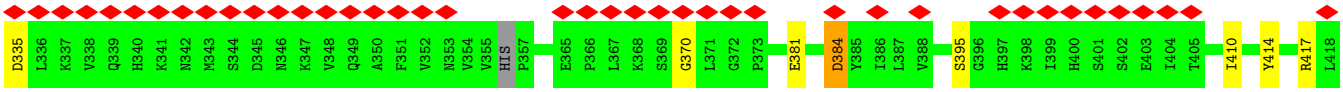
- Molecule 2: Nucleoporin 210

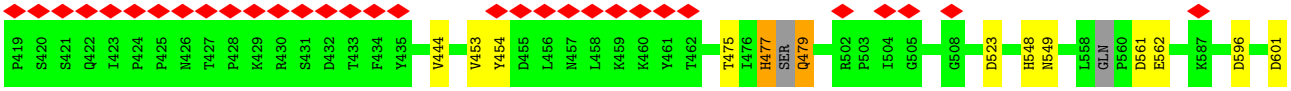
Chain 11:

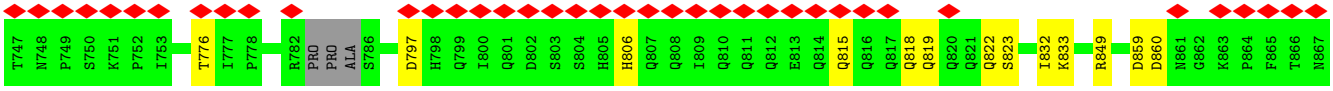


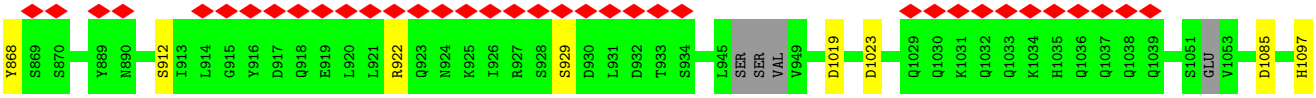


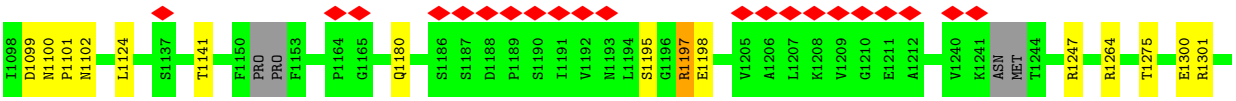


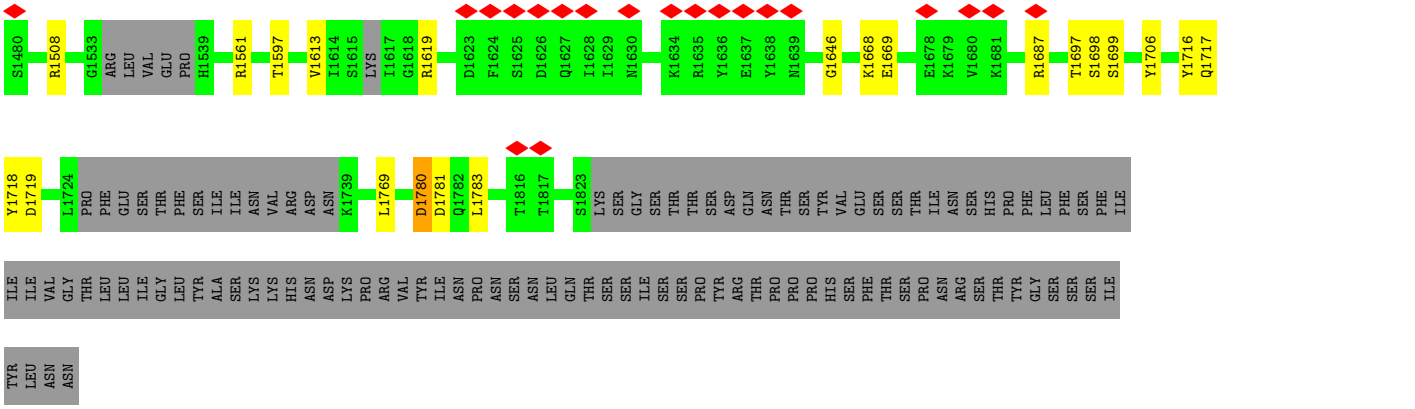






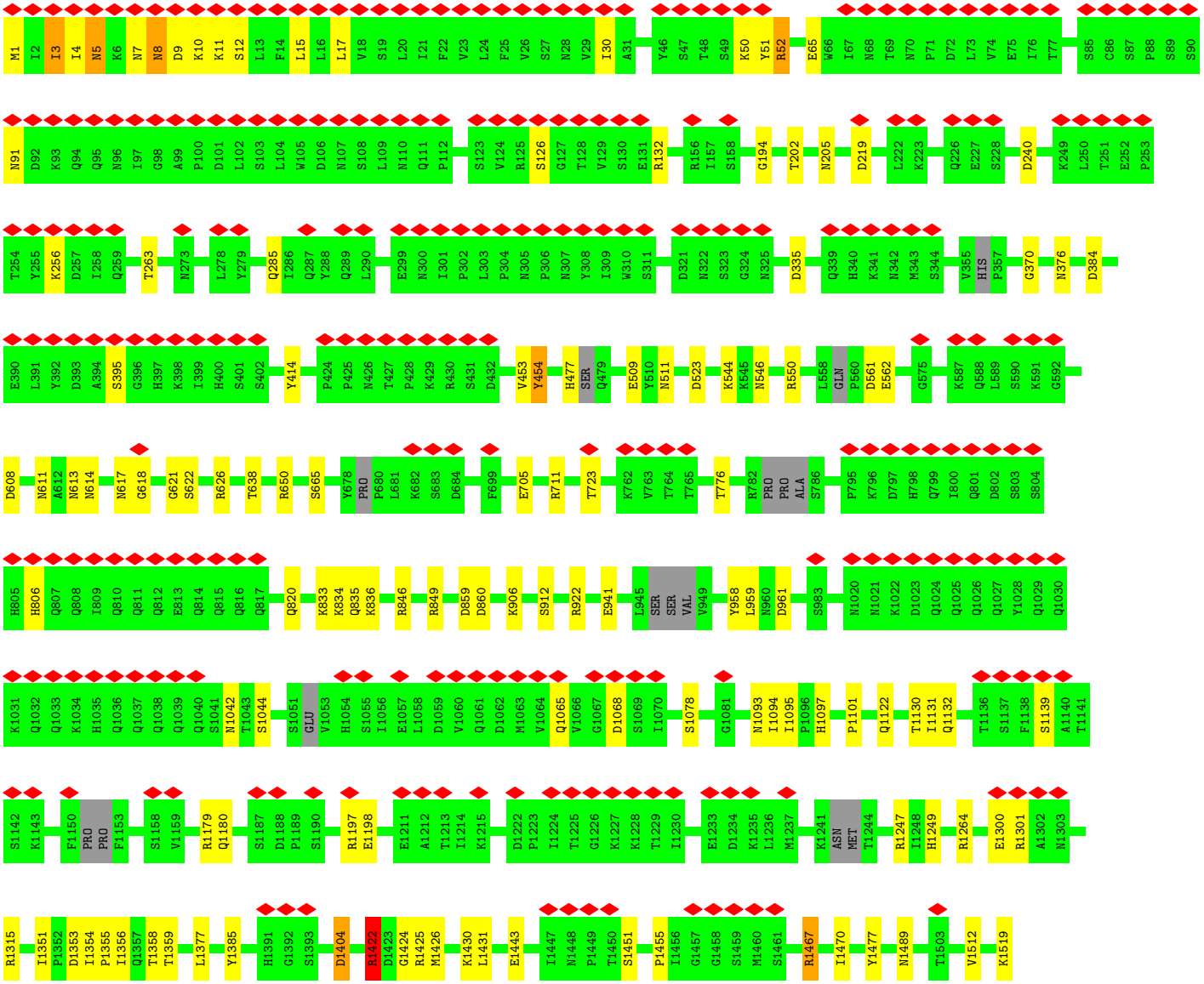


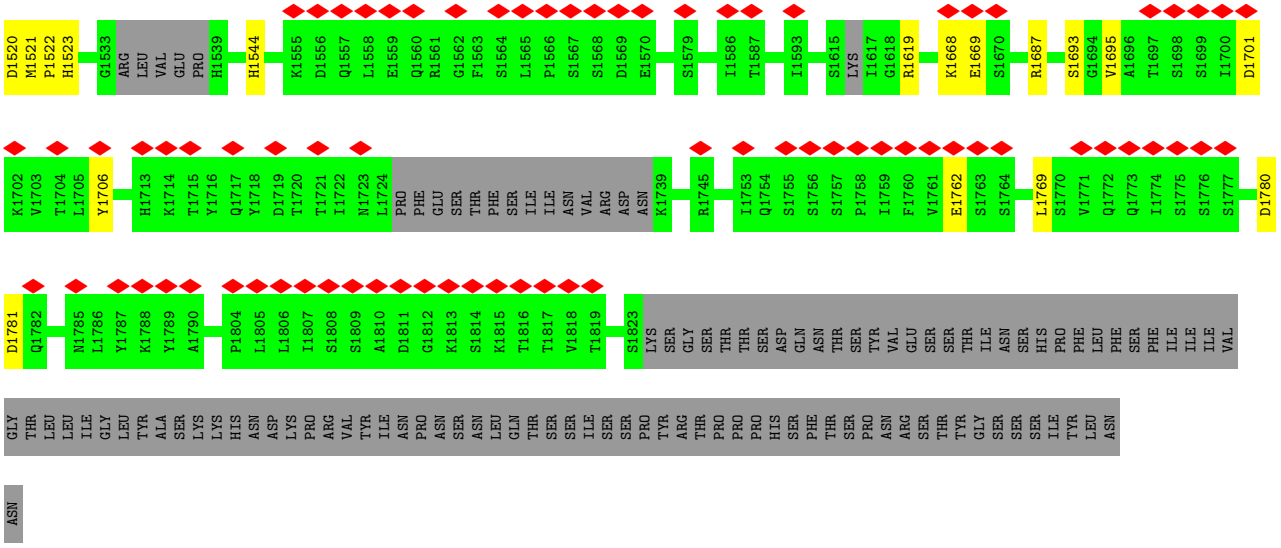




- Molecule 2: Nucleoporin 210

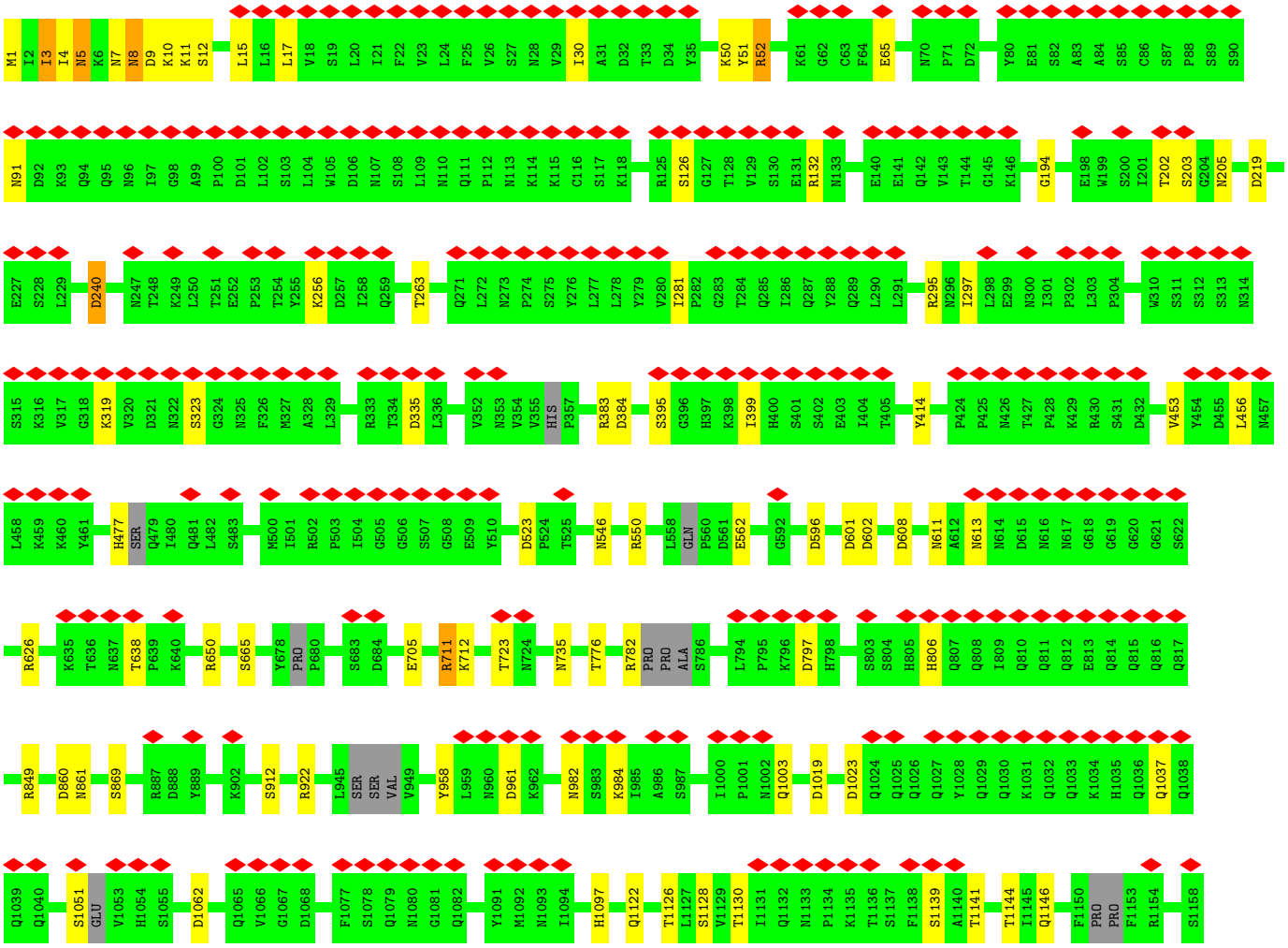
Chain 12:

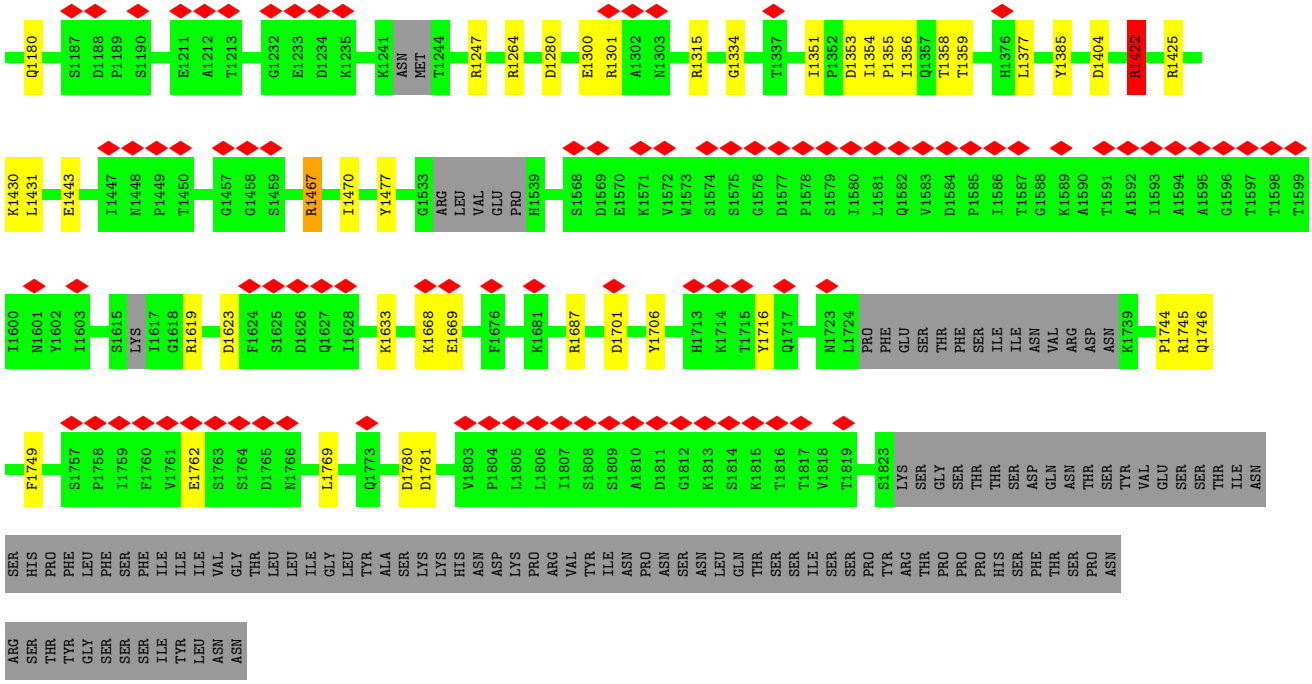




- Molecule 2: Nucleoporin 210

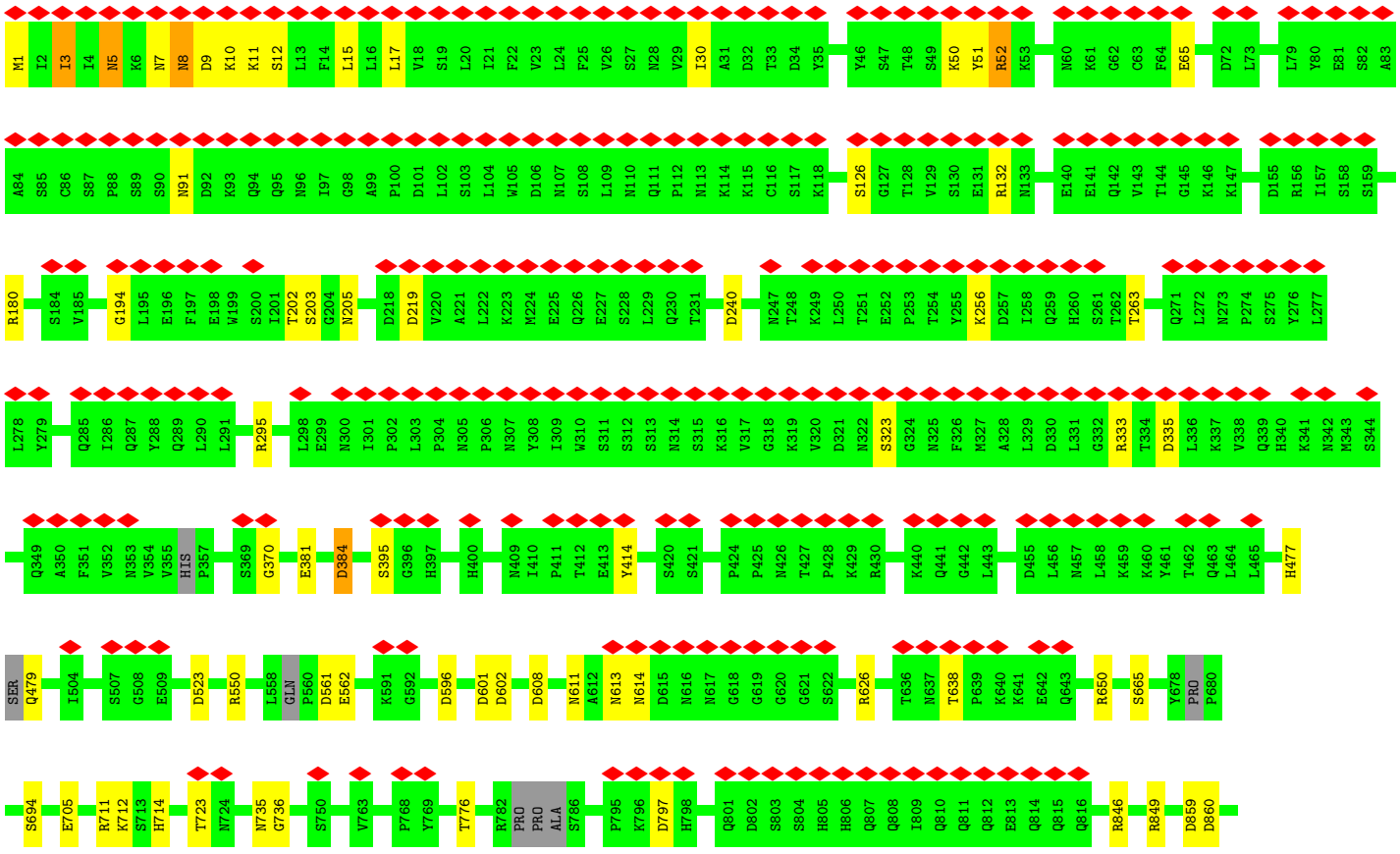
Chain 13:

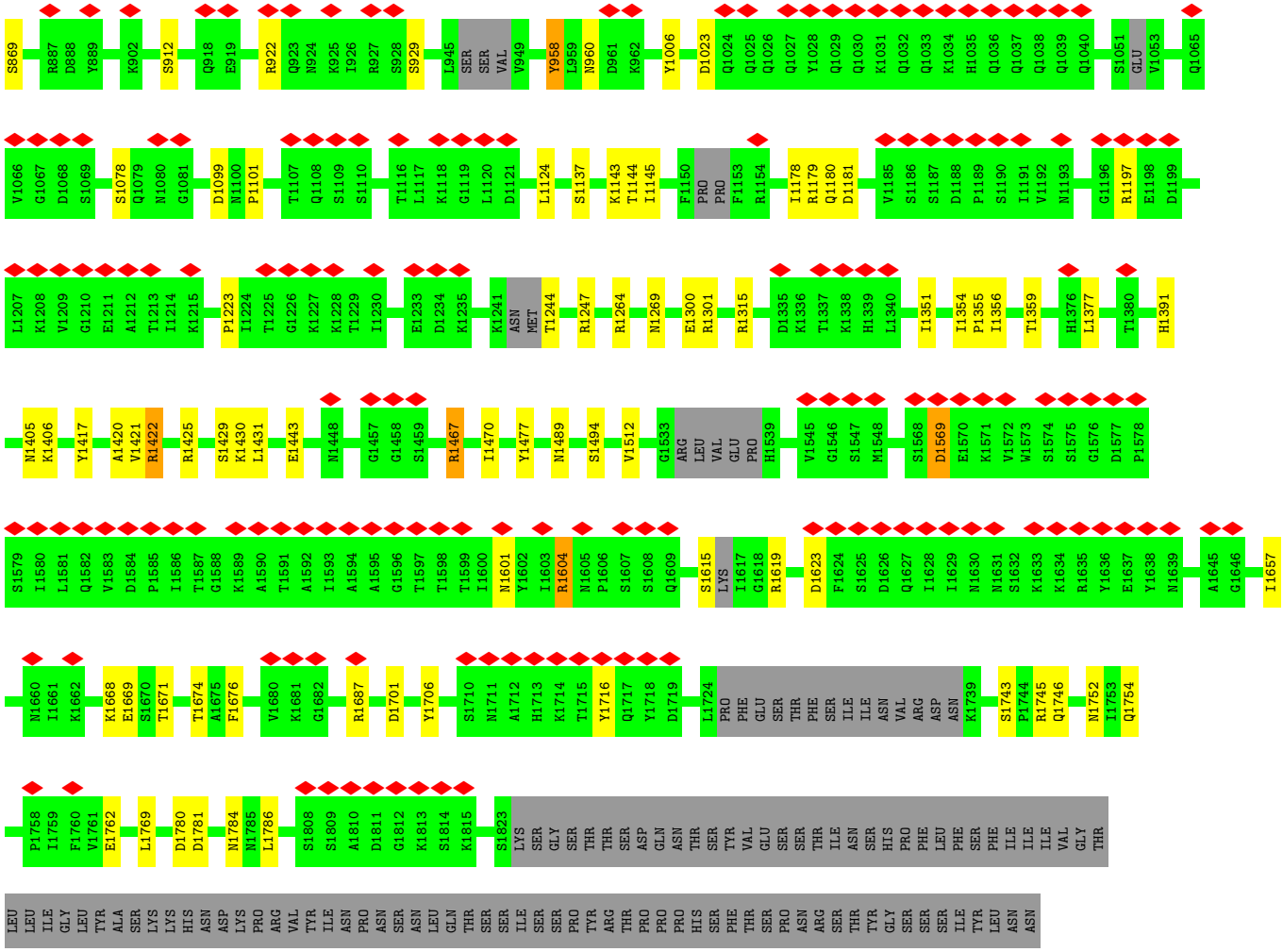




- Molecule 2: Nucleoporin 210

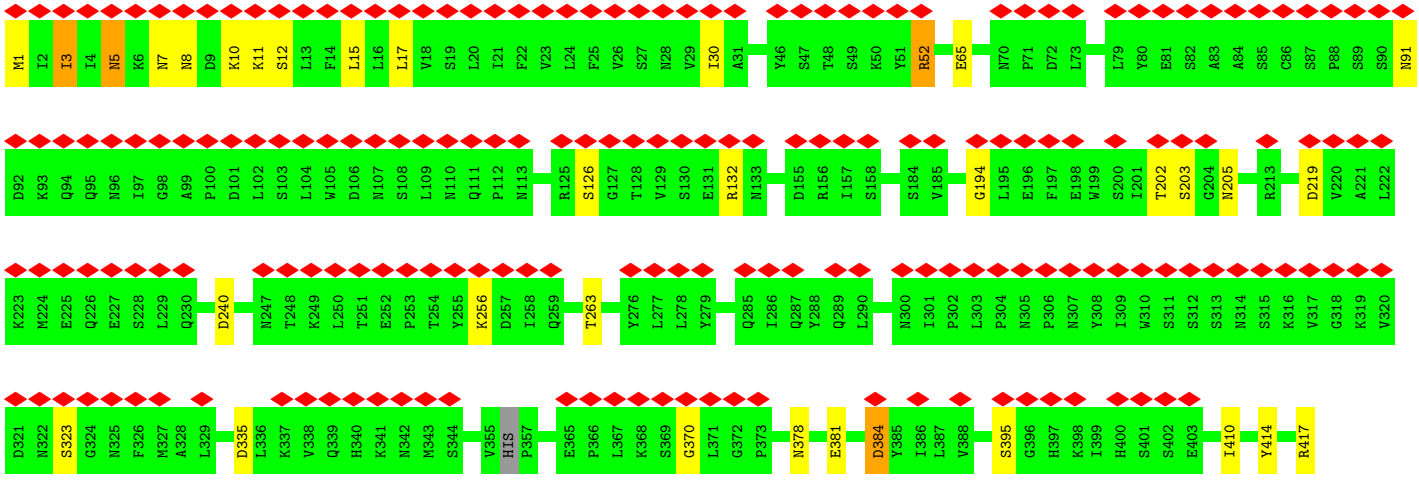
Chain 14:

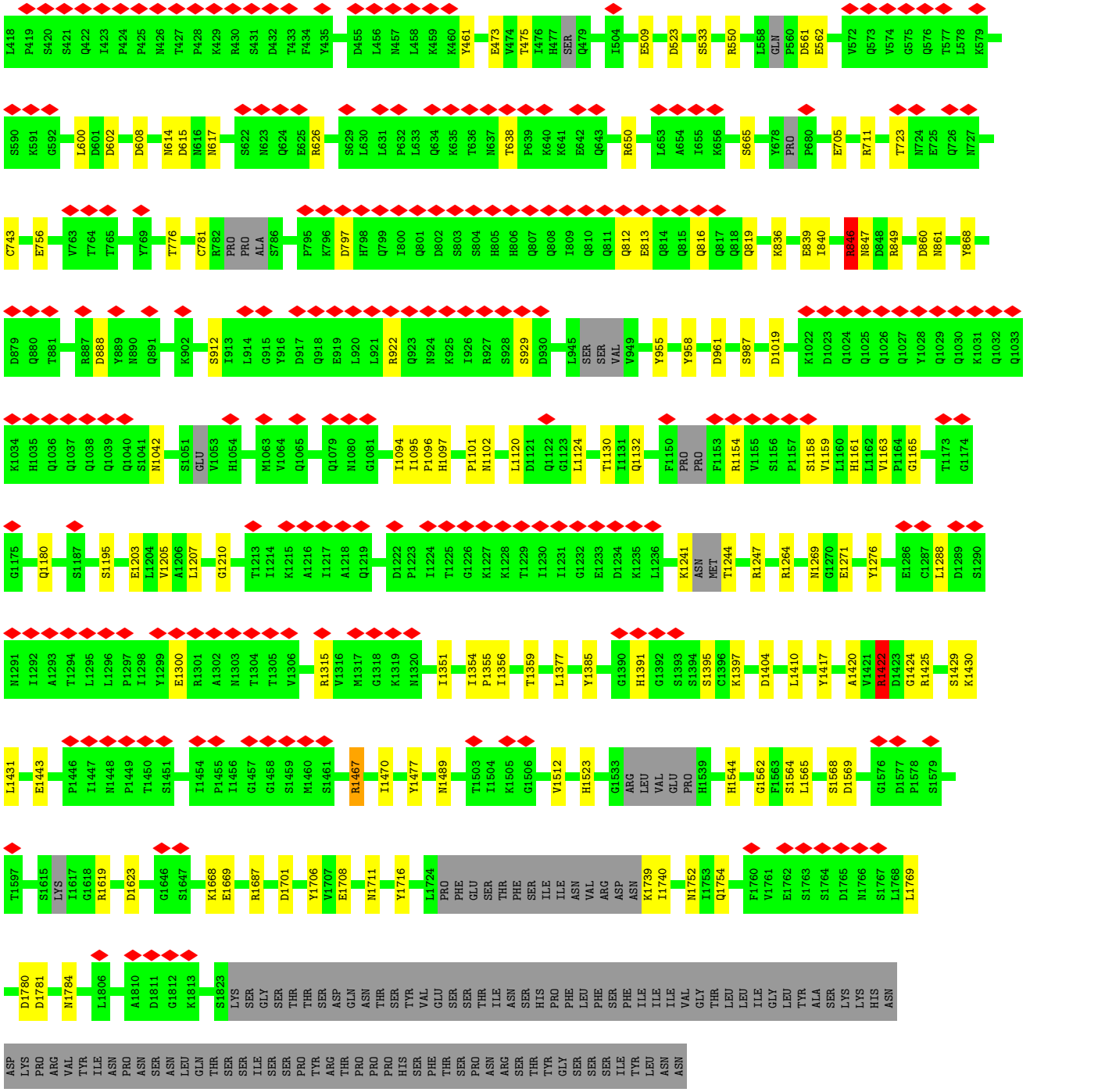




- Molecule 2: Nucleoporin 210

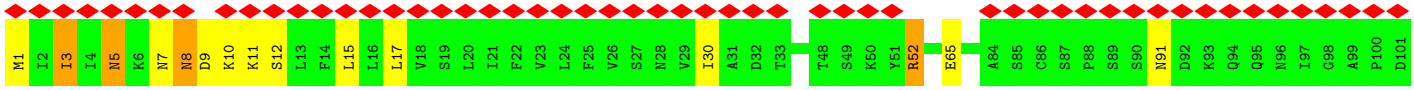
Chain 15:

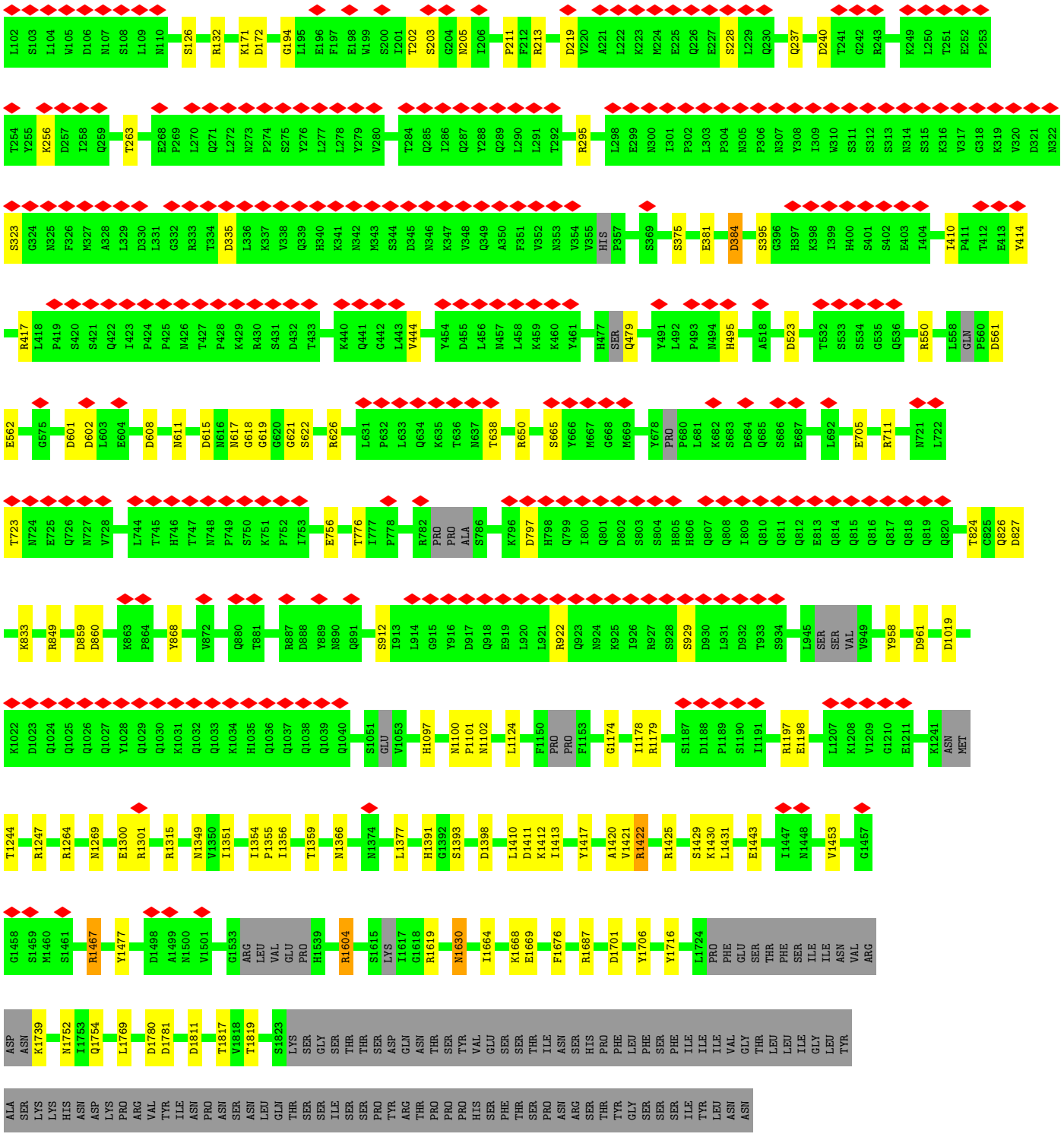




- Molecule 2: Nucleoporin 210

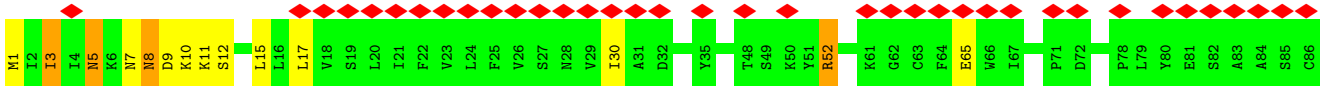
Chain 16:

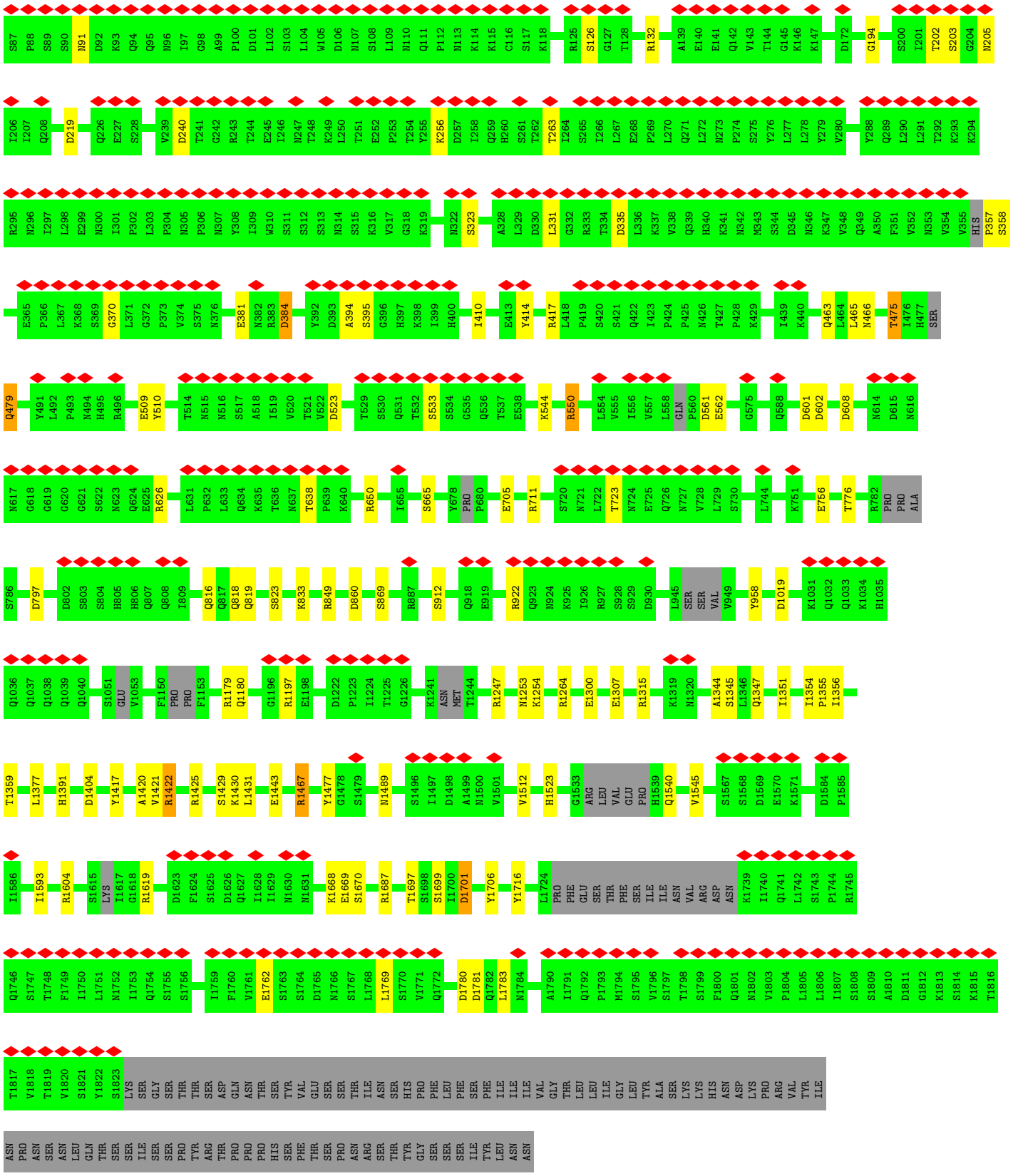




- Molecule 2: Nucleoporin 210

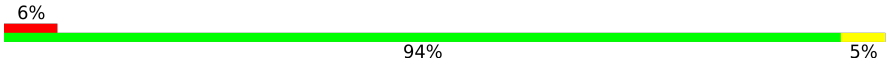
Chain 17:

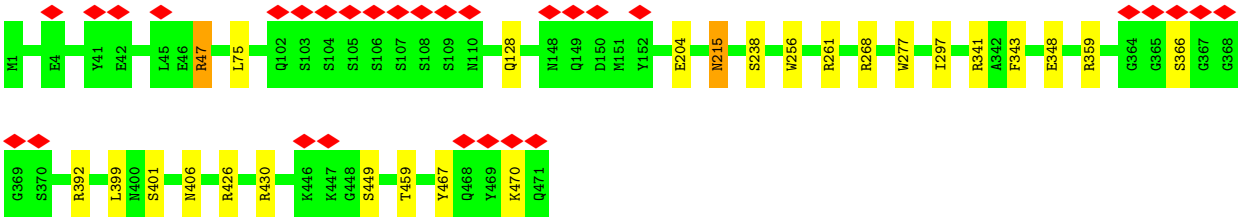




- Molecule 3: WD40 repeat-containing protein

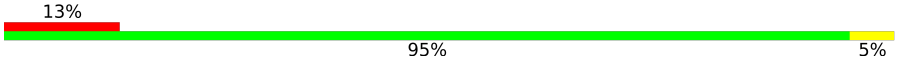
Chain 40:

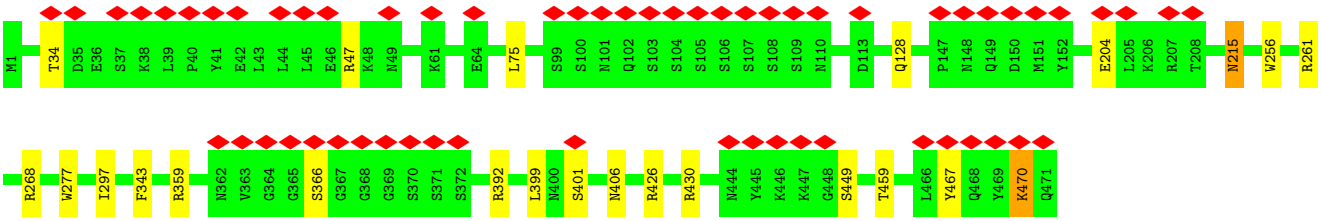




- Molecule 3: WD40 repeat-containing protein

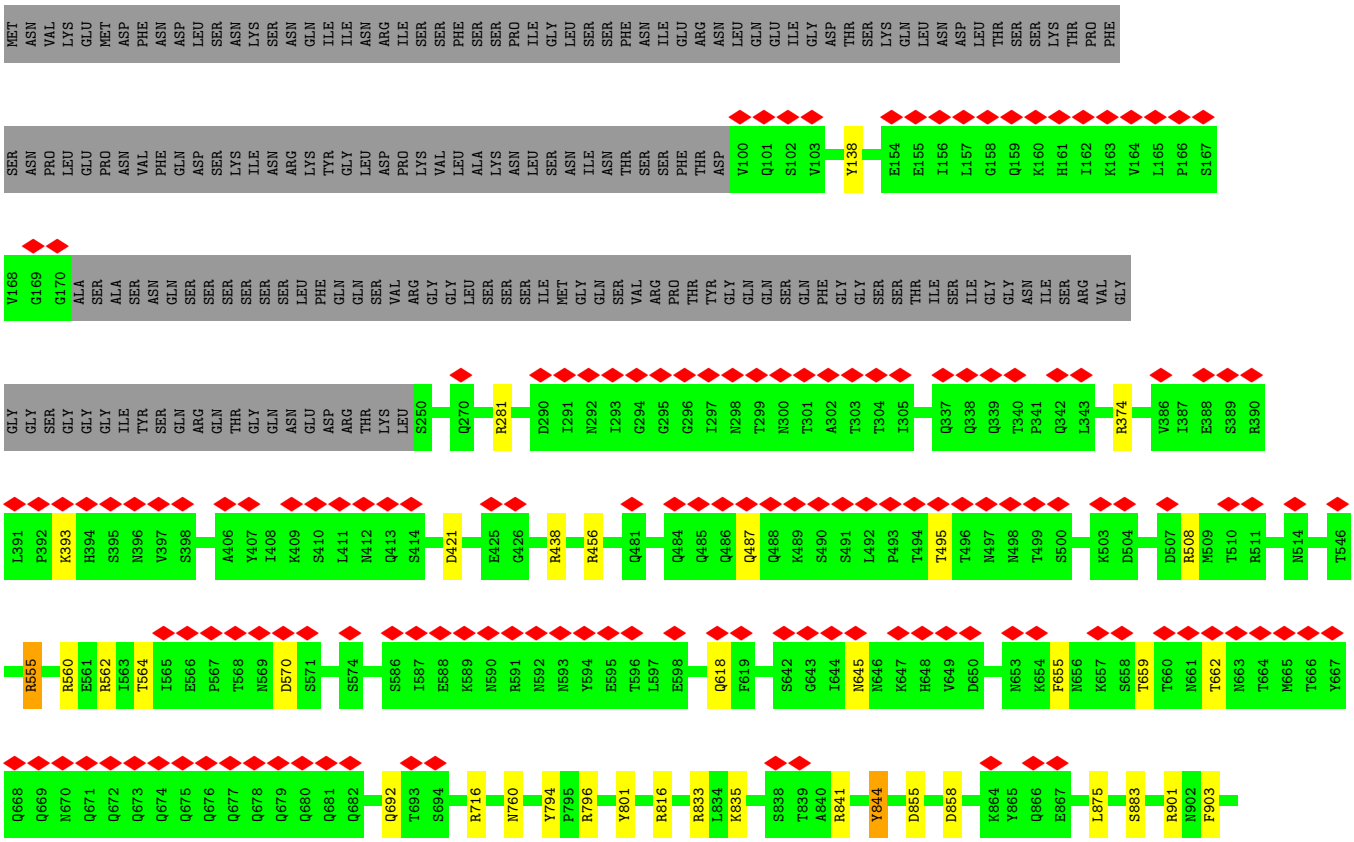
Chain 41:

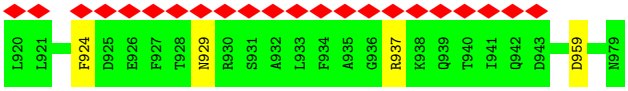




- Molecule 4: Nuclear pore protein

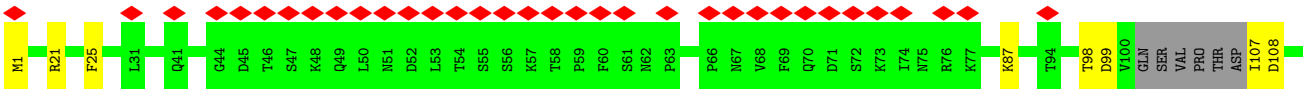
Chain A0:

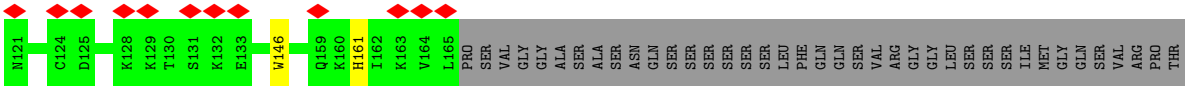


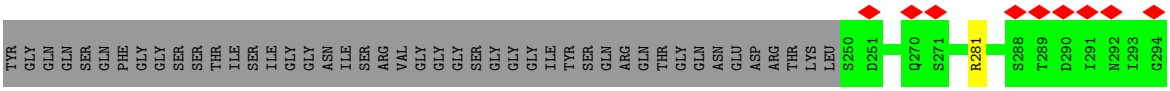


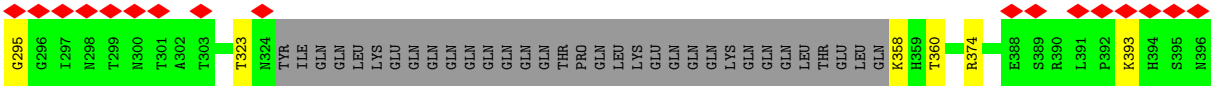
- Molecule 4: Nuclear pore protein

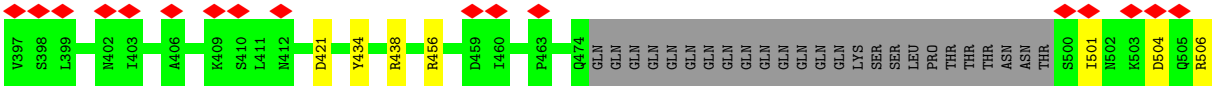
Chain A1:

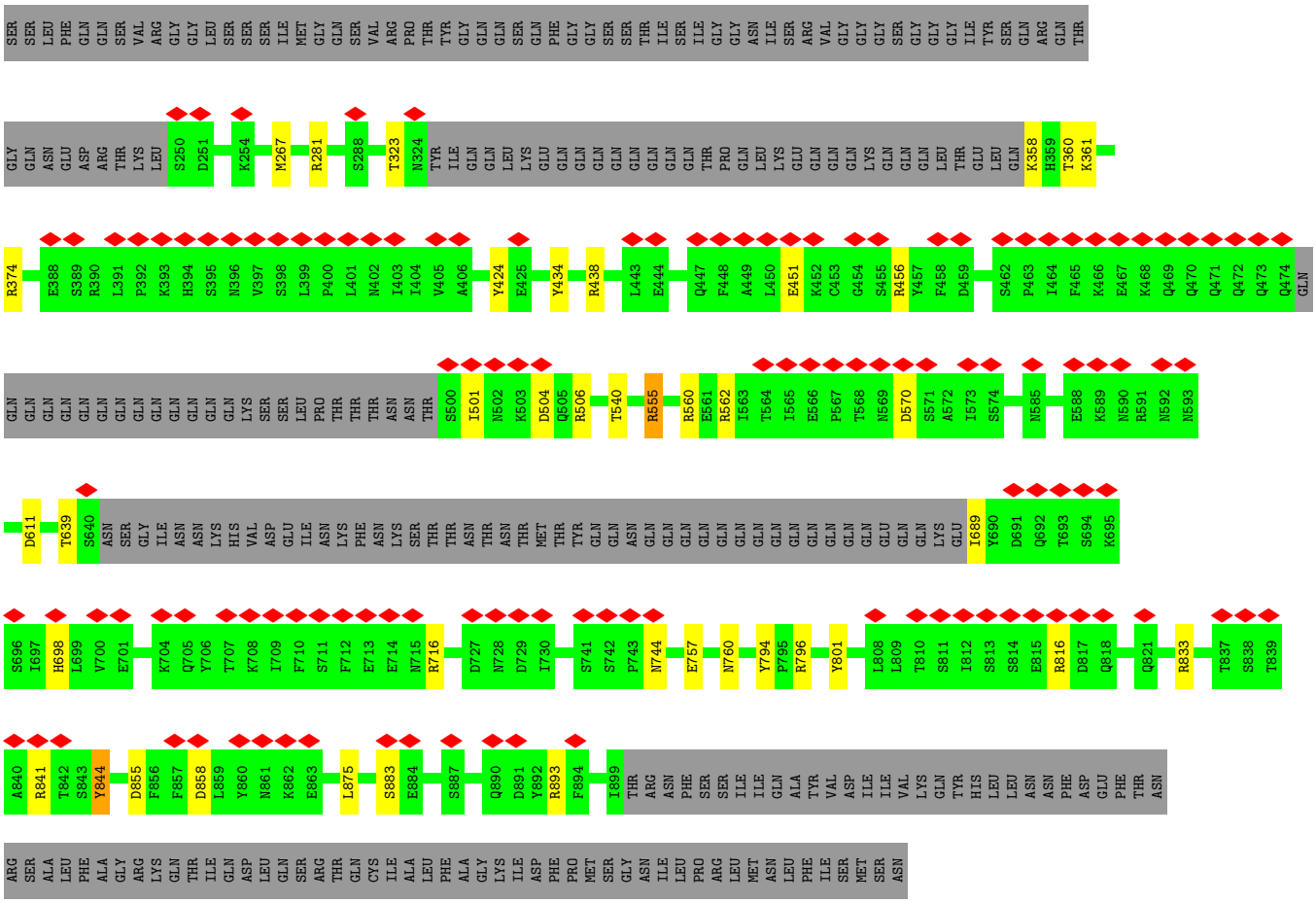






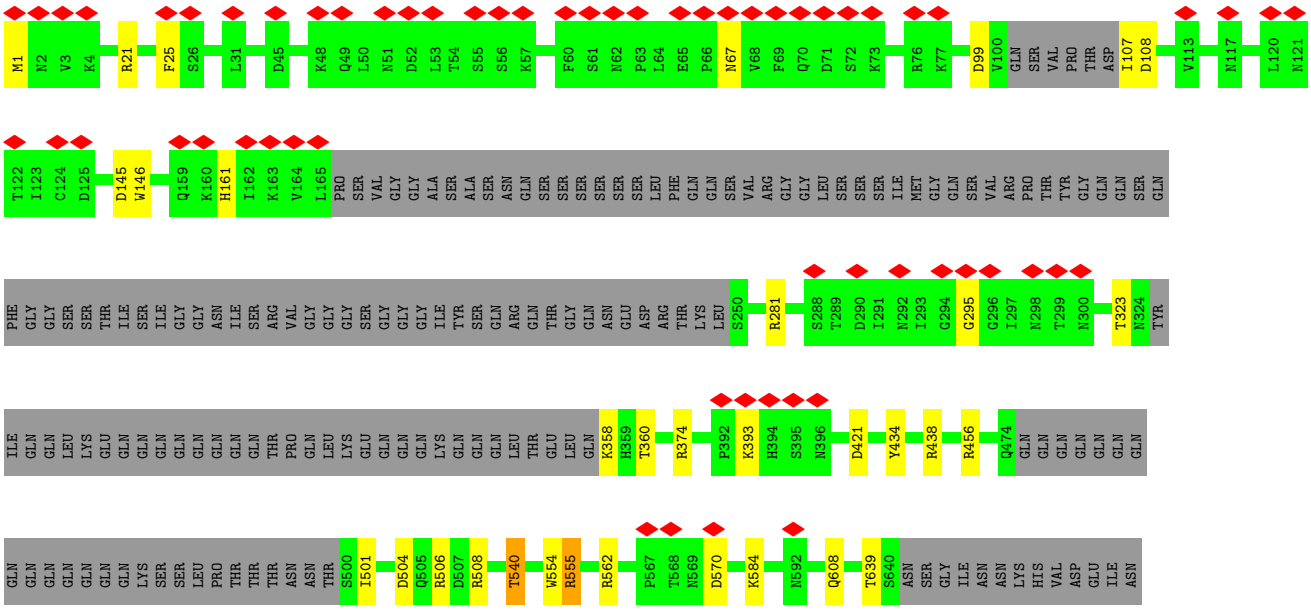


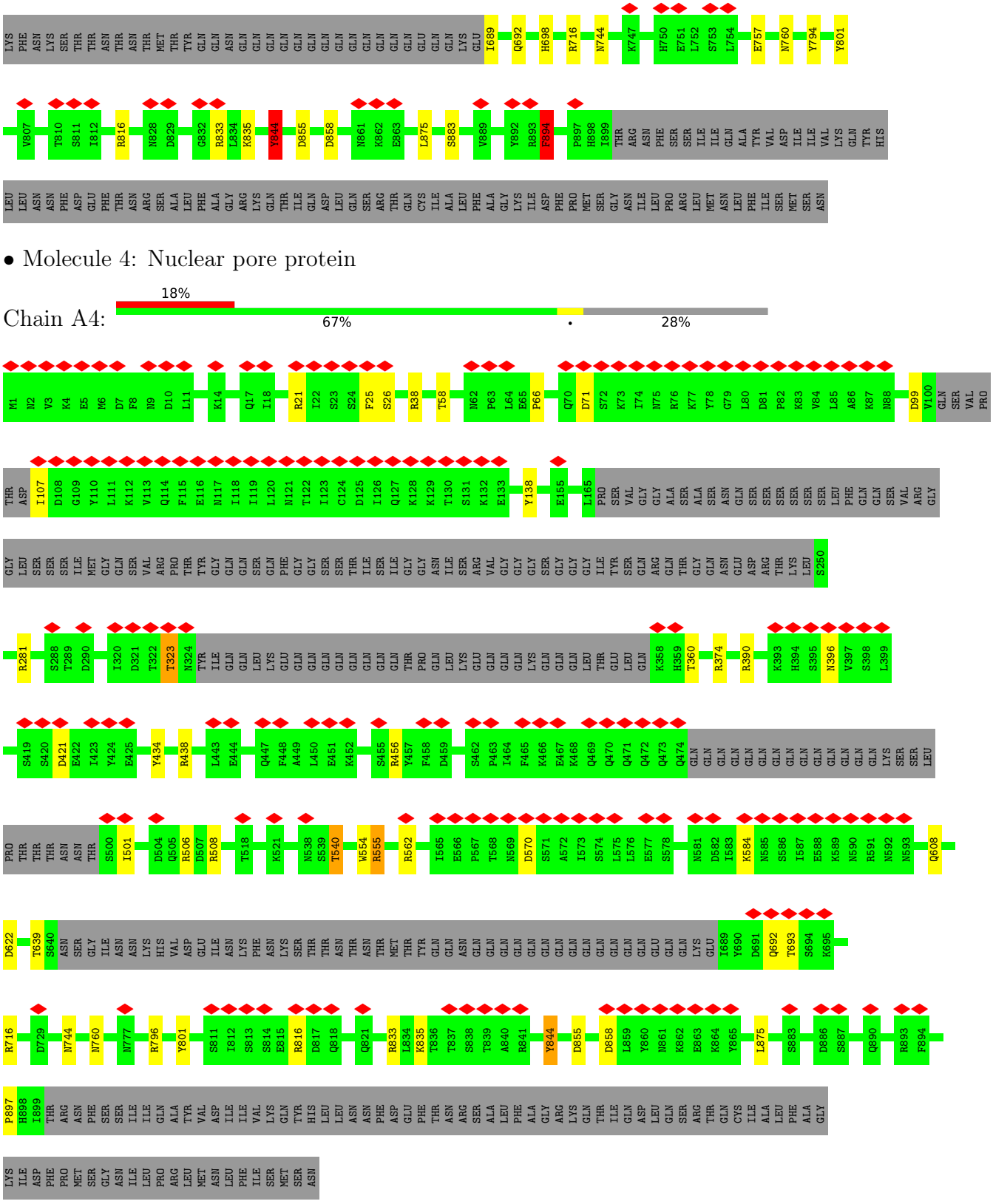

V397 S398 L399 N402 I403 A406 K409 S410 L411 N412 D421 Y434 R438 R456 D459 I460 P463 Q474 GLN GLN GLN GLN GLN GLN GLN GLN



• Molecule 4: Nuclear pore protein

Chain A3:



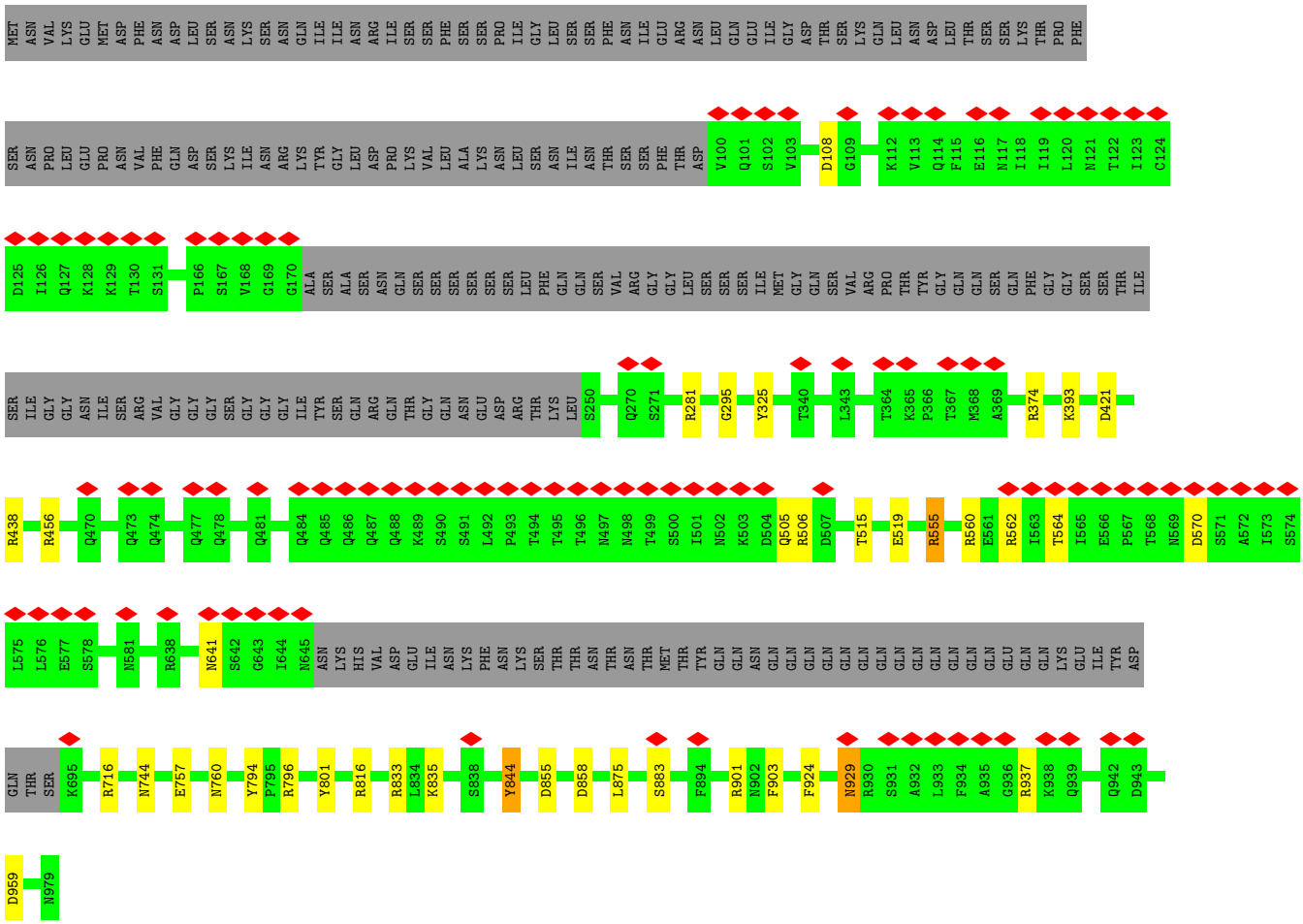


• Molecule 4: Nuclear pore protein

Chain A4: 18% 67% 28%

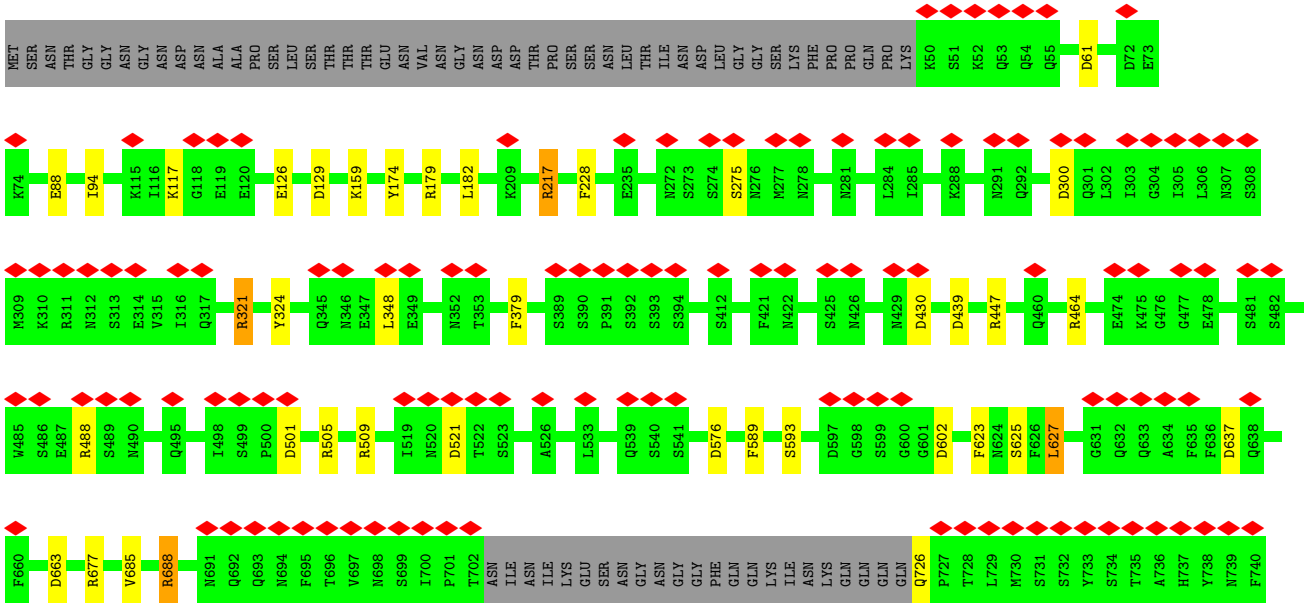
• Molecule 4: Nuclear pore protein

Chain A5: 11% 73% 23%



• Molecule 5: Nup188

Chain B0:



N741 E771 K772 G773 T780 V781 L782 I783 S784 L785 F786 K787 R788 G789 S790 F791 N792 H793 L794 Y795 D796 V797 E798 K799 R800 S801 S802 T803 T804 S805 S806 T807 S808 S809 T810 S811 S812 S813 S814 L815 S816 S817 S818 T819 F820 P821 L822 T823 K824 S825 I826 V827 K828 N831 I834 N835

Y852 F859 H860 L861 Q862 V863 I864 S865 D866 Y867 I870 S871 G872 N873 N874 N875 H876 N877 E878 T879 W880 E881 N882 I883 S884 E885 I886 F887 S888 A889 L890 D891 F892 I893 L894 N895 S899 T923 L924 S925 S926 L927 L928 D929 L930 E931 V932 L933 Q934 N935 T936 N937 K938 S939 I940

D941 R942 T943 S944 S945 I946 D947 N948 I949 L950 K951 S952 S953 L954 K955 F956 S957 K958 S959 R972 N979 N980 Q981 N982 N983 D984 N985 N986 N987 E988 ASN ASN ASN ASN ASN ASN ASN GLY ASP ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN GLU GLU ASN ASN ASN ASN ASN ASN ASP ASN

I1017 N1018 D1019 N1020 N1021 I1022 E1023 N1024 Y1025 E1026 N1027 E1028 N1032 F1041 F1042 I1043 VAL LYS GLN ASN GLU THR ASN LEU LEU ILE ASP GLN GLU ASP ARG ASN GLY LEU THR SER THR ILE VAL THR ASN SER ILE THR THR GLU THR ILE THR SER LYS THR D1080 Y1081 N1082 N1083 L1084 F1085

I1086 V1087 L1088 F1089 N1090 Y1091 I1092 N1093 I1094 I1095 S1096 D1097 C1098 Q1099 D1100 I1101 Q1102 I1103 L1104 S1105 C1106 E1107 I1108 L1109 R1117 S1121 N1122 L1128 D1132 E1133 P1134 L1137 M1138 I1147 S1157 L1158 Q1159 L1160 K1161 T1162 N1163 I1164 L1165 R1166 R1181 N1188 ASN ILE ASN ASN ASN

ASN ASN ASN ASN ASP D1199 S1200 G1201 G1202 D1203 F1209 R1217 N1218 V1219 S1220 I1221 N1222 D1223 N1224 S1225 E1226 F1227 S1228 Y1245 N1260 L1263 D1264 K1267 T1268 I1269 N1270 E1271 E1272 E1273 E1274 Q1275 E1276 E1277 E1278 S1279 I1280 I1281 N1282 E1283 E1284 L1285 T1310 T1311 A1312 T1313 T1314 T1315 V1316

G1317 N1318 L1319 V1320 C1321 S1322 T1323 L1324 S1325 N1326 N1327 K1328 W1329 N1330 E1331 I1332 F1333 K1334 N1335 N1336 K1337 N1345 Q1350 D1353 L1354 E1355 N1356 V1357 F1358 P1359 I1360 Q1361 K1362 I1363 R1364 D1365 Y1366 W1367 M1368 V1369 N1370 N1371 L1372 P1373 S1374 P1375 D1376 Q1377 Y1386 D1403 D1414 Q1415 Y1416 Y1417

L1418 E1419 L1420 L1421 I1422 Q1423 R1424 F1441 R1446 N1460 G1461 G1462 S1463 G1464 S1465 G1466 S1467 G1468 S1469 S1470 N1471 H1481 D1485 K1486 A1487 T1488 S1489 I1490 E1491 N1492 Q1493 S1494 I1495 K1496 T1497 R1501 E1526 S1527 V1528 D1529 I1530 E1531 I1532 L1533 S1534 K1535 N1538 T1568 S1569 Q1570 H1571

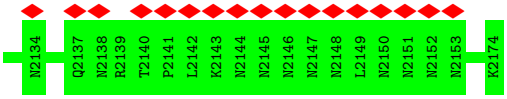
Q1572 Y1573 I1574 E1575 I1576 K1577 V1578 T1591 H1594 F1595 ARG VAL PRO PRO ILE SER SER MET ASP GLY THR THR THR THR THR SER GLY GLY ASN VAL GLY GLU GLY LYS THR ILE ASN GLY LYS Q1626 Y1639 R1647 L1648 D1649 P1650 N1651 A1652 L1653 I1654 N1659 N1660 L1661 L1662 E1663

N1664 L1665 A1666 K1667 K1670 N1671 N1674 M1675 V1676 Q1699 P1700 L1701 E1704 Q1705 L1706 L1707 D1708 N1709 R1710 Q1713 L1714 D1717 H1718 S1719 L1720 K1721 Y1722 L1723 Q1724 A1732 S1733 T1734 E1735 I1736 S1737 A1738 A1739 T1740 A1741 S1742 I1743 Y1744 G1745 G1746 I1747 N1748 Y1749 Y1750 F1751 HIS ASN ASN ASP

ASP ASP TYR ASP ASN HIS ARG Q1763 R1773 K1780 L1789 E1790 S1791 S1792 E1793 R1794 F1795 I1796 E1797 Q1798 Y1839 T1851 K1852 R1853 Y1854 Y1855 L1856 S1857 M1858 N1859 I1860 Y1861 R1862 S1880 E1881 L1882 N1883 N1887 P1891 I1892 T1893 K1894 N1895 E1896 K1897 H1898 K1899 N1900 L1901 V1902 Q1903 V1904

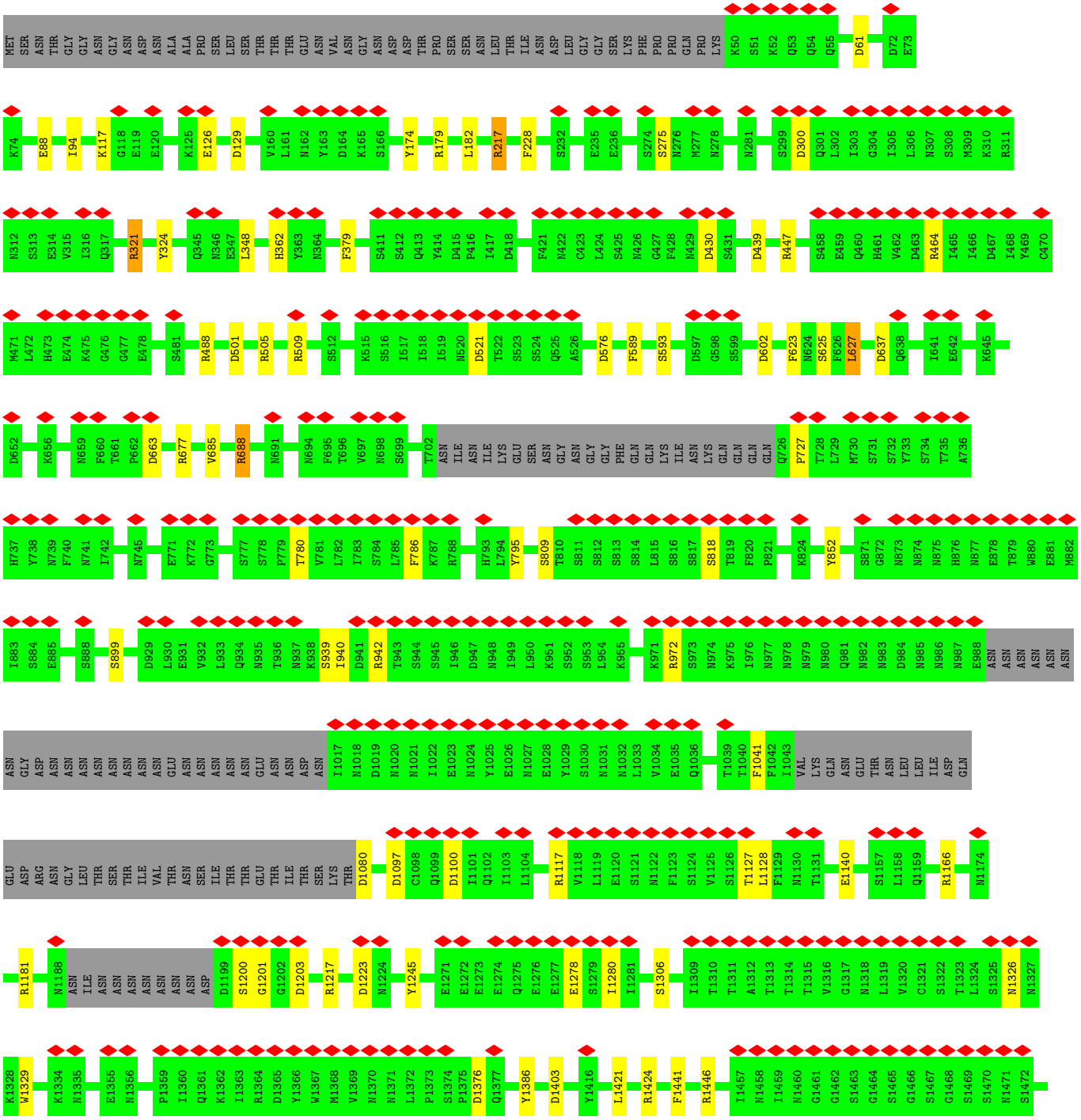
K1905 E1906 F1907 I1908 D1909 D1910 S1911 Q1912 R1913 L1914 Q1915 Q1916 Q1917 Q1918 L1919 Q1920 Q1921 Q1922 Q1923 Q1924 L1925 Q1926 Q1927 S1928 Q1929 L1930 Q1931 Q1932 S1933 T1934 P1935 Y1936 R1937 T1938 S1939 H1940 Y1941 Q1942 Q1943 Q1944 L1945 L1946 Q1947 L1948 Q1949 Q1950 Q1951 L1952 Q1953 K1954 Q1955 Q1956 Q1957 P1958 Q1959 Q1960 Q1961 R1989

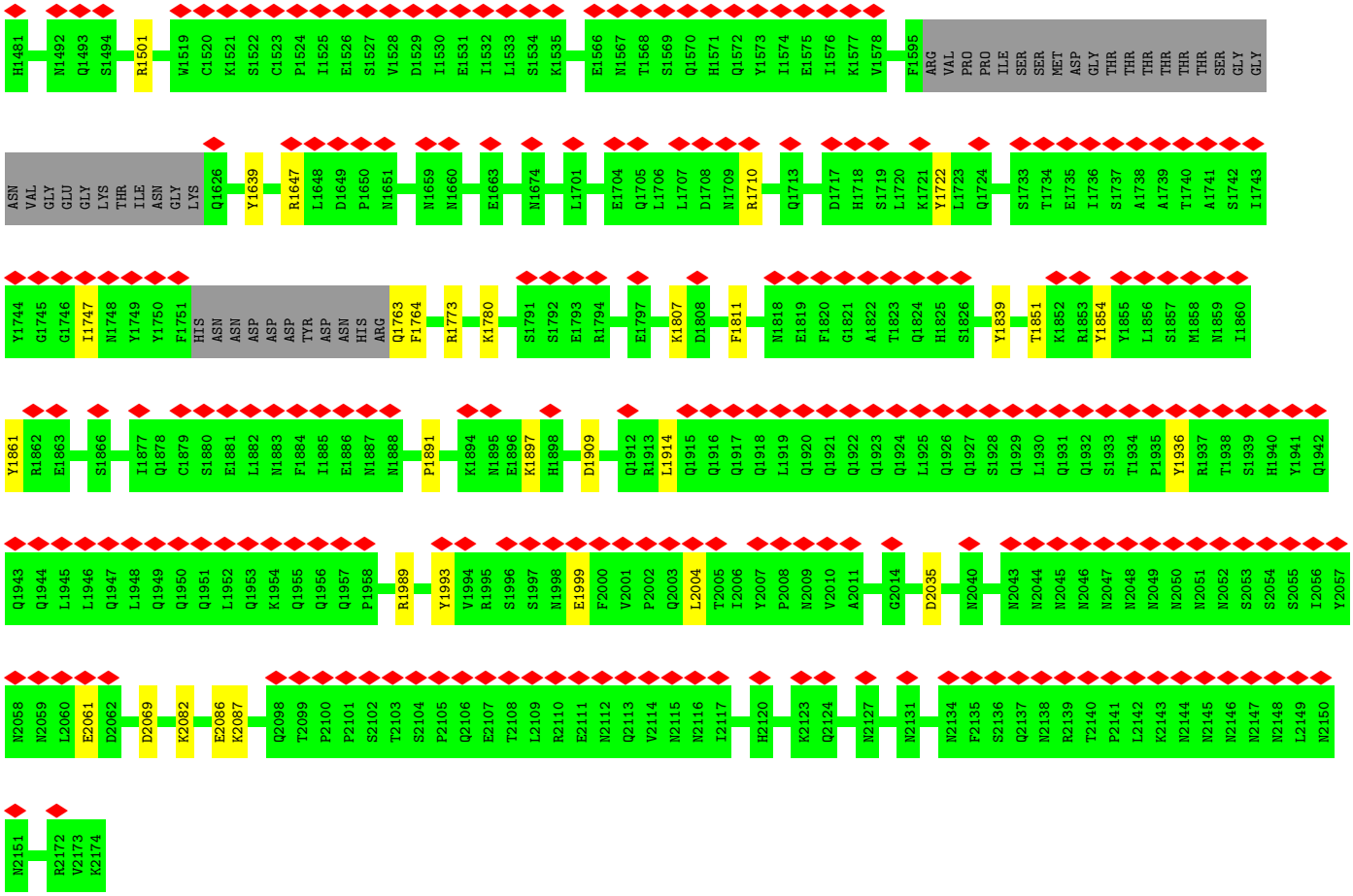
Y1993 S1996 S1997 N1998 E1999 F2000 V2001 P2002 Q2003 L2004 Q2021 D2035 N2046 N2047 N2048 N2049 N2050 N2051 N2052 S2053 S2054 S2055 I2056 Y2057 N2058 N2059 L2060 E2061 V2068 D2069 K2082 E2086 K2087 P2100 P2101 S2102 T2103 S2104 P2105 Q2106 E2107 T2108 L2109 R2110 E2111 N2112 Q2113 N2116 I2117 H2120



• Molecule 5: Nup188

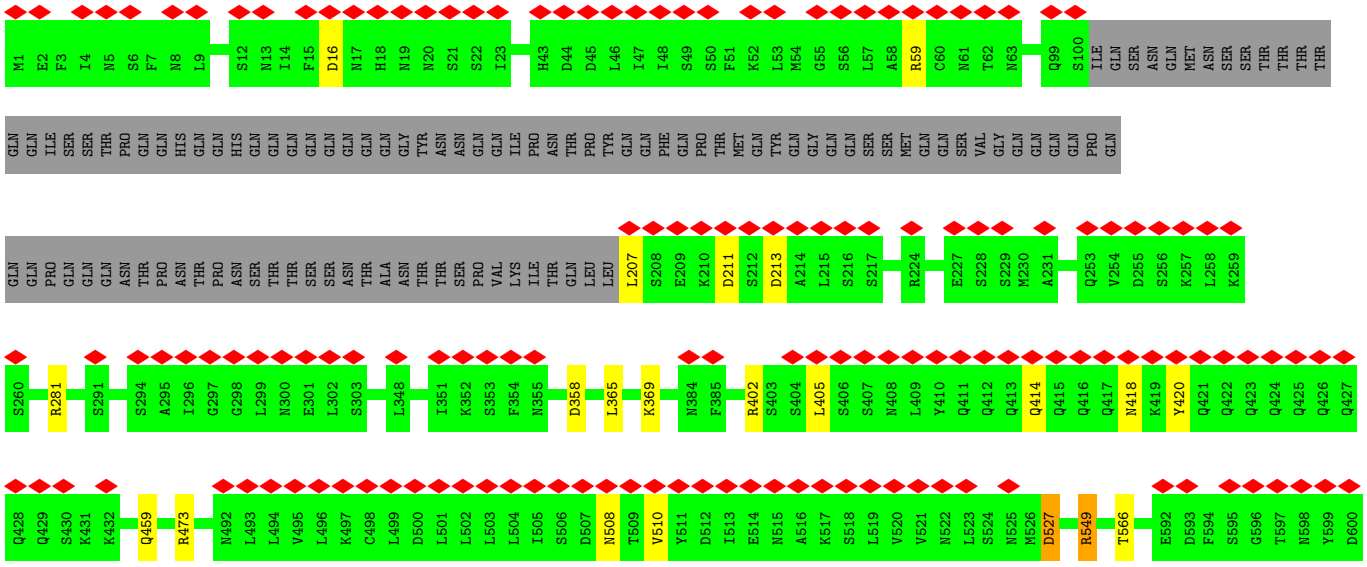
Chain B1:

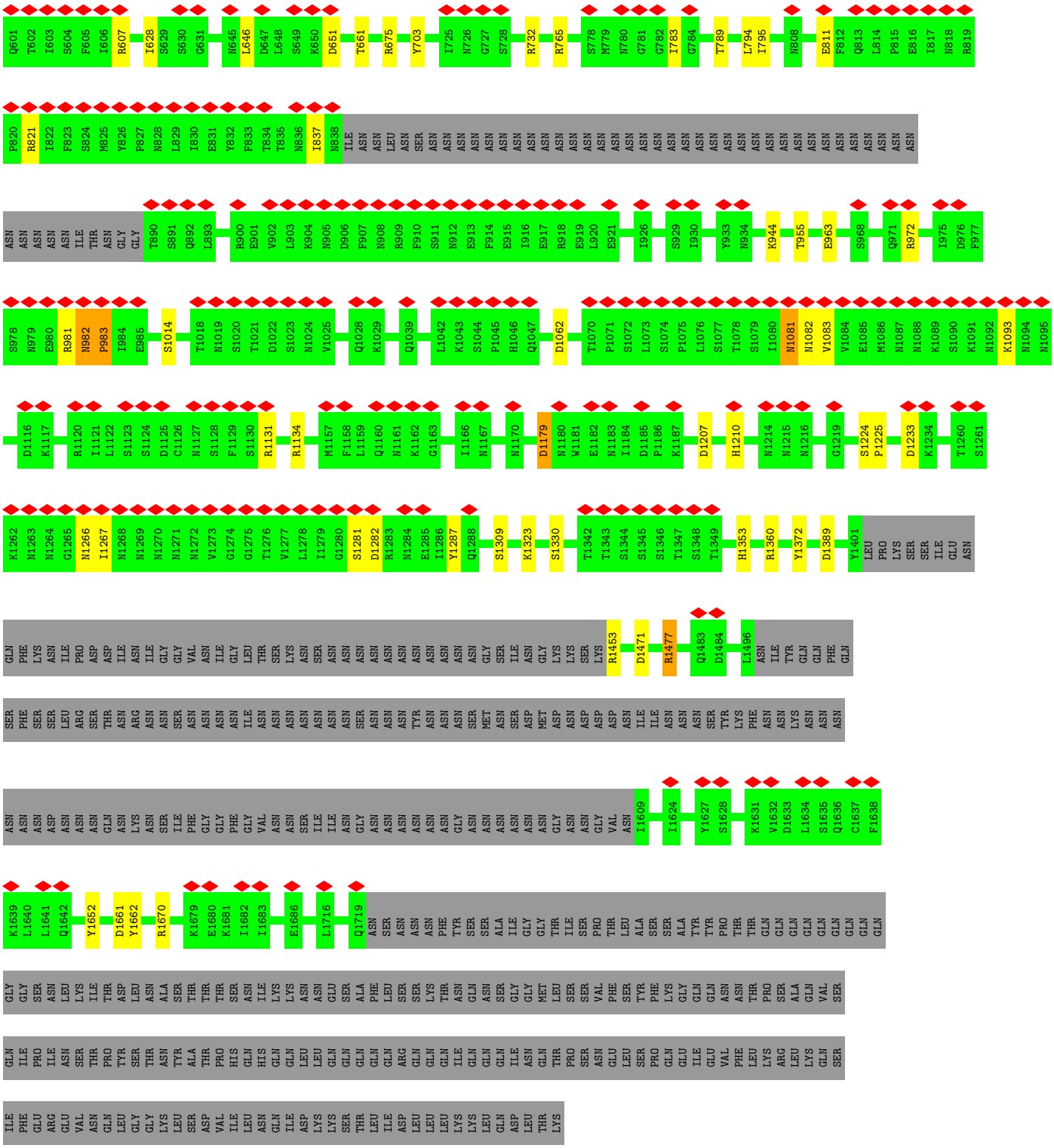


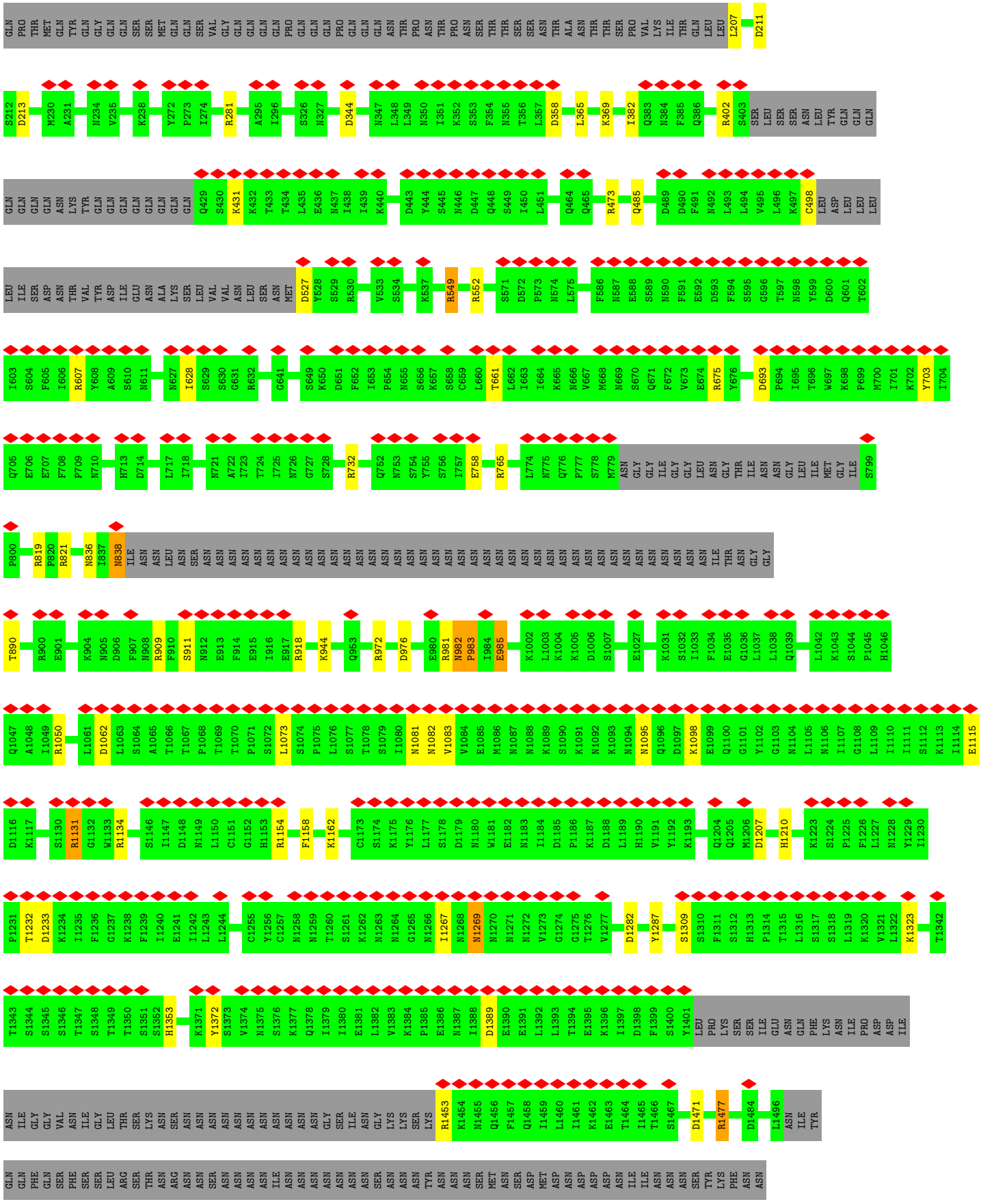


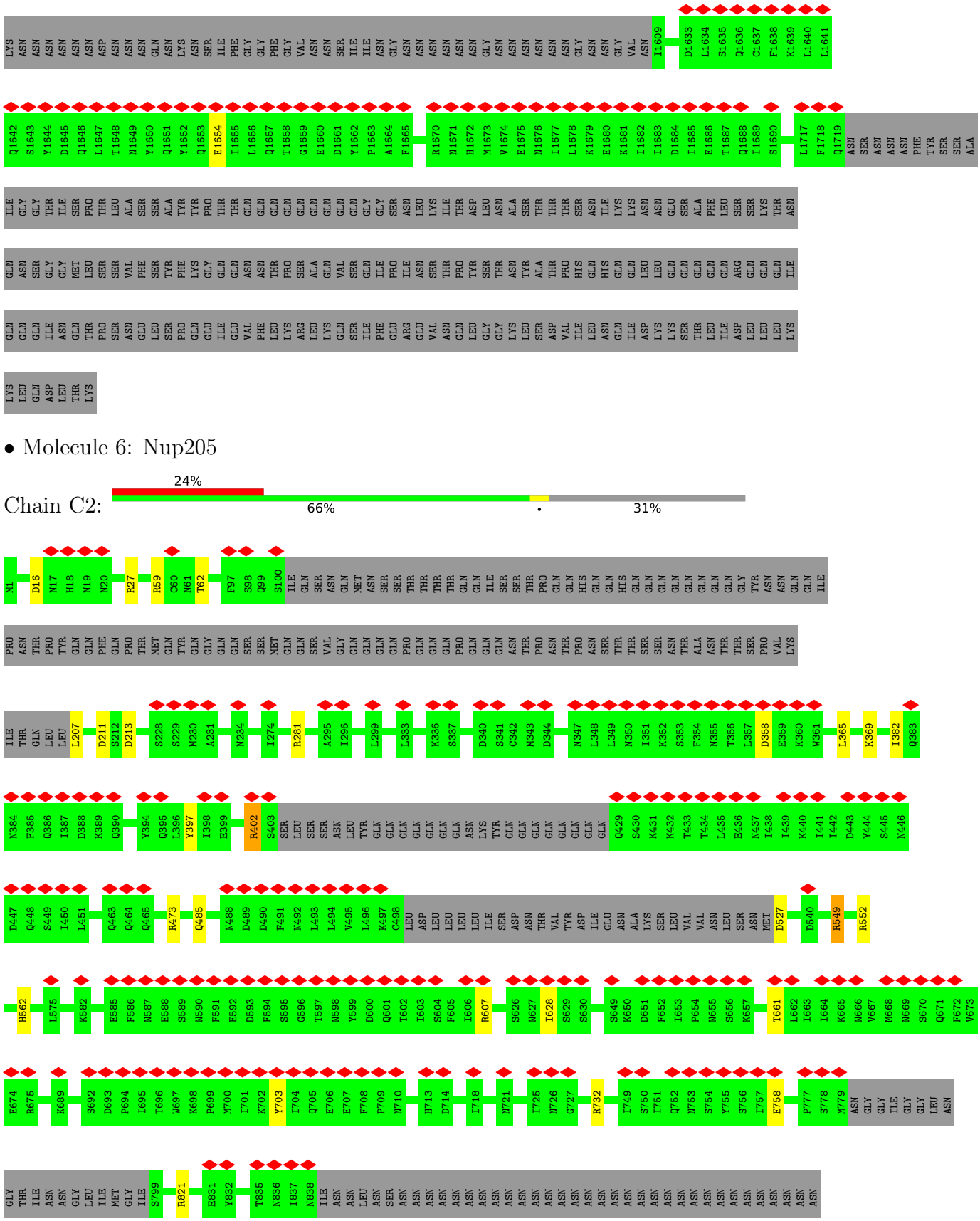
- Molecule 6: Nup205

Chain C0:




Q601 T602 I603 S604 F605 I606 R607 I628 S629 S630 G631 N645 L646 D647 L648 S649 K650 D651 T661 R675 Y703 I725 N726 G727 S728 R732 R765 S778 M779 N780 G781 G782 I783 G784 T789 L794 I795 N808 E811 F812 Q813 L814 P815 E816 I817 N818 R819
P820 R821 I822 F823 S824 M825 Y826 P827 N828 L829 I830 E831 Y832 F833 T834 T835 N836 I837 N838 ILE ASN ASN LEU ASN SER ASN ASN ASN

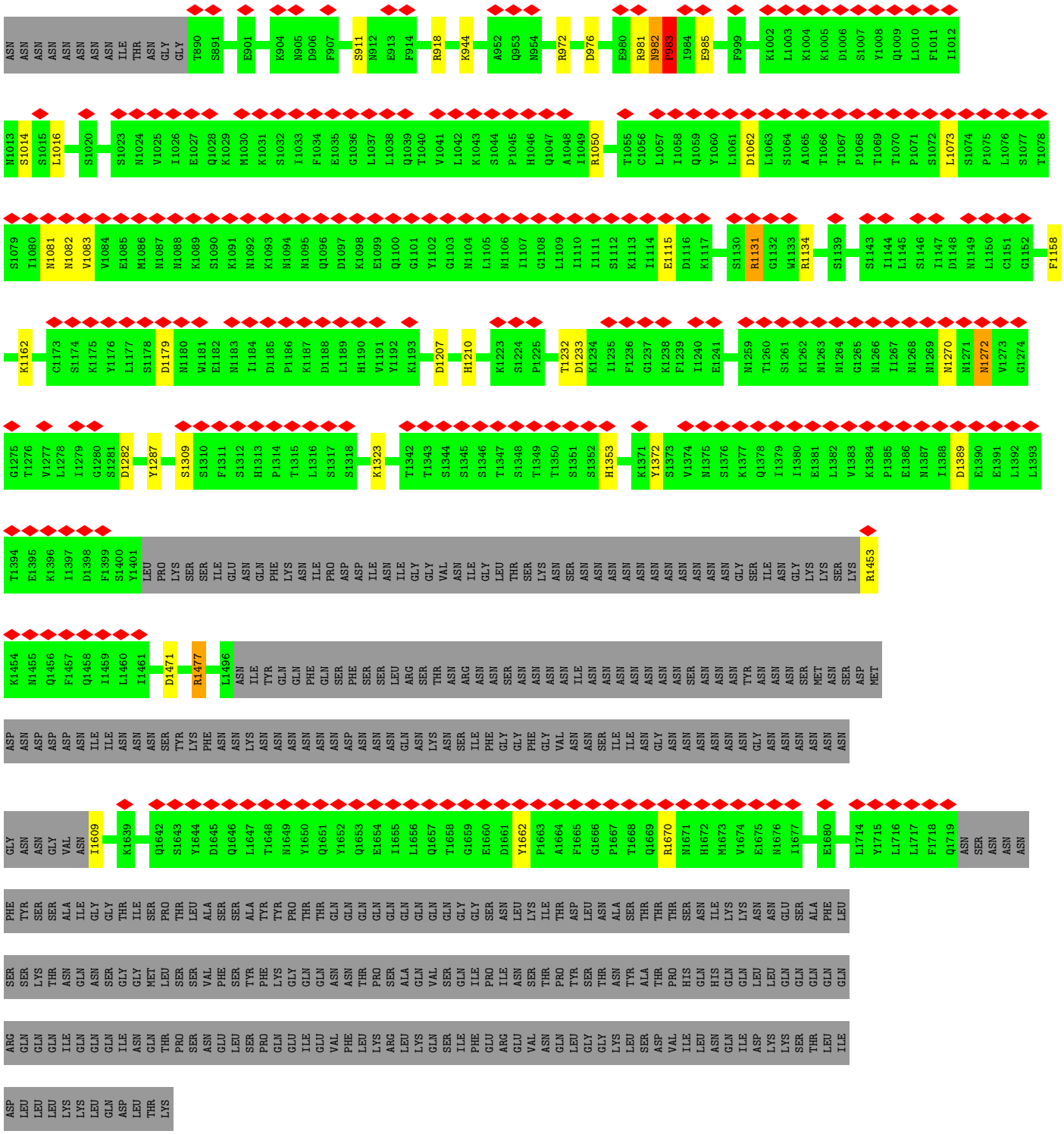

GLN PRO THR MET GLN TYR GLN GLY GLN GLN SER SER MET GLN GLN SER VAL GLY GLN GLN GLN GLN PRO GLN GLN GLN GLN GLN ASN THR PRO ASN THR PRO ASN SER THR THR SER SER ASN THR ALA ASN THR THR SER PRO VAL LYS ILE THR GLN LEU LEU L207 D211
S212 D213 M230 A231 N234 V235 K238 Y272 P273 I274 R281 A295 I296 S326 N327 D344 N347 L348 L349 N350 I351 K352 S353 F354 N355 T356 L357 D358 L365 K369 I382 Q383 N384 F385 Q386 R402 S403 SER LEU SER SER ASN LEU TYR GLN GLN GLN
GLN GLN GLN GLN LYS TYR GLN GLN GLN GLN GLN GLN Q429 S430 K431 K432 T433 T434 L435 E436 N437 I438 I439 K440 D443 Y444 S445 N446 D447 Q448 S449 I450 L451 Q464 Q465 R473 Q485 D489 D490 F491 N492 L493 L494 V495 L496 K497 C498 LEU ASP LEU LEU LEU
LEU ILE SER ASP ASN THR VAL TYR ASP ILE GLU ASN ALA LYS SER LEU VAL VAL ASN LEU SER ASN MET D527 Y528 S529 R530 V533 S534 K537 R549 R552 S571 D572 P573 N574 L575 F586 N587 E588 S589 N590 F591 E592 D593 F594 S595 G596 T597 N598 Y599 D600 Q601 T602
I603 S604 F605 I606 R607 Y608 A609 S610 N611 N627 I628 S629 S630 G631 R632 G641 S649 K650 D651 F652 I653 P654 N655 S656 K657 S658 C659 L660 T661 L662 I663 I664 K665 N666 V667 M668 N669 S670 Q671 F672 V673 E674 R675 Y676 D693 P694 I695 T696 W697 K698 P699 M700 I701 K702 Y703 I704
Q705 E706 E707 F708 P709 N710 H713 D714 L717 I718 N721 A722 I723 T724 I725 N726 G727 S728 R732 Q752 N753 S754 Y755 S756 I757 E758 R765 L774 N775 Q776 P777 S778 M779 ASN GLY GLY ILE GLY GLY LEU ASN GLY THR ILE ASN ASN GLY LEU ILE MET GLY ILE S799
P800 R819 P820 R821 N836 I837 N838 ILE ASN ASN LEU ASN SER ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ILE THR ASN GLY GLY
T890 R900 E901 K904 N905 D906 F907 N908 R909 F910 S911 N912 E913 F914 E915 I916 E917 R918 K944 Q963 R972 D976 E980 R981 N982 P983 I984 E985 K1002 L1003 K1004 K1005 D1006 S1007 E1027 K1031 S1032 I1033 F1034 E1035 G1036 L1037 L1038 Q1039 L1042 K1043 S1044 P1045 H1046
Q1047 A1048 I1049 R1050 L1061 D1062 L1063 S1064 A1065 T1066 T1067 P1068 T1069 T1070 P1071 S1072 L1073 S1074 P1075 L1076 S1077 T1078 S1079 I1080 N1081 N1082 V1083 V1084 E1085 M1086 N1087 N1088 K1089 S1090 K1091 N1092 K1093 N1094 N1095 Q1096 D1097 K1098 E1099 Q1100 G1101 Y1102 G1103 N1104 L1105 N1106 I1107 G1108 L1109 I1110 I1111 S1112 K1113 I1114 E1115
D1116 K1117 S1130 R1131 G1132 W1133 R1134 S1146 I1147 D1148 N1149 L1150 C1151 G1152 H1153 R1154 F1158 K1162 C1173 S1174 K1175 Y1176 L1177 S1178 D1179 N1180 W1181 E1182 N1183 I1184 D1185 P1186 K1187 D1188 L1189 H1190 V1191 Y1192 K1193 Q1204 Q1205 M1206 D1207 H1210 K1223 S1224 P1225 F1226 L1227 N1228 Y1229 I1230
P1231 T1232 D1233 K1234 I1235 F1236 G1237 K1238 F1239 I1240 E1241 I1242 L1243 L1244 C1255 Y1256 C1257 N1258 N1259 T1260 S1261 K1262 N1263 N1264 G1265 N1266 I1267 N1268 N1269 N1270 N1271 N1272 V1273 G1274 G1275 T1276 V1277 D1282 Y1287 S1309 S1310 F1311 S1312 H1313 P1314 T1315 L1316 S1317 S1318 L1319 K1320 V1321 L1322 K1323 T1342
T1343 S1344 S1345 S1346 T1347 S1348 T1349 T1350 S1351 S1352 H1353 K1371 Y1372 S1373 V1374 N1375 S1376 K1377 Q1378 I1379 I1380 E1381 L1382 V1383 K1384 P1385 E1386 N1387 I1388 D1389 E1390 E1391 L1392 L1393 T1394 E1395 K1396 I1397 D1398 F1399 S1400 Y1401 LEU PRO LYS SER SER ILE GLU ASN GLN PHE LYS ASN ILE PRO ASP ASP ILE
ASN ILE GLY GLY VAL ASN ILE GLY LEU THR SER LYS ASN SER ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN



- Molecule 6: Nup205

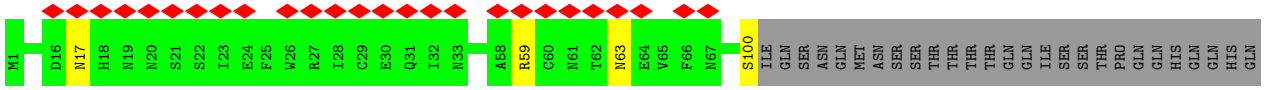
Chain C2:

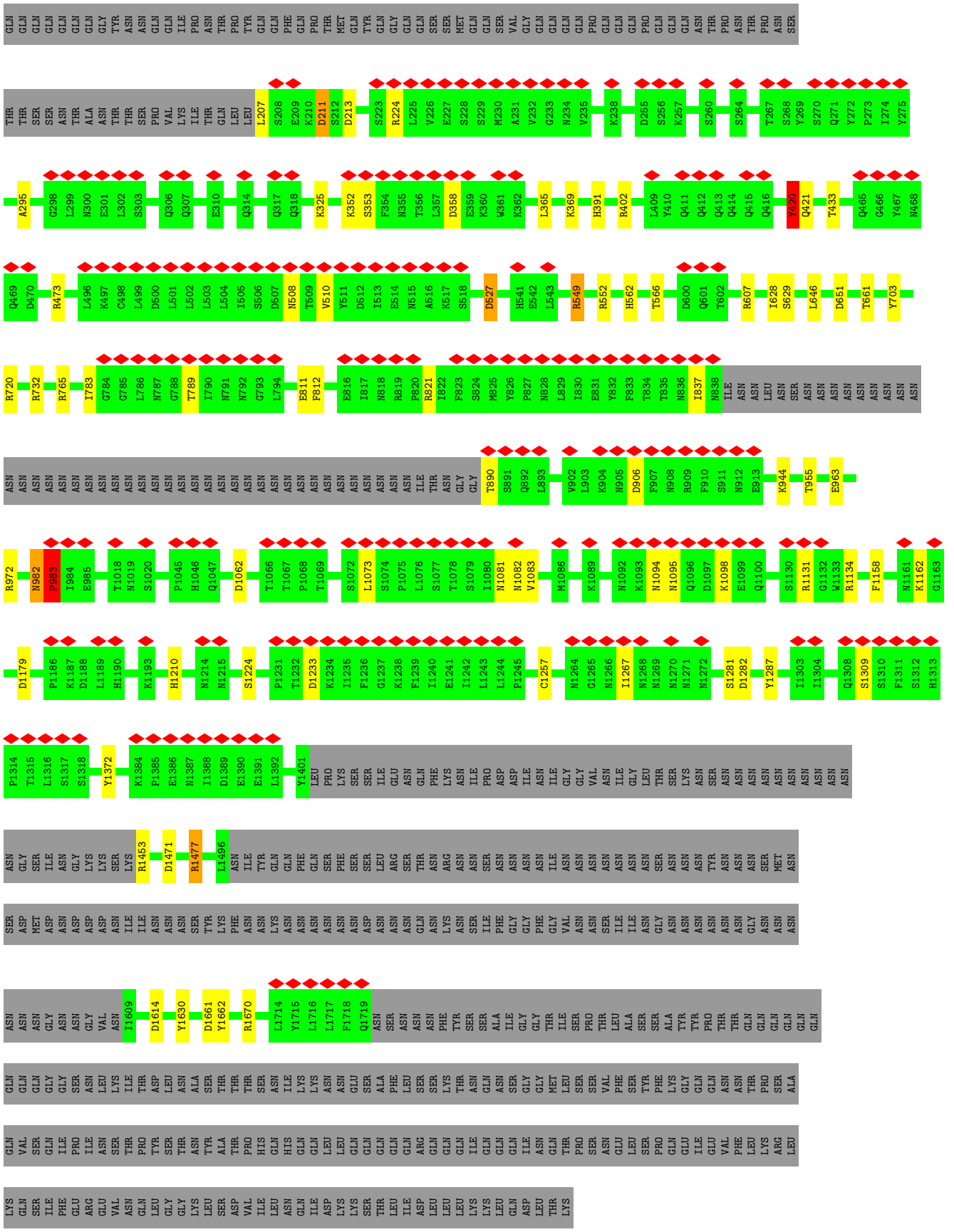
M1 D16 N17 H18 N19 N20 R27 R59 C60 M61 T62 F97 S98 Q99 S100 ILE GLN SER ASN GLN MET ASN SER SER THR THR THR GLN GLN ILE SER SER THR PRO GLN GLN HIS GLN GLN HIS GLN GLN GLN GLN GLN GLN GLN GLY TYR ASN ASN GLN ILE
PRO ASN THR PRO TYR GLN GLN PHE GLN PRO THR MET GLN TYR GLN GLY GLN GLN SER SER MET GLN GLN SER VAL GLY GLN GLN GLN PRO GLN GLN GLN PRO GLN GLN GLN ASN THR PRO ASN THR PRO ASN SER THR THR SER SER ASN THR ALA ASN THR THR SER PRO VAL LYS
ILE THR GLN LEU LEU L207 D211 S212 D213 S228 S229 M230 A231 N234 I274 R281 A295 I296 L299 L333 K336 S337 D340 S341 C342 M343 D344 N347 L348 L349 N350 I351 K352 S353 F354 N355 T356 L357 D358 E359 K360 W361 L365 K369 I382 Q383
N384 F385 Q386 I387 D388 K389 Q390 Y394 Q395 L396 Y397 I398 E399 R402 S403 SER LEU SER SER ASN LEU TYR GLN GLN GLN GLN GLN GLN GLN ASN LYS TYR GLN GLN GLN GLN GLN GLN GLN Q429 S430 K431 K432 T433 T434 L435 E436 N437 I438 I439 K440 I441 I442 D443 Y444 S445 N446
D447 Q448 S449 I450 L451 Q463 Q464 Q465 R473 Q485 N488 D489 D490 F491 N492 L493 L494 V495 L496 K497 C498 LEU ASP LEU LEU LEU LEU ILE SER ASP ASN THR VAL TYR ASP ILE GLU ASN ALA LYS SER LEU VAL VAL ASN LEU SER ASN MET D527 D540 R549 R552
H562 L575 K582 E585 F586 N587 E588 S589 N590 F591 E592 D593 F594 S595 G596 T597 N598 Y599 D600 Q601 T602 I603 S604 F605 I606 R607 S626 M627 I628 S629 S630 S649 K650 D651 F652 I653 P654 N655 S656 K657 T661 L662 I663 I664 K665 N666 V667 M668 N669 S670 Q671 F672 V673
E674 R675 K689 S692 D693 P694 I695 T696 W697 K698 P699 M700 I701 K702 Y703 I704 Q705 E706 E707 F708 P709 N710 H713 D714 I718 N721 I725 N726 G727 R732 I749 S750 I751 Q752 N753 S754 Y755 S756 I757 E758 P777 S778 M779 ASN GLY GLY ILE GLY LEU ASN
GLY THR ILE ASN ASN GLY LEU ILE MET GLY ILE S799 R821 E831 Y832 T835 N836 I837 N838 ILE ASN ASN LEU ASN SER ASN ASN ASN ASN ASN ASN



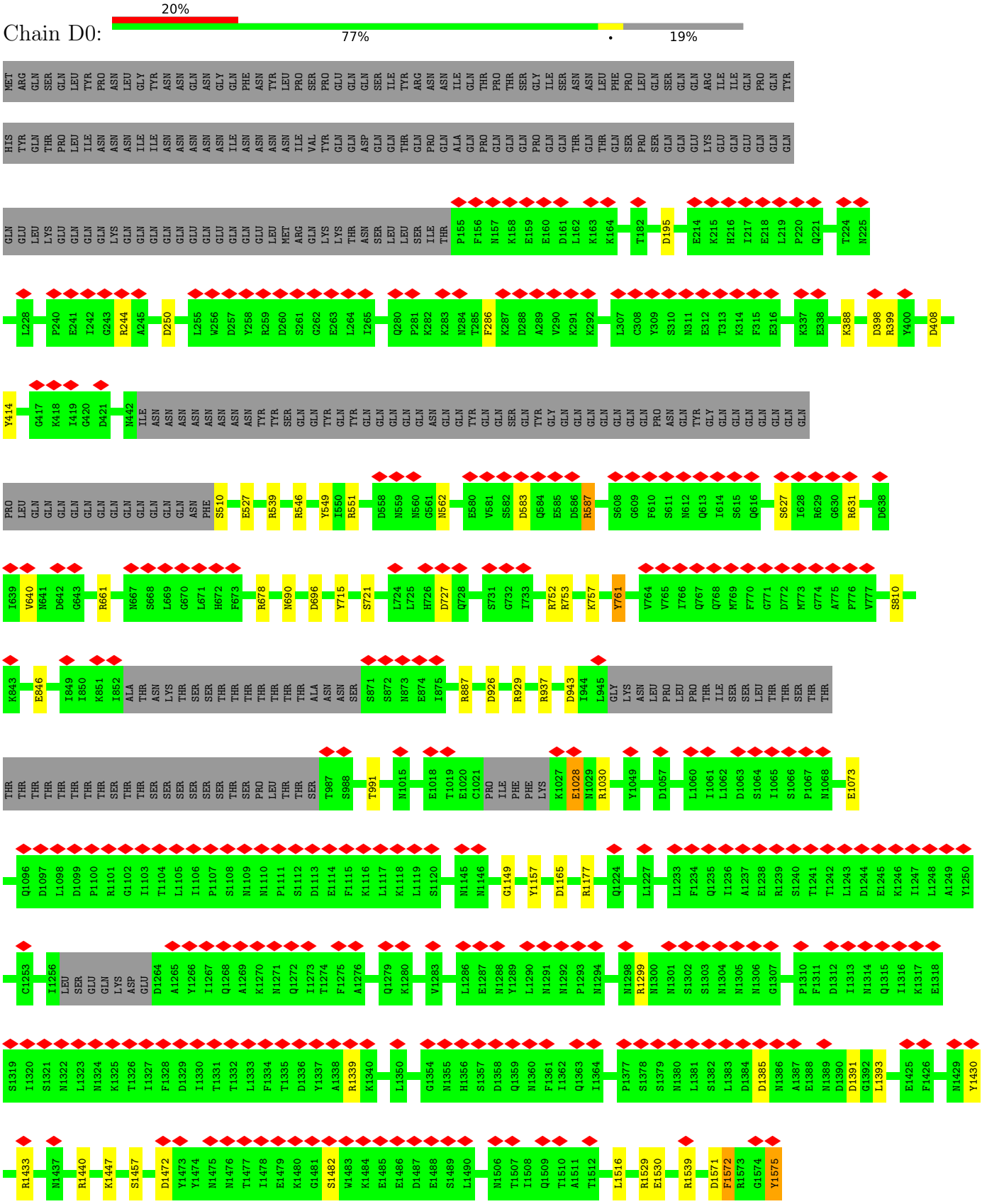
- Molecule 6: Nup205

Chain C3:



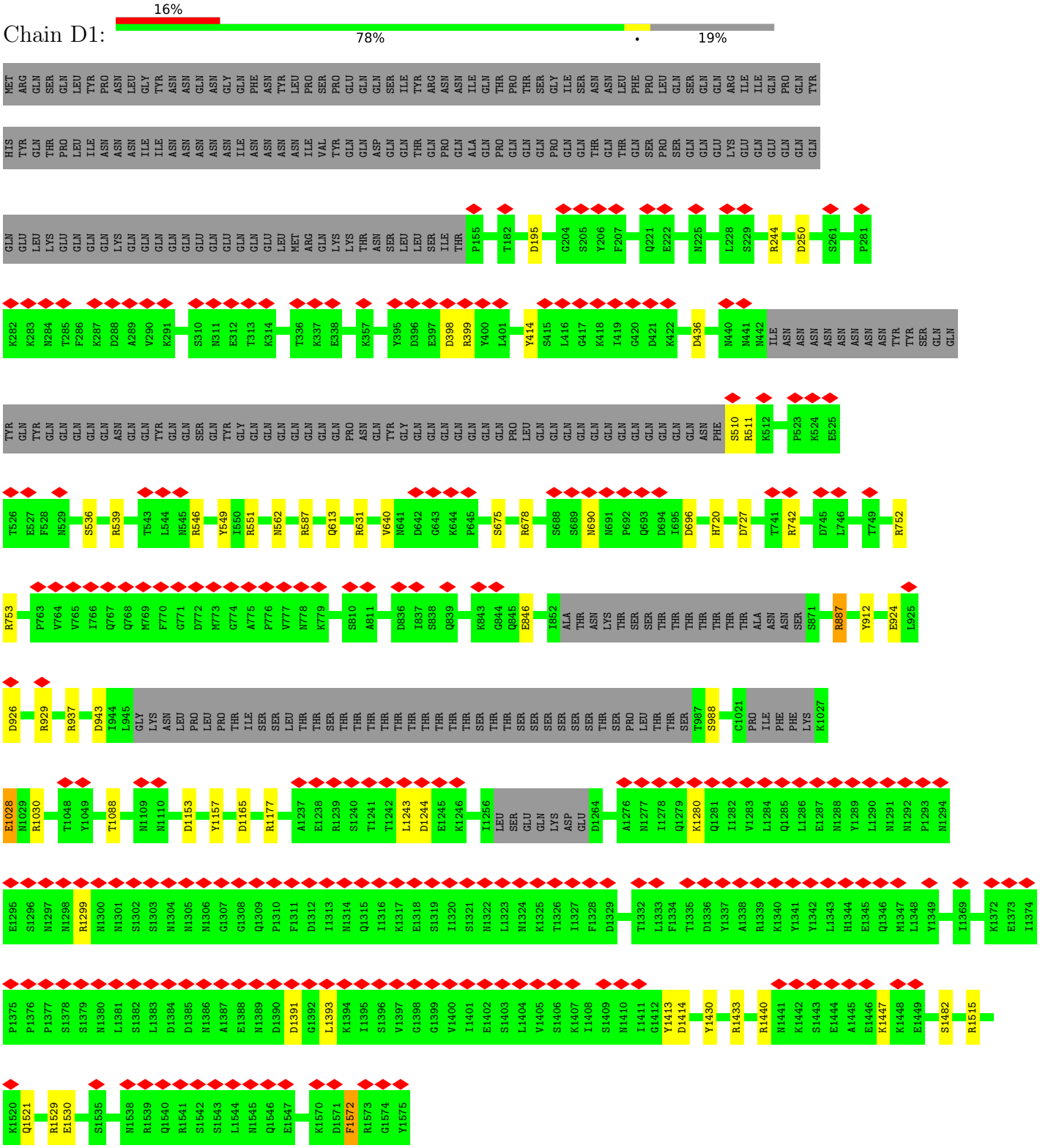

GLN GLN GLN GLN GLN GLN GLN GLY TYR ASN ASN GLN GLN ILE PRO ASN THR PRO TYR GLN GLN PHE GLN PRO THR MET GLN TYR GLN GLY GLN GLN SER SER MET GLN GLN SER VAL GLY GLN GLN GLN GLN PRO GLN GLN GLN PRO GLN GLN GLN GLN ASN THR PRO ASN THR PRO ASN SER
THR THR SER SER ASN THR ALA ASN THR THR SER PRO VAL LYS ILE THR GLN LEU LEU L207 S208 E209 K210 D211 S212 D213 S223 R224 L225 V226 E227 S228 S229 M230 A231 V232 G233 N234 Y235 K238 D255 S256 K257 S260 S264 T267 S268 Y269 S270 Q271 Y272 P273 I274 Y275
A295 G298 L299 N300 E301 L302 S303 Q306 Q307 E310 Q314 Q317 Q318 K325 K352 S353 F354 N355 T356 L357 D358 E359 K360 W361 K362 L365 K369 H391 R402 L409 Y410 Q411 Q412 Q413 Q414 Q415 Q416 Y420 Q421 T433 Q465 G466 Y467 N468
Q469 D470 R473 L496 K497 C498 L499 D500 L501 L502 L503 L504 I505 S506 D507 N508 T509 V510 Y511 D512 I513 E514 N515 A516 K517 S518 D527 H541 E542 L543 R549 R552 H562 T566 D600 Q601 T602 R607 I628 S629 L646 D651 T661 Y703
R720 R732 R765 I783 G784 G785 L786 N787 G788 T789 I790 N791 N792 G793 L794 E811 F812 E816 I817 N818 R819 P820 R821 I822 F823 S824 M825 Y826 P827 N828 L829 I830 E831 Y832 F833 T834 T835 N836 I837 N838 ILE ASN ASN LEU ASN SER ASN ASN ASN ASN ASN ASN
ASN ASN ASN ASN ASN ASN

Chain D0:



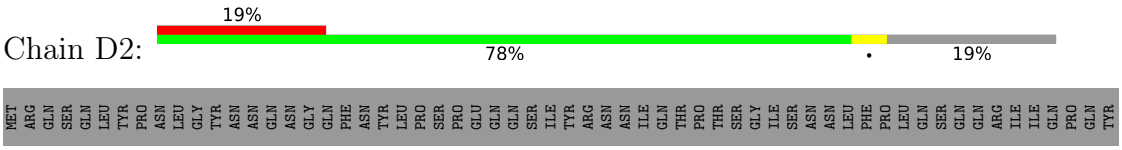
- Molecule 7: Nucleoporin 155

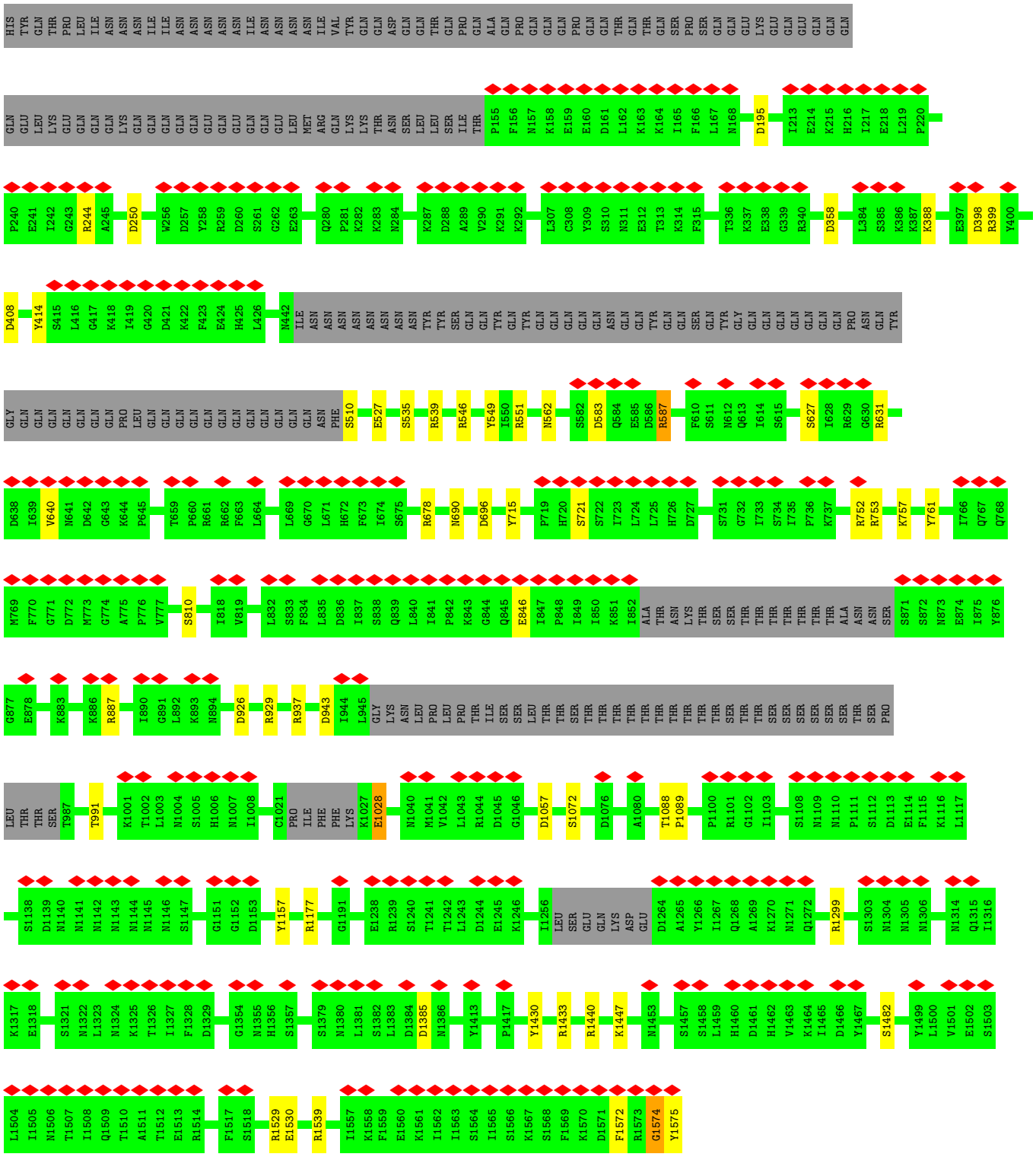
Chain D1:



• Molecule 7: Nucleoporin 155

Chain D2:





- Molecule 7: Nucleoporin 155

Chain D3:

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

GLN GLU LEU LYS GLU GLN GLN GLN LYS GLN GLN GLN GLN GLU GLN GLU GLN GLN GLU LEU MET ARG GLN LYS LYS THR ASN SER LEU LEU SER ILE THR P155 D178 A181 T182 I183 P184 D185 P186 T187 L188 L191 Y192 D195 P220 Q221 E222 I223 T224 N225 G226 Y227

L228 S229 T230 S231 E241 I242 G243 R244 D250 Q251 T252 D257 Y258 R259 D260 S261 G262 E263 L264 I265 S266 H267 N268 L269 S270 Q271 Q280 P281 K282 K283 N284 T285 F286 K287 D288 A289 V290 K291 K292 V293 F305 A306 L307 C308 Y309 S310 N311 E312 T313 K314 F315 E316 I317 L318 S319

T320 L321 T336 K337 E338 K357 D396 E397 D398 R399 Y400 Y414 K418 I419 D434 I435 D436 N442 ILE ASN ASN ASN ASN ASN ASN ASN ASN TYR TYR SER GLN GLN TYR GLN TYR GLN GLN GLN GLN GLN ASN GLN GLN TYR GLN GLN SER GLN TYR GLY GLN GLN GLN

GLN GLN GLN GLN PRO ASN GLN TYR GLY GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ASN PHE S510 R511 I521 S522 P523 K524 E525 T526 E527 F528 N529 S536 R539 R546 Y549 I550 R551 N562 N572 R587

Q613 R631 I639 V640 N641 D642 G643 K644 P645 T646 V647 Y648 Y649 K650 S675 R678 S689 N690 N691 P692 Q693 D694 I695 D696 S731 R742 R753 Y761 V765 I766 Q767 Q768 M769 F770 G771 D772 M773 G774 A775 P776 V777 N778 K779 N804 T809 S810 A811

G812 C813 S814 Y815 K843 I852 ALA THR ASN LYS THR SER SER THR THR THR THR THR THR THR ALA ASN ASN SER S871 E874 R887 Y912 K915 D919 E924 L925 D926 I927 K928 R929 K930 I931 D932 L933 R937 D943 I944 L945 GLY LYS ASN LEU PRO LEU

PRO THR ILE SER SER LEU THR THR SER THR THR THR THR THR THR THR THR SER SER THR THR SER SER SER SER SER SER SER THR SER PRO LEU THR THR SER T987 S988 C1021 PRO ILE PHE PHE LYS K1027 E1028 N1029 R1030 R1044 D1045 T1048 Y1049 F1050 T1051 D1057 T1088

G1149 D1153 D1165 R1177 N1200 K1222 H1223 Q1224 T1241 T1242 L1243 D1244 I1256 LEU SER GLU GLN LYS ASP GLU D1264 K1280 Q1281 I1282 V1283 L1284 Q1285 L1286 E1287 N1288 Y1289 L1290 N1291 N1292 P1293 N1294 E1295 S1296 N1297 N1298 R1299 P1310 F1311 D1312 I1313 N1314 Q1315 I1316 K1317 E1318

S1319 I1320 S1321 N1322 L1323 N1324 K1325 H1352 L1381 S1382 L1383 D1384 D1385 N1386 A1387 E1388 N1389 D1390 D1391 G1392 L1393 T1421 Y1430 R1433 R1440 K1447 K1464 D1472 S1482 T1510 R1515 K1520 R1529 E1530 R1539 S1542 S1543 Q1546 F1572 R1573 G1574 Y1575

- Molecule 8: NDC1

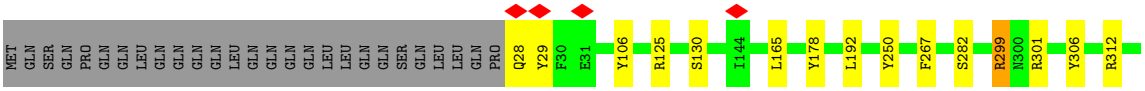
Chain E0:

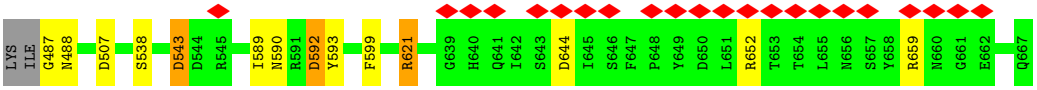
MET GLN SER GLN PRO GLN GLN LEU GLN GLN GLN GLN GLN LEU GLN GLN GLN GLN LEU LEU GLN GLN SER SER GLN LEU LEU GLN PRO Q28 Y29 S83 Y106 R125 S130 L165 Y178 T184 I185 Y250 F267 S282 R299 N300 R301 Y306 R312 D324

S325 P338 F350 R398 Y416 R431 N441 ILE LYS LYS GLU ASP ASP LYS ASN LYS ASN SER ASN ASN ASN ASN ASN ASN ASN ASN

- Molecule 8: NDC1

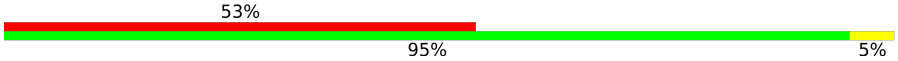
Chain E1:

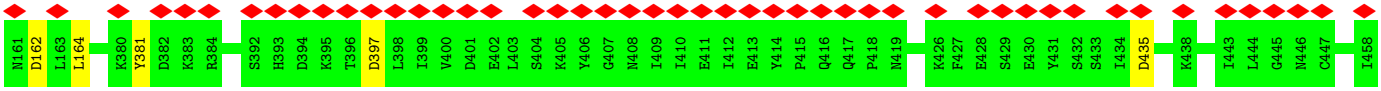




- Molecule 9: Nup35

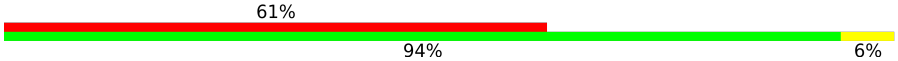
Chain F0:

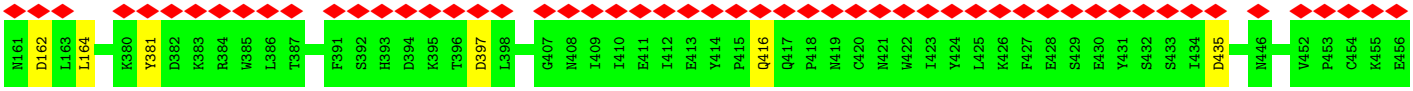


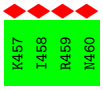


- Molecule 9: Nup35

Chain F1:

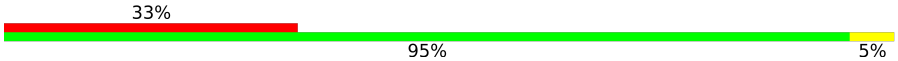


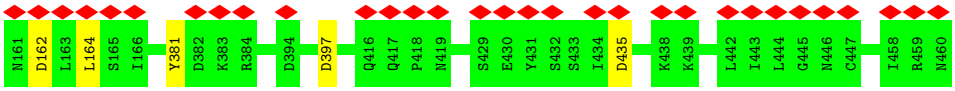




- Molecule 9: Nup35

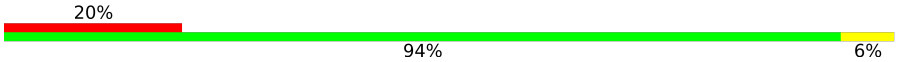
Chain F2:

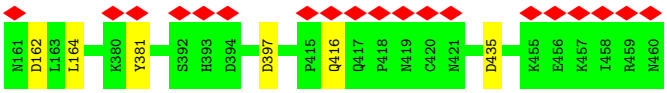




- Molecule 9: Nup35

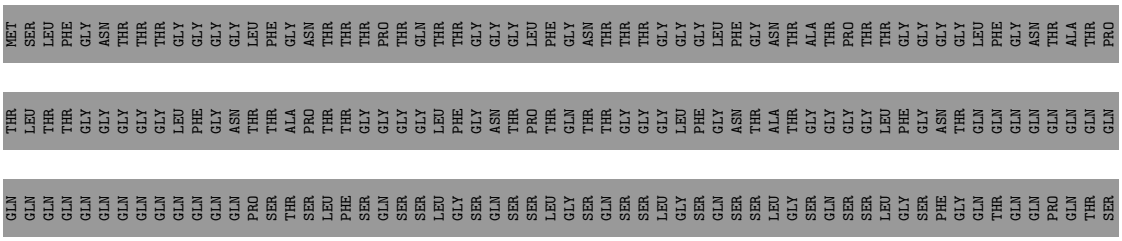
Chain F3:

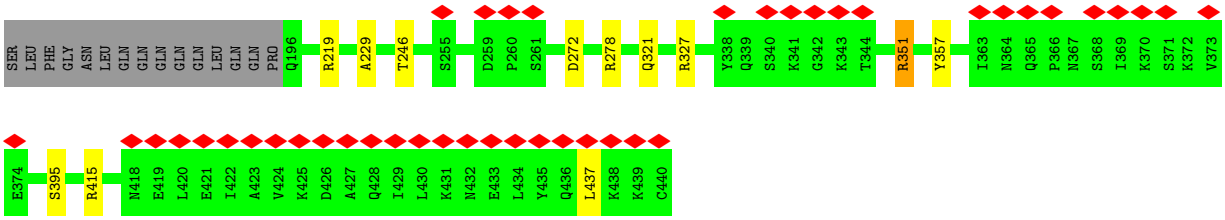




• Molecule 10: Nuclear pore complex protein nup54

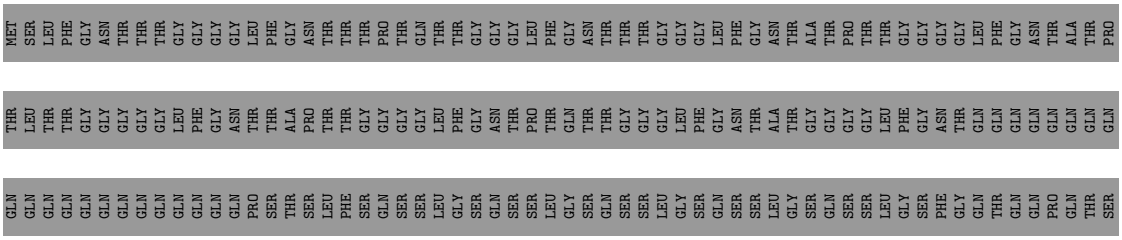
Chain H0:

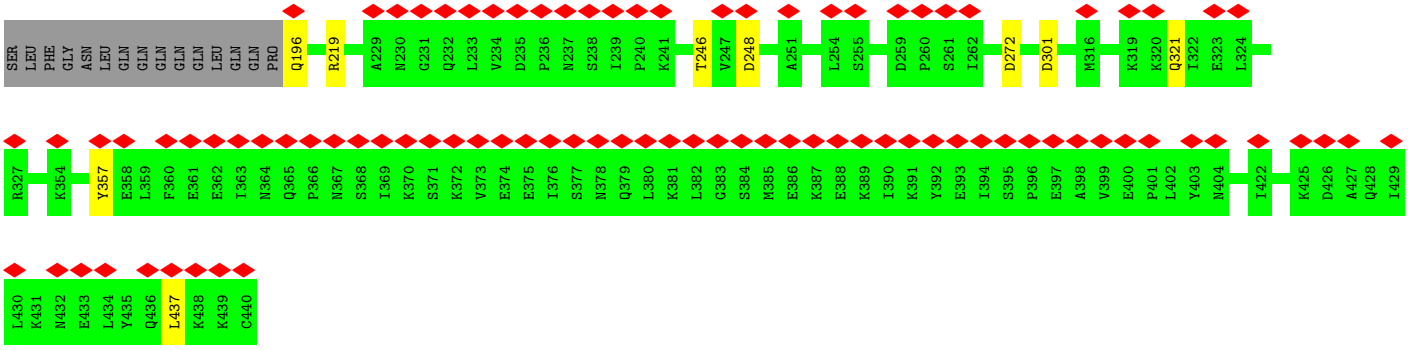




• Molecule 10: Nuclear pore complex protein nup54

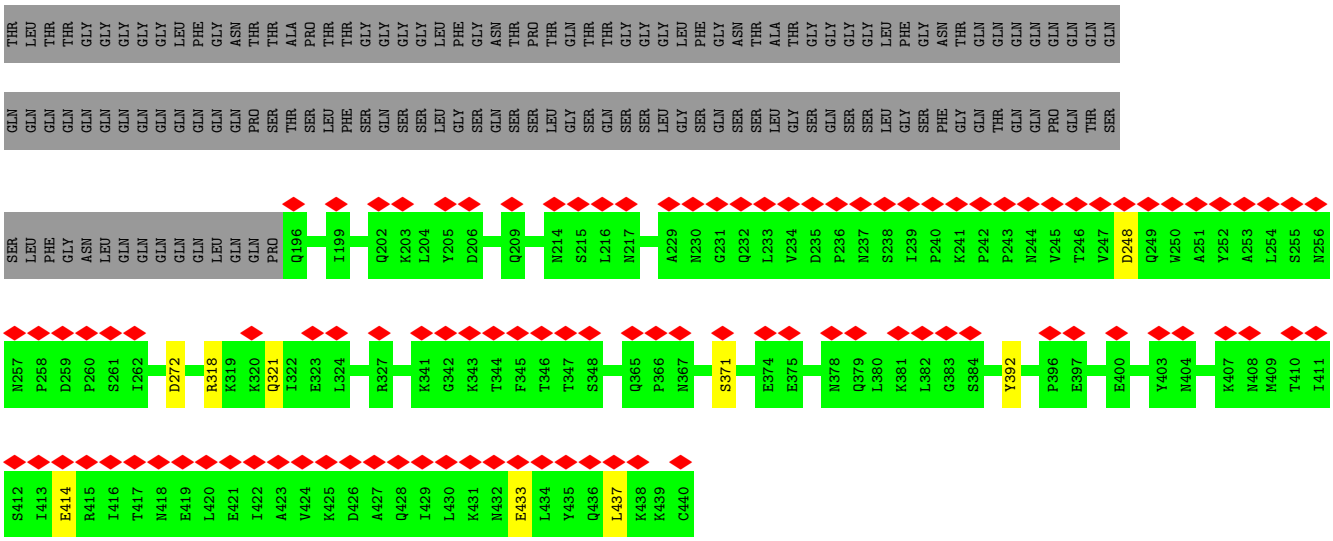
Chain H1:





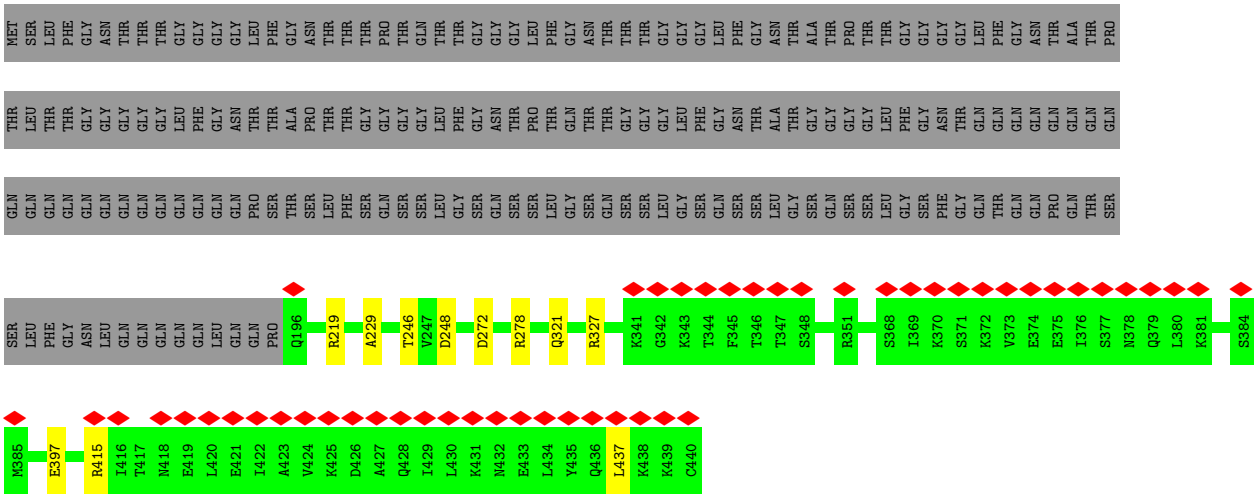
• Molecule 10: Nuclear pore complex protein nup54

Chain H2:



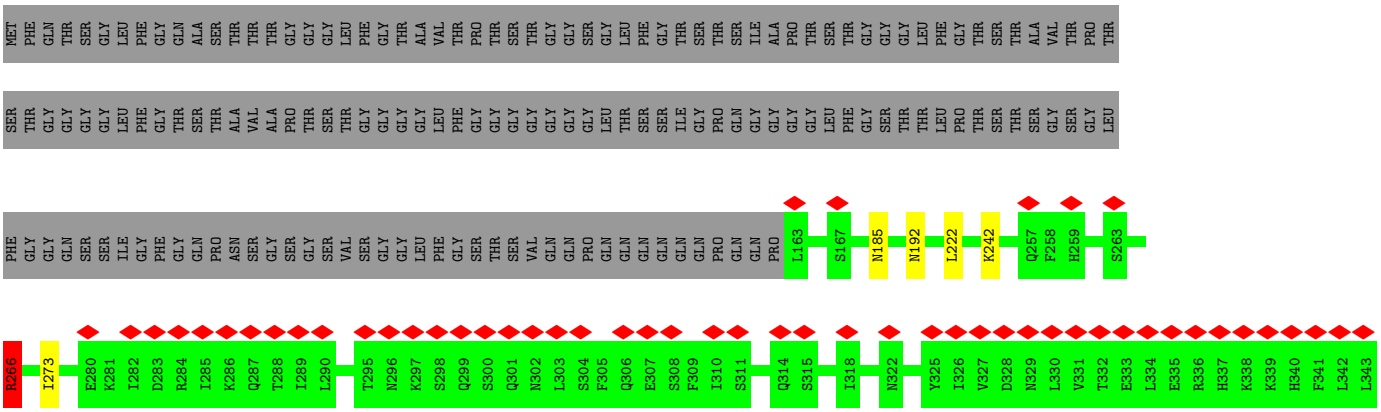
- Molecule 10: Nuclear pore complex protein nup54

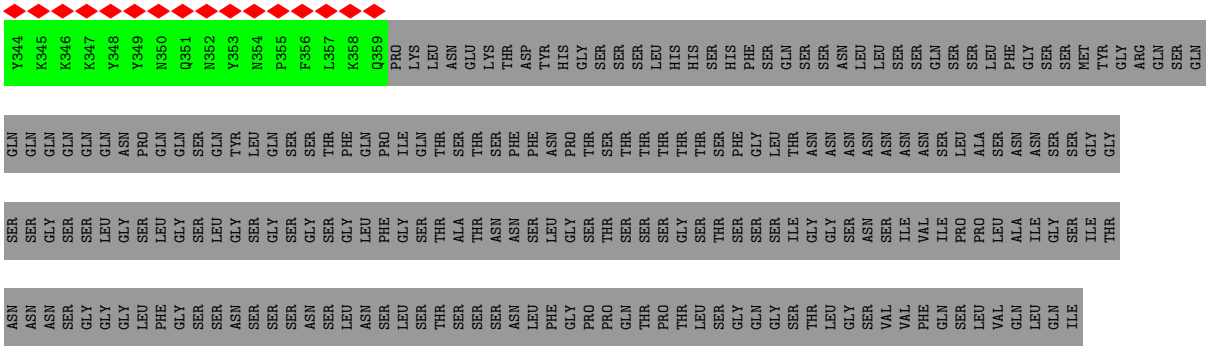
Chain H3:



- Molecule 11: Nup58

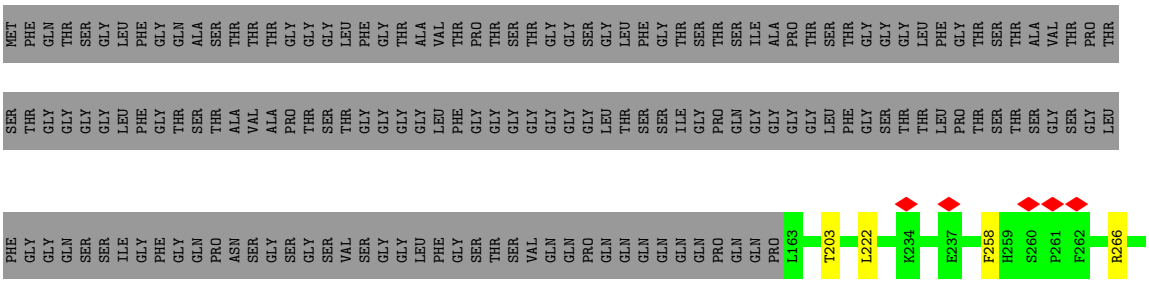
Chain I0:

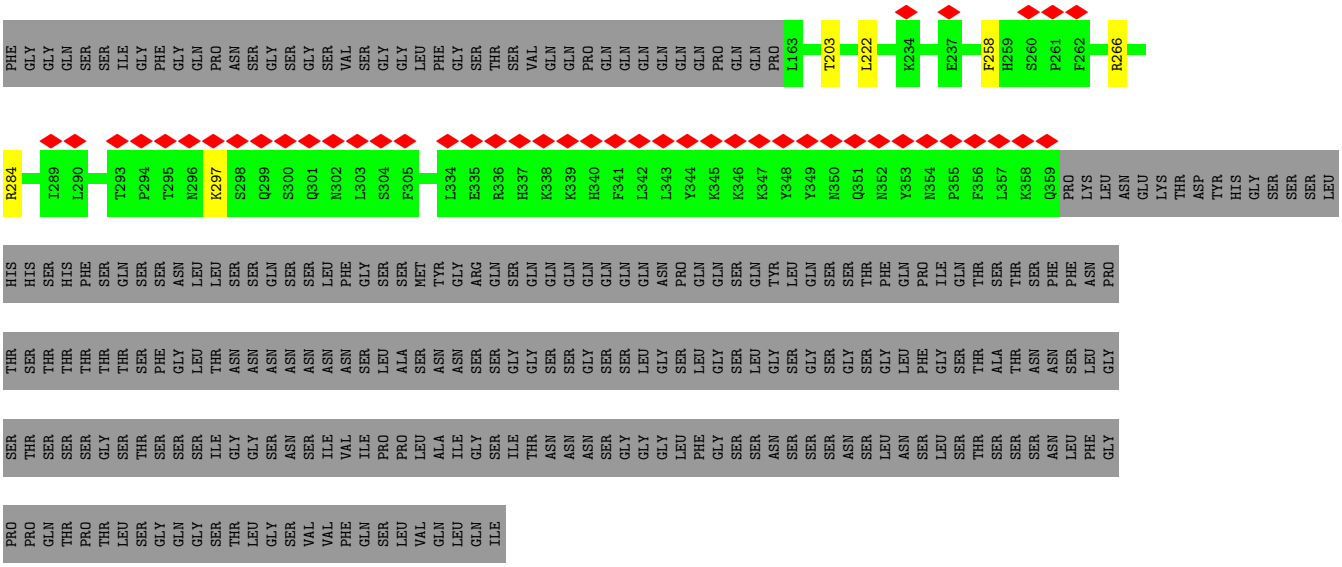




- Molecule 11: Nup58

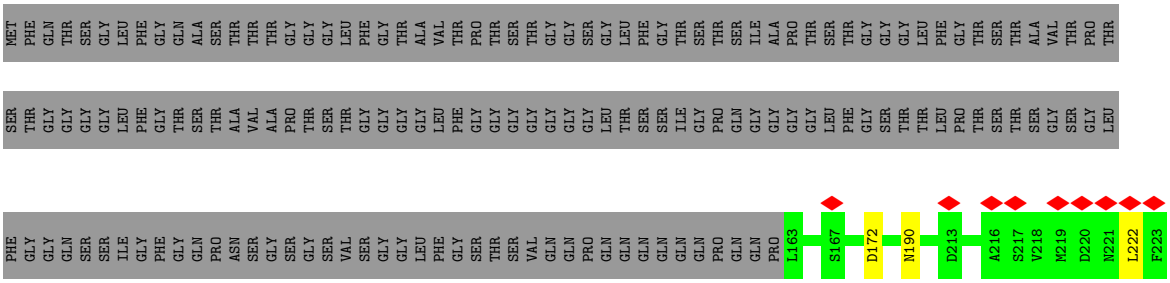
Chain I1:

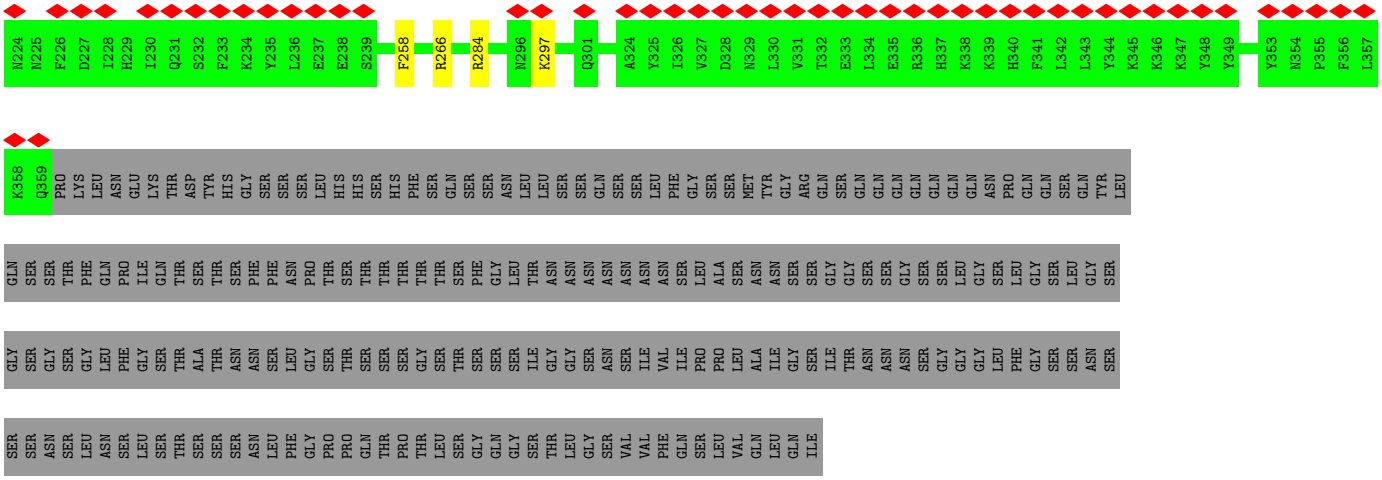




- Molecule 11: Nup58

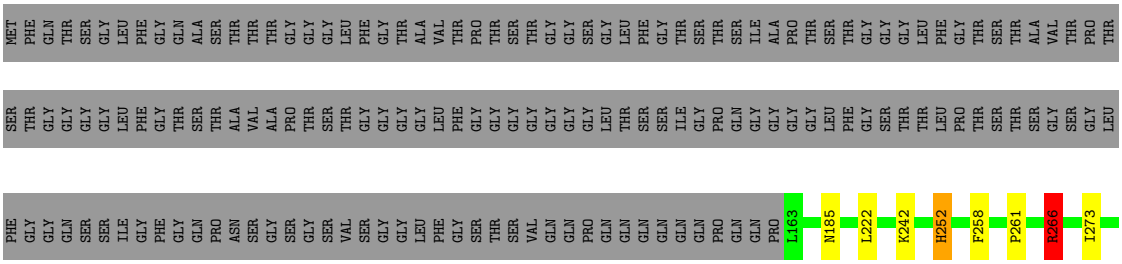
Chain I2:

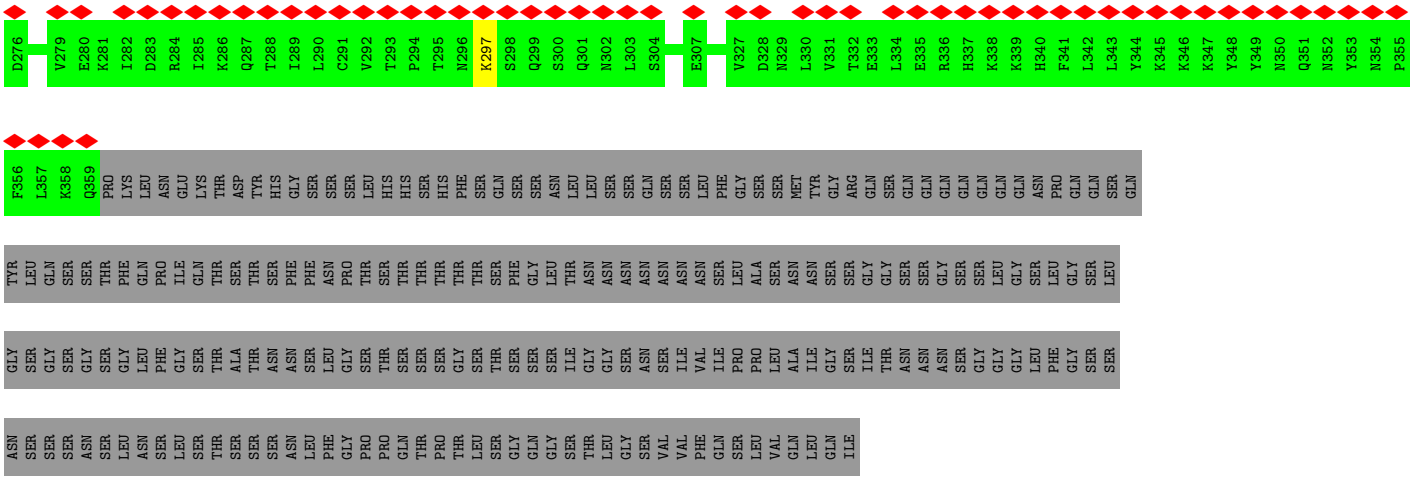




- Molecule 11: Nup58

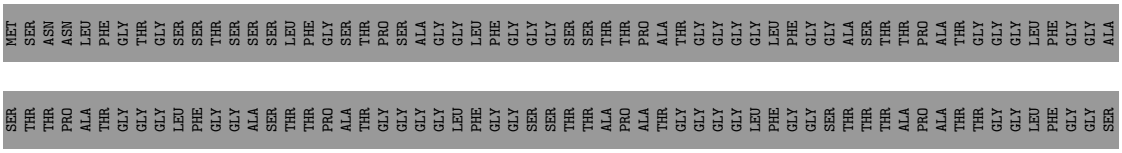
Chain I3:

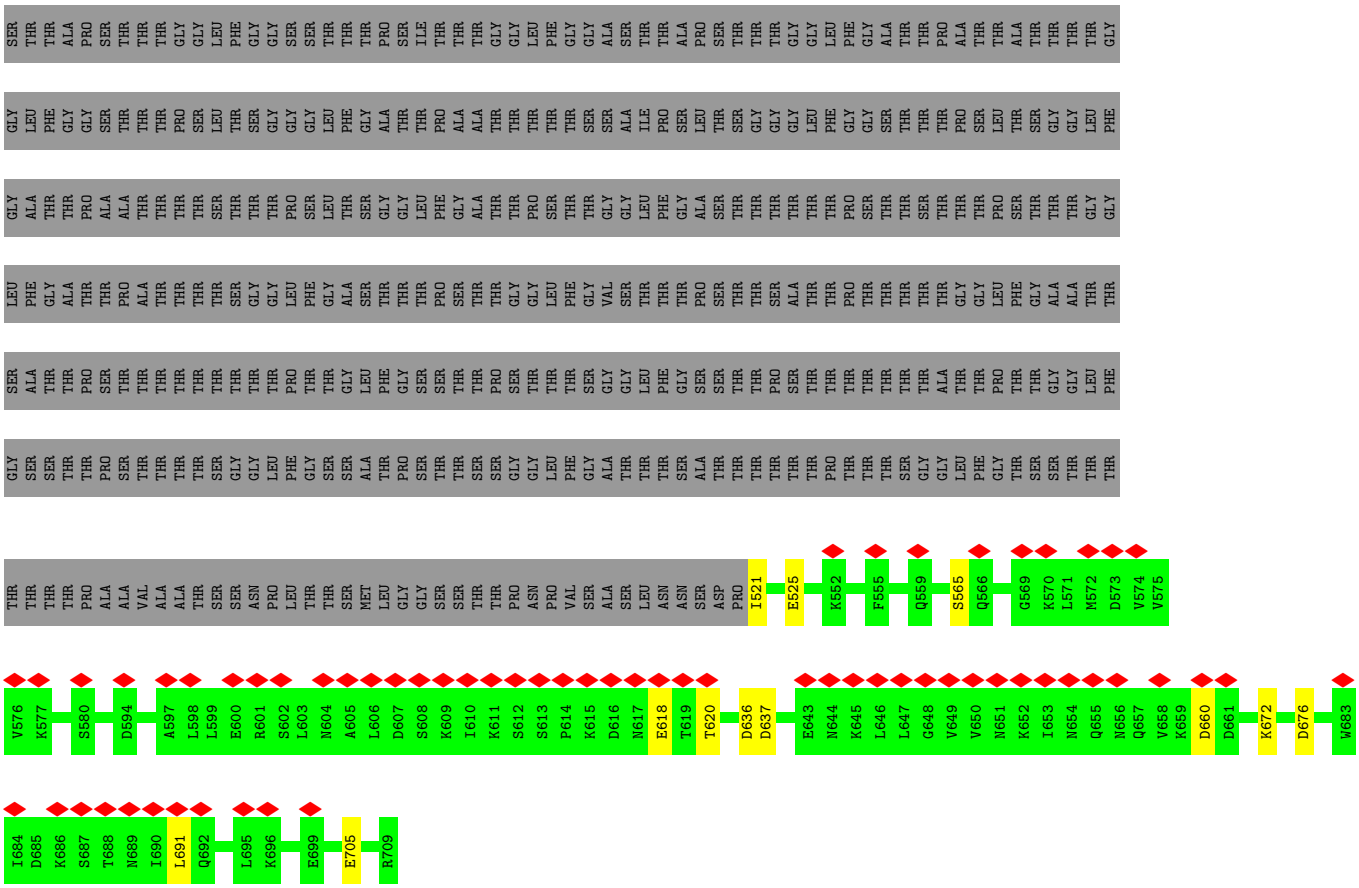




- Molecule 12: Nuclear pore protein

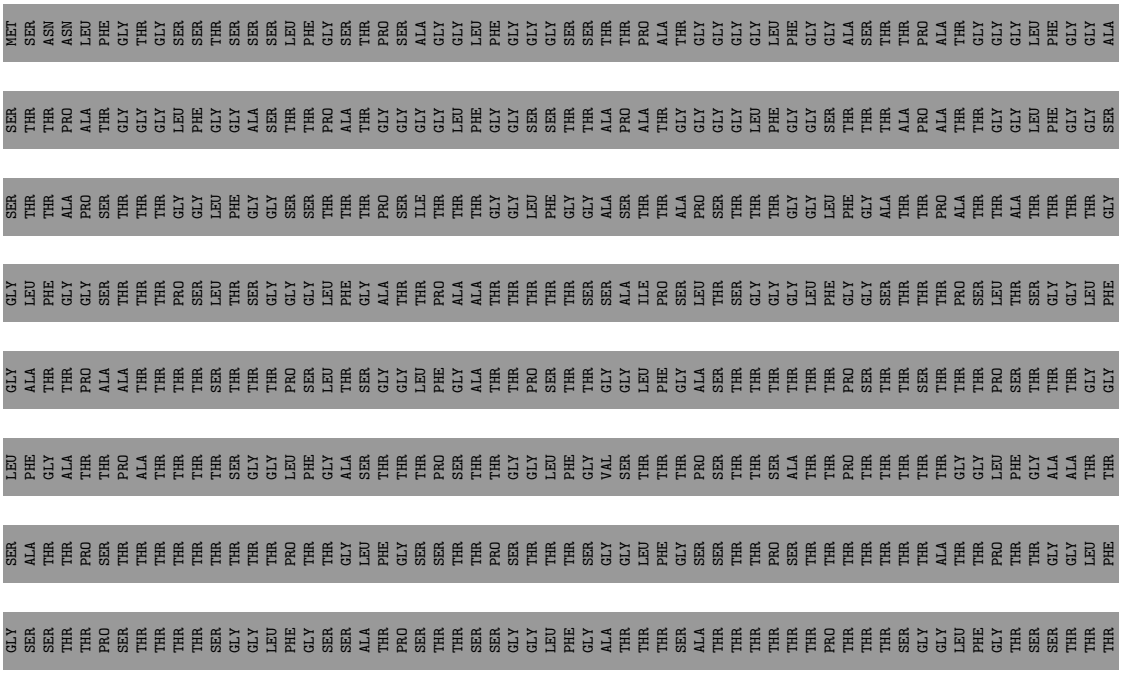
Chain J0:

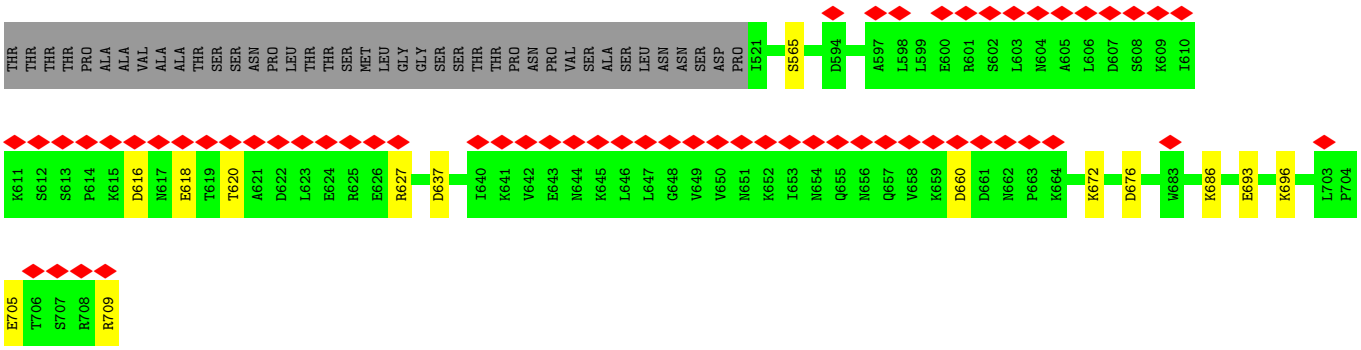




- Molecule 12: Nuclear pore protein

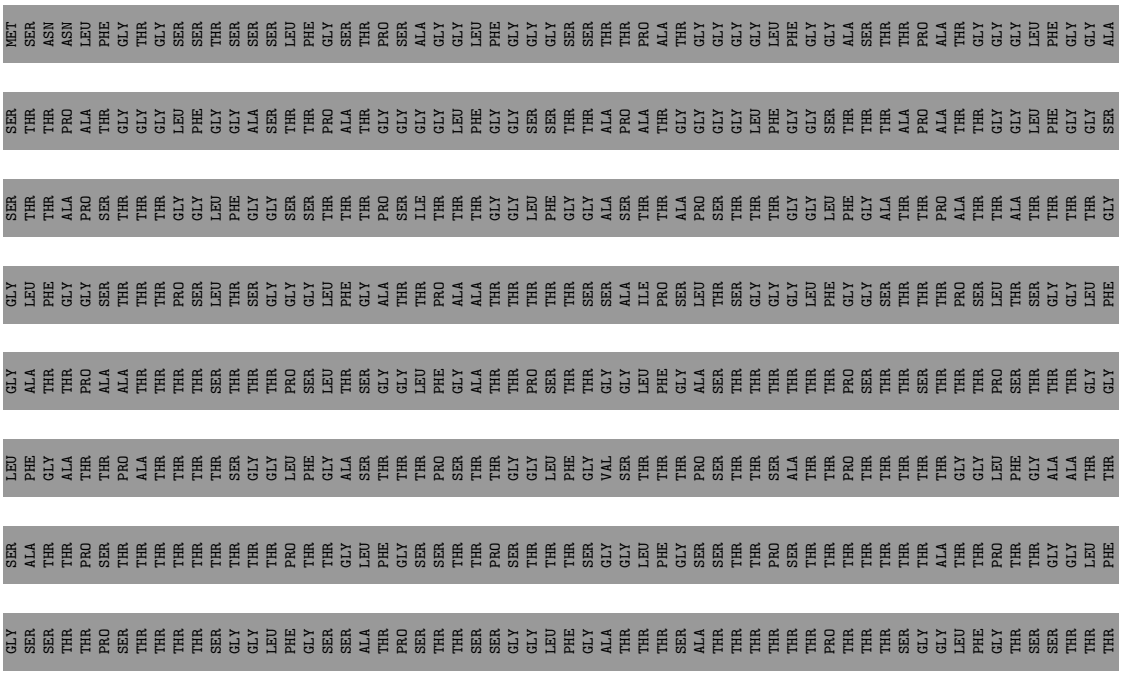
Chain J1:

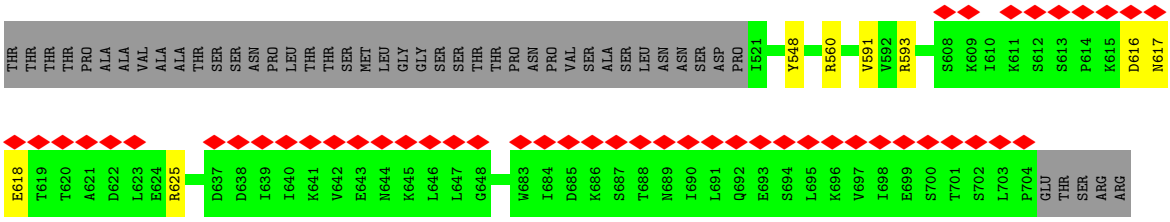




- Molecule 12: Nuclear pore protein

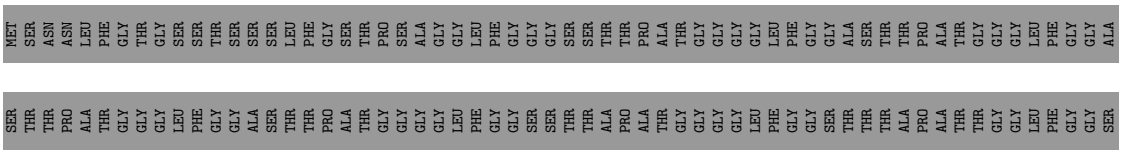
Chain J2:

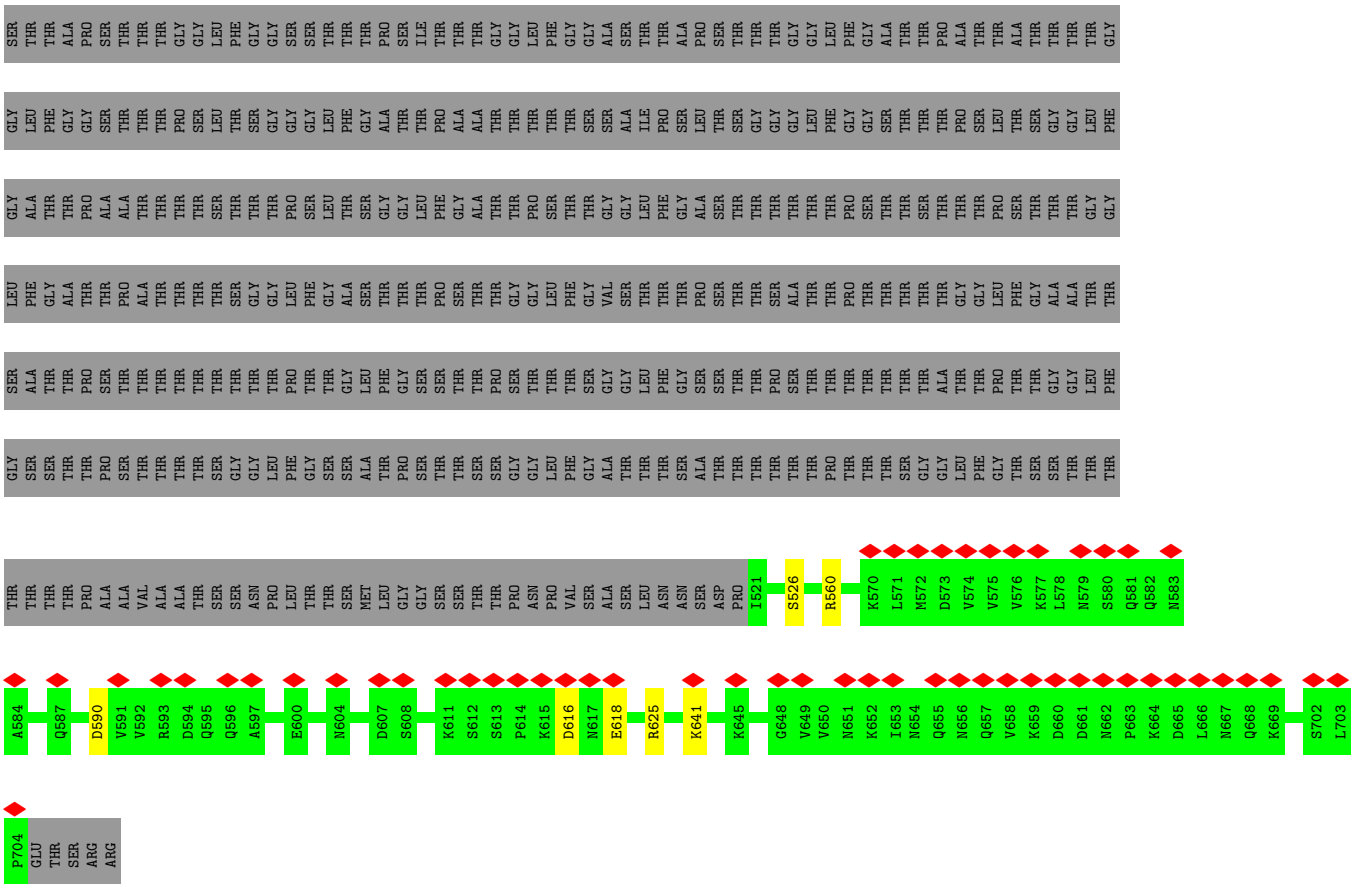




- Molecule 12: Nuclear pore protein

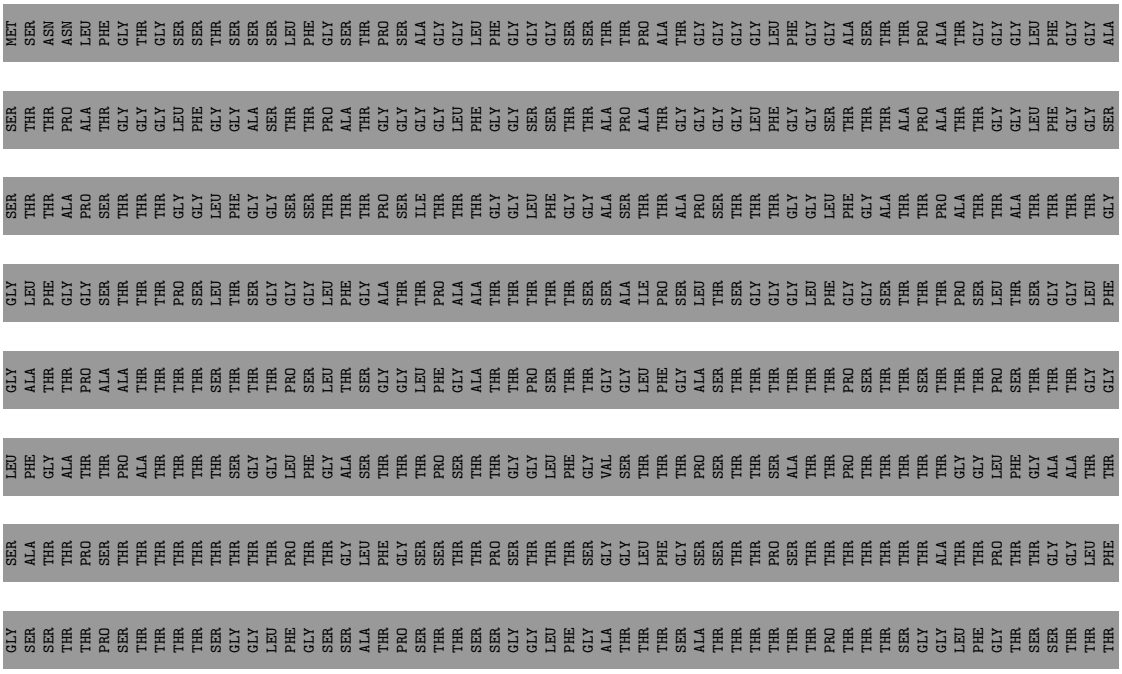
Chain J3:

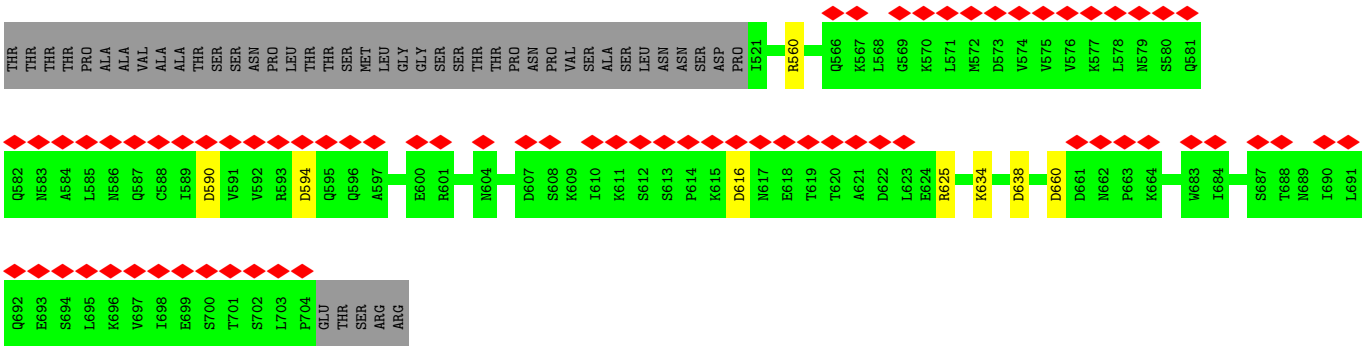




- Molecule 12: Nuclear pore protein

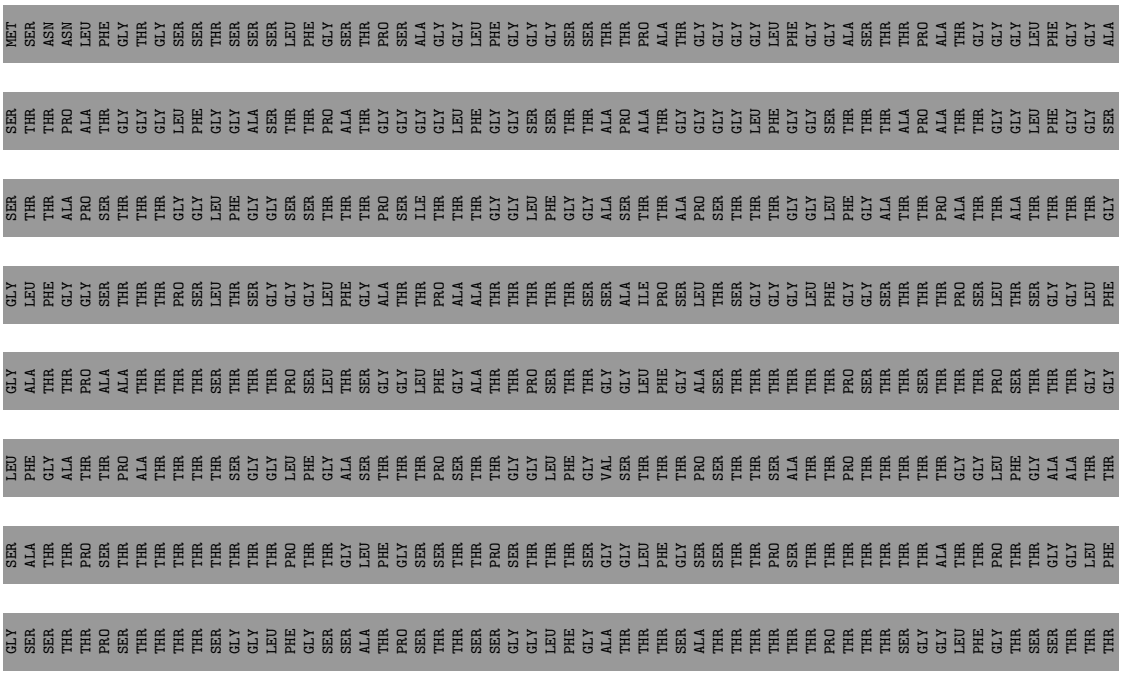
Chain J4:

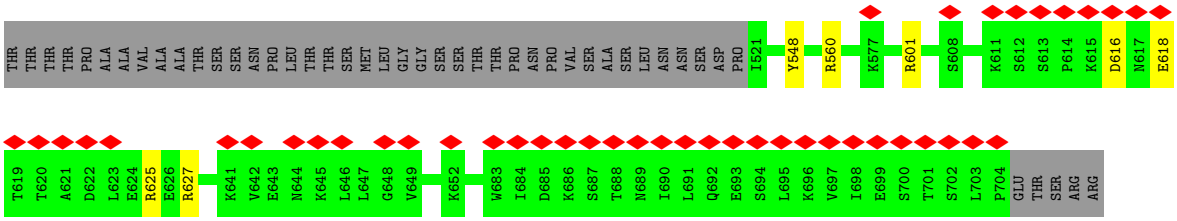




- Molecule 12: Nuclear pore protein

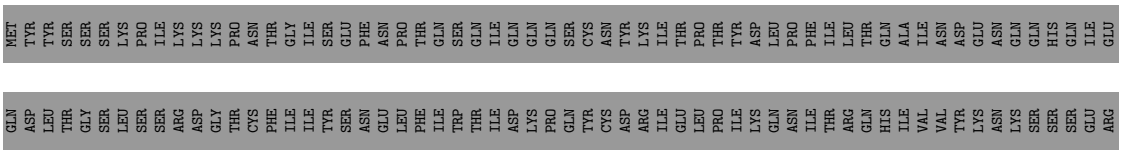
Chain J5:

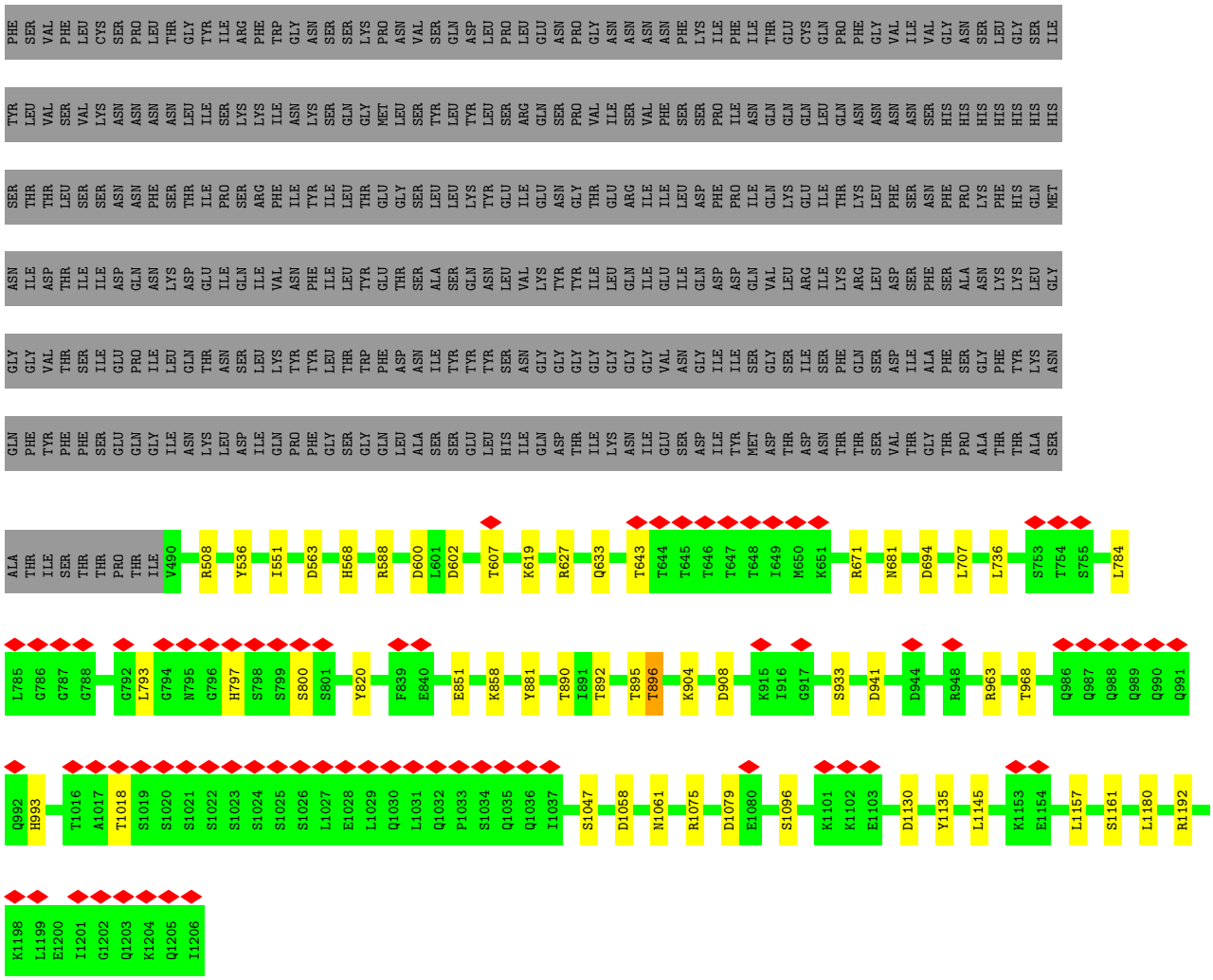




- Molecule 13: Nucleoporin 133

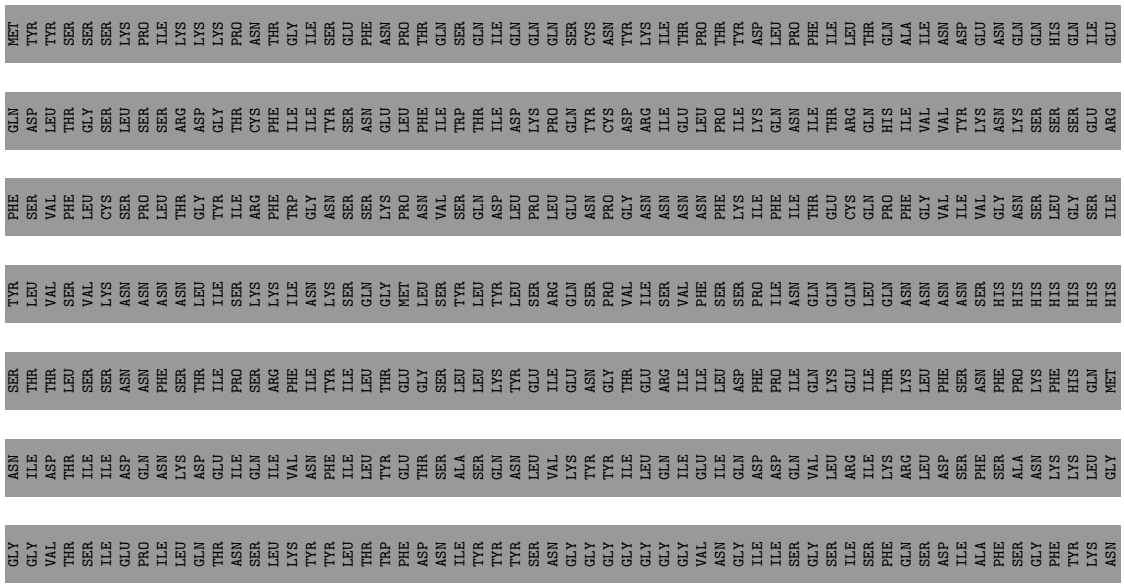
Chain K0:

