Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 01:02 PM EST

PDB ID	:	5WLC
EMDB ID	:	EMD-8859
Title	:	The complete structure of the small subunit processome
Authors	:	Barandun, J.; Chaker-Margot, M.; Hunziker, M.; Klinge, S.
Deposited on	:	2017-07-26
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

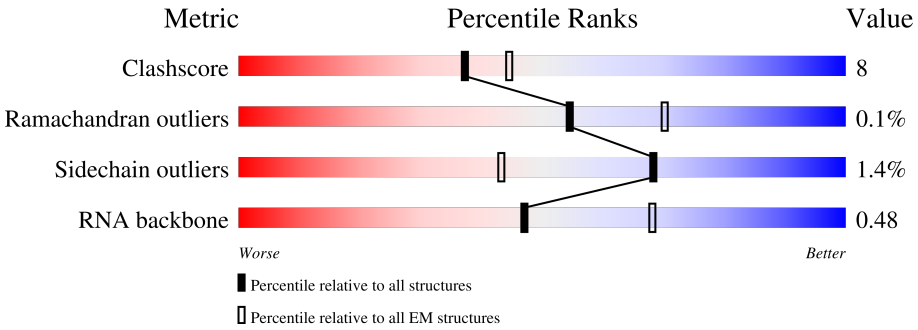
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	L0	700	5% 38% 26% 5% 30%
2	L1	1807	23% 30% 21% 6% 43%
3	L2	333	• 28% 18% • • 49%
4	L3	146	51% 64% 12% • 23%
5	L4	261	38% 63% 23% • 13%
6	L5	225	5% 76% 19% 5%
7	L6	236	38% 36% 11% • 52%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	L7	190	85% 68% 17% 13%
9	L8	200	61% 66% 18% 15%
10	L9	197	8% 71% 17% 11%
11	LC	143	73% 13% 13%
12	LD	156	67% 58% 22% 19%
13	LE	130	63% 82% 16%
14	LF	135	11% 53% 13% 33%
15	LG	67	73% 21% 6%
16	LH	896	7% 69% 23% 7%
17	LI	713	38% 58% 10% 32%
18	LJ	513	71% 24%
19	LK	575	19% 79%
20	LL	643	53% 21% 26%
21	LM	1769	20% 5% 76%
22	LN	776	9% 64% 23% 13%
23	LO	923	69% 21% 10%
24	LP	440	8% 68% 14% 18%
25	LQ	943	14% 63% 26% 10%
26	LR	817	69% 79% 11% 11%
27	LS	594	59% 22% 19%
28	LT	939	72% 19% 9%
29	LU	489	7% 69% 24% 7%
30	LV	707	42% 35% 16% 49%
31	LW	554	60% 19% 21%
32	LX	1056	49% 67% 9% 23%

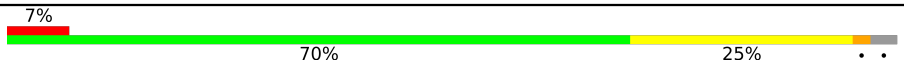
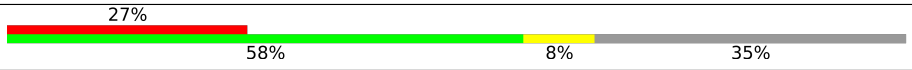
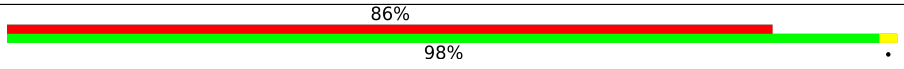
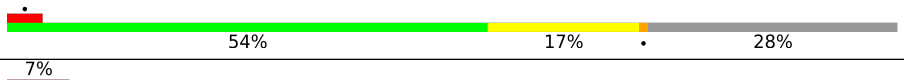
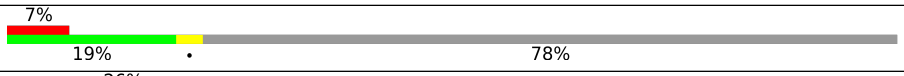
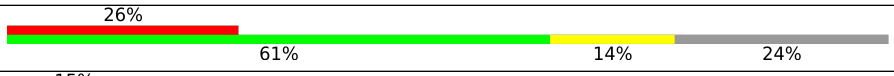
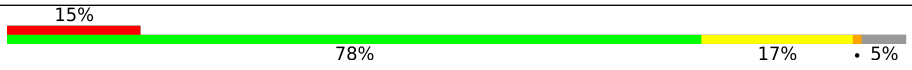
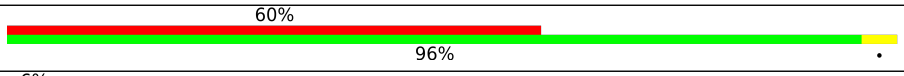
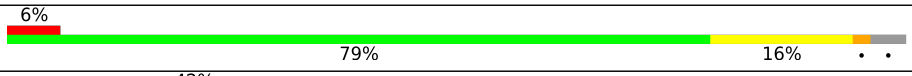
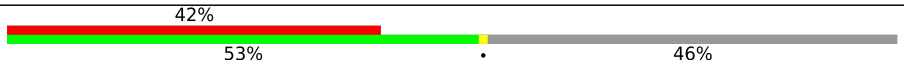
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	LY	1056	68% 69% 27%
33	LZ	183	70% 29%
34	NA	593	27% 7% 65%
35	NB	610	20% 77%
36	NC	357	15% 32% 6% 62%
37	ND	214	18% 31% 7% 62%
38	NE	346	41% 38% 8% 54%
39	NF	151	82% 82% 18%
40	NG	137	80% 70% 11% 19%
41	NH	1237	87% 86% 13%
42	NI	297	57% 56% 43%
43	NJ	1729	15% 15% 85%
44	NK	316	54% 54% 45%
45	SA	504	5% 60% 13% 27%
46	SB	511	12% 71% 12% 17%
47	SC	327	55% 18% 26%
47	SD	327	11% 50% 20% 30%
48	SE	126	81% 14%
48	SF	126	76% 20%
49	SG	573	7% 56% 19% 25%
50	SH	367	77% 21%
51	SI	1184	6% 50% 17% 32%
52	SJ	252	16% 67% 18% 14%
52	SK	252	7% 70% 20% 9%
53	SL	189	69% 23% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SM	290	
55	SN	274	
56	SO	274	
57	SP	982	
58	SQ	217	
59	SR	145	
60	SS	898	
61	ST	792	
62	SU	552	
63	SV	206	
64	SX	103	
65	SY	250	
66	SZ	483	