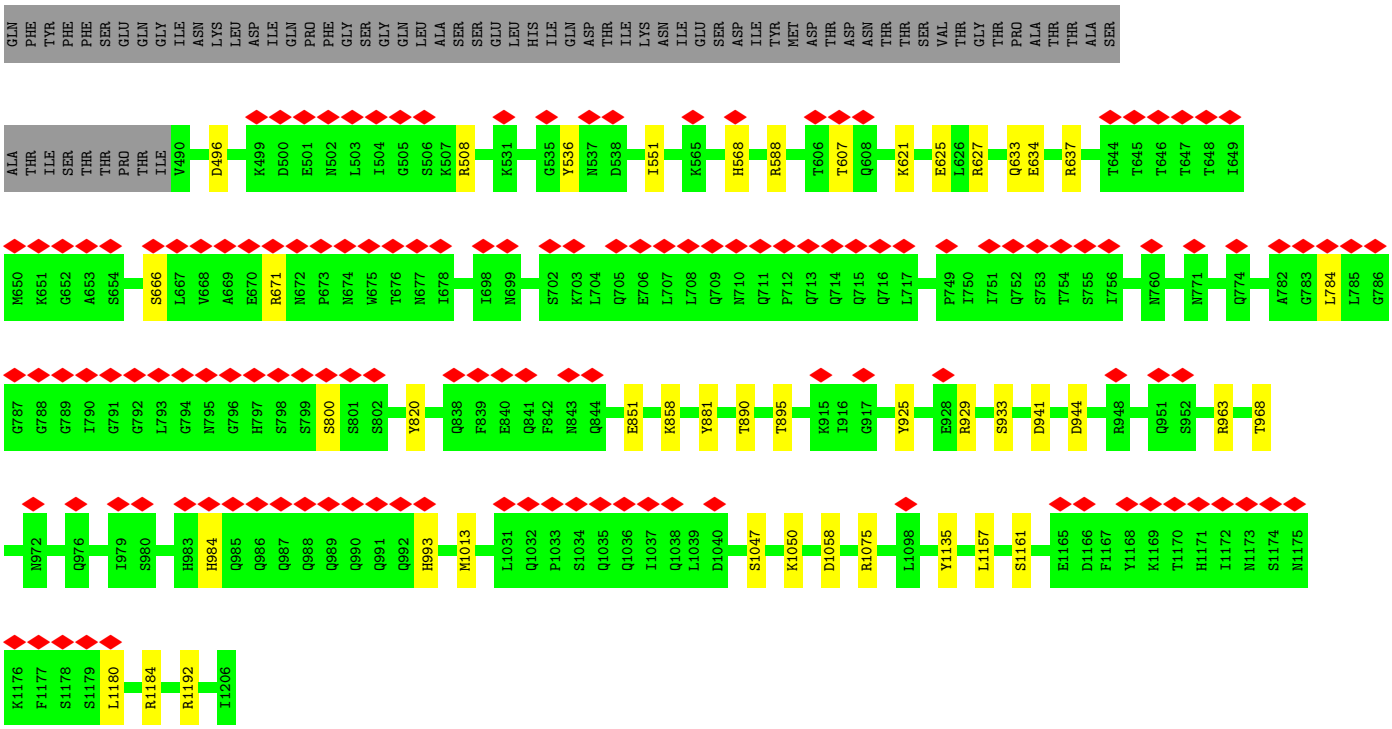




- Molecule 13: Nucleoporin 133

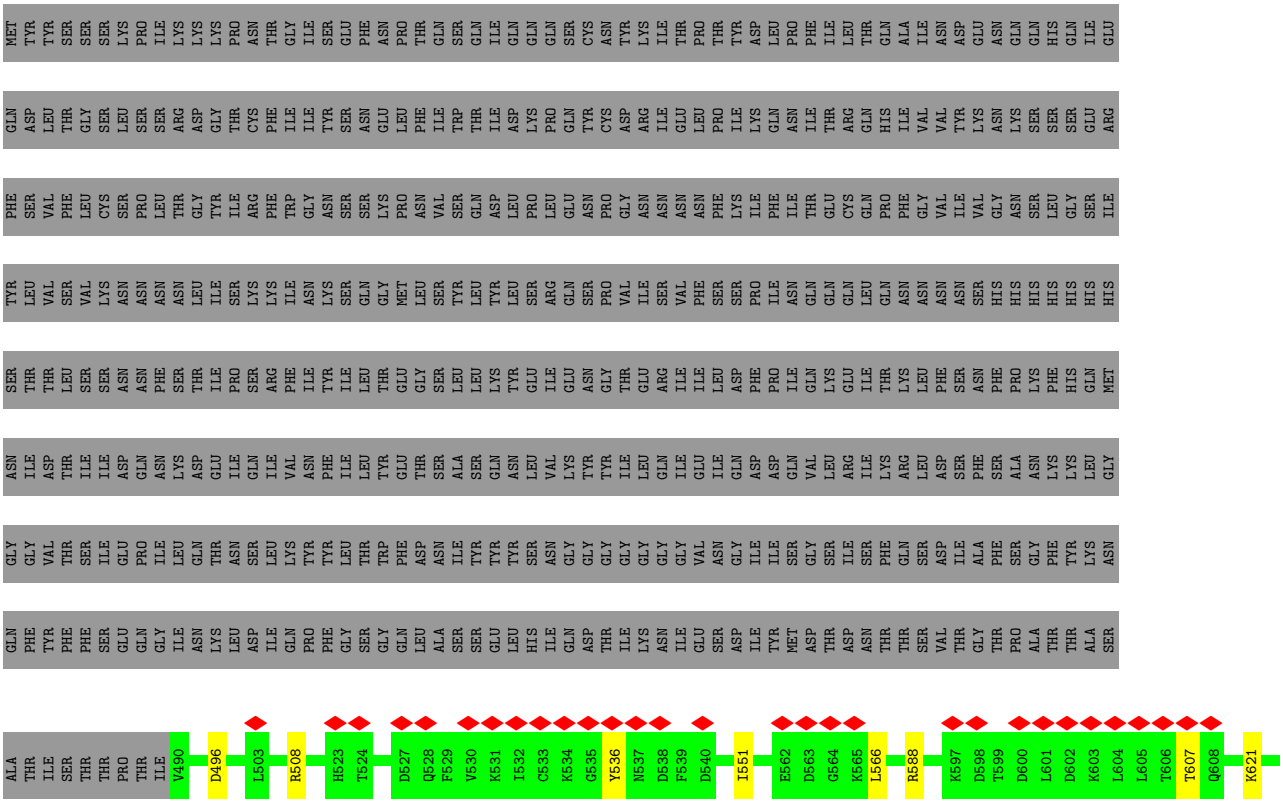
Chain K1:

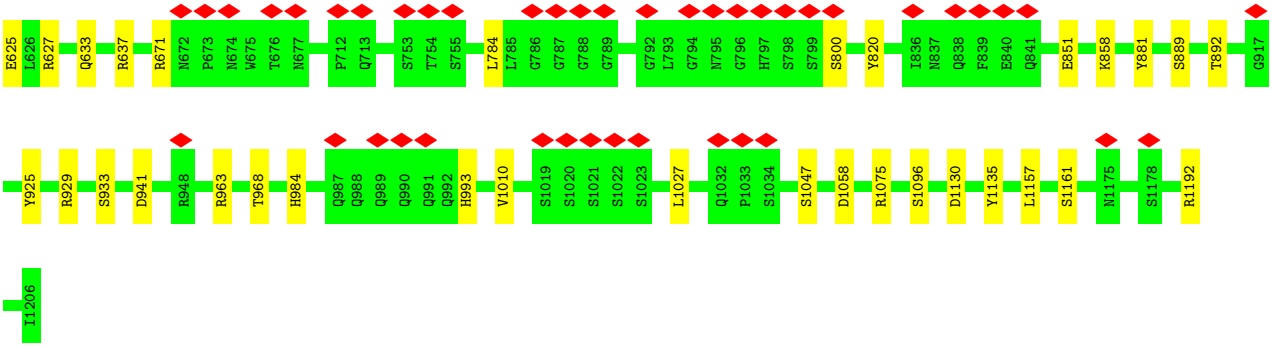




- Molecule 13: Nucleoporin 133

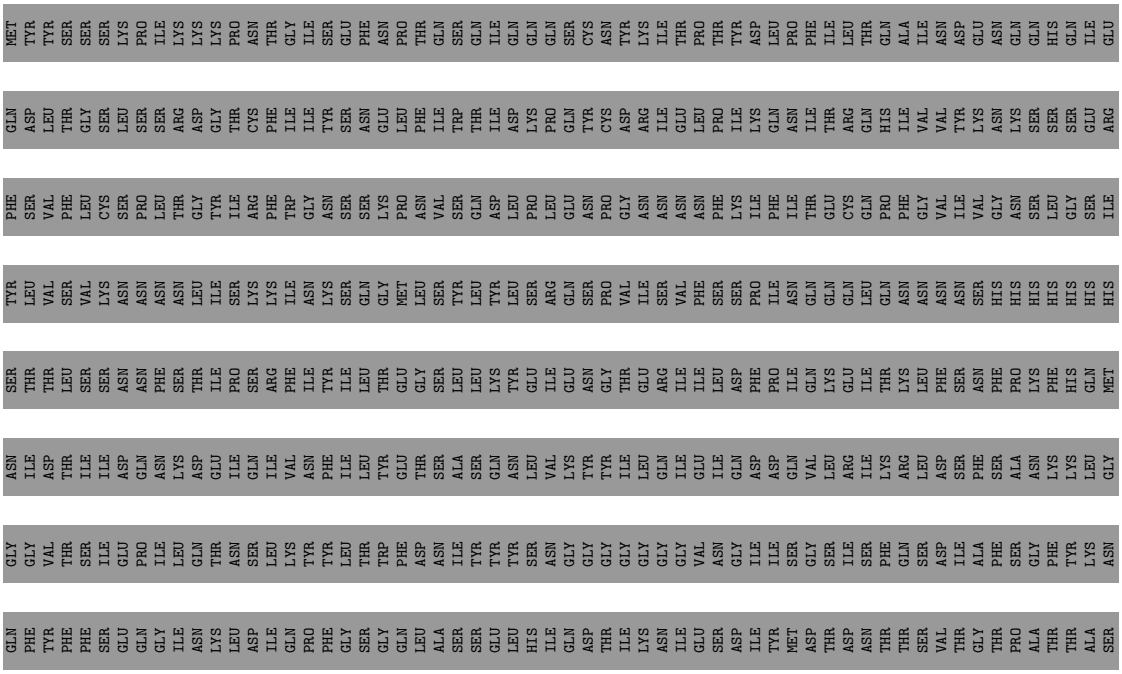
Chain K2:

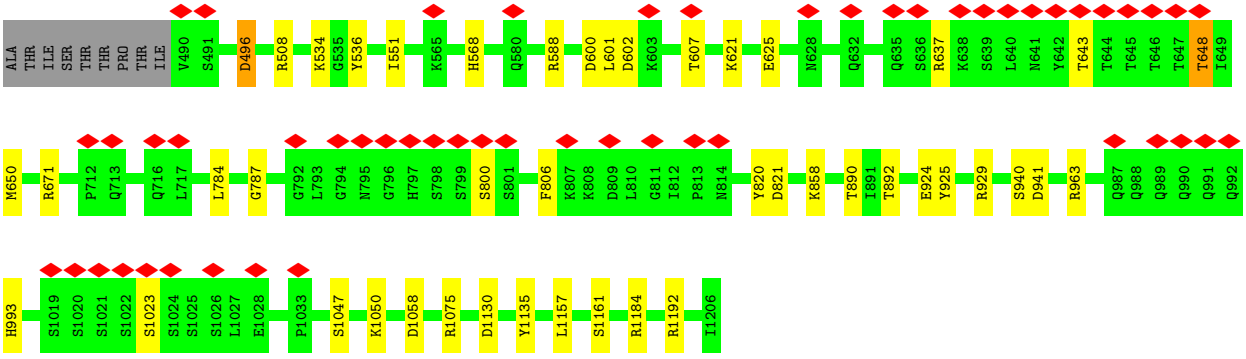




- Molecule 13: Nucleoporin 133

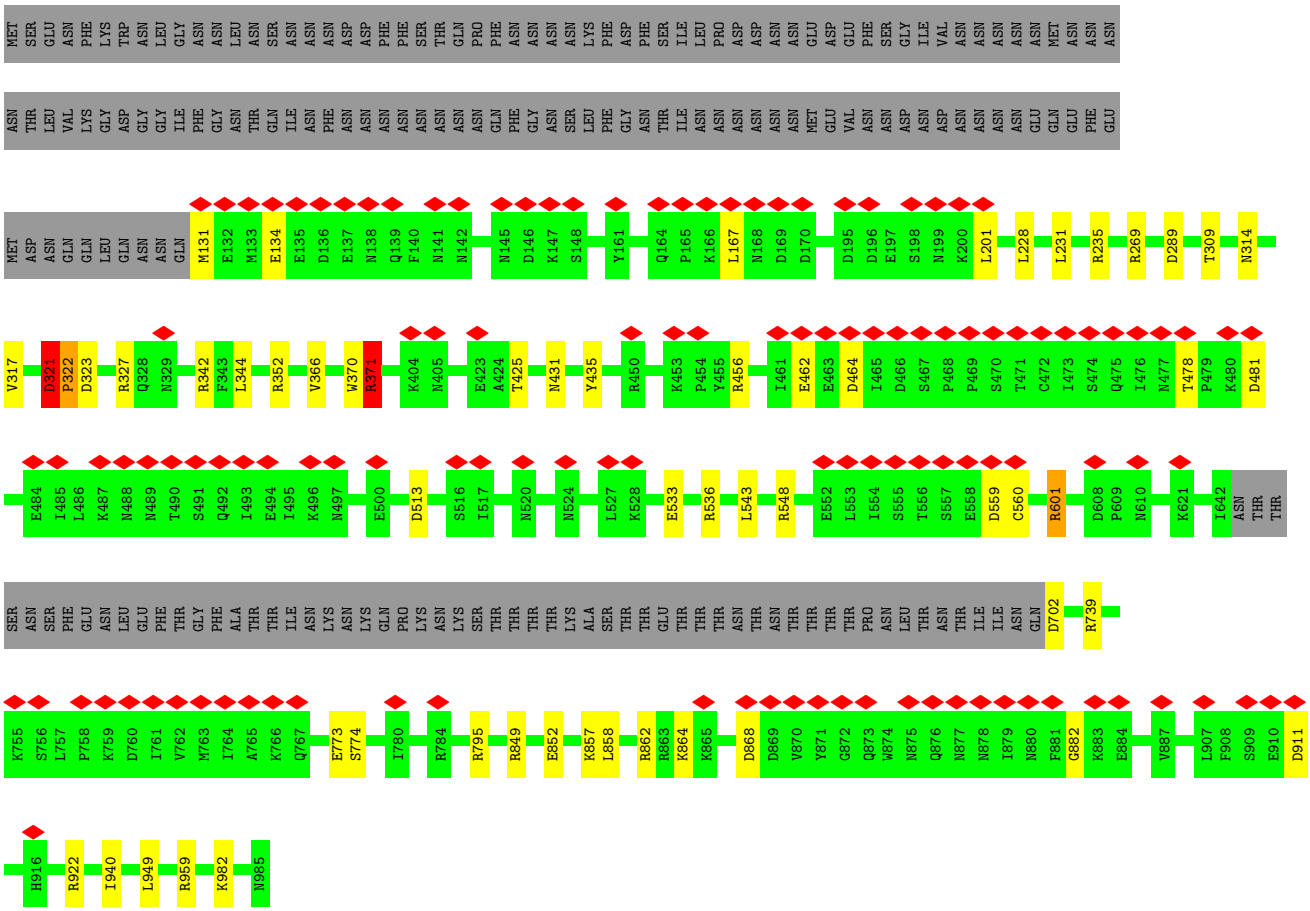
Chain K3:





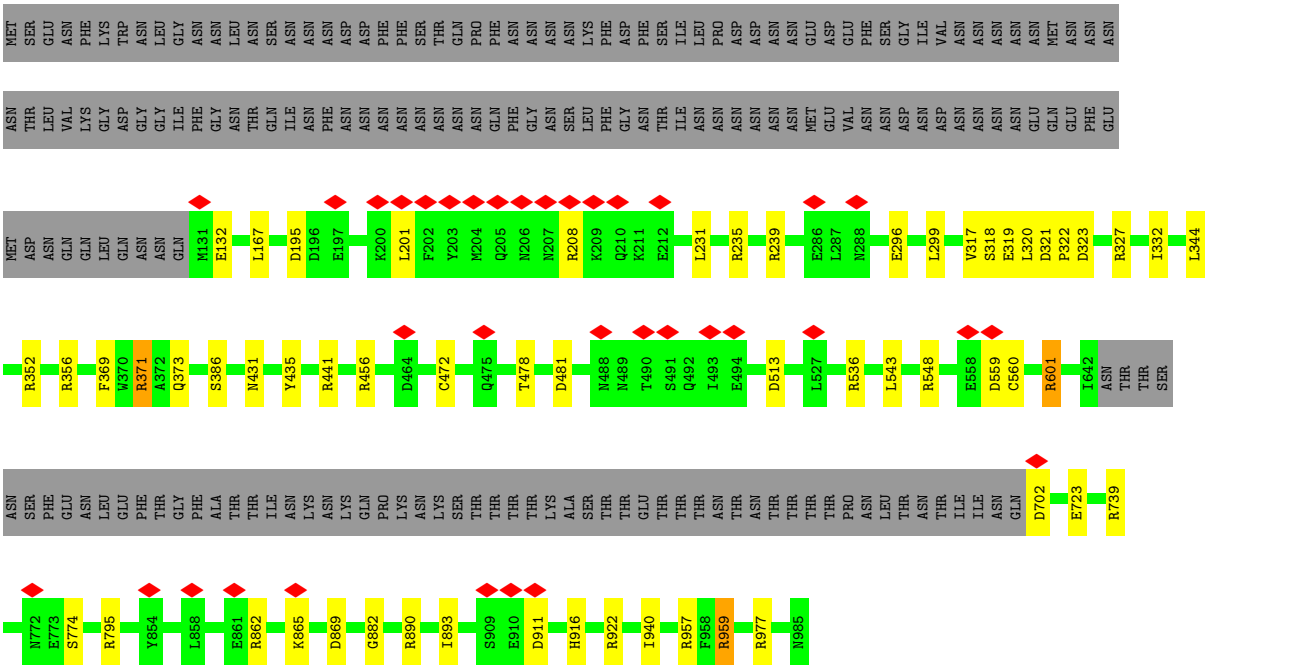
- Molecule 14: Nuclear pore complex protein

Chain L0:



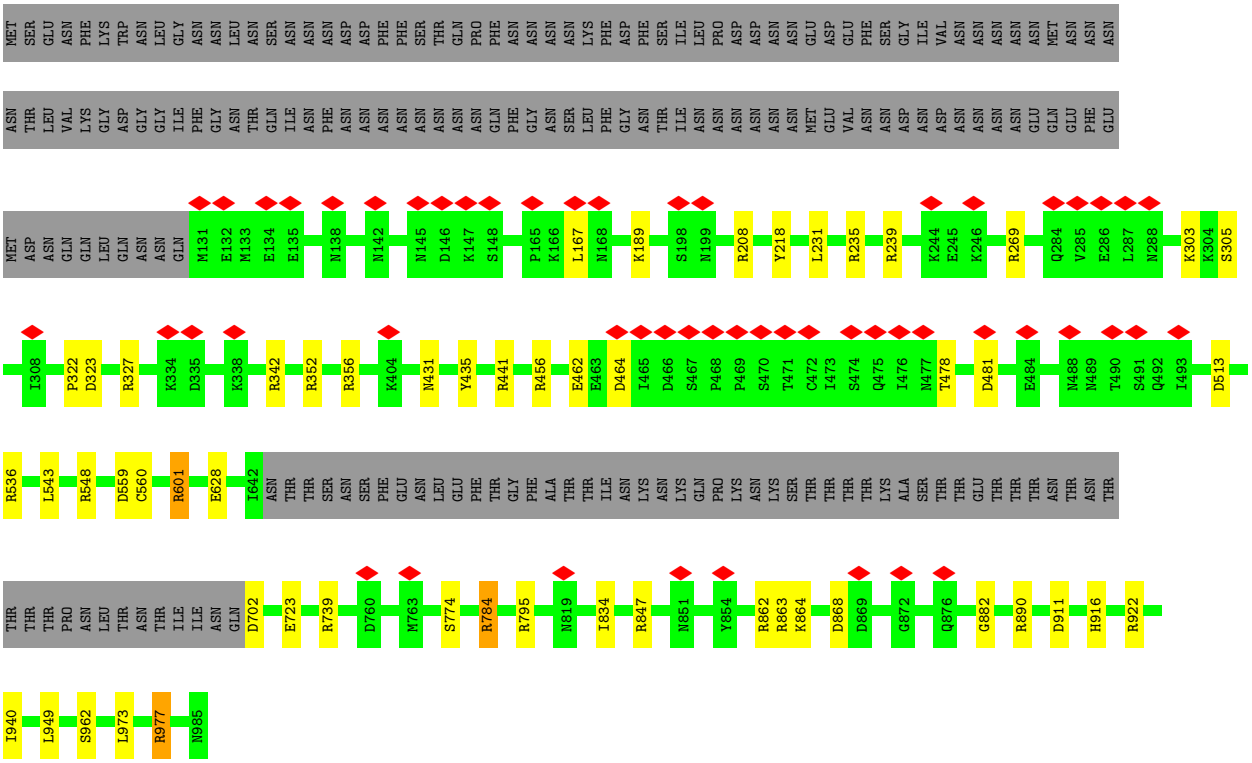
• Molecule 14: Nuclear pore complex protein

Chain L1: 75% 6% 19%



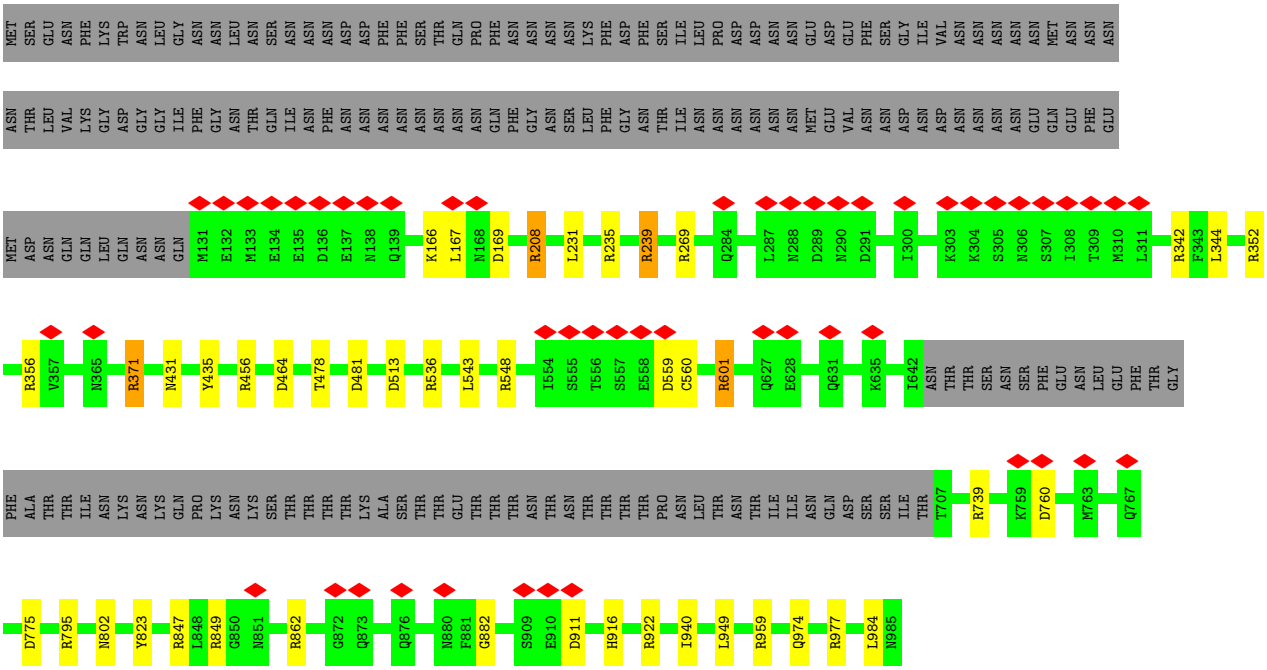
• Molecule 14: Nuclear pore complex protein

Chain L2:



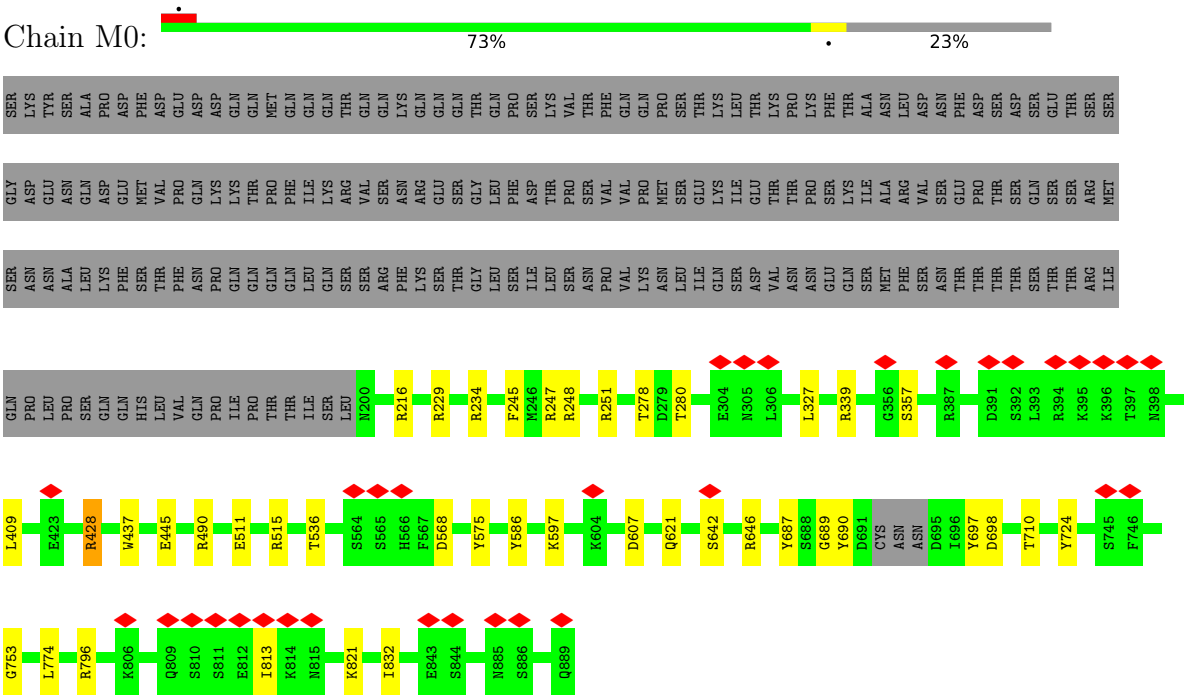
- Molecule 14: Nuclear pore complex protein

Chain L3:



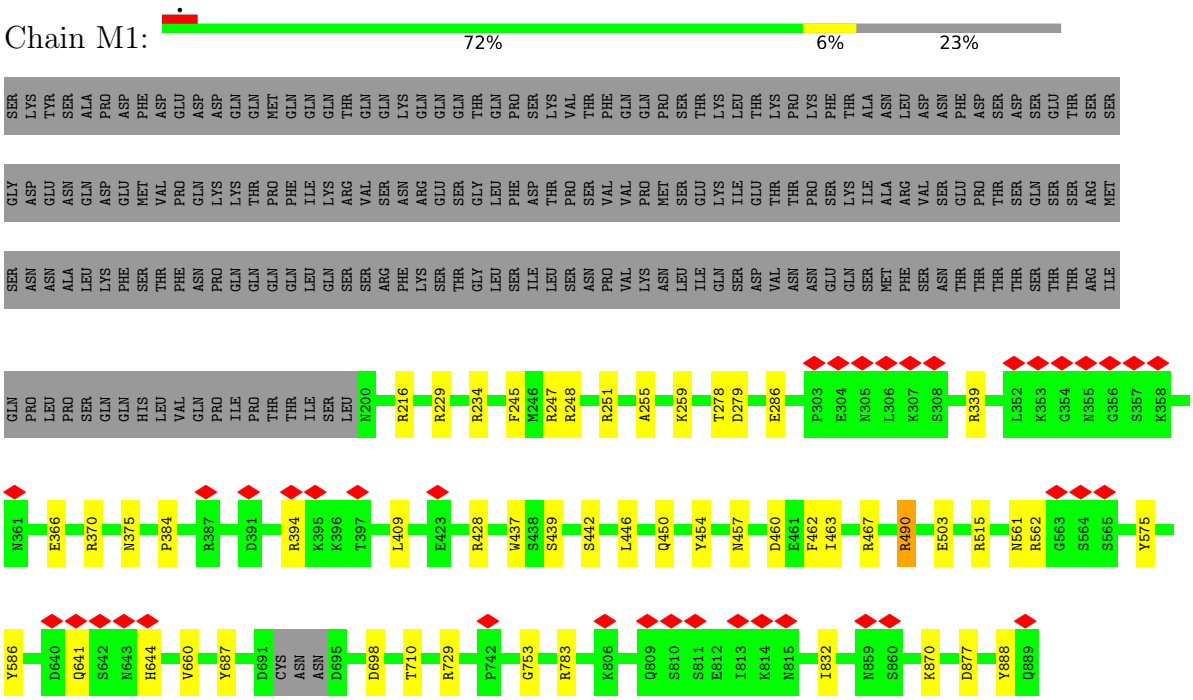
- Molecule 15: Nuclear pore complex protein Nup98-Nup96

Chain M0:



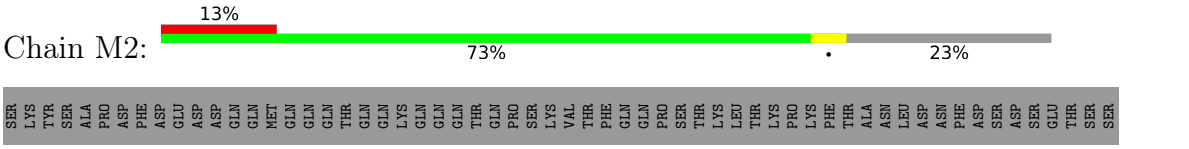
• Molecule 15: Nuclear pore complex protein Nup98-Nup96

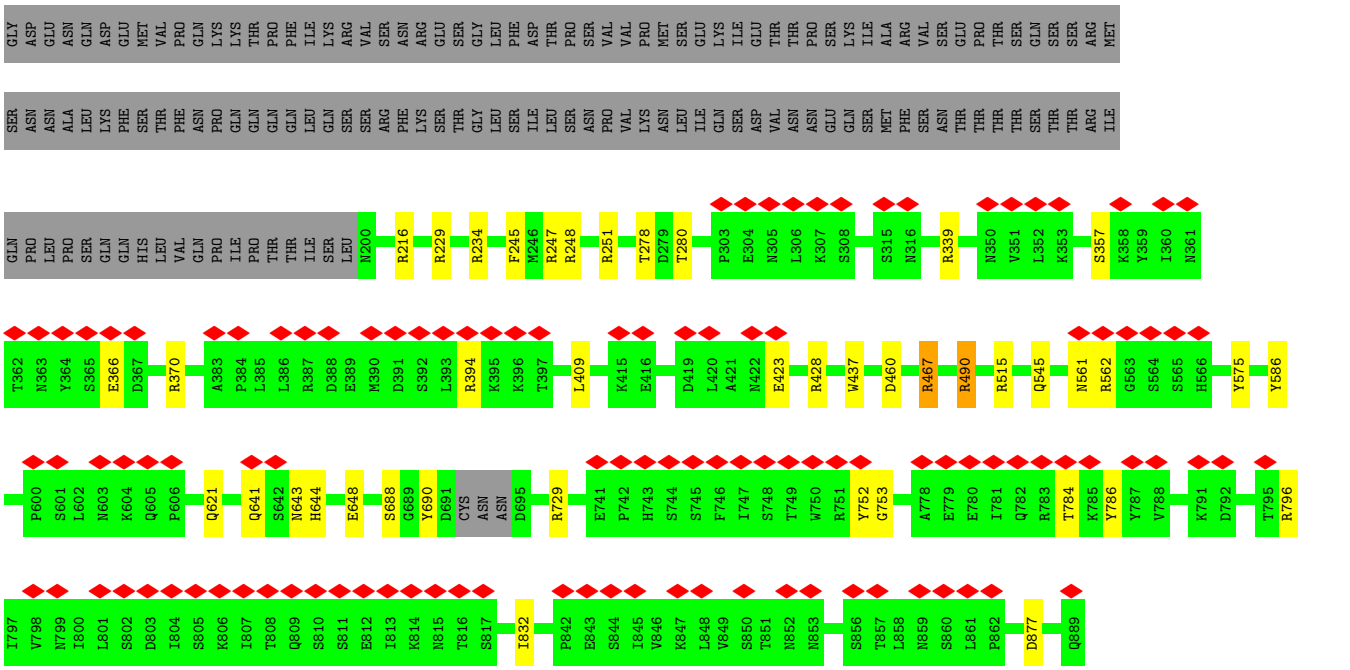
Chain M1:



• Molecule 15: Nuclear pore complex protein Nup98-Nup96

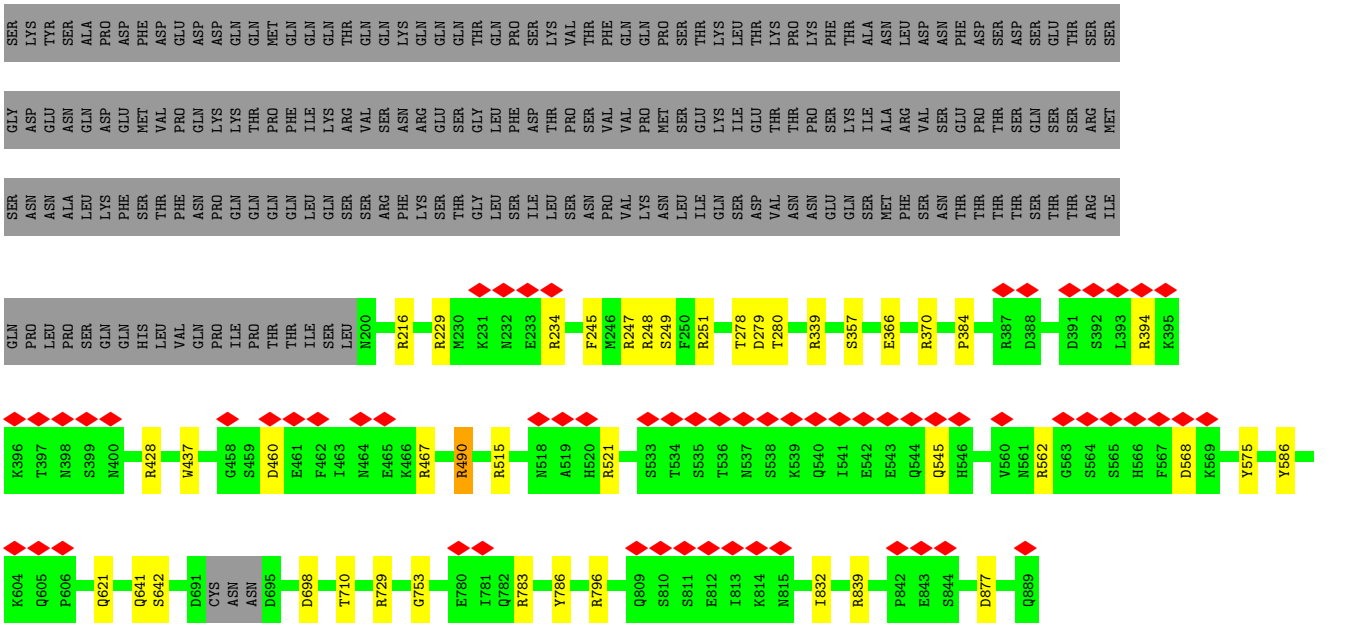
Chain M2:





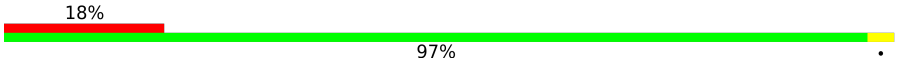
• Molecule 15: Nuclear pore complex protein Nup98-Nup96

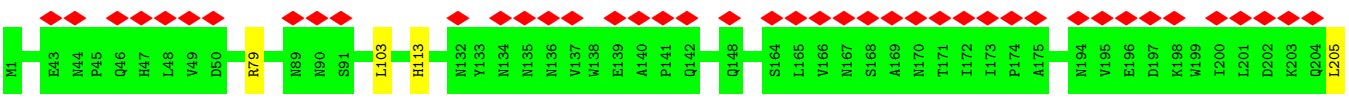
Chain M3:

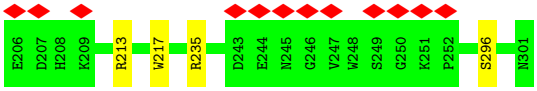


• Molecule 16: Protein SEC13 homolog

Chain N0:

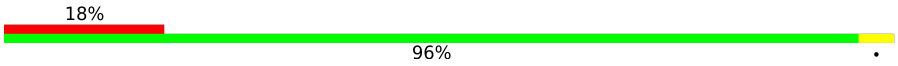


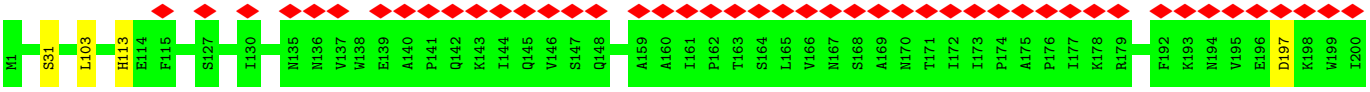


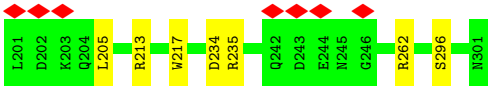


• Molecule 16: Protein SEC13 homolog

Chain N1:

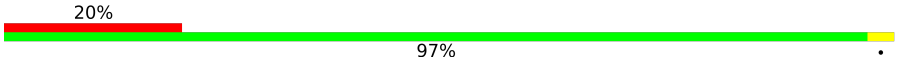


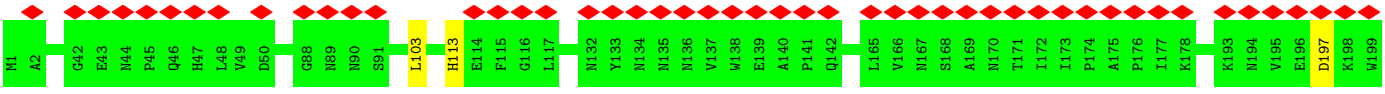


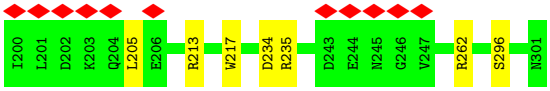


• Molecule 16: Protein SEC13 homolog

Chain N2:

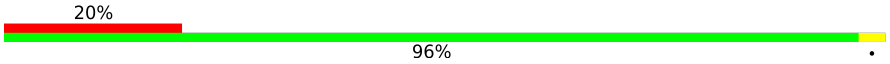


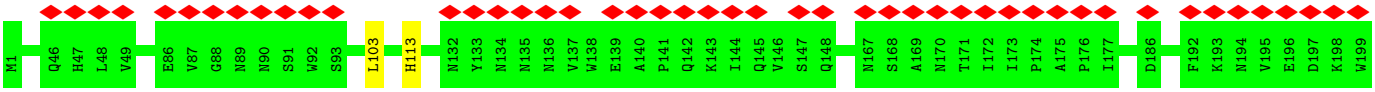


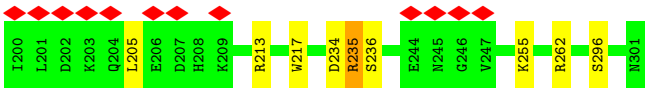


• Molecule 16: Protein SEC13 homolog

Chain N3:

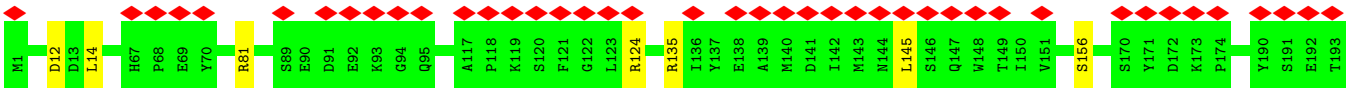


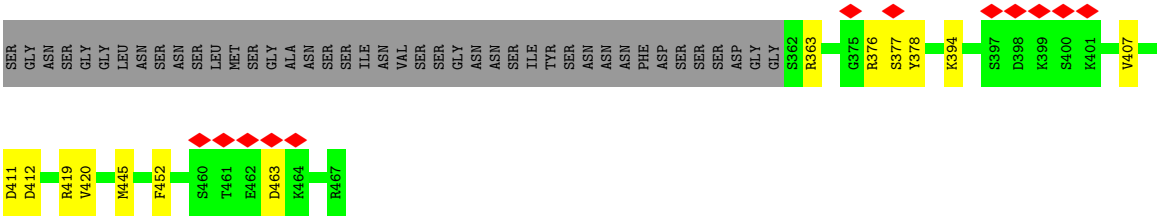




• Molecule 17: Seh1

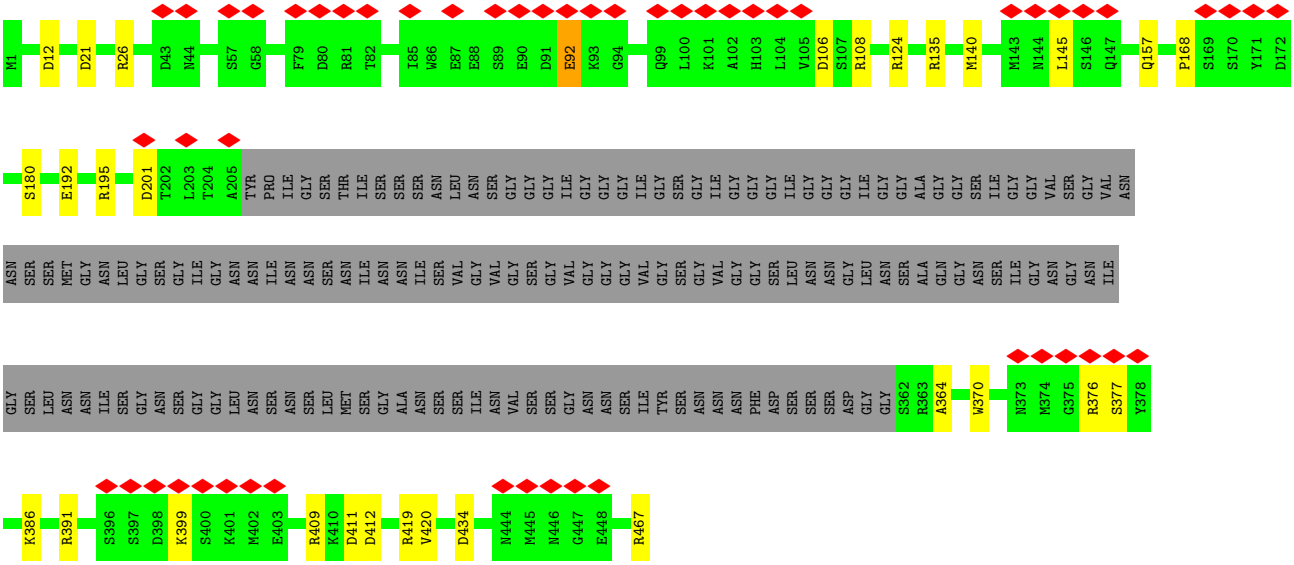
Chain O0:





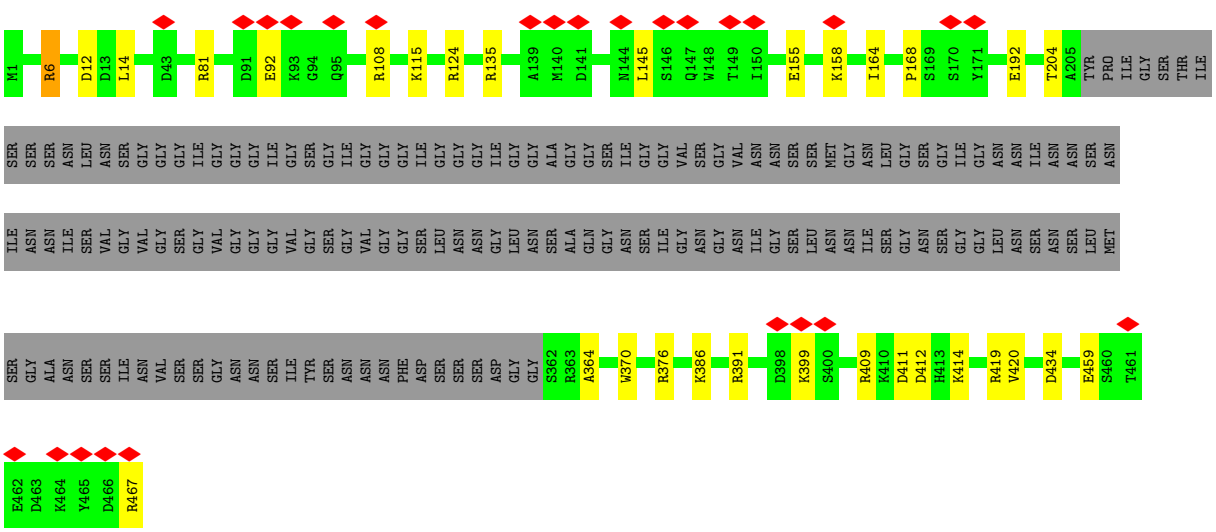
• Molecule 17: Seh1

Chain O1:



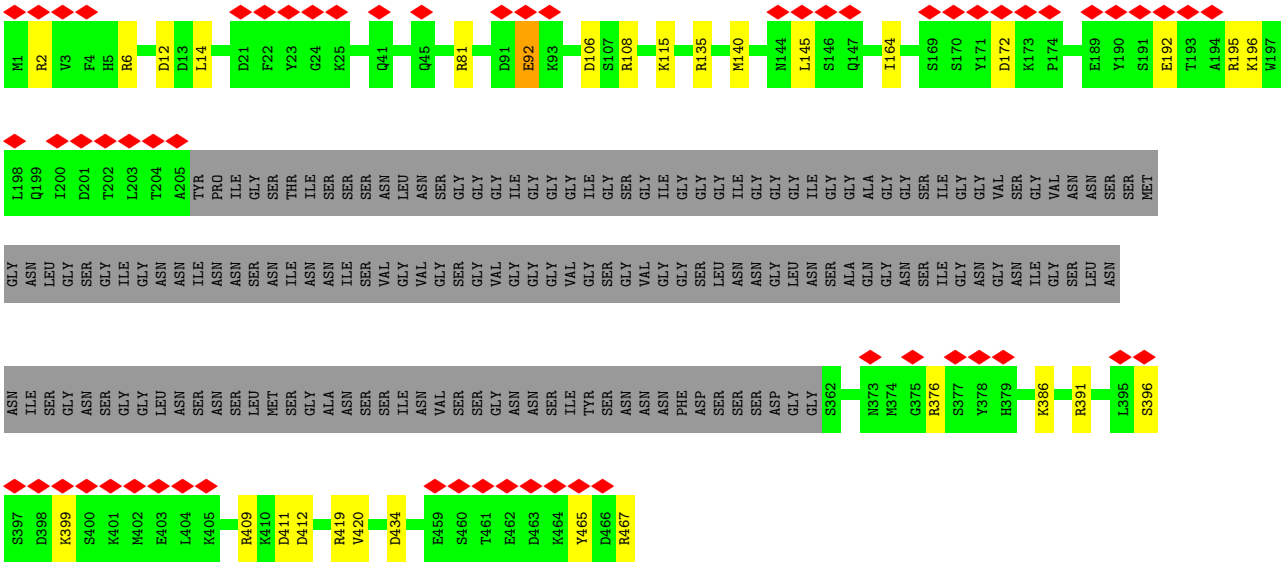
• Molecule 17: Seh1

Chain O2:



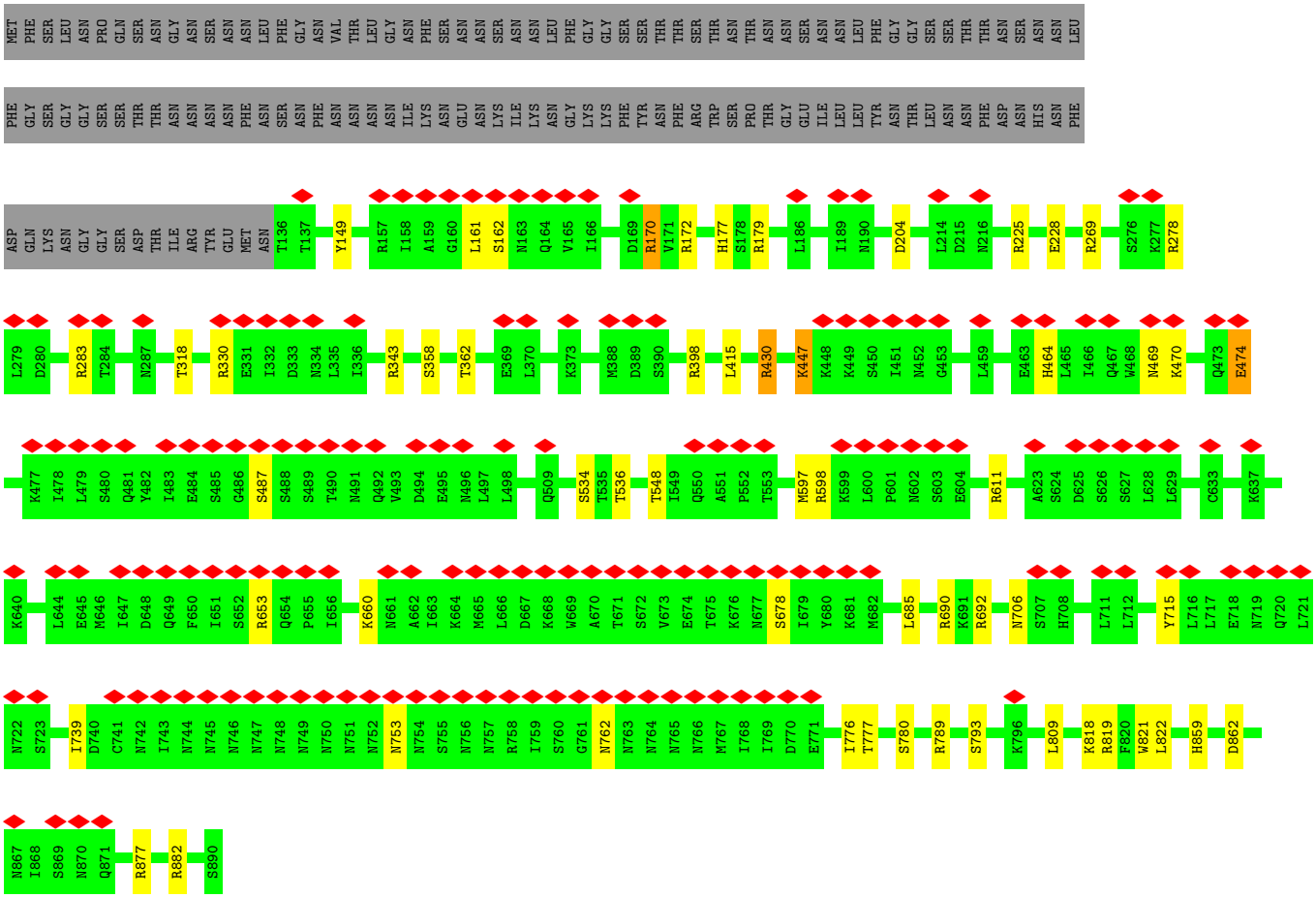
• Molecule 17: Seh1

Chain O3:



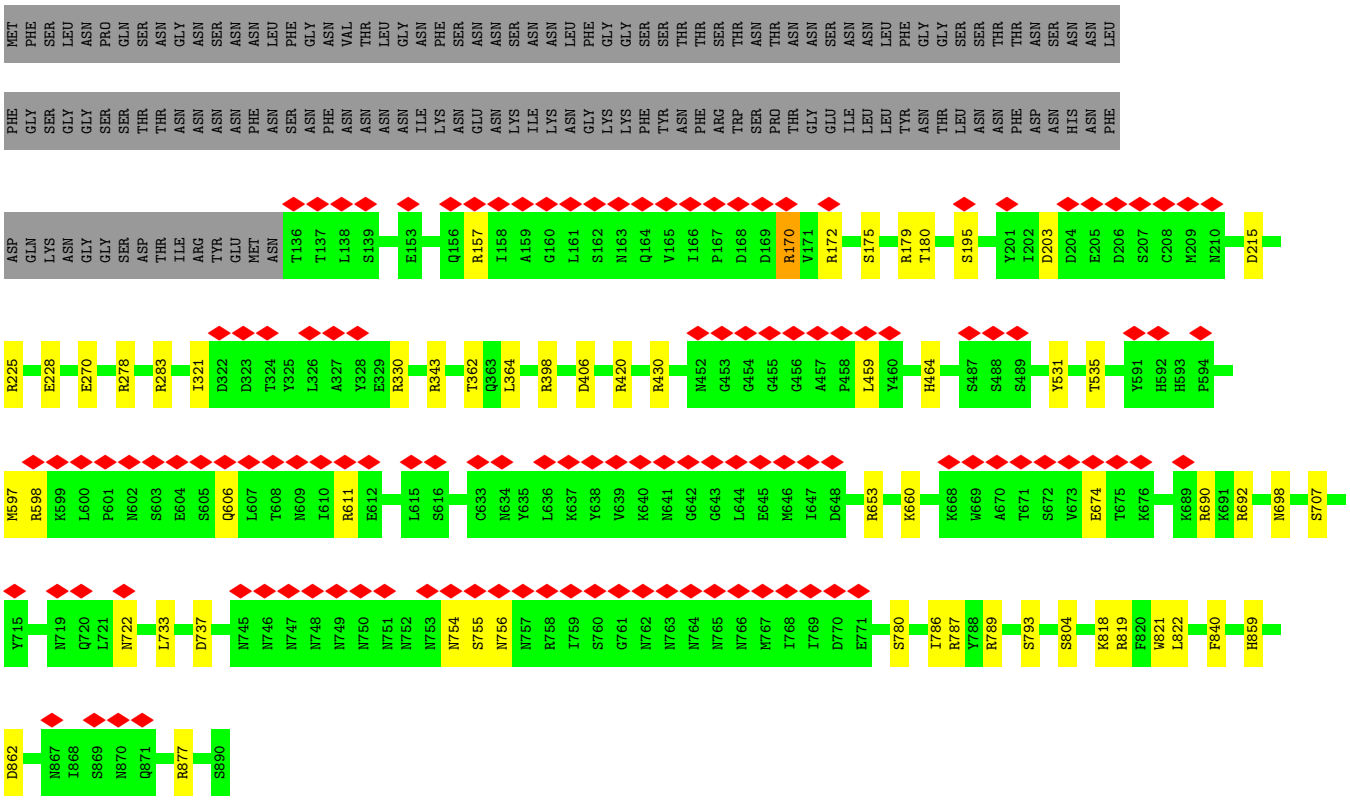
- Molecule 18: Nuclear pore complex protein nup85

Chain P0:



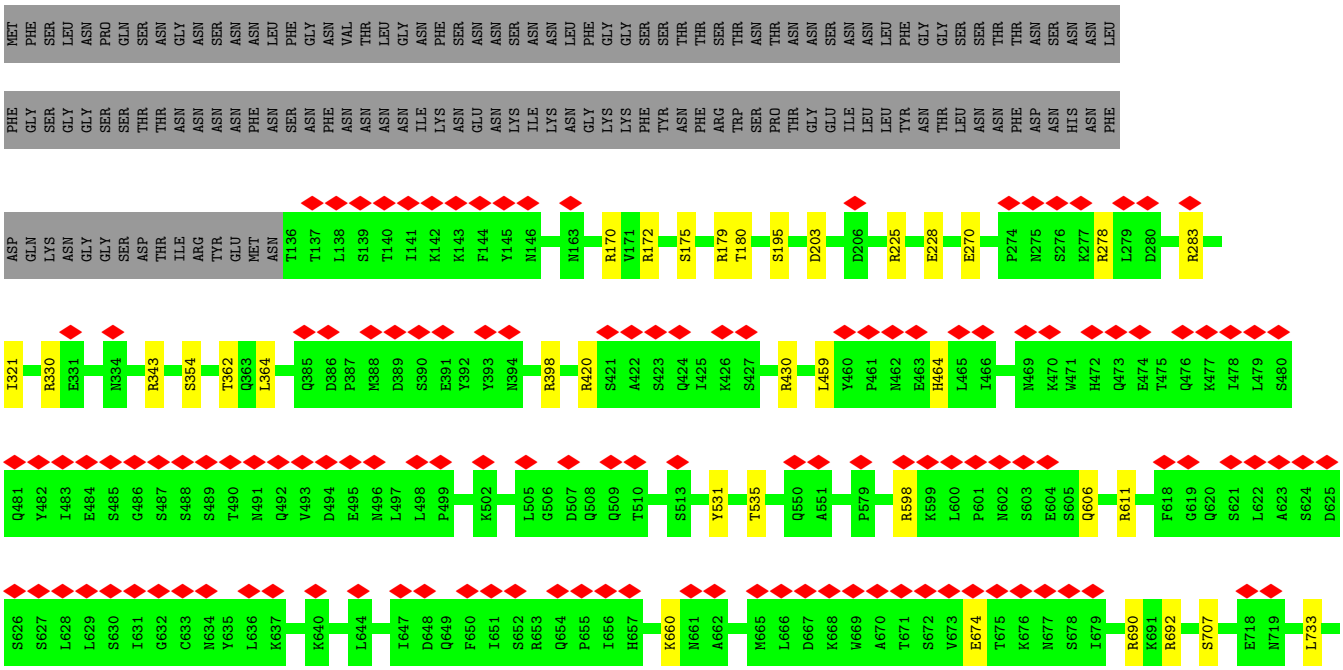
• Molecule 18: Nuclear pore complex protein nup85

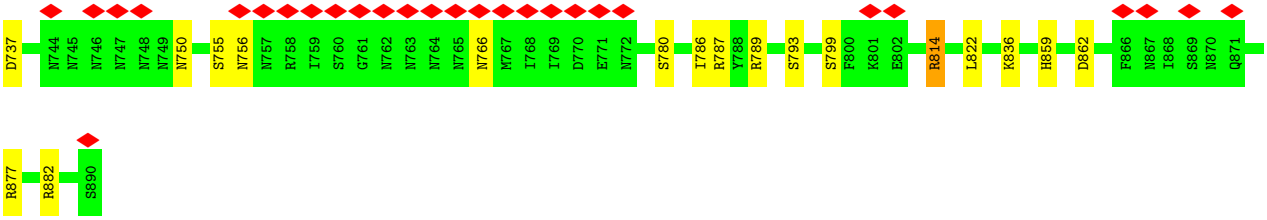
Chain P1:



• Molecule 18: Nuclear pore complex protein nup85

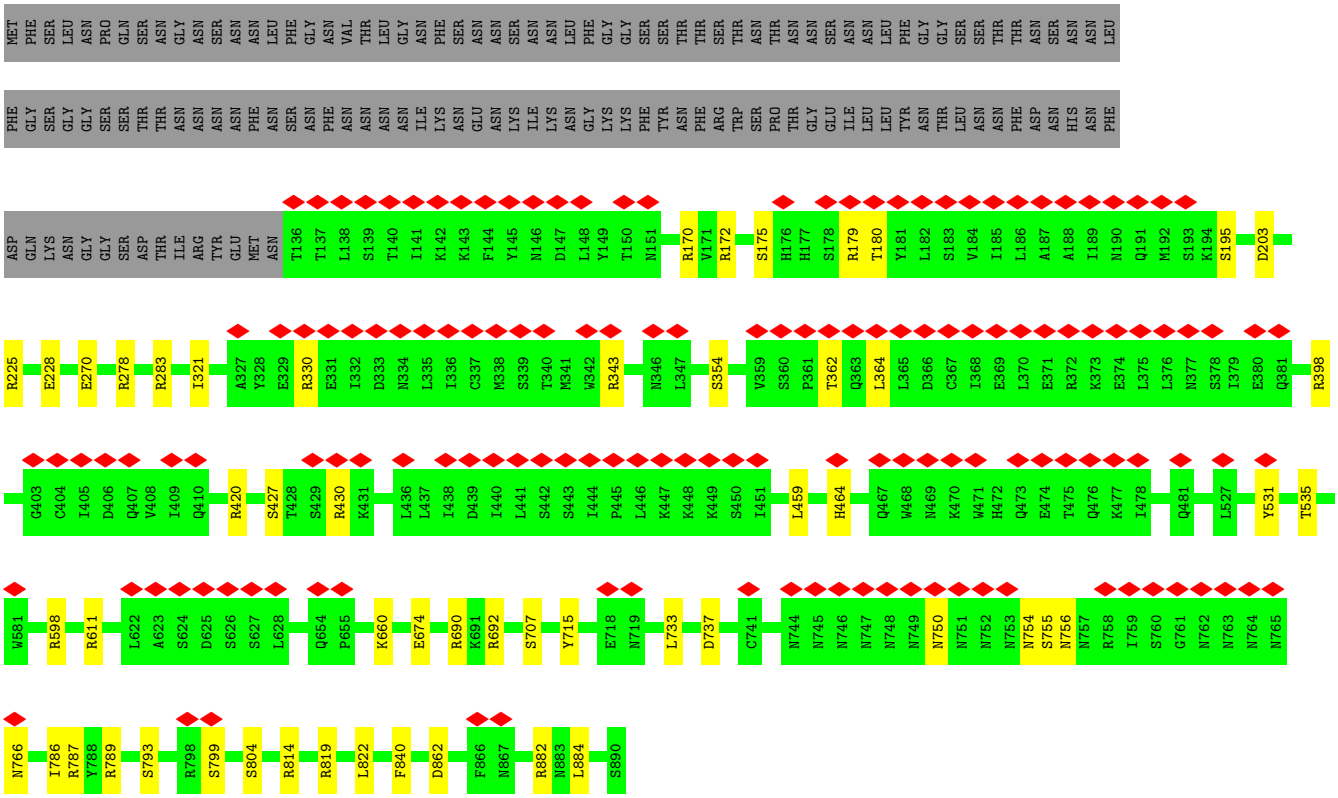
Chain P2:





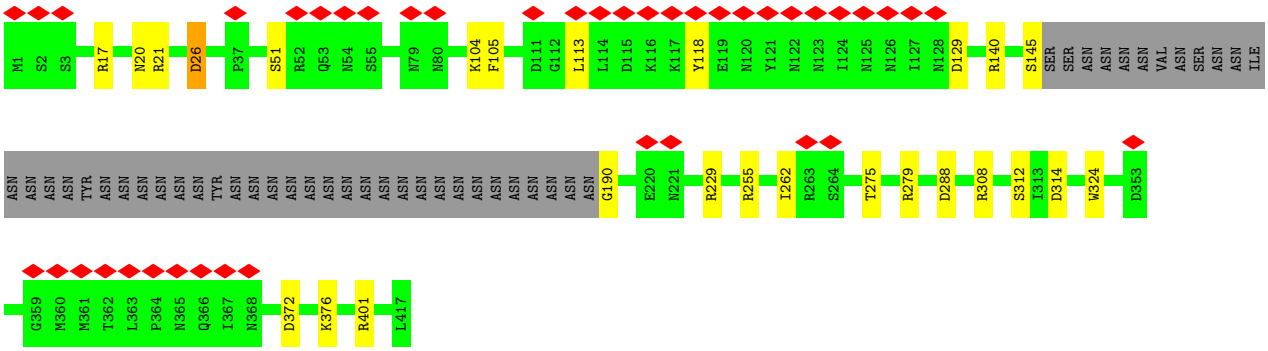
• Molecule 18: Nuclear pore complex protein nup85

Chain P3:



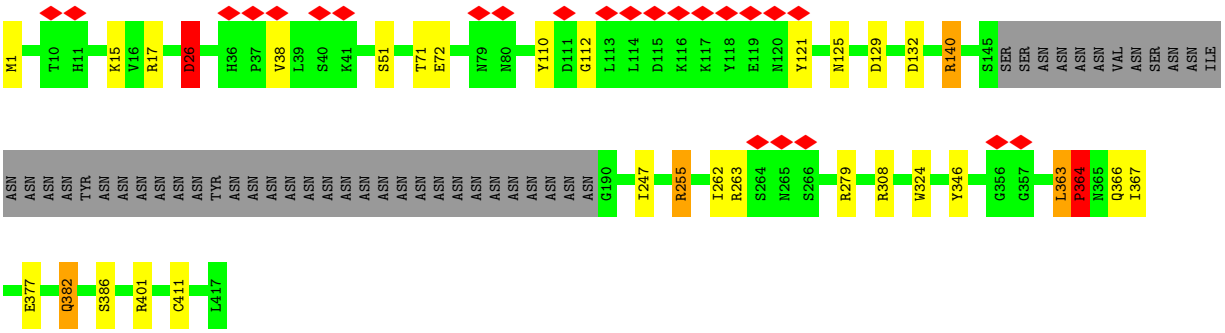
• Molecule 19: Nuclear pore complex protein nup43

Chain Q0:



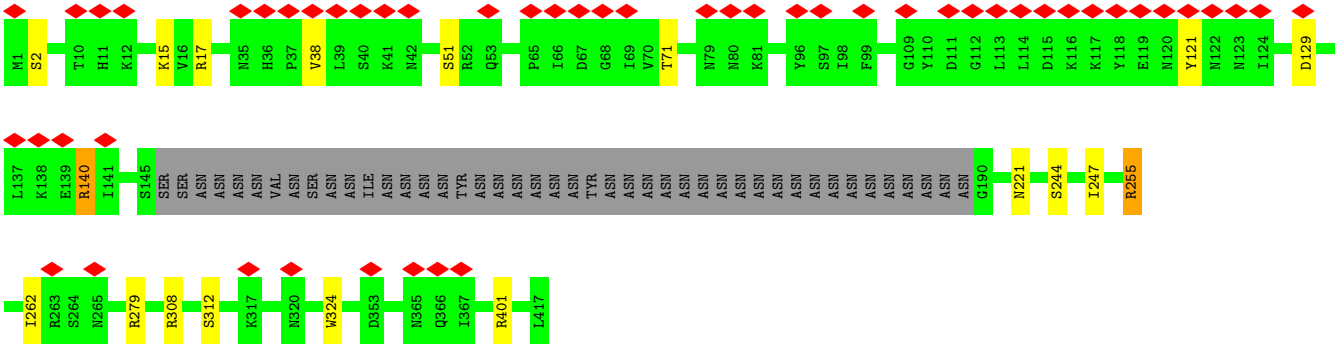
• Molecule 19: Nuclear pore complex protein nup43

Chain Q1:



- Molecule 19: Nuclear pore complex protein nup43

Chain Q2:


M1 S2 T10 H11 K12 K15 V16 R17 N35 H36 P37 V38 L39 S40 K41 N42 S51 R52 Q53 P65 I66 D67 G68 I69 V70 T71 N79 N80 K81 Y96 S97 I98 F99 G109 Y110 D111 G112 L113 L114 D115 K116 K117 Y118 E119 N120 Y121 N122 N123 I124 D129
L137 K138 E139 R140 I141 S145 SER SER ASN ASN ASN ASN VAL ASN SER ASN ASN ILE ASN ASN ASN ASN ASN TYR ASN ASN ASN ASN ASN TYR ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN

V101 S105 E119 S120 R124 I125 H126 F127 N128 N129 T130 S131 D143 T151 I152 S153 R158 I167 S170 D171 S172 R173 V174 G175 I176 K177 R178 K179 V180 E181 V182 D183 S184 F185 G186 S187 G188 S189 G190 N191 N192 N193 K194 R195 N196 Y197 K198 S199 S202 N203

L204 L205 N206 S207 N208 L209 D210 N211 Q212 W213 S214 R215 V216 R217 D222 S223 F224 E225 A234 S241 S242 G243 T247 S257 G258 K264 G270 Q271 G272 F273 F274 S275 S276 W277 K278 W279 G280 E281 K282 Q283 E284 W297 S298 N299 N312 N313 E346 N347 N348 N349

N350 N351 N352 N353 N354 I355 P356 T357 S358 P359 N360 I361 N362 S363 N364 Q365 Q366 Q367 Q368 Q369 Q370 Q371 N372 L373 S374 L375 I376 H377 Y383 Q384 R385 Q397 F398 N399 S400 E401 D412 K428 G429 K430 I449 K450 E451 Y454 N455 R456 G457 R458 I459 N460 R461 D462 D469

N470 K471 F472 D473 R474 N475 H476 F477 V478 D479 D480 N481 N482 F501 Q504 K505 L506 S507 T508 S509 N510 G511 N512 G513 N514 G515 N516 G517 N518 N519 N520 L521 E522 T549 I550 I551 E552 H553 S554 D555 E556 D557 S558 D559 Q560 P561 T562 D563 Q564 T565 Y566 Y567 Y568 N569 L570 R574

E588 Y589 D596 D597 H598 D601 F610 D611 N612 D613 N614 S615 L616 E617 S618 V619 V620 S621 N622 I623 L624 N625 Q626 E627 D628 F629 K630 F631 Q632 S633 N634 E635 Q636 W637 S638 I639 E661 R671 S697 N698 I699 I700 S701 D702 F705 Y706 N707 I708 I709 L710 N711 C712

F713 G714 S715 N716 S717 N718 V719 L720 V721 N722 D723 F724 L725 D735 R736 D740 R743 S744 F745 E746 Y747 E748 L749 S750 R751 Q752 N778 N779 N780 N781 I806 E807 N808 P809 I810 E811 T812 I813 N814 L815 I816 L817 K818 K819 F820 K821 E822 S825 N826 Q827 N828 D829 M830 V831

I832 Q833 L834 Q835 Q836 G837 Y838 K839 D842 D852 R883 G887 I888 D889 T890 K891 T892 T895 W916 F922 I923 K924 S925 F926 D927 N928 S929 T930 T931 S932 D933 I934 D935 K936 I937 L938 I939 S940 Q941 N942 Q943 Y944 G945 D946 D947 S948 D949 N950 N951 N952 N953 I954 N955

N956 N957 E958 Y959 Y960 E961 D962 Q963 Q964 Q965 Q966 T973 I974 S975 K976 N977 H1016 E1028 Q1031 Y1032 K1033 Q1034 L1035 M1036 E1037 F1038 L1039 Q1040 T1041 I1042 E1043 N1044 N1045 E1046 Y1065 S1066 K1067 E1080 D1107 I1108 P1109 I1110 D1111 N1112 R1113 M1114 M1115 N1116 Q1117 T1118 N1119 A1120 N1121

E1139 T1140 R1141 I1147 F1150 K1162 E1163 N1164 F1165 S1166 R1167 L1168 E1190 R1213 N1227 N1228 N1229 N1230 N1231 N1232 N1233 N1240 N1241 T1242 N1243 N1244 N1245 N1246 N1247 I1248 D1269 A1277 Q1278 D1279 L1280 N1281 K1282 R1297 R1301 I1316 E1317 G1320 D1329 L1334

P1353 D1366 I1367 R1368 S1369 T1370 N1371 I1372 Y1373 N1374 N1375 N1376 S1377 S1378 L1379 N1380 I1381 A1382 N1383 H1384 H1385 Q1386 K1412 E1413 I1414 E1415 K1416 E1417 Y1418 S1419 Y1420 Y1421 L1422 A1423 S1424 K1425 H1426 L1427 I1430 D1431 F1438 I1439 L1440 SER P1442 Q1443 Q1444 L1445 L1446 E1447 K1448 L1449 I1450 Q1451 Y1452

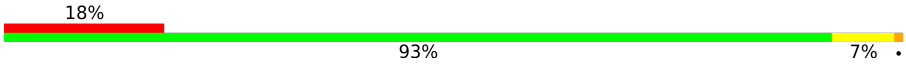
S1453 L1454 F1455 D1456 V1457 A1458 F1459 S1460 L1461 A1462 I1463 T1464 Q1465 E1466 I1467 D1468 L1469 G1470 A1471 I1472 F1473 E1474 S1475 F1476 A1477 S1478 K1479 C1480 V1481 Q1482 L1483 Q1484 L1485 N1486 P1487 Q1488 S1489 N1490 P1491 F1492 F1493 I1494 K1495 N1496 T1497 N1498 G1499 Y1500 G1503 A1509 R1543 S1546 D1547 K1548 D1549 F1550

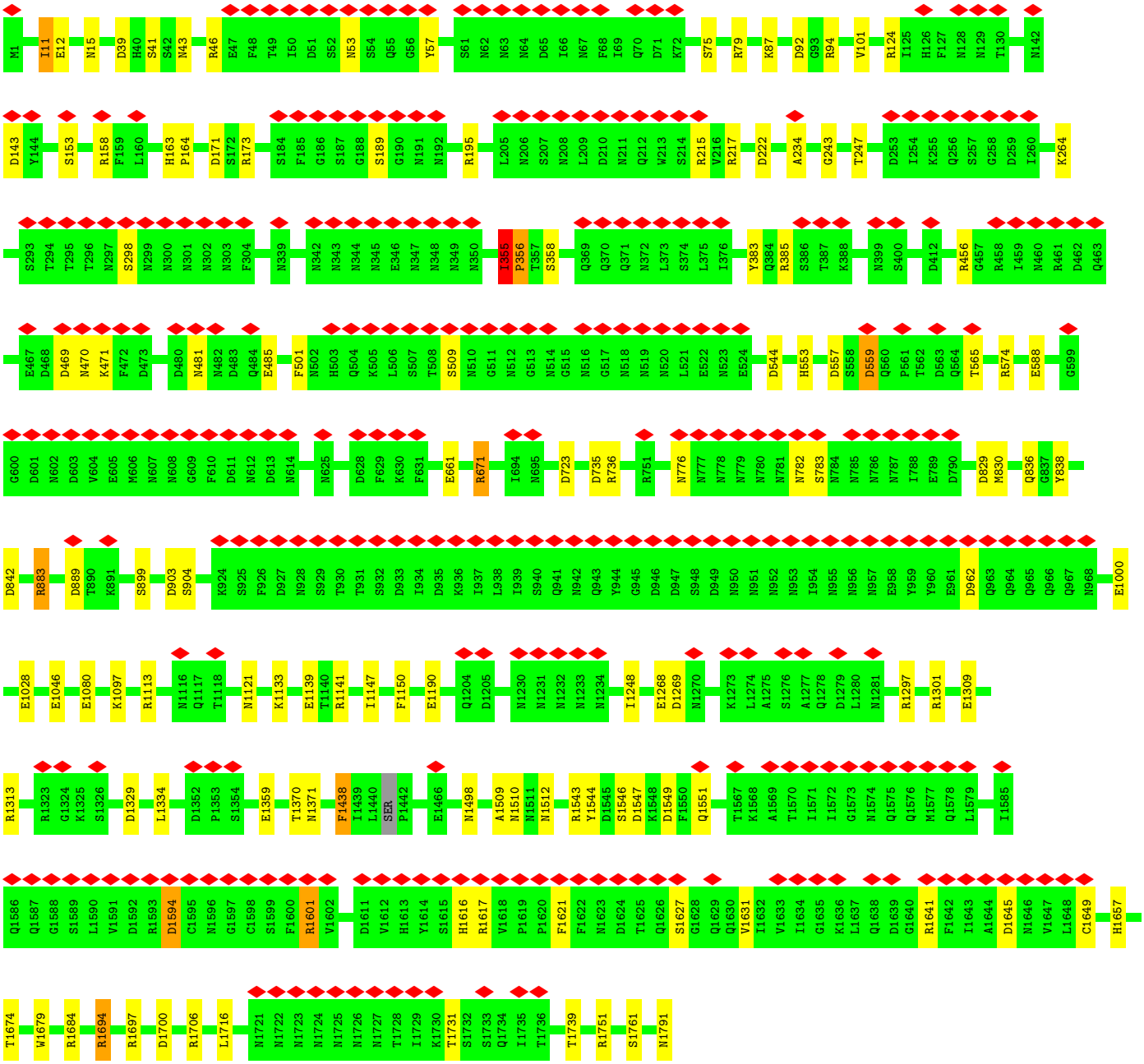
Q1551 I1572 G1573 N1574 Q1575 Q1576 Q1587 G1588 S1589 L1590 V1591 D1592 R1593 D1594 C1595 N1596 G1597 C1598 S1599 H1613 Y1614 S1615 H1616 R1617 V1618 P1619 P1620 D1624 S1627 G1628 Q1629 Q1630 V1631 Q1638 D1639 G1640 R1641 D1645 L1654 R1655 Y1656 L1659 V1660 T1663 Y1666 E1667 R1694

R1697 D1700 R1706 L1716 N1720 N1721 N1722 N1723 N1724 N1725 N1726 N1727 T1728 I1729 K1730 T1731 S1732 S1733 Q1734 T1735 T1739 R1751 S1761 T1764 N1791

- Molecule 20: Nup160

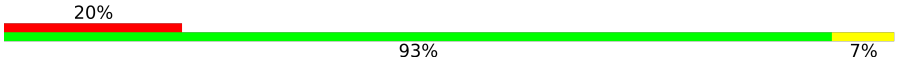
Chain R1:

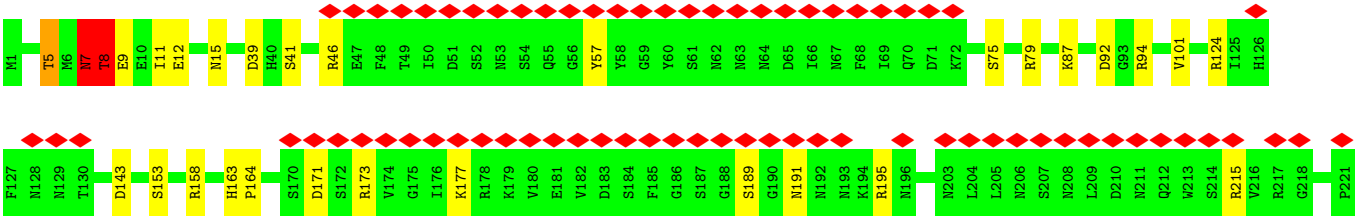




- Molecule 20: Nup160

Chain R2:





D222 S223 F224 E225 A234 S242 G243 S244 T247 K255 Q256 S257 G258 D259 I260 T261 V262 K263 K264 W279 K282 T296 N297 S298 N299 N300 N301 N302 N312 N322 D323 N338 N339 N342 N343 N344 N345 E346 N347 N348 N349 N350 N351 I355 P356 T357 S358

Q368 Q369 Q370 Q371 N372 L373 S374 L375 I376 H377 Y383 Q384 R385 Q397 F398 N399 S400 E401 D412 F413 S414 R423 K428 G429 K430 E451 R456 N470 E485 F501 L506 S507 T508 S509 N510 G511 N512 G513 N514 G515 N516 G517 N518 N519 N520 L521 E522 N523

N541 D544 D557 S558 D559 D563 Q564 T565 R574 E588 D594 D597 H598 G599 G600 D601 N602 D603 V604 E605 M606 N607 N608 G609 F610 D611 N612 D613 N614 S615 L616 E617 S618 V619 V620 S621 N622 I623 L624 N625 Q626 E627 D628 F629 K630 S633 E661 R671 I690

S691 N692 N693 I694 N695 N696 S697 N698 I699 I700 S701 D702 K729 N732 F733 I734 D735 R736 N778 N779 N780 N781 N782 S783 N784 N785 N786 N787 I788 E789 D790 N791 I792 N793 S825 N826 Q827 N828 D829 M830 V831 I832 Q833 Q836 G837 Y838 K839 D852 D889 S899 D903

S904 F926 D927 N928 S929 T930 T931 S932 D933 I934 D935 K936 I937 L938 I939 S940 Q941 N942 Q943 Y944 G945 D946 D947 S948 D949 N950 N951 N952 N953 I954 N955 N956 N957 E958 Y959 Y960 E961 D962 Q963 Q964 Q965 Q966 Q967 N968 Q969 Q970 Q971 F972 T973 N977 H1016 E1028 E1046 E1080

M1112 M1115 N1116 Q1117 T1118 N1119 E1139 T1140 R1141 I1147 F1150 K1162 E1163 R1167 E1190 D1205 N1227 N1228 N1229 N1230 N1231 N1232 N1233 N1234 N1235 N1236 N1237 T1238 N1239 N1240 N1241 T1242 N1243 N1244 N1245 N1246 N1247 I1248 D1269 R1297 R1301 R1323 G1324 K1325 S1326 I1327

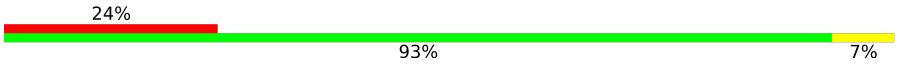
F1328 D1329 D1352 P1353 S1354 S1369 T1370 N1371 N1374 N1375 N1376 S1377 Q1433 F1438 I1439 I1440 SER P1442 E1466 I1467 D1468 Q1482 L1485 N1486 P1487 Q1488 S1489 K1495 N1496 T1497 S1502 G1503 R1543 S1546 D1547 K1548 D1549 F1550 Q1551 P1555 N1566 T1567 K1568 A1569 T1570 I1571 I1572

G1573 N1574 Q1575 Q1576 M1577 Q1578 G1588 V1591 D1592 R1593 D1594 C1595 N1596 R1601 S1615 H1616 R1617 F1621 S1627 Q1630 V1631 K1636 L1637 Q1638 D1639 N1646 C1649 L1654 R1655 R1684 R1694 R1697 D1700 H1711 L1716 N1721 N1724 N1725 N1726 N1727 T1728

I1729 K1730 T1731 K1738 T1739 R1751 S1762 I1763 I1764 N1791

- Molecule 20: Nup160

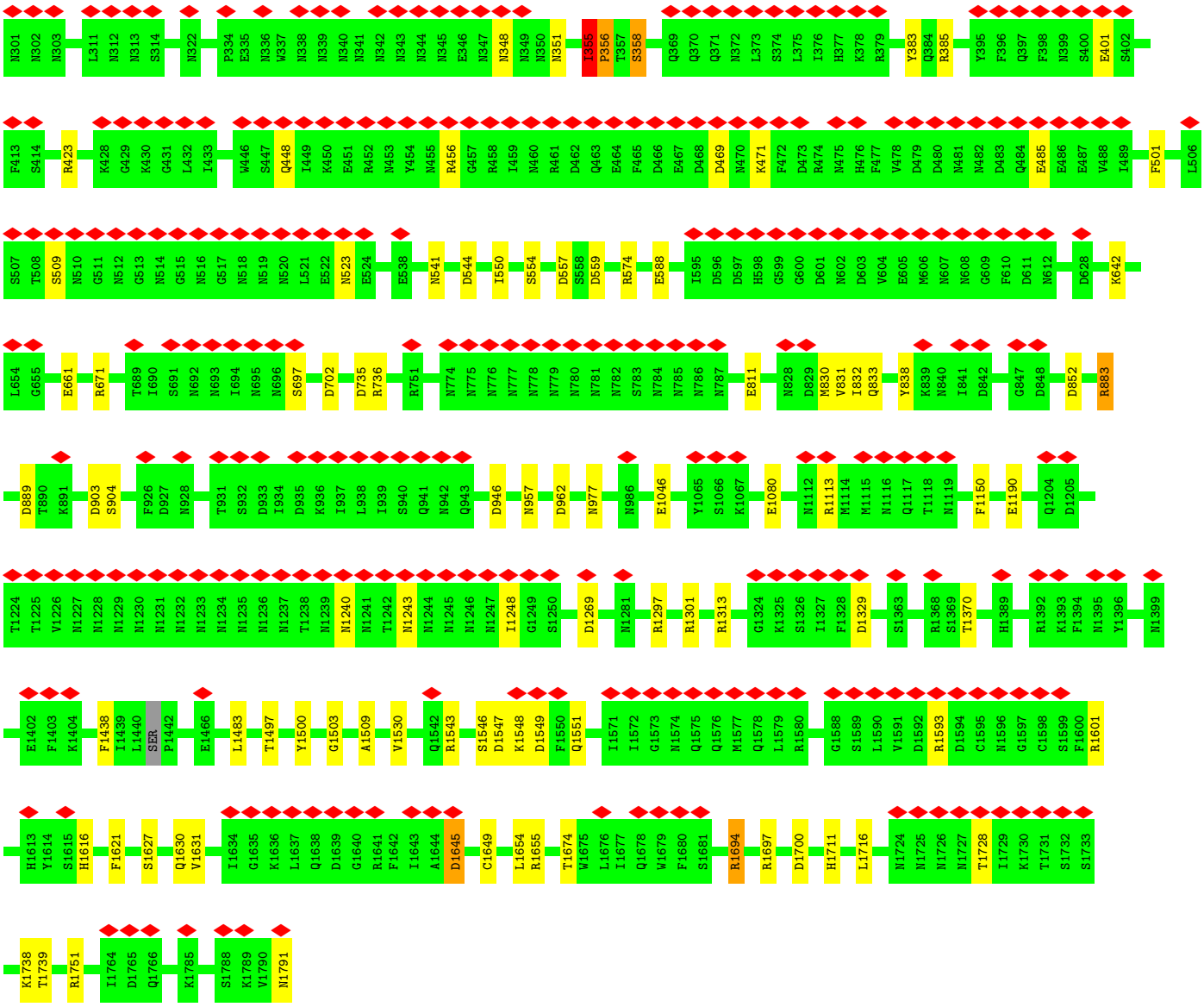
Chain R3:



M1 S2 D3 M6 I11 E12 D18 S36 D39 H40 S41 R46 S52 N53 S54 Q55 G56 Y57 Y58 G59 Y60 S61 N62 N63 N64 D65 I66 N67 F68 I69 Q70 D71 K72 F73 T74 S75 T76 P77 Y78 R79 K87 D92 G93 R94 L100 V101 N102 K103 S104 S105

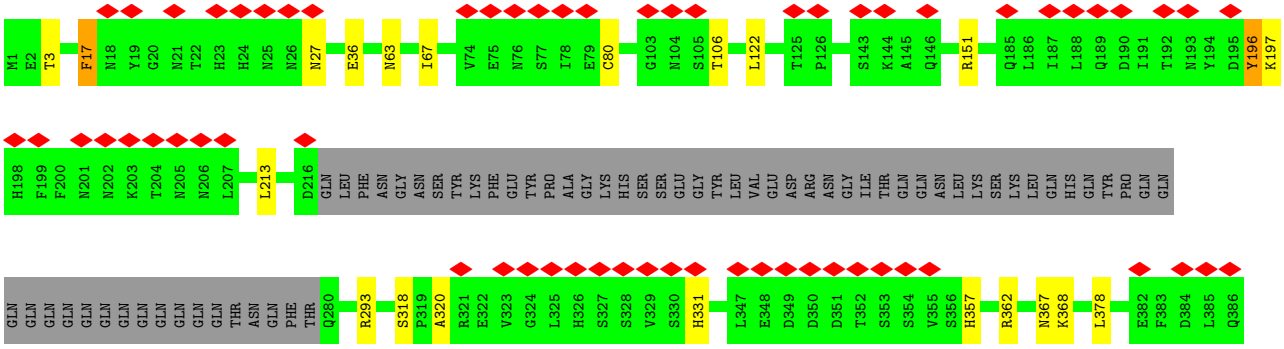
T106 H116 S117 L118 E119 S120 R124 N128 N129 T130 S131 I132 I133 G134 N142 D143 T150 T151 T152 S153 K154 T155 I156 Y157 R158 H163 P164 I167 E168 H169 S170 D171 S172 R173 V174 G175 I176 K177 R178 K179 V180 E181 S184 F185 G188 S189 G190 N191 N192 N193 K194

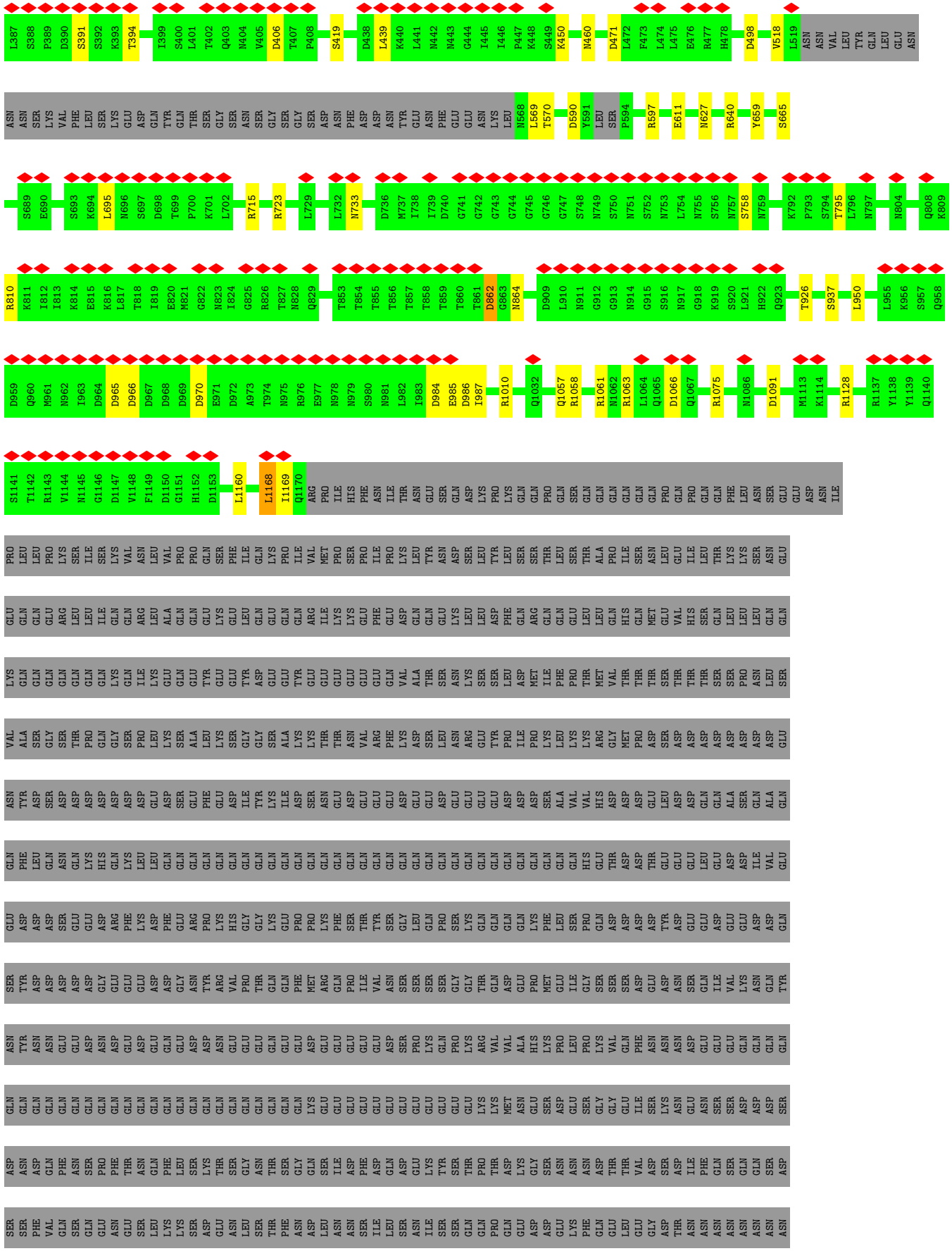
R195 N196 Y197 K198 V216 R217 G218 V219 L220 P221 D222 S223 F224 E225 P226 T227 V228 A234 T235 K236 I239 G240 S241 S242 G243 S244 G245 S246 T247 W248 L249 E250 L251 S252 D253 I254 K255 D259 I260 T261 V262 K263 K264 F265 E284 P285 V286 Q287 T295 T296 N297 S298 N299 N300

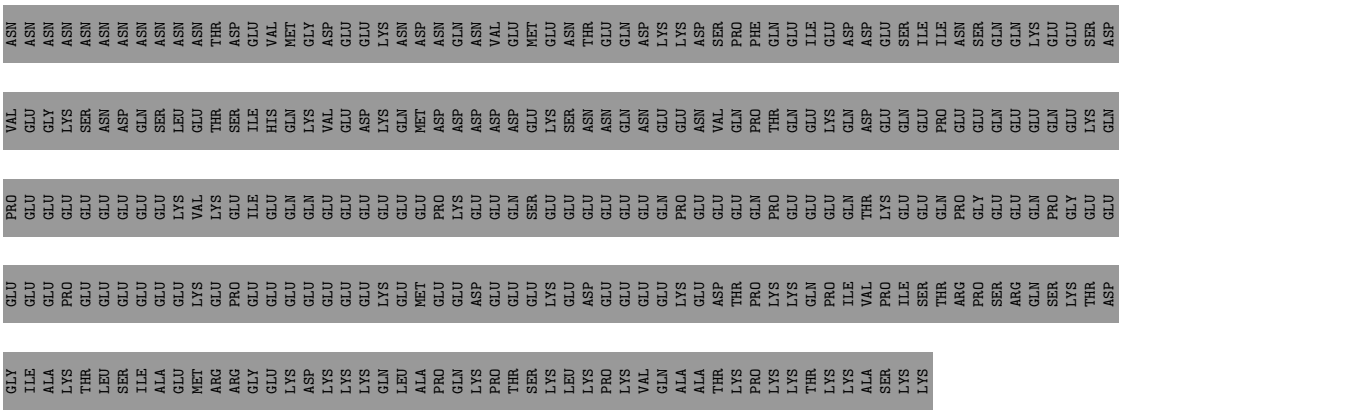


- Molecule 21: ELYS-like domain-containing protein

Chain T0:

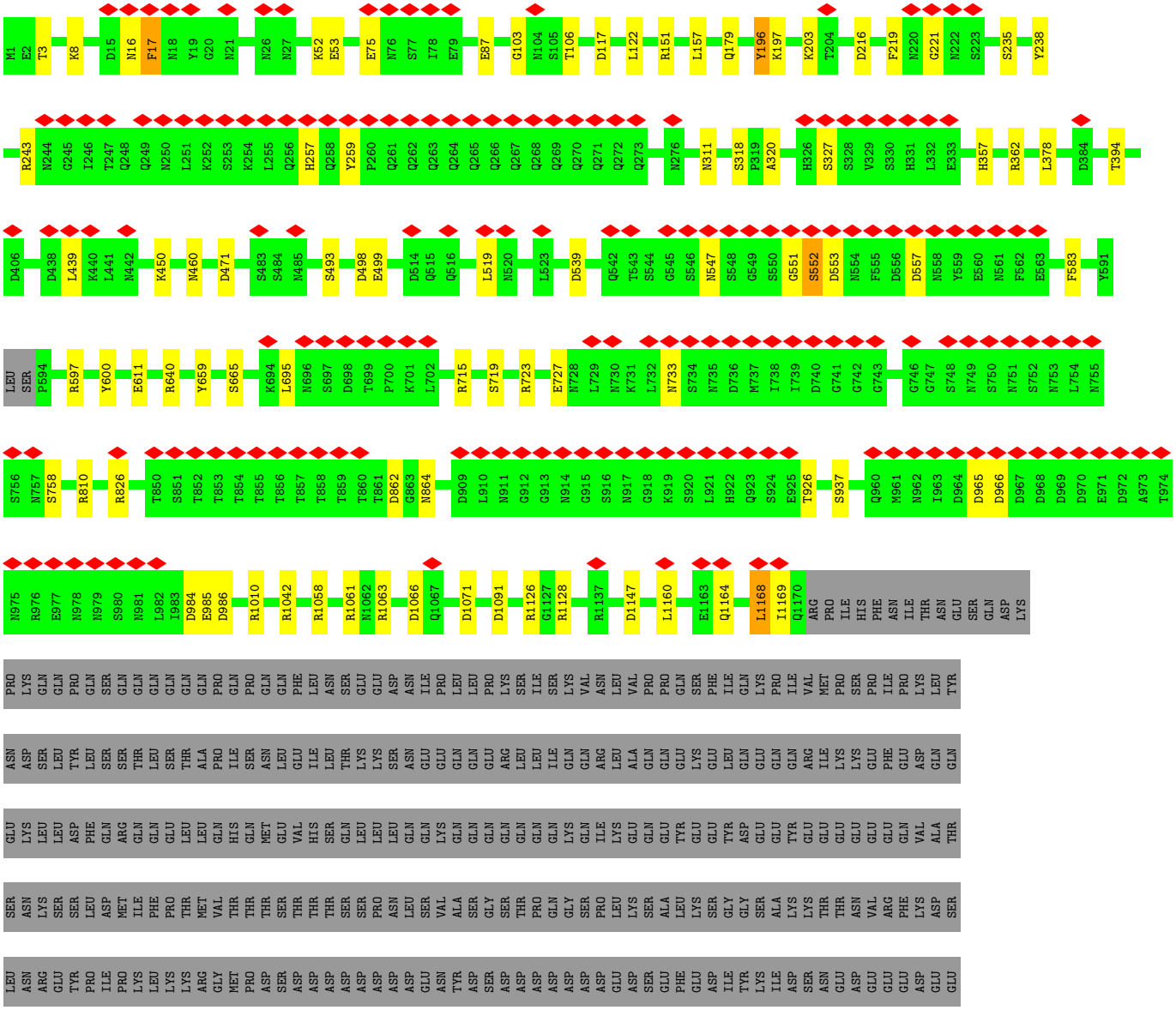


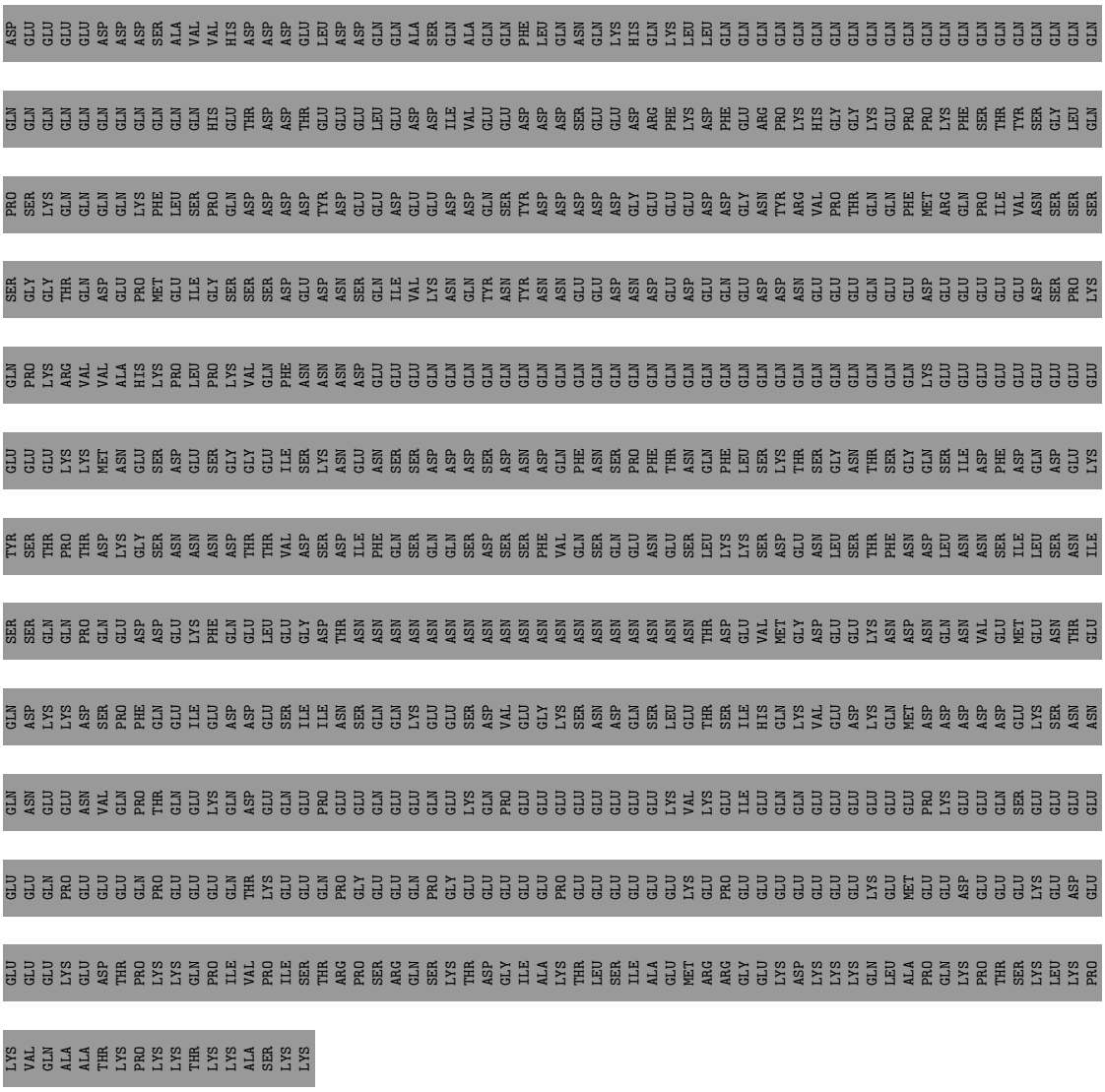

L387 S388 P389 D390 S391 S392 K393 T394 I399 S400 L401 T402 Q403 N404 V405 D406 T407 P408 S419 D438 L439 K440 L441 N442 N443 G444 I445 I446 P447 K448 S449 K450 N460 D471 L472 F473 L474 L475 E476 R477 H478 D498 V518 L519
ASN ASN VAL LEU TYR GLN LEU GLU ASN
ASN ASN SER LYS VAL PHE LEU SER LYS GLU ASP GLN TYR GLN THR SER GLY SER ASN SER GLY SER GLY SER ASP ASN PHE ASP ASP ASN TYR GLU ASN PHE GLU GLU ASN LYS LEU N568 L569 T570 D590 Y591 LEU SER P594 R597 E611 N627 R640 Y659 S665
S689 E690 S693 K694 L695 N696 S697 D698 T699 P700 K701 L702 R715 R723 L729 L732 N733 D736 M737 I738 I739 D740 G741 G742 G743 G744 G745 G746 G747 S748 N749 S750 N751 S752 N753 L754 N755 S756 N757 S758 N759 K792 P793 S794 T795 L796 N797 N804 Q808 K809
R810 K811 I812 I813 K814 E815 K816 L817 T818 I819 E820 M821 G822 N823 I824 G825 R826 T827 N828 Q829 T853 T854 T855 T856 T857 T858 T859 T860 T861 D862 G863 N864 D909 L910 N911 G912 G913 N914 G915 S916 N917 G918 K919 S920 L921 H922 Q923 T926 S937 L950 L955 K956 S957 Q958
D959 Q960 N961 N962 I963 D964 D965 D966 D967 D968 D969 D970 E971 D972 A973 T974 N975 R976 E977 N978 N979 S980 N981 L982 I983 D984 E985 D986 I987 R1010 Q1032 Q1057 R1058 R1061 N1062 R1063 L1064 Q1065 D1066 Q1067 R1075 M1086 D1091 M1113 K1114 R1128 R1137 Y1138 Y1139 Q1140
S1141 T1142 R1143 V1144 N1145 G1146 D1147 V1148 F1149 D1150 G1151 H1152 D1153 L1160 L1168 I1169 Q1170
ARG PRO ILE HIS PHE ASN ILE THR ASN GLU SER GLN ASP LYS PRO LYS GLN GLN PRO GLN SER GLN GLN GLN GLN GLN PRO GLN GLN PHE LEU ASN SER GLU GLU ASP ASN ILE
PRO LEU LEU PRO LYS SER ILE SER LYS VAL ASN LEU VAL PRO PRO GLN SER PHE ILE GLN LYS PRO ILE VAL MET PRO SER PRO ILE PRO LYS LEU TYR ASN ASP SER LEU TYR LEU SER SER THR LEU SER THR ALA PRO ILE SER ASN LEU GLU ILE ILE LEU THR LYS LYS SER ASN GLU
GLU GLN GLN GLU ARG LEU LEU ILE GLN GLN ARG LEU ALA GLN GLN GLU LYS GLU LEU GLN GLU GLN GLN ARG ILE LYS LYS GLU PHE GLU ASP GLN GLN GLU LYS LEU LEU ASP PHE GLN ARG GLN GLN GLU LEU LEU GLN HIS GLN MET GLU VAL HIS SER GLN LEU LEU LEU GLN GLN
LYS GLN GLN GLN GLN GLN GLN LYS GLN ILE LYS GLU GLN GLU TYR GLU GLU GLU GLU GLU GLN VAL ALA THR SER ASN LYS SER SER LEU ASP MET ILE PHE PRO THR MET VAL THR THR SER THR THR THR SER SER PRO ASN LEU SER
VAL ALA SER GLY SER THR PRO GLN GLY SER PRO LEU LYS SER ALA LEU LYS SER GLY GLY SER ALA LYS LYS THR THR ASN VAL ARG PHE LYS ASP SER LEU ASN ARG GLU TYR PRO ILE PRO LYS LEU LYS LYS ARG GLY MET PRO ASP SER ASP ASP ASP ASP ASP ASP ASP ASP
ASN TYR ASP SER ASP ASP ASP ASP ASP GLU ASP SER GLU PHE GLU ASP ILE TYR LYS ILE ASP SER ASN GLU ASP GLU GLU GLU ASP GLU GLU GLU GLU ASP ASP ASP SER ALA VAL VAL HIS HIS ASP ASP ASP GLU LEU ASP ASP GLN GLN ALA SER GLN ALA GLN
GLN PHE LEU GLN ASN GLN LYS HIS GLN LYS LEU LEU GLN GLN GLN GLN GLN GLN



• Molecule 21: ELYS-like domain-containing protein

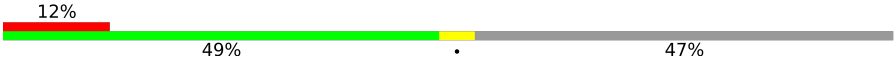
Chain T1:

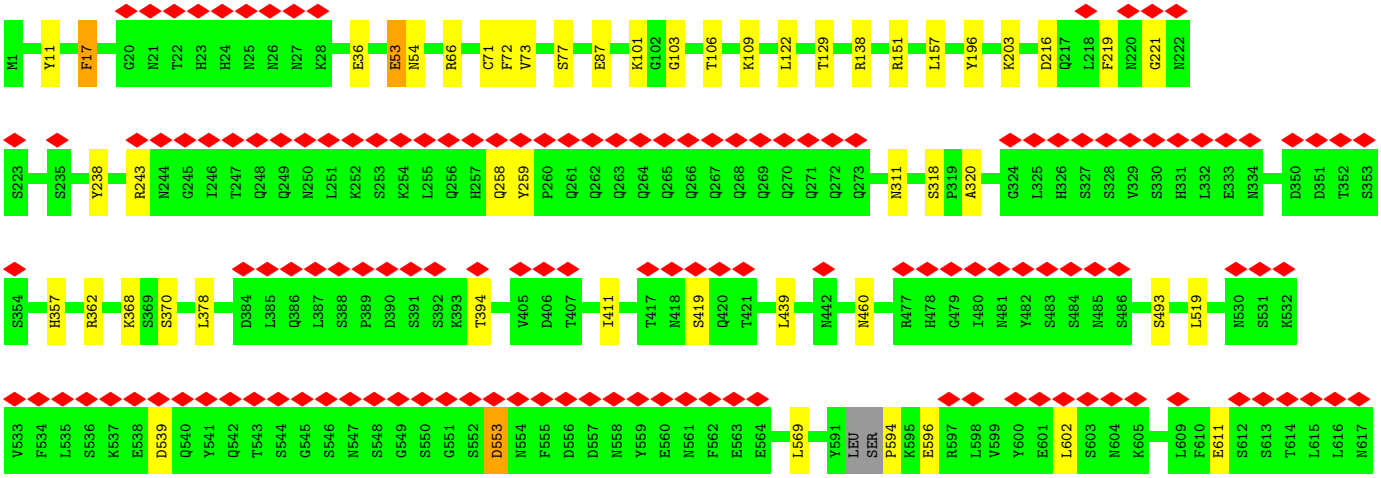


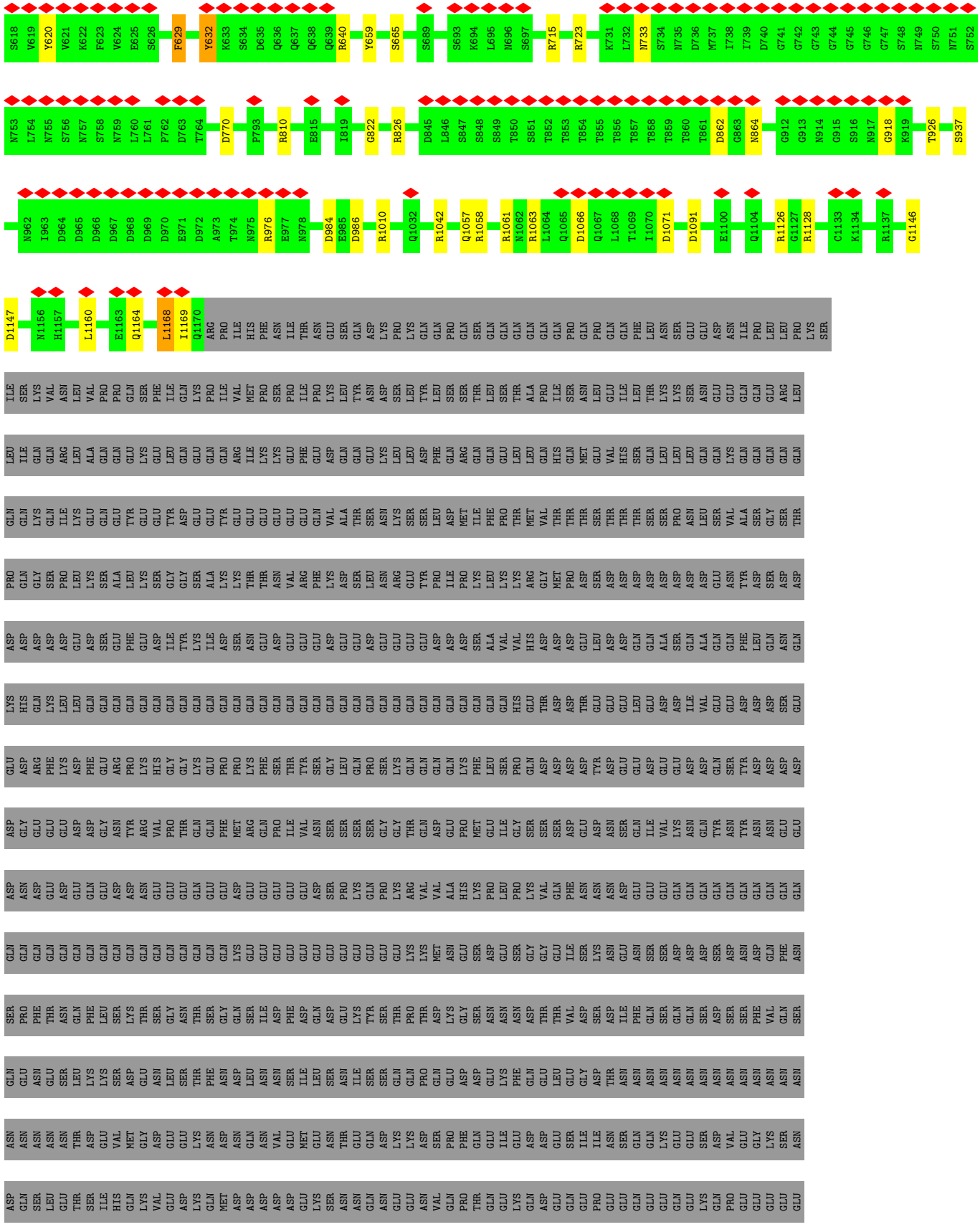


• Molecule 21: ELYS-like domain-containing protein

Chain T2:






S618 V619 Y620 V621 K622 F623 V624 E625 S626 F629 Y632 K633 S634 D635 Q636 Q637 Q638 Q639 R640 Y659 S665 S689 S693 K694 L695 N696 S697 R715 R723 K731 L732 N733 S734 N735 D736 M737 I738 I739 D740 G741 G742 G743 G744 G745 G746 G747 S748 N749 S750 N751 S752
N753 L754 N755 S756 N757 S758 N759 L760 L761 P762 D763 T764 D770 P793 R810 E815 I819 G822 R826 D845 L846 S847 S848 S849 T850 S851 T852 T853 T854 T855 T856 T857 T858 T859 T860 T861 D862 G863 N864 G912 G913 N914 G915 S916 N917 G918 K919 T926 S937
N962 I963 D964 D965 D966 D967 D968 D969 D970 E971 D972 A973 T974 N975 R976 E977 N978 D984 E985 D986 R1010 Q1032 R1042 Q1057 R1058 R1061 N1062 R1063 L1064 Q1065 D1066 Q1067 L1068 T1069 I1070 D1071 D1091 E1100 Q1104 R1126 G1127 R1128 C1133 K1134 R1137 G1146
D1147 N1156 H1157 L1160 E1163 Q1164 L1168 I1169 Q1170 ARG PRO ILE HIS PHE ASN ILE THR ASN GLU SER GLN ASP LYS PRO LYS GLN GLN PRO GLN SER GLN GLN GLN GLN GLN GLN GLN PRO GLN PRO GLN GLN PHE LEU ASN SER GLU GLU ASP ASN ILE PRO LEU LEU PRO LYS SER
ILE SER LYS VAL ASN LEU VAL PRO PRO GLN SER PHE ILE GLN LYS PRO ILE VAL MET PRO SER PRO ILE PRO LYS LEU TYR ASN ASP SER LEU TYR LEU SER SER THR LEU SER THR ALA PRO ILE SER ASN LEU GLU ILE LEU THR LYS SER GLU GLU GLN GLN GLU ARG LEU
LEU ILE GLN GLN ARG LEU ALA GLN GLN GLU LYS GLU LEU GLN GLN GLU GLN ARG ILE LYS LYS GLU PHE GLU ASP GLN GLN GLU LYS LEU LEU ASP PHE GLN ARG GLN GLN GLU LEU LEU GLN HIS GLN MET GLU VAL HIS SER GLN LEU LEU LEU GLN GLN LYS GLN GLN GLN GLN
GLN GLN LYS GLN ILE LYS GLU GLN GLU TYR GLU GLU TYR ASP GLU GLU TYR GLU GLU GLU GLU GLU GLN VAL ALA THR SER ASN LYS SER SER LEU ASP MET ILE PHE PRO THR MET VAL THR THR THR SER THR THR THR SER SER PRO ASN LEU SER VAL ALA SER GLY SER THR
PRO GLN GLY SER PRO LEU LYS SER ALA LEU LYS SER GLY GLY SER ALA LYS LYS THR THR ASN VAL ARG PHE LYS ASP SER LEU ASN ARG GLU TYR PRO ILE PRO LYS LEU LYS LYS ARG GLY MET PRO ASP SER ASP ASP ASP ASP ASP ASP ASP ASP GLU ASN TYR ASP SER SER ASP ASP
ASP ASP ASP ASP ASP GLU ASP SER GLU PHE GLU ASP ILE TYR LYS ILE ASP SER ASN GLU ASP GLU GLU GLU GLU ASP GLU GLU GLU GLU ASP ASP SER ALA VAL VAL HIS ASP ASP ASP GLU LEU ASP ASP GLN GLN ALA SER GLN ALA GLN GLN PHE LEU GLN ASN GLN
LYS HIS GLN LYS LEU LEU GLN GLN GLN GLN GLN GLN GLN

GLU GLU GLU LYS VAL LYS GLU ILE GLU GLN GLU GLU GLU GLU GLU GLU PRO LYS GLU GLU GLN SER GLU GLU GLU GLU GLN PRO GLU GLU GLU GLN PRO GLU GLU GLU GLN THR LYS GLU GLU GLN PRO GLY GLU GLU GLN PRO GLY GLU GLU GLU GLU GLU PRO GLU

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

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

- Molecule 21: ELYS-like domain-containing protein

Chain T3: 11% 48% • 47%

M1 E2 T3 Y11 I14 D15 N16 F17 N18 Y19 G20 N21 T22 H23 H24 N25 N26 N27 K28 Q29 E36 K52 E53 N63 E75 N76 S77 I78 E79 E87 G103 T106 L122 R138 R151 L157 Y196 N202 K203 T204 D216 Q217 L218 F219

N220 G221 N222 S223 Y224 K225 A230 G231 K232 H233 S234 S235 E236 G237 Y238 L239 V240 E241 D242 R243 N244 G245 I246 T247 Q248 Q249 N250 L251 K252 S253 K254 L255 Q256 H257 Q258 Y259 P260 Q261 Q262 Q263 Q264 Q265 Q266 Q267 Q268 Q269 Q270 Q271 Q272 Q273 Q274 T275 N276 Q277 N311 Y316 C317

S318 P319 A320 R321 E322 V323 G324 L325 H326 S327 S328 V329 S330 H331 L332 E333 N334 K335 T352 S353 S354 H357 R362 K368 S369 S370 L378 E382 F383 D384 L385 Q386 L387 S388 P389 D390 S391 T394 I395 N396 N397 L398 I399 S400 L401 T402 Q403 N404 V405 D406 T407 P408

I411 N418 S419 Q420 D438 L439 K440 L441 N442 N443 G444 N460 G479 I480 N481 Y482 S483 S484 N485 H492 S493 D498 L519 D539 Q540 Y541 Q542 T543 S544 G545 S546 N547 S548 G549 S550 G551 S552 D553 N554 F555 D556 D557 N558 Y559 E560 N561 E564 L569 F583

S584 Y591 LEU SER P594 E611 S612 S613 T614 N617 S618 V621 K622 E625 Y632 R640 Y659 S665 S689 E690 S693 K694 L695 N696 S697 D698 T699 P700 K701 R715 R723 N733 D740 G741 G742 G743 G744 G745 G746 G747 S748 N749 S750 N751 S752

D763 Y787 L790 F791 K792 P793 S794 T795 L796 N797 D798 R810 E820 R826 T852 T853 T854 T855 T856 T857 T858 T859 T860 T861 D862 D909 L910 N911 G912 G913 N914 G915 S916 N917 G918 K919 Q923 T926 S937 N962 I963 D964 D965 D966 D967 D968 D969 D970

E971 D972 A973 T974 N975 R976 E977 N978 N979 D984 E985 D986 I987 K988 S989 R1010 K1025 R1042 E1052 Q1057 R1058 R1061 N1062 R1063 L1064 Q1065 D1066 Q1067 D1071 D1091 R1126 G1127 R1128 V1144 N1145 G1146 D1147 L1160 L1168 I1169 Q1170 ARG PRO ILE HIS PHE ASN

ILE THR ASN GLU SER GLN ASP LYS PRO LYS GLN GLN PRO GLN SER GLN GLN GLN GLN GLN PRO GLN PRO GLN PRO GLN GLN PHE LEU ASN SER GLU GLU ASP ASN ILE PRO LEU LEU PRO LYS SER ILE SER LYS VAL ASN LEU VAL PRO PRO GLN SER PHE ILE GLN LYS PRO ILE VAL MET

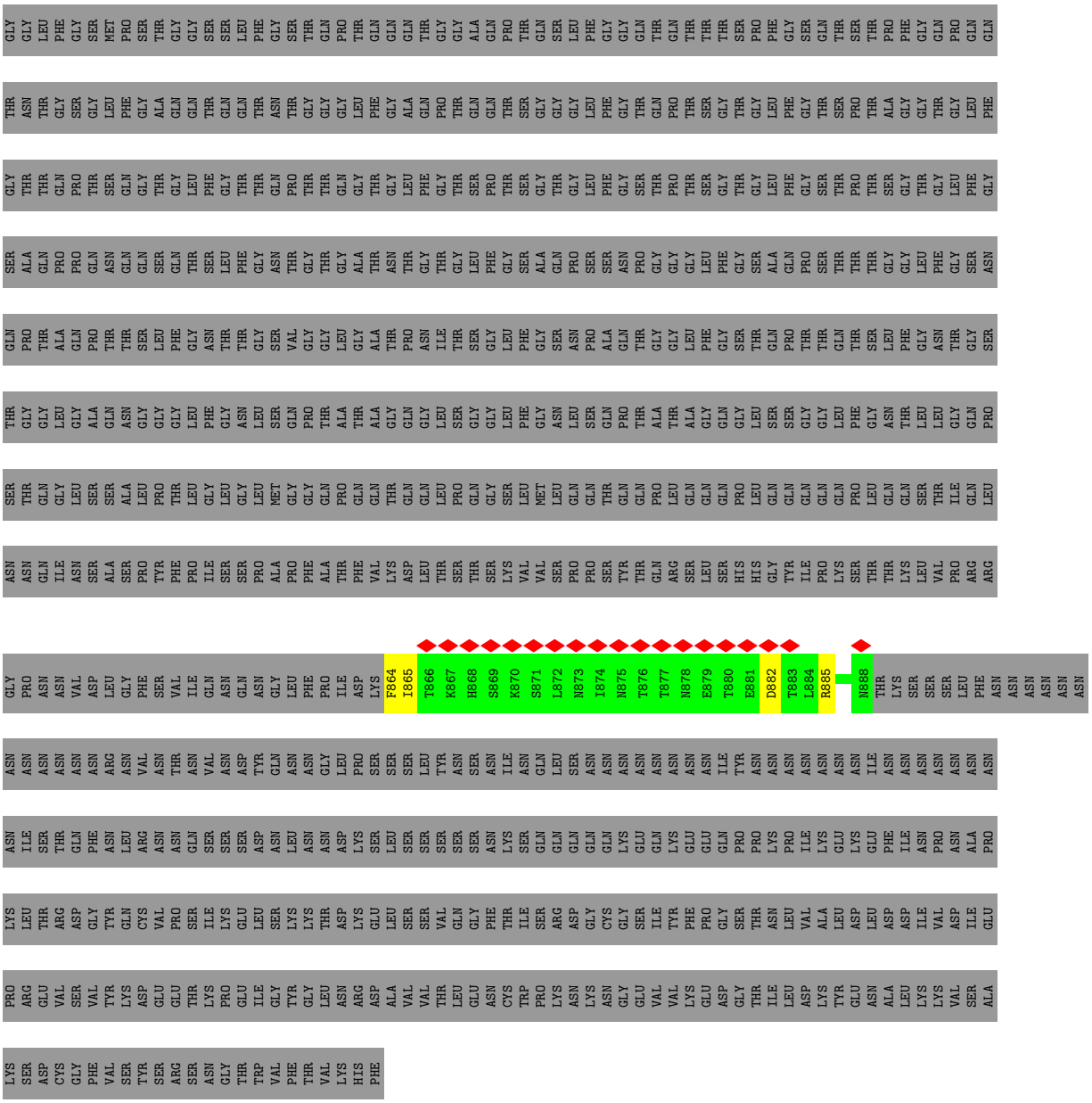
PRO SER PRO ILE PRO LYS LEU TYR ASN ASP SER LEU TYR LEU SER SER SER THR LEU SER THR ALA PRO ILE SER ASN LEU GLU ILE LEU THR LYS LYS SER ASN GLU GLU GLN GLN GLU ARG LEU LEU ILE GLN GLN GLN LYS GLU LEU GLN GLU GLN GLN GLU LYS GLU ARG ILE

LYS LYS GLU PHE GLU ASP GLN GLN GLU LYS GLN LEU LEU ASP PHE GLN ARG GLN GLN GLU GLU LEU LEU GLN HIS GLN MET GLU VAL HIS SER GLN LEU LEU LEU GLN GLN LYS GLN GLN GLN GLN GLN GLN GLN LYS GLN ILE LYS GLU GLN GLU GLU TYR GLU GLU TYR ASP GLU GLU GLU TYR GLU GLU

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

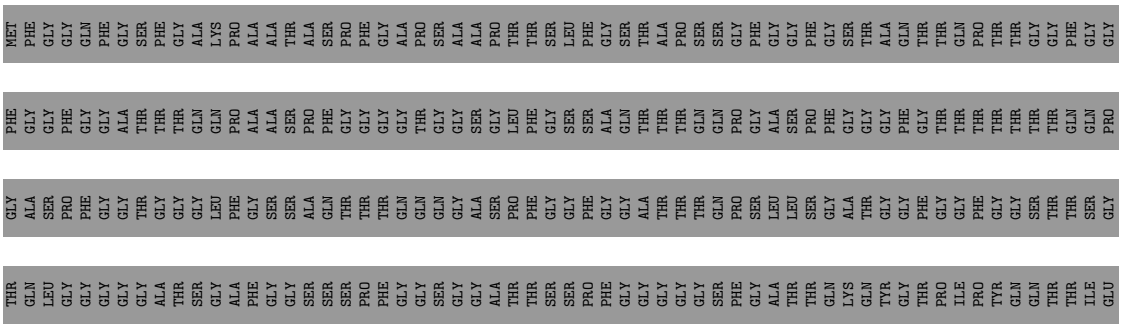
THR ASN VAL ARG PHE LYS ASP SER LEU ASN ARG GLU TYR PRO ILE PRO LYS LEU LYS LYS ARG GLY MET PRO ASP SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASN TYR ASP SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ILE TYR LYS ILE ASP LYS SER ASN

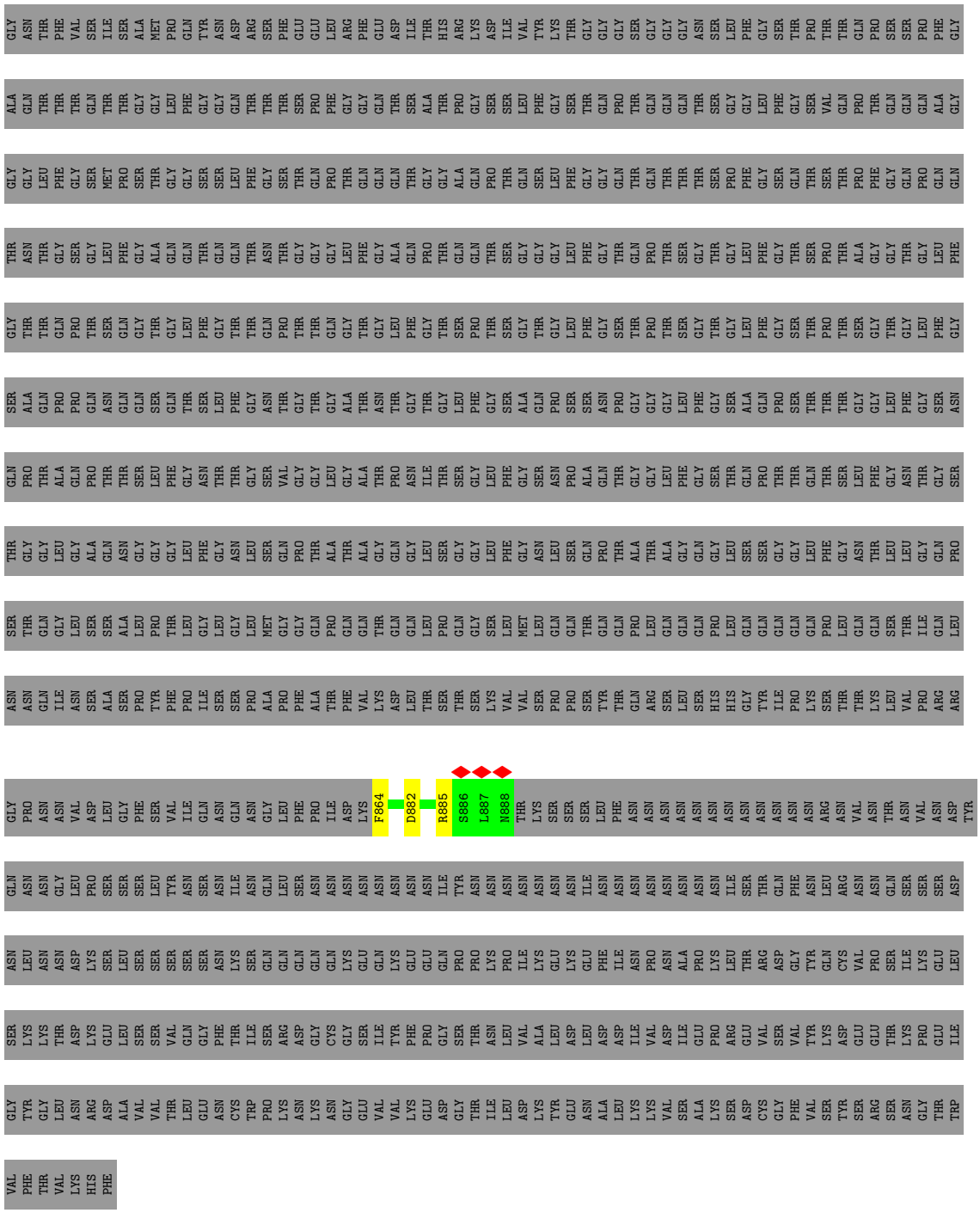
| | | |



• Molecule 22: Nuclear pore complex protein Nup98-Nup96

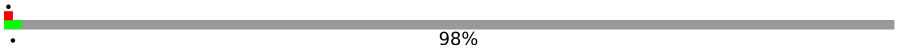
Chain U1: 98%

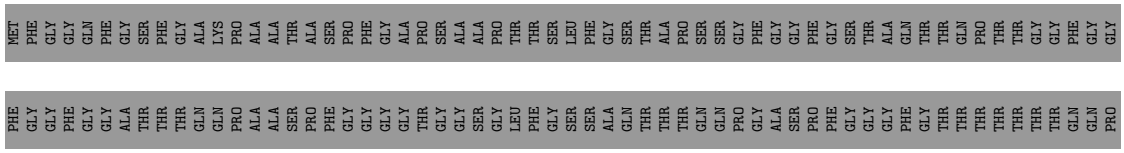


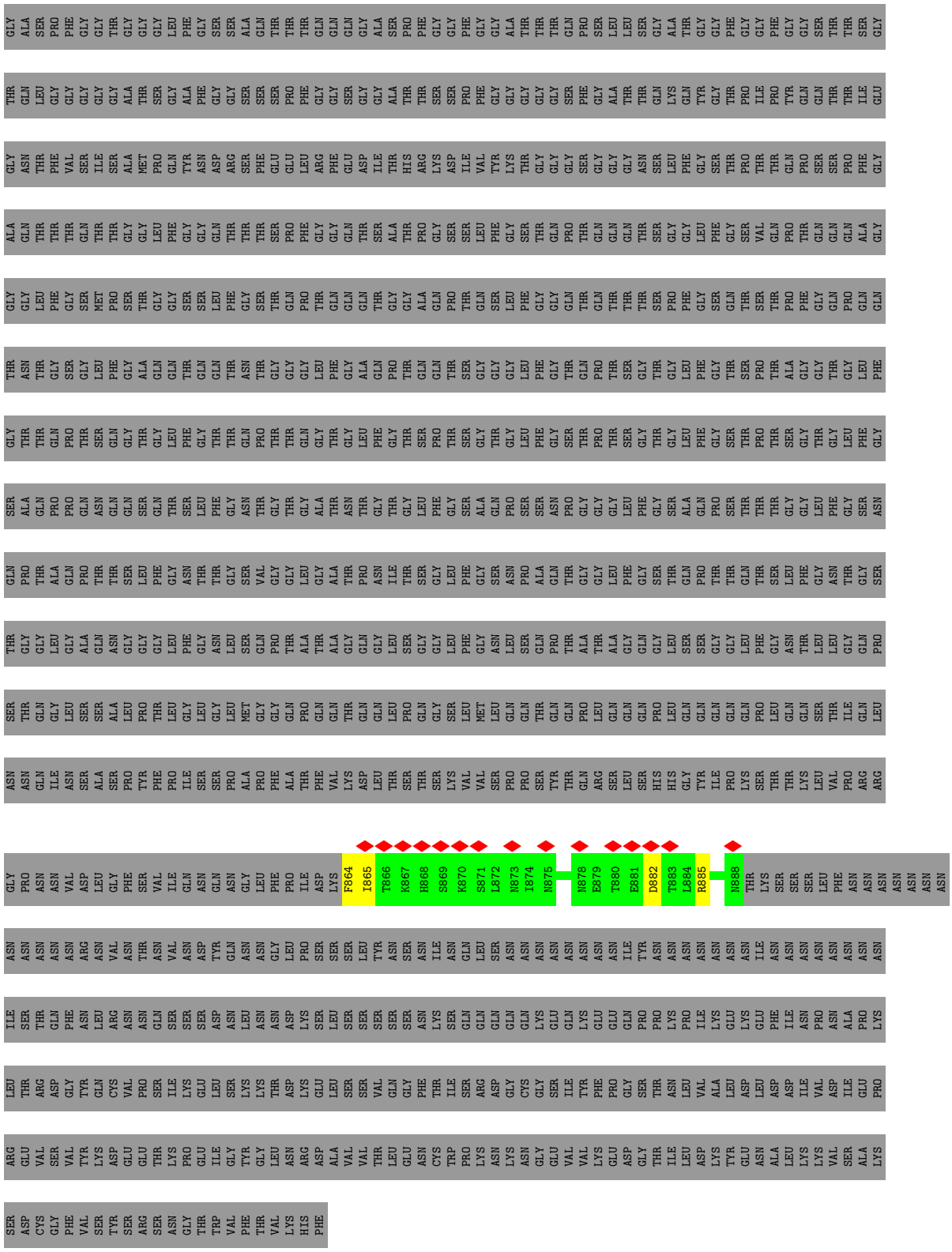


• Molecule 22: Nuclear pore complex protein Nup98-Nup96

Chain U2:

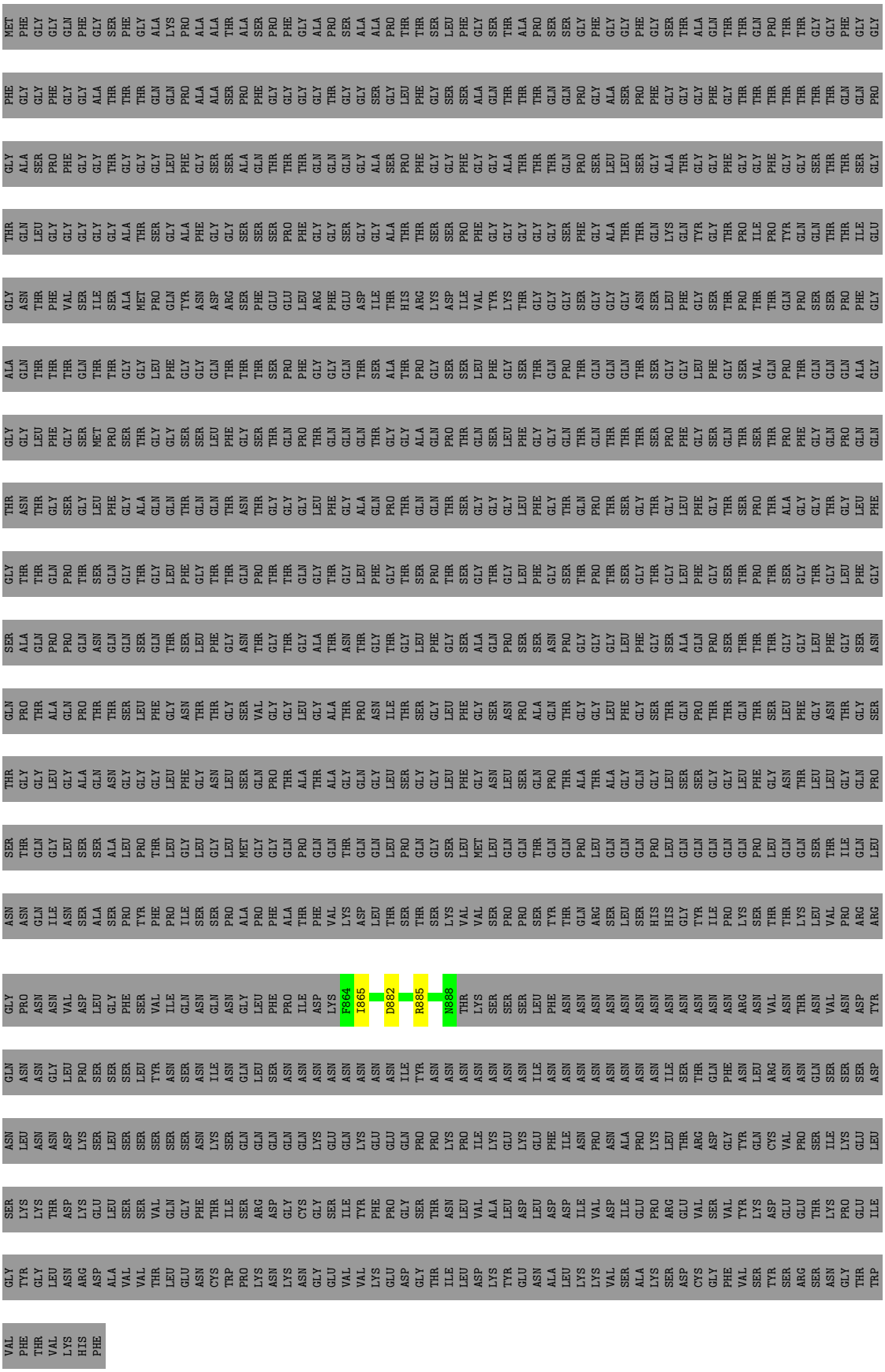






• Molecule 22: Nuclear pore complex protein Nup98-Nup96

Chain U3: 98%


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

Chain V0: 14% 85%

MET GLU SER GLN ASP ILE ASP TYR LEU LYS PHE ASN ASP PHE LYS SER ASP ILE GLU ASP PHE GLU ILE GLY GLN ASP ILE SER GLY TYR ASP ASN SER LYS ILE ASP PHE ASP SER ASN VAL ILE THR ILE SER ASN GLU TYR GLY ILE LEU LEU ILE VAL SER PRO GLU LEU ASN ASP

LEU LEU VAL THR PRO ILE GLU GLY LEU LEU ASN TYR ILE GLN SER ASN ASP GLN THR ASN ASP GLN THR THR ILE LEU SER CYS PRO THR ILE ILE LYS VAL GLY LYS VAL PHE GLU ILE PRO SER THR LYS THR SER PHE LYS ILE ASN LEU LEU PHE SER PRO ASN GLY ASP

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

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

ASN TYR GLU ASP GLU ASP GLU GLU GLU GLU GLU LEU ASN TYR TYR VAL SER SER ILE ASN LEU VAL VAL ALA ASP GLU PHE LEU LEU VAL GLN TYR TYR ILE VAL ARG MET ASP GLU TYR GLU ASP SER PRO ALA PHE LEU PHE ASP LEU LYS ASP GLU PHE GLN

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

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

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

PRO SER LEU PHE GLN GLN PRO GLN GLN PRO THR PRO THR THR SER ILE PHE GLN GLN GLN GLN ALA PRO PRO THR THR SER ILE ILE PHE GLN GLN GLN GLN GLN SER PRO THR THR SER ILE LEU GLN GLN GLN GLN ALA PRO THR THR SER

ILE PHE GLN GLN GLN GLN GLN GLN SER THR GLN GLN GLN GLN GLN LYS PRO LYS THR ILE PRO THR ILE SER PRO ILE LYS SER MET SER THR THR PHE THR ASN SER VAL SER THR ALA PRO SER GLN LYS GLN GLN GLN PRO SER GLN GLN GLN GLN SER GLN

GLN GLN PRO PHE LYS ARG GLN ASN SER ALA PRO THR PRO ILE SER THR PRO ILE SER THR PRO ILE ASN GLU LEU SER GLY ASN SER ASN VAL Y633 P634 M642 R677 E682 T701 K702 E706 E744 T747 Q748 Q749 Y750 S751 S752 T753 N754 Y755 K756 Q757

R762 N763 L797 E798 N799 N800 Q801 N802 N803 Q804 N805 N806 Q807 N808 N809 I810 E811 K812 E832 T833 N834 L835 R836 C837 E838 I839 E840 K841 I842 E843 K844 K845 L846 N847 K848 L849 K850 L851 N852 S874 R875 L876 S877 L878 E879 N880 N881 V882 N883 I884 L885 N886 D887 N888 G889 S890 GLY

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

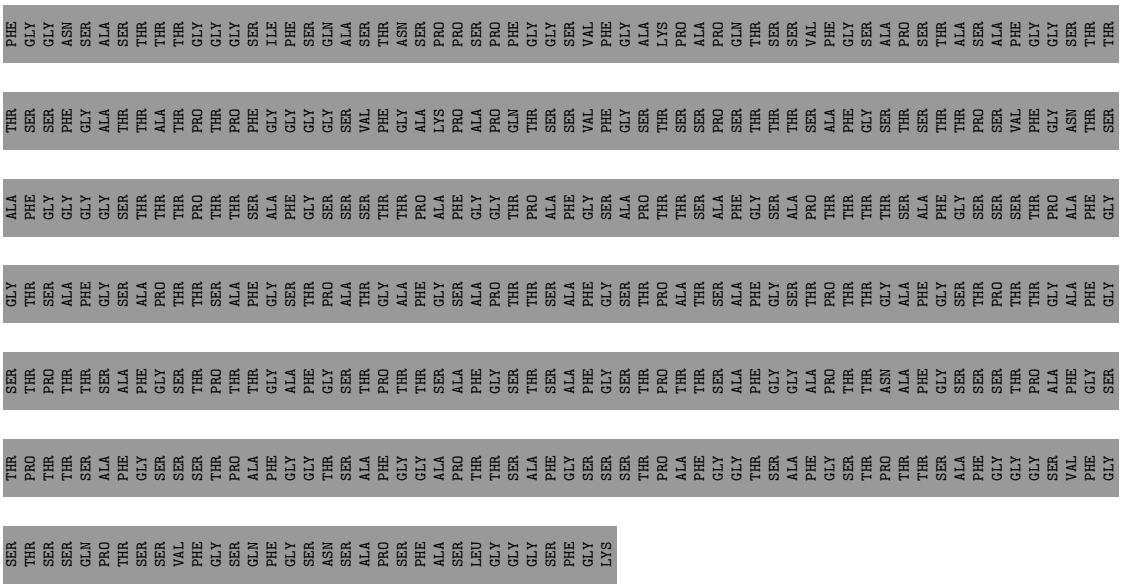
GLN PHE ASP ASP ILE ILE ASN ASN GLU TYR ASN ASN ASN ASN ASN ASN SER GLU ILE ILE GLU PRO PRO PRO ALA LEU ARG GLY ILE SER LEU SER LYS ARG LYS ASP ASN ALA PHE ALA ASN SER SER TYR LYS PHE THR SER ASN ILE THR PRO ILE LYS THR SER ILE

SER PRO SER SER THR THR SER SER PHE THR PRO THR SER HIS ILE SER PHE ALA SER THR ALA GLN ASN PHE ILE ASN ASN ASN ASN SER TYR ASP ASP TYR GLN ASP GLY ASN GLU GLU TYR ASP GLU ASP ASP ASP ASP ASP ASP GLU ASP GLU GLN TYR ASP GLU GLU TYR ILE

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

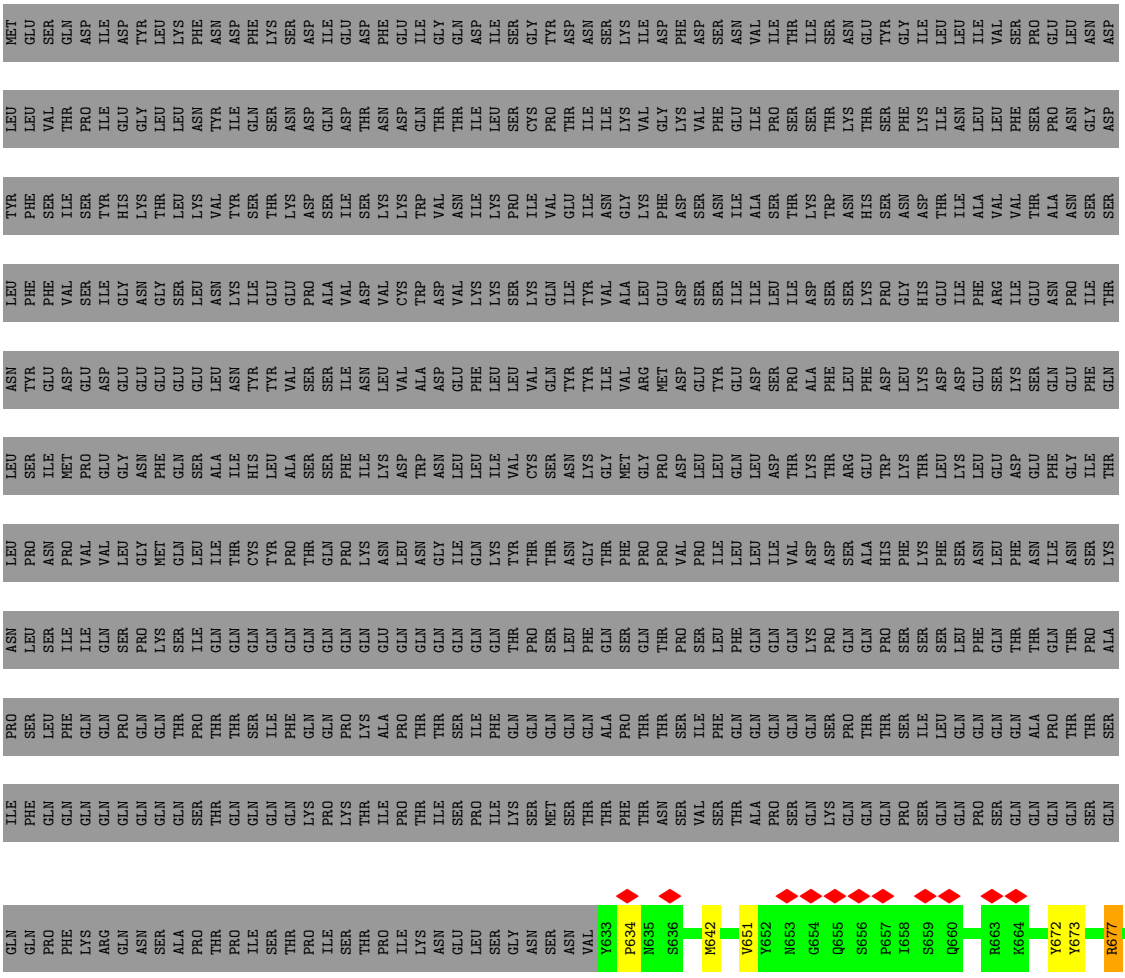
GLU ARG GLU THR ARG GLU LEU GLN ASP LYS LEU GLU ARG GLU GLU ARG GLU ALA LYS GLU LYS GLN LYS LYS LEU GLU ARG GLU ALA LYS GLU LYS GLN ALA ARG GLU LEU LYS GLU LYS GLN LYS GLU ALA LYS GLU ALA LYS GLU GLU LYS

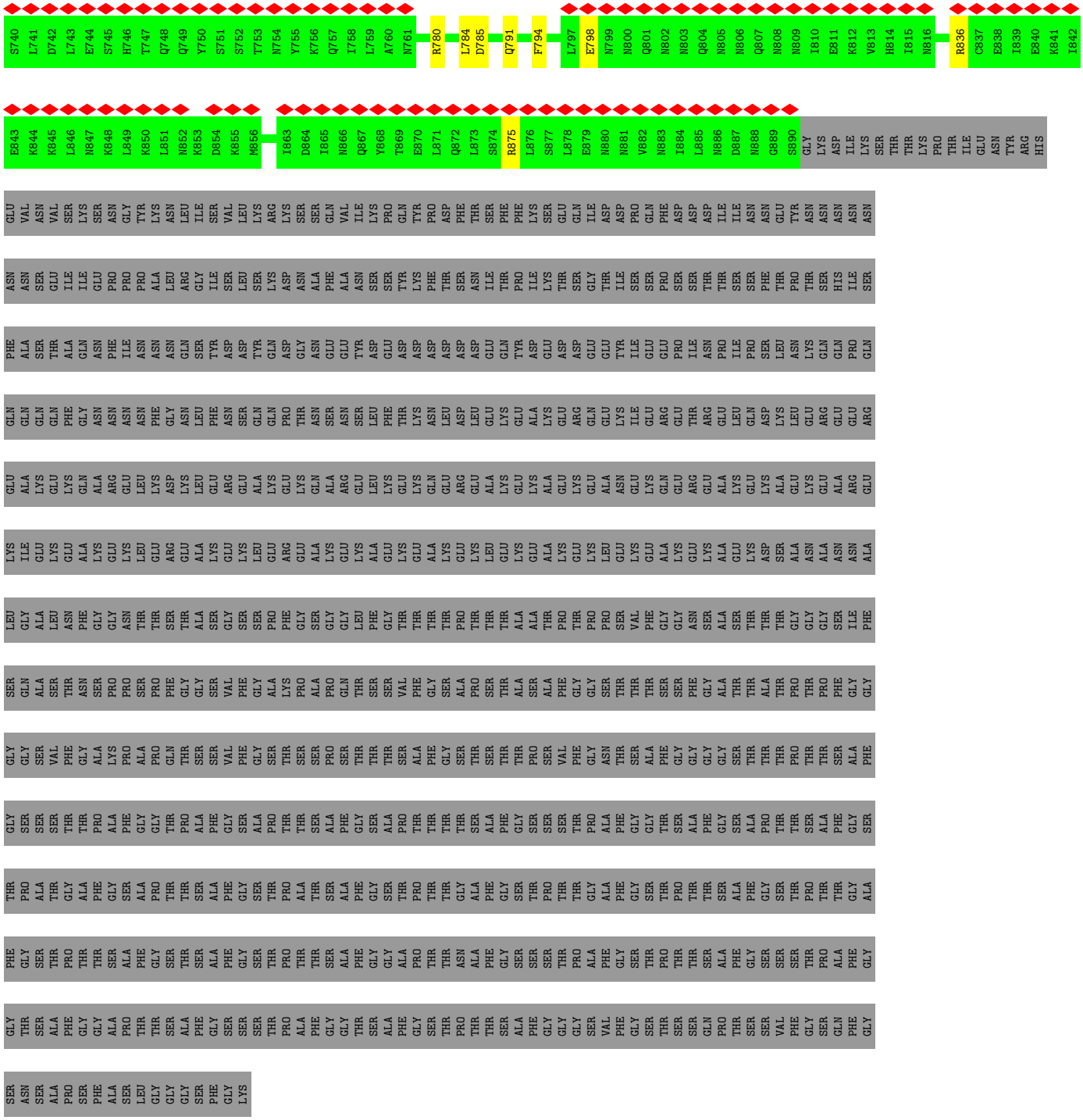
LYS GLN GLU ARG GLU ALA LYS GLU LYS ILE GLU LYS GLU LYS LYS GLU LYS ILE GLU LYS GLU ALA LYS LEU GLU LYS ARG GLU ALA LYS GLU LYS GLU ALA LYS GLU LYS GLU ALA LYS GLU LYS



• Molecule 23: WD40-like domain-containing protein

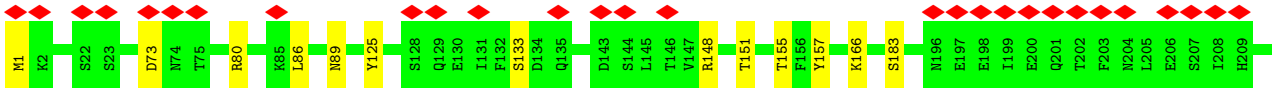
Chain V1:

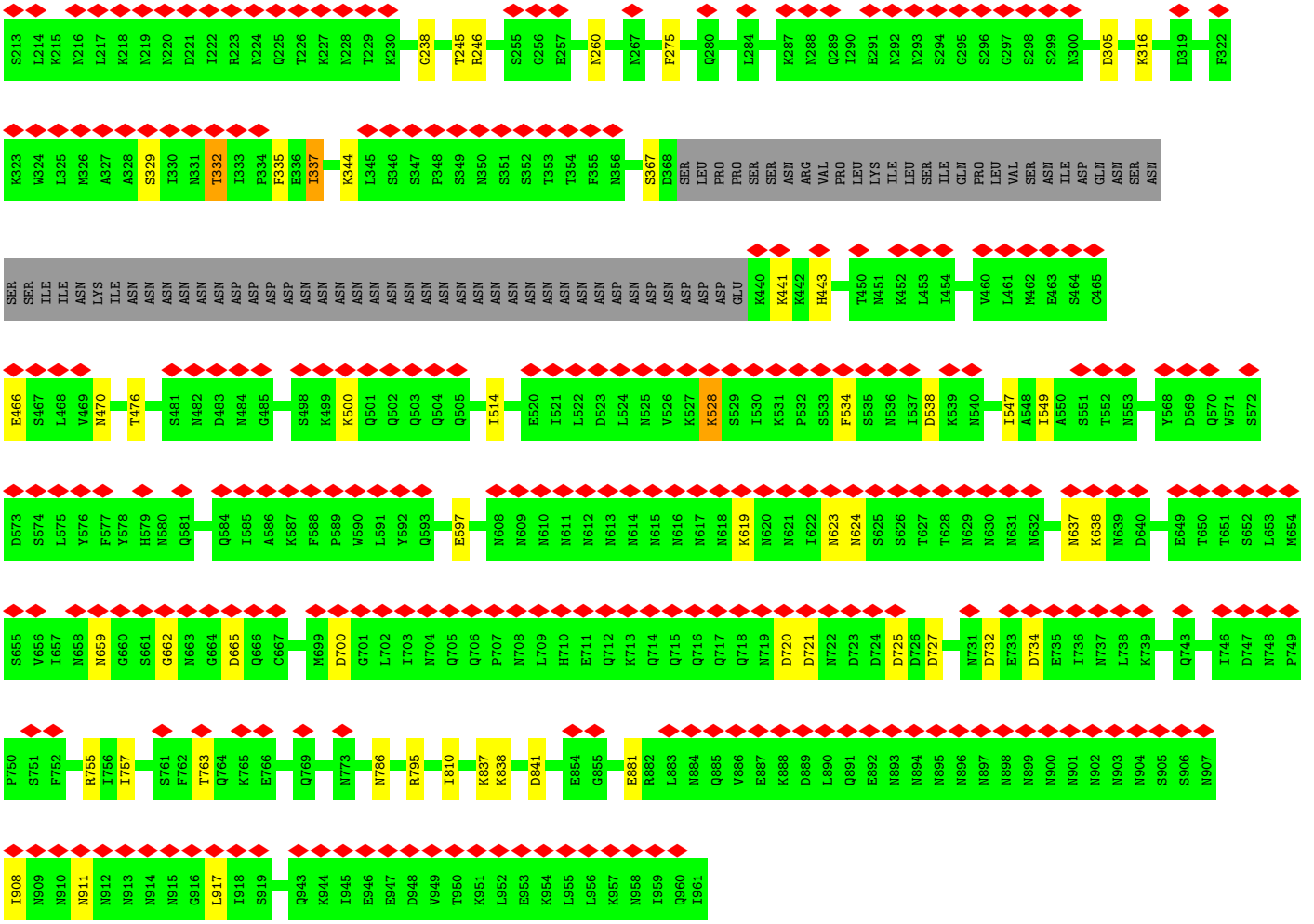




- Molecule 24: Nup88

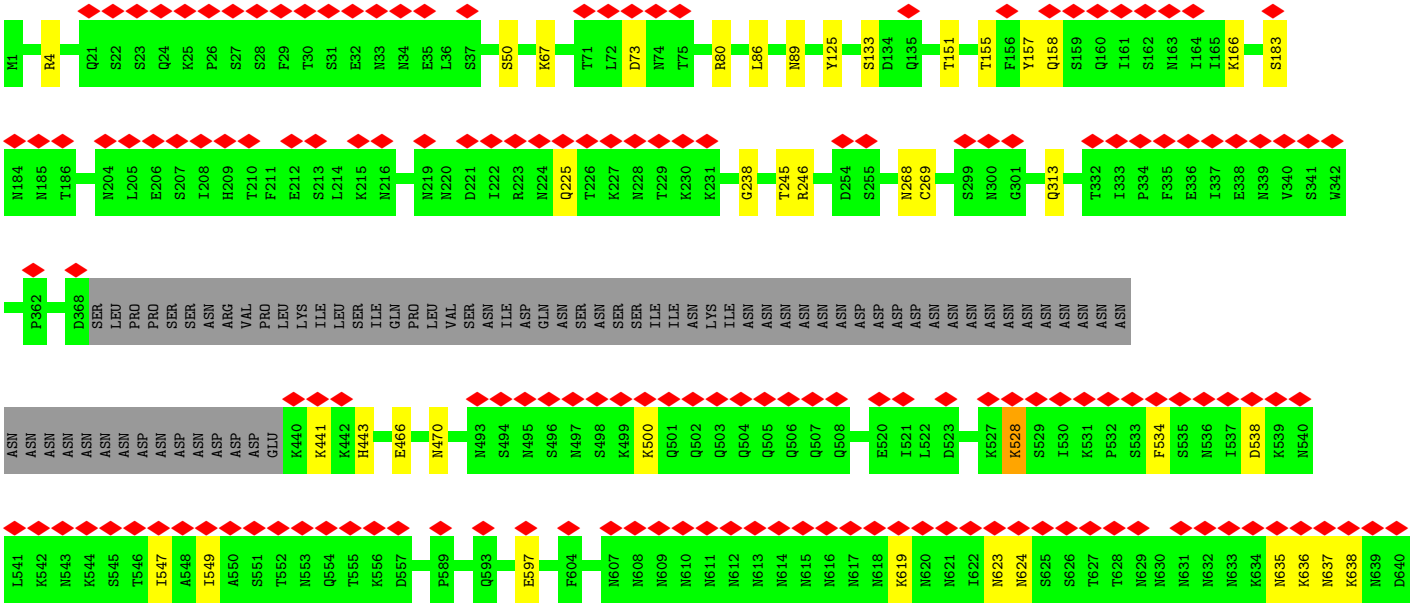
Chain W0:

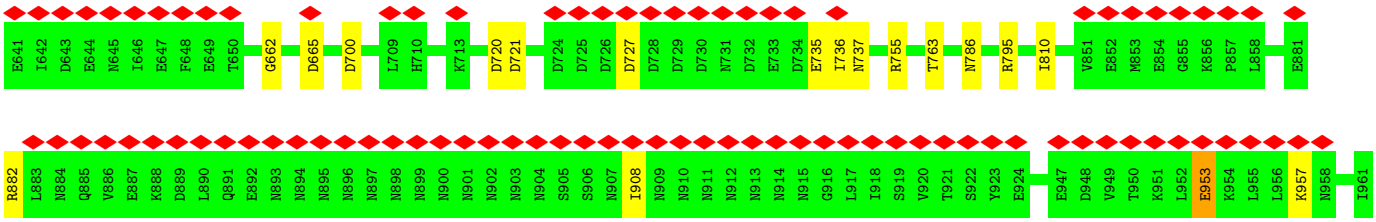




- Molecule 24: Nup88

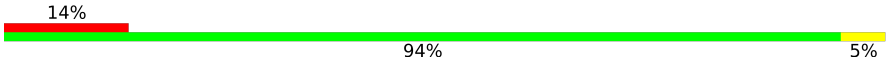
Chain W1:

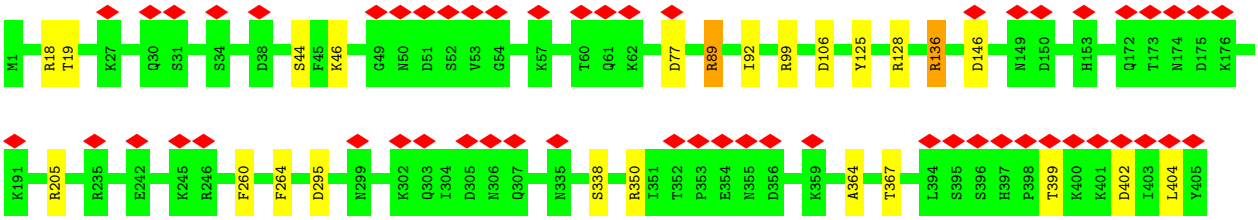




- Molecule 25: Nup205

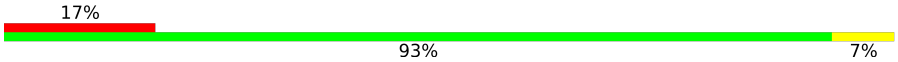
Chain X0:

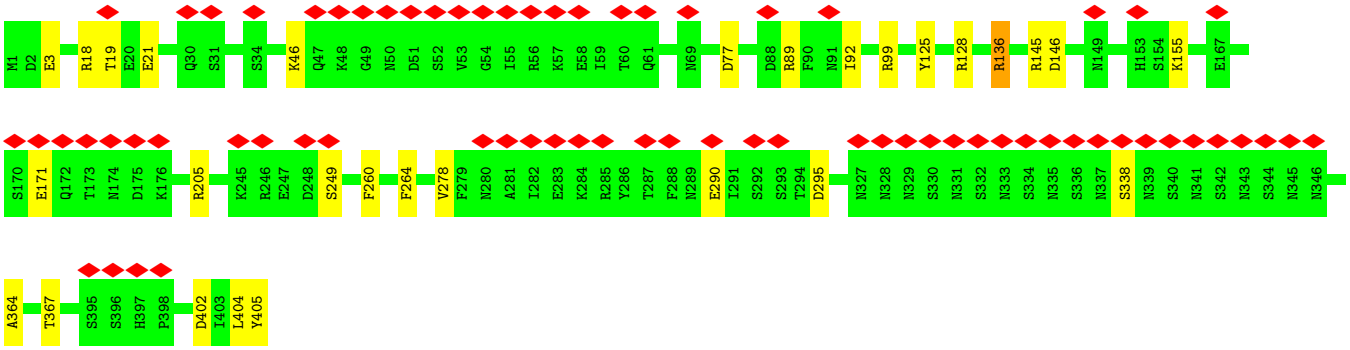




- Molecule 25: Nup205

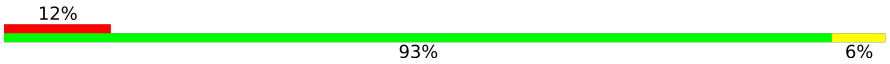
Chain X1:

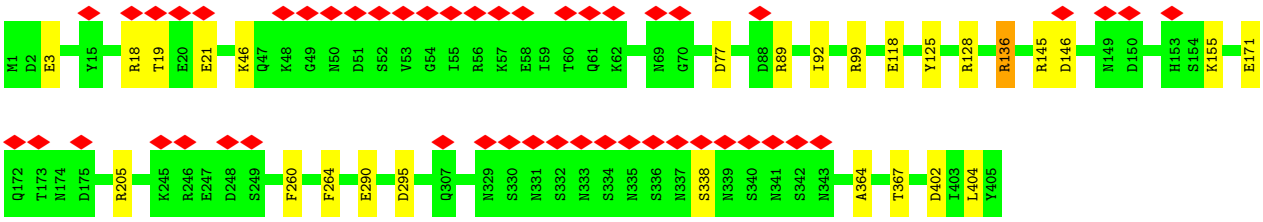




- Molecule 25: Nup205

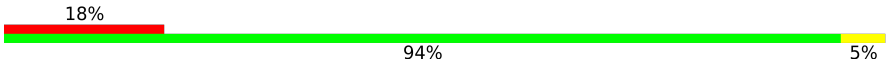
Chain X2:

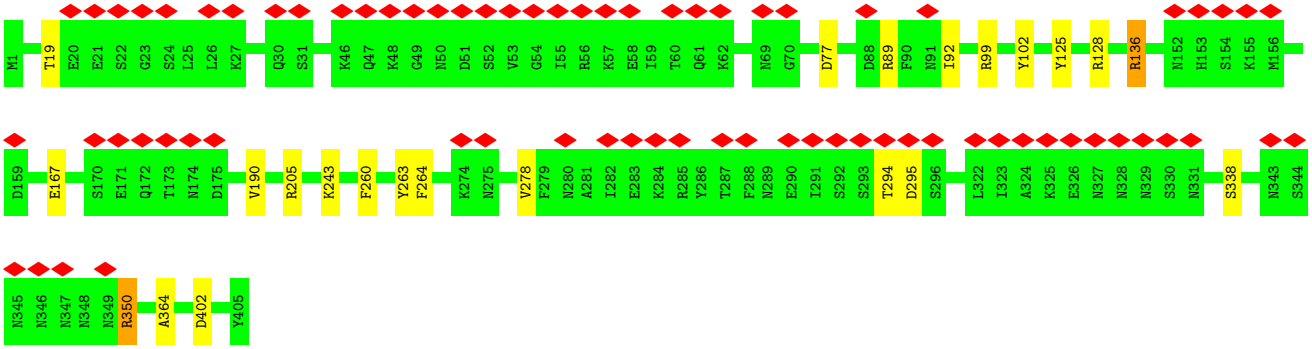




- Molecule 25: Nup205

Chain X3:




M1
T19
E20
E21
S22
G23
S24
L25
L26
K27
Q30
S31
K46
Q47
K48
G49
N50
D51
S52
V53
G54
I55
R56
K57
E58
I59
T60
Q61
K62
N69
G70
D77
D88
R89
F90
N91
I92
R99
Y102
Y125
R128
R136
N152
H153
S154
K155
M156
D159
E167
S170
E171
Q172
T173
N174
D175
V190
R205
K243
F260
Y263
F264
K274
N275
V278
F279
N280
A281
I282
E283
K284
R285
Y286
T287
F288
N289
E290
I291
S292
S293
T294
D295
S296
L322
I323
A324
K325
E326
N327
N328
N329
S330
N331
S338
N343
S344
N345
N346
N347
N348
N349
R350
A364
D402
Y405

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of subtomograms used	4921	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	130	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.923	Depositor
Minimum map value	-7.925	Depositor
Average map value	0.080	Depositor
Map value standard deviation	0.606	Depositor
Recommended contour level	1	Depositor
Map size (Å)	2088.9602, 2088.9602, 2088.9602	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	8.704, 8.704, 8.704	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	00	0.70	0/6572	0.95	9/8892 (0.1%)
1	01	0.70	0/6572	0.96	12/8892 (0.1%)
2	10	0.65	0/14245	0.94	20/19333 (0.1%)
2	11	0.65	0/14245	0.95	23/19333 (0.1%)
2	12	0.65	0/14245	0.95	24/19333 (0.1%)
2	13	0.65	0/14245	0.95	21/19333 (0.1%)
2	14	0.65	0/14245	0.95	26/19333 (0.1%)
2	15	0.64	0/14245	0.94	20/19333 (0.1%)
2	16	0.65	0/14245	0.95	21/19333 (0.1%)
2	17	0.65	0/14245	0.94	21/19333 (0.1%)
3	40	0.72	0/3904	0.99	8/5288 (0.2%)
3	41	0.72	0/3904	0.99	6/5288 (0.1%)
4	A0	0.69	0/6739	0.95	16/9102 (0.2%)
4	A1	0.70	0/5890	0.97	12/7954 (0.2%)
4	A2	0.70	0/5890	0.98	16/7954 (0.2%)
4	A3	0.96	6/5890 (0.1%)	0.97	11/7954 (0.1%)
4	A4	0.70	0/5890	0.97	13/7954 (0.2%)
4	A5	0.69	0/6315	0.95	12/8530 (0.1%)
5	B0	0.69	0/16413	0.94	30/22228 (0.1%)
5	B1	0.69	0/16413	0.94	30/22228 (0.1%)
6	C0	0.69	0/11548	0.94	21/15621 (0.1%)
6	C1	0.79	2/10984 (0.0%)	0.96	26/14854 (0.2%)
6	C2	0.69	0/10984	0.95	21/14854 (0.1%)
6	C3	0.91	6/11548 (0.1%)	0.95	21/15621 (0.1%)
7	D0	1.17	6/10606 (0.1%)	0.95	19/14350 (0.1%)
7	D1	0.69	0/10606	0.95	21/14350 (0.1%)
7	D2	0.69	0/10606	0.95	17/14350 (0.1%)
7	D3	0.91	1/10606 (0.0%)	0.96	23/14350 (0.2%)
8	E0	0.75	0/5087	0.95	11/6884 (0.2%)
8	E1	0.75	0/5087	0.96	10/6884 (0.1%)
9	F0	0.71	0/799	0.95	0/1077
9	F1	0.71	0/799	0.93	0/1077
9	F2	0.71	0/799	0.95	0/1077
9	F3	0.71	0/799	0.93	0/1077

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
10	H0	0.69	0/2073	0.95	3/2795 (0.1%)
10	H1	0.68	0/2073	0.95	2/2795 (0.1%)
10	H2	0.68	0/2073	0.94	1/2795 (0.0%)
10	H3	0.68	0/2073	0.94	3/2795 (0.1%)
11	I0	0.67	0/1646	0.90	1/2224 (0.0%)
11	I1	0.66	0/1646	0.89	2/2224 (0.1%)
11	I2	0.66	0/1646	0.90	2/2224 (0.1%)
11	I3	0.66	0/1646	0.89	1/2224 (0.0%)
12	J0	0.61	0/1541	0.99	1/2078 (0.0%)
12	J1	0.62	0/1541	1.01	3/2078 (0.1%)
12	J2	0.59	0/1496	1.00	3/2020 (0.1%)
12	J3	0.58	0/1496	0.99	2/2020 (0.1%)
12	J4	0.59	0/1496	0.99	2/2020 (0.1%)
12	J5	0.59	0/1496	1.02	5/2020 (0.2%)
13	K0	0.66	0/5914	0.91	8/7984 (0.1%)
13	K1	0.66	0/5914	0.94	11/7984 (0.1%)
13	K2	0.66	0/5914	0.93	10/7984 (0.1%)
13	K3	0.66	0/5914	0.94	13/7984 (0.2%)
14	L0	0.70	0/6704	0.98	17/9072 (0.2%)
14	L1	0.70	0/6704	1.00	18/9072 (0.2%)
14	L2	0.70	0/6704	0.99	19/9072 (0.2%)
14	L3	0.70	0/6669	1.00	23/9024 (0.3%)
15	M0	0.72	0/5775	0.97	13/7817 (0.2%)
15	M1	0.72	0/5775	1.00	15/7817 (0.2%)
15	M2	0.71	0/5775	0.99	16/7817 (0.2%)
15	M3	0.72	0/5775	1.00	20/7817 (0.3%)
16	N0	0.66	0/2443	0.97	2/3334 (0.1%)
16	N1	0.66	0/2443	0.99	3/3334 (0.1%)
16	N2	0.66	0/2443	0.99	3/3334 (0.1%)
16	N3	0.66	0/2443	0.99	3/3334 (0.1%)
17	O0	0.70	0/2602	1.09	6/3516 (0.2%)
17	O1	0.70	0/2602	1.12	12/3516 (0.3%)
17	O2	0.70	0/2602	1.10	8/3516 (0.2%)
17	O3	0.70	0/2602	1.09	9/3516 (0.3%)
18	P0	0.68	0/6227	0.97	20/8427 (0.2%)
18	P1	0.69	0/6227	1.00	22/8427 (0.3%)
18	P2	0.68	0/6227	0.99	22/8427 (0.3%)
18	P3	0.68	0/6227	0.99	20/8427 (0.2%)
19	Q0	0.67	0/3018	0.96	12/4087 (0.3%)
19	Q1	1.21	1/3018 (0.0%)	1.01	10/4087 (0.2%)
19	Q2	0.67	0/3018	0.95	6/4087 (0.1%)
19	Q3	0.67	0/3018	0.95	6/4087 (0.1%)
20	R0	0.71	0/14944	0.96	24/20198 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	R1	0.71	0/14944	0.98	30/20198 (0.1%)
20	R2	0.71	0/14944	0.97	25/20198 (0.1%)
20	R3	0.71	1/14943 (0.0%)	0.98	27/20195 (0.1%)
21	T0	0.72	0/8770	0.96	18/11860 (0.2%)
21	T1	0.72	0/9706	0.96	18/13124 (0.1%)
21	T2	1.05	6/9706 (0.1%)	0.98	22/13124 (0.2%)
21	T3	0.72	0/9706	0.97	18/13124 (0.1%)
22	U0	0.64	0/202	1.11	2/272 (0.7%)
22	U1	0.61	0/202	1.11	2/272 (0.7%)
22	U2	0.68	0/202	1.13	1/272 (0.4%)
22	U3	0.65	0/202	1.10	2/272 (0.7%)
23	V0	0.65	0/2143	0.90	4/2880 (0.1%)
23	V1	0.64	0/2143	0.92	3/2880 (0.1%)
24	W0	0.67	0/7392	0.94	5/10002 (0.0%)
24	W1	0.67	0/7392	0.94	7/10002 (0.1%)
25	X0	0.68	0/3365	0.95	8/4533 (0.2%)
25	X1	0.69	0/3365	0.97	8/4533 (0.2%)
25	X2	0.69	0/3365	0.98	7/4533 (0.2%)
25	X3	0.68	0/3365	0.96	8/4533 (0.2%)
All	All	0.72	29/590850 (0.0%)	0.96	1158/799571 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	00	0	9
1	01	0	10
2	10	0	22
2	11	0	25
2	12	0	23
2	13	0	20
2	14	0	25
2	15	0	22
2	16	0	21
2	17	0	22
3	40	0	3
3	41	0	4
4	A0	0	5
4	A1	0	13
4	A2	0	13

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A3	0	14
4	A4	0	9
4	A5	0	8
5	B0	0	14
5	B1	0	13
6	C0	3	16
6	C1	3	12
6	C2	3	15
6	C3	3	13
7	D0	0	10
7	D1	0	6
7	D2	0	9
7	D3	0	7
8	E0	0	10
8	E1	0	11
9	F0	0	3
9	F1	0	3
9	F2	0	3
9	F3	0	3
10	H0	0	3
10	H1	0	2
10	H2	0	1
10	H3	0	1
11	I0	0	1
11	I3	0	3
12	J2	0	2
12	J5	0	1
13	K1	0	1
13	K2	0	1
13	K3	0	5
14	L0	0	3
14	L1	0	5
14	L2	0	7
14	L3	0	4
15	M0	0	5
15	M1	0	2
15	M2	0	6
15	M3	0	4
16	N0	0	4
16	N1	0	3
16	N2	0	3
16	N3	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
17	O0	0	2
17	O1	0	1
17	O2	0	3
17	O3	0	3
18	P0	0	5
18	P1	0	5
18	P2	0	5
18	P3	0	6
19	Q0	0	1
19	Q1	0	6
19	Q2	0	1
19	Q3	0	2
20	R0	0	20
20	R1	0	17
20	R2	0	17
20	R3	0	17
21	T0	0	4
21	T1	0	12
21	T2	0	10
21	T3	0	13
23	V0	0	5
23	V1	0	4
24	W0	0	9
24	W1	0	8
25	X0	0	3
25	X1	0	2
25	X2	0	2
25	X3	0	4
All	All	12	673

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D3	1464	LYS	CD-CE	60.20	3.01	1.51
19	Q1	382	GLN	CB-CG	55.48	3.02	1.52
7	D0	1575	TYR	CE2-CZ	43.72	1.95	1.38
7	D0	1575	TYR	CE1-CZ	41.75	1.92	1.38
7	D0	1575	TYR	CG-CD1	41.12	1.92	1.39
7	D0	1575	TYR	CG-CD2	40.59	1.92	1.39
6	C1	1269	ASN	CG-ND2	39.04	2.30	1.32
21	T2	629	PHE	CG-CD1	36.05	1.92	1.38
7	D0	1575	TYR	CD2-CE2	35.65	1.92	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	T2	629	PHE	CG-CD2	35.63	1.92	1.38
7	D0	1575	TYR	CD1-CE1	35.00	1.91	1.39
21	T2	629	PHE	CE2-CZ	29.71	1.93	1.37
6	C3	420	TYR	CE1-CZ	28.75	1.75	1.38
21	T2	629	PHE	CE1-CZ	28.47	1.91	1.37
6	C3	420	TYR	CG-CD1	28.12	1.75	1.39
6	C3	420	TYR	CE2-CZ	27.57	1.74	1.38
6	C3	420	TYR	CG-CD2	26.77	1.74	1.39
21	T2	629	PHE	CD2-CE2	26.51	1.92	1.39
21	T2	629	PHE	CD1-CE1	25.78	1.90	1.39
4	A3	894	PHE	CG-CD2	23.89	1.74	1.38
6	C3	420	TYR	CD2-CE2	23.86	1.75	1.39
4	A3	894	PHE	CG-CD1	23.78	1.74	1.38
6	C3	420	TYR	CD1-CE1	23.62	1.74	1.39
4	A3	894	PHE	CE2-CZ	20.00	1.75	1.37
4	A3	894	PHE	CE1-CZ	20.00	1.75	1.37
4	A3	894	PHE	CD1-CE1	17.55	1.74	1.39
4	A3	894	PHE	CD2-CE2	17.48	1.74	1.39
20	R3	188	GLY	CA-C	7.77	1.64	1.51
6	C1	1269	ASN	CB-CG	6.62	1.66	1.51