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 196921 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 RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L0	488	10405	4650	1838	3429	488	0	0

- Molecule 2 is a RNA chain called 18S pre-rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	1025	21866	9773	3905	7163	1025	0	0

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L2	169	3585	1605	629	1182	169	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L2	200	C	G	conflict	GB 176452

- Molecule 4 is a protein called rpS18_uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L3	113	901	569	168	162	2	0	0

- Molecule 5 is a protein called rpS4_eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L4	228	1810	1158	330	319	3	0	0

- Molecule 6 is a protein called rpS5_uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	213	Total	C	N	O	S	0	0
			1669	1045	307	314	3		

- Molecule 7 is a protein called rpS6_eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	113	Total	C	N	O	S	0	0
			888	567	156	163	2		

- Molecule 8 is a protein called rpS7_eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L7	165	Total	C	N	O	0	0
			1321	854	227	240		

- Molecule 9 is a protein called rpS8_eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	170	Total	C	N	O	S	0	0
			1349	839	267	241	2		

- Molecule 10 is a protein called rpS9_uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	175	Total	C	N	O	S	0	0
			1415	895	273	246	1		

- Molecule 11 is a protein called rpS16_uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	LC	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 12 is a protein called rpS11_uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	127	Total	C	N	O	S	0	0
			1027	660	194	170	3		

- Molecule 13 is a protein called rpS22_uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	127	Total	C	N	O	S	0	0
			1003	640	183	177	3		

- Molecule 14 is a protein called rpS24_eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	LF	90	Total	C	N	O	0	0
			715	458	131	126		

- Molecule 15 is a protein called rpS28_eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 16 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	834	Total	C	N	O	S	0	0
			6633	4215	1121	1278	19		

- Molecule 17 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	487	Total	C	N	O	S	0	0
			2857	1763	529	562	3		

- Molecule 18 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 19 is a protein called Utp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	123	Total	C	N	O	S	0	0
			898	567	166	163	2		

- Molecule 20 is a protein called Utp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	475	Total	C	N	O	S	0	0
			3772	2400	649	710	13		

- Molecule 21 is a protein called Utp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	431	Total	C	N	O	S	0	0
			3443	2224	566	641	12		

- Molecule 22 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	678	Total	C	N	O	S	0	0
			5344	3384	930	1009	21		

- Molecule 23 is a protein called Utp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	834	Total	C	N	O	S	0	0
			6635	4223	1140	1253	19		

- Molecule 24 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	359	Total	C	N	O	S	0	0
			2709	1723	486	488	12		

- Molecule 25 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	848	Total	C	N	O	S	0	0
			6640	4244	1116	1253	27		

- Molecule 26 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	729	Total	C	N	O	S	0	0
			4144	2520	797	818	9		

- Molecule 27 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LS	481	Total	C	N	O	S	0	0
			3791	2399	668	714	10		

- Molecule 28 is a protein called Utp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	850	Total	C	N	O	S	0	0
			6697	4253	1154	1269	21		

- Molecule 29 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	457	Total	C	N	O	S	0	0
			3725	2328	679	702	16		

- Molecule 30 is a protein called Enp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	362	Total	C	N	O	S	0	0
			2840	1789	487	555	9		

- Molecule 31 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	438	Total	C	N	O	S	0	0
			3428	2163	601	652	12		

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	808	Total	C	N	O	S	0	0
			4583	2798	888	890	7		
32	LY	769	Total	C	N	O		0	0
			3823	2285	769	769			

- Molecule 33 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LZ	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 34 is a protein called Mpp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NA	207	Total	C	N	O	S	0	0
			1667	1034	297	332	4		

- Molecule 35 is a protein called Sas10.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	NB	142	Total	C	N	O	0	0
			1098	677	218	203		

- Molecule 36 is a protein called Lcp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NC	136	Total	C	N	O	S	0	0
			1125	674	231	217	3		

- Molecule 37 is a protein called Bud21.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	ND	81	Total	C	N	O	0	0
			600	373	122	105		

- Molecule 38 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NE	158	Total	C	N	O	S	0	0
			1192	731	246	212	3		

- Molecule 39 is a protein called rpS13_uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	NF	124	Total	C	N	O	0	0
			615	367	124	124		

- Molecule 40 is a protein called rpS14_uS11.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	NG	111	Total	C	N	O	0	0
			543	321	111	111		