All (1158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	R3	188	GLY	CA-C-O	-16.93	90.12	120.60
6	C1	1269	ASN	CB-CG-OD1	-14.99	91.61	121.60
12	J5	560	ARG	NE-CZ-NH1	11.57	126.09	120.30
13	K1	1184	ARG	NE-CZ-NH1	11.54	126.07	120.30
20	R1	574	ARG	NE-CZ-NH1	11.12	125.86	120.30
12	J4	560	ARG	NE-CZ-NH1	11.12	125.86	120.30
20	R3	574	ARG	NE-CZ-NH1	11.00	125.80	120.30
7	D1	244	ARG	NE-CZ-NH1	10.98	125.79	120.30
14	L3	456	ARG	NE-CZ-NH1	10.88	125.74	120.30
4	A0	555	ARG	NE-CZ-NH1	10.88	125.74	120.30
5	B0	1989	ARG	NE-CZ-NH1	10.83	125.71	120.30
7	D3	244	ARG	NE-CZ-NH1	10.76	125.68	120.30
7	D0	244	ARG	NE-CZ-NH1	10.74	125.67	120.30
13	K3	1075	ARG	NE-CZ-NH1	10.72	125.66	120.30
12	J3	560	ARG	NE-CZ-NH1	10.72	125.66	120.30
20	R2	574	ARG	NE-CZ-NH1	10.63	125.62	120.30
7	D2	244	ARG	NE-CZ-NH1	10.58	125.59	120.30
20	R0	1751	ARG	NE-CZ-NH1	10.46	125.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C3	732	ARG	NE-CZ-NH1	10.40	125.50	120.30
13	K2	1075	ARG	NE-CZ-NH1	10.33	125.47	120.30
17	O1	391	ARG	NE-CZ-NH1	10.32	125.46	120.30
20	R2	1751	ARG	NE-CZ-NH1	10.30	125.45	120.30
20	R3	1751	ARG	NE-CZ-NH1	10.29	125.45	120.30
5	B1	1989	ARG	NE-CZ-NH1	10.26	125.43	120.30
17	O3	467	ARG	NE-CZ-NH1	10.23	125.42	120.30
6	C0	732	ARG	NE-CZ-NH1	10.10	125.35	120.30
17	O1	135	ARG	NE-CZ-NH1	10.06	125.33	120.30
20	R1	1751	ARG	NE-CZ-NH1	10.05	125.33	120.30
17	O1	467	ARG	NE-CZ-NH1	10.04	125.32	120.30
13	K1	508	ARG	NE-CZ-NH1	10.01	125.31	120.30
13	K2	508	ARG	NE-CZ-NH1	9.98	125.29	120.30
6	C1	732	ARG	NE-CZ-NH1	9.82	125.21	120.30
17	O2	135	ARG	NE-CZ-NH1	9.82	125.21	120.30
18	P3	330	ARG	NE-CZ-NH1	9.80	125.20	120.30
6	C2	732	ARG	NE-CZ-NH1	9.79	125.20	120.30
17	O2	467	ARG	NE-CZ-NH1	9.79	125.19	120.30
20	R3	124	ARG	NE-CZ-NH1	9.77	125.19	120.30
18	P2	330	ARG	NE-CZ-NH1	9.76	125.18	120.30
21	T2	243	ARG	NE-CZ-NH1	9.71	125.16	120.30
12	J2	625	ARG	NE-CZ-NH1	9.63	125.12	120.30
17	O0	135	ARG	NE-CZ-NH1	9.62	125.11	120.30
7	D2	753	ARG	NE-CZ-NH1	9.56	125.08	120.30
12	J5	625	ARG	NE-CZ-NH1	9.53	125.07	120.30
6	C2	1134	ARG	NE-CZ-NH1	9.49	125.05	120.30
13	K0	1075	ARG	NE-CZ-NH1	9.45	125.03	120.30
18	P1	330	ARG	NE-CZ-NH1	9.43	125.02	120.30
20	R2	124	ARG	NE-CZ-NH1	9.41	125.01	120.30
11	I2	266	ARG	NE-CZ-NH1	9.38	124.99	120.30
4	A3	555	ARG	NE-CZ-NH1	9.37	124.98	120.30
23	V1	836	ARG	NE-CZ-NH1	9.37	124.98	120.30
7	D0	753	ARG	NE-CZ-NH1	9.36	124.98	120.30
6	C2	821	ARG	NE-CZ-NH1	9.36	124.98	120.30
4	A4	555	ARG	NE-CZ-NH1	9.34	124.97	120.30
13	K1	1075	ARG	NE-CZ-NH1	9.33	124.96	120.30
20	R1	124	ARG	NE-CZ-NH1	9.30	124.95	120.30
6	C1	1134	ARG	NE-CZ-NH1	9.22	124.91	120.30
6	C1	821	ARG	NE-CZ-NH1	9.19	124.90	120.30
4	A1	555	ARG	NE-CZ-NH1	9.19	124.89	120.30
3	40	341	ARG	NE-CZ-NH1	9.12	124.86	120.30
5	B1	1501	ARG	NE-CZ-NH1	9.10	124.85	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	T1	362	ARG	NE-CZ-NH1	9.08	124.84	120.30
7	D2	1299	ARG	NE-CZ-NH1	9.06	124.83	120.30
21	T3	243	ARG	NE-CZ-NH1	9.05	124.83	120.30
20	R0	124	ARG	NE-CZ-NH1	9.04	124.82	120.30
20	R1	1641	ARG	NE-CZ-NH1	9.02	124.81	120.30
12	J2	560	ARG	NE-CZ-NH1	9.01	124.80	120.30
3	40	268	ARG	NE-CZ-NH1	8.94	124.77	120.30
21	T2	362	ARG	NE-CZ-NH1	8.92	124.76	120.30
4	A2	555	ARG	NE-CZ-NH1	8.92	124.76	120.30
20	R0	574	ARG	NE-CZ-NH1	8.90	124.75	120.30
3	41	268	ARG	NE-CZ-NH1	8.87	124.73	120.30
4	A5	555	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	17	1179	ARG	NE-CZ-NH1	8.84	124.72	120.30
13	K1	963	ARG	NE-CZ-NH1	8.81	124.70	120.30
18	P0	789	ARG	NE-CZ-NH1	8.81	124.70	120.30
5	B0	1166	ARG	NE-CZ-NH1	8.79	124.69	120.30
20	R3	79	ARG	NE-CZ-NH1	8.76	124.68	120.30
13	K2	963	ARG	NE-CZ-NH1	8.76	124.68	120.30
13	K3	508	ARG	NE-CZ-NH1	8.75	124.68	120.30
18	P0	692	ARG	NE-CZ-NH1	8.75	124.68	120.30
15	M3	467	ARG	NE-CZ-NH1	8.75	124.68	120.30
12	J4	625	ARG	NE-CZ-NH1	8.75	124.67	120.30
7	D3	1030	ARG	NE-CZ-NH1	8.74	124.67	120.30
20	R0	1301	ARG	NE-CZ-NH1	8.74	124.67	120.30
5	B1	1166	ARG	NE-CZ-NH1	8.73	124.67	120.30
21	T3	362	ARG	NE-CZ-NH1	8.73	124.67	120.30
2	14	1604	ARG	NE-CZ-NH1	8.72	124.66	120.30
13	K3	963	ARG	NE-CZ-NH1	8.72	124.66	120.30
12	J3	625	ARG	NE-CZ-NH1	8.72	124.66	120.30
4	A4	716	ARG	NE-CZ-NH1	8.71	124.65	120.30
2	14	1179	ARG	NE-CZ-NH1	8.69	124.64	120.30
20	R2	79	ARG	NE-CZ-NH1	8.63	124.62	120.30
13	K0	963	ARG	NE-CZ-NH1	8.62	124.61	120.30
20	R0	456	ARG	NE-CZ-NH1	8.61	124.61	120.30
15	M2	467	ARG	NE-CZ-NH1	8.56	124.58	120.30
7	D1	753	ARG	NE-CZ-NH1	8.55	124.57	120.30
5	B0	1501	ARG	NE-CZ-NH1	8.52	124.56	120.30
17	O2	391	ARG	NE-CZ-NH1	8.52	124.56	120.30
18	P0	172	ARG	NE-CZ-NH1	8.52	124.56	120.30
20	R3	1301	ARG	NE-CZ-NH1	8.47	124.54	120.30
7	D3	1464	LYS	CD-CE-NZ	8.47	131.18	111.70
15	M1	229	ARG	NE-CZ-NH1	8.44	124.52	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D3	742	ARG	NE-CZ-NH1	8.40	124.50	120.30
21	T0	715	ARG	NE-CZ-NH1	8.39	124.50	120.30
15	M2	229	ARG	NE-CZ-NH1	8.39	124.49	120.30
19	Q1	382	GLN	CA-CB-CG	8.38	131.84	113.40
19	Q1	401	ARG	NE-CZ-NH1	8.38	124.49	120.30
4	A2	833	ARG	NE-CZ-NH1	8.37	124.48	120.30
13	K3	588	ARG	NE-CZ-NH1	8.36	124.48	120.30
20	R1	736	ARG	NE-CZ-NH1	8.36	124.48	120.30
4	A0	456	ARG	NE-CZ-NH1	8.35	124.47	120.30
5	B1	509	ARG	NE-CZ-NH1	8.34	124.47	120.30
18	P2	690	ARG	NE-CZ-NH1	8.34	124.47	120.30
7	D1	1515	ARG	NE-CZ-NH1	8.33	124.47	120.30
21	T0	362	ARG	NE-CZ-NH1	8.32	124.46	120.30
18	P1	690	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	01	722	ARG	NE-CZ-NH1	8.28	124.44	120.30
17	O0	419	ARG	NE-CZ-NH1	8.27	124.44	120.30
5	B0	509	ARG	NE-CZ-NH1	8.27	124.43	120.30
7	D1	1299	ARG	NE-CZ-NH1	8.24	124.42	120.30
22	U2	885	ARG	NE-CZ-NH1	8.23	124.41	120.30
6	C0	1134	ARG	NE-CZ-NH1	8.22	124.41	120.30
8	E1	301	ARG	NE-CZ-NH1	8.22	124.41	120.30
20	R1	79	ARG	NE-CZ-NH1	8.21	124.41	120.30
20	R2	1301	ARG	NE-CZ-NH1	8.21	124.41	120.30
4	A2	716	ARG	NE-CZ-NH1	8.19	124.39	120.30
7	D3	753	ARG	NE-CZ-NH1	8.18	124.39	120.30
4	A1	716	ARG	NE-CZ-NH1	8.15	124.38	120.30
8	E0	301	ARG	NE-CZ-NH1	8.15	124.37	120.30
4	A0	841	ARG	NE-CZ-NH1	8.14	124.37	120.30
4	A3	716	ARG	NE-CZ-NH1	8.13	124.36	120.30
7	D3	631	ARG	NE-CZ-NH1	8.11	124.35	120.30
13	K2	929	ARG	NE-CZ-NH1	8.10	124.35	120.30
18	P2	789	ARG	NE-CZ-NH1	8.10	124.35	120.30
4	A5	937	ARG	NE-CZ-NH1	8.10	124.35	120.30
13	K1	929	ARG	NE-CZ-NH1	8.09	124.34	120.30
5	B1	464	ARG	NE-CZ-NH1	8.05	124.33	120.30
20	R1	1301	ARG	NE-CZ-NH1	8.05	124.33	120.30
15	M3	428	ARG	NE-CZ-NH1	8.05	124.32	120.30
17	O3	391	ARG	NE-CZ-NH1	8.03	124.31	120.30
7	D2	631	ARG	NE-CZ-NH1	8.01	124.31	120.30
18	P3	690	ARG	NE-CZ-NH1	8.01	124.31	120.30
20	R2	1543	ARG	NE-CZ-NH1	8.01	124.31	120.30
22	U1	885	ARG	NE-CZ-NH1	8.01	124.30	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	P3	789	ARG	NE-CZ-NH1	8.00	124.30	120.30
21	T3	715	ARG	NE-CZ-NH1	7.99	124.30	120.30
20	R1	385	ARG	NE-CZ-NH1	7.99	124.30	120.30
20	R0	195	ARG	NE-CZ-NH1	7.98	124.29	120.30
20	R0	79	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	00	447	ARG	NE-CZ-NH2	-7.95	116.32	120.30
15	M0	229	ARG	NE-CZ-NH1	7.95	124.27	120.30
21	T1	243	ARG	NE-CZ-NH1	7.94	124.27	120.30
18	P3	278	ARG	NE-CZ-NH1	7.94	124.27	120.30
6	C1	819	ARG	NE-CZ-NH1	7.93	124.26	120.30
5	B0	464	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	T2	1061	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	11	1561	ARG	NE-CZ-NH1	7.92	124.26	120.30
11	I1	266	ARG	NE-CZ-NH1	7.91	124.26	120.30
7	D0	631	ARG	NE-CZ-NH1	7.91	124.25	120.30
21	T2	715	ARG	NE-CZ-NH1	7.91	124.25	120.30
25	X2	89	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	14	1301	ARG	NE-CZ-NH2	-7.90	116.35	120.30
18	P2	278	ARG	NE-CZ-NH1	7.90	124.25	120.30
23	V0	836	ARG	NE-CZ-NH1	7.90	124.25	120.30
4	A1	374	ARG	NE-CZ-NH1	7.89	124.25	120.30
18	P1	278	ARG	NE-CZ-NH1	7.89	124.24	120.30
7	D1	631	ARG	NE-CZ-NH1	7.88	124.24	120.30
4	A5	716	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	16	1301	ARG	NE-CZ-NH2	-7.87	116.37	120.30
4	A4	374	ARG	NE-CZ-NH1	7.86	124.23	120.30
20	R3	195	ARG	NE-CZ-NH1	7.84	124.22	120.30
21	T1	1061	ARG	NE-CZ-NH1	7.84	124.22	120.30
15	M3	229	ARG	NE-CZ-NH1	7.83	124.22	120.30
15	M0	796	ARG	NE-CZ-NH1	7.83	124.22	120.30
24	W0	755	ARG	NE-CZ-NH1	7.83	124.22	120.30
7	D2	551	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	13	1301	ARG	NE-CZ-NH2	-7.82	116.39	120.30
4	A3	374	ARG	NE-CZ-NH1	7.81	124.20	120.30
6	C3	821	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	16	1604	ARG	NE-CZ-NH1	7.80	124.20	120.30
22	U3	885	ARG	NE-CZ-NH1	7.80	124.20	120.30
13	K2	588	ARG	NE-CZ-NH1	7.80	124.20	120.30
14	L1	977	ARG	NE-CZ-NH1	7.79	124.19	120.30
21	T3	1010	ARG	NE-CZ-NH1	7.79	124.19	120.30
18	P1	172	ARG	NE-CZ-NH1	7.79	124.19	120.30
20	R2	94	ARG	NE-CZ-NH1	7.76	124.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O2	6	ARG	NE-CZ-NH1	7.76	124.18	120.30
21	T0	1010	ARG	NE-CZ-NH1	7.76	124.18	120.30
15	M1	339	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	01	6	ARG	NE-CZ-NH2	7.75	124.17	120.30
4	A0	716	ARG	NE-CZ-NH1	7.75	124.17	120.30
2	13	922	ARG	NE-CZ-NH1	7.74	124.17	120.30
6	C0	821	ARG	NE-CZ-NH1	7.74	124.17	120.30
6	C1	1269	ASN	CB-CG-ND2	7.74	135.27	116.70
18	P1	789	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	T1	715	ARG	NE-CZ-NH1	7.71	124.15	120.30
8	E0	659	ARG	NE-CZ-NH1	7.70	124.15	120.30
16	N1	262	ARG	NE-CZ-NH1	7.70	124.15	120.30
24	W1	755	ARG	NE-CZ-NH1	7.70	124.15	120.30
6	C0	981	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	11	1301	ARG	NE-CZ-NH2	-7.70	116.45	120.30
19	Q1	17	ARG	NE-CZ-NH1	7.69	124.15	120.30
19	Q2	17	ARG	NE-CZ-NH1	7.69	124.15	120.30
25	X1	89	ARG	NE-CZ-NH1	7.68	124.14	120.30
4	A4	456	ARG	NE-CZ-NH1	7.68	124.14	120.30
4	A2	374	ARG	NE-CZ-NH1	7.67	124.14	120.30
4	A0	937	ARG	NE-CZ-NH1	7.67	124.13	120.30
6	C2	1477	ARG	NE-CZ-NH1	7.66	124.13	120.30
22	U0	885	ARG	NE-CZ-NH1	7.65	124.12	120.30
2	11	1264	ARG	NE-CZ-NH1	7.64	124.12	120.30
4	A2	76	ARG	NE-CZ-NH1	7.64	124.12	120.30
15	M3	783	ARG	NE-CZ-NH1	7.63	124.11	120.30
13	K0	588	ARG	NE-CZ-NH1	7.63	124.11	120.30
2	17	922	ARG	NE-CZ-NH1	7.60	124.10	120.30
17	O1	376	ARG	NE-CZ-NH1	7.60	124.10	120.30
15	M0	339	ARG	NE-CZ-NH1	7.60	124.10	120.30
21	T3	1061	ARG	NE-CZ-NH1	7.59	124.09	120.30
6	C3	1477	ARG	NE-CZ-NH1	7.59	124.09	120.30
6	C1	1477	ARG	NE-CZ-NH1	7.58	124.09	120.30
12	J5	627	ARG	NE-CZ-NH1	7.58	124.09	120.30
20	R3	1694	ARG	NE-CZ-NH1	7.58	124.09	120.30
16	N2	262	ARG	NE-CZ-NH1	7.57	124.08	120.30
21	T0	151	ARG	NE-CZ-NH1	7.55	124.08	120.30
15	M3	796	ARG	NE-CZ-NH1	7.55	124.07	120.30
19	Q3	17	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	16	922	ARG	NE-CZ-NH1	7.54	124.07	120.30
7	D0	551	ARG	NE-CZ-NH1	7.54	124.07	120.30
18	P0	690	ARG	NE-CZ-NH1	7.54	124.07	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O3	419	ARG	NE-CZ-NH1	7.53	124.07	120.30
4	A1	456	ARG	NE-CZ-NH1	7.53	124.06	120.30
4	A4	833	ARG	NE-CZ-NH1	7.53	124.06	120.30
17	O3	135	ARG	NE-CZ-NH1	7.51	124.05	120.30
4	A3	456	ARG	NE-CZ-NH1	7.50	124.05	120.30
25	X0	89	ARG	NE-CZ-NH1	7.50	124.05	120.30
5	B1	942	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	01	447	ARG	NE-CZ-NH2	-7.49	116.56	120.30
18	P2	343	ARG	NE-CZ-NH1	7.49	124.04	120.30
20	R2	1694	ARG	NE-CZ-NH1	7.49	124.04	120.30
18	P3	343	ARG	NE-CZ-NH1	7.47	124.04	120.30
4	A5	374	ARG	NE-CZ-NH1	7.47	124.03	120.30
4	A5	562	ARG	NE-CZ-NH1	7.46	124.03	120.30
15	M3	247	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	01	260	ARG	NE-CZ-NH1	7.45	124.02	120.30
7	D0	1030	ARG	NE-CZ-NH1	7.44	124.02	120.30
15	M2	247	ARG	NE-CZ-NH1	7.44	124.02	120.30
21	T2	1010	ARG	NE-CZ-NH1	7.41	124.00	120.30
6	C0	1477	ARG	NE-CZ-NH1	7.40	124.00	120.30
20	R0	1543	ARG	NE-CZ-NH1	7.40	124.00	120.30
14	L0	327	ARG	NE-CZ-NH1	7.40	124.00	120.30
21	T1	1010	ARG	NE-CZ-NH1	7.40	124.00	120.30
5	B0	1181	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	12	922	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	16	1264	ARG	NE-CZ-NH1	7.38	123.99	120.30
13	K0	508	ARG	NE-CZ-NH1	7.37	123.98	120.30
14	L0	536	ARG	NE-CZ-NH1	7.37	123.98	120.30
8	E0	299	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	10	550	ARG	NE-CZ-NH1	7.35	123.97	120.30
8	E1	299	ARG	NE-CZ-NH1	7.34	123.97	120.30
21	T0	1061	ARG	NE-CZ-NH1	7.34	123.97	120.30
5	B1	1424	ARG	NE-CZ-NH1	7.33	123.97	120.30
5	B0	1424	ARG	NE-CZ-NH1	7.33	123.96	120.30
20	R2	1697	ARG	NE-CZ-NH1	7.32	123.96	120.30
20	R1	1706	ARG	NE-CZ-NH1	7.32	123.96	120.30
20	R0	94	ARG	NE-CZ-NH1	7.31	123.95	120.30
17	O0	363	ARG	NE-CZ-NH1	7.31	123.95	120.30
17	O2	419	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	00	6	ARG	NE-CZ-NH2	7.30	123.95	120.30
14	L0	371	ARG	NE-CZ-NH1	7.29	123.95	120.30
8	E1	659	ARG	NE-CZ-NH1	7.29	123.95	120.30
14	L1	456	ARG	NE-CZ-NH1	7.29	123.95	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	15	550	ARG	NE-CZ-NH1	7.27	123.94	120.30
21	T1	151	ARG	NE-CZ-NH1	7.27	123.94	120.30
21	T0	1128	ARG	NE-CZ-NH2	-7.25	116.67	120.30
6	C3	1134	ARG	NE-CZ-NH1	7.25	123.92	120.30
14	L1	536	ARG	NE-CZ-NH1	7.25	123.92	120.30
21	T3	1042	ARG	NE-CZ-NH1	7.25	123.92	120.30
15	M1	247	ARG	NE-CZ-NH1	7.24	123.92	120.30
20	R2	456	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	01	326	ARG	NE-CZ-NH1	7.22	123.91	120.30
16	N3	213	ARG	NE-CZ-NH1	7.22	123.91	120.30
19	Q1	382	GLN	CB-CG-CD	7.21	130.36	111.60
14	L0	456	ARG	NE-CZ-NH1	7.21	123.91	120.30
17	O1	195	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	00	260	ARG	NE-CZ-NH1	7.21	123.90	120.30
2	17	1264	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	10	1264	ARG	NE-CZ-NH1	7.20	123.90	120.30
5	B0	942	ARG	NE-CZ-NH1	7.20	123.90	120.30
20	R3	94	ARG	NE-CZ-NH1	7.18	123.89	120.30
5	B1	447	ARG	NE-CZ-NH1	7.16	123.88	120.30
16	N3	262	ARG	NE-CZ-NH1	7.16	123.88	120.30
3	41	430	ARG	NE-CZ-NH1	7.16	123.88	120.30
15	M2	729	ARG	NE-CZ-NH1	7.14	123.87	120.30
18	P0	343	ARG	NE-CZ-NH1	7.14	123.87	120.30
13	K3	929	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	40	430	ARG	NE-CZ-NH1	7.13	123.87	120.30
15	M3	729	ARG	NE-CZ-NH1	7.13	123.86	120.30
15	M2	339	ARG	NE-CZ-NH1	7.12	123.86	120.30
15	M1	729	ARG	NE-CZ-NH1	7.12	123.86	120.30
20	R1	94	ARG	NE-CZ-NH1	7.10	123.85	120.30
7	D1	551	ARG	NE-CZ-NH1	7.10	123.85	120.30
6	C3	607	ARG	NE-CZ-NH1	7.10	123.85	120.30
15	M0	247	ARG	NE-CZ-NH1	7.09	123.84	120.30
4	A0	374	ARG	NE-CZ-NH1	7.08	123.84	120.30
20	R2	385	ARG	NE-CZ-NH1	7.08	123.84	120.30
18	P1	343	ARG	NE-CZ-NH1	7.08	123.84	120.30
19	Q0	255	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	T3	138	ARG	NE-CZ-NH2	7.08	123.84	120.30
2	13	1264	ARG	NE-CZ-NH1	7.08	123.84	120.30
6	C0	607	ARG	NE-CZ-NH1	7.08	123.84	120.30
19	Q1	263	ARG	NE-CZ-NH1	7.07	123.84	120.30
21	T2	138	ARG	NE-CZ-NH2	7.07	123.83	120.30
20	R0	1694	ARG	NE-CZ-NH1	7.07	123.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N2	213	ARG	NE-CZ-NH1	7.07	123.83	120.30
18	P0	170	ARG	NE-CZ-NH1	7.05	123.83	120.30
25	X3	89	ARG	NE-CZ-NH1	7.05	123.83	120.30
5	B0	447	ARG	NE-CZ-NH1	7.05	123.82	120.30
5	B1	677	ARG	NE-CZ-NH1	7.05	123.83	120.30
14	L2	739	ARG	NE-CZ-NH1	7.05	123.83	120.30
4	A2	456	ARG	NE-CZ-NH1	7.04	123.82	120.30
17	O3	6	ARG	NE-CZ-NH1	7.04	123.82	120.30
20	R1	1697	ARG	NE-CZ-NH1	7.03	123.81	120.30
4	A1	833	ARG	NE-CZ-NH1	7.02	123.81	120.30
25	X1	128	ARG	NE-CZ-NH1	7.01	123.81	120.30
20	R1	1694	ARG	NE-CZ-NH1	7.00	123.80	120.30
18	P2	170	ARG	NE-CZ-NH1	6.99	123.80	120.30
2	17	550	ARG	NE-CZ-NH1	6.99	123.80	120.30
5	B1	1424	ARG	CD-NE-CZ	6.99	133.38	123.60
6	C2	607	ARG	NE-CZ-NH1	6.98	123.79	120.30
5	B0	677	ARG	NE-CZ-NH1	6.98	123.79	120.30
25	X2	128	ARG	NE-CZ-NH1	6.98	123.79	120.30
20	R1	1113	ARG	NE-CZ-NH1	6.97	123.78	120.30
20	R1	158	ARG	NE-CZ-NH1	6.94	123.77	120.30
4	A3	833	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	16	550	ARG	NE-CZ-NH1	6.92	123.76	120.30
20	R2	158	ARG	NE-CZ-NH1	6.92	123.76	120.30
5	B0	324	TYR	CB-CG-CD2	-6.90	116.86	121.00
7	D2	587	ARG	NE-CZ-NH1	6.89	123.75	120.30
6	C1	59	ARG	NE-CZ-NH1	6.89	123.75	120.30
5	B0	439	ASP	CB-CG-OD1	6.89	124.50	118.30
1	01	188	ARG	NE-CZ-NH1	6.88	123.74	120.30
20	R3	1593	ARG	NE-CZ-NH1	6.88	123.74	120.30
14	L2	536	ARG	NE-CZ-NH1	6.87	123.74	120.30
18	P2	179	ARG	NE-CZ-NH1	6.87	123.74	120.30
18	P1	179	ARG	NE-CZ-NH1	6.87	123.73	120.30
5	B1	439	ASP	CB-CG-OD1	6.87	124.48	118.30
7	D0	587	ARG	NE-CZ-NH1	6.86	123.73	120.30
10	H3	327	ARG	NE-CZ-NH2	6.86	123.73	120.30
14	L3	536	ARG	NE-CZ-NH1	6.86	123.73	120.30
10	H0	327	ARG	NE-CZ-NH2	6.85	123.72	120.30
14	L3	548	ARG	NE-CZ-NH1	6.84	123.72	120.30
4	A3	562	ARG	NE-CZ-NH1	6.84	123.72	120.30
14	L0	601	ARG	NE-CZ-NH1	6.83	123.71	120.30
14	L2	548	ARG	NE-CZ-NH1	6.82	123.71	120.30
4	A4	562	ARG	NE-CZ-NH1	6.82	123.71	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L1	601	ARG	NE-CZ-NH1	6.81	123.71	120.30
6	C3	1670	ARG	NE-CZ-NH1	6.81	123.70	120.30
2	12	550	ARG	NE-CZ-NH1	6.80	123.70	120.30
6	C1	607	ARG	NE-CZ-NH1	6.80	123.70	120.30
13	K0	627	ARG	NE-CZ-NH2	-6.80	116.90	120.30
4	A4	281	ARG	NE-CZ-NH1	6.79	123.70	120.30
7	D3	1299	ARG	NE-CZ-NH1	6.79	123.70	120.30
6	C2	59	ARG	NE-CZ-NH1	6.79	123.69	120.30
19	Q0	140	ARG	NE-CZ-NH1	6.79	123.69	120.30
18	P1	430	ARG	NE-CZ-NH1	6.78	123.69	120.30
14	L2	456	ARG	NE-CZ-NH1	6.78	123.69	120.30
5	B1	324	TYR	CB-CG-CD2	-6.77	116.94	121.00
14	L0	795	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	15	626	ARG	NE-CZ-NH1	6.77	123.68	120.30
3	40	426	ARG	NE-CZ-NH1	6.77	123.68	120.30
18	P1	420	ARG	NE-CZ-NH1	6.77	123.68	120.30
5	B0	1424	ARG	CD-NE-CZ	6.76	133.07	123.60
4	A5	438	ARG	NE-CZ-NH1	6.76	123.68	120.30
17	O1	419	ARG	NE-CZ-NH1	6.75	123.68	120.30
25	X3	128	ARG	NE-CZ-NH1	6.75	123.67	120.30
4	A2	562	ARG	NE-CZ-NH1	6.75	123.67	120.30
15	M2	796	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	12	1264	ARG	NE-CZ-NH1	6.74	123.67	120.30
3	41	426	ARG	NE-CZ-NH1	6.74	123.67	120.30
18	P3	179	ARG	NE-CZ-NH1	6.74	123.67	120.30
20	R3	1697	ARG	NE-CZ-NH1	6.74	123.67	120.30
4	A5	281	ARG	NE-CZ-NH1	6.74	123.67	120.30
21	T0	640	ARG	NE-CZ-NH1	6.74	123.67	120.30
13	K1	588	ARG	NE-CZ-NH1	6.73	123.67	120.30
4	A1	562	ARG	NE-CZ-NH1	6.72	123.66	120.30
14	L2	601	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	14	1264	ARG	NE-CZ-NH1	6.71	123.66	120.30
7	D3	551	ARG	NE-CZ-NH1	6.71	123.65	120.30
13	K3	496	ASP	CB-CG-OD1	6.71	124.33	118.30
4	A0	562	ARG	NE-CZ-NH1	6.70	123.65	120.30
5	B0	688	ARG	NE-CZ-NH1	6.70	123.65	120.30
5	B1	505	ARG	NE-CZ-NH1	6.69	123.64	120.30
20	R2	736	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	17	132	ARG	NE-CZ-NH1	6.68	123.64	120.30
21	T3	640	ARG	NE-CZ-NH1	6.68	123.64	120.30
4	A5	833	ARG	NE-CZ-NH1	6.67	123.64	120.30
6	C0	1670	ARG	NE-CZ-NH1	6.67	123.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A1	281	ARG	NE-CZ-NH1	6.67	123.64	120.30
7	D0	937	ARG	NE-CZ-NH1	6.67	123.63	120.30
15	M3	490	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	15	132	ARG	NE-CZ-NH1	6.67	123.63	120.30
18	P3	225	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	16	132	ARG	NE-CZ-NH1	6.66	123.63	120.30
18	P1	225	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	T3	810	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	14	626	ARG	NE-CZ-NH1	6.66	123.63	120.30
15	M2	428	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	10	922	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	11	922	ARG	NE-CZ-NH1	6.65	123.62	120.30
4	A3	281	ARG	NE-CZ-NH1	6.65	123.62	120.30
14	L1	548	ARG	NE-CZ-NH1	6.63	123.62	120.30
7	D2	937	ARG	NE-CZ-NH1	6.63	123.62	120.30
13	K0	671	ARG	NE-CZ-NH1	6.63	123.62	120.30
13	K2	627	ARG	NE-CZ-NH2	-6.63	116.99	120.30
4	A0	438	ARG	NE-CZ-NH1	6.62	123.61	120.30
4	A2	281	ARG	NE-CZ-NH1	6.62	123.61	120.30
5	B0	505	ARG	NE-CZ-NH1	6.61	123.61	120.30
18	P2	430	ARG	NE-CZ-NH1	6.61	123.61	120.30
25	X0	128	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	14	132	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	16	626	ARG	NE-CZ-NH1	6.60	123.60	120.30
20	R1	456	ARG	NE-CZ-NH1	6.60	123.60	120.30
4	A0	796	ARG	NE-CZ-NH1	6.59	123.59	120.30
14	L3	795	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	11	626	ARG	NE-CZ-NH1	6.58	123.59	120.30
11	I0	266	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	14	922	ARG	NE-CZ-NH1	6.58	123.59	120.30
18	P0	225	ARG	NE-CZ-NH1	6.57	123.58	120.30
4	A5	456	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	00	188	ARG	NE-CZ-NH1	6.56	123.58	120.30
6	C0	1131	ARG	NE-CZ-NH2	6.56	123.58	120.30
2	11	1508	ARG	NE-CZ-NH1	6.55	123.58	120.30
21	T2	1042	ARG	NE-CZ-NH1	6.55	123.58	120.30
5	B1	464	ARG	NE-CZ-NH2	-6.55	117.03	120.30
21	T0	293	ARG	NE-CZ-NH1	6.55	123.58	120.30
4	A0	281	ARG	NE-CZ-NH1	6.55	123.57	120.30
15	M3	339	ARG	NE-CZ-NH1	6.55	123.57	120.30
20	R3	158	ARG	NE-CZ-NH1	6.54	123.57	120.30
13	K1	671	ARG	NE-CZ-NH1	6.54	123.57	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M0	216	ARG	NE-CZ-NH1	6.54	123.57	120.30
14	L0	548	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	14	550	ARG	NE-CZ-NH1	6.53	123.56	120.30
2	17	626	ARG	NE-CZ-NH1	6.52	123.56	120.30
8	E1	125	ARG	NE-CZ-NH1	6.52	123.56	120.30
6	C3	402	ARG	NE-CZ-NH1	6.51	123.56	120.30
15	M3	575	TYR	CB-CG-CD2	-6.51	117.09	121.00
18	P2	225	ARG	NE-CZ-NH1	6.51	123.56	120.30
16	N0	213	ARG	NE-CZ-NH1	6.51	123.55	120.30
18	P3	430	ARG	NE-CZ-NH1	6.51	123.55	120.30
2	13	132	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	13	626	ARG	NE-CZ-NH1	6.50	123.55	120.30
15	M2	575	TYR	CB-CG-CD2	-6.49	117.10	121.00
20	R3	385	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	15	1467	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	11	132	ARG	NE-CZ-NH1	6.49	123.54	120.30
4	A1	816	ARG	NE-CZ-NH1	6.49	123.54	120.30
4	A0	901	ARG	NE-CZ-NH1	6.48	123.54	120.30
5	B0	464	ARG	NE-CZ-NH2	-6.48	117.06	120.30
14	L0	269	ARG	NE-CZ-NH2	6.48	123.54	120.30
13	K3	671	ARG	NE-CZ-NH1	6.47	123.54	120.30
15	M2	490	ARG	NE-CZ-NH1	6.47	123.53	120.30
6	C0	59	ARG	NE-CZ-NH1	6.46	123.53	120.30
6	C0	402	ARG	NE-CZ-NH1	6.46	123.53	120.30
15	M1	575	TYR	CB-CG-CD2	-6.46	117.12	121.00
20	R1	215	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	11	1247	ARG	NE-CZ-NH1	6.45	123.52	120.30
6	C0	1360	ARG	NE-CZ-NH1	6.45	123.52	120.30
20	R3	1543	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	T1	640	ARG	NE-CZ-NH1	6.44	123.52	120.30
4	A1	882	GLU	CA-CB-CG	6.43	127.55	113.40
2	14	849	ARG	NE-CZ-NH1	6.43	123.51	120.30
2	10	626	ARG	NE-CZ-NH1	6.42	123.51	120.30
18	P0	430	ARG	NE-CZ-NH1	6.42	123.51	120.30
20	R0	158	ARG	NE-CZ-NH1	6.42	123.51	120.30
20	R0	736	ARG	NE-CZ-NH1	6.42	123.51	120.30
14	L1	739	ARG	NE-CZ-NH1	6.41	123.50	120.30
14	L1	352	ARG	NE-CZ-NH1	6.41	123.50	120.30
25	X0	99	ARG	NE-CZ-NH1	6.41	123.50	120.30
18	P0	330	ARG	NE-CZ-NH1	6.40	123.50	120.30
5	B1	688	ARG	NE-CZ-NH1	6.39	123.50	120.30
19	Q0	229	ARG	NE-CZ-NH1	6.39	123.50	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	P3	598	ARG	NE-CZ-NH1	6.39	123.50	120.30
2	12	650	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	01	618	TYR	CB-CG-CD2	-6.39	117.17	121.00
2	12	626	ARG	NE-CZ-NH1	6.39	123.49	120.30
14	L0	922	ARG	NE-CZ-NH1	6.38	123.49	120.30
16	N1	213	ARG	NE-CZ-NH1	6.38	123.49	120.30
15	M3	248	ARG	NE-CZ-NH1	6.37	123.49	120.30
20	R3	1297	ARG	NE-CZ-NH1	6.37	123.49	120.30
15	M0	575	TYR	CB-CG-CD2	-6.37	117.18	121.00
20	R2	1593	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	12	132	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	16	650	ARG	NE-CZ-NH1	6.36	123.48	120.30
4	A3	21	ARG	NE-CZ-NH1	6.35	123.48	120.30
4	A3	816	ARG	NE-CZ-NH1	6.35	123.48	120.30
14	L3	352	ARG	NE-CZ-NH1	6.35	123.47	120.30
13	K1	637	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	T1	597	ARG	NE-CZ-NH1	6.34	123.47	120.30
15	M1	248	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	T3	1128	ARG	NE-CZ-NH1	6.33	123.47	120.30
18	P0	882	ARG	NE-CZ-NH1	6.33	123.46	120.30
7	D0	1299	ARG	NE-CZ-NH1	6.32	123.46	120.30
18	P3	170	ARG	NE-CZ-NH1	6.32	123.46	120.30
7	D1	1529	ARG	NE-CZ-NH1	6.31	123.46	120.30
13	K1	627	ARG	NE-CZ-NH2	-6.31	117.14	120.30
20	R3	1313	ARG	NE-CZ-NH2	-6.31	117.14	120.30
13	K2	671	ARG	NE-CZ-NH1	6.31	123.45	120.30
12	J1	637	ASP	CB-CG-OD2	-6.29	112.64	118.30
6	C2	549	ARG	NE-CZ-NH1	6.29	123.45	120.30
7	D3	937	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	T1	1128	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	15	650	ARG	NE-CZ-NH1	6.28	123.44	120.30
20	R0	1697	ARG	NE-CZ-NH1	6.28	123.44	120.30
7	D3	1464	LYS	CG-CD-CE	6.28	130.74	111.90
2	13	650	ARG	NE-CZ-NH1	6.27	123.44	120.30
21	T2	1128	ARG	NE-CZ-NH2	-6.27	117.16	120.30
15	M2	248	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	17	650	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	00	618	TYR	CB-CG-CD2	-6.26	117.24	121.00
2	15	1315	ARG	NE-CZ-NH1	6.25	123.43	120.30
14	L0	352	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	00	326	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	T0	1075	ARG	NE-CZ-NH1	6.24	123.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	11	1619	ARG	NE-CZ-NH1	6.23	123.42	120.30
4	A1	21	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	15	1467	ARG	NE-CZ-NH2	-6.22	117.19	120.30
7	D3	399	ARG	NE-CZ-NH1	6.22	123.41	120.30
18	P3	611	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	10	650	ARG	NE-CZ-NH1	6.22	123.41	120.30
18	P3	819	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	01	238	ARG	NE-CZ-NH1	6.21	123.41	120.30
8	E0	125	ARG	NE-CZ-NH1	6.21	123.41	120.30
11	I3	266	ARG	NE-CZ-NH1	6.20	123.40	120.30
7	D1	937	ARG	NE-CZ-NH1	6.20	123.40	120.30
25	X2	18	ARG	NE-CZ-NH1	6.20	123.40	120.30
14	L0	739	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	10	132	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	T1	810	ARG	NE-CZ-NH1	6.19	123.39	120.30
19	Q2	401	ARG	NE-CZ-NH1	6.19	123.39	120.30
21	T3	151	ARG	NE-CZ-NH1	6.19	123.39	120.30
7	D1	399	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	10	711	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	15	1264	ARG	NE-CZ-NH1	6.17	123.39	120.30
10	H1	301	ASP	CB-CG-OD1	6.17	123.85	118.30
18	P2	611	ARG	NE-CZ-NH1	6.17	123.38	120.30
21	T2	1126	ARG	NE-CZ-NH1	6.17	123.38	120.30
4	A0	833	ARG	NE-CZ-NH1	6.15	123.38	120.30
4	A5	796	ARG	NE-CZ-NH1	6.15	123.38	120.30
14	L2	352	ARG	NE-CZ-NH1	6.15	123.37	120.30
21	T0	597	ARG	NE-CZ-NH1	6.15	123.37	120.30
2	11	650	ARG	NE-CZ-NH1	6.15	123.37	120.30
6	C2	1287	TYR	CB-CG-CD2	-6.14	117.31	121.00
18	P2	882	ARG	NE-CZ-NH1	6.14	123.37	120.30
25	X1	18	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	17	1315	ARG	NE-CZ-NH1	6.14	123.37	120.30
18	P0	170	ARG	NE-CZ-NH2	-6.14	117.23	120.30
13	K3	1192	ARG	NE-CZ-NH1	6.13	123.37	120.30
4	A4	796	ARG	NE-CZ-NH1	6.13	123.37	120.30
13	K2	1192	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	12	1619	ARG	NE-CZ-NH1	6.12	123.36	120.30
6	C1	549	ARG	NE-CZ-NH1	6.12	123.36	120.30
8	E1	543	ASP	CB-CG-OD1	6.12	123.80	118.30
5	B1	1117	ARG	NE-CZ-NH1	6.11	123.36	120.30
6	C3	765	ARG	NE-CZ-NH1	6.11	123.36	120.30
18	P2	598	ARG	NE-CZ-NH1	6.11	123.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N2	235	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	14	1619	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	17	1619	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	C2	1131	ARG	NE-CZ-NH2	6.10	123.35	120.30
21	T2	151	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	16	1422	ARG	NE-CZ-NH1	6.10	123.35	120.30
20	R0	385	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	C2	402	ARG	NE-CZ-NH1	6.09	123.34	120.30
21	T1	826	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	16	1477	TYR	CB-CG-CD2	-6.09	117.35	121.00
2	17	1477	TYR	CB-CG-CD2	-6.08	117.35	121.00
6	C1	1131	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	12	1477	TYR	CB-CG-CD2	-6.08	117.35	121.00
14	L3	601	ARG	NE-CZ-NH1	6.08	123.34	120.30
15	M1	216	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	11	1422	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	T2	1128	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	10	1467	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	14	1247	ARG	NE-CZ-NH1	6.07	123.34	120.30
18	P1	787	ARG	NE-CZ-NH2	6.07	123.33	120.30
5	B1	1181	ARG	NE-CZ-NH1	6.07	123.33	120.30
20	R3	736	ARG	NE-CZ-NH1	6.07	123.33	120.30
4	A3	438	ARG	NE-CZ-NH1	6.06	123.33	120.30
7	D0	399	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	16	1247	ARG	NE-CZ-NH1	6.06	123.33	120.30
13	K1	1192	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	14	650	ARG	NE-CZ-NH1	6.05	123.33	120.30
6	C1	1287	TYR	CB-CG-CD2	-6.05	117.37	121.00
18	P2	420	ARG	NE-CZ-NH1	6.05	123.32	120.30
18	P1	611	ARG	NE-CZ-NH1	6.04	123.32	120.30
19	Q1	255	ARG	NE-CZ-NH1	6.04	123.32	120.30
20	R0	46	ARG	NE-CZ-NH1	6.04	123.32	120.30
25	X3	205	ARG	NE-CZ-NH2	-6.04	117.28	120.30
20	R1	1297	ARG	NE-CZ-NH1	6.04	123.32	120.30
4	A2	38	ARG	NE-CZ-NH1	6.04	123.32	120.30
21	T3	1126	ARG	NE-CZ-NH1	6.04	123.32	120.30
4	A1	438	ARG	NE-CZ-NH1	6.03	123.32	120.30
5	B0	1117	ARG	NE-CZ-NH1	6.03	123.31	120.30
14	L0	959	ARG	NE-CZ-NH1	6.03	123.31	120.30
4	A4	390	ARG	NE-CZ-NH1	6.02	123.31	120.30
7	D2	1529	ARG	NE-CZ-NH1	6.02	123.31	120.30
20	R1	173	ARG	NE-CZ-NH1	6.01	123.31	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	12	1467	ARG	NE-CZ-NH1	6.01	123.31	120.30
7	D2	929	ARG	NE-CZ-NH1	6.01	123.31	120.30
18	P1	598	ARG	NE-CZ-NH1	6.01	123.31	120.30
20	R1	1601	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	00	238	ARG	NE-CZ-NH1	6.01	123.30	120.30
18	P3	420	ARG	NE-CZ-NH1	6.00	123.30	120.30
15	M2	216	ARG	NE-CZ-NH1	6.00	123.30	120.30
14	L0	959	ARG	NE-CZ-NH2	-5.99	117.30	120.30
2	15	1477	TYR	CB-CG-CD2	-5.99	117.41	121.00
14	L1	208	ARG	NE-CZ-NH2	-5.99	117.31	120.30
21	T1	1063	ARG	NE-CZ-NH1	5.98	123.29	120.30
15	M0	724	TYR	CB-CG-CD2	-5.98	117.41	121.00
20	R0	671	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	17	1422	ARG	NE-CZ-NH1	5.97	123.29	120.30
18	P2	283	ARG	NE-CZ-NH1	5.97	123.29	120.30
19	Q0	401	ARG	NE-CZ-NH1	5.97	123.29	120.30
19	Q0	21	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	10	1422	ARG	NE-CZ-NH1	5.96	123.28	120.30
4	A4	38	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	14	1422	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	11	1477	TYR	CB-CG-CD2	-5.96	117.42	121.00
5	B0	321	ARG	NE-CZ-NH1	5.96	123.28	120.30
5	B0	972	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	16	1619	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	14	1477	TYR	CB-CG-CD2	-5.95	117.43	121.00
14	L3	208	ARG	NE-CZ-NH2	-5.95	117.33	120.30
20	R2	1297	ARG	NE-CZ-NH1	5.95	123.27	120.30
5	B1	1647	ARG	NE-CZ-NH1	5.95	123.27	120.30
18	P3	170	ARG	CD-NE-CZ	5.95	131.92	123.60
6	C1	473	ARG	NE-CZ-NH1	5.94	123.27	120.30
17	O0	376	ARG	NE-CZ-NH1	5.94	123.27	120.30
25	X1	99	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	13	1477	TYR	CB-CG-CD2	-5.93	117.44	121.00
14	L2	977	ARG	NE-CZ-NH1	5.93	123.27	120.30
4	A2	21	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	11	1301	ARG	CD-NE-CZ	5.93	131.90	123.60
2	15	1619	ARG	NE-CZ-NH1	5.93	123.27	120.30
18	P2	172	ARG	NE-CZ-NH1	5.93	123.26	120.30
21	T1	723	ARG	NE-CZ-NH1	5.93	123.26	120.30
7	D3	1057	ASP	CB-CG-OD2	-5.93	112.97	118.30
20	R2	671	ARG	NE-CZ-NH1	5.92	123.26	120.30
4	A2	796	ARG	NE-CZ-NH1	5.92	123.26	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L3	959	ARG	NE-CZ-NH1	5.91	123.26	120.30
15	M1	562	ARG	NE-CZ-NH1	5.91	123.26	120.30
17	O1	108	ARG	NE-CZ-NH1	5.91	123.25	120.30
21	T3	723	ARG	NE-CZ-NH1	5.91	123.25	120.30
14	L0	235	ARG	NE-CZ-NH1	5.90	123.25	120.30
16	N3	235	ARG	NE-CZ-NH1	5.90	123.25	120.30
20	R2	195	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	17	1467	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	12	1422	ARG	NE-CZ-NH1	5.90	123.25	120.30
10	H2	318	ARG	NE-CZ-NH1	5.90	123.25	120.30
14	L3	371	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	14	1301	ARG	CD-NE-CZ	5.90	131.86	123.60
2	12	1315	ARG	NE-CZ-NH1	5.90	123.25	120.30
4	A4	816	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	11	711	ARG	NE-CZ-NH1	5.89	123.25	120.30
4	A2	816	ARG	NE-CZ-NH1	5.89	123.25	120.30
25	X1	125	TYR	CB-CG-CD2	-5.89	117.46	121.00
6	C3	1131	ARG	NE-CZ-NH2	5.89	123.24	120.30
17	O2	409	ARG	NE-CZ-NH1	5.89	123.25	120.30
21	T2	810	ARG	NE-CZ-NH1	5.89	123.25	120.30
6	C3	552	ARG	NE-CZ-NH1	5.89	123.24	120.30
20	R1	671	ARG	NE-CZ-NH1	5.89	123.24	120.30
25	X2	125	TYR	CB-CG-CD2	-5.89	117.47	121.00
20	R3	671	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	T2	826	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	13	1422	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	13	1467	ARG	NE-CZ-NH1	5.88	123.24	120.30
7	D2	1440	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	13	1301	ARG	CD-NE-CZ	5.88	131.83	123.60
2	13	1619	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	14	1467	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	16	1467	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	10	1477	TYR	CB-CG-CD2	-5.87	117.48	121.00
14	L1	959	ARG	NE-CZ-NH1	5.87	123.24	120.30
2	10	1619	ARG	NE-CZ-NH1	5.87	123.24	120.30
19	Q0	279	ARG	NE-CZ-NH1	5.87	123.24	120.30
6	C3	473	ARG	NE-CZ-NH1	5.87	123.23	120.30
4	A5	816	ARG	NE-CZ-NH1	5.87	123.23	120.30
14	L1	795	ARG	NE-CZ-NH1	5.86	123.23	120.30
25	X2	99	ARG	NE-CZ-NH1	5.86	123.23	120.30
7	D0	1529	ARG	NE-CZ-NH1	5.86	123.23	120.30
19	Q1	26	ASP	CB-CG-OD2	-5.86	113.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	X3	99	ARG	NE-CZ-NH1	5.85	123.23	120.30
5	B0	1647	ARG	NE-CZ-NH1	5.85	123.22	120.30
14	L3	862	ARG	NE-CZ-NH1	5.85	123.22	120.30
4	A2	438	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	13	1315	ARG	NE-CZ-NH1	5.84	123.22	120.30
15	M3	216	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	T1	1126	ARG	NE-CZ-NH1	5.84	123.22	120.30
7	D0	539	ARG	NE-CZ-NH1	5.84	123.22	120.30
7	D3	929	ARG	NE-CZ-NH1	5.84	123.22	120.30
7	D3	1515	ARG	NE-CZ-NH1	5.84	123.22	120.30
5	B1	1424	ARG	NE-CZ-NH2	-5.84	117.38	120.30
13	K2	637	ARG	NE-CZ-NH1	5.83	123.21	120.30
18	P1	283	ARG	NE-CZ-NH1	5.83	123.21	120.30
7	D2	399	ARG	NE-CZ-NH1	5.83	123.21	120.30
20	R1	1601	ARG	NE-CZ-NH1	5.83	123.21	120.30
6	C0	473	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	15	922	ARG	NE-CZ-NH1	5.82	123.21	120.30
18	P3	283	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	10	1315	ARG	NE-CZ-NH1	5.81	123.21	120.30
2	16	1301	ARG	CD-NE-CZ	5.81	131.74	123.60
20	R2	46	ARG	NE-CZ-NH1	5.81	123.21	120.30
7	D2	539	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	T0	1063	ARG	NE-CZ-NH1	5.81	123.20	120.30
19	Q3	140	ARG	NE-CZ-NH1	5.81	123.20	120.30
5	B1	217	ARG	NE-CZ-NH1	5.80	123.20	120.30
19	Q1	279	ARG	NE-CZ-NH1	5.80	123.20	120.30
7	D1	929	ARG	NE-CZ-NH1	5.80	123.20	120.30
6	C1	402	ARG	NE-CZ-NH1	5.80	123.20	120.30
6	C1	552	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	11	1315	ARG	NE-CZ-NH1	5.79	123.20	120.30
14	L3	977	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	11	1467	ARG	NE-CZ-NH1	5.79	123.19	120.30
23	V1	672	TYR	CB-CG-CD2	-5.79	117.53	121.00
14	L2	235	ARG	NE-CZ-NH1	5.78	123.19	120.30
5	B0	217	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	T1	723	ARG	NE-CZ-NH2	-5.78	117.41	120.30
22	U0	885	ARG	NE-CZ-NH2	-5.78	117.41	120.30
6	C2	473	ARG	NE-CZ-NH1	5.77	123.19	120.30
8	E1	621	ARG	NE-CZ-NH1	5.77	123.19	120.30
13	K0	536	TYR	CB-CG-CD2	-5.77	117.54	121.00
13	K3	536	TYR	CB-CG-CD2	-5.76	117.54	121.00
2	16	1315	ARG	NE-CZ-NH1	5.76	123.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	12	1467	ARG	NE-CZ-NH2	-5.75	117.42	120.30
5	B1	321	ARG	NE-CZ-NH1	5.75	123.18	120.30
15	M0	248	ARG	NE-CZ-NH1	5.75	123.17	120.30
6	C2	552	ARG	NE-CZ-NH1	5.75	123.17	120.30
21	T2	723	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	15	1422	ARG	NE-CZ-NH1	5.74	123.17	120.30
13	K1	536	TYR	CB-CG-CD2	-5.74	117.56	121.00
24	W1	882	ARG	NE-CZ-NH1	5.74	123.17	120.30
18	P3	882	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	11	1301	ARG	NE-CZ-NH1	5.73	123.17	120.30
21	T3	723	ARG	NE-CZ-NH2	-5.73	117.43	120.30
21	T3	1058	ARG	NE-CZ-NH1	5.73	123.17	120.30
18	P2	170	ARG	CD-NE-CZ	5.73	131.62	123.60
19	Q2	140	ARG	NE-CZ-NH1	5.72	123.16	120.30
5	B1	972	ARG	NE-CZ-NH1	5.72	123.16	120.30
7	D2	1433	ARG	NE-CZ-NH1	5.72	123.16	120.30
19	Q3	401	ARG	NE-CZ-NH1	5.72	123.16	120.30
7	D1	1030	ARG	NE-CZ-NH1	5.72	123.16	120.30
5	B0	1424	ARG	NE-CZ-NH2	-5.72	117.44	120.30
20	R3	46	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	15	1247	ARG	NE-CZ-NH1	5.71	123.16	120.30
23	V1	875	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	12	846	ARG	NE-CZ-NH1	5.71	123.15	120.30
5	B0	179	ARG	NE-CZ-NH1	5.71	123.15	120.30
12	J2	593	ARG	NE-CZ-NH1	5.70	123.15	120.30
6	C0	765	ARG	NE-CZ-NH1	5.69	123.15	120.30
7	D0	929	ARG	NE-CZ-NH1	5.69	123.15	120.30
18	P2	877	ARG	NE-CZ-NH1	5.69	123.14	120.30
20	R1	195	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	10	1179	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	D0	678	ARG	NE-CZ-NH1	5.68	123.14	120.30
18	P0	179	ARG	NE-CZ-NH1	5.68	123.14	120.30
18	P0	283	ARG	NE-CZ-NH1	5.68	123.14	120.30
13	K0	1192	ARG	NE-CZ-NH1	5.68	123.14	120.30
18	P2	170	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	13	1247	ARG	NE-CZ-NH1	5.67	123.14	120.30
20	R2	215	ARG	NE-CZ-NH1	5.67	123.14	120.30
14	L3	235	ARG	NE-CZ-NH1	5.66	123.13	120.30
15	M3	234	ARG	NE-CZ-NH1	5.66	123.13	120.30
7	D1	539	ARG	NE-CZ-NH1	5.66	123.13	120.30
4	A4	438	ARG	NE-CZ-NH1	5.65	123.13	120.30
13	K2	536	TYR	CB-CG-CD2	-5.65	117.61	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	T0	1128	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	13	1301	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	14	1301	ARG	NE-CZ-NH1	5.64	123.12	120.30
4	A4	21	ARG	NE-CZ-NH1	5.64	123.12	120.30
14	L0	862	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	00	225	ARG	NE-CZ-NH1	5.63	123.11	120.30
14	L1	356	ARG	NE-CZ-NH1	5.63	123.12	120.30
6	C0	972	ARG	NE-CZ-NH1	5.63	123.11	120.30
2	12	1301	ARG	NE-CZ-NH1	5.63	123.11	120.30
2	14	1315	ARG	NE-CZ-NH1	5.63	123.11	120.30
6	C1	972	ARG	NE-CZ-NH1	5.63	123.11	120.30
12	J0	637	ASP	CB-CG-OD2	-5.62	113.24	118.30
6	C2	1134	ARG	CD-NE-CZ	5.62	131.47	123.60
2	12	1	MET	C-N-CA	5.62	135.74	121.70
2	10	1	MET	C-N-CA	5.61	135.73	121.70
20	R1	1684	ARG	NE-CZ-NH1	5.61	123.11	120.30
8	E0	431	ARG	NE-CZ-NH1	5.61	123.11	120.30
15	M1	251	ARG	NE-CZ-NH1	5.61	123.10	120.30
18	P2	787	ARG	NE-CZ-NH2	5.60	123.10	120.30
2	16	1	MET	C-N-CA	5.59	135.68	121.70
24	W0	80	ARG	NE-CZ-NH1	5.59	123.09	120.30
5	B1	179	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	15	1	MET	C-N-CA	5.58	135.66	121.70
14	L2	269	ARG	NE-CZ-NH1	5.58	123.09	120.30
5	B1	1710	ARG	NE-CZ-NH1	5.58	123.09	120.30
17	O0	124	ARG	CD-NE-CZ	5.58	131.41	123.60
2	13	1	MET	C-N-CA	5.58	135.65	121.70
6	C3	972	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	10	1467	ARG	NE-CZ-NH2	-5.58	117.51	120.30
18	P3	398	ARG	NE-CZ-NH1	5.58	123.09	120.30
8	E1	652	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	T2	1058	ARG	NE-CZ-NH1	5.58	123.09	120.30
6	C3	720	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	11	1	MET	C-N-CA	5.57	135.63	121.70
2	17	1	MET	C-N-CA	5.57	135.63	121.70
7	D1	1440	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	14	1	MET	C-N-CA	5.57	135.62	121.70
14	L3	847	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	11	384	ASP	CB-CG-OD2	5.57	123.31	118.30
20	R1	46	ARG	NE-CZ-NH1	5.57	123.08	120.30
24	W0	125	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	12	1301	ARG	NE-CZ-NH2	-5.56	117.52	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L3	269	ARG	NE-CZ-NH1	5.56	123.08	120.30
7	D1	587	ARG	NE-CZ-NH1	5.56	123.08	120.30
8	E0	621	ARG	NE-CZ-NH1	5.56	123.08	120.30
11	I1	284	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	12	1247	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	16	1467	ARG	NE-CZ-NH2	-5.55	117.52	120.30
21	T2	1063	ARG	NE-CZ-NH1	5.55	123.08	120.30
23	V0	875	ARG	NE-CZ-NH2	-5.55	117.52	120.30
21	T3	826	ARG	NE-CZ-NH1	5.55	123.08	120.30
18	P2	398	ARG	NE-CZ-NH1	5.55	123.08	120.30
7	D2	678	ARG	NE-CZ-NH1	5.55	123.08	120.30
14	L3	922	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	17	1467	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	C0	1287	TYR	CB-CG-CD2	-5.54	117.68	121.00
10	H0	415	ARG	NE-CZ-NH1	5.54	123.07	120.30
14	L2	784	ARG	NE-CZ-NH2	-5.53	117.53	120.30
15	M0	646	ARG	NE-CZ-NH1	5.53	123.06	120.30
6	C2	1670	ARG	NE-CZ-NH1	5.53	123.06	120.30
20	R0	1297	ARG	NE-CZ-NH1	5.53	123.06	120.30
20	R1	1617	ARG	NE-CZ-NH1	5.53	123.06	120.30
5	B0	129	ASP	CB-CG-OD1	5.53	123.27	118.30
20	R0	1617	ARG	CD-NE-CZ	5.53	131.34	123.60
18	P1	157	ARG	NE-CZ-NH1	5.52	123.06	120.30
17	O1	124	ARG	CD-NE-CZ	5.52	131.33	123.60
13	K3	637	ARG	NE-CZ-NH1	5.52	123.06	120.30
18	P0	398	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	15	1404	ASP	CB-CG-OD2	-5.52	113.34	118.30
20	R3	1601	ARG	NE-CZ-NH2	-5.51	117.54	120.30
2	13	1467	ARG	NE-CZ-NH2	-5.51	117.55	120.30
21	T2	723	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	T2	640	ARG	NE-CZ-NH1	5.50	123.05	120.30
14	L3	739	ARG	NE-CZ-NH1	5.50	123.05	120.30
15	M1	783	ARG	NE-CZ-NH1	5.50	123.05	120.30
10	H1	219	ARG	NE-CZ-NH1	5.50	123.05	120.30
7	D0	1433	ARG	NE-CZ-NH1	5.49	123.05	120.30
5	B0	1710	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	10	357	PRO	CA-N-CD	-5.49	103.82	111.50
19	Q0	17	ARG	NE-CZ-NH1	5.49	123.04	120.30
25	X1	136	ARG	NE-CZ-NH1	5.49	123.04	120.30
5	B1	129	ASP	CB-CG-OD1	5.48	123.23	118.30
6	C3	549	ARG	NE-CZ-NH1	5.48	123.04	120.30
23	V0	762	ARG	NE-CZ-NH1	5.48	123.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C3	224	ARG	NE-CZ-NH1	5.47	123.04	120.30
6	C1	1134	ARG	CD-NE-CZ	5.47	131.25	123.60
2	15	608	ASP	CB-CG-OD1	5.47	123.22	118.30
7	D0	1440	ARG	NE-CZ-NH1	5.47	123.03	120.30
5	B0	1773	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	14	1467	ARG	NE-CZ-NH2	-5.46	117.57	120.30
7	D1	752	ARG	NE-CZ-NH1	5.46	123.03	120.30
18	P1	170	ARG	NE-CZ-NH1	5.46	123.03	120.30
6	C0	1134	ARG	CD-NE-CZ	5.45	131.24	123.60
14	L2	208	ARG	NE-CZ-NH2	-5.45	117.57	120.30
16	N1	235	ARG	NE-CZ-NH1	5.45	123.03	120.30
18	P1	877	ARG	NE-CZ-NH1	5.45	123.03	120.30
11	I2	284	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	17	384	ASP	CB-CG-OD2	5.45	123.20	118.30
2	15	384	ASP	CB-CG-OD2	5.45	123.20	118.30
14	L2	795	ARG	NE-CZ-NH1	5.45	123.02	120.30
18	P3	692	ARG	NE-CZ-NH1	5.45	123.02	120.30
15	M2	234	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	14	711	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	12	1179	ARG	NE-CZ-NH1	5.44	123.02	120.30
5	B0	688	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
14	L2	922	ARG	NE-CZ-NH1	5.43	123.02	120.30
17	O3	81	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	14	608	ASP	CB-CG-OD1	5.43	123.19	118.30
14	L0	342	ARG	NE-CZ-NH1	5.43	123.02	120.30
18	P0	611	ARG	NE-CZ-NH1	5.43	123.01	120.30
2	15	846	ARG	CD-NE-CZ	5.42	131.19	123.60
5	B1	688	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	14	384	ASP	CB-CG-OD2	5.42	123.17	118.30
5	B1	488	ARG	NE-CZ-NH1	5.42	123.01	120.30
4	A0	816	ARG	NE-CZ-NH1	5.41	123.01	120.30
5	B0	488	ARG	NE-CZ-NH1	5.41	123.01	120.30
20	R0	173	ARG	NE-CZ-NH1	5.41	123.01	120.30
19	Q0	308	ARG	NE-CZ-NH1	5.41	123.01	120.30
25	X3	125	TYR	CB-CG-CD2	-5.41	117.76	121.00
8	E0	543	ASP	CB-CG-OD1	5.40	123.16	118.30
25	X0	136	ARG	NE-CZ-NH1	5.40	123.00	120.30
15	M2	562	ARG	NE-CZ-NH1	5.40	123.00	120.30
8	E1	398	ARG	CD-NE-CZ	5.39	131.15	123.60
18	P1	819	ARG	NE-CZ-NH1	5.39	122.99	120.30
15	M2	515	ARG	CD-NE-CZ	5.38	131.14	123.60
15	M3	515	ARG	CD-NE-CZ	5.38	131.14	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	13	1404	ASP	CB-CG-OD2	-5.38	113.46	118.30
14	L1	922	ARG	NE-CZ-NH1	5.38	122.99	120.30
25	X0	125	TYR	CB-CG-CD2	-5.38	117.77	121.00
7	D1	1433	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	17	1604	ARG	NE-CZ-NH1	5.38	122.99	120.30
5	B1	688	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
25	X2	136	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	13	550	ARG	NE-CZ-NH1	5.37	122.99	120.30
20	R1	1543	ARG	NE-CZ-NH1	5.37	122.99	120.30
20	R3	173	ARG	NE-CZ-NH1	5.37	122.98	120.30
21	T1	1058	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	12	849	ARG	NE-CZ-NH1	5.37	122.98	120.30
15	M2	394	ARG	NE-CZ-NH1	5.36	122.98	120.30
19	Q0	21	ARG	NE-CZ-NH2	-5.36	117.62	120.30
6	C0	983	PRO	CA-N-CD	-5.36	103.99	111.50
14	L1	959	ARG	NE-CZ-NH2	-5.36	117.62	120.30
14	L2	327	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	16	608	ASP	CB-CG-OD1	5.36	123.12	118.30
2	10	1	MET	CA-C-N	5.36	128.99	117.20
2	17	608	ASP	CB-CG-OD1	5.36	123.12	118.30
4	A2	844	TYR	CB-CG-CD2	-5.36	117.79	121.00
2	16	1301	ARG	NE-CZ-NH1	5.35	122.98	120.30
7	D3	1440	ARG	NE-CZ-NH1	5.35	122.98	120.30
14	L3	342	ARG	NE-CZ-NH1	5.35	122.98	120.30
4	A5	560	ARG	NE-CZ-NH1	5.35	122.97	120.30
7	D3	539	ARG	NE-CZ-NH1	5.35	122.97	120.30
12	J1	627	ARG	NE-CZ-NH1	5.35	122.97	120.30
15	M2	251	ARG	NE-CZ-NH1	5.35	122.97	120.30
20	R2	173	ARG	NE-CZ-NH1	5.35	122.97	120.30
12	J1	709	ARG	NE-CZ-NH1	5.34	122.97	120.30
14	L3	356	ARG	NE-CZ-NH1	5.34	122.97	120.30
25	X3	136	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	16	384	ASP	CB-CG-OD2	5.34	123.11	118.30
14	L1	208	ARG	CD-NE-CZ	5.34	131.08	123.60
19	Q2	255	ARG	NE-CZ-NH1	5.34	122.97	120.30
4	A0	508	ARG	NE-CZ-NH1	5.34	122.97	120.30
15	M1	490	ARG	NE-CZ-NH1	5.34	122.97	120.30
17	O1	201	ASP	CB-CG-OD2	-5.34	113.50	118.30
20	R3	423	ARG	NE-CZ-NH1	5.33	122.97	120.30
24	W1	80	ARG	NE-CZ-NH1	5.33	122.97	120.30
6	C2	981	ARG	NE-CZ-NH1	5.33	122.97	120.30
20	R0	1213	ARG	NE-CZ-NH2	-5.33	117.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C1	981	ARG	NE-CZ-NH1	5.33	122.97	120.30
15	M1	888	TYR	CB-CG-CD2	-5.33	117.80	121.00
18	P1	692	ARG	NE-CZ-NH1	5.33	122.96	120.30
20	R2	1601	ARG	NE-CZ-NH2	-5.33	117.64	120.30
10	H3	219	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	13	608	ASP	CB-CG-OD1	5.33	123.09	118.30
6	C0	607	ARG	NH1-CZ-NH2	-5.32	113.54	119.40
17	O1	409	ARG	NE-CZ-NH1	5.32	122.96	120.30
19	Q1	308	ARG	NE-CZ-NH1	5.32	122.96	120.30
7	D3	678	ARG	NE-CZ-NH1	5.32	122.96	120.30
13	K3	963	ARG	NE-CZ-NH2	-5.32	117.64	120.30
15	M3	562	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	11	608	ASP	CB-CG-OD1	5.31	123.08	118.30
2	13	1	MET	CA-C-N	5.31	128.89	117.20
2	10	608	ASP	CB-CG-OD1	5.31	123.08	118.30
2	12	608	ASP	CB-CG-OD1	5.31	123.08	118.30
10	H0	219	ARG	NE-CZ-NH1	5.31	122.95	120.30
14	L3	959	ARG	NE-CZ-NH2	-5.30	117.65	120.30
18	P0	269	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	15	711	ARG	NE-CZ-NH2	5.30	122.95	120.30
6	C2	983	PRO	CA-N-CD	-5.30	104.08	111.50
7	D3	587	ARG	NE-CZ-NH1	5.30	122.95	120.30
6	C0	281	ARG	NE-CZ-NH1	5.30	122.95	120.30
20	R0	1706	ARG	NE-CZ-NH1	5.30	122.95	120.30
16	N0	235	ARG	NE-CZ-NH1	5.29	122.95	120.30
21	T2	976	ARG	NE-CZ-NH1	5.29	122.95	120.30
25	X3	350	ARG	NE-CZ-NH2	5.29	122.95	120.30
20	R2	423	ARG	NE-CZ-NH1	5.29	122.94	120.30
24	W1	125	TYR	CB-CG-CD2	-5.29	117.83	121.00
15	M3	251	ARG	NE-CZ-NH1	5.29	122.94	120.30
15	M1	515	ARG	CD-NE-CZ	5.29	131.00	123.60
25	X3	205	ARG	NE-CZ-NH1	5.29	122.94	120.30
15	M1	234	ARG	NE-CZ-NH1	5.28	122.94	120.30
17	O3	2	ARG	NE-CZ-NH1	5.28	122.94	120.30
18	P1	398	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	12	1	MET	CA-C-N	5.28	128.82	117.20
2	17	1701	ASP	CB-CG-OD2	-5.28	113.55	118.30
7	D1	678	ARG	NE-CZ-NH1	5.28	122.94	120.30
15	M0	234	ARG	NE-CZ-NH1	5.28	122.94	120.30
18	P2	692	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	T1	1042	ARG	NE-CZ-NH1	5.28	122.94	120.30
19	Q3	308	ARG	NE-CZ-NH1	5.27	122.94	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C1	983	PRO	CA-N-CD	-5.26	104.13	111.50
2	11	1467	ARG	NE-CZ-NH2	-5.26	117.67	120.30
24	W0	148	ARG	NE-CZ-NH1	5.26	122.93	120.30
17	O2	124	ARG	CD-NE-CZ	5.26	130.96	123.60
18	P1	653	ARG	NE-CZ-NH1	5.26	122.93	120.30
18	P3	172	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	11	1404	ASP	CB-CG-OD2	-5.25	113.57	118.30
5	B1	1773	ARG	NE-CZ-NH1	5.25	122.92	120.30
5	B0	688	ARG	NE-CZ-NH2	5.25	122.92	120.30
24	W0	795	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	14	1	MET	CA-C-N	5.25	128.74	117.20
2	17	1	MET	CA-C-N	5.25	128.74	117.20
10	H3	415	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	11	1	MET	CA-C-N	5.25	128.74	117.20
14	L1	235	ARG	NE-CZ-NH1	5.25	122.92	120.30
21	T0	810	ARG	NE-CZ-NH1	5.25	122.92	120.30
21	T1	1128	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	01	415	ARG	NE-CZ-NH1	5.24	122.92	120.30
6	C3	1134	ARG	CD-NE-CZ	5.24	130.93	123.60
20	R2	1655	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	01	225	ARG	NE-CZ-NH1	5.24	122.92	120.30
5	B0	1909	ASP	CB-CG-OD1	5.24	123.01	118.30
6	C2	972	ARG	NE-CZ-NH1	5.23	122.91	120.30
18	P0	278	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	12	1404	ASP	CB-CG-OD2	-5.23	113.59	118.30
14	L1	235	ARG	NE-CZ-NH2	-5.23	117.69	120.30
20	R1	217	ARG	NE-CZ-NH1	5.23	122.91	120.30
21	T2	66	ARG	NE-CZ-NH1	5.23	122.91	120.30
21	T3	976	ARG	NE-CZ-NH1	5.22	122.91	120.30
15	M1	394	ARG	NE-CZ-NH1	5.22	122.91	120.30
7	D1	1177	ARG	NE-CZ-NH1	5.22	122.91	120.30
14	L3	849	ARG	NE-CZ-NH1	5.22	122.91	120.30
18	P1	170	ARG	CD-NE-CZ	5.22	130.90	123.60
20	R2	1684	ARG	NE-CZ-NH1	5.22	122.91	120.30
7	D1	887	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	12	849	ARG	CD-NE-CZ	5.21	130.89	123.60
8	E0	617	ARG	CD-NE-CZ	5.21	130.89	123.60
19	Q2	279	ARG	NE-CZ-NH1	5.21	122.90	120.30
6	C1	1654	GLU	OE1-CD-OE2	-5.20	117.06	123.30
21	T3	1063	ARG	NE-CZ-NH1	5.20	122.90	120.30
25	X0	18	ARG	NE-CZ-NH2	5.20	122.90	120.30
7	D1	742	ARG	NE-CZ-NH1	5.20	122.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L2	342	ARG	NE-CZ-NH1	5.20	122.90	120.30
7	D2	752	ARG	NE-CZ-NH1	5.20	122.90	120.30
15	M0	515	ARG	CD-NE-CZ	5.20	130.88	123.60
2	16	1	MET	CA-C-N	5.20	128.63	117.20
14	L1	957	ARG	NE-CZ-NH1	5.20	122.90	120.30
20	R3	883	ARG	NE-CZ-NH2	5.20	122.90	120.30
3	40	392	ARG	NE-CZ-NH1	5.19	122.90	120.30
7	D3	887	ARG	NE-CZ-NH1	5.19	122.90	120.30
25	X0	18	ARG	NE-CZ-NH1	5.19	122.90	120.30
15	M3	839	ARG	CD-NE-CZ	5.19	130.87	123.60
2	17	1247	ARG	NE-CZ-NH1	5.19	122.89	120.30
19	Q0	279	ARG	CD-NE-CZ	5.19	130.86	123.60
8	E0	398	ARG	CD-NE-CZ	5.18	130.85	123.60
5	B1	1909	ASP	CB-CG-OD1	5.18	122.96	118.30
7	D3	1177	ARG	NE-CZ-NH1	5.18	122.89	120.30
8	E0	652	ARG	NE-CZ-NH1	5.18	122.89	120.30
13	K3	1184	ARG	NE-CZ-NH1	5.18	122.89	120.30
15	M0	428	ARG	NE-CZ-NH1	5.18	122.89	120.30
20	R2	1617	ARG	NE-CZ-NH1	5.17	122.89	120.30
6	C2	27	ARG	NE-CZ-NH1	5.17	122.89	120.30
17	O0	419	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
7	D3	1529	ARG	NE-CZ-NH1	5.17	122.89	120.30
6	C0	675	ARG	NE-CZ-NH2	5.17	122.88	120.30
8	E1	431	ARG	NE-CZ-NH1	5.17	122.88	120.30
6	C2	1050	ARG	NE-CZ-NH1	5.17	122.88	120.30
25	X0	205	ARG	NE-CZ-NH1	5.17	122.88	120.30
25	X1	205	ARG	NE-CZ-NH1	5.16	122.88	120.30
19	Q2	308	ARG	NE-CZ-NH1	5.16	122.88	120.30
7	D2	1177	ARG	NE-CZ-NH1	5.16	122.88	120.30
18	P0	653	ARG	NE-CZ-NH1	5.16	122.88	120.30
14	L2	863	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	15	1	MET	CA-C-N	5.15	128.54	117.20
20	R1	385	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
18	P2	814	ARG	NE-CZ-NH1	5.15	122.88	120.30
4	A1	560	ARG	NE-CZ-NH1	5.15	122.88	120.30
20	R0	1442	PRO	CA-N-CD	-5.15	104.29	111.50
23	V0	875	ARG	NE-CZ-NH1	5.15	122.88	120.30
6	C3	651	ASP	CB-CG-OD1	5.15	122.93	118.30
15	M3	394	ARG	NE-CZ-NH1	5.15	122.87	120.30
21	T0	862	ASP	CB-CG-OD2	-5.15	113.67	118.30
14	L2	356	ARG	NE-CZ-NH1	5.14	122.87	120.30
7	D1	511	ARG	NE-CZ-NH1	5.14	122.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A2	893	ARG	CD-NE-CZ	5.14	130.80	123.60
14	L2	441	ARG	NE-CZ-NH1	5.14	122.87	120.30
15	M3	521	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	40	467	TYR	CB-CG-CD2	-5.13	117.92	121.00
24	W1	4	ARG	NE-CZ-NH1	5.13	122.86	120.30
3	41	359	ARG	NE-CZ-NH1	5.13	122.86	120.30
6	C1	1050	ARG	NE-CZ-NH1	5.13	122.86	120.30
18	P0	330	ARG	CD-NE-CZ	5.13	130.78	123.60
24	W1	795	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	13	383	ARG	NE-CZ-NH1	5.12	122.86	120.30
20	R3	1113	ARG	NE-CZ-NH1	5.12	122.86	120.30
6	C3	607	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
3	41	467	TYR	CB-CG-CD2	-5.12	117.93	121.00
20	R3	456	ARG	NE-CZ-NH1	5.12	122.86	120.30
21	T0	590	ASP	CB-CG-OD1	5.12	122.90	118.30
2	17	1404	ASP	CB-CG-OD2	-5.11	113.70	118.30
13	K3	821	ASP	CB-CG-OD1	5.11	122.90	118.30
2	12	454	TYR	CB-CG-CD1	-5.11	117.93	121.00
6	C3	1287	TYR	CB-CG-CD2	-5.11	117.94	121.00
4	A0	560	ARG	NE-CZ-NH1	5.10	122.85	120.30
21	T2	632	TYR	CB-CG-CD1	-5.10	117.94	121.00
14	L2	208	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	14	333	ARG	NE-CZ-NH1	5.09	122.85	120.30
3	41	392	ARG	NE-CZ-NH1	5.09	122.85	120.30
6	C3	59	ARG	NE-CZ-NH1	5.09	122.85	120.30
17	O1	26	ARG	NE-CZ-NH1	5.09	122.85	120.30
21	T0	723	ARG	NE-CZ-NH1	5.09	122.85	120.30
6	C0	549	ARG	NE-CZ-NH1	5.09	122.84	120.30
20	R0	354	ASN	C-N-CA	5.08	134.41	121.70
6	C1	765	ARG	NE-CZ-NH1	5.08	122.84	120.30
7	D0	752	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	10	1247	ARG	NE-CZ-NH1	5.08	122.84	120.30
6	C1	27	ARG	NE-CZ-NH1	5.08	122.84	120.30
7	D0	1177	ARG	NE-CZ-NH1	5.07	122.84	120.30
7	D0	1339	ARG	NE-CZ-NH1	5.07	122.84	120.30
18	P3	787	ARG	NE-CZ-NH2	5.07	122.83	120.30
7	D0	661	ARG	NE-CZ-NH1	5.07	122.83	120.30
15	M0	251	ARG	NE-CZ-NH1	5.07	122.83	120.30
21	T0	1058	ARG	NE-CZ-NH1	5.07	122.83	120.30
17	O3	409	ARG	NE-CZ-NH1	5.06	122.83	120.30
7	D3	511	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	01	722	ARG	NH1-CZ-NH2	-5.06	113.84	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	X2	205	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	40	47	ARG	NE-CZ-NH1	5.06	122.83	120.30
14	L1	441	ARG	NE-CZ-NH1	5.06	122.83	120.30
20	R1	883	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	T2	71	CYS	CA-CB-SG	-5.05	104.90	114.00
8	E0	312	ARG	NE-CZ-NH1	5.05	122.83	120.30
6	C2	281	ARG	NE-CZ-NH1	5.05	122.83	120.30
19	Q3	255	ARG	NE-CZ-NH1	5.05	122.83	120.30
15	M3	783	ARG	CD-NE-CZ	5.04	130.66	123.60
19	Q0	255	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	00	415	ARG	NE-CZ-NH1	5.04	122.82	120.30
6	C2	607	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
18	P0	819	ARG	NE-CZ-NH2	5.04	122.82	120.30
20	R3	1655	ARG	NE-CZ-NH1	5.04	122.82	120.30
21	T0	1010	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
12	J5	560	ARG	NE-CZ-NH2	-5.04	117.78	120.30
20	R0	215	ARG	NE-CZ-NH1	5.04	122.82	120.30
24	W1	246	ARG	NE-CZ-NH1	5.04	122.82	120.30
6	C3	983	PRO	CA-N-CD	-5.04	104.45	111.50
12	J5	601	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	40	359	ARG	NE-CZ-NH1	5.04	122.82	120.30
7	D3	1433	ARG	NE-CZ-NH1	5.04	122.82	120.30
4	A3	844	TYR	CB-CG-CD2	-5.04	117.98	121.00
25	X1	405	TYR	CB-CG-CD2	-5.04	117.98	121.00
4	A2	560	ARG	NE-CZ-NH1	5.03	122.82	120.30
6	C1	909	ARG	NE-CZ-NH2	-5.03	117.78	120.30
20	R3	1601	ARG	NE-CZ-NH1	5.03	122.81	120.30
4	A0	456	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
19	Q0	129	ASP	CB-CG-OD1	5.02	122.82	118.30
19	Q3	279	ARG	NE-CZ-NH1	5.02	122.81	120.30
7	D2	551	ARG	NE-CZ-NH2	-5.02	117.79	120.30
20	R1	1313	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	14	180	ARG	NE-CZ-NH1	5.02	122.81	120.30
8	E1	312	ARG	NE-CZ-NH1	5.02	122.81	120.30
14	L3	239	ARG	NE-CZ-NH1	5.02	122.81	120.30
22	U3	885	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	01	633	ARG	NE-CZ-NH1	5.02	122.81	120.30
14	L3	166	LYS	CB-CA-C	5.02	120.44	110.40
19	Q1	140	ARG	NE-CZ-NH1	5.02	122.81	120.30
14	L3	208	ARG	CD-NE-CZ	5.01	130.62	123.60
17	O2	376	ARG	NE-CZ-NH1	5.01	122.81	120.30
6	C1	675	ARG	NE-CZ-NH2	5.01	122.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U1	885	ARG	NE-CZ-NH2	-5.01	117.79	120.30
2	10	1012	ARG	NE-CZ-NH1	5.01	122.81	120.30
17	O3	376	ARG	NE-CZ-NH1	5.01	122.81	120.30
17	O1	26	ARG	NE-CZ-NH2	-5.01	117.80	120.30
6	C1	281	ARG	NE-CZ-NH1	5.00	122.80	120.30
14	L0	849	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C0	316	ILE	CB
6	C0	982	ASN	CA
6	C0	983	PRO	CA
6	C1	316	ILE	CB
6	C1	982	ASN	CA
6	C1	983	PRO	CA
6	C2	316	ILE	CB
6	C2	982	ASN	CA
6	C2	983	PRO	CA
6	C3	316	ILE	CB
6	C3	982	ASN	CA
6	C3	983	PRO	CA

All (673) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	00	116	TYR	Sidechain
1	00	388	ASP	Peptide
1	00	405	TYR	Sidechain
1	00	465	THR	Peptide
1	00	466	THR	Peptide
1	00	511	SER	Peptide
1	00	646	ILE	Peptide
1	00	657	ILE	Peptide
1	00	720	TYR	Sidechain
1	01	116	TYR	Sidechain
1	01	388	ASP	Peptide
1	01	405	TYR	Sidechain
1	01	462	SER	Peptide
1	01	465	THR	Peptide
1	01	466	THR	Peptide
1	01	511	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	01	646	ILE	Peptide
1	01	657	ILE	Peptide
1	01	720	TYR	Sidechain
2	10	10	LYS	Peptide
2	10	11	LYS	Peptide
2	10	1180	GLN	Peptide
2	10	1422	ARG	Sidechain
2	10	15	LEU	Peptide
2	10	1544	HIS	Sidechain
2	10	1561	ARG	Sidechain
2	10	1657	ILE	Peptide
2	10	1687	ARG	Sidechain
2	10	17	LEU	Peptide
2	10	1716	TYR	Sidechain
2	10	202	THR	Peptide
2	10	3	ILE	Peptide
2	10	370	GLY	Peptide
2	10	4	ILE	Peptide
2	10	414	TYR	Sidechain
2	10	5	ASN	Peptide
2	10	52	ARG	Sidechain
2	10	7	ASN	Peptide
2	10	8	ASN	Peptide
2	10	849	ARG	Sidechain
2	10	860	ASP	Peptide
2	11	10	LYS	Peptide
2	11	11	LYS	Peptide
2	11	1180	GLN	Peptide
2	11	1422	ARG	Sidechain
2	11	15	LEU	Peptide
2	11	1687	ARG	Sidechain
2	11	17	LEU	Peptide
2	11	1716	TYR	Sidechain
2	11	194	GLY	Peptide
2	11	202	THR	Peptide
2	11	285	GLN	Peptide
2	11	3	ILE	Peptide
2	11	370	GLY	Peptide
2	11	4	ILE	Peptide
2	11	414	TYR	Sidechain
2	11	477	HIS	Sidechain
2	11	479	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	11	5	ASN	Peptide
2	11	52	ARG	Sidechain
2	11	7	ASN	Peptide
2	11	8	ASN	Peptide
2	11	849	ARG	Sidechain
2	11	860	ASP	Peptide
2	11	868	TYR	Sidechain
2	11	929	SER	Peptide
2	12	10	LYS	Peptide
2	12	11	LYS	Peptide
2	12	1180	GLN	Peptide
2	12	1422	ARG	Sidechain
2	12	1451	SER	Peptide
2	12	1455	PRO	Peptide
2	12	15	LEU	Peptide
2	12	1544	HIS	Sidechain
2	12	1687	ARG	Sidechain
2	12	17	LEU	Peptide
2	12	194	GLY	Peptide
2	12	202	THR	Peptide
2	12	285	GLN	Peptide
2	12	3	ILE	Peptide
2	12	370	GLY	Peptide
2	12	4	ILE	Peptide
2	12	414	TYR	Sidechain
2	12	5	ASN	Peptide
2	12	52	ARG	Sidechain
2	12	7	ASN	Peptide
2	12	8	ASN	Peptide
2	12	860	ASP	Peptide
2	12	958	TYR	Sidechain
2	13	10	LYS	Peptide
2	13	11	LYS	Peptide
2	13	1180	GLN	Peptide
2	13	1422	ARG	Sidechain
2	13	15	LEU	Peptide
2	13	1687	ARG	Sidechain
2	13	17	LEU	Peptide
2	13	1716	TYR	Sidechain
2	13	194	GLY	Peptide
2	13	202	THR	Peptide
2	13	3	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	13	4	ILE	Peptide
2	13	414	TYR	Sidechain
2	13	5	ASN	Peptide
2	13	52	ARG	Sidechain
2	13	7	ASN	Peptide
2	13	8	ASN	Peptide
2	13	849	ARG	Sidechain
2	13	860	ASP	Peptide
2	13	958	TYR	Sidechain
2	14	10	LYS	Peptide
2	14	11	LYS	Peptide
2	14	1180	GLN	Peptide
2	14	1181	ASP	Peptide
2	14	1422	ARG	Sidechain
2	14	15	LEU	Peptide
2	14	1569	ASP	Peptide
2	14	1604	ARG	Sidechain
2	14	1657	ILE	Peptide
2	14	1687	ARG	Sidechain
2	14	17	LEU	Peptide
2	14	1716	TYR	Sidechain
2	14	194	GLY	Peptide
2	14	202	THR	Peptide
2	14	3	ILE	Peptide
2	14	370	GLY	Peptide
2	14	414	TYR	Sidechain
2	14	5	ASN	Peptide
2	14	52	ARG	Sidechain
2	14	7	ASN	Peptide
2	14	8	ASN	Peptide
2	14	846	ARG	Sidechain
2	14	860	ASP	Peptide
2	14	929	SER	Peptide
2	14	958	TYR	Sidechain
2	15	10	LYS	Peptide
2	15	11	LYS	Peptide
2	15	1180	GLN	Peptide
2	15	1422	ARG	Sidechain
2	15	15	LEU	Peptide
2	15	1687	ARG	Sidechain
2	15	17	LEU	Peptide
2	15	194	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	15	202	THR	Peptide
2	15	3	ILE	Peptide
2	15	370	GLY	Peptide
2	15	414	TYR	Sidechain
2	15	461	TYR	Sidechain
2	15	5	ASN	Peptide
2	15	52	ARG	Sidechain
2	15	7	ASN	Peptide
2	15	849	ARG	Sidechain
2	15	860	ASP	Peptide
2	15	868	TYR	Sidechain
2	15	929	SER	Peptide
2	15	955	TYR	Sidechain
2	15	958	TYR	Sidechain
2	16	10	LYS	Peptide
2	16	11	LYS	Peptide
2	16	1422	ARG	Sidechain
2	16	15	LEU	Peptide
2	16	1687	ARG	Sidechain
2	16	17	LEU	Peptide
2	16	1716	TYR	Sidechain
2	16	194	GLY	Peptide
2	16	202	THR	Peptide
2	16	3	ILE	Peptide
2	16	414	TYR	Sidechain
2	16	479	GLN	Peptide
2	16	5	ASN	Peptide
2	16	52	ARG	Sidechain
2	16	7	ASN	Peptide
2	16	8	ASN	Peptide
2	16	849	ARG	Sidechain
2	16	860	ASP	Peptide
2	16	868	TYR	Sidechain
2	16	929	SER	Peptide
2	16	958	TYR	Sidechain
2	17	10	LYS	Peptide
2	17	11	LYS	Peptide
2	17	1180	GLN	Peptide
2	17	1422	ARG	Sidechain
2	17	15	LEU	Peptide
2	17	1687	ARG	Sidechain
2	17	17	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	17	1716	TYR	Sidechain
2	17	194	GLY	Peptide
2	17	202	THR	Peptide
2	17	3	ILE	Peptide
2	17	370	GLY	Peptide
2	17	414	TYR	Sidechain
2	17	479	GLN	Peptide
2	17	5	ASN	Peptide
2	17	52	ARG	Sidechain
2	17	550	ARG	Sidechain
2	17	7	ASN	Peptide
2	17	8	ASN	Peptide
2	17	849	ARG	Sidechain
2	17	860	ASP	Peptide
2	17	958	TYR	Sidechain
3	40	256	TRP	Peptide
3	40	47	ARG	Sidechain
3	40	470	LYS	Peptide
3	41	256	TRP	Peptide
3	41	34	THR	Peptide
3	41	47	ARG	Sidechain
3	41	470	LYS	Peptide
4	A0	487	GLN	Peptide
4	A0	555	ARG	Sidechain
4	A0	794	TYR	Sidechain
4	A0	801	TYR	Sidechain
4	A0	844	TYR	Sidechain
4	A1	1	MET	Peptide
4	A1	161	HIS	Sidechain
4	A1	25	PHE	Peptide
4	A1	323	THR	Peptide
4	A1	358	LYS	Peptide
4	A1	434	TYR	Sidechain
4	A1	506	ARG	Sidechain
4	A1	508	ARG	Sidechain
4	A1	555	ARG	Sidechain
4	A1	794	TYR	Sidechain
4	A1	801	TYR	Sidechain
4	A1	844	TYR	Sidechain
4	A1	99	ASP	Peptide
4	A2	107	ILE	Peptide
4	A2	25	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	A2	323	THR	Peptide
4	A2	358	LYS	Peptide
4	A2	424	TYR	Sidechain
4	A2	434	TYR	Sidechain
4	A2	506	ARG	Sidechain
4	A2	555	ARG	Sidechain
4	A2	61	SER	Peptide
4	A2	794	TYR	Sidechain
4	A2	801	TYR	Sidechain
4	A2	841	ARG	Sidechain
4	A2	844	TYR	Sidechain
4	A3	1	MET	Peptide
4	A3	161	HIS	Sidechain
4	A3	25	PHE	Peptide
4	A3	323	THR	Peptide
4	A3	358	LYS	Peptide
4	A3	434	TYR	Sidechain
4	A3	506	ARG	Sidechain
4	A3	508	ARG	Sidechain
4	A3	555	ARG	Sidechain
4	A3	794	TYR	Sidechain
4	A3	801	TYR	Sidechain
4	A3	844	TYR	Sidechain
4	A3	894	PHE	Sidechain
4	A3	99	ASP	Peptide
4	A4	107	ILE	Peptide
4	A4	25	PHE	Peptide
4	A4	323	THR	Peptide
4	A4	434	TYR	Sidechain
4	A4	506	ARG	Sidechain
4	A4	508	ARG	Sidechain
4	A4	555	ARG	Sidechain
4	A4	801	TYR	Sidechain
4	A4	844	TYR	Sidechain
4	A5	325	TYR	Sidechain
4	A5	506	ARG	Sidechain
4	A5	519	GLU	Peptide
4	A5	555	ARG	Sidechain
4	A5	794	TYR	Sidechain
4	A5	801	TYR	Sidechain
4	A5	844	TYR	Sidechain
4	A5	901	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
5	B0	1217	ARG	Peptide
5	B0	1386	TYR	Sidechain
5	B0	1446	ARG	Sidechain
5	B0	159	LYS	Peptide
5	B0	1639	TYR	Sidechain
5	B0	174	TYR	Sidechain
5	B0	1861	TYR	Sidechain
5	B0	2061	GLU	Peptide
5	B0	217	ARG	Sidechain
5	B0	275	SER	Peptide
5	B0	321	ARG	Sidechain
5	B0	589	PHE	Sidechain
5	B0	795	TYR	Sidechain
5	B0	852	TYR	Sidechain
5	B1	1217	ARG	Peptide
5	B1	1386	TYR	Sidechain
5	B1	1446	ARG	Sidechain
5	B1	1639	TYR	Sidechain
5	B1	174	TYR	Sidechain
5	B1	1861	TYR	Sidechain
5	B1	2061	GLU	Peptide
5	B1	217	ARG	Sidechain
5	B1	275	SER	Peptide
5	B1	321	ARG	Sidechain
5	B1	589	PHE	Sidechain
5	B1	795	TYR	Sidechain
5	B1	852	TYR	Sidechain
6	C0	1014	SER	Peptide
6	C0	1081	ASN	Peptide
6	C0	1082	ASN	Peptide
6	C0	1083	VAL	Peptide
6	C0	1266	ASN	Peptide
6	C0	1267	ILE	Peptide
6	C0	1372	TYR	Sidechain
6	C0	1453	ARG	Sidechain
6	C0	1652	TYR	Sidechain
6	C0	1662	TYR	Sidechain
6	C0	459	GLN	Peptide
6	C0	628	ILE	Peptide
6	C0	703	TYR	Sidechain
6	C0	794	LEU	Peptide
6	C0	837	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	C0	982	ASN	Peptide
6	C1	1082	ASN	Peptide
6	C1	1083	VAL	Peptide
6	C1	1154	ARG	Sidechain
6	C1	1267	ILE	Peptide
6	C1	1372	TYR	Sidechain
6	C1	1453	ARG	Sidechain
6	C1	431	LYS	Peptide
6	C1	628	ILE	Peptide
6	C1	703	TYR	Sidechain
6	C1	836	ASN	Peptide
6	C1	918	ARG	Sidechain
6	C1	982	ASN	Peptide
6	C2	1014	SER	Peptide
6	C2	1016	LEU	Peptide
6	C2	1082	ASN	Peptide
6	C2	1083	VAL	Peptide
6	C2	1232	THR	Peptide
6	C2	1272	ASN	Peptide
6	C2	1372	TYR	Sidechain
6	C2	1453	ARG	Sidechain
6	C2	1662	TYR	Sidechain
6	C2	397	TYR	Sidechain
6	C2	402	ARG	Sidechain
6	C2	628	ILE	Peptide
6	C2	703	TYR	Sidechain
6	C2	918	ARG	Sidechain
6	C2	982	ASN	Peptide
6	C3	1082	ASN	Peptide
6	C3	1083	VAL	Peptide
6	C3	1267	ILE	Peptide
6	C3	1372	TYR	Sidechain
6	C3	1453	ARG	Sidechain
6	C3	1630	TYR	Sidechain
6	C3	1662	TYR	Sidechain
6	C3	295	ALA	Peptide
6	C3	420	TYR	Sidechain
6	C3	628	ILE	Peptide
6	C3	703	TYR	Sidechain
6	C3	812	PHE	Peptide
6	C3	982	ASN	Peptide
7	D0	1430	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
7	D0	1539	ARG	Sidechain
7	D0	1571	ASP	Peptide
7	D0	286	PHE	Peptide
7	D0	546	ARG	Peptide
7	D0	549	TYR	Sidechain
7	D0	587	ARG	Sidechain
7	D0	757	LYS	Peptide
7	D0	761	TYR	Sidechain
7	D0	887	ARG	Sidechain
7	D1	1413	TYR	Sidechain
7	D1	1430	TYR	Sidechain
7	D1	546	ARG	Peptide
7	D1	549	TYR	Sidechain
7	D1	887	ARG	Sidechain
7	D1	912	TYR	Sidechain
7	D2	1057	ASP	Sidechain
7	D2	1430	TYR	Sidechain
7	D2	1539	ARG	Sidechain
7	D2	1574	GLY	Peptide
7	D2	546	ARG	Peptide
7	D2	549	TYR	Sidechain
7	D2	587	ARG	Sidechain
7	D2	757	LYS	Peptide
7	D2	887	ARG	Sidechain
7	D3	1430	TYR	Sidechain
7	D3	546	ARG	Peptide
7	D3	549	TYR	Sidechain
7	D3	761	TYR	Sidechain
7	D3	779	LYS	Peptide
7	D3	887	ARG	Sidechain
7	D3	912	TYR	Sidechain
8	E0	106	TYR	Sidechain
8	E0	250	TYR	Sidechain
8	E0	267	PHE	Sidechain
8	E0	28	GLN	Peptide
8	E0	29	TYR	Peptide
8	E0	299	ARG	Sidechain
8	E0	306	TYR	Sidechain
8	E0	487	GLY	Peptide
8	E0	592	ASP	Peptide
8	E0	599	PHE	Peptide
8	E1	106	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	E1	250	TYR	Sidechain
8	E1	267	PHE	Sidechain
8	E1	28	GLN	Peptide
8	E1	29	TYR	Peptide
8	E1	299	ARG	Sidechain
8	E1	306	TYR	Sidechain
8	E1	334	GLN	Peptide
8	E1	487	GLY	Peptide
8	E1	592	ASP	Peptide
8	E1	599	PHE	Peptide
9	F0	162	ASP	Peptide
9	F0	164	LEU	Peptide
9	F0	381	TYR	Sidechain
9	F1	162	ASP	Peptide
9	F1	164	LEU	Peptide
9	F1	381	TYR	Sidechain
9	F2	162	ASP	Peptide
9	F2	164	LEU	Peptide
9	F2	381	TYR	Sidechain
9	F3	162	ASP	Peptide
9	F3	164	LEU	Peptide
9	F3	381	TYR	Sidechain
10	H0	278	ARG	Sidechain
10	H0	351	ARG	Sidechain
10	H0	357	TYR	Sidechain
10	H1	196	GLN	Peptide
10	H1	357	TYR	Sidechain
10	H2	392	TYR	Sidechain
10	H3	278	ARG	Sidechain
11	I0	266	ARG	Sidechain
11	I3	252	HIS	Sidechain
11	I3	261	PRO	Peptide
11	I3	266	ARG	Sidechain
12	J2	548	TYR	Sidechain
12	J2	617	ASN	Peptide
12	J5	548	TYR	Sidechain
13	K1	925	TYR	Sidechain
13	K2	925	TYR	Sidechain
13	K3	1023	SER	Peptide
13	K3	648	THR	Peptide
13	K3	806	PHE	Peptide
13	K3	925	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
13	K3	940	SER	Peptide
14	L0	321	ASP	Peptide
14	L0	371	ARG	Sidechain
14	L0	601	ARG	Sidechain
14	L1	239	ARG	Sidechain
14	L1	371	ARG	Sidechain
14	L1	601	ARG	Sidechain
14	L1	862	ARG	Sidechain
14	L1	890	ARG	Peptide
14	L2	239	ARG	Sidechain
14	L2	601	ARG	Sidechain
14	L2	628	GLU	Peptide
14	L2	834	ILE	Peptide
14	L2	862	ARG	Sidechain
14	L2	890	ARG	Peptide
14	L2	977	ARG	Sidechain
14	L3	239	ARG	Sidechain
14	L3	601	ARG	Sidechain
14	L3	823	TYR	Sidechain
14	L3	984	LEU	Peptide
15	M0	586	TYR	Sidechain
15	M0	642	SER	Peptide
15	M0	687	TYR	Sidechain
15	M0	690	TYR	Peptide
15	M0	697	TYR	Sidechain
15	M1	586	TYR	Sidechain
15	M1	687	TYR	Sidechain
15	M2	467	ARG	Sidechain
15	M2	586	TYR	Sidechain
15	M2	643	ASN	Peptide
15	M2	690	TYR	Peptide
15	M2	752	TYR	Sidechain
15	M2	786	TYR	Sidechain
15	M3	279	ASP	Peptide
15	M3	586	TYR	Sidechain
15	M3	642	SER	Peptide
15	M3	786	TYR	Sidechain
16	N0	113	HIS	Sidechain
16	N0	205	LEU	Peptide
16	N0	296	SER	Peptide
16	N0	79	ARG	Sidechain
16	N1	113	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
16	N1	205	LEU	Peptide
16	N1	296	SER	Peptide
16	N2	113	HIS	Sidechain
16	N2	205	LEU	Peptide
16	N2	296	SER	Peptide
16	N3	113	HIS	Sidechain
16	N3	205	LEU	Peptide
16	N3	296	SER	Peptide
17	O0	411	ASP	Peptide
17	O0	81	ARG	Sidechain
17	O1	386	LYS	Peptide
17	O2	108	ARG	Peptide
17	O2	386	LYS	Peptide
17	O2	81	ARG	Sidechain
17	O3	108	ARG	Peptide
17	O3	386	LYS	Peptide
17	O3	465	TYR	Peptide
18	P0	149	TYR	Sidechain
18	P0	161	LEU	Peptide
18	P0	715	TYR	Sidechain
18	P0	753	ASN	Peptide
18	P0	877	ARG	Sidechain
18	P1	170	ARG	Sidechain
18	P1	531	TYR	Sidechain
18	P1	754	ASN	Peptide
18	P1	755	SER	Peptide
18	P1	756	ASN	Peptide
18	P2	531	TYR	Sidechain
18	P2	750	ASN	Peptide
18	P2	755	SER	Peptide
18	P2	756	ASN	Peptide
18	P2	814	ARG	Sidechain
18	P3	531	TYR	Sidechain
18	P3	715	TYR	Sidechain
18	P3	750	ASN	Peptide
18	P3	755	SER	Peptide
18	P3	756	ASN	Peptide
18	P3	814	ARG	Sidechain
19	Q0	113	LEU	Peptide
19	Q1	140	ARG	Sidechain
19	Q1	346	TYR	Sidechain
19	Q1	364	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
19	Q1	366	GLN	Peptide
19	Q1	38	VAL	Peptide
19	Q1	411	CYS	Peptide
19	Q2	38	VAL	Peptide
19	Q3	140	ARG	Sidechain
19	Q3	38	VAL	Peptide
20	R0	11	ILE	Peptide
20	R0	1141	ARG	Sidechain
20	R0	12	GLU	Peptide
20	R0	1500	TYR	Sidechain
20	R0	1546	SER	Peptide
20	R0	1551	GLN	Peptide
20	R0	1628	GLY	Peptide
20	R0	1631	VAL	Peptide
20	R0	1694	ARG	Sidechain
20	R0	348	ASN	Peptide
20	R0	351	ASN	Peptide
20	R0	355	ILE	Peptide
20	R0	566	TYR	Sidechain
20	R0	589	TYR	Sidechain
20	R0	6	MET	Peptide
20	R0	7	ASN	Peptide
20	R0	75	SER	Peptide
20	R0	830	MET	Peptide
20	R0	883	ARG	Sidechain
20	R0	9	GLU	Peptide
20	R1	11	ILE	Peptide
20	R1	1141	ARG	Sidechain
20	R1	12	GLU	Peptide
20	R1	1498	ASN	Peptide
20	R1	1544	TYR	Sidechain
20	R1	1546	SER	Peptide
20	R1	1551	GLN	Peptide
20	R1	1601	ARG	Sidechain
20	R1	1631	VAL	Peptide
20	R1	1694	ARG	Sidechain
20	R1	355	ILE	Peptide
20	R1	553	HIS	Peptide
20	R1	671	ARG	Sidechain
20	R1	75	SER	Peptide
20	R1	783	SER	Peptide
20	R1	830	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
20	R1	883	ARG	Sidechain
20	R2	11	ILE	Peptide
20	R2	1141	ARG	Sidechain
20	R2	1163	GLU	Sidechain
20	R2	12	GLU	Peptide
20	R2	1546	SER	Peptide
20	R2	1551	GLN	Peptide
20	R2	1631	VAL	Peptide
20	R2	1694	ARG	Sidechain
20	R2	348	ASN	Peptide
20	R2	355	ILE	Peptide
20	R2	5	THR	Peptide
20	R2	7	ASN	Peptide
20	R2	75	SER	Peptide
20	R2	8	THR	Peptide
20	R2	830	MET	Peptide
20	R2	9	GLU	Peptide
20	R2	947	ASP	Peptide
20	R3	11	ILE	Peptide
20	R3	12	GLU	Peptide
20	R3	142	ASN	Peptide
20	R3	1546	SER	Peptide
20	R3	1551	GLN	Peptide
20	R3	1631	VAL	Peptide
20	R3	1645	ASP	Peptide
20	R3	1694	ARG	Sidechain
20	R3	184	SER	Peptide
20	R3	189	SER	Peptide
20	R3	348	ASN	Peptide
20	R3	355	ILE	Peptide
20	R3	6	MET	Peptide
20	R3	75	SER	Peptide
20	R3	830	MET	Peptide
20	R3	831	VAL	Peptide
20	R3	883	ARG	Sidechain
21	T0	17	PHE	Peptide
21	T0	196	TYR	Sidechain
21	T0	518	VAL	Peptide
21	T0	659	TYR	Sidechain
21	T1	1147	ASP	Peptide
21	T1	17	PHE	Peptide
21	T1	196	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	T1	216	ASP	Peptide
21	T1	238	TYR	Sidechain
21	T1	259	TYR	Sidechain
21	T1	547	ASN	Peptide
21	T1	552	SER	Peptide
21	T1	600	TYR	Sidechain
21	T1	659	TYR	Sidechain
21	T1	8	LYS	Peptide
21	T1	87	GLU	Peptide
21	T2	1147	ASP	Peptide
21	T2	17	PHE	Peptide
21	T2	196	TYR	Sidechain
21	T2	216	ASP	Peptide
21	T2	238	TYR	Sidechain
21	T2	258	GLN	Peptide
21	T2	259	TYR	Sidechain
21	T2	620	TYR	Sidechain
21	T2	659	TYR	Sidechain
21	T2	87	GLU	Peptide
21	T3	1	MET	Peptide
21	T3	11	TYR	Sidechain
21	T3	1147	ASP	Peptide
21	T3	17	PHE	Peptide
21	T3	196	TYR	Sidechain
21	T3	216	ASP	Peptide
21	T3	238	TYR	Sidechain
21	T3	259	TYR	Sidechain
21	T3	331	HIS	Sidechain
21	T3	547	ASN	Peptide
21	T3	552	SER	Peptide
21	T3	659	TYR	Sidechain
21	T3	87	GLU	Peptide
23	V0	677	ARG	Sidechain,Peptide
23	V0	750	TYR	Sidechain
23	V0	763	ASN	Peptide
23	V0	875	ARG	Sidechain
23	V1	673	TYR	Sidechain
23	V1	677	ARG	Sidechain,Peptide
23	V1	780	ARG	Sidechain
24	W0	332	THR	Peptide
24	W0	441	LYS	Peptide
24	W0	443	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
24	W0	619	LYS	Peptide
24	W0	623	ASN	Peptide
24	W0	637	ASN	Peptide
24	W0	638	LYS	Peptide
24	W0	732	ASP	Peptide
24	W0	908	ILE	Peptide
24	W1	441	LYS	Peptide
24	W1	443	HIS	Sidechain
24	W1	619	LYS	Peptide
24	W1	623	ASN	Peptide
24	W1	636	LYS	Peptide
24	W1	637	ASN	Peptide
24	W1	638	LYS	Peptide
24	W1	908	ILE	Peptide
25	X0	136	ARG	Sidechain
25	X0	350	ARG	Sidechain
25	X0	89	ARG	Sidechain
25	X1	136	ARG	Sidechain
25	X1	145	ARG	Peptide
25	X2	136	ARG	Sidechain
25	X2	145	ARG	Peptide
25	X3	102	TYR	Sidechain
25	X3	136	ARG	Sidechain
25	X3	263	TYR	Sidechain
25	X3	350	ARG	Sidechain

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	00	6455	0	6412	5	0
1	01	6455	0	6412	7	0
2	10	13985	0	14006	207	0
2	11	13985	0	14005	289	0
2	12	13985	0	14004	321	0
2	13	13985	0	14008	256	0
2	14	13985	0	14003	290	0
2	15	13985	0	14005	286	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	16	13985	0	13999	245	0
2	17	13985	0	14006	188	0
3	40	3808	0	3732	3	0
3	41	3808	0	3732	3	0
4	A0	6619	0	6534	2	0
4	A1	5782	0	5734	8	0
4	A2	5782	0	5734	5	0
4	A3	5782	0	5734	37	0
4	A4	5782	0	5734	7	0
4	A5	6200	0	6149	4	0
5	B0	16130	0	16059	10	0
5	B1	16130	0	16059	11	0
6	C0	11337	0	11328	4	0
6	C1	10779	0	10772	31	0
6	C2	10779	0	10772	8	0
6	C3	11337	0	11328	40	0
7	D0	10402	0	10363	27	0
7	D1	10402	0	10363	1	0
7	D2	10402	0	10363	3	0
7	D3	10402	0	10363	27	0
8	E0	4959	0	4988	1	0
8	E1	4959	0	4988	2	0
9	F0	783	0	779	0	0
9	F1	783	0	779	0	0
9	F2	783	0	779	0	0
9	F3	783	0	779	0	0
10	H0	2036	0	2058	0	0
10	H1	2036	0	2058	0	0
10	H2	2036	0	2058	0	0
10	H3	2036	0	2058	1	0
11	I0	1617	0	1630	2	0
11	I1	1617	0	1630	0	0
11	I2	1617	0	1630	1	0
11	I3	1617	0	1630	2	0
12	J0	1528	0	1557	2	0
12	J1	1528	0	1557	5	0
12	J2	1483	0	1513	1	0
12	J3	1483	0	1513	2	0
12	J4	1483	0	1513	1	0
12	J5	1483	0	1513	0	0
13	K0	5814	0	5920	4	0
13	K1	5814	0	5920	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K2	5814	0	5920	13	0
13	K3	5814	0	5920	4	0
14	L0	6582	0	6514	9	0
14	L1	6582	0	6513	109	0
14	L2	6582	0	6511	14	0
14	L3	6547	0	6482	2	0
15	M0	5650	0	5643	7	0
15	M1	5650	0	5638	107	0
15	M2	5650	0	5643	2	0
15	M3	5650	0	5643	3	0
16	N0	2375	0	2291	1	0
16	N1	2375	0	2291	1	0
16	N2	2375	0	2291	2	0
16	N3	2375	0	2291	3	0
17	O0	2537	0	2434	1	0
17	O1	2537	0	2434	2	0
17	O2	2537	0	2434	4	0
17	O3	2537	0	2434	2	0
18	P0	6121	0	6123	8	0
18	P1	6121	0	6123	5	0
18	P2	6121	0	6123	3	0
18	P3	6121	0	6123	4	0
19	Q0	2962	0	2898	4	0
19	Q1	2962	0	2898	37	0
19	Q2	2962	0	2898	5	0
19	Q3	2962	0	2898	3	0
20	R0	14662	0	14189	11	0
20	R1	14662	0	14189	12	0
20	R2	14662	0	14189	11	0
20	R3	14662	0	14188	38	0
21	T0	8600	0	8524	5	0
21	T1	9517	0	9352	4	0
21	T2	9517	0	9352	34	0
21	T3	9517	0	9352	4	0
22	U0	201	0	199	0	0
22	U1	201	0	199	0	0
22	U2	201	0	199	0	0
22	U3	201	0	199	0	0
23	V0	2120	0	2120	2	0
23	V1	2120	0	2120	5	0
24	W0	7264	0	7125	12	0
24	W1	7264	0	7125	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	X0	3312	0	3315	2	0
25	X1	3312	0	3315	1	0
25	X2	3312	0	3315	1	0
25	X3	3312	0	3315	2	0
All	All	579851	0	575855	1608	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 1.