- Molecule 41 is a protein called Utp22.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	NH	1082	Total 5362	C 3198	N 1082	O 1082	0	0

- Molecule 42 is a protein called Rrp7.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	NI	169	Total 841	C 503	N 169	O 169	0	0

- Molecule 43 is a protein called Rrp5.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	NJ	265	Total 1314	C 784	N 265	O 265	0	0

- Molecule 44 is a protein called Krr1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	NK	175	Total 868	C 518	N 175	O 175	0	0

- Molecule 45 is a protein called Nop56.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SA	370	Total 2854	C 1815	N 490	O 541	S 8	0	0

- Molecule 46 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SB	425	Total 2937	C 1824	N 533	O 572	S 8	0	0

- Molecule 47 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SC	242	Total 1881	C 1193	N 338	O 340	S 10	0	0
47	SD	228	Total 1782	C 1131	N 320	O 321	S 10	0	0

- Molecule 48 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SE	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
48	SF	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 49 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SG	429	Total	C	N	O	S	0	0
			3428	2185	596	637	10		

- Molecule 50 is a protein called Rcl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SH	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 51 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SI	802	Total	C	N	O	S	0	0
			6412	4108	1142	1133	29		

- Molecule 52 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SJ	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
52	SK	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 53 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SL	174	Total	C	N	O	S	0	0
			1395	890	255	240	10		

- Molecule 54 is a protein called Imp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SM	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 55 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SN	247	Total	C	N	O	S	0	0
			2006	1284	356	358	8		

- Molecule 56 is a protein called Pno1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SO	179	Total	C	N	O	S	0	0
			998	606	199	192	1		

- Molecule 57 is a protein called Utp20.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	SP	982	Total	C	N	O	0	0
			4910	2946	982	982		

- Molecule 58 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SQ	135	Total	C	N	O	S	0	0
			1137	721	211	201	4		

- Molecule 59 is a protein called rpS23_uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SR	104	Total	C	N	O	S	0	0
			792	506	145	139	2		

- Molecule 60 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SS	197	Total	C	N	O	S	0	0
			1466	905	282	277	2		

- Molecule 61 is a protein called Nop14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	ST	599	Total	C	N	O	S	0	0
			4473	2830	809	823	11		

- Molecule 62 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SU	526	Total	C	N	O	S	0	0
			3781	2422	650	697	12		

- Molecule 63 is a protein called Rrt14.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	SV	63	Total	C	N	O	0	0
			381	234	69	78		

- Molecule 64 is a protein called Unassigned peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	SX	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 65 is a protein called Utp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SY	241	Total	C	N	O	S	0	0
			2016	1251	388	370	7		

- Molecule 66 is a protein called Enp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	SZ	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 67 is ZINC ION (three-letter code: ZN) (formula: Zn).

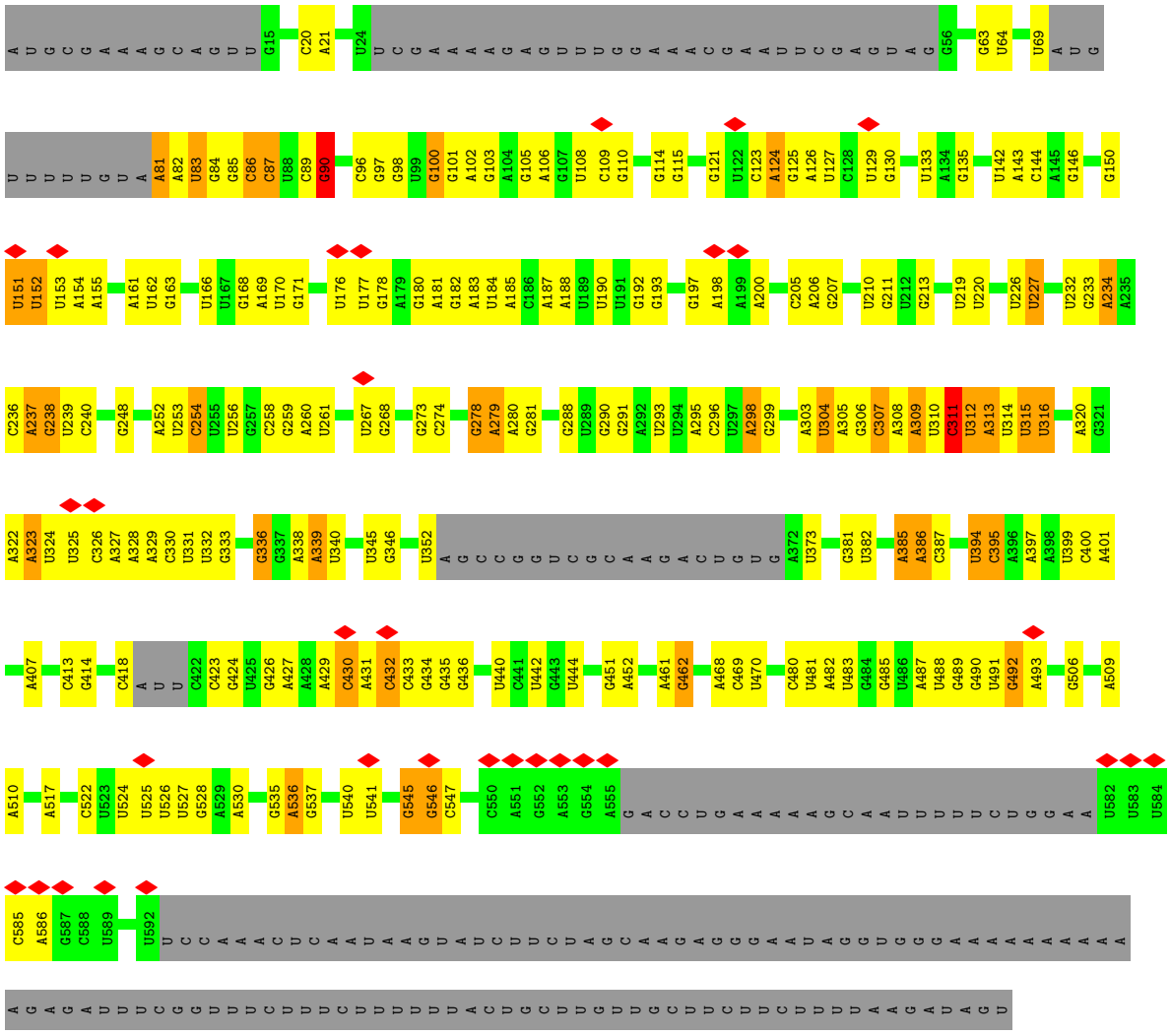
Mol	Chain	Residues	Atoms		AltConf
67	SL	1	Total	Zn	0
			1	1	