All (1608) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:894:PHE:CZ	4:A3:894:PHE:CE2	1.75	1.70
6:C3:420:TYR:CG	6:C3:420:TYR:CD1	1.75	1.70
4:A3:894:PHE:CZ	4:A3:894:PHE:CE1	1.75	1.68
6:C3:420:TYR:CE2	6:C3:420:TYR:CD2	1.75	1.68
4:A3:894:PHE:CD2	4:A3:894:PHE:CG	1.74	1.67
6:C3:420:TYR:CD1	6:C3:420:TYR:CE1	1.74	1.67
6:C3:420:TYR:CE1	6:C3:420:TYR:CZ	1.75	1.64
14:L1:369:PHE:HB3	15:M1:446:LEU:CD2	1.17	1.58
2:12:1521:MET:CG	2:13:1097:HIS:CG	1.86	1.58
21:T2:629:PHE:CE1	21:T2:629:PHE:CZ	1.91	1.58
21:T2:629:PHE:CD2	21:T2:629:PHE:CG	1.92	1.58
2:10:1664:ILE:CD1	2:14:1784:ASN:HD21	1.12	1.57
21:T2:629:PHE:CE1	21:T2:629:PHE:CD1	1.90	1.57
7:D0:1575:TYR:CG	7:D0:1575:TYR:CD1	1.92	1.57
21:T2:629:PHE:CD2	21:T2:629:PHE:CE2	1.92	1.57
7:D0:1575:TYR:CZ	7:D0:1575:TYR:CE1	1.92	1.56
2:10:1593:ILE:HG22	2:14:1674:THR:CB	1.31	1.55
7:D0:1575:TYR:CD1	7:D0:1575:TYR:CE1	1.91	1.55
2:10:1593:ILE:CG2	2:14:1674:THR:CG2	1.80	1.55
2:11:1411:ASP:CB	2:12:1132:GLN:CB	1.83	1.55
7:D0:1575:TYR:CZ	7:D0:1575:TYR:CE2	1.95	1.54
2:11:818:GLN:CB	2:12:617:ASN:HD21	1.21	1.54
2:11:1699:SER:CA	2:16:1739:LYS:HE3	1.31	1.54
7:D0:1575:TYR:CG	7:D0:1575:TYR:CD2	1.91	1.54
2:11:833:LYS:CD	2:12:611:ASN:HB3	1.32	1.54
7:D0:1575:TYR:CE2	7:D0:1575:TYR:CD2	1.92	1.54
14:L1:327:ARG:HD2	15:M1:467:ARG:CZ	1.39	1.53
21:T2:629:PHE:CG	21:T2:629:PHE:CD1	1.92	1.53
2:11:833:LYS:HD3	2:12:611:ASN:CB	1.34	1.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T2:629:PHE:CZ	21:T2:629:PHE:CE2	1.93	1.53
2:11:1411:ASP:CB	2:12:1132:GLN:HB2	1.06	1.52
2:10:1593:ILE:CG2	2:14:1674:THR:HG22	1.31	1.52
2:12:833:LYS:HD3	2:13:711:ARG:CD	1.36	1.50
2:12:1521:MET:HG2	2:13:1097:HIS:CG	1.01	1.50
14:L1:323:ASP:CB	15:M1:428:ARG:HD3	1.40	1.48
2:11:818:GLN:HB3	2:12:617:ASN:ND2	1.22	1.44
2:14:295:ARG:NH2	2:15:473:GLU:HG3	1.30	1.44
2:12:1521:MET:CG	2:13:1097:HIS:CD2	1.99	1.43
2:15:1205:VAL:HG11	2:15:1565:LEU:N	1.19	1.43
2:10:819:GLN:HB3	2:11:615:ASP:CG	1.35	1.43
2:12:1521:MET:HG2	2:13:1097:HIS:CB	1.47	1.42
14:L1:369:PHE:CB	15:M1:446:LEU:HD22	1.49	1.42
14:L1:323:ASP:N	15:M1:428:ARG:CD	1.78	1.42
2:12:1522:PRO:C	2:13:1144:THR:CG2	1.88	1.42
2:10:822:GLN:NE2	2:11:614:ASN:HD21	1.13	1.42
2:14:735:ASN:HD21	2:15:840:ILE:CD1	1.32	1.42
2:14:1143:LYS:CB	2:15:1159:VAL:HB	1.38	1.42
2:14:1143:LYS:HB3	2:15:1159:VAL:CB	1.46	1.41
2:12:1065:GLN:CD	2:13:1037:GLN:HE22	1.20	1.41
2:12:1523:HIS:N	2:13:1144:THR:CG2	1.81	1.41
2:11:1699:SER:CA	2:16:1739:LYS:CE	1.98	1.40
2:15:1205:VAL:CB	2:15:1564:SER:HB2	1.51	1.40
2:10:1664:ILE:HD12	2:14:1784:ASN:ND2	1.34	1.40
2:15:1205:VAL:CG1	2:15:1565:LEU:H	1.34	1.39
2:16:1178:ILE:CG2	2:17:1345:SER:O	1.67	1.39
2:12:1065:GLN:NE2	2:13:1037:GLN:CD	1.76	1.39
2:14:735:ASN:CG	2:15:840:ILE:HB	1.42	1.38
14:L1:323:ASP:HB3	15:M1:428:ARG:CB	1.51	1.38
2:10:1593:ILE:HG22	2:14:1674:THR:CG2	0.91	1.38
2:11:1699:SER:HA	2:16:1739:LYS:CE	1.49	1.38
13:K2:889:SER:HB2	14:L2:847:ARG:NH2	1.05	1.37
2:11:818:GLN:CB	2:12:617:ASN:ND2	1.82	1.37
2:11:1412:LYS:NZ	2:12:1094:ILE:N	1.70	1.37
14:L1:373:GLN:CG	15:M1:446:LEU:HD12	1.54	1.37
2:14:735:ASN:ND2	2:15:840:ILE:HD12	1.37	1.36
14:L1:369:PHE:CB	15:M1:446:LEU:CD2	2.02	1.36
2:11:1102:ASN:ND2	2:14:1425:ARG:HH11	1.25	1.35
2:11:1102:ASN:ND2	2:14:1425:ARG:NH1	1.74	1.35
2:11:1411:ASP:CG	2:12:1132:GLN:CB	1.77	1.34
2:14:295:ARG:CZ	2:15:473:GLU:CG	2.04	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:11:1411:ASP:OD1	2:12:1132:GLN:CB	1.73	1.34
2:11:1412:LYS:HZ3	2:12:1094:ILE:N	0.85	1.34
2:12:833:LYS:NZ	2:13:711:ARG:NH1	1.73	1.34
2:14:295:ARG:CZ	2:15:473:GLU:HG3	1.57	1.34
2:11:1366:ASN:ND2	2:12:1139:SER:OG	1.59	1.33
2:11:1699:SER:HB3	2:16:1739:LYS:CG	1.58	1.33
2:11:1406:LYS:NZ	2:14:1405:ASN:HB2	1.42	1.33
2:14:735:ASN:CB	2:15:840:ILE:HB	1.59	1.32
2:14:1178:ILE:HG22	2:15:1269:ASN:CG	1.33	1.31
2:10:1469:ASP:HB2	2:11:1099:ASP:O	1.19	1.31
13:K2:889:SER:CB	14:L2:847:ARG:NH2	1.93	1.31
2:11:1406:LYS:HZ1	2:14:1405:ASN:CB	1.42	1.31
2:11:1412:LYS:HZ3	2:12:1093:ASN:C	1.31	1.31
2:14:613:ASN:ND2	2:15:819:GLN:OE1	1.60	1.31
2:11:1699:SER:CB	2:16:1739:LYS:HE2	1.59	1.30
2:16:211:PRO:HG3	2:17:331:LEU:CD1	1.62	1.30
2:11:1102:ASN:HD21	2:14:1425:ARG:NH1	1.28	1.30
14:L1:319:GLU:HG2	15:M1:463:ILE:CG1	1.60	1.30
2:12:833:LYS:HZ2	2:13:711:ARG:NH1	1.25	1.29
14:L1:323:ASP:CA	15:M1:428:ARG:HD3	1.60	1.29
2:11:1412:LYS:NZ	2:12:1093:ASN:C	1.85	1.29
2:14:295:ARG:NH1	2:15:473:GLU:CG	1.95	1.29
2:11:822:GLN:HE22	2:12:617:ASN:CB	1.44	1.29
2:16:622:SER:OG	2:17:823:SER:HB3	1.30	1.29
2:12:1523:HIS:HB2	2:13:1126:THR:CG2	1.62	1.28
14:L1:323:ASP:CB	15:M1:428:ARG:CD	2.12	1.28
2:10:1664:ILE:CD1	2:14:1784:ASN:ND2	1.91	1.28
2:10:1668:LYS:NZ	2:14:1752:ASN:HB2	1.48	1.28
2:11:1412:LYS:CE	2:12:1093:ASN:O	1.81	1.28
2:16:211:PRO:CG	2:17:331:LEU:CD1	2.09	1.28
2:11:1412:LYS:N	2:12:1095:ILE:HD12	1.46	1.27
2:12:833:LYS:CD	2:13:711:ARG:HD3	1.62	1.27
2:13:1745:ARG:HD2	2:17:1699:SER:OG	1.20	1.27
2:16:211:PRO:CG	2:17:331:LEU:HD11	1.62	1.27
2:15:614:ASN:O	2:16:833:LYS:HD2	1.29	1.27
2:15:1241:LYS:O	2:15:1269:ASN:ND2	1.66	1.27
2:11:1411:ASP:OD1	2:12:1132:GLN:HB3	1.09	1.26
2:11:1717:GLN:HB2	2:15:1754:GLN:OE1	1.29	1.26
2:11:1699:SER:CB	2:16:1739:LYS:CE	2.13	1.25
14:L1:373:GLN:CG	15:M1:446:LEU:CD1	2.14	1.25
2:10:1701:ASP:HB2	2:14:1746:GLN:OE1	1.31	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:735:ASN:ND2	2:15:840:ILE:CD1	1.94	1.25
2:11:833:LYS:CG	2:12:611:ASN:O	1.84	1.25
2:11:1411:ASP:HB3	2:12:1132:GLN:CB	1.46	1.25
2:16:619:GLY:CA	2:17:816:GLN:HA	1.64	1.24
2:11:818:GLN:CA	2:12:617:ASN:HD21	1.50	1.24
14:L1:319:GLU:CG	15:M1:463:ILE:HG12	1.67	1.24
2:10:822:GLN:CD	2:11:614:ASN:ND2	1.92	1.24
2:14:1178:ILE:CG2	2:15:1269:ASN:CG	2.06	1.24
2:10:1593:ILE:C	2:14:1674:THR:CG2	2.07	1.22
14:L1:319:GLU:CD	15:M1:463:ILE:HG12	1.60	1.22
2:11:1398:ASP:O	2:12:1095:ILE:HG12	1.37	1.22
2:12:820:GLN:NE2	2:13:613:ASN:ND2	1.85	1.22
2:12:834:LYS:O	2:13:712:LYS:CE	1.88	1.21
2:14:1178:ILE:CG2	2:15:1269:ASN:OD1	1.88	1.21
2:16:611:ASN:HD21	2:17:833:LYS:CG	1.52	1.21
2:11:833:LYS:HG2	2:12:611:ASN:O	1.03	1.21
2:13:1745:ARG:CD	2:17:1699:SER:OG	1.87	1.21
2:16:1097:HIS:CE1	2:17:1523:HIS:CE1	2.29	1.21
2:10:822:GLN:OE1	2:11:614:ASN:ND2	1.74	1.21
2:12:834:LYS:O	2:13:712:LYS:HE3	1.33	1.21
14:L1:373:GLN:HG2	15:M1:446:LEU:CD1	1.68	1.21
2:10:1593:ILE:CG2	2:14:1674:THR:CB	2.06	1.21
14:L1:327:ARG:CD	15:M1:467:ARG:CZ	2.18	1.21
2:14:735:ASN:CG	2:15:840:ILE:CB	2.09	1.20
2:10:819:GLN:CD	2:11:614:ASN:C	1.95	1.19
2:11:1413:ILE:HG13	2:12:1097:HIS:CE1	1.77	1.19
2:10:819:GLN:NE2	2:11:614:ASN:O	1.74	1.19
2:12:1523:HIS:CA	2:13:1144:THR:HG21	1.71	1.19
14:L1:319:GLU:OE2	15:M1:463:ILE:HG12	1.38	1.19
2:11:1412:LYS:CE	2:12:1093:ASN:C	2.11	1.19
13:K2:889:SER:CB	14:L2:847:ARG:HH22	1.52	1.19
2:10:1668:LYS:NZ	2:14:1752:ASN:CB	1.92	1.19
2:15:1205:VAL:HG21	2:15:1565:LEU:O	1.37	1.19
2:16:1097:HIS:NE2	2:17:1523:HIS:NE2	1.89	1.19
2:11:1717:GLN:CB	2:15:1754:GLN:OE1	1.90	1.18
2:14:1494:SER:CB	2:15:1288:LEU:HD11	1.72	1.18
2:14:1143:LYS:HG2	2:15:1159:VAL:N	1.53	1.18
2:10:1668:LYS:HZ1	2:14:1752:ASN:CB	1.52	1.17
2:12:1522:PRO:HD2	2:13:1128:SER:OG	1.43	1.17
2:16:1097:HIS:NE2	2:17:1523:HIS:CE1	2.13	1.17
2:11:1411:ASP:HB3	2:12:1132:GLN:CA	1.75	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:614:ASN:OD1	2:15:816:GLN:NE2	1.78	1.16
2:12:1523:HIS:CB	2:13:1126:THR:HG22	1.76	1.16
4:A3:894:PHE:CZ	7:D3:1464:LYS:CE	2.28	1.16
2:11:822:GLN:NE2	2:12:617:ASN:CB	2.09	1.16
2:10:1579:SER:HB3	2:14:1676:PHE:CD1	1.78	1.16
2:10:1701:ASP:CB	2:14:1746:GLN:OE1	1.91	1.15
2:11:1411:ASP:CA	2:12:1132:GLN:HB2	1.77	1.15
2:12:833:LYS:CD	2:13:711:ARG:CD	2.18	1.15
2:15:1096:PRO:CD	2:16:1412:LYS:NZ	2.09	1.15
4:A3:894:PHE:CD2	7:D3:1464:LYS:CE	2.30	1.15
14:L1:323:ASP:CA	15:M1:428:ARG:CD	2.20	1.15
2:10:1706:TYR:OH	2:14:1786:LEU:CD1	1.95	1.15
2:11:822:GLN:NE2	2:12:617:ASN:HB3	1.59	1.15
6:C3:420:TYR:CD1	19:Q1:382:GLN:CB	2.30	1.15
6:C3:420:TYR:CD2	19:Q1:382:GLN:CG	2.30	1.15
2:11:1412:LYS:HE2	2:12:1093:ASN:O	1.01	1.14
2:14:295:ARG:CZ	2:15:473:GLU:CD	2.12	1.14
2:11:1411:ASP:CG	2:12:1132:GLN:HB2	1.48	1.14
2:14:735:ASN:ND2	2:15:840:ILE:CB	2.11	1.14
2:16:618:GLY:O	2:17:816:GLN:HG2	1.46	1.14
2:10:822:GLN:CD	2:11:614:ASN:HD21	1.50	1.14
4:A3:894:PHE:CE1	7:D3:1464:LYS:CD	2.30	1.14
6:C3:420:TYR:CE1	19:Q1:382:GLN:CG	2.30	1.14
6:C3:420:TYR:CZ	19:Q1:382:GLN:CB	2.31	1.14
4:A3:894:PHE:CE2	7:D3:1464:LYS:CE	2.29	1.14
6:C3:420:TYR:CE1	19:Q1:382:GLN:CB	2.30	1.14
14:L1:323:ASP:HB3	15:M1:428:ARG:CD	1.74	1.14
2:12:1522:PRO:C	2:13:1144:THR:HG21	1.56	1.14
4:A3:894:PHE:CE1	7:D3:1464:LYS:CE	2.30	1.14
14:L1:386:SER:HB3	15:M1:439:SER:OG	1.47	1.14
2:10:1706:TYR:OH	2:14:1786:LEU:HD13	1.47	1.13
2:12:1523:HIS:N	2:13:1144:THR:HG21	1.49	1.13
2:14:735:ASN:CG	2:15:840:ILE:CG1	2.17	1.13
6:C3:420:TYR:CE2	19:Q1:382:GLN:CG	2.32	1.13
6:C3:420:TYR:CZ	19:Q1:382:GLN:CG	2.30	1.13
4:A3:894:PHE:CE2	7:D3:1464:LYS:CD	2.31	1.13
4:A3:894:PHE:CD2	7:D3:1464:LYS:CD	2.32	1.13
6:C3:420:TYR:CE2	19:Q1:382:GLN:CB	2.31	1.13
4:A3:894:PHE:CD1	7:D3:1464:LYS:CE	2.31	1.13
6:C3:420:TYR:CD1	19:Q1:382:GLN:CG	2.31	1.13
4:A3:894:PHE:CZ	7:D3:1464:LYS:CD	2.30	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:894:PHE:CG	7:D3:1464:LYS:CD	2.32	1.12
4:A3:894:PHE:CG	7:D3:1464:LYS:CE	2.30	1.12
4:A3:894:PHE:CD1	7:D3:1464:LYS:CD	2.31	1.12
14:L1:323:ASP:HB3	15:M1:428:ARG:CG	1.78	1.12
2:11:1697:THR:HG21	2:16:1817:THR:O	1.47	1.12
2:11:1699:SER:HB2	2:16:1739:LYS:CE	1.78	1.12
6:C3:420:TYR:CG	19:Q1:382:GLN:CG	2.32	1.12
6:C3:420:TYR:CD2	19:Q1:382:GLN:CB	2.32	1.12
6:C3:420:TYR:CG	19:Q1:382:GLN:CB	2.31	1.12
2:10:819:GLN:CD	2:11:614:ASN:O	1.87	1.12
2:10:1593:ILE:CG2	2:14:1674:THR:HB	1.74	1.12
2:15:1096:PRO:HD3	2:16:1412:LYS:HZ3	1.02	1.12
2:16:1178:ILE:CD1	2:17:1347:GLN:HG3	1.78	1.12
2:14:735:ASN:HB3	2:15:840:ILE:HB	1.31	1.11
2:15:1096:PRO:CD	2:16:1412:LYS:HZ3	1.60	1.11
2:14:295:ARG:NH1	2:15:473:GLU:CD	2.04	1.11
2:12:1521:MET:HG3	2:13:1097:HIS:CD2	1.85	1.11
14:L1:327:ARG:HD2	15:M1:467:ARG:NH2	1.65	1.11
2:11:1699:SER:CB	2:16:1739:LYS:CG	2.28	1.11
2:14:735:ASN:ND2	2:15:840:ILE:HB	1.65	1.11
2:15:1205:VAL:HG11	2:15:1564:SER:C	1.70	1.11
14:L1:373:GLN:HG2	15:M1:446:LEU:HD11	1.33	1.11
2:10:1715:THR:OG1	2:14:1671:THR:OG1	1.69	1.10
2:16:171:LYS:HE3	2:17:465:LEU:HD21	1.19	1.10
14:L1:323:ASP:N	15:M1:428:ARG:HD3	1.49	1.10
6:C1:1269:ASN:CG	7:D0:1575:TYR:CD2	2.24	1.10
20:R3:188:GLY:C	21:T2:629:PHE:CD2	2.25	1.10
6:C1:1269:ASN:CG	7:D0:1575:TYR:CE1	2.25	1.10
2:12:1522:PRO:C	2:13:1144:THR:HG23	1.61	1.10
2:16:611:ASN:HD21	2:17:833:LYS:HG2	1.03	1.10
2:16:1178:ILE:HG22	2:17:1345:SER:O	1.40	1.10
2:11:818:GLN:C	2:12:617:ASN:ND2	2.05	1.09
14:L1:369:PHE:HB3	15:M1:446:LEU:HD21	1.17	1.09
14:L1:323:ASP:HB3	15:M1:428:ARG:HB3	1.28	1.09
2:16:622:SER:OG	2:17:823:SER:CB	1.99	1.09
20:R3:188:GLY:C	21:T2:629:PHE:CD1	2.25	1.09
20:R3:188:GLY:C	21:T2:629:PHE:CE1	2.25	1.09
2:11:822:GLN:CD	2:12:617:ASN:HB3	1.72	1.09
2:12:1101:PRO:HG2	2:15:1424:GLY:O	1.52	1.09
6:C1:1269:ASN:CG	7:D0:1575:TYR:CD1	2.25	1.09
6:C1:1269:ASN:ND2	7:D0:1575:TYR:CG	2.20	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:15:1095:ILE:N	2:16:1411:ASP:OD2	1.61	1.08
20:R3:188:GLY:C	21:T2:629:PHE:CG	2.26	1.08
2:11:1404:ASP:OD1	2:14:1406:LYS:HE3	1.52	1.08
2:15:1205:VAL:CG1	2:15:1565:LEU:N	2.02	1.08
2:16:619:GLY:HA2	2:17:816:GLN:HA	1.33	1.08
20:R3:188:GLY:C	21:T2:629:PHE:CE2	2.27	1.08
6:C1:1269:ASN:CG	7:D0:1575:TYR:CG	2.26	1.08
2:14:1178:ILE:HG22	2:15:1269:ASN:OD1	0.92	1.08
2:15:1096:PRO:HD2	2:16:1412:LYS:NZ	1.63	1.08
2:15:1205:VAL:HB	2:15:1564:SER:CB	1.83	1.08
2:12:1523:HIS:HB2	2:13:1126:THR:HG22	1.30	1.07
2:14:1223:PRO:HB2	2:15:1210:GLY:HA2	1.36	1.07
6:C1:1269:ASN:ND2	7:D0:1575:TYR:CD2	2.23	1.07
6:C1:1269:ASN:ND2	7:D0:1575:TYR:CD1	2.21	1.07
14:L1:386:SER:HB3	15:M1:439:SER:CB	1.84	1.07
20:R3:189:SER:N	21:T2:629:PHE:CG	2.22	1.07
2:11:822:GLN:OE1	2:12:617:ASN:HB3	1.51	1.07
2:16:1178:ILE:HG23	2:17:1345:SER:O	1.36	1.07
6:C1:1269:ASN:ND2	7:D0:1575:TYR:CE1	2.23	1.07
2:10:1664:ILE:HD11	2:14:1784:ASN:HD21	1.20	1.07
2:10:819:GLN:CB	2:11:615:ASP:CG	2.23	1.06
6:C1:1269:ASN:ND2	7:D0:1575:TYR:CE2	2.24	1.06
2:10:822:GLN:NE2	2:11:614:ASN:ND2	1.97	1.06
2:12:1521:MET:SD	2:13:1097:HIS:CD2	2.47	1.06
2:12:1523:HIS:HA	2:13:1144:THR:HG21	1.37	1.06
6:C1:1269:ASN:ND2	7:D0:1575:TYR:CZ	2.23	1.06
20:R3:188:GLY:C	21:T2:629:PHE:CZ	2.28	1.06
2:11:1699:SER:CB	2:16:1739:LYS:HG2	1.85	1.06
2:14:735:ASN:OD1	2:15:840:ILE:HG13	1.55	1.06
6:C1:1269:ASN:CG	7:D0:1575:TYR:CE2	2.27	1.06
2:15:614:ASN:O	2:16:833:LYS:CD	2.02	1.05
2:10:822:GLN:OE1	2:11:614:ASN:CG	1.95	1.05
2:12:1068:ASP:OD2	2:13:1037:GLN:HG2	1.53	1.05
6:C1:1269:ASN:CG	7:D0:1575:TYR:CZ	2.29	1.05
20:R3:189:SER:N	21:T2:629:PHE:CD1	2.23	1.05
2:11:1398:ASP:O	2:12:1095:ILE:CG1	2.04	1.05
2:12:834:LYS:HG2	2:13:712:LYS:NZ	1.70	1.05
2:14:613:ASN:ND2	2:15:819:GLN:CD	2.09	1.05
2:13:1351:ILE:HD13	2:17:1425:ARG:NH1	1.70	1.05
2:14:295:ARG:NH1	2:15:473:GLU:HG2	1.71	1.05
2:15:1205:VAL:CG1	2:15:1564:SER:HB2	1.86	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:11:822:GLN:HE22	2:12:617:ASN:HB2	1.13	1.04
20:R3:189:SER:N	21:T2:629:PHE:CE1	2.25	1.04
2:13:984:LYS:HE2	2:15:1395:SER:OG	1.56	1.04
2:16:171:LYS:HE3	2:17:465:LEU:CD2	1.87	1.04
20:R3:189:SER:N	21:T2:629:PHE:CD2	2.24	1.04
2:11:1412:LYS:HA	2:12:1130:THR:HB	1.36	1.04
2:13:1744:PRO:HG2	2:17:1783:LEU:CD2	1.88	1.04
20:R3:189:SER:N	21:T2:629:PHE:CZ	2.25	1.03
2:10:819:GLN:HB3	2:11:615:ASP:OD1	1.55	1.03
2:10:1351:ILE:HD13	2:14:1425:ARG:NH1	1.72	1.03
2:16:1178:ILE:HD11	2:17:1347:GLN:CG	1.88	1.03
20:R3:189:SER:N	21:T2:629:PHE:CE2	2.26	1.03
2:11:1411:ASP:CB	2:12:1132:GLN:CA	2.23	1.03
2:12:1351:ILE:HD13	2:16:1425:ARG:NH1	1.71	1.03
2:16:1097:HIS:CE1	2:17:1523:HIS:ND1	2.26	1.03
14:L1:323:ASP:CG	15:M1:428:ARG:HD3	1.77	1.03
2:16:211:PRO:HG3	2:17:331:LEU:HD12	1.05	1.02
2:10:1701:ASP:CG	2:14:1746:GLN:OE1	1.97	1.02
14:L1:323:ASP:CB	15:M1:428:ARG:HB3	1.88	1.02
2:12:1068:ASP:CG	2:13:1037:GLN:HG2	1.80	1.02
2:15:1130:THR:O	2:16:1411:ASP:OD2	1.78	1.02
2:12:1522:PRO:O	2:13:1144:THR:HG21	1.56	1.02
2:14:1101:PRO:HD2	2:15:1523:HIS:HB3	1.39	1.02
2:12:1065:GLN:HE22	2:13:1037:GLN:CD	1.43	1.01
2:11:1699:SER:HA	2:16:1739:LYS:CD	1.90	1.01
2:11:1699:SER:N	2:16:1739:LYS:HG3	1.75	1.01
2:12:834:LYS:HG2	2:13:712:LYS:HZ1	1.23	1.01
2:12:1523:HIS:N	2:13:1144:THR:HG22	1.70	1.01
2:13:1744:PRO:HG2	2:17:1783:LEU:HD21	1.04	1.01
2:11:1699:SER:C	2:16:1739:LYS:HE3	1.81	1.01
2:16:211:PRO:HG2	2:17:331:LEU:CD1	1.80	1.01
2:11:818:GLN:C	2:12:617:ASN:HD21	1.61	1.00
2:11:1412:LYS:HE2	2:12:1093:ASN:C	1.74	1.00
2:10:819:GLN:CB	2:11:615:ASP:OD2	2.10	1.00
2:10:1593:ILE:HG23	2:14:1674:THR:HG22	1.40	1.00
2:11:1351:ILE:HD13	2:15:1425:ARG:NH1	1.76	1.00
2:12:509:GLU:OE1	2:13:297:ILE:HG21	1.61	1.00
2:16:618:GLY:C	2:17:816:GLN:HG2	1.82	1.00
2:10:1593:ILE:C	2:14:1674:THR:HG21	1.76	1.00
2:12:1523:HIS:CA	2:13:1144:THR:CG2	2.35	1.00
2:14:1143:LYS:HG2	2:15:1159:VAL:H	1.20	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1664:ILE:HD12	2:14:1784:ASN:CG	1.82	0.99
2:13:984:LYS:HB3	2:15:1397:LYS:HB3	1.41	0.99
2:10:1469:ASP:CB	2:11:1099:ASP:O	2.09	0.99
2:16:619:GLY:HA3	2:17:819:GLN:HB2	1.45	0.99
2:10:1593:ILE:HG22	2:14:1674:THR:HG21	1.41	0.99
2:10:1593:ILE:HG21	2:14:1674:THR:HB	1.41	0.99
2:12:836:LYS:HE3	2:13:712:LYS:HB3	1.44	0.99
2:11:1102:ASN:HD21	2:14:1425:ARG:CZ	1.76	0.99
14:L1:319:GLU:HG2	15:M1:463:ILE:HG13	1.40	0.99
2:11:1406:LYS:HZ1	2:14:1405:ASN:HB2	0.87	0.98
13:K2:889:SER:HB2	14:L2:847:ARG:HH21	1.22	0.98
2:11:819:GLN:HG3	2:12:617:ASN:OD1	1.62	0.98
14:L1:323:ASP:N	15:M1:428:ARG:HD2	1.78	0.98
2:16:622:SER:CB	2:17:823:SER:HB3	1.92	0.98
2:10:1757:SER:HA	2:14:1745:ARG:HH22	1.24	0.98
6:C3:420:TYR:CE2	19:Q1:382:GLN:HG2	1.97	0.98
2:12:1426:MET:CE	2:15:1101:PRO:HG3	1.93	0.98
2:16:211:PRO:HG2	2:17:331:LEU:HD11	0.98	0.98
2:16:228:SER:HB3	2:17:331:LEU:O	1.62	0.98
2:14:735:ASN:OD1	2:15:840:ILE:CG1	2.12	0.98
2:14:735:ASN:ND2	2:15:840:ILE:CG1	2.26	0.98
2:10:1717:GLN:HE22	2:14:1784:ASN:C	1.65	0.98
2:11:1699:SER:CA	2:16:1739:LYS:HG3	1.94	0.98
2:16:1178:ILE:HD11	2:17:1347:GLN:CD	1.83	0.98
2:15:1132:GLN:NE2	2:16:1366:ASN:HB3	1.77	0.97
14:L1:323:ASP:CB	15:M1:428:ARG:CB	2.41	0.97
2:11:1413:ILE:CG1	2:12:1097:HIS:CE1	2.33	0.97
6:C3:420:TYR:CE1	19:Q1:382:GLN:HG3	1.99	0.97
2:12:1521:MET:HG2	2:13:1097:HIS:CD2	1.72	0.97
2:16:213:ARG:CD	2:17:394:ALA:HB2	1.94	0.97
6:C3:420:TYR:CG	19:Q1:382:GLN:HB2	2.00	0.97
2:10:822:GLN:HE22	2:11:614:ASN:HD21	1.09	0.97
4:A3:894:PHE:CZ	7:D3:1464:LYS:HE2	1.95	0.97
14:L1:319:GLU:CG	15:M1:463:ILE:CG1	2.35	0.96
2:12:1521:MET:HG2	2:13:1097:HIS:HB3	1.45	0.96
2:10:1717:GLN:NE2	2:14:1784:ASN:O	1.98	0.96
2:15:1205:VAL:HB	2:15:1564:SER:HB2	0.96	0.96
4:A3:894:PHE:CD1	7:D3:1464:LYS:HD3	1.98	0.96
2:14:1143:LYS:CG	2:15:1159:VAL:N	2.14	0.96
2:14:613:ASN:CG	2:15:819:GLN:OE1	2.03	0.95
2:11:1404:ASP:HA	2:14:1406:LYS:CE	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1664:ILE:HD12	2:14:1784:ASN:HD21	0.88	0.95
2:11:1412:LYS:NZ	2:12:1094:ILE:C	2.19	0.95
2:15:1205:VAL:HG11	2:15:1564:SER:CA	1.96	0.95
2:16:611:ASN:ND2	2:17:833:LYS:HG2	1.80	0.95
2:10:819:GLN:HB3	2:11:615:ASP:OD2	1.67	0.95
2:13:1746:GLN:OE1	2:17:1670:SER:HA	1.66	0.95
2:16:213:ARG:NE	2:17:394:ALA:HB2	1.80	0.95
2:12:1521:MET:CG	2:13:1097:HIS:HB3	1.94	0.95
2:13:1746:GLN:HE22	2:17:1670:SER:CA	1.80	0.94
14:L1:319:GLU:OE2	15:M1:463:ILE:CG1	2.15	0.94
2:10:1579:SER:CB	2:14:1676:PHE:CD1	2.51	0.94
14:L1:373:GLN:HG3	15:M1:446:LEU:CD1	1.82	0.94
2:12:1522:PRO:O	2:13:1144:THR:CG2	2.12	0.94
2:10:1668:LYS:HZ3	2:14:1752:ASN:HB2	1.13	0.94
14:L1:299:LEU:HD11	15:M1:457:ASN:HB3	1.47	0.94
2:14:1101:PRO:CD	2:15:1523:HIS:HB3	1.98	0.94
2:16:619:GLY:HA3	2:17:816:GLN:HA	1.50	0.94
14:L1:369:PHE:HB3	15:M1:446:LEU:HD22	1.06	0.93
2:10:1469:ASP:HB2	2:11:1099:ASP:C	1.89	0.93
2:15:1132:GLN:HE22	2:16:1366:ASN:HB3	1.28	0.93
2:16:172:ASP:OD1	2:17:465:LEU:HD22	1.69	0.93
2:11:1699:SER:CA	2:16:1739:LYS:CG	2.46	0.93
2:15:1096:PRO:O	2:16:1412:LYS:HB3	1.69	0.93
2:11:1412:LYS:H	2:12:1095:ILE:HD12	1.22	0.93
2:12:1359:THR:HG21	2:16:1356:ILE:HG23	1.51	0.93
2:12:1519:LYS:NZ	2:13:1139:SER:OG	2.01	0.92
2:10:1717:GLN:HE21	2:14:1754:GLN:NE2	1.68	0.92
2:13:1351:ILE:HD13	2:17:1425:ARG:HH12	1.32	0.92
14:L1:386:SER:CB	15:M1:503:GLU:OE2	2.18	0.92
2:12:833:LYS:CG	2:13:711:ARG:HD2	2.01	0.91
2:10:1717:GLN:HB3	2:14:1754:GLN:NE2	1.85	0.91
2:12:1351:ILE:HD13	2:16:1425:ARG:HH12	1.33	0.91
2:12:1404:ASP:OD1	2:14:1137:SER:O	1.86	0.91
2:16:1097:HIS:CE1	2:17:1523:HIS:CG	2.58	0.91
4:A3:894:PHE:CD2	7:D3:1464:LYS:HE3	2.02	0.91
6:C3:420:TYR:CE2	19:Q1:382:GLN:HB3	2.05	0.91
14:L1:369:PHE:HB2	15:M1:446:LEU:HD22	1.49	0.91
2:10:1338:LYS:NZ	2:11:1197:ARG:HH12	1.68	0.91
2:10:1594:ALA:N	2:14:1674:THR:HG21	1.83	0.91
6:C3:420:TYR:CD2	19:Q1:382:GLN:HB3	2.03	0.91
2:11:832:ILE:O	2:12:614:ASN:ND2	2.03	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:11:1699:SER:HB3	2:16:1739:LYS:HG2	0.92	0.91
2:11:1783:LEU:HD21	2:16:1752:ASN:HB3	1.52	0.91
2:11:1366:ASN:OD1	2:12:1132:GLN:NE2	2.04	0.91
2:12:820:GLN:NE2	2:13:613:ASN:HD21	1.63	0.91
2:16:1178:ILE:CD1	2:17:1347:GLN:CG	2.45	0.91
6:C3:420:TYR:CD1	19:Q1:382:GLN:HB2	2.07	0.90
2:11:1412:LYS:HZ2	2:12:1094:ILE:C	1.73	0.90
2:15:1130:THR:CB	2:16:1411:ASP:O	2.19	0.90
2:16:213:ARG:NH1	2:17:357:PRO:O	2.05	0.90
2:11:1699:SER:HB2	2:16:1739:LYS:HE2	0.91	0.90
2:13:1744:PRO:CG	2:17:1783:LEU:HD21	1.98	0.90
4:A3:894:PHE:CD2	7:D3:1464:LYS:HD2	2.03	0.90
2:12:834:LYS:C	2:13:712:LYS:HE3	1.92	0.90
14:L1:373:GLN:NE2	15:M1:442:SER:HB2	1.87	0.90
2:11:1354:ILE:O	2:15:1430:LYS:HG3	1.71	0.90
2:12:835:GLN:C	2:13:712:LYS:HE2	1.92	0.90
2:15:1205:VAL:HG13	2:15:1565:LEU:H	1.35	0.90
2:12:1523:HIS:CB	2:13:1126:THR:CG2	2.40	0.90
2:15:1205:VAL:CG2	2:15:1565:LEU:O	2.20	0.90
2:14:295:ARG:NH2	2:15:473:GLU:CG	2.21	0.90
2:12:834:LYS:C	2:13:712:LYS:CE	2.39	0.89
4:A3:894:PHE:CE2	7:D3:1464:LYS:HE3	2.02	0.89
14:L1:321:ASP:HA	15:M1:450:GLN:OE1	1.72	0.89
14:L1:373:GLN:HG3	15:M1:446:LEU:HD12	0.91	0.89
2:15:1205:VAL:CG1	2:15:1564:SER:CA	2.50	0.89
2:11:1398:ASP:O	2:12:1095:ILE:CD1	2.21	0.89
2:13:1359:THR:HG21	2:17:1356:ILE:HG23	1.51	0.89
2:16:617:ASN:O	2:17:819:GLN:NE2	2.05	0.89
14:L1:322:PRO:HD3	15:M1:450:GLN:OE1	1.71	0.89
20:R3:188:GLY:HA2	21:T2:629:PHE:CZ	2.07	0.89
2:11:1102:ASN:ND2	2:14:1425:ARG:HD2	1.88	0.89
2:11:1412:LYS:N	2:12:1095:ILE:CD1	2.34	0.89
2:16:228:SER:CB	2:17:331:LEU:O	2.20	0.89
2:12:836:LYS:HE3	2:13:712:LYS:CB	1.95	0.89
2:14:295:ARG:HH12	2:15:473:GLU:HG2	1.32	0.89
2:12:820:GLN:NE2	2:13:613:ASN:CG	2.25	0.89
6:C1:1269:ASN:CB	7:D0:1575:TYR:CG	2.55	0.89
2:10:1359:THR:HG21	2:14:1356:ILE:HG23	1.55	0.88
2:10:1717:GLN:HE22	2:14:1784:ASN:CA	1.85	0.88
2:11:818:GLN:HB3	2:12:617:ASN:HD22	1.36	0.88
14:L1:323:ASP:CA	15:M1:428:ARG:HD2	2.02	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:16:295:ARG:NH1	2:17:463:GLN:NE2	2.21	0.88
2:12:1426:MET:HE2	2:15:1101:PRO:HG3	1.54	0.88
20:R3:188:GLY:CA	21:T2:629:PHE:CZ	2.57	0.88
2:10:1351:ILE:HD13	2:14:1425:ARG:HH12	1.35	0.88
2:12:833:LYS:CE	2:13:711:ARG:CZ	2.52	0.88
2:13:1633:LYS:NZ	2:17:1545:VAL:HG13	1.89	0.88
2:14:735:ASN:HD21	2:15:840:ILE:HD12	0.73	0.88
6:C3:420:TYR:CZ	19:Q1:382:GLN:HG3	2.08	0.88
2:14:735:ASN:CB	2:15:840:ILE:CB	2.49	0.88
2:14:1494:SER:HB2	2:15:1288:LEU:HD11	1.56	0.88
2:14:735:ASN:CG	2:15:840:ILE:HD12	1.95	0.87
4:A3:894:PHE:CG	7:D3:1464:LYS:HD2	2.06	0.87
2:11:1404:ASP:HA	2:14:1406:LYS:HE2	1.56	0.87
2:12:1068:ASP:OD2	2:13:1037:GLN:CG	2.22	0.87
2:12:1523:HIS:HB3	2:13:1126:THR:HG22	1.56	0.87
2:15:1205:VAL:CG1	2:15:1564:SER:CB	2.52	0.87
2:10:1668:LYS:HZ3	2:14:1752:ASN:CB	1.69	0.87
2:12:1068:ASP:OD2	2:13:1037:GLN:NE2	2.06	0.87
14:L1:318:SER:OG	15:M1:462:PHE:HB3	1.74	0.87
14:L1:369:PHE:HB3	15:M1:446:LEU:HD23	1.51	0.87
2:11:1359:THR:HG21	2:15:1356:ILE:HG23	1.56	0.87
2:13:1746:GLN:NE2	2:17:1669:GLU:O	2.07	0.87
2:11:1412:LYS:NZ	2:12:1094:ILE:CA	2.36	0.87
2:12:1521:MET:SD	2:13:1097:HIS:HD2	1.94	0.87
2:14:295:ARG:NE	2:15:473:GLU:OE2	2.09	0.86
2:13:1746:GLN:NE2	2:17:1670:SER:HA	1.89	0.86
2:15:1094:ILE:O	2:16:1412:LYS:NZ	2.07	0.86
2:11:815:GLN:O	2:12:617:ASN:OD1	1.94	0.86
2:10:1593:ILE:O	2:14:1674:THR:CG2	2.23	0.86
2:12:833:LYS:HZ2	2:13:711:ARG:HH11	1.20	0.86
2:16:295:ARG:CZ	2:17:463:GLN:HE21	1.89	0.85
2:14:1223:PRO:CB	2:15:1210:GLY:HA2	2.05	0.85
2:11:1406:LYS:HZ1	2:14:1405:ASN:CG	1.79	0.85
2:14:735:ASN:HB3	2:15:840:ILE:CB	2.04	0.85
2:16:611:ASN:ND2	2:17:833:LYS:CG	2.36	0.85
2:12:833:LYS:HZ3	2:13:711:ARG:NH1	1.71	0.85
2:16:1097:HIS:NE2	2:17:1523:HIS:CD2	2.43	0.85
2:13:1354:ILE:O	2:17:1430:LYS:HG3	1.76	0.85
2:15:1130:THR:HB	2:16:1411:ASP:O	1.74	0.85
2:10:1593:ILE:CB	2:14:1674:THR:CG2	2.54	0.85
2:12:833:LYS:NZ	2:13:711:ARG:CZ	2.38	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C1:1269:ASN:CG	6:C1:1269:ASN:ND2	2.30	0.85
2:10:1715:THR:HG21	2:14:1671:THR:H	1.41	0.84
2:13:1746:GLN:CD	2:17:1669:GLU:O	2.15	0.84
2:11:1718:TYR:HE2	2:15:1752:ASN:HD22	1.19	0.84
2:10:1717:GLN:NE2	2:14:1754:GLN:HE21	1.73	0.84
2:13:1745:ARG:HD2	2:17:1699:SER:HG	1.03	0.84
2:15:1095:ILE:HG21	2:16:1412:LYS:N	1.91	0.84
2:16:1097:HIS:CD2	2:17:1523:HIS:CD2	2.66	0.84
2:10:1706:TYR:OH	2:14:1786:LEU:HD11	1.75	0.84
14:L1:386:SER:OG	15:M1:503:GLU:OE2	1.96	0.84
2:11:1404:ASP:CA	2:14:1406:LYS:HE3	2.06	0.83
2:10:1813:LYS:NZ	2:14:1743:SER:OG	2.10	0.83
2:13:1003:GLN:NE2	2:15:1397:LYS:O	2.11	0.83
2:14:295:ARG:HH22	2:15:473:GLU:HG3	1.38	0.83
2:11:1699:SER:HA	2:16:1739:LYS:HE3	0.85	0.83
2:11:1412:LYS:H	2:12:1095:ILE:CD1	1.92	0.83
4:A3:894:PHE:CE1	7:D3:1464:LYS:HE2	2.10	0.83
2:11:1697:THR:CG2	2:16:1817:THR:O	2.25	0.83
14:L1:327:ARG:CD	15:M1:467:ARG:NH1	2.41	0.83
2:11:1412:LYS:HG2	2:12:1130:THR:O	1.78	0.83
2:15:1205:VAL:CB	2:15:1564:SER:CB	2.48	0.83
2:11:833:LYS:HD3	2:12:611:ASN:CA	2.07	0.83
2:11:1699:SER:CB	2:16:1819:THR:OG1	2.27	0.83
2:12:376:ASN:OD1	2:13:240:ASP:OD2	1.97	0.82
2:10:1385:TYR:HE1	2:14:1391:HIS:HE2	1.26	0.82
2:12:1520:ASP:OD1	2:13:1130:THR:HG21	1.79	0.82
2:13:1351:ILE:CD1	2:17:1425:ARG:HH12	1.92	0.82
2:16:1097:HIS:HE2	2:17:1523:HIS:CE1	1.85	0.82
2:14:735:ASN:HB3	2:15:840:ILE:O	1.79	0.82
2:15:1097:HIS:HE1	2:16:1411:ASP:O	1.34	0.82
14:L1:319:GLU:OE2	15:M1:463:ILE:HG23	1.79	0.82
2:11:1351:ILE:HD13	2:15:1425:ARG:HH12	1.44	0.82
2:14:614:ASN:OD1	2:15:816:GLN:CD	2.18	0.82
2:11:1411:ASP:HB3	2:12:1132:GLN:HA	1.61	0.82
2:11:1404:ASP:OD1	2:14:1406:LYS:CE	2.27	0.82
2:11:1411:ASP:N	2:12:1132:GLN:HB2	1.94	0.82
2:13:1745:ARG:HD2	2:17:1699:SER:CB	2.09	0.82
2:14:1178:ILE:HG23	2:15:1244:THR:OG1	1.80	0.81
14:L1:386:SER:CB	15:M1:439:SER:CB	2.57	0.81
2:12:1354:ILE:O	2:16:1430:LYS:HG3	1.81	0.81
2:14:1143:LYS:HG3	2:15:1158:SER:OG	1.78	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R3:189:SER:HA	21:T2:629:PHE:CD1	2.15	0.81
2:11:833:LYS:HA	2:12:613:ASN:HB2	1.60	0.81
2:14:1078:SER:O	2:15:1154:ARG:NH2	2.13	0.81
2:10:819:GLN:OE1	2:11:615:ASP:HA	1.80	0.81
2:15:1096:PRO:HD3	2:16:1412:LYS:NZ	1.82	0.81
14:L1:323:ASP:OD1	15:M1:428:ARG:HD3	1.79	0.81
14:L1:327:ARG:HD2	15:M1:467:ARG:NE	1.94	0.81
2:11:1646:GLY:HA3	2:15:1740:ILE:HG23	1.63	0.81
2:15:614:ASN:C	2:16:833:LYS:HD2	2.01	0.81
2:16:211:PRO:CG	2:17:331:LEU:HD12	1.89	0.81
13:K2:889:SER:HB2	14:L2:847:ARG:HH22	1.00	0.81
2:10:1579:SER:CB	2:14:1676:PHE:HD1	1.92	0.81
2:12:1351:ILE:CD1	2:16:1425:ARG:HH12	1.93	0.81
2:11:1411:ASP:N	2:12:1132:GLN:CD	2.24	0.80
2:12:833:LYS:NZ	2:13:711:ARG:HH12	1.74	0.80
2:16:1178:ILE:CG1	2:17:1347:GLN:HG3	2.10	0.80
2:12:1065:GLN:HE21	2:13:1037:GLN:CD	1.62	0.80
2:12:1522:PRO:CD	2:13:1128:SER:OG	2.28	0.80
2:12:1065:GLN:CD	2:13:1037:GLN:NE2	1.96	0.80
2:13:1746:GLN:CD	2:17:1670:SER:HA	2.02	0.80
2:16:618:GLY:C	2:17:816:GLN:CG	2.50	0.80
2:12:833:LYS:CE	2:13:711:ARG:NH1	2.45	0.80
6:C3:420:TYR:CD2	19:Q1:382:GLN:HG2	2.15	0.80
2:11:1717:GLN:HB3	2:15:1754:GLN:OE1	1.80	0.80
2:12:833:LYS:HG2	2:13:711:ARG:HD2	1.63	0.79
2:15:1095:ILE:HG23	2:16:1398:ASP:O	1.81	0.79
2:14:613:ASN:ND2	2:15:816:GLN:HA	1.97	0.79
2:14:614:ASN:ND2	2:15:813:GLU:HA	1.96	0.79
2:16:1102:ASN:OD1	2:17:1254:LYS:HE2	1.82	0.79
14:L1:386:SER:HB2	15:M1:503:GLU:OE2	1.81	0.79
2:10:1668:LYS:HZ1	2:14:1752:ASN:HB3	1.48	0.79
2:12:834:LYS:O	2:13:712:LYS:HE2	1.80	0.79
14:L1:321:ASP:N	15:M1:454:TYR:CE1	2.51	0.79
2:10:1338:LYS:HZ2	2:11:1197:ARG:HH12	1.28	0.79
2:10:1593:ILE:CB	2:14:1674:THR:HG22	2.11	0.79
20:R3:188:GLY:C	20:R3:189:SER:N	2.36	0.79
2:12:835:GLN:O	2:13:712:LYS:HE2	1.83	0.79
2:16:611:ASN:HD21	2:17:833:LYS:HG3	1.47	0.79
2:12:1523:HIS:HA	2:13:1144:THR:CG2	2.10	0.79
2:14:1178:ILE:O	2:15:1269:ASN:OD1	1.99	0.79
4:A3:894:PHE:CE1	7:D3:1464:LYS:HD3	2.11	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:1523:HIS:HB2	2:13:1126:THR:CB	2.13	0.79
2:11:1406:LYS:NZ	2:14:1405:ASN:CB	2.19	0.78
14:L1:369:PHE:O	15:M1:446:LEU:HD13	1.83	0.78
2:10:1351:ILE:CD1	2:14:1425:ARG:HH12	1.95	0.78
2:13:984:LYS:CE	2:15:1395:SER:OG	2.32	0.78
2:13:1746:GLN:HE22	2:17:1670:SER:HA	1.43	0.78
2:14:613:ASN:HD22	2:15:816:GLN:HA	1.47	0.78
2:15:1207:LEU:HB3	2:15:1562:GLY:O	1.83	0.78
14:L1:323:ASP:OD1	15:M1:428:ARG:CD	2.31	0.78
2:12:1520:ASP:OD1	2:13:1130:THR:CG2	2.30	0.78
2:11:1699:SER:CA	2:16:1739:LYS:CD	2.58	0.78
2:15:1165:GLY:O	2:15:1565:LEU:HD11	1.84	0.78
2:13:1745:ARG:HD3	2:17:1697:THR:OG1	1.84	0.78
2:15:614:ASN:O	2:16:833:LYS:CE	2.31	0.78
2:16:619:GLY:HA2	2:17:816:GLN:CA	2.11	0.78
20:R3:188:GLY:CA	21:T2:629:PHE:CE2	2.67	0.78
2:15:1207:LEU:O	2:15:1562:GLY:HA2	1.83	0.77
14:L1:299:LEU:CD1	15:M1:457:ASN:HB3	2.13	0.77
2:15:1096:PRO:HD2	2:16:1412:LYS:HZ2	1.46	0.77
2:14:1494:SER:OG	2:15:1288:LEU:HD11	1.82	0.77
20:R3:188:GLY:O	21:T2:629:PHE:CG	2.37	0.77
2:12:833:LYS:HE2	2:13:711:ARG:CZ	2.15	0.77
2:14:613:ASN:OD1	2:15:819:GLN:OE1	2.02	0.77
2:11:1406:LYS:HZ2	2:14:1405:ASN:HB2	1.47	0.77
2:16:618:GLY:O	2:17:816:GLN:CG	2.30	0.77
2:10:1706:TYR:CE1	2:14:1786:LEU:HD21	2.20	0.77
2:12:1522:PRO:HD3	2:13:1141:THR:HG21	1.66	0.77
2:12:834:LYS:C	2:13:712:LYS:HE2	2.04	0.77
2:15:1205:VAL:HG12	2:15:1564:SER:HA	1.67	0.77
2:10:1698:SER:O	2:14:1745:ARG:HD3	1.85	0.77
2:11:1404:ASP:HA	2:14:1406:LYS:HE3	1.61	0.77
2:12:1426:MET:HE1	2:15:1101:PRO:HG3	1.64	0.77
2:13:1745:ARG:CD	2:17:1699:SER:HG	1.82	0.76
2:12:509:GLU:OE1	2:13:297:ILE:CG2	2.34	0.76
2:10:1717:GLN:HE22	2:14:1784:ASN:HA	1.50	0.76
2:14:1006:TYR:HE2	2:15:1120:LEU:O	1.69	0.76
6:C1:1269:ASN:OD1	7:D0:1575:TYR:CZ	2.37	0.76
14:L1:299:LEU:HD11	15:M1:457:ASN:CB	2.14	0.76
16:N2:103:LEU:HD22	20:R2:1739:THR:HG23	1.66	0.76
2:12:1521:MET:HG3	2:13:1097:HIS:CG	2.07	0.76
2:11:1102:ASN:HD21	2:14:1425:ARG:HD2	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1354:ILE:O	2:14:1430:LYS:HG3	1.86	0.76
2:10:1813:LYS:CE	2:14:1743:SER:HB3	2.16	0.76
2:16:295:ARG:CZ	2:17:463:GLN:NE2	2.48	0.76
2:11:1412:LYS:HE3	2:12:1093:ASN:ND2	2.01	0.76
2:12:1101:PRO:CG	2:15:1424:GLY:O	2.34	0.76
2:13:1633:LYS:NZ	2:17:1545:VAL:CG1	2.49	0.76
2:16:237:GLN:HE22	2:17:466:ASN:HD22	1.34	0.75
2:10:819:GLN:NE2	2:11:614:ASN:C	2.25	0.75
2:10:1717:GLN:NE2	2:14:1754:GLN:NE2	2.32	0.75
2:12:1385:TYR:HE1	2:16:1391:HIS:HE2	1.33	0.75
2:15:1095:ILE:CD1	2:16:1410:LEU:HB3	2.16	0.75
2:10:1715:THR:CB	2:14:1671:THR:OG1	2.35	0.75
2:13:1745:ARG:HB2	2:17:1699:SER:OG	1.85	0.75
2:15:1097:HIS:CE1	2:16:1411:ASP:O	2.24	0.75
2:15:1130:THR:HB	2:16:1411:ASP:HB2	1.69	0.75
2:16:171:LYS:CE	2:17:465:LEU:HD21	2.08	0.75
6:C1:1269:ASN:CB	7:D0:1575:TYR:CD1	2.70	0.75
2:13:1745:ARG:CB	2:17:1699:SER:OG	2.35	0.75
16:N3:103:LEU:HD22	20:R3:1739:THR:HG23	1.67	0.75
2:11:1351:ILE:CD1	2:15:1425:ARG:HH12	1.99	0.74
14:L1:320:LEU:C	15:M1:454:TYR:HE1	1.89	0.74
14:L1:327:ARG:HD3	15:M1:467:ARG:NH1	2.02	0.74
2:10:1717:GLN:HE21	2:14:1754:GLN:HE21	1.31	0.74
2:12:906:LYS:NZ	2:13:735:ASN:HB3	2.02	0.74
4:A3:894:PHE:CZ	7:D3:1464:LYS:CG	2.70	0.74
2:14:295:ARG:NE	2:15:473:GLU:CD	2.40	0.74
2:15:1130:THR:CG2	2:16:1411:ASP:HB2	2.17	0.74
2:10:1593:ILE:HG22	2:14:1674:THR:HG22	0.93	0.74
2:14:735:ASN:OD1	2:15:840:ILE:CD1	2.35	0.74
2:11:1719:ASP:OD2	2:15:1784:ASN:OD1	2.06	0.73
2:10:1438:PRO:HG3	2:11:1097:HIS:HD2	1.53	0.73
2:12:1523:HIS:HB2	2:13:1126:THR:HG21	1.64	0.73
2:10:1706:TYR:CE1	2:14:1786:LEU:CD2	2.70	0.73
2:14:1178:ILE:O	2:15:1244:THR:HG21	1.87	0.73
2:16:1179:ARG:HG2	2:17:1344:ALA:HB1	1.69	0.73
20:R3:189:SER:CA	21:T2:629:PHE:CG	2.71	0.73
2:11:1102:ASN:HD21	2:14:1425:ARG:CD	2.00	0.73
2:12:1377:LEU:CD1	2:16:1356:ILE:HD11	2.19	0.73
2:10:819:GLN:OE1	2:11:614:ASN:O	2.06	0.73
14:L1:323:ASP:HB3	15:M1:428:ARG:HB2	1.67	0.73
2:10:1377:LEU:CD1	2:14:1356:ILE:HD11	2.19	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:11:1699:SER:CB	2:16:1739:LYS:CD	2.67	0.73
16:N1:103:LEU:HD22	20:R1:1739:THR:HG23	1.71	0.73
2:11:1411:ASP:HB3	2:12:1132:GLN:HB2	1.13	0.73
2:11:1411:ASP:OD2	2:12:1093:ASN:O	2.07	0.73
2:10:819:GLN:CB	2:11:615:ASP:OD1	2.35	0.72
2:13:1377:LEU:CD1	2:17:1356:ILE:HD11	2.18	0.72
2:14:295:ARG:CD	2:15:473:GLU:OE2	2.37	0.72
2:11:1412:LYS:HZ3	2:12:1094:ILE:H	1.25	0.72
2:12:1522:PRO:HD2	2:13:1128:SER:CB	2.19	0.72
2:14:1101:PRO:HD2	2:15:1523:HIS:CB	2.19	0.72
2:16:619:GLY:CA	2:17:819:GLN:HB2	2.19	0.72
6:C1:1269:ASN:HB2	7:D0:1575:TYR:CD1	2.23	0.72
2:14:295:ARG:HD3	2:15:473:GLU:OE2	1.89	0.72
2:14:613:ASN:HD22	2:15:816:GLN:CA	2.03	0.72
2:15:1205:VAL:CG1	2:15:1564:SER:HA	2.18	0.72
2:11:818:GLN:HB2	2:12:617:ASN:ND2	2.00	0.72
2:12:836:LYS:HZ2	2:13:712:LYS:HA	1.55	0.72
2:12:1068:ASP:OD1	2:13:1037:GLN:HG2	1.88	0.72
2:13:982:ASN:OD1	2:15:1397:LYS:NZ	2.21	0.72
2:15:1132:GLN:CD	2:16:1366:ASN:OD1	2.27	0.72
2:15:1165:GLY:O	2:15:1565:LEU:CD1	2.37	0.72
2:10:1253:ASN:ND2	2:11:1124:LEU:O	2.16	0.72
2:16:611:ASN:OD1	2:17:833:LYS:HA	1.90	0.72
2:16:617:ASN:OD1	2:17:816:GLN:N	2.21	0.72
13:K2:889:SER:HB3	14:L2:847:ARG:HH22	1.52	0.72
2:12:833:LYS:CG	2:13:711:ARG:CD	2.63	0.72
2:10:1717:GLN:HB3	2:14:1754:GLN:HE22	1.55	0.72
2:11:833:LYS:CE	2:12:611:ASN:HB3	2.20	0.72
2:15:1095:ILE:HG21	2:16:1412:LYS:H	1.53	0.72
2:16:1178:ILE:HD11	2:17:1347:GLN:HG3	1.56	0.72
20:R3:189:SER:CA	21:T2:629:PHE:CD1	2.72	0.72
2:11:1411:ASP:HB3	2:12:1132:GLN:CG	2.20	0.71
2:16:1178:ILE:HG12	2:17:1347:GLN:HG3	1.70	0.71
2:10:1254:LYS:CG	2:11:1100:ASN:HB2	2.20	0.71
2:11:1377:LEU:CD1	2:15:1356:ILE:HD11	2.20	0.71
2:13:1633:LYS:HZ1	2:17:1545:VAL:HG13	1.55	0.71
2:10:1717:GLN:NE2	2:14:1784:ASN:C	2.43	0.71
2:10:1757:SER:CA	2:14:1745:ARG:HH22	2.00	0.71
2:12:509:GLU:CD	2:13:297:ILE:HG21	2.10	0.71
2:13:1003:GLN:HE21	2:15:1410:LEU:HD11	1.55	0.71
2:15:1130:THR:CB	2:16:1411:ASP:HB2	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1593:ILE:O	2:14:1674:THR:HG23	1.89	0.71
2:12:1521:MET:CG	2:13:1097:HIS:CB	2.32	0.71
2:16:213:ARG:HG2	2:17:394:ALA:CB	2.20	0.71
2:13:1745:ARG:CG	2:17:1699:SER:OG	2.39	0.71
18:P0:358:SER:H	24:W0:337:ILE:HD11	1.54	0.71
2:12:1356:ILE:HG23	2:16:1359:THR:HG21	1.72	0.71
2:14:1143:LYS:CB	2:15:1159:VAL:CB	2.11	0.71
2:16:172:ASP:OD1	2:17:465:LEU:CD2	2.38	0.70
2:15:1095:ILE:CG2	2:16:1412:LYS:N	2.47	0.70
2:15:1132:GLN:NE2	2:16:1366:ASN:CB	2.53	0.70
2:10:1664:ILE:HD12	2:14:1784:ASN:OD1	1.92	0.70
2:12:820:GLN:HE22	2:13:613:ASN:ND2	1.86	0.70
6:C3:420:TYR:CG	19:Q1:382:GLN:CD	2.64	0.70
2:13:982:ASN:OD1	2:15:1397:LYS:HE2	1.92	0.70
2:11:1406:LYS:NZ	2:14:1405:ASN:ND2	2.40	0.70
2:13:1385:TYR:HE1	2:17:1391:HIS:HE2	1.35	0.70
2:15:1097:HIS:HB3	2:16:1413:ILE:HB	1.72	0.70
14:L1:322:PRO:C	15:M1:428:ARG:CD	2.60	0.70
2:10:819:GLN:NE2	2:11:614:ASN:CA	2.51	0.70
2:13:1356:ILE:HG23	2:17:1359:THR:HG21	1.73	0.70
6:C1:1269:ASN:OD1	7:D0:1575:TYR:CE2	2.44	0.70
6:C3:420:TYR:CE1	19:Q1:382:GLN:CA	2.73	0.70
2:12:1065:GLN:NE2	2:13:1037:GLN:NE2	0.75	0.70
2:14:735:ASN:ND2	2:15:840:ILE:CG2	2.55	0.70
6:C3:420:TYR:CZ	19:Q1:382:GLN:HA	2.26	0.70
2:12:941:GLU:OE1	2:13:735:ASN:ND2	2.25	0.69
2:16:615:ASP:OD2	2:17:818:GLN:OE1	2.10	0.69
2:11:833:LYS:CD	2:12:611:ASN:O	2.40	0.69
2:13:982:ASN:OD1	2:15:1397:LYS:CE	2.39	0.69
20:R2:7:ASN:HA	20:R2:8:THR:HG23	1.73	0.69
2:11:1613:VAL:CG1	2:15:1739:LYS:HD2	2.23	0.69
2:14:614:ASN:CG	2:15:816:GLN:HB2	2.13	0.69
2:11:1385:TYR:HE1	2:15:1391:HIS:HE2	1.37	0.69
2:13:1470:ILE:HG21	2:17:1425:ARG:HH22	1.56	0.69
2:15:1130:THR:HG22	2:16:1411:ASP:HB2	1.73	0.69
2:15:1241:LYS:O	2:15:1271:GLU:OE1	2.11	0.69
2:12:1065:GLN:HE21	2:13:1037:GLN:NE2	0.38	0.68
2:12:906:LYS:HZ3	2:13:735:ASN:HB3	1.57	0.68
2:16:622:SER:OG	2:17:823:SER:CA	2.41	0.68
2:17:475:THR:HG1	2:17:479:GLN:N	1.90	0.68
2:10:1385:TYR:CE1	2:14:1391:HIS:NE2	2.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:1470:ILE:HG21	2:16:1425:ARG:HH22	1.57	0.68
2:14:1178:ILE:CG2	2:15:1244:THR:HG1	2.06	0.68
2:10:1717:GLN:NE2	2:14:1784:ASN:HA	2.08	0.68
17:O0:378:TYR:CG	17:O0:394:LYS:HE3	2.28	0.68
14:L1:321:ASP:N	15:M1:454:TYR:CZ	2.57	0.68
2:11:1406:LYS:NZ	2:14:1405:ASN:CG	2.44	0.68
2:12:1065:GLN:HE21	2:13:1037:GLN:HE21	0.69	0.68
2:10:1757:SER:HA	2:14:1745:ARG:NH2	2.03	0.68
2:11:1354:ILE:HB	2:15:1430:LYS:HG2	1.76	0.68
2:10:1470:ILE:HG21	2:14:1425:ARG:HH22	1.58	0.68
2:15:1241:LYS:C	2:15:1269:ASN:HD22	1.97	0.68
2:16:1097:HIS:CE1	2:17:1523:HIS:CD2	2.82	0.68
2:12:1065:GLN:HE22	2:13:1037:GLN:NE2	1.19	0.67
2:16:1100:ASN:HA	2:17:1253:ASN:CG	2.13	0.67
6:C3:420:TYR:CZ	19:Q1:382:GLN:CA	2.76	0.67
14:L1:373:GLN:HE22	15:M1:442:SER:HB2	1.59	0.67
2:10:1338:LYS:NZ	2:11:1197:ARG:NH1	2.43	0.67
2:11:1406:LYS:HZ1	2:14:1405:ASN:ND2	1.92	0.67
14:L1:369:PHE:CA	15:M1:446:LEU:HD22	2.24	0.67
2:11:1404:ASP:CG	2:14:1406:LYS:HE3	2.13	0.67
2:12:544:LYS:HG2	2:13:295:ARG:HH11	1.59	0.67
2:14:295:ARG:NH1	2:15:473:GLU:OE1	2.27	0.67
2:10:1356:ILE:HD11	2:14:1377:LEU:HD13	1.77	0.67
14:L1:320:LEU:CA	15:M1:454:TYR:HE1	2.08	0.67
4:A3:894:PHE:CE2	7:D3:1464:LYS:HG2	2.30	0.67
2:10:1356:ILE:HG23	2:14:1359:THR:HG21	1.75	0.67
14:L1:319:GLU:OE2	15:M1:463:ILE:CG2	2.42	0.67
2:11:1356:ILE:HD11	2:15:1377:LEU:HD13	1.77	0.67
2:13:1003:GLN:NE2	2:15:1410:LEU:HD11	2.10	0.67
2:15:1163:VAL:HG22	2:15:1271:GLU:HG2	1.76	0.66
2:16:237:GLN:NE2	2:17:466:ASN:ND2	2.43	0.66
2:13:1356:ILE:HD11	2:17:1377:LEU:HD13	1.77	0.66
2:14:1494:SER:HB3	2:15:1288:LEU:HD11	1.76	0.66
4:A3:894:PHE:CE2	7:D3:1464:LYS:CG	2.78	0.66
20:R3:188:GLY:O	21:T2:629:PHE:CD1	2.49	0.66
2:15:1095:ILE:HD13	2:16:1410:LEU:CB	2.23	0.66
2:11:1412:LYS:CE	2:12:1094:ILE:CA	2.74	0.66
2:11:1470:ILE:HG21	2:15:1425:ARG:HH22	1.60	0.66
2:13:1745:ARG:CD	2:17:1697:THR:OG1	2.43	0.66
2:16:213:ARG:HG2	2:17:394:ALA:HB1	1.75	0.66
2:16:1178:ILE:HD13	2:17:1347:GLN:HG3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:714:HIS:ND1	2:15:836:LYS:HE3	2.10	0.66
2:11:1597:THR:HG21	2:15:1739:LYS:NZ	2.11	0.66
2:12:1377:LEU:HD13	2:16:1356:ILE:HD11	1.78	0.66
2:16:228:SER:OG	2:17:331:LEU:O	2.12	0.66
2:15:1544:HIS:HE1	2:15:1711:ASN:HB3	1.61	0.65
2:10:1813:LYS:CE	2:14:1743:SER:CB	2.74	0.65
2:10:819:GLN:C	2:11:615:ASP:OD2	2.34	0.65
2:10:1593:ILE:CA	2:14:1674:THR:CG2	2.74	0.65
2:10:1698:SER:HB2	2:14:1745:ARG:CZ	2.27	0.65
2:12:833:LYS:HD3	2:13:711:ARG:NE	2.09	0.65
2:10:1377:LEU:HD13	2:14:1356:ILE:HD11	1.77	0.65
2:11:819:GLN:OE1	2:12:618:GLY:O	2.11	0.65
2:11:1613:VAL:HG13	2:15:1739:LYS:HD2	1.77	0.65
2:10:819:GLN:HB2	2:11:615:ASP:OD2	1.94	0.65
2:14:614:ASN:ND2	2:15:816:GLN:HB2	2.12	0.65
14:L1:321:ASP:N	15:M1:454:TYR:HE1	1.94	0.65
4:A3:894:PHE:CD1	7:D3:1464:LYS:NZ	2.64	0.65
2:10:1254:LYS:HG3	2:11:1100:ASN:HB2	1.79	0.65
2:10:1593:ILE:C	2:14:1674:THR:HG22	2.01	0.64
2:11:1597:THR:HG21	2:15:1739:LYS:HZ2	1.61	0.64
2:13:1377:LEU:HD13	2:17:1356:ILE:HD11	1.78	0.64
2:11:1411:ASP:H	2:12:1132:GLN:CB	2.09	0.64
2:15:1096:PRO:O	2:16:1412:LYS:CB	2.43	0.64
2:16:1097:HIS:CD2	2:17:1523:HIS:NE2	2.63	0.64
2:12:833:LYS:HD3	2:13:711:ARG:HD3	0.68	0.64
2:16:1102:ASN:HD21	2:17:1254:LYS:HG2	1.63	0.64
16:N0:103:LEU:HD22	20:R0:1739:THR:HG23	1.80	0.64
2:10:1593:ILE:CA	2:14:1674:THR:HG22	2.28	0.64
2:12:1356:ILE:HD11	2:16:1377:LEU:HD13	1.79	0.64
2:12:1385:TYR:CE1	2:16:1391:HIS:NE2	2.62	0.64
2:14:1223:PRO:HB2	2:15:1210:GLY:CA	2.21	0.64
2:15:1095:ILE:HD13	2:16:1410:LEU:HB3	1.76	0.64
18:P0:447:LYS:HE3	18:P0:464:HIS:CD2	2.33	0.64
2:10:1593:ILE:CG2	2:14:1674:THR:HG21	2.10	0.64
2:11:822:GLN:HE22	2:12:617:ASN:HB3	1.24	0.64
2:11:1411:ASP:N	2:12:1132:GLN:CB	2.61	0.64
2:11:1470:ILE:HG21	2:15:1425:ARG:NH2	2.12	0.64
14:L1:369:PHE:O	15:M1:446:LEU:CD1	2.46	0.64
2:11:1699:SER:O	2:16:1739:LYS:HE3	1.98	0.63
2:15:1205:VAL:HG11	2:15:1564:SER:CB	2.26	0.63
2:11:1385:TYR:CE1	2:15:1391:HIS:NE2	2.65	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:11:1412:LYS:CE	2:12:1094:ILE:N	2.50	0.63
2:16:213:ARG:NE	2:17:394:ALA:CB	2.59	0.63
2:13:1470:ILE:HG21	2:17:1425:ARG:NH2	2.14	0.63
14:L1:319:GLU:OE2	15:M1:463:ILE:CB	2.47	0.63
2:11:1351:ILE:CD1	2:15:1425:ARG:NH1	2.56	0.63
2:14:295:ARG:CZ	2:15:473:GLU:OE2	2.42	0.63
2:13:1385:TYR:CE1	2:17:1391:HIS:NE2	2.64	0.62
2:10:1706:TYR:HE1	2:14:1786:LEU:HD22	1.62	0.62
2:11:1102:ASN:ND2	2:14:1425:ARG:CZ	2.49	0.62
2:11:1411:ASP:H	2:12:1132:GLN:HB2	1.64	0.62
2:12:820:GLN:CD	2:13:611:ASN:HA	2.20	0.62
14:L1:369:PHE:C	15:M1:446:LEU:HD22	2.19	0.62
2:11:1412:LYS:HA	2:12:1130:THR:CB	2.20	0.62
2:12:1470:ILE:HG21	2:16:1425:ARG:NH2	2.15	0.62
2:16:619:GLY:HA3	2:17:819:GLN:CB	2.23	0.62
2:12:544:LYS:HA	2:13:295:ARG:NH1	2.14	0.62
2:11:1411:ASP:HB2	2:12:1130:THR:HG22	1.82	0.62
2:11:822:GLN:NE2	2:12:617:ASN:HB2	1.94	0.62
2:14:1144:THR:O	2:15:1159:VAL:HG11	1.99	0.62
2:10:1715:THR:HG21	2:14:1671:THR:OG1	2.00	0.62
2:10:1706:TYR:HE1	2:14:1786:LEU:CD2	2.11	0.61
2:14:1178:ILE:HG23	2:15:1244:THR:HG1	1.65	0.61
2:10:1715:THR:HG1	2:14:1671:THR:HG1	1.20	0.61
14:L1:386:SER:O	15:M1:439:SER:OG	2.15	0.61
2:11:1377:LEU:CD2	2:15:1355:PRO:HD2	2.30	0.61
2:16:622:SER:CB	2:17:823:SER:CB	2.70	0.61
2:12:1249:HIS:HE1	2:13:1146:GLN:NE2	1.98	0.61
2:12:1522:PRO:HG2	2:13:1128:SER:CB	2.30	0.61
2:16:237:GLN:NE2	2:17:466:ASN:HD22	1.98	0.61
2:12:820:GLN:NE2	2:13:611:ASN:HA	2.16	0.61
2:13:1003:GLN:HE21	2:15:1410:LEU:CD1	2.13	0.61
2:11:1780:ASP:HB3	2:16:1754:GLN:HE22	1.66	0.61
15:M3:280:THR:HG21	15:M3:621:GLN:HE21	1.66	0.61
2:10:1470:ILE:HG21	2:14:1425:ARG:NH2	2.15	0.60
2:13:1633:LYS:HZ2	2:17:1545:VAL:CG1	2.12	0.60
2:10:1338:LYS:HZ1	2:11:1197:ARG:HH12	1.49	0.60
2:16:1102:ASN:ND2	2:17:1254:LYS:HG2	2.15	0.60
2:10:1714:LYS:NZ	2:14:1784:ASN:HA	2.16	0.60
2:10:1813:LYS:HE3	2:14:1743:SER:HB3	1.82	0.60
2:12:544:LYS:HZ1	2:13:297:ILE:HD11	1.66	0.60
2:11:822:GLN:NE2	2:12:617:ASN:HD22	1.99	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1714:LYS:HZ2	2:14:1784:ASN:HA	1.67	0.60
2:14:735:ASN:HB3	2:15:840:ILE:CA	2.31	0.60
2:10:1594:ALA:N	2:14:1674:THR:CG2	2.53	0.60
2:11:1404:ASP:CB	2:14:1406:LYS:HE3	2.31	0.60
2:11:1783:LEU:CD2	2:16:1752:ASN:HB3	2.30	0.60
2:12:1520:ASP:HB3	2:13:1130:THR:OG1	2.02	0.60
2:14:735:ASN:ND2	2:15:840:ILE:HG21	2.16	0.60
2:11:1431:LEU:HD21	2:15:1417:TYR:CD1	2.36	0.60
2:12:1520:ASP:HA	2:13:1130:THR:OG1	2.00	0.60
2:12:1522:PRO:HG3	2:13:1141:THR:HG22	1.84	0.60
2:12:1354:ILE:HD12	2:16:1429:SER:HA	1.84	0.60
2:11:1102:ASN:HD21	2:14:1425:ARG:NE	2.00	0.60
2:11:1377:LEU:HD13	2:15:1356:ILE:HD11	1.83	0.59
2:12:833:LYS:HZ3	2:13:711:ARG:CZ	2.11	0.59
2:13:984:LYS:HB3	2:15:1397:LYS:CB	2.11	0.59
2:16:213:ARG:CG	2:17:394:ALA:HB2	2.31	0.59
2:16:621:GLY:HA2	2:17:819:GLN:O	2.01	0.59
14:L1:320:LEU:C	15:M1:454:TYR:CE1	2.74	0.59
2:11:1783:LEU:HD21	2:16:1752:ASN:CB	2.28	0.59
2:14:735:ASN:OD1	2:15:840:ILE:HD12	1.98	0.59
4:A3:894:PHE:CG	7:D3:1464:LYS:NZ	2.70	0.59
14:L1:321:ASP:OD1	15:M1:454:TYR:CZ	2.56	0.59
2:10:1706:TYR:CE1	2:14:1786:LEU:HD22	2.36	0.59
2:14:714:HIS:ND1	2:15:836:LYS:CE	2.66	0.59
2:12:1065:GLN:NE2	2:13:1037:GLN:HE22	0.20	0.59
2:14:1143:LYS:CG	2:15:1158:SER:OG	2.49	0.59
2:15:1203:GLU:OE1	2:15:1568:SER:N	2.35	0.59
2:10:822:GLN:HE22	2:11:614:ASN:ND2	1.82	0.59
2:12:1523:HIS:CA	2:13:1144:THR:HG22	2.23	0.59
2:14:1006:TYR:CE2	2:15:1120:LEU:O	2.55	0.59
2:10:1254:LYS:CE	2:11:1100:ASN:OD1	2.48	0.59
2:12:544:LYS:NZ	2:13:297:ILE:HD11	2.18	0.59
2:12:834:LYS:O	2:13:712:LYS:CG	2.51	0.59
2:12:1426:MET:HE2	2:15:1101:PRO:CG	2.27	0.59
2:13:1431:LEU:HD21	2:17:1417:TYR:CD1	2.38	0.59
14:L1:373:GLN:NE2	15:M1:442:SER:CB	2.62	0.59
2:10:1469:ASP:OD2	2:11:1101:PRO:CD	2.51	0.58
2:16:1179:ARG:CG	2:17:1344:ALA:HB1	2.32	0.58
2:12:836:LYS:CG	2:13:712:LYS:HB3	2.33	0.58
2:12:1431:LEU:HD21	2:16:1417:TYR:CD1	2.38	0.58
2:10:1354:ILE:HD12	2:14:1429:SER:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1431:LEU:HD21	2:14:1417:TYR:CD1	2.38	0.58
2:10:1593:ILE:CB	2:14:1674:THR:HG21	2.25	0.58
2:13:984:LYS:NZ	2:15:1395:SER:HA	2.18	0.58
2:10:1579:SER:HB2	2:14:1676:PHE:HD1	1.67	0.58
2:11:1404:ASP:CA	2:14:1406:LYS:CE	2.68	0.58
2:14:295:ARG:CD	2:15:473:GLU:CD	2.72	0.58
2:14:735:ASN:CG	2:15:840:ILE:HG13	2.04	0.58
14:L1:299:LEU:HD11	15:M1:457:ASN:CG	2.23	0.58
2:10:1715:THR:CG2	2:14:1671:THR:OG1	2.51	0.58
2:11:1597:THR:CG2	2:15:1739:LYS:HZ2	2.16	0.58
2:13:1633:LYS:HZ1	2:17:1545:VAL:CG1	2.12	0.58
2:13:984:LYS:CB	2:15:1397:LYS:HB3	2.13	0.58
2:13:1359:THR:CG2	2:17:1356:ILE:HG23	2.31	0.58
2:10:1594:ALA:HB2	2:14:1674:THR:CG2	2.34	0.58
2:12:820:GLN:HE21	2:13:613:ASN:ND2	1.95	0.58
2:12:1520:ASP:CA	2:13:1130:THR:OG1	2.52	0.58
2:12:1522:PRO:CA	2:13:1144:THR:HG23	2.32	0.58
2:15:1244:THR:HG23	2:15:1269:ASN:HD21	1.68	0.58
15:M0:280:THR:HG21	15:M0:621:GLN:NE2	2.18	0.57
2:13:1354:ILE:HD12	2:17:1429:SER:HA	1.85	0.57
2:12:820:GLN:HE21	2:13:613:ASN:CG	2.02	0.57
6:C3:420:TYR:CD1	19:Q1:382:GLN:CD	2.77	0.57
14:L1:299:LEU:CD2	15:M1:457:ASN:ND2	2.67	0.57
14:L1:373:GLN:HE22	15:M1:442:SER:CB	2.16	0.57
2:12:1523:HIS:HB2	2:13:1126:THR:HB	1.86	0.57
4:A3:146:TRP:CE3	5:B1:2087:LYS:HE2	2.39	0.57
21:T2:596:GLU:CD	21:T2:596:GLU:H	2.07	0.57
2:16:611:ASN:ND2	2:17:833:LYS:HG3	2.12	0.57
2:10:1523:HIS:CE1	2:11:1141:THR:HG21	2.40	0.57
2:10:1594:ALA:HB2	2:14:1674:THR:OG1	2.04	0.57
14:L1:320:LEU:HB2	15:M1:454:TYR:CD1	2.40	0.57
2:10:1593:ILE:C	2:14:1674:THR:HG23	2.16	0.57
2:14:1099:ASP:O	2:15:1523:HIS:HA	2.05	0.57
4:A1:146:TRP:CE3	5:B0:2087:LYS:HE2	2.39	0.57
2:11:1354:ILE:HD12	2:15:1429:SER:HA	1.87	0.57
6:C1:1232:THR:HG1	6:C2:1609:ILE:N	2.03	0.57
2:11:1356:ILE:HG23	2:15:1359:THR:HG21	1.85	0.56
2:12:836:LYS:NZ	2:13:712:LYS:HA	2.19	0.56
14:L1:327:ARG:CD	15:M1:467:ARG:NH2	2.47	0.56
20:R0:1416:LYS:HE2	20:R0:1465:GLN:HA	1.86	0.56
2:11:833:LYS:HB3	2:12:613:ASN:ND2	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:735:ASN:HD21	2:15:840:ILE:HD13	1.55	0.56
2:14:735:ASN:HB3	2:15:840:ILE:C	2.24	0.56
2:14:1144:THR:O	2:15:1159:VAL:CG1	2.54	0.56
15:M3:280:THR:HG21	15:M3:621:GLN:NE2	2.20	0.56
2:10:1438:PRO:CG	2:11:1097:HIS:HD2	2.19	0.56
2:11:833:LYS:HA	2:12:613:ASN:CB	2.33	0.56
2:12:1521:MET:HG3	2:13:1097:HIS:NE2	2.20	0.56
2:14:614:ASN:CG	2:15:816:GLN:NE2	2.57	0.56
2:10:285:GLN:HA	2:10:456:LEU:HD11	1.87	0.56
2:11:1102:ASN:HD22	2:14:1425:ARG:HH11	1.41	0.56
2:11:1366:ASN:ND2	2:12:1139:SER:CB	2.65	0.56
13:K2:1010:VAL:CG1	14:L2:973:LEU:HD21	2.34	0.56
2:10:1469:ASP:HB2	2:11:1099:ASP:CA	2.34	0.56
2:13:1351:ILE:CD1	2:17:1425:ARG:NH1	2.53	0.56
2:14:614:ASN:CG	2:15:813:GLU:HA	2.25	0.56
2:16:1097:HIS:HE1	2:17:1523:HIS:ND1	1.98	0.56
2:10:1593:ILE:CG2	2:14:1674:THR:CA	2.82	0.56
2:15:1130:THR:OG1	2:16:1411:ASP:O	2.22	0.56
2:16:237:GLN:HE22	2:17:466:ASN:ND2	2.00	0.56
2:16:213:ARG:HD3	2:17:394:ALA:HB2	1.84	0.56
2:12:1068:ASP:OD2	2:13:1037:GLN:CD	2.44	0.56
2:11:1699:SER:HA	2:16:1739:LYS:CG	2.25	0.56
2:12:836:LYS:HG3	2:13:712:LYS:HB3	1.88	0.56
14:L1:386:SER:CB	15:M1:439:SER:HB2	2.35	0.56
14:L1:319:GLU:CD	15:M1:463:ILE:CG1	2.54	0.56
14:L1:320:LEU:HB2	15:M1:454:TYR:CE1	2.42	0.55
2:10:1717:GLN:CB	2:14:1754:GLN:NE2	2.65	0.55
2:14:614:ASN:CG	2:15:816:GLN:CD	2.63	0.55
2:15:617:ASN:HD21	2:16:824:THR:HA	1.70	0.55
2:11:1425:ARG:NH1	2:15:1351:ILE:HD13	2.21	0.55
2:12:820:GLN:CD	2:13:613:ASN:HD21	2.09	0.55
2:16:1097:HIS:HE1	2:17:1523:HIS:CE1	2.16	0.55
2:12:1695:VAL:HG21	2:16:1664:ILE:HD11	1.88	0.55
2:14:613:ASN:HD22	2:15:816:GLN:N	2.05	0.55
2:16:622:SER:HB3	2:17:823:SER:HB3	1.83	0.55
14:L1:321:ASP:HA	15:M1:450:GLN:CD	2.27	0.55
2:15:614:ASN:O	2:16:833:LYS:NZ	2.39	0.55
4:A3:894:PHE:CZ	7:D3:1464:LYS:HG2	2.40	0.55
2:12:511:ASN:HD21	2:13:295:ARG:NH1	2.04	0.55
20:R3:188:GLY:HA2	21:T2:629:PHE:CE2	2.41	0.55
2:11:819:GLN:N	2:12:617:ASN:ND2	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:1520:ASP:CG	2:13:1130:THR:HG21	2.27	0.55
2:14:613:ASN:ND2	2:15:819:GLN:NE2	2.54	0.55
3:40:204:GLU:CD	3:40:204:GLU:H	2.11	0.55
2:12:1520:ASP:OD1	2:13:1130:THR:HG23	2.05	0.55
2:10:1356:ILE:HD11	2:14:1377:LEU:CD1	2.36	0.55
2:11:1391:HIS:HE2	2:15:1385:TYR:HE1	1.53	0.55
6:C1:1269:ASN:HB3	7:D0:1575:TYR:CG	2.38	0.55
14:L1:299:LEU:HD21	15:M1:457:ASN:ND2	2.21	0.55
2:12:1521:MET:CB	2:13:1097:HIS:HB3	2.36	0.54
4:A4:835:LYS:CE	4:A4:844:TYR:CE1	2.89	0.54
2:11:1358:THR:HG23	2:15:1431:LEU:HB2	1.87	0.54
2:12:511:ASN:HD21	2:13:295:ARG:HH12	1.56	0.54
14:L1:319:GLU:HG2	15:M1:463:ILE:CD1	2.34	0.54
2:11:1597:THR:CG2	2:15:1739:LYS:NZ	2.69	0.54
2:12:1522:PRO:HD3	2:13:1141:THR:CG2	2.36	0.54
2:10:1254:LYS:HE2	2:11:1100:ASN:OD1	1.70	0.54
2:10:1354:ILE:HB	2:14:1430:LYS:HG2	1.89	0.54
2:12:835:GLN:O	2:13:712:LYS:CE	2.55	0.54
2:12:1377:LEU:HD11	2:16:1356:ILE:HD11	1.90	0.54
2:13:1356:ILE:HD11	2:17:1377:LEU:CD1	2.37	0.54
2:15:1163:VAL:HG21	2:15:1276:TYR:HB3	1.88	0.54
2:11:1411:ASP:HB3	2:12:1139:SER:HB3	1.89	0.54
4:A4:835:LYS:HE2	4:A4:844:TYR:CE1	2.43	0.54
1:00:244:TYR:CD2	1:00:248:ILE:HD11	2.43	0.54
2:10:1355:PRO:HG2	2:14:1377:LEU:HD21	1.89	0.54
2:10:1425:ARG:NH1	2:14:1351:ILE:HD13	2.22	0.54
2:10:1813:LYS:HE2	2:14:1743:SER:HB3	1.87	0.54
2:11:1470:ILE:CG2	2:15:1425:ARG:HH22	2.19	0.54
14:L1:327:ARG:CZ	15:M1:467:ARG:CD	2.86	0.54
2:11:1377:LEU:HD11	2:15:1356:ILE:HD11	1.88	0.54
2:12:1470:ILE:CG2	2:16:1425:ARG:HH22	2.20	0.54
2:13:1354:ILE:HB	2:17:1430:LYS:HG2	1.89	0.54
2:14:295:ARG:HD3	2:15:473:GLU:CD	2.28	0.54
2:10:1438:PRO:HG3	2:11:1097:HIS:CD2	2.39	0.54
2:12:833:LYS:CD	2:13:711:ARG:NE	2.69	0.54
15:M0:280:THR:HG21	15:M0:621:GLN:HE21	1.71	0.54
2:10:1254:LYS:CG	2:11:1100:ASN:CB	2.82	0.54
2:10:1354:ILE:CD1	2:14:1420:ALA:O	2.56	0.54
2:10:1385:TYR:HE1	2:14:1391:HIS:NE2	2.01	0.54
2:13:984:LYS:HZ1	2:15:1395:SER:HA	1.72	0.54
2:13:1377:LEU:HD11	2:17:1356:ILE:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R0:355:ILE:H	20:R0:356:PRO:CD	2.20	0.54
2:13:1470:ILE:CG2	2:17:1425:ARG:HH22	2.19	0.53
2:13:1745:ARG:HB2	2:17:1699:SER:CB	2.37	0.53
2:13:1746:GLN:HE22	2:17:1670:SER:C	2.11	0.53
14:L2:882:GLY:HA3	14:L2:940:ILE:HD11	1.89	0.53
1:01:244:TYR:CD2	1:01:248:ILE:HD11	2.43	0.53
2:12:1356:ILE:HD11	2:16:1377:LEU:CD1	2.38	0.53
2:12:1425:ARG:NH1	2:16:1351:ILE:HD13	2.24	0.53
2:13:1746:GLN:OE1	2:17:1669:GLU:O	2.26	0.53
20:R3:87:LYS:HE3	20:R3:92:ASP:CG	2.29	0.53
2:11:1398:ASP:O	2:12:1095:ILE:HD13	2.07	0.53
2:11:1613:VAL:HG13	2:15:1739:LYS:CD	2.38	0.53
12:J1:693:GLU:CB	23:V1:784:LEU:HD11	2.39	0.53
2:10:1422:ARG:HB2	2:14:1354:ILE:HD11	1.90	0.53
2:10:1438:PRO:CB	2:11:1097:HIS:CD2	2.91	0.53
2:16:619:GLY:CA	2:17:816:GLN:CA	2.60	0.53
6:C1:985:GLU:CD	6:C1:985:GLU:H	2.10	0.53
13:K2:1010:VAL:HG11	14:L2:973:LEU:HD21	1.90	0.53
17:O3:195:ARG:HH12	20:R3:1530:VAL:HG21	1.73	0.53
2:15:617:ASN:HB2	2:16:826:GLN:HB2	1.88	0.53
2:10:1706:TYR:HH	2:14:1786:LEU:CD1	2.17	0.53
2:15:617:ASN:HB2	2:16:826:GLN:CB	2.17	0.53
2:12:1693:SER:O	2:16:1676:PHE:HB3	2.09	0.53
14:L1:299:LEU:CD1	15:M1:457:ASN:ND2	2.72	0.53
2:10:1377:LEU:HD11	2:14:1356:ILE:HD11	1.90	0.53
2:13:1358:THR:HG23	2:17:1431:LEU:HB2	1.90	0.53
2:15:617:ASN:ND2	2:16:824:THR:HA	2.23	0.53
2:10:1358:THR:HG23	2:14:1431:LEU:HB2	1.91	0.52
2:11:823:SER:HB3	2:12:621:GLY:HA2	1.90	0.52
2:12:820:GLN:HE22	2:13:613:ASN:CG	2.08	0.52
2:11:1699:SER:OG	2:16:1819:THR:OG1	2.27	0.52
2:12:1354:ILE:HB	2:16:1430:LYS:HG2	1.90	0.52
6:C2:985:GLU:CD	6:C2:985:GLU:H	2.12	0.52
2:10:1469:ASP:CB	2:11:1099:ASP:HA	2.39	0.52
2:10:1593:ILE:CA	2:14:1674:THR:HG21	2.39	0.52
2:11:1699:SER:HB2	2:16:1819:THR:OG1	2.08	0.52
2:12:1426:MET:CE	2:15:1101:PRO:CG	2.79	0.52
2:12:1353:ASP:OD1	2:16:1430:LYS:HE2	2.09	0.52
2:12:1354:ILE:CD1	2:16:1420:ALA:O	2.57	0.52
2:12:1358:THR:HG23	2:16:1431:LEU:HB2	1.91	0.52
2:13:1353:ASP:OD1	2:17:1430:LYS:HE2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:15:1095:ILE:HD11	2:16:1410:LEU:HB3	1.91	0.52
14:L1:323:ASP:HA	15:M1:428:ARG:HD2	1.90	0.52
2:11:1412:LYS:HE3	2:12:1093:ASN:HD22	1.70	0.52
2:11:1699:SER:O	2:16:1739:LYS:CE	2.56	0.52
2:13:1425:ARG:NH1	2:17:1351:ILE:HD13	2.24	0.52
14:L1:318:SER:O	15:M1:462:PHE:HB2	2.09	0.52
2:15:1096:PRO:C	2:16:1412:LYS:HB3	2.27	0.52
2:10:1359:THR:CG2	2:14:1356:ILE:HG23	2.36	0.52
20:R1:247:THR:HG21	20:R1:264:LYS:HE2	1.91	0.52
2:10:1353:ASP:OD1	2:14:1430:LYS:HE2	2.10	0.52
2:10:1701:ASP:OD2	2:14:1746:GLN:OE1	2.25	0.52
2:15:615:ASP:C	2:16:826:GLN:OE1	2.44	0.52
5:B0:1780:LYS:CE	5:B0:1839:TYR:CZ	2.93	0.52
14:L1:322:PRO:C	15:M1:428:ARG:HD2	2.27	0.52
21:T0:36:GLU:OE1	21:T0:368:LYS:HE2	2.09	0.52
2:12:833:LYS:HE2	2:13:711:ARG:NE	2.24	0.52
5:B1:1780:LYS:CE	5:B1:1839:TYR:CZ	2.93	0.52
2:12:834:LYS:O	2:13:712:LYS:HG3	2.11	0.51
2:11:832:ILE:O	2:12:614:ASN:CG	2.47	0.51
2:12:835:GLN:N	2:13:712:LYS:HE2	2.25	0.51
2:12:833:LYS:CE	2:13:711:ARG:NE	2.74	0.51
2:15:1132:GLN:HE22	2:16:1366:ASN:CB	2.12	0.51
2:12:1430:LYS:HG3	2:16:1354:ILE:O	2.09	0.51
2:12:1522:PRO:CB	2:13:1144:THR:HG23	2.39	0.51
2:12:1355:PRO:HG2	2:16:1377:LEU:HD21	1.91	0.51
5:B0:1891:PRO:O	5:B0:1897:LYS:HE3	2.10	0.51
2:10:1430:LYS:HG3	2:14:1354:ILE:O	2.11	0.51
2:14:614:ASN:HD21	2:15:813:GLU:HA	1.71	0.51
13:K3:621:LYS:HE2	13:K3:625:GLU:OE1	2.11	0.51
2:10:1470:ILE:CG2	2:14:1425:ARG:HH22	2.21	0.51
2:11:1411:ASP:CB	2:12:1139:SER:HB3	2.41	0.51
2:12:1520:ASP:CB	2:13:1130:THR:OG1	2.59	0.51
2:13:1746:GLN:NE2	2:17:1670:SER:CA	2.52	0.51
11:I0:242:LYS:HZ1	11:I0:273:ILE:HD13	1.76	0.51
15:M1:366:GLU:CD	15:M1:370:ARG:HE	2.14	0.51
2:11:1356:ILE:HD11	2:15:1377:LEU:CD1	2.40	0.51
2:11:1699:SER:CB	2:16:1739:LYS:HG3	2.20	0.50
2:12:1359:THR:CG2	2:16:1356:ILE:HG23	2.32	0.50
2:12:1522:PRO:CD	2:13:1128:SER:CB	2.88	0.50
12:J1:693:GLU:HB3	23:V1:784:LEU:HD11	1.93	0.50
20:R1:87:LYS:HE3	20:R1:92:ASP:OD1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:835:GLN:CA	2:13:712:LYS:HE2	2.41	0.50
2:12:1522:PRO:HG2	2:13:1128:SER:HB3	1.92	0.50
2:14:614:ASN:OD1	2:15:816:GLN:HB2	2.12	0.50
2:16:1178:ILE:O	2:17:1345:SER:N	2.44	0.50
13:K3:820:TYR:CD2	13:K3:858:LYS:HE3	2.46	0.50
2:11:1354:ILE:CD1	2:15:1420:ALA:O	2.60	0.50
2:13:1354:ILE:CD1	2:17:1420:ALA:O	2.59	0.50
2:16:213:ARG:HE	2:17:394:ALA:HB2	1.72	0.50
2:11:1354:ILE:HD11	2:15:1422:ARG:HB2	1.94	0.50
2:13:1746:GLN:HE22	2:17:1670:SER:N	2.08	0.50
2:14:1143:LYS:HB3	2:15:1159:VAL:HB	0.57	0.50
4:A4:835:LYS:HE3	4:A4:844:TYR:CE1	2.46	0.50
14:L0:882:GLY:HA3	14:L0:940:ILE:HD11	1.93	0.50
3:41:277:TRP:CZ2	3:41:297:ILE:HD13	2.47	0.50
21:T0:357:HIS:HB3	21:T0:378:LEU:HD11	1.93	0.50
2:11:1411:ASP:CB	2:12:1130:THR:HG22	2.41	0.50
2:15:1101:PRO:HB2	2:16:1393:SER:HB2	1.94	0.50
3:40:277:TRP:CZ2	3:40:297:ILE:HD13	2.47	0.50
15:M2:280:THR:HG21	15:M2:621:GLN:NE2	2.27	0.50
2:11:1613:VAL:HG11	2:15:1739:LYS:HD2	1.94	0.50
2:12:834:LYS:HG2	2:13:712:LYS:CE	2.39	0.50
20:R2:355:ILE:H	20:R2:356:PRO:CD	2.25	0.50
2:11:822:GLN:NE2	2:12:617:ASN:ND2	2.60	0.49
2:11:1783:LEU:CD2	2:16:1752:ASN:CB	2.90	0.49
13:K0:820:TYR:CD2	13:K0:858:LYS:HE3	2.46	0.49
14:L1:882:GLY:HA3	14:L1:940:ILE:HD11	1.94	0.49
20:R1:355:ILE:H	20:R1:356:PRO:CD	2.24	0.49
2:10:1469:ASP:HB2	2:11:1099:ASP:HA	1.92	0.49
2:11:1359:THR:CG2	2:15:1356:ILE:HG23	2.35	0.49
2:12:1422:ARG:HB2	2:16:1354:ILE:HD11	1.92	0.49
2:13:477:HIS:CG	2:13:546:ASN:HD22	2.30	0.49
14:L1:369:PHE:CB	15:M1:446:LEU:HD23	2.19	0.49
5:B1:1891:PRO:O	5:B1:1897:LYS:HE3	2.11	0.49
14:L3:882:GLY:HA3	14:L3:940:ILE:HD11	1.92	0.49
18:P0:660:LYS:HE3	19:Q0:324:TRP:CD2	2.47	0.49
2:10:1354:ILE:HD13	2:14:1420:ALA:O	2.13	0.49
2:12:1354:ILE:HD13	2:16:1420:ALA:O	2.13	0.49
2:12:1522:PRO:CG	2:13:1128:SER:CB	2.91	0.49
2:10:819:GLN:OE1	2:11:614:ASN:C	2.42	0.49
2:11:1411:ASP:HB2	2:12:1131:ILE:C	2.31	0.49
2:13:1377:LEU:CD2	2:17:1355:PRO:HD2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:834:LYS:HG2	2:13:712:LYS:HZ2	1.70	0.49
4:A5:835:LYS:CE	4:A5:844:TYR:CE1	2.96	0.49
5:B1:1780:LYS:HE2	5:B1:1839:TYR:CE1	2.48	0.49
19:Q1:110:TYR:CZ	19:Q1:112:GLY:HA3	2.48	0.49
2:11:819:GLN:HG3	2:12:617:ASN:CG	2.31	0.49
2:11:823:SER:CB	2:12:621:GLY:HA2	2.43	0.49
2:12:1351:ILE:CD1	2:16:1425:ARG:NH1	2.54	0.49
4:A1:835:LYS:CE	4:A1:844:TYR:CE1	2.96	0.49
4:A3:689:ILE:N	4:A3:698:HIS:HD1	2.10	0.49
2:10:1338:LYS:HZ1	2:11:1197:ARG:NH1	2.07	0.49
2:15:1241:LYS:C	2:15:1271:GLU:OE1	2.51	0.49
2:16:1178:ILE:HG23	2:17:1345:SER:C	2.23	0.49
4:A0:835:LYS:HE3	4:A0:844:TYR:CZ	2.48	0.49
4:A1:835:LYS:HE3	4:A1:844:TYR:CE1	2.48	0.49
5:B0:627:LEU:HD22	5:B0:688:ARG:HD2	1.95	0.49
2:15:1097:HIS:HD2	2:16:1413:ILE:O	1.91	0.48
2:16:213:ARG:HD3	2:17:358:SER:HB2	1.94	0.48
14:L1:386:SER:HB2	15:M1:439:SER:HB2	1.94	0.48
17:O3:115:LYS:HE2	17:O3:164:ILE:O	2.13	0.48
2:10:1438:PRO:CG	2:11:1097:HIS:CD2	2.96	0.48
2:13:1745:ARG:CD	2:17:1697:THR:CB	2.83	0.48
4:A1:689:ILE:N	4:A1:698:HIS:HD1	2.10	0.48
18:P1:660:LYS:HE3	19:Q1:324:TRP:CE3	2.48	0.48
20:R3:355:ILE:H	20:R3:356:PRO:CD	2.25	0.48
1:00:345:LYS:HE2	1:00:387:THR:HB	1.96	0.48
2:10:819:GLN:C	2:11:615:ASP:OD1	2.51	0.48
2:10:1593:ILE:O	2:14:1674:THR:HG22	2.05	0.48
2:12:1424:GLY:HA2	2:15:1102:ASN:HD22	1.78	0.48
14:L0:370:TRP:CE3	15:M0:428:ARG:HD2	2.49	0.48
2:10:1254:LYS:HG2	2:11:1100:ASN:CG	2.33	0.48
2:12:1523:HIS:HE1	2:13:1097:HIS:HB3	1.77	0.48
2:15:1132:GLN:NE2	2:16:1366:ASN:CG	2.66	0.48
2:15:1132:GLN:OE1	2:16:1366:ASN:OD1	2.31	0.48
2:15:1668:LYS:HE3	2:15:1706:TYR:CG	2.49	0.48
18:P0:162:SER:CB	18:P0:170:ARG:HH22	2.25	0.48
14:L1:323:ASP:CB	15:M1:428:ARG:CG	2.59	0.48
2:10:819:GLN:HA	2:11:614:ASN:HD22	1.78	0.48
2:11:819:GLN:N	2:12:617:ASN:CG	2.66	0.48
2:16:619:GLY:N	2:17:816:GLN:HG2	2.27	0.48
20:R2:87:LYS:HE3	20:R2:92:ASP:OD1	2.14	0.48
2:10:819:GLN:O	2:11:615:ASP:OD1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:13:1633:LYS:HD3	2:17:1593:ILE:HG22	1.94	0.48
4:A4:138:TYR:CE1	6:C2:1323:LYS:HE3	2.49	0.48
20:R3:469:ASP:OD2	20:R3:471:LYS:HE3	2.14	0.48
16:N3:103:LEU:HD21	20:R3:1738:LYS:HB2	1.95	0.48
20:R3:1483:LEU:HG	20:R3:1530:VAL:HG22	1.96	0.48
2:14:1124:LEU:CD1	2:15:1269:ASN:HB3	2.43	0.48
2:10:1469:ASP:OD2	2:11:1101:PRO:HD2	2.13	0.47
2:11:819:GLN:N	2:12:617:ASN:OD1	2.47	0.47
2:11:1102:ASN:HD21	2:14:1425:ARG:HH11	0.88	0.47
4:A2:138:TYR:CE1	6:C1:1323:LYS:HE3	2.49	0.47
5:B0:1780:LYS:HE2	5:B0:1839:TYR:CE1	2.49	0.47
5:B1:126:GLU:CD	5:B1:126:GLU:H	2.18	0.47
20:R0:87:LYS:HE3	20:R0:92:ASP:OD1	2.13	0.47
2:14:477:HIS:HD1	2:14:479:GLN:N	2.11	0.47
15:M3:366:GLU:CD	15:M3:370:ARG:HE	2.18	0.47
20:R0:355:ILE:H	20:R0:356:PRO:HD3	1.79	0.47
1:01:345:LYS:HE2	1:01:387:THR:HB	1.96	0.47
2:10:1351:ILE:CD1	2:14:1425:ARG:NH1	2.55	0.47
2:11:1430:LYS:CG	2:15:1354:ILE:HB	2.44	0.47
2:16:213:ARG:HG2	2:17:394:ALA:HB2	1.89	0.47
2:11:1412:LYS:CA	2:12:1130:THR:HB	2.26	0.47
2:12:1065:GLN:NE2	2:13:1037:GLN:HE21	1.42	0.47
2:13:1355:PRO:HG2	2:17:1377:LEU:HD21	1.95	0.47
4:A3:835:LYS:CE	4:A3:844:TYR:CE1	2.97	0.47
4:A5:835:LYS:HE3	4:A5:844:TYR:CE1	2.49	0.47
2:10:819:GLN:C	2:11:615:ASP:CG	2.73	0.47
2:10:1307:GLU:H	2:10:1307:GLU:CD	2.18	0.47
2:11:823:SER:HB2	2:12:622:SER:H	1.80	0.47
2:11:1377:LEU:HD21	2:15:1355:PRO:HD2	1.96	0.47
2:14:614:ASN:OD1	2:15:816:GLN:CG	2.62	0.47
5:B0:126:GLU:CD	5:B0:126:GLU:H	2.18	0.47
5:B1:1763:GLN:HA	10:H3:397:GLU:OE2	2.15	0.47
6:C3:325:LYS:HE2	6:C3:391:HIS:HA	1.96	0.47
16:N2:103:LEU:HD21	20:R2:1738:LYS:HB2	1.97	0.47
2:13:1354:ILE:HD13	2:17:1420:ALA:O	2.14	0.47
4:A3:835:LYS:HE3	4:A3:844:TYR:CE1	2.50	0.47
5:B1:627:LEU:HD22	5:B1:688:ARG:HD2	1.96	0.47
19:Q0:104:LYS:HE2	19:Q0:105:PHE:CZ	2.50	0.47
2:10:1354:ILE:HB	2:14:1430:LYS:CG	2.45	0.47
2:12:1695:VAL:HG21	2:16:1664:ILE:CD1	2.45	0.47
2:16:213:ARG:HE	2:17:394:ALA:CB	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T3:357:HIS:HB3	21:T3:378:LEU:HD11	1.96	0.47
25:X3:260:PHE:CD2	25:X3:364:ALA:HB1	2.49	0.47
2:11:1412:LYS:CA	2:12:1095:ILE:CD1	2.73	0.47
6:C3:1158:PHE:CE2	6:C3:1162:LYS:HE2	2.50	0.47
21:T2:11:TYR:HH	21:T2:594:PRO:N	2.13	0.47
2:12:477:HIS:CG	2:12:546:ASN:HD22	2.33	0.46
17:O2:115:LYS:HE2	17:O2:164:ILE:O	2.14	0.46
2:15:1130:THR:HB	2:16:1411:ASP:C	2.33	0.46
12:J1:686:LYS:HE3	23:V1:785:ASP:OD1	2.16	0.46
14:L1:344:LEU:HD21	14:L1:371:ARG:NH1	2.31	0.46
2:12:1249:HIS:CE1	2:13:1146:GLN:HE22	2.33	0.46
2:14:1101:PRO:CG	2:15:1523:HIS:HB3	2.45	0.46
6:C1:1269:ASN:HB2	7:D0:1575:TYR:CG	2.49	0.46
18:P0:447:LYS:HE3	18:P0:464:HIS:CG	2.49	0.46
19:Q3:15:LYS:HE3	19:Q3:71:THR:O	2.16	0.46
20:R2:247:THR:HG21	20:R2:264:LYS:HE2	1.97	0.46
21:T1:52:LYS:HE2	21:T1:53:GLU:OE1	2.15	0.46
2:13:1422:ARG:HB2	2:17:1354:ILE:HD11	1.97	0.46
2:16:619:GLY:C	2:17:819:GLN:CB	2.84	0.46
11:I3:242:LYS:HZ1	11:I3:273:ILE:HD13	1.81	0.46
2:11:1430:LYS:HG3	2:15:1354:ILE:HB	1.98	0.46
2:11:1699:SER:CB	2:16:1819:THR:HG1	2.28	0.46
2:12:1519:LYS:O	2:13:1141:THR:HG21	2.15	0.46
2:15:743:CYS:HG	2:15:781:CYS:HG	1.60	0.46
2:10:819:GLN:HE21	2:11:614:ASN:CA	2.28	0.46
2:10:1489:ASN:H	2:10:1512:VAL:HG23	1.81	0.46
2:11:833:LYS:CB	2:12:613:ASN:ND2	2.66	0.46
5:B1:623:PHE:CE1	5:B1:685:VAL:HG21	2.51	0.46
2:10:1241:LYS:O	2:10:1244:THR:HG23	2.16	0.46
2:12:1521:MET:SD	2:13:1097:HIS:HB3	2.55	0.46
2:13:1430:LYS:HG3	2:17:1354:ILE:O	2.15	0.46
5:B0:623:PHE:CE1	5:B0:685:VAL:HG21	2.51	0.46
18:P0:818:LYS:HA	18:P0:821:TRP:CD1	2.51	0.46
21:T3:52:LYS:HE2	21:T3:53:GLU:OE1	2.15	0.46
2:12:1489:ASN:H	2:12:1512:VAL:HG23	1.81	0.46
2:14:1145:ILE:HA	2:15:1161:HIS:NE2	2.31	0.46
6:C2:382:ILE:HD12	6:C2:485:GLN:HE22	1.81	0.46
2:12:836:LYS:CE	2:13:712:LYS:HB3	2.32	0.46
2:14:735:ASN:HD22	2:15:840:ILE:CG2	2.29	0.46
2:16:1100:ASN:HA	2:17:1253:ASN:OD1	2.15	0.46
4:A3:894:PHE:CD2	4:A3:894:PHE:CB	2.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L1:132:GLU:CD	14:L1:132:GLU:H	2.18	0.46
14:L1:296:GLU:HA	14:L1:299:LEU:HB3	1.98	0.46
4:A0:138:TYR:CE1	6:C0:1323:LYS:HE3	2.51	0.46
21:T2:357:HIS:HB3	21:T2:378:LEU:HD11	1.98	0.46
1:01:770:LYS:HE3	23:V1:791:GLN:O	2.15	0.45
2:12:477:HIS:CD2	2:12:546:ASN:HD22	2.34	0.45
2:16:1178:ILE:HD13	2:17:1347:GLN:HB2	1.98	0.45
7:D2:388:LYS:HE3	7:D2:408:ASP:OD2	2.16	0.45
19:Q1:15:LYS:HE3	19:Q1:71:THR:O	2.16	0.45
19:Q2:15:LYS:HE3	19:Q2:71:THR:O	2.16	0.45
2:11:1354:ILE:HD13	2:15:1420:ALA:O	2.15	0.45
2:14:614:ASN:OD1	2:15:812:GLN:O	2.34	0.45
12:J0:521:ILE:HA	12:J0:525:GLU:OE2	2.16	0.45
14:L1:299:LEU:HD13	15:M1:457:ASN:HD22	1.81	0.45
2:11:1698:SER:C	2:16:1739:LYS:HG3	2.35	0.45
2:13:1749:PHE:HE2	2:17:1669:GLU:H	1.63	0.45
17:O2:6:ARG:HH21	17:O2:459:GLU:CD	2.20	0.45
24:W0:466:GLU:CD	24:W0:528:LYS:HZ1	2.20	0.45
2:15:1207:LEU:CG	2:15:1564:SER:HB3	2.45	0.45
6:C1:382:ILE:HD12	6:C1:485:GLN:HE22	1.82	0.45
16:N3:236:SER:HB3	16:N3:255:LYS:HE2	1.98	0.45
2:12:1354:ILE:HB	2:16:1430:LYS:CG	2.47	0.45
2:14:1145:ILE:HA	2:15:1161:HIS:HE2	1.81	0.45
2:15:1544:HIS:NE2	2:15:1716:TYR:HE1	2.15	0.45
6:C1:498:CYS:C	12:J3:641:LYS:HE2	2.37	0.45
6:C1:1073:LEU:HD12	6:C1:1073:LEU:H	1.81	0.45
19:Q1:363:LEU:HD22	19:Q1:364:PRO:HD3	1.99	0.45
21:T0:196:TYR:CE1	21:T0:197:LYS:HE3	2.51	0.45
2:12:833:LYS:HZ3	2:13:711:ARG:HH12	1.52	0.45
2:14:958:TYR:CE1	2:14:960:ASN:HB2	2.51	0.45
12:J2:591:VAL:HG22	12:J3:526:SER:CB	2.46	0.45
18:P2:660:LYS:HE3	19:Q2:324:TRP:CE3	2.52	0.45
2:10:1355:PRO:HD2	2:14:1377:LEU:CD2	2.45	0.45
2:11:1354:ILE:HB	2:15:1430:LYS:CG	2.43	0.45
19:Q1:15:LYS:HZ2	19:Q1:72:GLU:CD	2.20	0.45
2:10:1153:PHE:HA	2:10:1173:THR:O	2.17	0.45
2:10:1377:LEU:CD2	2:14:1355:PRO:HD2	2.47	0.45
2:10:1430:LYS:CG	2:14:1354:ILE:HB	2.47	0.45
2:11:1398:ASP:HA	2:12:1093:ASN:HD21	1.81	0.45
2:13:1354:ILE:HB	2:17:1430:LYS:CG	2.47	0.45
13:K2:889:SER:CB	14:L2:847:ARG:CZ	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L0:864:LYS:HE2	14:L0:868:ASP:OD2	2.17	0.45
18:P1:660:LYS:HE3	19:Q1:324:TRP:CD2	2.51	0.45
14:L0:344:LEU:HD21	14:L0:371:ARG:NH1	2.32	0.45
21:T0:196:TYR:CZ	21:T0:197:LYS:HE3	2.52	0.45
2:10:820:GLN:N	2:11:615:ASP:OD2	2.50	0.45
6:C2:1073:LEU:HD12	6:C2:1073:LEU:H	1.81	0.45
14:L1:299:LEU:HD11	15:M1:457:ASN:ND2	2.31	0.45
18:P1:733:LEU:HD21	18:P1:786:ILE:HG23	1.97	0.45
19:Q1:26:ASP:HB3	19:Q1:51:SER:HB3	1.99	0.45
2:12:820:GLN:CD	2:13:613:ASN:ND2	2.61	0.44
2:12:834:LYS:CG	2:13:712:LYS:NZ	2.61	0.44
2:12:1668:LYS:HE3	2:12:1706:TYR:CG	2.52	0.44
2:15:1130:THR:HB	2:16:1411:ASP:CB	2.44	0.44
2:16:619:GLY:HA2	2:17:816:GLN:HG2	1.98	0.44
18:P2:733:LEU:HD21	18:P2:786:ILE:HG23	1.99	0.44
25:X0:260:PHE:CD2	25:X0:364:ALA:HB1	2.52	0.44
2:15:1489:ASN:H	2:15:1512:VAL:HG23	1.83	0.44
2:16:410:ILE:HD12	2:16:417:ARG:HE	1.82	0.44
2:10:1668:LYS:HE3	2:10:1706:TYR:CG	2.52	0.44
2:12:1377:LEU:CD2	2:16:1355:PRO:HD2	2.47	0.44
2:12:1523:HIS:CE1	2:13:1097:HIS:C	2.91	0.44
2:13:281:ILE:HG21	2:13:399:ILE:HD13	2.00	0.44
2:14:1144:THR:O	2:15:1161:HIS:NE2	2.47	0.44
2:16:295:ARG:NH1	2:17:463:GLN:HE21	1.95	0.44
2:16:619:GLY:HA2	2:17:816:GLN:CB	2.46	0.44
18:P3:660:LYS:HE3	19:Q3:324:TRP:CD2	2.52	0.44
2:12:1355:PRO:HD2	2:16:1377:LEU:CD2	2.48	0.44
2:16:622:SER:OG	2:17:823:SER:HA	2.17	0.44
4:A1:87:LYS:HE3	4:A4:66:PRO:HB2	1.99	0.44
6:C3:207:LEU:HA	6:C3:211:ASP:OD2	2.17	0.44
2:10:1594:ALA:HB2	2:14:1674:THR:HG23	2.00	0.44
2:12:1520:ASP:HB3	2:13:1130:THR:HG21	1.99	0.44
11:I0:242:LYS:NZ	11:I0:273:ILE:HG21	2.32	0.44
11:I2:190:ASN:HA	11:I3:252:HIS:CE1	2.53	0.44
14:L3:344:LEU:HD21	14:L3:371:ARG:NH1	2.33	0.44
15:M0:813:ILE:O	15:M0:821:LYS:HE2	2.17	0.44
18:P2:660:LYS:HE3	19:Q2:324:TRP:CD2	2.53	0.44
20:R3:190:GLY:N	21:T2:629:PHE:CD2	2.85	0.44
23:V0:701:THR:HG23	24:W0:810:ILE:HD11	1.99	0.44
2:12:906:LYS:HZ3	2:13:735:ASN:CB	2.27	0.44
14:L1:865:LYS:HE2	14:L1:869:ASP:OD2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W0:238:GLY:HA3	24:W0:245:THR:HG22	1.99	0.44
2:10:50:LYS:HE3	2:10:51:TYR:CE2	2.53	0.44
2:14:1124:LEU:HD12	2:15:1269:ASN:HA	1.73	0.44
7:D1:1243:LEU:HD11	7:D1:1280:LYS:HE2	2.00	0.44
12:J1:672:LYS:HE2	12:J1:676:ASP:OD2	2.18	0.44
21:T2:36:GLU:CD	21:T2:368:LYS:HE2	2.38	0.44
2:12:544:LYS:NZ	2:13:297:ILE:CD1	2.80	0.44
2:12:1430:LYS:CG	2:16:1354:ILE:HB	2.48	0.44
2:15:410:ILE:HD12	2:15:417:ARG:HE	1.83	0.44
4:A5:835:LYS:HE3	4:A5:844:TYR:CZ	2.53	0.44
6:C1:838:ASN:O	6:C1:890:THR:HA	2.18	0.44
7:D0:388:LYS:HE3	7:D0:408:ASP:OD2	2.17	0.44
20:R0:247:THR:HG21	20:R0:264:LYS:HE2	2.00	0.44
20:R3:1621:PHE:CD2	20:R3:1649:CYS:HB2	2.53	0.44
2:11:1406:LYS:NZ	2:14:1405:ASN:HD22	2.11	0.44
2:14:712:LYS:NZ	2:15:861:ASN:O	2.48	0.44
2:16:619:GLY:N	2:17:816:GLN:HA	2.27	0.44
2:17:1668:LYS:HE3	2:17:1706:TYR:CG	2.53	0.44
4:A4:584:LYS:HE3	4:A4:608:GLN:OE1	2.18	0.44
4:A5:835:LYS:HE2	4:A5:844:TYR:CE1	2.53	0.44
18:P3:804:SER:HB2	18:P3:840:PHE:CE1	2.53	0.44
19:Q1:247:ILE:HD11	19:Q1:262:ILE:HD11	1.99	0.44
5:B0:2082:LYS:HE2	5:B0:2086:GLU:OE1	2.18	0.43
6:C3:365:LEU:HD11	6:C3:369:LYS:HE3	2.00	0.43
2:11:833:LYS:CD	2:12:611:ASN:CB	2.26	0.43
13:K1:820:TYR:CD2	13:K1:858:LYS:HE3	2.53	0.43
20:R0:469:ASP:OD2	20:R0:471:LYS:HE3	2.17	0.43
20:R3:87:LYS:HE3	20:R3:92:ASP:OD2	2.18	0.43
24:W1:953:GLU:CD	24:W1:957:LYS:HZ1	2.21	0.43
2:13:319:LYS:HB3	2:13:456:LEU:HD13	1.99	0.43
2:16:1178:ILE:HD13	2:17:1347:GLN:CB	2.49	0.43
14:L0:370:TRP:CD2	15:M0:428:ARG:HD2	2.53	0.43
15:M2:366:GLU:CD	15:M2:370:ARG:HE	2.20	0.43
2:11:822:GLN:CD	2:12:617:ASN:CB	2.60	0.43
2:12:820:GLN:NE2	2:13:613:ASN:OD1	2.41	0.43
2:12:833:LYS:CD	2:13:711:ARG:NH1	2.81	0.43
2:13:984:LYS:CE	2:15:1397:LYS:CE	2.73	0.43
2:14:614:ASN:HD21	2:15:813:GLU:CA	2.31	0.43
6:C1:1095:ASN:HA	6:C1:1098:LYS:HZ2	1.83	0.43
20:R1:1621:PHE:CD2	20:R1:1649:CYS:HB2	2.53	0.43
1:00:263:PHE:CD2	1:00:324:VAL:HG22	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:736:GLY:HA2	2:15:839:GLU:CG	2.48	0.43
2:16:1668:LYS:HE3	2:16:1706:TYR:CG	2.54	0.43
4:A1:540:THR:HG22	4:A1:554:TRP:CE2	2.53	0.43
19:Q0:314:ASP:CG	19:Q0:376:LYS:HZ3	2.22	0.43
21:T1:357:HIS:HB3	21:T1:378:LEU:HD11	2.00	0.43
1:00:244:TYR:CG	1:00:248:ILE:HD11	2.54	0.43
2:10:819:GLN:CA	2:11:615:ASP:OD1	2.66	0.43
5:B1:2082:LYS:HE2	5:B1:2086:GLU:OE1	2.18	0.43
6:C3:421:GLN:CD	19:Q1:1:MET:HA	2.39	0.43
12:J0:672:LYS:HE2	12:J0:676:ASP:OD2	2.19	0.43
2:10:1430:LYS:HG2	2:14:1354:ILE:HB	2.00	0.43
2:11:1668:LYS:HE3	2:11:1706:TYR:CG	2.54	0.43
4:A2:112:LYS:HE2	4:A2:116:GLU:OE1	2.18	0.43
14:L1:318:SER:HB2	15:M1:462:PHE:CG	2.53	0.43
25:X1:260:PHE:CD2	25:X1:364:ALA:HB1	2.54	0.43
2:12:833:LYS:CB	2:13:711:ARG:HD2	2.48	0.43
2:13:50:LYS:HE3	2:13:51:TYR:CE2	2.54	0.43
2:14:1178:ILE:O	2:15:1244:THR:CG2	2.63	0.43
2:15:1132:GLN:NE2	2:16:1366:ASN:OD1	2.52	0.43
3:41:204:GLU:H	3:41:204:GLU:CD	2.21	0.43
4:A3:835:LYS:HE2	4:A3:844:TYR:CE1	2.53	0.43
13:K2:621:LYS:HE2	13:K2:625:GLU:OE2	2.18	0.43
14:L1:386:SER:HB3	15:M1:439:SER:HB3	1.90	0.43
20:R1:355:ILE:H	20:R1:356:PRO:HD3	1.84	0.43
2:10:1813:LYS:CE	2:14:1743:SER:OG	2.66	0.43
2:12:50:LYS:HE3	2:12:51:TYR:CE2	2.54	0.43
6:C2:1158:PHE:CZ	6:C2:1162:LYS:HE2	2.54	0.43
14:L1:323:ASP:OD1	15:M1:428:ARG:CG	2.66	0.43
2:12:1443:GLU:CD	2:12:1467:ARG:HE	2.23	0.43
2:14:614:ASN:HA	2:15:816:GLN:HE22	1.33	0.43
2:17:410:ILE:HD12	2:17:417:ARG:HE	1.84	0.43
6:C0:414:GLN:NE2	6:C0:418:ASN:HD21	2.15	0.43
12:J4:634:LYS:HE2	12:J4:638:ASP:OD2	2.19	0.43
18:P3:660:LYS:HE3	19:Q3:324:TRP:CE3	2.54	0.43
2:10:1443:GLU:CD	2:10:1467:ARG:HE	2.23	0.42
2:13:1354:ILE:HD11	2:17:1421:VAL:C	2.40	0.42
2:13:1668:LYS:HE3	2:13:1706:TYR:CG	2.53	0.42
2:16:1102:ASN:OD1	2:17:1254:LYS:CE	2.61	0.42
4:A1:584:LYS:HE3	4:A1:608:GLN:OE1	2.19	0.42
14:L2:864:LYS:HE2	14:L2:868:ASP:OD2	2.19	0.42
18:P3:733:LEU:HD21	18:P3:786:ILE:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:16:1443:GLU:CD	2:16:1467:ARG:HE	2.22	0.42
4:A1:835:LYS:HE2	4:A1:844:TYR:CE1	2.54	0.42
13:K2:820:TYR:CD2	13:K2:858:LYS:HE3	2.53	0.42
18:P0:739:ILE:HD11	18:P0:776:ILE:HD12	2.01	0.42
2:10:819:GLN:NE2	2:11:614:ASN:HA	2.31	0.42
2:16:213:ARG:HH12	2:17:357:PRO:N	2.18	0.42
13:K0:619:LYS:HZ3	13:K0:694:ASP:CG	2.22	0.42
14:L0:131:MET:HA	14:L0:134:GLU:OE1	2.20	0.42
2:12:1521:MET:SD	2:13:1097:HIS:CB	3.06	0.42
2:13:782:ARG:NH1	2:13:861:ASN:HD21	2.17	0.42
14:L1:323:ASP:CG	15:M1:428:ARG:CD	2.60	0.42
20:R2:355:ILE:H	20:R2:356:PRO:HD3	1.85	0.42
21:T3:36:GLU:CD	21:T3:368:LYS:HE2	2.40	0.42
1:01:244:TYR:CG	1:01:248:ILE:HD11	2.55	0.42
2:11:1443:GLU:CD	2:11:1467:ARG:HE	2.23	0.42
2:12:1354:ILE:HD11	2:16:1421:VAL:C	2.40	0.42
2:12:1520:ASP:HB3	2:13:1130:THR:CB	2.49	0.42
2:13:1430:LYS:CG	2:17:1354:ILE:HB	2.49	0.42
2:13:1443:GLU:CD	2:13:1467:ARG:HE	2.23	0.42
4:A3:540:THR:HG22	4:A3:554:TRP:CE2	2.54	0.42
14:L0:322:PRO:HG2	15:M0:428:ARG:CD	2.50	0.42
20:R1:1097:LYS:HA	20:R1:1133:LYS:HE2	2.01	0.42
25:X2:260:PHE:CD2	25:X2:364:ALA:HB1	2.54	0.42
2:12:833:LYS:HZ2	2:13:711:ARG:HH12	1.34	0.42
13:K0:904:LYS:HE2	13:K0:908:ASP:OD2	2.20	0.42
20:R0:1139:GLU:HA	20:R0:1147:ILE:HD11	2.01	0.42
21:T3:1025:LYS:HZ1	21:T3:1052:GLU:CD	2.23	0.42
23:V0:702:LYS:HE2	23:V0:706:GLU:OE1	2.20	0.42
2:11:833:LYS:CE	2:12:611:ASN:CB	2.92	0.42
2:14:1668:LYS:HE3	2:14:1706:TYR:CG	2.54	0.42
2:15:1095:ILE:HG23	2:16:1412:LYS:HE3	1.73	0.42
6:C3:420:TYR:CD1	19:Q1:382:GLN:NE2	2.87	0.42
14:L1:369:PHE:C	15:M1:446:LEU:HD13	2.40	0.42
24:W1:466:GLU:CD	24:W1:528:LYS:HZ1	2.23	0.42
2:11:833:LYS:HD3	2:12:611:ASN:HB3	0.51	0.42
2:14:1494:SER:CB	2:15:1288:LEU:CD1	2.67	0.42
23:V1:701:THR:HG23	24:W1:810:ILE:HD11	2.01	0.42
24:W1:166:LYS:HE3	24:W1:183:SER:HA	2.01	0.42
4:A2:689:ILE:N	4:A2:698:HIS:HD1	2.18	0.42
17:O1:168:PRO:HD2	17:O1:370:TRP:CD1	2.55	0.42
19:Q0:145:SER:O	19:Q0:190:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R0:36:SER:HB3	20:R0:39:ASP:CG	2.40	0.42
2:10:1706:TYR:HH	2:14:1786:LEU:HD13	1.72	0.42
2:12:1521:MET:SD	2:13:1097:HIS:CG	2.98	0.42
6:C1:758:GLU:CD	6:C1:758:GLU:H	2.23	0.42
13:K1:621:LYS:HE2	13:K1:625:GLU:OE2	2.20	0.42
13:K3:534:LYS:HE3	13:K3:601:LEU:HD23	2.02	0.42
19:Q2:247:ILE:HD11	19:Q2:262:ILE:HD11	2.02	0.42
20:R0:1630:GLN:HE22	20:R0:1654:LEU:CD1	2.33	0.42
20:R1:163:HIS:CD2	20:R1:164:PRO:HD2	2.55	0.42
20:R2:1621:PHE:CD2	20:R2:1649:CYS:HB2	2.55	0.42
2:12:1519:LYS:HZ3	2:12:1520:ASP:CG	2.24	0.41
4:A2:112:LYS:HE2	4:A2:116:GLU:CD	2.40	0.41
5:B0:1147:ILE:HG23	5:B0:1209:PHE:HB2	2.02	0.41
5:B1:1780:LYS:HE2	5:B1:1839:TYR:CZ	2.55	0.41
6:C2:365:LEU:HD11	6:C2:369:LYS:HE3	2.02	0.41
14:L0:321:ASP:HB2	14:L0:322:PRO:HD3	2.01	0.41
20:R3:1630:GLN:HE22	20:R3:1654:LEU:HD11	1.85	0.41
24:W1:238:GLY:HA3	24:W1:245:THR:HG22	2.02	0.41
1:01:263:PHE:CD2	1:01:324:VAL:HG22	2.55	0.41
2:11:1366:ASN:OD1	2:12:1132:GLN:CD	2.59	0.41
2:11:1425:ARG:HH22	2:15:1470:ILE:HG21	1.86	0.41
2:16:619:GLY:CA	2:17:819:GLN:CB	2.92	0.41
5:B0:1780:LYS:HE2	5:B0:1839:TYR:CZ	2.54	0.41
18:P1:818:LYS:HA	18:P1:821:TRP:CD1	2.55	0.41
20:R3:36:SER:HB3	20:R3:39:ASP:CG	2.41	0.41
20:R3:189:SER:HA	21:T2:629:PHE:CG	2.50	0.41
24:W0:166:LYS:HE3	24:W0:183:SER:HA	2.02	0.41
2:16:1244:THR:HG23	2:16:1269:ASN:HD21	1.86	0.41
2:17:1443:GLU:CD	2:17:1467:ARG:HE	2.23	0.41
4:A4:540:THR:HG22	4:A4:554:TRP:CE2	2.55	0.41
6:C3:420:TYR:CE1	19:Q1:382:GLN:HA	2.55	0.41
7:D2:715:TYR:CE1	7:D2:721:SER:HB3	2.55	0.41
14:L1:318:SER:HG	15:M1:462:PHE:HB3	1.81	0.41
19:Q1:363:LEU:CD2	19:Q1:364:PRO:HD3	2.50	0.41
2:10:822:GLN:OE1	2:11:614:ASN:OD1	2.32	0.41
2:10:1254:LYS:CE	2:11:1099:ASP:O	2.64	0.41
2:11:50:LYS:HE3	2:11:51:TYR:CE2	2.56	0.41
2:11:410:ILE:HD12	2:11:417:ARG:HE	1.84	0.41
2:13:1003:GLN:NE2	2:15:1410:LEU:CD1	2.78	0.41
2:13:1355:PRO:HD2	2:17:1377:LEU:CD2	2.50	0.41
2:14:1443:GLU:CD	2:14:1467:ARG:HE	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:15:1544:HIS:CE1	2:15:1711:ASN:HB3	2.48	0.41
6:C1:1158:PHE:CZ	6:C1:1162:LYS:HE2	2.55	0.41
6:C2:758:GLU:H	6:C2:758:GLU:CD	2.24	0.41
6:C3:352:LYS:HG2	6:C3:353:SER:H	1.85	0.41
13:K2:1010:VAL:HG12	14:L2:973:LEU:HD21	2.00	0.41
17:O1:157:GLN:HE22	17:O1:180:SER:HB2	1.86	0.41
18:P0:470:LYS:HE2	18:P0:474:GLU:OE2	2.19	0.41
20:R0:1425:LYS:HE2	20:R0:1500:TYR:CZ	2.55	0.41
20:R1:1139:GLU:HA	20:R1:1147:ILE:HD11	2.01	0.41
20:R2:1630:GLN:HE22	20:R2:1654:LEU:HD11	1.86	0.41
2:10:819:GLN:OE1	2:11:615:ASP:CA	2.59	0.41
2:11:1646:GLY:HA3	2:15:1740:ILE:HG12	2.01	0.41
2:16:1453:VAL:CG1	2:16:1604:ARG:HH22	2.34	0.41
2:17:1489:ASN:H	2:17:1512:VAL:HG23	1.86	0.41
3:41:261:ARG:HH21	8:E1:621:ARG:NE	2.18	0.41
6:C3:837:ILE:O	6:C3:890:THR:HA	2.20	0.41
17:O2:155:GLU:OE2	17:O2:158:LYS:HE2	2.20	0.41
19:Q2:140:ARG:CZ	19:Q2:221:ASN:HA	2.51	0.41
20:R2:1139:GLU:HA	20:R2:1147:ILE:HD11	2.02	0.41
17:O2:168:PRO:HD2	17:O2:370:TRP:CD1	2.54	0.41
21:T1:196:TYR:CZ	21:T1:197:LYS:HE3	2.56	0.41
1:01:70:GLU:HG2	1:01:102:PHE:CE1	2.56	0.41
2:11:477:HIS:CE1	2:11:549:ASN:HA	2.55	0.41
2:16:619:GLY:CA	2:17:816:GLN:HG2	2.51	0.41
6:C0:1225:PRO:CG	24:W0:316:LYS:HE2	2.50	0.41
8:E1:393:ARG:CZ	8:E1:538:SER:HB3	2.50	0.41
13:K3:621:LYS:HE2	13:K3:625:GLU:CD	2.41	0.41
24:W0:476:THR:HG22	24:W0:514:ILE:HD13	2.03	0.41
2:10:1356:ILE:O	2:14:1430:LYS:HD2	2.21	0.41
2:10:1698:SER:HB2	2:14:1745:ARG:NH1	2.35	0.41
2:12:1356:ILE:O	2:16:1430:LYS:HD2	2.21	0.41
2:13:984:LYS:HZ3	2:15:1395:SER:CA	2.34	0.41
2:13:1746:GLN:NE2	2:17:1669:GLU:C	2.73	0.41
2:15:743:CYS:SG	2:15:781:CYS:SG	3.16	0.41
4:A2:267:MET:HA	4:A2:361:LYS:HE2	2.02	0.41
4:A3:584:LYS:HE3	4:A3:608:GLN:OE1	2.20	0.41
20:R2:163:HIS:CD2	20:R2:164:PRO:HD2	2.55	0.41
20:R3:355:ILE:H	20:R3:356:PRO:HD3	1.85	0.41
24:W0:332:THR:HG21	24:W0:335:PHE:CE1	2.55	0.41
1:00:70:GLU:HG2	1:00:102:PHE:CE1	2.55	0.41
1:01:779:ASP:O	12:J1:696:LYS:HE2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:1354:ILE:HD11	2:14:1421:VAL:C	2.41	0.41
2:10:1717:GLN:HE21	2:14:1754:GLN:HE22	1.61	0.41
2:12:1521:MET:HG3	2:13:1097:HIS:CE1	2.56	0.41
2:14:1244:THR:HG23	2:14:1269:ASN:HD21	1.86	0.41
2:15:846:ARG:HH12	2:15:1042:ASN:HB2	1.85	0.41
2:15:1443:GLU:CD	2:15:1467:ARG:HE	2.24	0.41
2:16:295:ARG:NH2	2:17:463:GLN:HG2	2.36	0.41
2:16:618:GLY:C	2:17:816:GLN:HG3	2.36	0.41
2:17:1307:GLU:H	2:17:1307:GLU:CD	2.23	0.41
6:C1:365:LEU:HD11	6:C1:369:LYS:HE3	2.02	0.41
6:C3:1095:ASN:HA	6:C3:1098:LYS:HZ2	1.86	0.41
7:D0:715:TYR:CE1	7:D0:721:SER:HB3	2.55	0.41
7:D3:1352:HIS:HA	7:D3:1421:THR:HG21	2.03	0.41
13:K2:1027:LEU:CD1	14:L2:962:SER:HA	2.51	0.41
15:M1:870:LYS:HZ2	20:R1:1268:GLU:CD	2.25	0.41
20:R1:1657:HIS:HB3	20:R1:1679:TRP:CH2	2.56	0.41
20:R3:163:HIS:CD2	20:R3:164:PRO:HD2	2.56	0.41
20:R3:550:ILE:HG22	20:R3:642:LYS:HE3	2.03	0.41
21:T0:450:LYS:HE2	21:T0:471:ASP:OD2	2.21	0.41
2:11:1404:ASP:N	2:14:1406:LYS:HE3	2.36	0.41
2:11:1718:TYR:CE2	2:15:1752:ASN:ND2	2.82	0.41
2:16:295:ARG:HH12	2:17:463:GLN:NE2	2.15	0.41
7:D2:1088:THR:HB	7:D2:1089:PRO:HD3	2.02	0.41
14:L1:386:SER:CB	15:M1:439:SER:OG	2.40	0.41
21:T2:72:PHE:CD1	21:T2:109:LYS:NZ	2.89	0.41
24:W0:246:ARG:HD2	24:W0:275:PHE:CZ	2.56	0.41
2:10:1254:LYS:CG	2:11:1100:ASN:CG	2.90	0.40
2:10:1715:THR:CG2	2:14:1671:THR:HG1	2.34	0.40
3:40:261:ARG:HH21	8:E0:621:ARG:NE	2.19	0.40
14:L1:318:SER:OG	15:M1:462:PHE:CB	2.58	0.40
18:P1:804:SER:HB2	18:P1:840:PHE:CE1	2.56	0.40
24:W0:659:ASN:HD21	24:W0:757:ILE:HD12	1.86	0.40
24:W0:837:LYS:HE2	24:W0:841:ASP:OD1	2.22	0.40
24:W1:50:SER:O	24:W1:67:LYS:HE3	2.21	0.40
2:10:1425:ARG:HH22	2:14:1470:ILE:HG21	1.86	0.40
2:13:984:LYS:NZ	2:15:1395:SER:OG	2.53	0.40
2:14:1489:ASN:H	2:14:1512:VAL:HG23	1.87	0.40
2:16:1178:ILE:CD1	2:17:1347:GLN:CB	2.98	0.40
6:C3:1073:LEU:HD12	6:C3:1073:LEU:H	1.85	0.40
15:M0:597:LYS:HE3	15:M0:607:ASP:OD1	2.21	0.40
20:R1:469:ASP:OD2	20:R1:471:LYS:HE3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:10:327:MET:HA	2:10:456:LEU:HD13	2.02	0.40
2:10:1813:LYS:HE3	2:14:1743:SER:CB	2.45	0.40
2:11:1780:ASP:CB	2:16:1754:GLN:HE22	2.34	0.40
2:12:833:LYS:CD	2:13:711:ARG:CZ	2.99	0.40
2:16:1101:PRO:HD2	2:17:1253:ASN:OD1	2.20	0.40
13:K0:820:TYR:CG	13:K0:858:LYS:HE3	2.57	0.40
21:T1:450:LYS:HE3	21:T1:471:ASP:OD1	2.21	0.40
24:W0:332:THR:HG23	24:W0:344:LYS:HB2	2.02	0.40
25:X0:260:PHE:CG	25:X0:364:ALA:HB1	2.56	0.40
2:13:984:LYS:HZ3	2:15:1395:SER:C	2.24	0.40
2:14:50:LYS:HE3	2:14:51:TYR:CE2	2.57	0.40
2:14:611:ASN:HA	2:15:819:GLN:HB3	2.04	0.40
6:C0:365:LEU:HD11	6:C0:369:LYS:HE3	2.03	0.40
15:M1:255:ALA:HB3	15:M1:259:LYS:HB2	2.03	0.40
25:X3:190:VAL:O	25:X3:243:LYS:HE2	2.22	0.40
2:10:819:GLN:CA	2:11:614:ASN:HD22	2.34	0.40
2:14:1143:LYS:HE3	2:15:1158:SER:HB2	1.20	0.40
2:17:510:TYR:O	2:17:544:LYS:HE3	2.21	0.40
5:B1:1807:LYS:HE3	5:B1:1811:PHE:CE2	2.57	0.40
14:L0:852:GLU:HB2	14:L0:857:LYS:HE3	2.03	0.40
14:L2:189:LYS:HE2	14:L2:218:TYR:CE2	2.57	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	00	778/3566 (22%)	712 (92%)	56 (7%)	10 (1%)	10 43
1	01	778/3566 (22%)	714 (92%)	54 (7%)	10 (1%)	10 43
2	10	1762/1916 (92%)	1651 (94%)	101 (6%)	10 (1%)	22 60
2	11	1762/1916 (92%)	1638 (93%)	114 (6%)	10 (1%)	22 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	1762/1916 (92%)	1642 (93%)	109 (6%)	11 (1%)	22	60
2	13	1762/1916 (92%)	1642 (93%)	108 (6%)	12 (1%)	19	57
2	14	1762/1916 (92%)	1644 (93%)	108 (6%)	10 (1%)	22	60
2	15	1762/1916 (92%)	1659 (94%)	95 (5%)	8 (0%)	25	64
2	16	1762/1916 (92%)	1634 (93%)	116 (7%)	12 (1%)	19	57
2	17	1762/1916 (92%)	1643 (93%)	107 (6%)	12 (1%)	19	57
3	40	469/471 (100%)	432 (92%)	33 (7%)	4 (1%)	14	52
3	41	469/471 (100%)	433 (92%)	33 (7%)	3 (1%)	22	60
4	A0	797/979 (81%)	755 (95%)	39 (5%)	3 (0%)	30	68
4	A1	691/979 (71%)	647 (94%)	41 (6%)	3 (0%)	30	68
4	A2	691/979 (71%)	654 (95%)	36 (5%)	1 (0%)	48	83
4	A3	691/979 (71%)	649 (94%)	38 (6%)	4 (1%)	22	60
4	A4	691/979 (71%)	648 (94%)	41 (6%)	2 (0%)	37	73
4	A5	746/979 (76%)	708 (95%)	34 (5%)	4 (0%)	25	64
5	B0	1973/2174 (91%)	1834 (93%)	125 (6%)	14 (1%)	19	57
5	B1	1973/2174 (91%)	1837 (93%)	121 (6%)	15 (1%)	16	55
6	C0	1389/1916 (72%)	1303 (94%)	75 (5%)	11 (1%)	16	55
6	C1	1311/1916 (68%)	1236 (94%)	71 (5%)	4 (0%)	37	73
6	C2	1311/1916 (68%)	1232 (94%)	73 (6%)	6 (0%)	25	64
6	C3	1389/1916 (72%)	1300 (94%)	79 (6%)	10 (1%)	19	57
7	D0	1271/1575 (81%)	1186 (93%)	75 (6%)	10 (1%)	16	55
7	D1	1271/1575 (81%)	1189 (94%)	72 (6%)	10 (1%)	16	55
7	D2	1271/1575 (81%)	1183 (93%)	81 (6%)	7 (1%)	22	60
7	D3	1271/1575 (81%)	1185 (93%)	76 (6%)	10 (1%)	16	55
8	E0	591/667 (89%)	550 (93%)	35 (6%)	6 (1%)	13	49
8	E1	591/667 (89%)	550 (93%)	36 (6%)	5 (1%)	16	55
9	F0	91/95 (96%)	88 (97%)	3 (3%)	0	100	100
9	F1	91/95 (96%)	88 (97%)	2 (2%)	1 (1%)	12	47
9	F2	91/95 (96%)	87 (96%)	4 (4%)	0	100	100
9	F3	91/95 (96%)	88 (97%)	2 (2%)	1 (1%)	12	47
10	H0	243/440 (55%)	234 (96%)	7 (3%)	2 (1%)	16	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H1	243/440 (55%)	234 (96%)	8 (3%)	1 (0%)	30	68
10	H2	243/440 (55%)	234 (96%)	9 (4%)	0	100	100
10	H3	243/440 (55%)	235 (97%)	6 (2%)	2 (1%)	16	55
11	I0	195/581 (34%)	187 (96%)	8 (4%)	0	100	100
11	I1	195/581 (34%)	186 (95%)	8 (4%)	1 (0%)	25	64
11	I2	195/581 (34%)	187 (96%)	7 (4%)	1 (0%)	25	64
11	I3	195/581 (34%)	188 (96%)	6 (3%)	1 (0%)	25	64
12	J0	187/709 (26%)	180 (96%)	6 (3%)	1 (0%)	25	64
12	J1	187/709 (26%)	182 (97%)	4 (2%)	1 (0%)	25	64
12	J2	182/709 (26%)	177 (97%)	5 (3%)	0	100	100
12	J3	182/709 (26%)	178 (98%)	4 (2%)	0	100	100
12	J4	182/709 (26%)	179 (98%)	3 (2%)	0	100	100
12	J5	182/709 (26%)	178 (98%)	4 (2%)	0	100	100
13	K0	715/1206 (59%)	672 (94%)	40 (6%)	3 (0%)	30	68
13	K1	715/1206 (59%)	675 (94%)	39 (6%)	1 (0%)	48	83
13	K2	715/1206 (59%)	671 (94%)	42 (6%)	2 (0%)	37	73
13	K3	715/1206 (59%)	670 (94%)	42 (6%)	3 (0%)	30	68
14	L0	792/985 (80%)	744 (94%)	44 (6%)	4 (0%)	25	64
14	L1	792/985 (80%)	749 (95%)	39 (5%)	4 (0%)	25	64
14	L2	792/985 (80%)	748 (94%)	41 (5%)	3 (0%)	30	68
14	L3	787/985 (80%)	739 (94%)	48 (6%)	0	100	100
15	M0	683/889 (77%)	651 (95%)	29 (4%)	3 (0%)	30	68
15	M1	683/889 (77%)	639 (94%)	40 (6%)	4 (1%)	22	60
15	M2	683/889 (77%)	643 (94%)	36 (5%)	4 (1%)	22	60
15	M3	683/889 (77%)	645 (94%)	34 (5%)	4 (1%)	22	60
16	N0	299/301 (99%)	280 (94%)	19 (6%)	0	100	100
16	N1	299/301 (99%)	278 (93%)	21 (7%)	0	100	100
16	N2	299/301 (99%)	279 (93%)	20 (7%)	0	100	100
16	N3	299/301 (99%)	281 (94%)	17 (6%)	1 (0%)	37	73
17	O0	307/467 (66%)	296 (96%)	8 (3%)	3 (1%)	13	49
17	O1	307/467 (66%)	284 (92%)	18 (6%)	5 (2%)	8	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O2	307/467 (66%)	288 (94%)	16 (5%)	3 (1%)	13	49
17	O3	307/467 (66%)	289 (94%)	15 (5%)	3 (1%)	13	49
18	P0	753/890 (85%)	717 (95%)	31 (4%)	5 (1%)	19	57
18	P1	753/890 (85%)	706 (94%)	42 (6%)	5 (1%)	19	57
18	P2	753/890 (85%)	707 (94%)	40 (5%)	6 (1%)	16	55
18	P3	753/890 (85%)	705 (94%)	45 (6%)	3 (0%)	30	68
19	Q0	369/417 (88%)	346 (94%)	22 (6%)	1 (0%)	37	73
19	Q1	369/417 (88%)	339 (92%)	25 (7%)	5 (1%)	9	41
19	Q2	369/417 (88%)	341 (92%)	27 (7%)	1 (0%)	37	73
19	Q3	369/417 (88%)	339 (92%)	29 (8%)	1 (0%)	37	73
20	R0	1786/1791 (100%)	1598 (90%)	165 (9%)	23 (1%)	10	43
20	R1	1786/1791 (100%)	1588 (89%)	169 (10%)	29 (2%)	8	38
20	R2	1786/1791 (100%)	1596 (89%)	159 (9%)	31 (2%)	7	37
20	R3	1784/1791 (100%)	1586 (89%)	171 (10%)	27 (2%)	8	40
21	T0	1049/2221 (47%)	962 (92%)	76 (7%)	11 (1%)	13	49
21	T1	1164/2221 (52%)	1046 (90%)	100 (9%)	18 (2%)	8	40
21	T2	1164/2221 (52%)	1038 (89%)	105 (9%)	21 (2%)	7	35
21	T3	1164/2221 (52%)	1041 (89%)	101 (9%)	22 (2%)	6	32
22	U0	23/1164 (2%)	21 (91%)	1 (4%)	1 (4%)	2	17
22	U1	23/1164 (2%)	22 (96%)	1 (4%)	0	100	100
22	U2	23/1164 (2%)	21 (91%)	1 (4%)	1 (4%)	2	17
22	U3	23/1164 (2%)	21 (91%)	1 (4%)	1 (4%)	2	17
23	V0	256/1704 (15%)	246 (96%)	7 (3%)	3 (1%)	11	44
23	V1	256/1704 (15%)	246 (96%)	9 (4%)	1 (0%)	30	68
24	W0	886/961 (92%)	792 (89%)	84 (10%)	10 (1%)	12	47
24	W1	886/961 (92%)	789 (89%)	86 (10%)	11 (1%)	11	44
25	X0	403/405 (100%)	380 (94%)	21 (5%)	2 (0%)	25	64
25	X1	403/405 (100%)	380 (94%)	20 (5%)	3 (1%)	19	57
25	X2	403/405 (100%)	380 (94%)	21 (5%)	2 (0%)	25	64
25	X3	403/405 (100%)	377 (94%)	25 (6%)	1 (0%)	44	78
All	All	71065/105914 (67%)	66051 (93%)	4470 (6%)	544 (1%)	19	55

All (544) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	00	466	THR
1	01	466	THR
2	10	1300	GLU
2	12	1300	GLU
2	13	1300	GLU
2	14	1300	GLU
2	16	1300	GLU
4	A0	929	ASN
4	A1	501	ILE
4	A2	501	ILE
4	A3	501	ILE
4	A4	501	ILE
4	A5	929	ASN
5	B0	663	ASP
5	B1	663	ASP
6	C1	1115	GLU
6	C1	1131	ARG
6	C2	1115	GLU
6	C2	1131	ARG
7	D0	1028	GLU
7	D0	1385	ASP
7	D1	1028	GLU
8	E0	593	TYR
8	E1	593	TYR
14	L0	201	LEU
14	L1	201	LEU
18	P1	270	GLU
18	P1	459	LEU
18	P2	459	LEU
19	Q1	125	ASN
19	Q1	364	PRO
20	R0	356	PRO
20	R3	184	SER
20	R3	356	PRO
20	R3	957	ASN
20	R3	977	ASN
21	T0	391	SER
21	T1	17	PHE
21	T1	179	GLN
21	T1	219	PHE
21	T2	17	PHE
21	T2	53	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	T2	219	PHE
21	T2	553	ASP
21	T3	219	PHE
21	T3	391	SER
23	V0	701	THR
24	W1	549	ILE
1	00	364	ASP
2	11	1197	ARG
2	11	1300	GLU
2	11	1669	GLU
2	12	1042	ASN
2	16	256	LYS
2	16	1197	ARG
3	40	215	ASN
4	A0	393	LYS
4	A3	67	ASN
5	B0	1201	GLY
5	B0	1245	TYR
5	B1	1201	GLY
5	B1	1245	TYR
6	C0	405	LEU
6	C1	1081	ASN
6	C2	1081	ASN
6	C2	1270	ASN
6	C3	1081	ASN
7	D0	250	ASP
7	D0	1572	PHE
7	D1	250	ASP
7	D2	250	ASP
7	D2	1028	GLU
7	D2	1385	ASP
7	D3	250	ASP
7	D3	731	SER
7	D3	1572	PHE
8	E0	589	ILE
8	E0	592	ASP
8	E1	589	ILE
8	E1	592	ASP
15	M0	689	GLY
15	M1	644	HIS
17	O0	145	LEU
17	O2	364	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P2	270	GLU
19	Q0	26	ASP
20	R0	298	SER
20	R0	977	ASN
20	R0	1548	LYS
20	R0	1549	ASP
20	R1	53	ASN
20	R1	298	SER
20	R1	836	GLN
20	R1	1046	GLU
20	R1	1509	ALA
20	R1	1627	SER
20	R2	7	ASN
20	R2	234	ALA
20	R2	836	GLN
20	R3	234	ALA
20	R3	1549	ASP
21	T0	17	PHE
21	T0	733	ASN
21	T0	1169	ILE
21	T1	75	GLU
21	T1	460	ASN
21	T1	733	ASN
21	T1	1169	ILE
21	T2	103	GLY
21	T2	221	GLY
21	T3	17	PHE
21	T3	221	GLY
21	T3	370	SER
21	T3	733	ASN
21	T3	1168	LEU
21	T3	1169	ILE
22	U2	865	ILE
24	W0	549	ILE
24	W0	721	ASP
24	W0	734	ASP
24	W1	500	LYS
24	W1	721	ASP
25	X1	46	LYS
25	X1	338	SER
25	X2	46	LYS
25	X2	338	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	X3	338	SER
1	00	212	ASP
1	00	282	SER
1	00	470	SER
1	00	522	ASP
1	01	282	SER
1	01	338	ASP
1	01	470	SER
1	01	522	ASP
1	01	647	ASN
1	01	776	ASN
2	10	52	ARG
2	10	1669	GLU
2	11	52	ARG
2	11	256	LYS
2	12	52	ARG
2	12	256	LYS
2	12	959	LEU
2	13	52	ARG
2	13	256	LYS
2	13	1280	ASP
2	14	52	ARG
2	14	256	LYS
2	14	1197	ARG
2	15	52	ARG
2	15	256	LYS
2	15	1669	GLU
2	16	52	ARG
2	17	52	ARG
2	17	256	LYS
2	17	1197	ARG
3	41	215	ASN
4	A1	295	GLY
4	A3	295	GLY
5	B0	117	LYS
5	B0	939	SER
5	B0	1200	SER
5	B0	1278	GLU
5	B0	2004	LEU
5	B1	117	LYS
5	B1	809	SER
5	B1	939	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B1	1200	SER
5	B1	1278	GLU
5	B1	2004	LEU
6	C0	508	ASN
6	C0	811	GLU
6	C0	1081	ASN
6	C2	1272	ASN
6	C3	508	ASN
6	C3	811	GLU
7	D1	536	SER
7	D1	613	GLN
7	D2	1482	SER
7	D3	536	SER
8	E0	324	ASP
8	E0	488	ASN
8	E1	324	ASP
8	E1	488	ASN
10	H0	246	THR
10	H1	246	THR
10	H3	246	THR
11	I2	297	LYS
14	L0	322	PRO
14	L2	462	GLU
15	M0	753	GLY
15	M1	641	GLN
15	M2	641	GLN
15	M2	753	GLY
15	M3	641	GLN
15	M3	753	GLY
17	O1	364	ALA
17	O2	399	LYS
17	O3	92	GLU
17	O3	399	LYS
18	P2	606	GLN
18	P2	859	HIS
18	P3	270	GLU
18	P3	459	LEU
19	Q1	363	LEU
19	Q2	255	ARG
19	Q3	255	ARG
20	R0	41	SER
20	R0	234	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R0	243	GLY
20	R0	355	ILE
20	R0	1046	GLU
20	R0	1240	ASN
20	R0	1509	ALA
20	R0	1627	SER
20	R1	153	SER
20	R1	234	ALA
20	R1	243	GLY
20	R1	355	ILE
20	R1	1248	ILE
20	R1	1371	ASN
20	R1	1512	ASN
20	R1	1549	ASP
20	R1	1594	ASP
20	R2	8	THR
20	R2	243	GLY
20	R2	298	SER
20	R2	355	ILE
20	R2	356	PRO
20	R2	485	GLU
20	R2	833	GLN
20	R2	1046	GLU
20	R2	1248	ILE
20	R2	1549	ASP
20	R3	355	ILE
20	R3	697	SER
20	R3	1548	LYS
21	T0	67	ILE
21	T0	320	ALA
21	T0	439	LEU
21	T0	1168	LEU
21	T1	221	GLY
21	T1	551	GLY
21	T2	77	SER
21	T2	370	SER
21	T2	460	ASN
21	T2	733	ASN
21	T2	1168	LEU
21	T3	419	SER
21	T3	439	LEU
21	T3	551	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	T3	583	PHE
21	T3	795	THR
24	W0	528	LYS
24	W0	662	GLY
24	W1	225	GLN
24	W1	528	LYS
24	W1	662	GLY
25	X0	338	SER
1	00	646	ILE
1	00	648	ASN
2	10	9	ASP
2	10	711	ARG
2	10	723	THR
2	10	1197	ARG
2	11	9	ASP
2	11	723	THR
2	12	9	ASP
2	12	723	THR
2	12	1197	ARG
2	12	1669	GLU
2	13	9	ASP
2	13	723	THR
2	13	1669	GLU
2	14	9	ASP
2	14	723	THR
2	15	723	THR
2	15	1300	GLU
2	16	9	ASP
2	16	203	SER
2	16	723	THR
2	16	1630	ASN
2	17	9	ASP
2	17	602	ASP
2	17	723	THR
3	40	401	SER
4	A5	641	ASN
6	C0	510	VAL
6	C0	1179	ASP
6	C1	983	PRO
6	C3	527	ASP
7	D0	1391	ASP
7	D0	1393	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D0	1482	SER
7	D1	1391	ASP
7	D1	1447	LYS
7	D1	1482	SER
7	D1	1572	PHE
7	D2	535	SER
7	D2	1447	LYS
7	D3	613	GLN
7	D3	1391	ASP
7	D3	1447	LYS
13	K0	800	SER
13	K0	896	THR
13	K1	800	SER
14	L1	472	CYS
14	L2	303	LYS
15	M1	753	GLY
15	M2	688	SER
15	M3	545	GLN
17	O0	377	SER
17	O1	145	LEU
18	P0	447	LYS
18	P0	487	SER
18	P0	598	ARG
18	P0	762	ASN
18	P1	215	ASP
18	P1	597	MET
18	P2	766	ASN
20	R0	153	SER
20	R0	598	HIS
20	R0	1243	ASN
20	R0	1438	PHE
20	R0	1503	GLY
20	R1	356	PRO
20	R1	782	ASN
20	R1	1121	ASN
20	R2	41	SER
20	R2	153	SER
20	R2	177	LYS
20	R2	509	SER
20	R2	697	SER
20	R2	778	ASN
20	R2	1162	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R3	41	SER
20	R3	243	GLY
20	R3	298	SER
20	R3	485	GLU
20	R3	509	SER
20	R3	1046	GLU
20	R3	1240	ASN
20	R3	1509	ALA
20	R3	1627	SER
21	T0	460	ASN
21	T1	320	ALA
21	T1	583	PHE
21	T1	1168	LEU
21	T2	203	LYS
21	T2	320	ALA
21	T3	103	GLY
21	T3	320	ALA
21	T3	790	LEU
21	T3	916	SER
21	T3	1146	GLY
24	W0	367	SER
25	X0	46	LYS
1	00	656	ILE
1	01	646	ILE
2	10	256	LYS
2	11	203	SER
2	11	711	ARG
2	12	711	ARG
2	13	203	SER
2	14	869	SER
2	14	1669	GLU
2	15	847	ASN
2	16	1669	GLU
2	17	711	ARG
2	17	1300	GLU
3	40	238	SER
3	40	366	SER
3	41	366	SER
3	41	401	SER
4	A1	393	LYS
4	A3	393	LYS
4	A5	393	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B0	899	SER
5	B1	727	PRO
5	B1	1306	SER
6	C0	646	LEU
6	C2	983	PRO
6	C3	17	ASN
6	C3	646	LEU
6	C3	1257	CYS
7	D0	1447	LYS
7	D1	1153	ASP
7	D1	1393	LEU
10	H0	229	ALA
10	H3	229	ALA
11	I3	297	LYS
12	J0	618	GLU
12	J1	618	GLU
13	K2	800	SER
13	K3	800	SER
14	L0	462	GLU
14	L1	893	ILE
15	M0	536	THR
15	M2	545	GLN
17	O0	445	MET
17	O1	92	GLU
17	O1	377	SER
17	O1	399	LYS
17	O3	145	LEU
18	P0	430	ARG
18	P2	836	LYS
19	Q1	255	ARG
20	R0	838	TYR
20	R0	957	ASN
20	R0	1248	ILE
20	R1	15	ASN
20	R1	41	SER
20	R1	43	ASN
20	R1	171	ASP
20	R1	485	GLU
20	R1	509	SER
20	R1	776	ASN
20	R1	1438	PHE
20	R2	15	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R2	171	ASP
20	R2	191	ASN
20	R2	559	ASP
20	R2	957	ASN
20	R2	977	ASN
20	R2	1240	ASN
20	R2	1627	SER
20	R3	11	ILE
20	R3	61	SER
20	R3	153	SER
21	T0	367	ASN
21	T0	419	SER
21	T1	103	GLY
21	T1	203	LYS
21	T1	311	ASN
21	T1	327	SER
21	T1	439	LEU
21	T1	1164	GLN
21	T2	311	ASN
21	T2	439	LEU
21	T2	1146	GLY
21	T2	1169	ILE
21	T3	311	ASN
21	T3	327	SER
21	T3	460	ASN
21	T3	584	SER
22	U0	865	ILE
24	W0	534	PHE
24	W1	158	GLN
24	W1	534	PHE
24	W1	635	ASN
1	00	647	ASN
1	01	364	ASP
2	10	203	SER
2	13	711	ARG
2	13	869	SER
2	14	203	SER
2	15	203	SER
2	16	711	ARG
2	17	203	SER
2	17	869	SER
2	17	1540	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A0	495	THR
4	A5	295	GLY
5	B0	809	SER
5	B1	899	SER
6	C0	527	ASP
6	C0	783	ILE
6	C3	783	ILE
7	D0	1073	GLU
7	D3	1393	LEU
7	D3	1482	SER
8	E0	83	SER
9	F1	416	GLN
9	F3	416	GLN
11	I1	297	LYS
13	K3	650	MET
14	L0	982	LYS
16	N3	235	ARG
17	O2	145	LEU
18	P1	606	GLN
18	P3	766	ASN
19	Q1	367	ILE
20	R0	189	SER
20	R1	189	SER
20	R1	559	ASP
20	R2	189	SER
20	R3	833	GLN
20	R3	1243	ASN
20	R3	1248	ILE
21	T2	419	SER
21	T2	1164	GLN
22	U3	865	ILE
24	W0	500	LYS
24	W0	911	ASN
25	X1	249	SER
1	01	656	ILE
5	B0	940	ILE
5	B0	1495	ILE
5	B1	940	ILE
6	C3	510	VAL
6	C3	983	PRO
7	D3	1149	GLY
21	T2	822	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	V0	634	PRO
23	V1	634	PRO
24	W0	547	ILE
24	W1	547	ILE
2	13	1334	GLY
5	B0	1747	ILE
5	B1	1747	ILE
6	C0	983	PRO
7	D2	1574	GLY
15	M1	384	PRO
20	R0	358	SER
20	R2	358	SER
20	R3	358	SER
20	R3	1503	GLY
24	W1	736	ILE
2	10	30	ILE
2	12	30	ILE
20	R1	358	SER
20	R2	1503	GLY
20	R3	832	ILE
2	11	30	ILE
2	13	30	ILE
2	14	30	ILE
2	16	1174	GLY
2	17	30	ILE
4	A4	897	PRO
5	B0	1280	ILE
5	B1	1280	ILE
6	C0	795	ILE
7	D0	1149	GLY
13	K0	1096	SER
14	L1	332	ILE
14	L2	322	PRO
15	M3	384	PRO
23	V0	810	ILE
2	15	30	ILE
2	16	30	ILE
13	K2	1096	SER
13	K3	787	GLY
21	T2	918	GLY

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	00	753/3306 (23%)	737 (98%)	16 (2%)	48	66
1	01	753/3306 (23%)	731 (97%)	22 (3%)	37	56
2	10	1627/1749 (93%)	1586 (98%)	41 (2%)	42	61
2	11	1627/1749 (93%)	1580 (97%)	47 (3%)	37	56
2	12	1627/1749 (93%)	1591 (98%)	36 (2%)	47	65
2	13	1627/1749 (93%)	1587 (98%)	40 (2%)	42	61
2	14	1627/1749 (93%)	1587 (98%)	40 (2%)	42	61
2	15	1627/1749 (93%)	1581 (97%)	46 (3%)	38	57
2	16	1627/1749 (93%)	1583 (97%)	44 (3%)	40	58
2	17	1627/1749 (93%)	1591 (98%)	36 (2%)	47	65
3	40	430/430 (100%)	421 (98%)	9 (2%)	48	66
3	41	430/430 (100%)	421 (98%)	9 (2%)	48	66
4	A0	757/914 (83%)	740 (98%)	17 (2%)	47	65
4	A1	666/914 (73%)	649 (97%)	17 (3%)	41	59
4	A2	666/914 (73%)	650 (98%)	16 (2%)	44	62
4	A3	666/914 (73%)	649 (97%)	17 (3%)	41	59
4	A4	666/914 (73%)	647 (97%)	19 (3%)	37	56
4	A5	708/914 (78%)	691 (98%)	17 (2%)	44	62
5	B0	1908/2076 (92%)	1863 (98%)	45 (2%)	44	62
5	B1	1908/2076 (92%)	1862 (98%)	46 (2%)	44	62
6	C0	1329/1812 (73%)	1297 (98%)	32 (2%)	44	62
6	C1	1265/1812 (70%)	1238 (98%)	27 (2%)	48	66
6	C2	1265/1812 (70%)	1239 (98%)	26 (2%)	48	66
6	C3	1329/1812 (73%)	1296 (98%)	33 (2%)	42	61
7	D0	1197/1480 (81%)	1171 (98%)	26 (2%)	47	65
7	D1	1197/1480 (81%)	1171 (98%)	26 (2%)	47	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D2	1197/1480 (81%)	1173 (98%)	24 (2%)	50	68
7	D3	1197/1480 (81%)	1168 (98%)	29 (2%)	44	62
8	E0	565/637 (89%)	555 (98%)	10 (2%)	54	71
8	E1	565/637 (89%)	552 (98%)	13 (2%)	45	64
9	F0	90/90 (100%)	88 (98%)	2 (2%)	47	65
9	F1	90/90 (100%)	88 (98%)	2 (2%)	47	65
9	F2	90/90 (100%)	88 (98%)	2 (2%)	47	65
9	F3	90/90 (100%)	88 (98%)	2 (2%)	47	65
10	H0	232/377 (62%)	227 (98%)	5 (2%)	47	65
10	H1	232/377 (62%)	228 (98%)	4 (2%)	56	72
10	H2	232/377 (62%)	225 (97%)	7 (3%)	36	55
10	H3	232/377 (62%)	228 (98%)	4 (2%)	56	72
11	I0	192/493 (39%)	188 (98%)	4 (2%)	48	66
11	I1	192/493 (39%)	189 (98%)	3 (2%)	58	73
11	I2	192/493 (39%)	189 (98%)	3 (2%)	58	73
11	I3	192/493 (39%)	188 (98%)	4 (2%)	48	66
12	J0	180/553 (32%)	174 (97%)	6 (3%)	33	52
12	J1	180/553 (32%)	175 (97%)	5 (3%)	38	57
12	J2	175/553 (32%)	173 (99%)	2 (1%)	70	80
12	J3	175/553 (32%)	172 (98%)	3 (2%)	56	72
12	J4	175/553 (32%)	171 (98%)	4 (2%)	45	64
12	J5	175/553 (32%)	173 (99%)	2 (1%)	70	80
13	K0	684/1136 (60%)	649 (95%)	35 (5%)	20	41
13	K1	684/1136 (60%)	658 (96%)	26 (4%)	28	49
13	K2	684/1136 (60%)	664 (97%)	20 (3%)	37	56
13	K3	684/1136 (60%)	663 (97%)	21 (3%)	35	54
14	L0	754/932 (81%)	727 (96%)	27 (4%)	30	50
14	L1	754/932 (81%)	736 (98%)	18 (2%)	44	62
14	L2	754/932 (81%)	734 (97%)	20 (3%)	40	58
14	L3	749/932 (80%)	729 (97%)	20 (3%)	40	58
15	M0	646/841 (77%)	632 (98%)	14 (2%)	47	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	M1	646/841 (77%)	631 (98%)	15 (2%)	45	64
15	M2	646/841 (77%)	632 (98%)	14 (2%)	47	65
15	M3	646/841 (77%)	634 (98%)	12 (2%)	52	69
16	N0	262/262 (100%)	261 (100%)	1 (0%)	89	91
16	N1	262/262 (100%)	258 (98%)	4 (2%)	60	75
16	N2	262/262 (100%)	259 (99%)	3 (1%)	70	80
16	N3	262/262 (100%)	260 (99%)	2 (1%)	79	85
17	O0	278/383 (73%)	269 (97%)	9 (3%)	34	53
17	O1	278/383 (73%)	268 (96%)	10 (4%)	30	50
17	O2	278/383 (73%)	268 (96%)	10 (4%)	30	50
17	O3	278/383 (73%)	265 (95%)	13 (5%)	22	44
18	P0	713/834 (86%)	691 (97%)	22 (3%)	35	54
18	P1	713/834 (86%)	692 (97%)	21 (3%)	37	56
18	P2	713/834 (86%)	694 (97%)	19 (3%)	40	58
18	P3	713/834 (86%)	692 (97%)	21 (3%)	37	56
19	Q0	348/392 (89%)	339 (97%)	9 (3%)	41	59
19	Q1	348/392 (89%)	342 (98%)	6 (2%)	56	72
19	Q2	348/392 (89%)	342 (98%)	6 (2%)	56	72
19	Q3	348/392 (89%)	345 (99%)	3 (1%)	75	83
20	R0	1686/1687 (100%)	1630 (97%)	56 (3%)	33	52
20	R1	1686/1687 (100%)	1637 (97%)	49 (3%)	37	56
20	R2	1686/1687 (100%)	1637 (97%)	49 (3%)	37	56
20	R3	1686/1687 (100%)	1635 (97%)	51 (3%)	36	55
21	T0	991/2106 (47%)	954 (96%)	37 (4%)	29	49
21	T1	1094/2106 (52%)	1056 (96%)	38 (4%)	31	51
21	T2	1094/2106 (52%)	1061 (97%)	33 (3%)	36	55
21	T3	1094/2106 (52%)	1054 (96%)	40 (4%)	29	49
22	U0	25/911 (3%)	23 (92%)	2 (8%)	10	29
22	U1	25/911 (3%)	23 (92%)	2 (8%)	10	29
22	U2	25/911 (3%)	23 (92%)	2 (8%)	10	29
22	U3	25/911 (3%)	24 (96%)	1 (4%)	27	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V0	251/1497 (17%)	248 (99%)	3 (1%)	67	78
23	V1	251/1497 (17%)	246 (98%)	5 (2%)	50	68
24	W0	857/928 (92%)	831 (97%)	26 (3%)	36	55
24	W1	857/928 (92%)	834 (97%)	23 (3%)	40	58
25	X0	388/388 (100%)	376 (97%)	12 (3%)	35	54
25	X1	388/388 (100%)	373 (96%)	15 (4%)	27	48
25	X2	388/388 (100%)	373 (96%)	15 (4%)	27	48
25	X3	388/388 (100%)	379 (98%)	9 (2%)	45	64
All	All	67169/97038 (69%)	65410 (97%)	1759 (3%)	42	59

All (1759) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	00	46	ASP
1	00	205	ASP
1	00	213	TYR
1	00	338	ASP
1	00	343	ASP
1	00	394	PHE
1	00	435	CYS
1	00	463	THR
1	00	464	THR
1	00	467	THR
1	00	468	THR
1	00	471	SER
1	00	608	ASP
1	00	650	ASN
1	00	695	ASP
1	00	760	ASP
1	01	46	ASP
1	01	192	HIS
1	01	205	ASP
1	01	213	TYR
1	01	338	ASP
1	01	343	ASP
1	01	364	ASP
1	01	394	PHE
1	01	435	CYS
1	01	463	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	01	464	THR
1	01	467	THR
1	01	468	THR
1	01	471	SER
1	01	509	GLN
1	01	561	SER
1	01	608	ASP
1	01	644	ASN
1	01	649	ASN
1	01	650	ASN
1	01	760	ASP
1	01	762	ASP
2	10	3	ILE
2	10	5	ASN
2	10	8	ASN
2	10	12	SER
2	10	65	GLU
2	10	91	ASN
2	10	126	SER
2	10	219	ASP
2	10	240	ASP
2	10	245	GLU
2	10	263	THR
2	10	323	SER
2	10	335	ASP
2	10	384	ASP
2	10	395	SER
2	10	441	GLN
2	10	453	VAL
2	10	454	TYR
2	10	475	THR
2	10	523	ASP
2	10	561	ASP
2	10	596	ASP
2	10	601	ASP
2	10	602	ASP
2	10	638	THR
2	10	665	SER
2	10	719	VAL
2	10	776	THR
2	10	797	ASP
2	10	806	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	10	827	ASP
2	10	859	ASP
2	10	912	SER
2	10	1019	ASP
2	10	1023	ASP
2	10	1085	ASP
2	10	1198	GLU
2	10	1698	SER
2	10	1769	LEU
2	10	1780	ASP
2	10	1781	ASP
2	11	3	ILE
2	11	5	ASN
2	11	8	ASN
2	11	12	SER
2	11	65	GLU
2	11	91	ASN
2	11	126	SER
2	11	205	ASN
2	11	219	ASP
2	11	240	ASP
2	11	263	THR
2	11	323	SER
2	11	327	MET
2	11	335	ASP
2	11	381	GLU
2	11	384	ASP
2	11	395	SER
2	11	444	VAL
2	11	453	VAL
2	11	454	TYR
2	11	475	THR
2	11	479	GLN
2	11	523	ASP
2	11	548	HIS
2	11	561	ASP
2	11	562	GLU
2	11	596	ASP
2	11	601	ASP
2	11	638	THR
2	11	665	SER
2	11	705	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	11	776	THR
2	11	797	ASP
2	11	806	HIS
2	11	859	ASP
2	11	912	SER
2	11	1019	ASP
2	11	1023	ASP
2	11	1085	ASP
2	11	1195	SER
2	11	1198	GLU
2	11	1275	THR
2	11	1349	ASN
2	11	1452	THR
2	11	1769	LEU
2	11	1780	ASP
2	11	1781	ASP
2	12	3	ILE
2	12	5	ASN
2	12	8	ASN
2	12	12	SER
2	12	65	GLU
2	12	91	ASN
2	12	126	SER
2	12	205	ASN
2	12	219	ASP
2	12	240	ASP
2	12	263	THR
2	12	335	ASP
2	12	384	ASP
2	12	395	SER
2	12	453	VAL
2	12	454	TYR
2	12	523	ASP
2	12	561	ASP
2	12	562	GLU
2	12	638	THR
2	12	665	SER
2	12	705	GLU
2	12	776	THR
2	12	806	HIS
2	12	859	ASP
2	12	912	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	12	961	ASP
2	12	1044	SER
2	12	1078	SER
2	12	1122	GLN
2	12	1198	GLU
2	12	1701	ASP
2	12	1762	GLU
2	12	1769	LEU
2	12	1780	ASP
2	12	1781	ASP
2	13	3	ILE
2	13	5	ASN
2	13	8	ASN
2	13	12	SER
2	13	65	GLU
2	13	91	ASN
2	13	126	SER
2	13	205	ASN
2	13	219	ASP
2	13	240	ASP
2	13	263	THR
2	13	323	SER
2	13	335	ASP
2	13	384	ASP
2	13	395	SER
2	13	453	VAL
2	13	523	ASP
2	13	562	GLU
2	13	596	ASP
2	13	601	ASP
2	13	602	ASP
2	13	638	THR
2	13	665	SER
2	13	705	GLU
2	13	776	THR
2	13	797	ASP
2	13	806	HIS
2	13	912	SER
2	13	961	ASP
2	13	1019	ASP
2	13	1023	ASP
2	13	1051	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	13	1062	ASP
2	13	1122	GLN
2	13	1623	ASP
2	13	1701	ASP
2	13	1762	GLU
2	13	1769	LEU
2	13	1780	ASP
2	13	1781	ASP
2	14	3	ILE
2	14	5	ASN
2	14	8	ASN
2	14	12	SER
2	14	65	GLU
2	14	91	ASN
2	14	126	SER
2	14	205	ASN
2	14	219	ASP
2	14	240	ASP
2	14	263	THR
2	14	323	SER
2	14	335	ASP
2	14	381	GLU
2	14	384	ASP
2	14	395	SER
2	14	523	ASP
2	14	561	ASP
2	14	562	GLU
2	14	596	ASP
2	14	601	ASP
2	14	602	ASP
2	14	638	THR
2	14	665	SER
2	14	694	SER
2	14	705	GLU
2	14	776	THR
2	14	797	ASP
2	14	859	ASP
2	14	912	SER
2	14	1023	ASP
2	14	1569	ASP
2	14	1601	ASN
2	14	1615	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	14	1623	ASP
2	14	1701	ASP
2	14	1762	GLU
2	14	1769	LEU
2	14	1780	ASP
2	14	1781	ASP
2	15	3	ILE
2	15	5	ASN
2	15	8	ASN
2	15	12	SER
2	15	65	GLU
2	15	91	ASN
2	15	126	SER
2	15	205	ASN
2	15	219	ASP
2	15	240	ASP
2	15	263	THR
2	15	323	SER
2	15	335	ASP
2	15	378	ASN
2	15	381	GLU
2	15	384	ASP
2	15	395	SER
2	15	475	THR
2	15	509	GLU
2	15	523	ASP
2	15	533	SER
2	15	561	ASP
2	15	562	GLU
2	15	600	LEU
2	15	602	ASP
2	15	638	THR
2	15	665	SER
2	15	705	GLU
2	15	756	GLU
2	15	776	THR
2	15	797	ASP
2	15	846	ARG
2	15	888	ASP
2	15	912	SER
2	15	961	ASP
2	15	987	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	15	1019	ASP
2	15	1124	LEU
2	15	1195	SER
2	15	1569	ASP
2	15	1623	ASP
2	15	1701	ASP
2	15	1708	GLU
2	15	1769	LEU
2	15	1780	ASP
2	15	1781	ASP
2	16	3	ILE
2	16	5	ASN
2	16	8	ASN
2	16	12	SER
2	16	65	GLU
2	16	91	ASN
2	16	126	SER
2	16	205	ASN
2	16	219	ASP
2	16	240	ASP
2	16	263	THR
2	16	323	SER
2	16	335	ASP
2	16	375	SER
2	16	381	GLU
2	16	384	ASP
2	16	395	SER
2	16	444	VAL
2	16	495	HIS
2	16	523	ASP
2	16	561	ASP
2	16	562	GLU
2	16	601	ASP
2	16	602	ASP
2	16	638	THR
2	16	665	SER
2	16	705	GLU
2	16	756	GLU
2	16	776	THR
2	16	797	ASP
2	16	827	ASP
2	16	859	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	16	912	SER
2	16	961	ASP
2	16	1019	ASP
2	16	1124	LEU
2	16	1198	GLU
2	16	1349	ASN
2	16	1630	ASN
2	16	1701	ASP
2	16	1769	LEU
2	16	1780	ASP
2	16	1781	ASP
2	16	1811	ASP
2	17	3	ILE
2	17	5	ASN
2	17	8	ASN
2	17	12	SER
2	17	65	GLU
2	17	91	ASN
2	17	126	SER
2	17	205	ASN
2	17	219	ASP
2	17	240	ASP
2	17	263	THR
2	17	323	SER
2	17	335	ASP
2	17	381	GLU
2	17	384	ASP
2	17	395	SER
2	17	475	THR
2	17	509	GLU
2	17	523	ASP
2	17	533	SER
2	17	561	ASP
2	17	562	GLU
2	17	601	ASP
2	17	638	THR
2	17	665	SER
2	17	705	GLU
2	17	756	GLU
2	17	776	THR
2	17	797	ASP
2	17	912	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	17	1019	ASP
2	17	1701	ASP
2	17	1762	GLU
2	17	1769	LEU
2	17	1780	ASP
2	17	1781	ASP
3	40	75	LEU
3	40	128	GLN
3	40	215	ASN
3	40	343	PHE
3	40	348	GLU
3	40	399	LEU
3	40	406	ASN
3	40	449	SER
3	40	459	THR
3	41	75	LEU
3	41	128	GLN
3	41	215	ASN
3	41	343	PHE
3	41	399	LEU
3	41	406	ASN
3	41	449	SER
3	41	459	THR
3	41	470	LYS
4	A0	421	ASP
4	A0	564	THR
4	A0	570	ASP
4	A0	618	GLN
4	A0	645	ASN
4	A0	655	PHE
4	A0	659	THR
4	A0	662	THR
4	A0	692	GLN
4	A0	760	ASN
4	A0	855	ASP
4	A0	858	ASP
4	A0	875	LEU
4	A0	883	SER
4	A0	903	PHE
4	A0	924	PHE
4	A0	959	ASP
4	A1	98	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A1	107	ILE
4	A1	108	ASP
4	A1	360	THR
4	A1	421	ASP
4	A1	504	ASP
4	A1	540	THR
4	A1	570	ASP
4	A1	639	THR
4	A1	692	GLN
4	A1	744	ASN
4	A1	757	GLU
4	A1	760	ASN
4	A1	855	ASP
4	A1	858	ASP
4	A1	875	LEU
4	A1	886	ASP
4	A2	26	SER
4	A2	58	THR
4	A2	360	THR
4	A2	451	GLU
4	A2	504	ASP
4	A2	540	THR
4	A2	570	ASP
4	A2	611	ASP
4	A2	639	THR
4	A2	744	ASN
4	A2	757	GLU
4	A2	760	ASN
4	A2	855	ASP
4	A2	858	ASP
4	A2	875	LEU
4	A2	883	SER
4	A3	107	ILE
4	A3	108	ASP
4	A3	145	ASP
4	A3	360	THR
4	A3	421	ASP
4	A3	504	ASP
4	A3	540	THR
4	A3	570	ASP
4	A3	639	THR
4	A3	692	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A3	744	ASN
4	A3	757	GLU
4	A3	760	ASN
4	A3	855	ASP
4	A3	858	ASP
4	A3	875	LEU
4	A3	883	SER
4	A4	26	SER
4	A4	58	THR
4	A4	71	ASP
4	A4	99	ASP
4	A4	323	THR
4	A4	360	THR
4	A4	396	ASN
4	A4	421	ASP
4	A4	540	THR
4	A4	570	ASP
4	A4	622	ASP
4	A4	639	THR
4	A4	692	GLN
4	A4	693	THR
4	A4	744	ASN
4	A4	760	ASN
4	A4	855	ASP
4	A4	858	ASP
4	A4	875	LEU
4	A5	108	ASP
4	A5	421	ASP
4	A5	505	GLN
4	A5	515	THR
4	A5	564	THR
4	A5	570	ASP
4	A5	744	ASN
4	A5	757	GLU
4	A5	760	ASN
4	A5	855	ASP
4	A5	858	ASP
4	A5	875	LEU
4	A5	883	SER
4	A5	903	PHE
4	A5	924	PHE
4	A5	929	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A5	959	ASP
5	B0	61	ASP
5	B0	88	GLU
5	B0	94	ILE
5	B0	182	LEU
5	B0	228	PHE
5	B0	300	ASP
5	B0	348	LEU
5	B0	379	PHE
5	B0	430	ASP
5	B0	501	ASP
5	B0	521	ASP
5	B0	576	ASP
5	B0	593	SER
5	B0	602	ASP
5	B0	625	SER
5	B0	627	LEU
5	B0	637	ASP
5	B0	726	GLN
5	B0	780	THR
5	B0	786	PHE
5	B0	818	SER
5	B0	1023	GLU
5	B0	1041	PHE
5	B0	1080	ASP
5	B0	1081	TYR
5	B0	1083	ASN
5	B0	1097	ASP
5	B0	1100	ASP
5	B0	1128	LEU
5	B0	1203	ASP
5	B0	1223	ASP
5	B0	1326	ASN
5	B0	1329	TRP
5	B0	1376	ASP
5	B0	1403	ASP
5	B0	1421	LEU
5	B0	1441	PHE
5	B0	1722	TYR
5	B0	1851	THR
5	B0	1854	TYR
5	B0	1914	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B0	1936	TYR
5	B0	1993	TYR
5	B0	2035	ASP
5	B0	2069	ASP
5	B1	61	ASP
5	B1	88	GLU
5	B1	94	ILE
5	B1	182	LEU
5	B1	228	PHE
5	B1	300	ASP
5	B1	348	LEU
5	B1	362	HIS
5	B1	379	PHE
5	B1	430	ASP
5	B1	501	ASP
5	B1	521	ASP
5	B1	576	ASP
5	B1	593	SER
5	B1	602	ASP
5	B1	625	SER
5	B1	627	LEU
5	B1	637	ASP
5	B1	780	THR
5	B1	786	PHE
5	B1	818	SER
5	B1	1041	PHE
5	B1	1080	ASP
5	B1	1097	ASP
5	B1	1100	ASP
5	B1	1127	THR
5	B1	1128	LEU
5	B1	1140	GLU
5	B1	1203	ASP
5	B1	1223	ASP
5	B1	1326	ASN
5	B1	1329	TRP
5	B1	1376	ASP
5	B1	1403	ASP
5	B1	1421	LEU
5	B1	1441	PHE
5	B1	1722	TYR
5	B1	1764	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B1	1851	THR
5	B1	1854	TYR
5	B1	1914	LEU
5	B1	1936	TYR
5	B1	1993	TYR
5	B1	1999	GLU
5	B1	2035	ASP
5	B1	2069	ASP
6	C0	16	ASP
6	C0	207	LEU
6	C0	211	ASP
6	C0	213	ASP
6	C0	358	ASP
6	C0	420	TYR
6	C0	527	ASP
6	C0	549	ARG
6	C0	566	THR
6	C0	651	ASP
6	C0	661	THR
6	C0	789	THR
6	C0	944	LYS
6	C0	955	THR
6	C0	963	GLU
6	C0	982	ASN
6	C0	1062	ASP
6	C0	1093	LYS
6	C0	1179	ASP
6	C0	1207	ASP
6	C0	1210	HIS
6	C0	1224	SER
6	C0	1233	ASP
6	C0	1281	SER
6	C0	1282	ASP
6	C0	1309	SER
6	C0	1330	SER
6	C0	1353	HIS
6	C0	1389	ASP
6	C0	1471	ASP
6	C0	1477	ARG
6	C0	1661	ASP
6	C1	16	ASP
6	C1	62	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C1	207	LEU
6	C1	211	ASP
6	C1	213	ASP
6	C1	344	ASP
6	C1	358	ASP
6	C1	527	ASP
6	C1	549	ARG
6	C1	661	THR
6	C1	693	ASP
6	C1	838	ASN
6	C1	911	SER
6	C1	944	LYS
6	C1	976	ASP
6	C1	982	ASN
6	C1	985	GLU
6	C1	1062	ASP
6	C1	1207	ASP
6	C1	1210	HIS
6	C1	1233	ASP
6	C1	1282	ASP
6	C1	1309	SER
6	C1	1353	HIS
6	C1	1389	ASP
6	C1	1471	ASP
6	C1	1477	ARG
6	C2	16	ASP
6	C2	62	THR
6	C2	207	LEU
6	C2	211	ASP
6	C2	213	ASP
6	C2	358	ASP
6	C2	527	ASP
6	C2	549	ARG
6	C2	562	HIS
6	C2	661	THR
6	C2	911	SER
6	C2	944	LYS
6	C2	976	ASP
6	C2	982	ASN
6	C2	983	PRO
6	C2	1062	ASP
6	C2	1179	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C2	1207	ASP
6	C2	1210	HIS
6	C2	1233	ASP
6	C2	1282	ASP
6	C2	1309	SER
6	C2	1353	HIS
6	C2	1389	ASP
6	C2	1471	ASP
6	C2	1477	ARG
6	C3	63	ASN
6	C3	100	SER
6	C3	211	ASP
6	C3	213	ASP
6	C3	358	ASP
6	C3	420	TYR
6	C3	433	THR
6	C3	527	ASP
6	C3	549	ARG
6	C3	562	HIS
6	C3	566	THR
6	C3	629	SER
6	C3	661	THR
6	C3	789	THR
6	C3	906	ASP
6	C3	944	LYS
6	C3	955	THR
6	C3	963	GLU
6	C3	982	ASN
6	C3	983	PRO
6	C3	1062	ASP
6	C3	1094	ASN
6	C3	1179	ASP
6	C3	1210	HIS
6	C3	1224	SER
6	C3	1233	ASP
6	C3	1281	SER
6	C3	1282	ASP
6	C3	1309	SER
6	C3	1471	ASP
6	C3	1477	ARG
6	C3	1614	ASP
6	C3	1661	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D0	195	ASP
7	D0	398	ASP
7	D0	414	TYR
7	D0	510	SER
7	D0	527	GLU
7	D0	562	ASN
7	D0	583	ASP
7	D0	627	SER
7	D0	640	VAL
7	D0	690	ASN
7	D0	696	ASP
7	D0	727	ASP
7	D0	761	TYR
7	D0	810	SER
7	D0	846	GLU
7	D0	926	ASP
7	D0	943	ASP
7	D0	991	THR
7	D0	1028	GLU
7	D0	1157	TYR
7	D0	1165	ASP
7	D0	1457	SER
7	D0	1472	ASP
7	D0	1516	LEU
7	D0	1530	GLU
7	D0	1572	PHE
7	D1	195	ASP
7	D1	398	ASP
7	D1	414	TYR
7	D1	436	ASP
7	D1	510	SER
7	D1	562	ASN
7	D1	640	VAL
7	D1	675	SER
7	D1	690	ASN
7	D1	696	ASP
7	D1	720	HIS
7	D1	727	ASP
7	D1	846	GLU
7	D1	924	GLU
7	D1	926	ASP
7	D1	943	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D1	988	SER
7	D1	1028	GLU
7	D1	1088	THR
7	D1	1157	TYR
7	D1	1165	ASP
7	D1	1244	ASP
7	D1	1414	ASP
7	D1	1521	GLN
7	D1	1530	GLU
7	D1	1572	PHE
7	D2	195	ASP
7	D2	358	ASP
7	D2	398	ASP
7	D2	414	TYR
7	D2	510	SER
7	D2	527	GLU
7	D2	562	ASN
7	D2	583	ASP
7	D2	627	SER
7	D2	640	VAL
7	D2	690	ASN
7	D2	696	ASP
7	D2	761	TYR
7	D2	810	SER
7	D2	846	GLU
7	D2	926	ASP
7	D2	943	ASP
7	D2	991	THR
7	D2	1028	GLU
7	D2	1072	SER
7	D2	1157	TYR
7	D2	1530	GLU
7	D2	1572	PHE
7	D2	1575	TYR
7	D3	178	ASP
7	D3	195	ASP
7	D3	284	ASN
7	D3	398	ASP
7	D3	414	TYR
7	D3	434	ASP
7	D3	436	ASP
7	D3	510	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D3	527	GLU
7	D3	562	ASN
7	D3	640	VAL
7	D3	675	SER
7	D3	690	ASN
7	D3	696	ASP
7	D3	874	GLU
7	D3	924	GLU
7	D3	926	ASP
7	D3	943	ASP
7	D3	988	SER
7	D3	1028	GLU
7	D3	1051	THR
7	D3	1088	THR
7	D3	1153	ASP
7	D3	1165	ASP
7	D3	1244	ASP
7	D3	1472	ASP
7	D3	1510	THR
7	D3	1530	GLU
7	D3	1572	PHE
8	E0	130	SER
8	E0	165	LEU
8	E0	178	TYR
8	E0	282	SER
8	E0	324	ASP
8	E0	350	PHE
8	E0	416	TYR
8	E0	507	ASP
8	E0	590	ASN
8	E0	644	ASP
8	E1	130	SER
8	E1	165	LEU
8	E1	178	TYR
8	E1	192	LEU
8	E1	282	SER
8	E1	324	ASP
8	E1	350	PHE
8	E1	389	SER
8	E1	416	TYR
8	E1	507	ASP
8	E1	543	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	E1	590	ASN
8	E1	644	ASP
9	F0	397	ASP
9	F0	435	ASP
9	F1	397	ASP
9	F1	435	ASP
9	F2	397	ASP
9	F2	435	ASP
9	F3	397	ASP
9	F3	435	ASP
10	H0	272	ASP
10	H0	321	GLN
10	H0	351	ARG
10	H0	395	SER
10	H0	437	LEU
10	H1	248	ASP
10	H1	272	ASP
10	H1	321	GLN
10	H1	437	LEU
10	H2	248	ASP
10	H2	272	ASP
10	H2	321	GLN
10	H2	371	SER
10	H2	414	GLU
10	H2	433	GLU
10	H2	437	LEU
10	H3	248	ASP
10	H3	272	ASP
10	H3	321	GLN
10	H3	437	LEU
11	I0	185	ASN
11	I0	192	ASN
11	I0	222	LEU
11	I0	266	ARG
11	I1	203	THR
11	I1	222	LEU
11	I1	258	PHE
11	I2	172	ASP
11	I2	222	LEU
11	I2	258	PHE
11	I3	185	ASN
11	I3	222	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I3	258	PHE
11	I3	266	ARG
12	J0	565	SER
12	J0	620	THR
12	J0	636	ASP
12	J0	660	ASP
12	J0	691	LEU
12	J0	705	GLU
12	J1	565	SER
12	J1	616	ASP
12	J1	620	THR
12	J1	660	ASP
12	J1	705	GLU
12	J2	616	ASP
12	J2	618	GLU
12	J3	590	ASP
12	J3	616	ASP
12	J3	618	GLU
12	J4	590	ASP
12	J4	594	ASP
12	J4	616	ASP
12	J4	660	ASP
12	J5	616	ASP
12	J5	618	GLU
13	K0	551	ILE
13	K0	563	ASP
13	K0	568	HIS
13	K0	600	ASP
13	K0	602	ASP
13	K0	607	THR
13	K0	633	GLN
13	K0	643	THR
13	K0	681	ASN
13	K0	707	LEU
13	K0	736	LEU
13	K0	784	LEU
13	K0	793	LEU
13	K0	797	HIS
13	K0	851	GLU
13	K0	881	TYR
13	K0	890	THR
13	K0	892	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	K0	895	THR
13	K0	896	THR
13	K0	933	SER
13	K0	941	ASP
13	K0	968	THR
13	K0	993	HIS
13	K0	1018	THR
13	K0	1047	SER
13	K0	1058	ASP
13	K0	1061	ASN
13	K0	1079	ASP
13	K0	1130	ASP
13	K0	1135	TYR
13	K0	1145	LEU
13	K0	1157	LEU
13	K0	1161	SER
13	K0	1180	LEU
13	K1	496	ASP
13	K1	551	ILE
13	K1	568	HIS
13	K1	607	THR
13	K1	633	GLN
13	K1	634	GLU
13	K1	666	SER
13	K1	784	LEU
13	K1	851	GLU
13	K1	881	TYR
13	K1	890	THR
13	K1	895	THR
13	K1	933	SER
13	K1	941	ASP
13	K1	944	ASP
13	K1	968	THR
13	K1	984	HIS
13	K1	993	HIS
13	K1	1013	MET
13	K1	1047	SER
13	K1	1050	LYS
13	K1	1058	ASP
13	K1	1135	TYR
13	K1	1157	LEU
13	K1	1161	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	K1	1180	LEU
13	K2	496	ASP
13	K2	551	ILE
13	K2	566	LEU
13	K2	607	THR
13	K2	633	GLN
13	K2	784	LEU
13	K2	851	GLU
13	K2	881	TYR
13	K2	892	THR
13	K2	933	SER
13	K2	941	ASP
13	K2	968	THR
13	K2	984	HIS
13	K2	993	HIS
13	K2	1047	SER
13	K2	1058	ASP
13	K2	1130	ASP
13	K2	1135	TYR
13	K2	1157	LEU
13	K2	1161	SER
13	K3	496	ASP
13	K3	551	ILE
13	K3	568	HIS
13	K3	600	ASP
13	K3	602	ASP
13	K3	607	THR
13	K3	643	THR
13	K3	648	THR
13	K3	784	LEU
13	K3	890	THR
13	K3	892	THR
13	K3	924	GLU
13	K3	941	ASP
13	K3	993	HIS
13	K3	1047	SER
13	K3	1050	LYS
13	K3	1058	ASP
13	K3	1130	ASP
13	K3	1135	TYR
13	K3	1157	LEU
13	K3	1161	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L0	167	LEU
14	L0	228	LEU
14	L0	231	LEU
14	L0	289	ASP
14	L0	309	THR
14	L0	314	ASN
14	L0	317	VAL
14	L0	321	ASP
14	L0	323	ASP
14	L0	366	VAL
14	L0	425	THR
14	L0	431	ASN
14	L0	435	TYR
14	L0	464	ASP
14	L0	478	THR
14	L0	481	ASP
14	L0	513	ASP
14	L0	533	GLU
14	L0	543	LEU
14	L0	559	ASP
14	L0	560	CYS
14	L0	702	ASP
14	L0	773	GLU
14	L0	774	SER
14	L0	858	LEU
14	L0	911	ASP
14	L0	949	LEU
14	L1	167	LEU
14	L1	195	ASP
14	L1	231	LEU
14	L1	317	VAL
14	L1	431	ASN
14	L1	435	TYR
14	L1	478	THR
14	L1	481	ASP
14	L1	513	ASP
14	L1	543	LEU
14	L1	559	ASP
14	L1	560	CYS
14	L1	702	ASP
14	L1	723	GLU
14	L1	774	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L1	911	ASP
14	L1	916	HIS
14	L1	959	ARG
14	L2	167	LEU
14	L2	231	LEU
14	L2	305	SER
14	L2	323	ASP
14	L2	431	ASN
14	L2	435	TYR
14	L2	464	ASP
14	L2	478	THR
14	L2	481	ASP
14	L2	513	ASP
14	L2	543	LEU
14	L2	559	ASP
14	L2	560	CYS
14	L2	702	ASP
14	L2	723	GLU
14	L2	774	SER
14	L2	784	ARG
14	L2	911	ASP
14	L2	916	HIS
14	L2	949	LEU
14	L3	167	LEU
14	L3	169	ASP
14	L3	208	ARG
14	L3	231	LEU
14	L3	431	ASN
14	L3	435	TYR
14	L3	464	ASP
14	L3	478	THR
14	L3	481	ASP
14	L3	513	ASP
14	L3	543	LEU
14	L3	559	ASP
14	L3	560	CYS
14	L3	760	ASP
14	L3	775	ASP
14	L3	802	ASN
14	L3	911	ASP
14	L3	916	HIS
14	L3	949	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L3	974	GLN
15	M0	245	PHE
15	M0	278	THR
15	M0	327	LEU
15	M0	357	SER
15	M0	409	LEU
15	M0	437	TRP
15	M0	445	GLU
15	M0	490	ARG
15	M0	511	GLU
15	M0	568	ASP
15	M0	698	ASP
15	M0	710	THR
15	M0	774	LEU
15	M0	832	ILE
15	M1	245	PHE
15	M1	278	THR
15	M1	279	ASP
15	M1	286	GLU
15	M1	375	ASN
15	M1	409	LEU
15	M1	437	TRP
15	M1	460	ASP
15	M1	490	ARG
15	M1	561	ASN
15	M1	660	VAL
15	M1	698	ASP
15	M1	710	THR
15	M1	832	ILE
15	M1	877	ASP
15	M2	245	PHE
15	M2	278	THR
15	M2	357	SER
15	M2	409	LEU
15	M2	423	GLU
15	M2	437	TRP
15	M2	460	ASP
15	M2	490	ARG
15	M2	561	ASN
15	M2	644	HIS
15	M2	648	GLU
15	M2	784	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M2	832	ILE
15	M2	877	ASP
15	M3	245	PHE
15	M3	249	SER
15	M3	278	THR
15	M3	357	SER
15	M3	437	TRP
15	M3	460	ASP
15	M3	490	ARG
15	M3	568	ASP
15	M3	698	ASP
15	M3	710	THR
15	M3	832	ILE
15	M3	877	ASP
16	N0	217	TRP
16	N1	31	SER
16	N1	197	ASP
16	N1	217	TRP
16	N1	234	ASP
16	N2	197	ASP
16	N2	217	TRP
16	N2	234	ASP
16	N3	217	TRP
16	N3	234	ASP
17	O0	12	ASP
17	O0	14	LEU
17	O0	156	SER
17	O0	203	LEU
17	O0	407	VAL
17	O0	412	ASP
17	O0	420	VAL
17	O0	452	PHE
17	O0	463	ASP
17	O1	12	ASP
17	O1	21	ASP
17	O1	92	GLU
17	O1	106	ASP
17	O1	140	MET
17	O1	192	GLU
17	O1	411	ASP
17	O1	412	ASP
17	O1	420	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	O1	434	ASP
17	O2	12	ASP
17	O2	14	LEU
17	O2	92	GLU
17	O2	192	GLU
17	O2	204	THR
17	O2	411	ASP
17	O2	412	ASP
17	O2	414	LYS
17	O2	420	VAL
17	O2	434	ASP
17	O3	12	ASP
17	O3	14	LEU
17	O3	92	GLU
17	O3	106	ASP
17	O3	140	MET
17	O3	172	ASP
17	O3	192	GLU
17	O3	196	LYS
17	O3	396	SER
17	O3	411	ASP
17	O3	412	ASP
17	O3	420	VAL
17	O3	434	ASP
18	P0	177	HIS
18	P0	204	ASP
18	P0	228	GLU
18	P0	318	THR
18	P0	362	THR
18	P0	415	LEU
18	P0	469	ASN
18	P0	474	GLU
18	P0	534	SER
18	P0	536	THR
18	P0	548	THR
18	P0	597	MET
18	P0	678	SER
18	P0	685	LEU
18	P0	706	ASN
18	P0	777	THR
18	P0	780	SER
18	P0	793	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P0	809	LEU
18	P0	822	LEU
18	P0	859	HIS
18	P0	862	ASP
18	P1	175	SER
18	P1	180	THR
18	P1	195	SER
18	P1	203	ASP
18	P1	228	GLU
18	P1	321	ILE
18	P1	362	THR
18	P1	364	LEU
18	P1	406	ASP
18	P1	464	HIS
18	P1	535	THR
18	P1	674	GLU
18	P1	698	ASN
18	P1	707	SER
18	P1	722	ASN
18	P1	737	ASP
18	P1	780	SER
18	P1	793	SER
18	P1	822	LEU
18	P1	859	HIS
18	P1	862	ASP
18	P2	175	SER
18	P2	180	THR
18	P2	195	SER
18	P2	203	ASP
18	P2	228	GLU
18	P2	321	ILE
18	P2	354	SER
18	P2	362	THR
18	P2	364	LEU
18	P2	464	HIS
18	P2	535	THR
18	P2	674	GLU
18	P2	707	SER
18	P2	737	ASP
18	P2	780	SER
18	P2	793	SER
18	P2	799	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P2	822	LEU
18	P2	862	ASP
18	P3	175	SER
18	P3	180	THR
18	P3	195	SER
18	P3	203	ASP
18	P3	228	GLU
18	P3	321	ILE
18	P3	354	SER
18	P3	362	THR
18	P3	364	LEU
18	P3	427	SER
18	P3	464	HIS
18	P3	535	THR
18	P3	674	GLU
18	P3	707	SER
18	P3	737	ASP
18	P3	754	ASN
18	P3	793	SER
18	P3	799	SER
18	P3	822	LEU
18	P3	862	ASP
18	P3	884	LEU
19	Q0	20	ASN
19	Q0	26	ASP
19	Q0	51	SER
19	Q0	118	TYR
19	Q0	262	ILE
19	Q0	275	THR
19	Q0	288	ASP
19	Q0	312	SER
19	Q0	372	ASP
19	Q1	26	ASP
19	Q1	121	TYR
19	Q1	129	ASP
19	Q1	132	ASP
19	Q1	377	GLU
19	Q1	386	SER
19	Q2	2	SER
19	Q2	51	SER
19	Q2	121	TYR
19	Q2	129	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q2	244	SER
19	Q2	312	SER
19	Q3	2	SER
19	Q3	121	TYR
19	Q3	312	SER
20	R0	3	ASP
20	R0	11	ILE
20	R0	13	ASN
20	R0	57	TYR
20	R0	101	VAL
20	R0	143	ASP
20	R0	216	VAL
20	R0	222	ASP
20	R0	241	SER
20	R0	358	SER
20	R0	373	LEU
20	R0	383	TYR
20	R0	412	ASP
20	R0	462	ASP
20	R0	481	ASN
20	R0	501	PHE
20	R0	549	THR
20	R0	555	ASP
20	R0	557	ASP
20	R0	558	SER
20	R0	559	ASP
20	R0	565	THR
20	R0	570	LEU
20	R0	588	GLU
20	R0	597	ASP
20	R0	601	ASP
20	R0	661	GLU
20	R0	702	ASP
20	R0	722	ASN
20	R0	735	ASP
20	R0	838	TYR
20	R0	842	ASP
20	R0	852	ASP
20	R0	889	ASP
20	R0	947	ASP
20	R0	962	ASP
20	R0	1028	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R0	1042	ILE
20	R0	1080	GLU
20	R0	1150	PHE
20	R0	1190	GLU
20	R0	1240	ASN
20	R0	1269	ASP
20	R0	1329	ASP
20	R0	1334	LEU
20	R0	1438	PHE
20	R0	1497	THR
20	R0	1547	ASP
20	R0	1550	PHE
20	R0	1616	HIS
20	R0	1645	ASP
20	R0	1700	ASP
20	R0	1716	LEU
20	R0	1728	THR
20	R0	1761	SER
20	R0	1791	ASN
20	R1	11	ILE
20	R1	39	ASP
20	R1	57	TYR
20	R1	101	VAL
20	R1	143	ASP
20	R1	222	ASP
20	R1	383	TYR
20	R1	470	ASN
20	R1	481	ASN
20	R1	501	PHE
20	R1	544	ASP
20	R1	557	ASP
20	R1	559	ASP
20	R1	565	THR
20	R1	588	GLU
20	R1	661	GLU
20	R1	723	ASP
20	R1	735	ASP
20	R1	829	ASP
20	R1	838	TYR
20	R1	842	ASP
20	R1	889	ASP
20	R1	899	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R1	903	ASP
20	R1	904	SER
20	R1	962	ASP
20	R1	1000	GLU
20	R1	1028	GLU
20	R1	1080	GLU
20	R1	1150	PHE
20	R1	1190	GLU
20	R1	1269	ASP
20	R1	1309	GLU
20	R1	1329	ASP
20	R1	1334	LEU
20	R1	1359	GLU
20	R1	1370	THR
20	R1	1438	PHE
20	R1	1510	ASN
20	R1	1547	ASP
20	R1	1594	ASP
20	R1	1616	HIS
20	R1	1645	ASP
20	R1	1674	THR
20	R1	1700	ASP
20	R1	1716	LEU
20	R1	1731	THR
20	R1	1761	SER
20	R1	1791	ASN
20	R2	5	THR
20	R2	8	THR
20	R2	39	ASP
20	R2	57	TYR
20	R2	101	VAL
20	R2	143	ASP
20	R2	222	ASP
20	R2	259	ASP
20	R2	351	ASN
20	R2	383	TYR
20	R2	470	ASN
20	R2	501	PHE
20	R2	523	ASN
20	R2	541	ASN
20	R2	544	ASP
20	R2	557	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R2	559	ASP
20	R2	588	GLU
20	R2	594	ASP
20	R2	612	ASN
20	R2	661	GLU
20	R2	702	ASP
20	R2	735	ASP
20	R2	838	TYR
20	R2	852	ASP
20	R2	889	ASP
20	R2	899	SER
20	R2	903	ASP
20	R2	904	SER
20	R2	946	ASP
20	R2	948	SER
20	R2	962	ASP
20	R2	1028	GLU
20	R2	1080	GLU
20	R2	1150	PHE
20	R2	1190	GLU
20	R2	1269	ASP
20	R2	1329	ASP
20	R2	1370	THR
20	R2	1438	PHE
20	R2	1502	SER
20	R2	1547	ASP
20	R2	1615	SER
20	R2	1646	ASN
20	R2	1700	ASP
20	R2	1711	HIS
20	R2	1716	LEU
20	R2	1728	THR
20	R2	1791	ASN
20	R3	3	ASP
20	R3	18	ASP
20	R3	57	TYR
20	R3	101	VAL
20	R3	143	ASP
20	R3	184	SER
20	R3	185	PHE
20	R3	222	ASP
20	R3	259	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R3	351	ASN
20	R3	358	SER
20	R3	383	TYR
20	R3	401	GLU
20	R3	448	GLN
20	R3	501	PHE
20	R3	523	ASN
20	R3	541	ASN
20	R3	544	ASP
20	R3	554	SER
20	R3	557	ASP
20	R3	559	ASP
20	R3	588	GLU
20	R3	661	GLU
20	R3	702	ASP
20	R3	735	ASP
20	R3	811	GLU
20	R3	838	TYR
20	R3	852	ASP
20	R3	889	ASP
20	R3	903	ASP
20	R3	904	SER
20	R3	946	ASP
20	R3	962	ASP
20	R3	1080	GLU
20	R3	1150	PHE
20	R3	1190	GLU
20	R3	1269	ASP
20	R3	1329	ASP
20	R3	1370	THR
20	R3	1438	PHE
20	R3	1497	THR
20	R3	1500	TYR
20	R3	1547	ASP
20	R3	1616	HIS
20	R3	1645	ASP
20	R3	1674	THR
20	R3	1700	ASP
20	R3	1711	HIS
20	R3	1716	LEU
20	R3	1728	THR
20	R3	1791	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	T0	3	THR
21	T0	27	ASN
21	T0	63	ASN
21	T0	80	CYS
21	T0	106	THR
21	T0	122	LEU
21	T0	213	LEU
21	T0	318	SER
21	T0	331	HIS
21	T0	394	THR
21	T0	406	ASP
21	T0	498	ASP
21	T0	569	LEU
21	T0	570	THR
21	T0	611	GLU
21	T0	627	ASN
21	T0	665	SER
21	T0	695	LEU
21	T0	758	SER
21	T0	795	THR
21	T0	862	ASP
21	T0	864	ASN
21	T0	926	THR
21	T0	937	SER
21	T0	950	LEU
21	T0	965	ASP
21	T0	966	ASP
21	T0	970	ASP
21	T0	984	ASP
21	T0	985	GLU
21	T0	986	ASP
21	T0	987	ILE
21	T0	1057	GLN
21	T0	1066	ASP
21	T0	1091	ASP
21	T0	1160	LEU
21	T0	1168	LEU
21	T1	3	THR
21	T1	16	ASN
21	T1	106	THR
21	T1	117	ASP
21	T1	122	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	T1	157	LEU
21	T1	235	SER
21	T1	257	HIS
21	T1	318	SER
21	T1	394	THR
21	T1	493	SER
21	T1	498	ASP
21	T1	499	GLU
21	T1	519	LEU
21	T1	539	ASP
21	T1	552	SER
21	T1	553	ASP
21	T1	557	ASP
21	T1	611	GLU
21	T1	665	SER
21	T1	695	LEU
21	T1	719	SER
21	T1	727	GLU
21	T1	758	SER
21	T1	862	ASP
21	T1	864	ASN
21	T1	926	THR
21	T1	937	SER
21	T1	965	ASP
21	T1	966	ASP
21	T1	984	ASP
21	T1	985	GLU
21	T1	986	ASP
21	T1	1066	ASP
21	T1	1071	ASP
21	T1	1091	ASP
21	T1	1160	LEU
21	T1	1168	LEU
21	T2	53	GLU
21	T2	54	ASN
21	T2	73	VAL
21	T2	101	LYS
21	T2	106	THR
21	T2	122	LEU
21	T2	129	THR
21	T2	157	LEU
21	T2	318	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	T2	394	THR
21	T2	411	ILE
21	T2	493	SER
21	T2	519	LEU
21	T2	539	ASP
21	T2	553	ASP
21	T2	569	LEU
21	T2	602	LEU
21	T2	611	GLU
21	T2	632	TYR
21	T2	665	SER
21	T2	770	ASP
21	T2	862	ASP
21	T2	864	ASN
21	T2	926	THR
21	T2	937	SER
21	T2	984	ASP
21	T2	986	ASP
21	T2	1057	GLN
21	T2	1066	ASP
21	T2	1071	ASP
21	T2	1091	ASP
21	T2	1160	LEU
21	T2	1168	LEU
21	T3	3	THR
21	T3	16	ASN
21	T3	25	ASN
21	T3	63	ASN
21	T3	75	GLU
21	T3	106	THR
21	T3	122	LEU
21	T3	157	LEU
21	T3	257	HIS
21	T3	318	SER
21	T3	394	THR
21	T3	411	ILE
21	T3	492	HIS
21	T3	493	SER
21	T3	498	ASP
21	T3	519	LEU
21	T3	539	ASP
21	T3	552	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	T3	553	ASP
21	T3	557	ASP
21	T3	569	LEU
21	T3	611	GLU
21	T3	665	SER
21	T3	695	LEU
21	T3	763	ASP
21	T3	795	THR
21	T3	798	ASP
21	T3	820	GLU
21	T3	926	THR
21	T3	937	SER
21	T3	984	ASP
21	T3	986	ASP
21	T3	987	ILE
21	T3	989	SER
21	T3	1057	GLN
21	T3	1066	ASP
21	T3	1071	ASP
21	T3	1091	ASP
21	T3	1160	LEU
21	T3	1168	LEU
22	U0	864	PHE
22	U0	882	ASP
22	U1	864	PHE
22	U1	882	ASP
22	U2	864	PHE
22	U2	882	ASP
22	U3	882	ASP
23	V0	642	MET
23	V0	677	ARG
23	V0	682	GLU
23	V1	642	MET
23	V1	651	VAL
23	V1	677	ARG
23	V1	794	PHE
23	V1	798	GLU
24	W0	1	MET
24	W0	73	ASP
24	W0	86	LEU
24	W0	89	ASN
24	W0	133	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W0	151	THR
24	W0	155	THR
24	W0	157	TYR
24	W0	260	ASN
24	W0	305	ASP
24	W0	329	SER
24	W0	337	ILE
24	W0	470	ASN
24	W0	538	ASP
24	W0	597	GLU
24	W0	624	ASN
24	W0	665	ASP
24	W0	700	ASP
24	W0	720	ASP
24	W0	725	ASP
24	W0	727	ASP
24	W0	763	THR
24	W0	786	ASN
24	W0	838	LYS
24	W0	881	GLU
24	W0	917	LEU
24	W1	73	ASP
24	W1	86	LEU
24	W1	89	ASN
24	W1	133	SER
24	W1	151	THR
24	W1	155	THR
24	W1	157	TYR
24	W1	268	ASN
24	W1	269	CYS
24	W1	313	GLN
24	W1	470	ASN
24	W1	538	ASP
24	W1	597	GLU
24	W1	624	ASN
24	W1	665	ASP
24	W1	700	ASP
24	W1	720	ASP
24	W1	727	ASP
24	W1	735	GLU
24	W1	737	ASN
24	W1	763	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W1	786	ASN
24	W1	953	GLU
25	X0	19	THR
25	X0	44	SER
25	X0	77	ASP
25	X0	92	ILE
25	X0	106	ASP
25	X0	146	ASP
25	X0	264	PHE
25	X0	295	ASP
25	X0	367	THR
25	X0	399	THR
25	X0	402	ASP
25	X0	404	LEU
25	X1	3	GLU
25	X1	19	THR
25	X1	21	GLU
25	X1	77	ASP
25	X1	92	ILE
25	X1	146	ASP
25	X1	155	LYS
25	X1	171	GLU
25	X1	264	PHE
25	X1	278	VAL
25	X1	290	GLU
25	X1	295	ASP
25	X1	367	THR
25	X1	402	ASP
25	X1	404	LEU
25	X2	3	GLU
25	X2	19	THR
25	X2	21	GLU
25	X2	77	ASP
25	X2	92	ILE
25	X2	118	GLU
25	X2	146	ASP
25	X2	155	LYS
25	X2	171	GLU
25	X2	264	PHE
25	X2	290	GLU
25	X2	295	ASP
25	X2	367	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	X2	402	ASP
25	X2	404	LEU
25	X3	19	THR
25	X3	77	ASP
25	X3	92	ILE
25	X3	167	GLU
25	X3	264	PHE
25	X3	278	VAL
25	X3	294	THR
25	X3	295	ASP
25	X3	402	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	01	357	ASN
2	10	285	GLN
2	10	1523	HIS
2	10	1540	GLN
2	10	1544	HIS
2	10	1717	GLN
2	11	611	ASN
2	11	614	ASN
2	11	822	GLN
2	11	1097	HIS
2	11	1102	ASN
2	11	1349	ASN
2	11	1540	GLN
2	11	1784	ASN
2	12	285	GLN
2	12	376	ASN
2	12	378	ASN
2	12	511	ASN
2	12	617	ASN
2	12	820	GLN
2	12	1065	GLN
2	12	1079	GLN
2	12	1093	ASN
2	12	1249	HIS
2	12	1523	HIS
2	12	1540	GLN
2	13	285	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	13	613	ASN
2	13	735	ASN
2	13	861	ASN
2	13	1003	GLN
2	13	1037	GLN
2	13	1079	GLN
2	13	1540	GLN
2	13	1717	GLN
2	13	1746	GLN
2	14	376	ASN
2	14	614	ASN
2	14	735	ASN
2	14	1269	ASN
2	14	1405	ASN
2	14	1540	GLN
2	14	1754	GLN
2	14	1784	ASN
2	14	1785	ASN
2	15	816	GLN
2	15	1102	ASN
2	15	1132	GLN
2	15	1269	ASN
2	15	1540	GLN
2	16	285	GLN
2	16	325	ASN
2	16	611	ASN
2	16	1079	GLN
2	16	1269	ASN
2	16	1349	ASN
2	16	1540	GLN
2	16	1754	GLN
2	17	463	GLN
2	17	466	ASN
2	17	1269	ASN
3	40	216	GLN
3	40	337	GLN
3	41	216	GLN
3	41	337	GLN
4	A0	917	GLN
4	A1	382	GLN
4	A1	601	GLN
4	A2	382	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	601	GLN
4	A2	849	GLN
4	A3	382	GLN
4	A3	601	GLN
4	A4	382	GLN
4	A4	601	GLN
4	A4	849	GLN
4	A5	645	ASN
5	B0	694	ASN
5	B0	1517	HIS
5	B0	1929	GLN
5	B0	1975	ASN
5	B1	694	ASN
5	B1	1517	HIS
5	B1	1929	GLN
5	B1	1975	ASN
6	C0	414	GLN
6	C0	515	ASN
6	C0	1047	GLN
6	C0	1676	ASN
6	C1	752	GLN
6	C1	838	ASN
6	C2	752	GLN
6	C3	414	GLN
6	C3	1047	GLN
7	D0	267	HIS
7	D1	267	HIS
7	D2	216	HIS
7	D3	267	HIS
8	E0	419	GLN
8	E1	419	GLN
10	H0	404	ASN
10	H1	196	GLN
10	H2	196	GLN
10	H2	404	ASN
11	I0	192	ASN
11	I0	196	ASN
13	K0	631	ASN
13	K1	631	ASN
13	K2	631	ASN
13	K3	631	ASN
14	L1	266	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L1	373	GLN
14	L3	431	ASN
14	L3	821	ASN
15	M0	455	HIS
15	M1	773	GLN
15	M2	773	GLN
15	M3	776	ASN
17	O2	157	GLN
17	O3	157	GLN
18	P0	472	HIS
18	P0	849	GLN
18	P2	309	ASN
18	P3	309	ASN
19	Q1	245	ASN
20	R0	950	ASN
20	R0	1510	ASN
20	R0	1630	GLN
20	R0	1646	ASN
20	R1	470	ASN
20	R1	950	ASN
20	R1	1361	ASN
20	R2	405	GLN
20	R2	612	ASN
20	R2	950	ASN
20	R3	7	ASN
20	R3	405	GLN
20	R3	470	ASN
20	R3	482	ASN
20	R3	782	ASN
21	T0	396	ASN
21	T0	962	ASN
21	T1	575	ASN
21	T2	396	ASN
21	T3	63	ASN
21	T3	396	ASN
24	W0	659	ASN
24	W1	659	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	F2	1
9	F0	1
9	F3	1
9	F1	1
20	R3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F2	174:GLU	C	380:LYS	N	105.57
1	F0	174:GLU	C	380:LYS	N	100.31
1	F3	174:GLU	C	380:LYS	N	42.15
1	F1	174:GLU	C	380:LYS	N	41.08
1	R3	188:GLY	C	189:SER	N	2.36

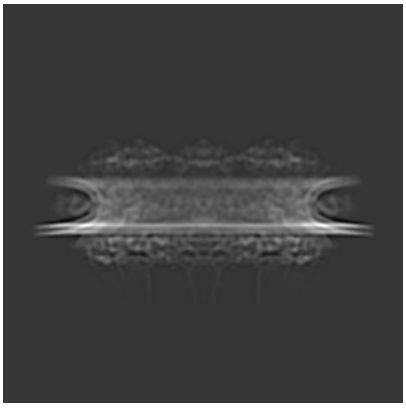
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19137. These allow visual inspection of the internal detail of the map and identification of artifacts.

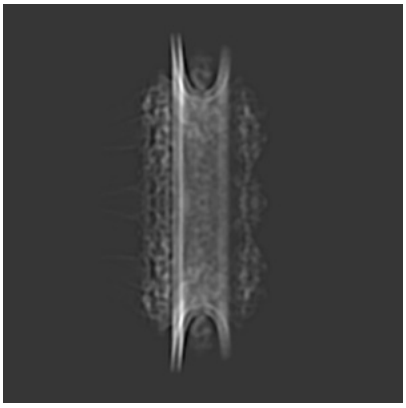
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

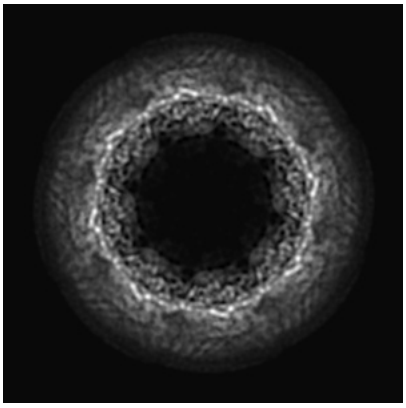
6.1.1 Primary map



X



Y



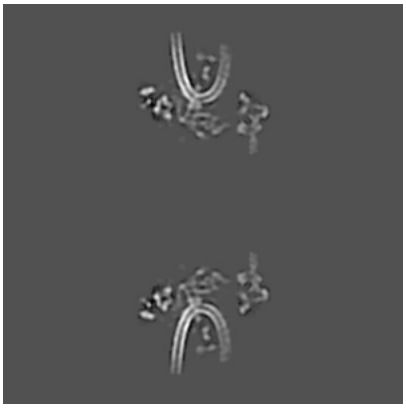
Z

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

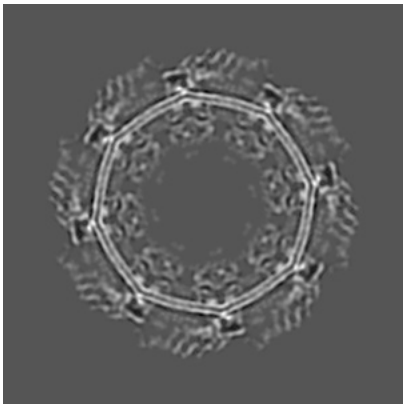
6.2 Central slices (i)

6.2.1 Primary map

X Index: 120



Y Index: 120



Z Index: 120

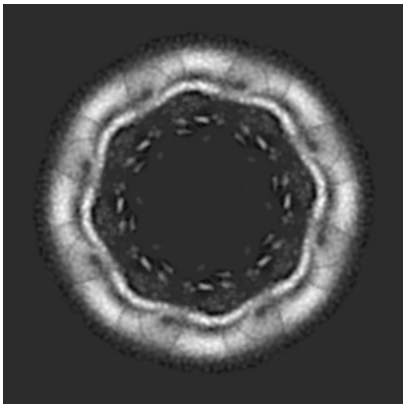
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 59

Y Index: 181

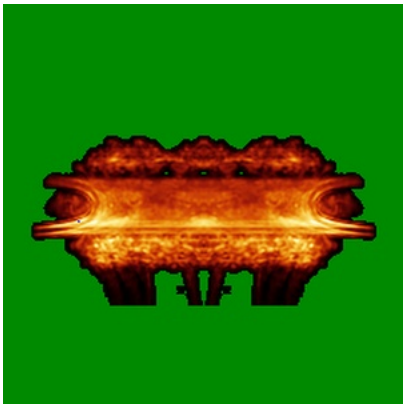


Z Index: 107

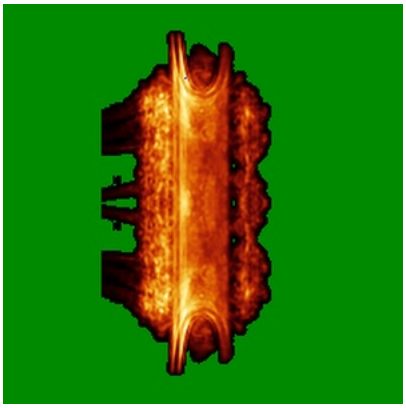
The images above show the largest variance slices of the map in three orthogonal directions.

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

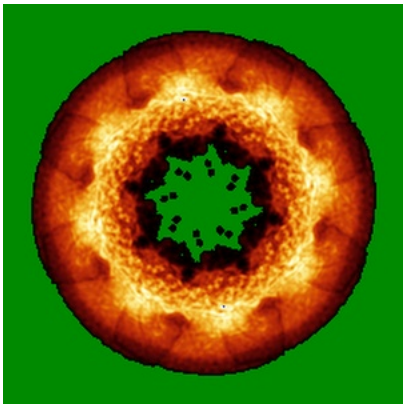
6.4.1 Primary map



X



Y

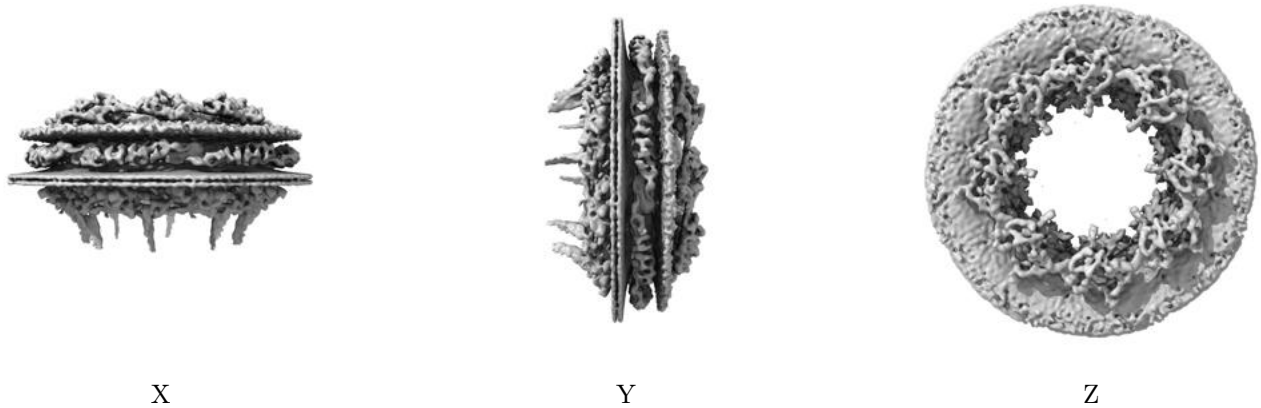


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

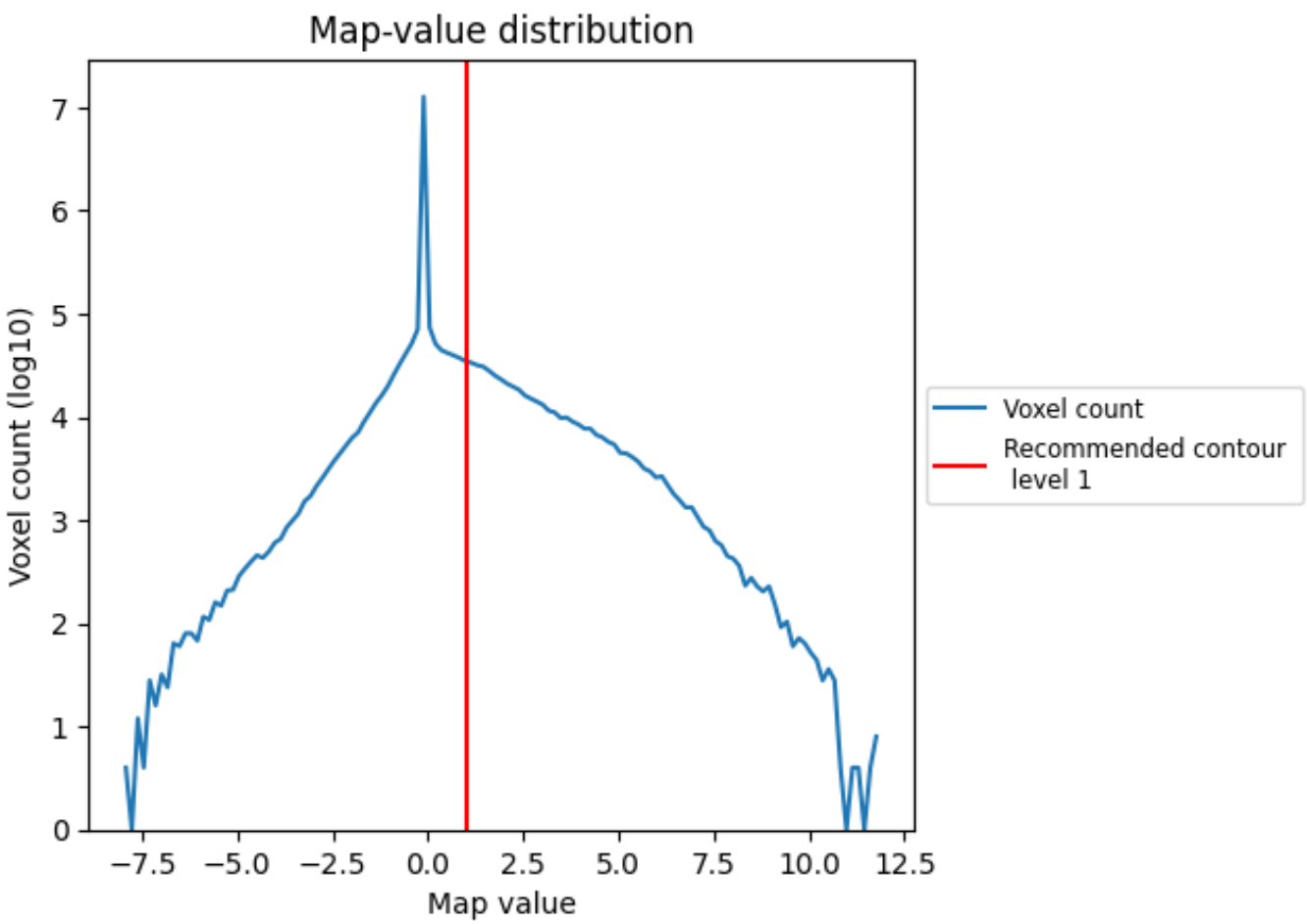
6.6 Mask visualisation (i)

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

7 Map analysis (i)

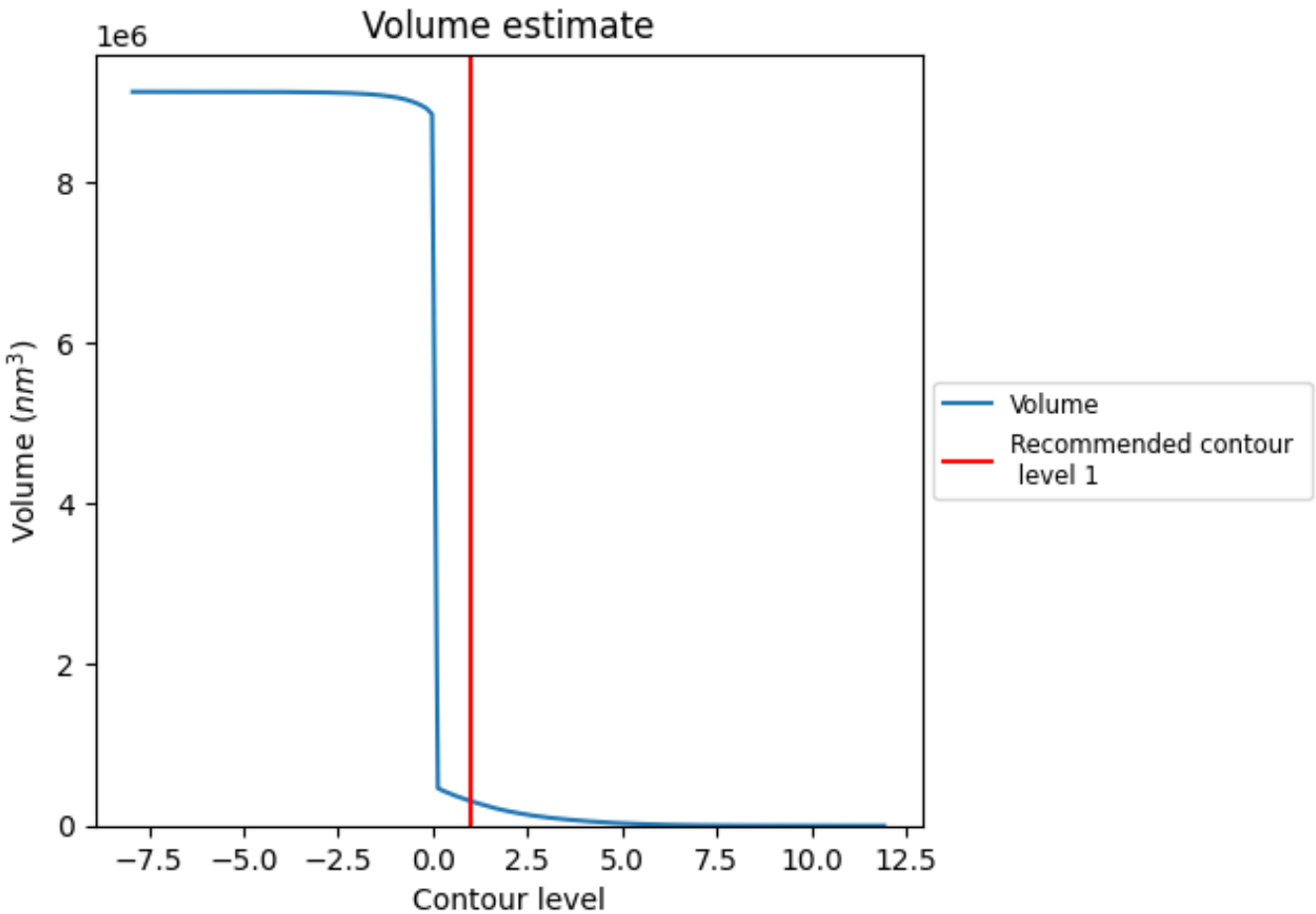
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

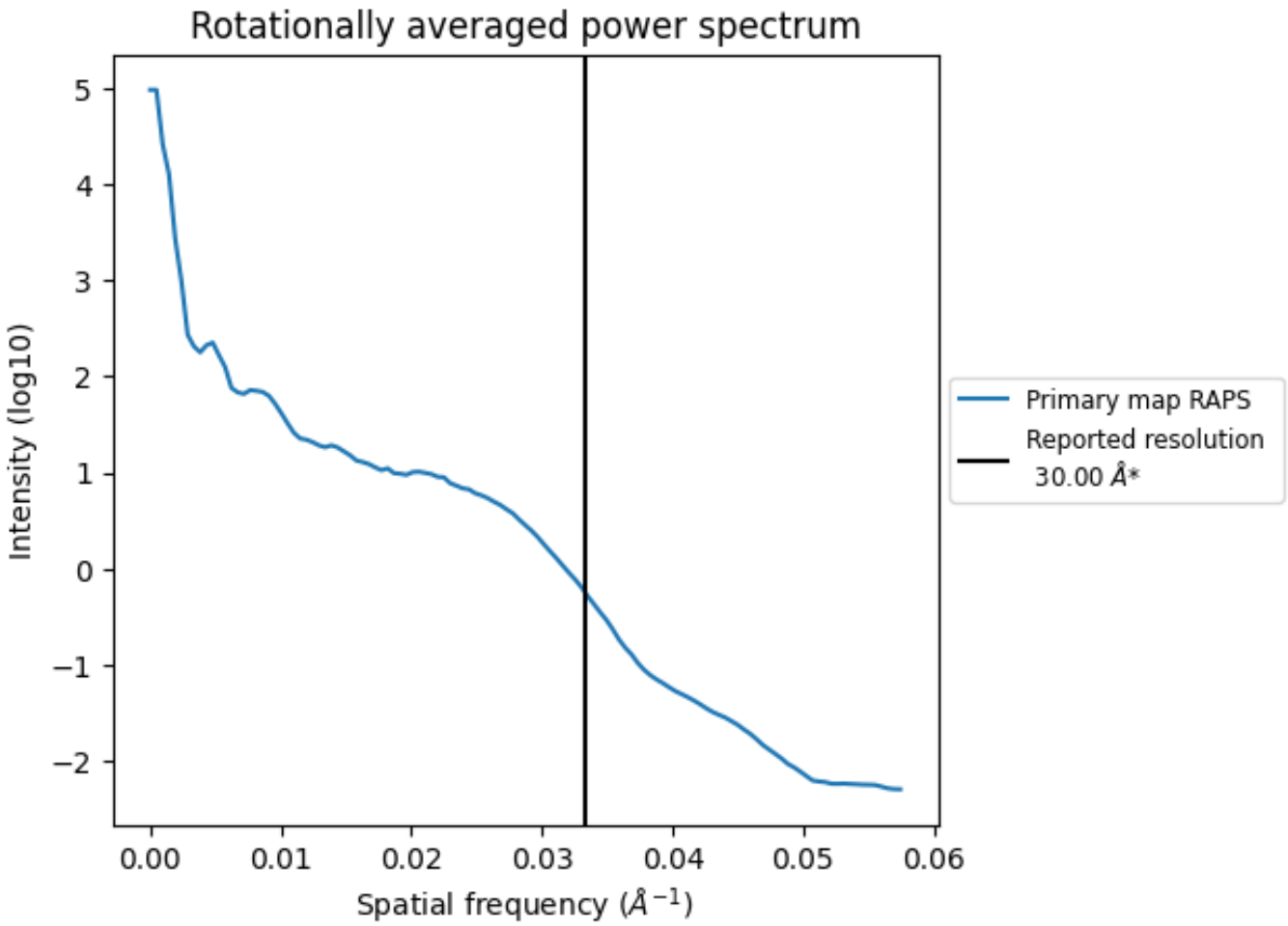
7.2 Volume estimate (i)



The volume at the recommended contour level is 306272 nm^3; this corresponds to an approximate mass of 276664 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 0.033 Å^{-1}

8 Fourier-Shell correlation (i)

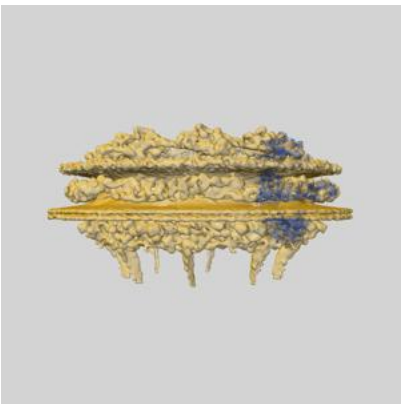
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

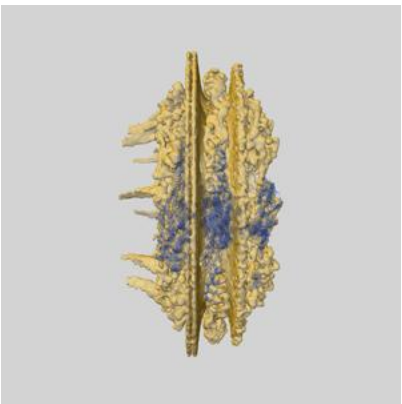
This section contains information regarding the fit between EMDB map EMD-19137 and PDB model 9HCJ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlays

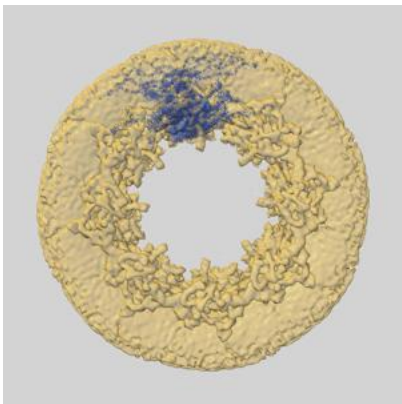
9.1.1 Map-model overlay (i)



X

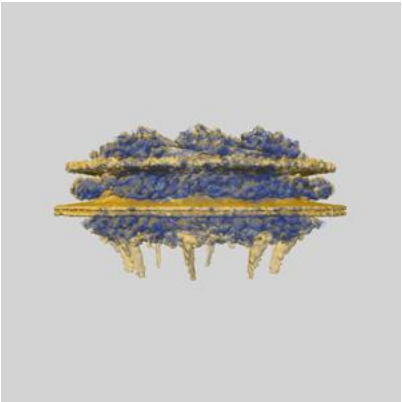


Y

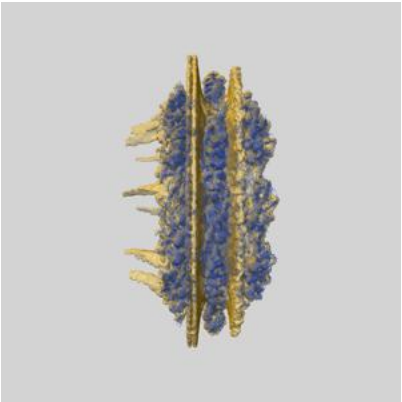


Z

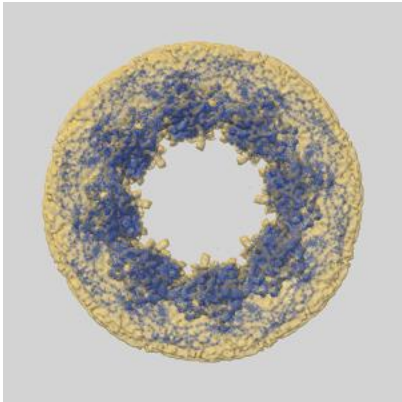
9.1.2 Map-model assembly overlay (i)



X



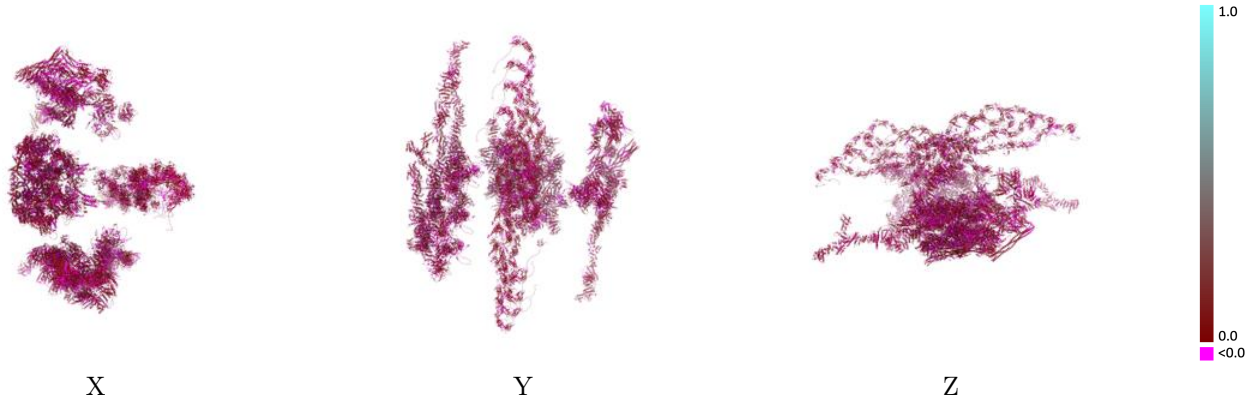
Y



Z

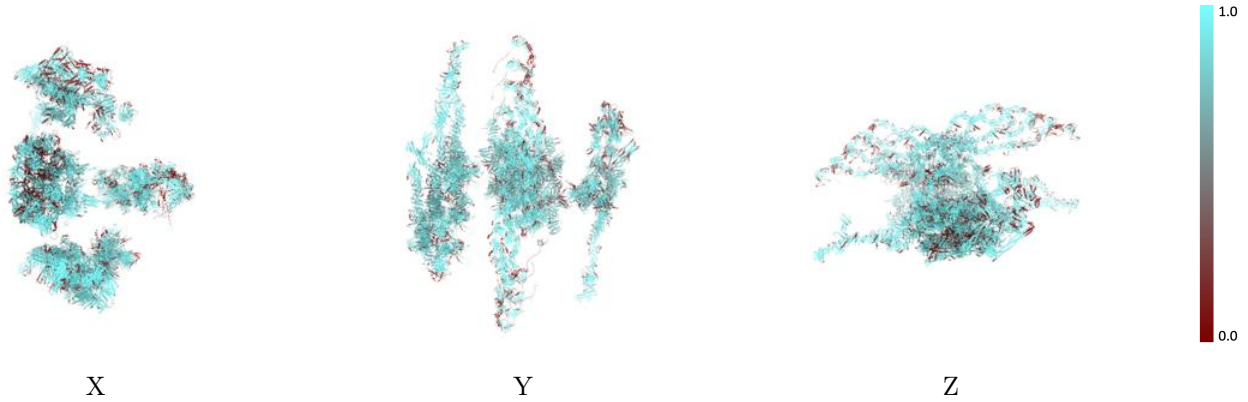
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



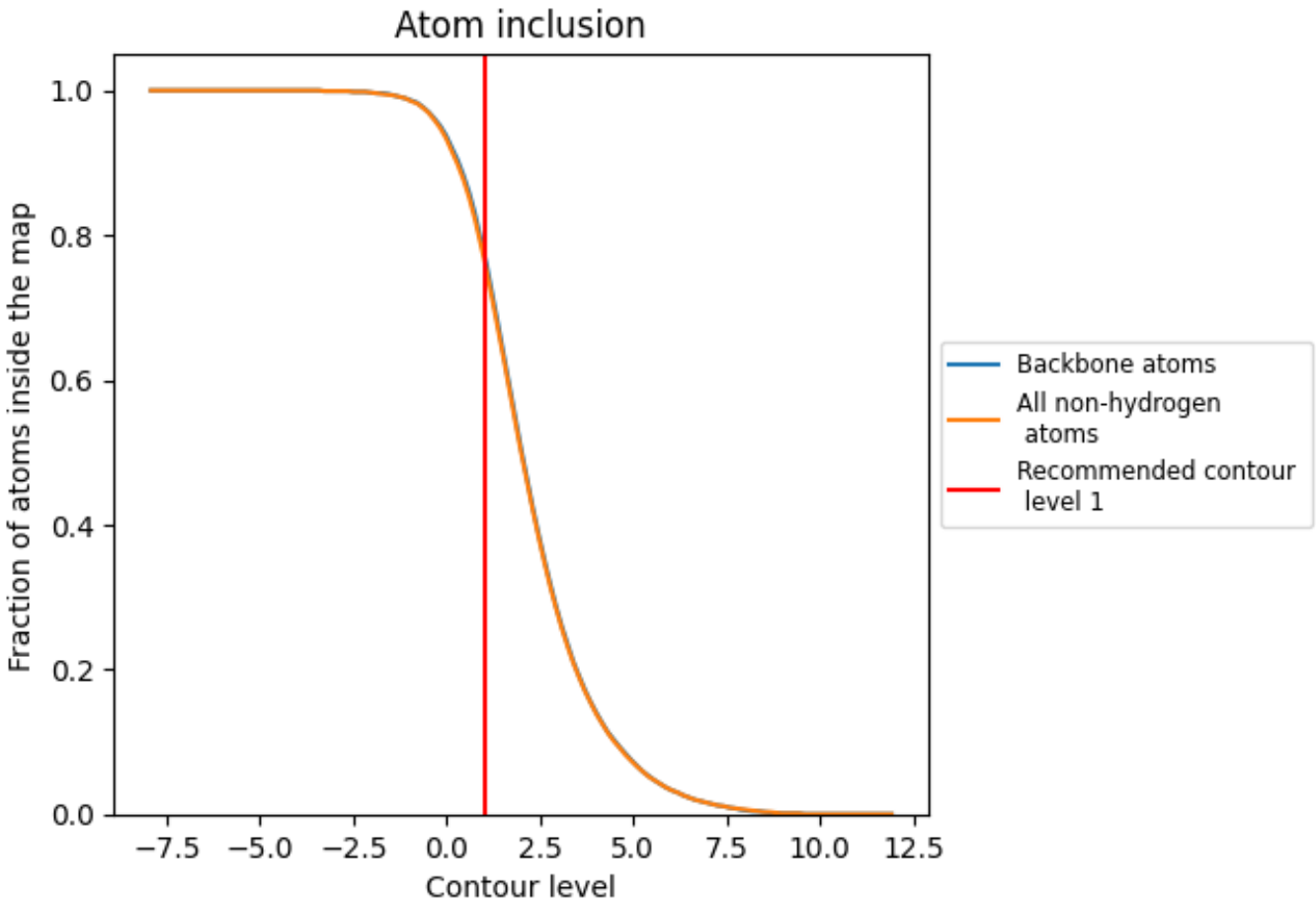
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.0360
00	0.6780	0.0380
01	0.6090	0.0190
10	0.6520	0.0370
11	0.7700	0.0400
12	0.7790	0.0390
13	0.7610	0.0410
14	0.7200	0.0440
15	0.7400	0.0420
16	0.7840	0.0470
17	0.7490	0.0440
40	0.9400	0.0270
41	0.8650	0.0250
A0	0.7710	0.0380
A1	0.8070	0.0440
A2	0.6840	0.0390
A3	0.8660	0.0480
A4	0.7220	0.0380
A5	0.8570	0.0390
B0	0.6480	0.0350
B1	0.6940	0.0380
C0	0.7230	0.0300
C1	0.6330	0.0300
C2	0.6320	0.0330
C3	0.8030	0.0320
D0	0.7360	0.0390
D1	0.7930	0.0370
D2	0.7420	0.0400
D3	0.8230	0.0390
E0	0.9640	0.0210
E1	0.9500	0.0240
F0	0.4410	0.0500
F1	0.3390	0.0320
F2	0.6040	0.0660
F3	0.7740	0.0540

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
H0	0.8130	0.0500
H1	0.6180	0.0330
H2	0.5600	0.0340
H3	0.7960	0.0460
I0	0.6270	0.0370
I1	0.7170	0.0440
I2	0.6620	0.0440
I3	0.6780	0.0350
J0	0.6460	0.0180
J1	0.6590	0.0370
J2	0.7160	0.0300
J3	0.6730	0.0420
J4	0.5930	0.0280
J5	0.7530	0.0500
K0	0.8910	0.0490
K1	0.7930	0.0330
K2	0.8890	0.0510
K3	0.9070	0.0570
L0	0.8280	0.0370
L1	0.9430	0.0530
L2	0.9120	0.0430
L3	0.9130	0.0460
M0	0.9330	0.0570
M1	0.9350	0.0530
M2	0.8130	0.0410
M3	0.9000	0.0450
N0	0.7990	0.0290
N1	0.8060	0.0120
N2	0.7800	0.0230
N3	0.7870	0.0300
O0	0.8110	0.0190
O1	0.8190	0.0150
O2	0.9000	0.0360
O3	0.7940	0.0190
P0	0.7480	0.0320
P1	0.8160	0.0250
P2	0.7700	0.0280
P3	0.7910	0.0270
Q0	0.8710	0.0400
Q1	0.9220	0.0340
Q2	0.8370	0.0260
Q3	0.8320	0.0410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
R0	0.6700	0.0140
R1	0.8030	0.0250
R2	0.7840	0.0250
R3	0.7530	0.0160
T0	0.7680	0.0410
T1	0.8360	0.0330
T2	0.7650	0.0260
T3	0.7870	0.0390
U0	0.2510	0.0030
U1	0.8540	0.0450
U2	0.3670	-0.0300
U3	0.9550	0.0510
V0	0.7420	0.0500
V1	0.5880	0.0240
W0	0.6320	0.0200
W1	0.6970	0.0250
X0	0.8470	0.0390
X1	0.8110	0.0550
X2	0.8650	0.0530
X3	0.8060	0.0470