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.

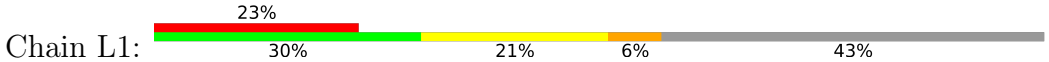
• Molecule 1: 5' ETS

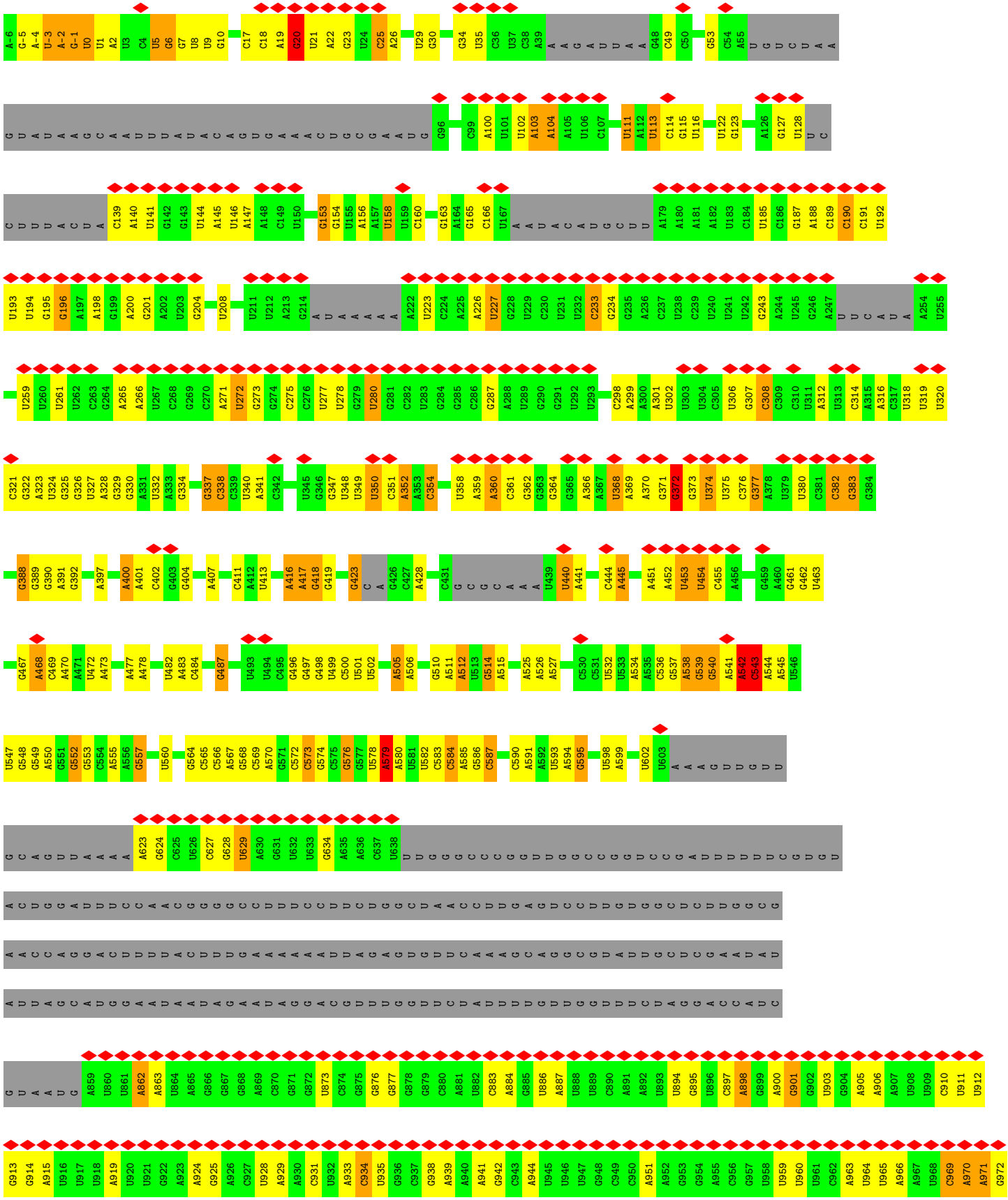
Chain L0:

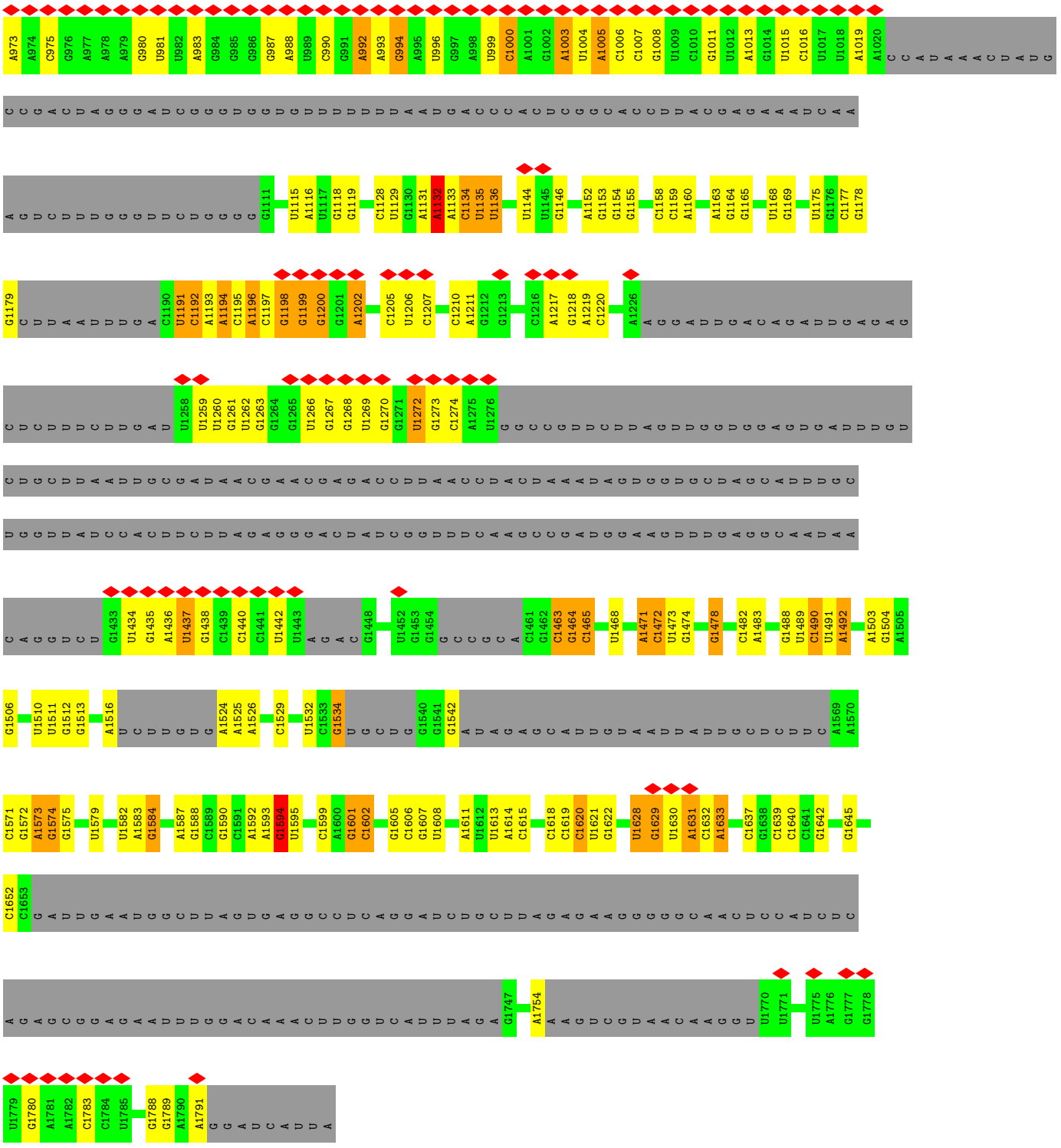


• Molecule 2: 18S pre-rRNA

Chain L1:

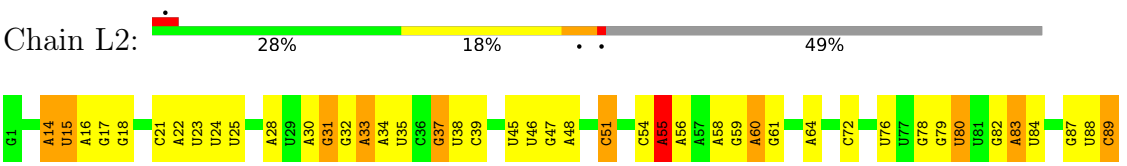


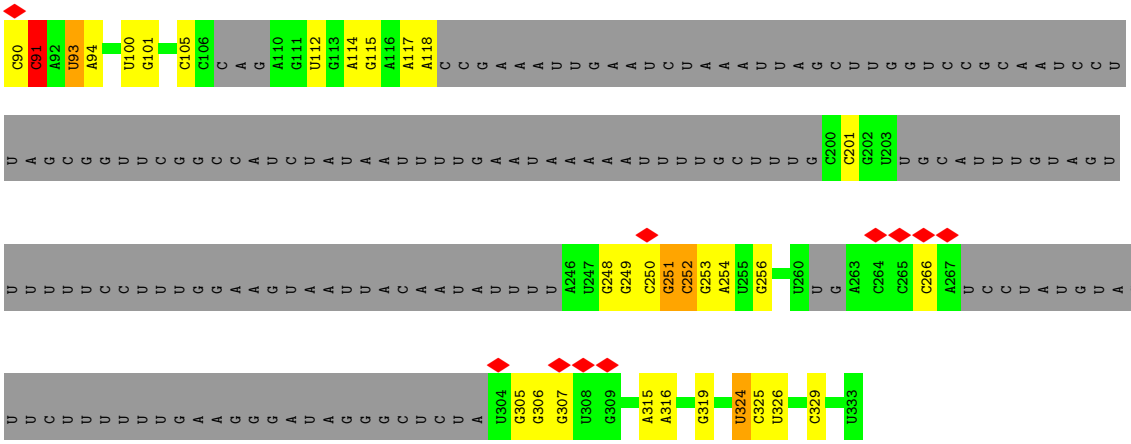




• Molecule 3: U3 snoRNA

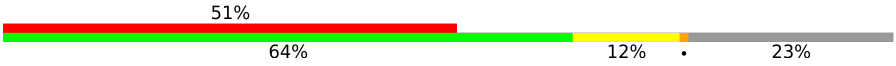
Chain L2:

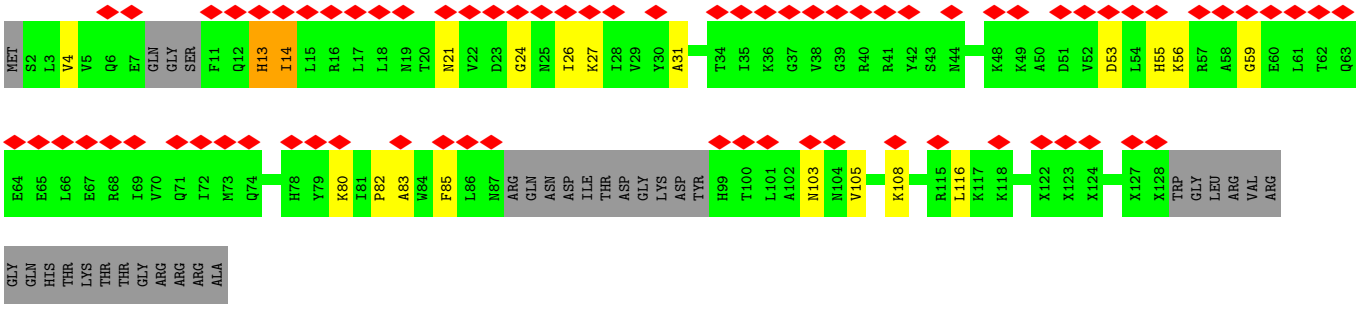




• Molecule 4: rpS18_uS13

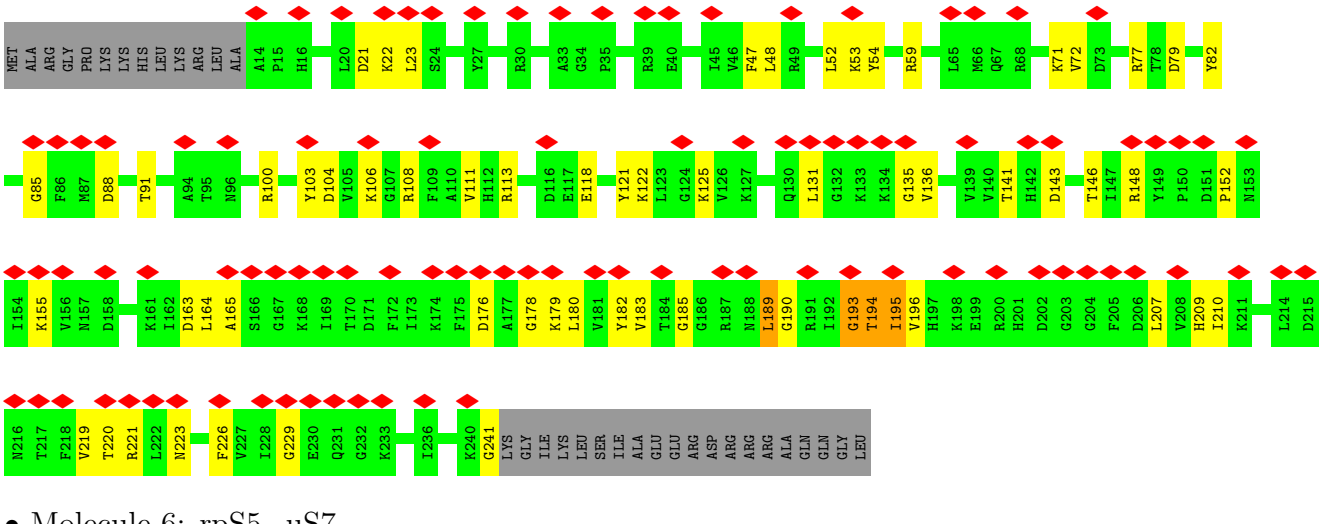
Chain L3:





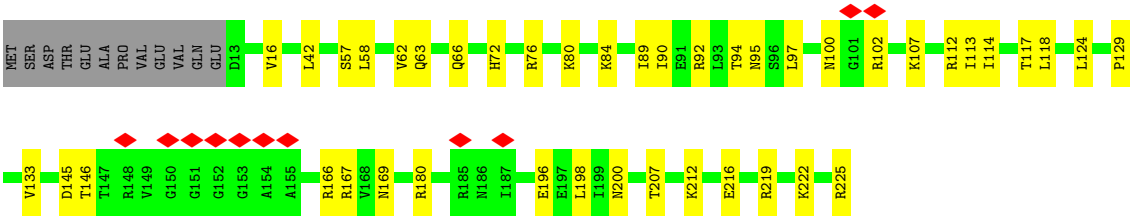
• Molecule 5: rpS4_eS4

Chain L4:



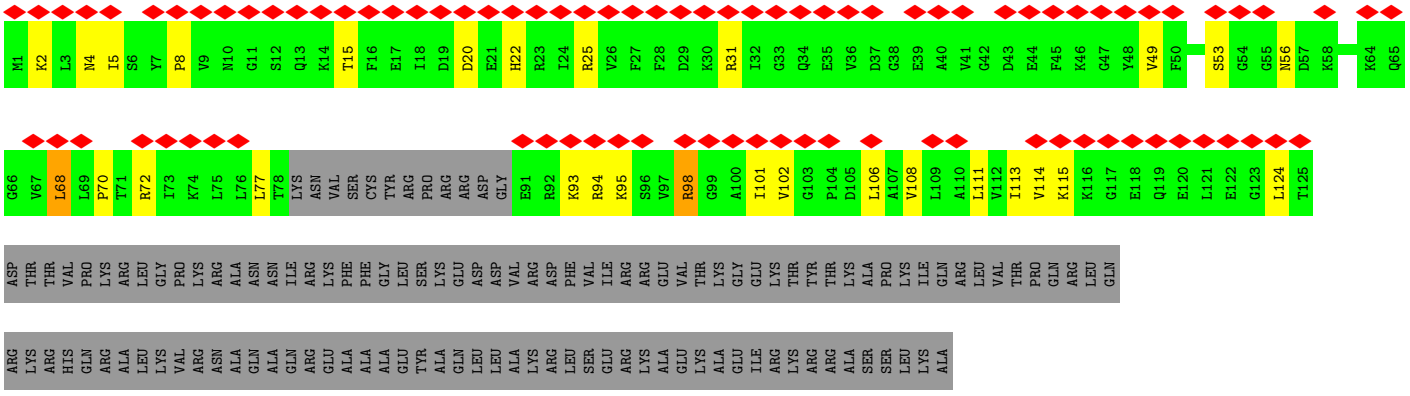
• Molecule 6: rpS5_uS7

Chain L5:



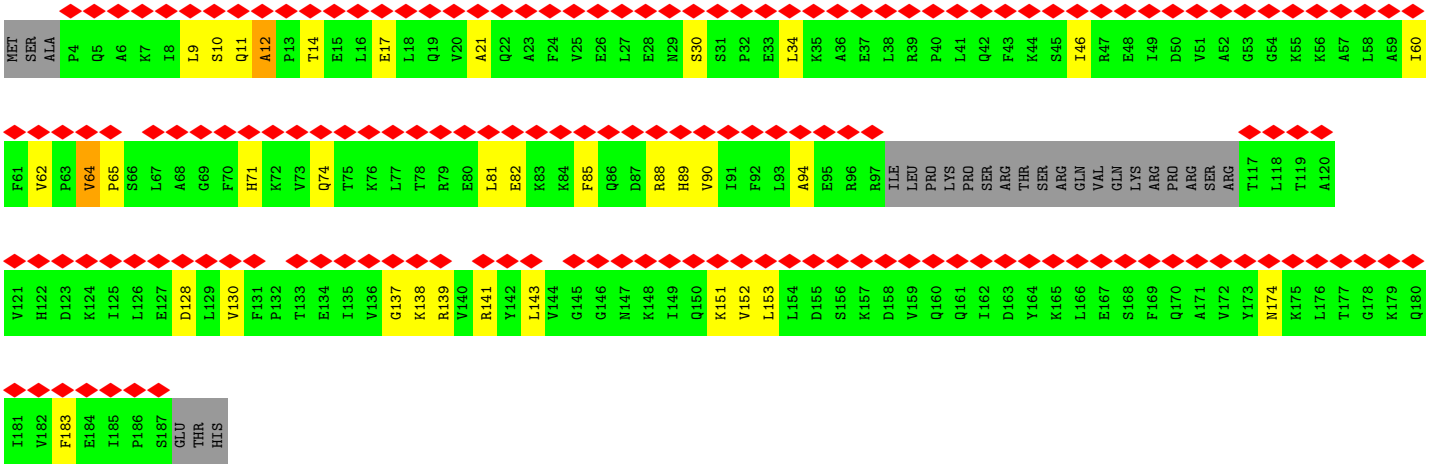
• Molecule 7: rpS6_eS6

Chain L6:



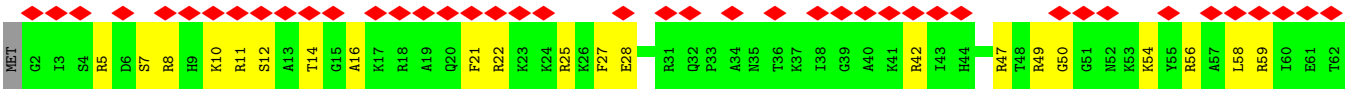
• Molecule 8: rpS7_eS7

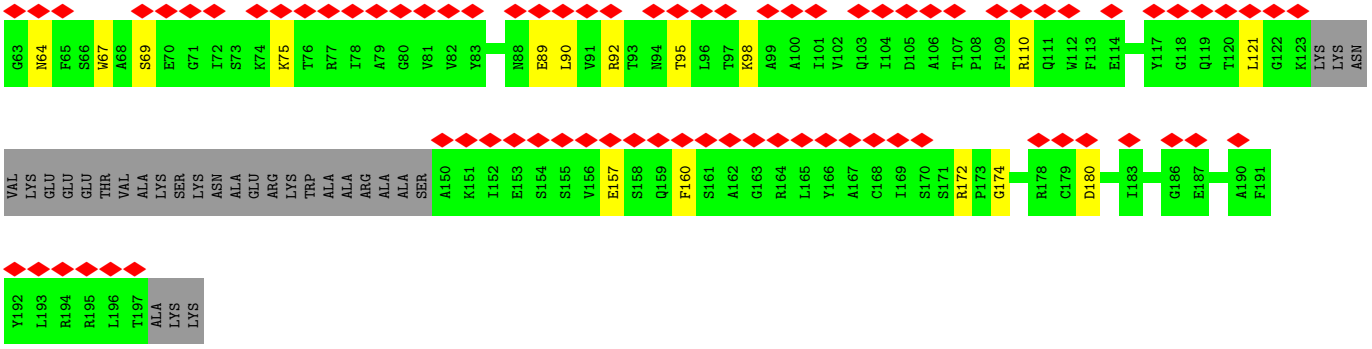
Chain L7:



• Molecule 9: rpS8_eS8

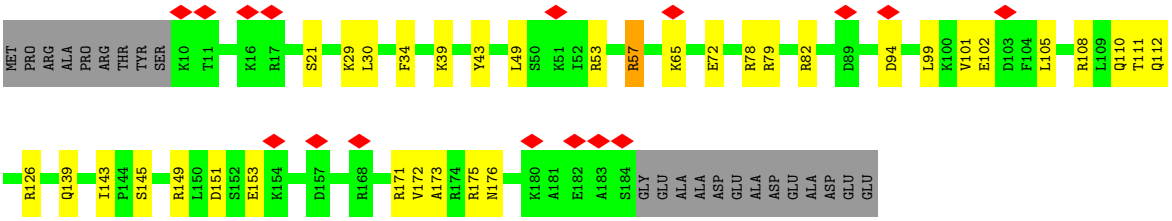
Chain L8:





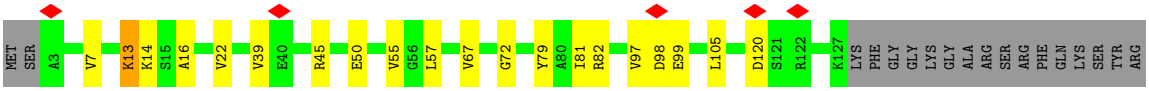
• Molecule 10: rpS9_uS4

Chain L9:



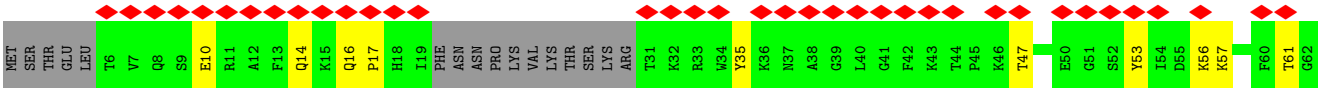
• Molecule 11: rpS16_uS9

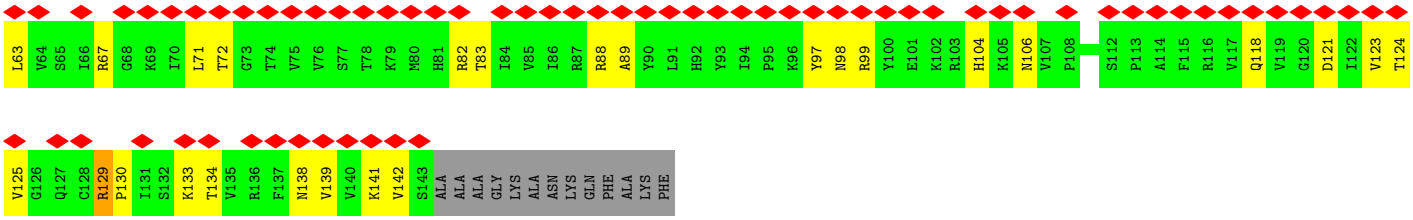
Chain LC:



• Molecule 12: rpS11_uS17

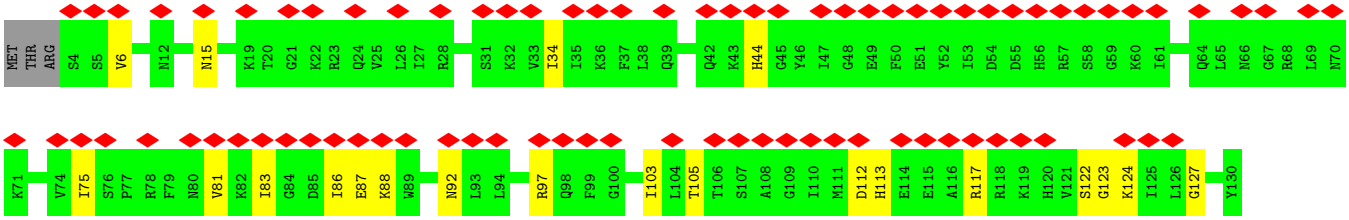
Chain LD:





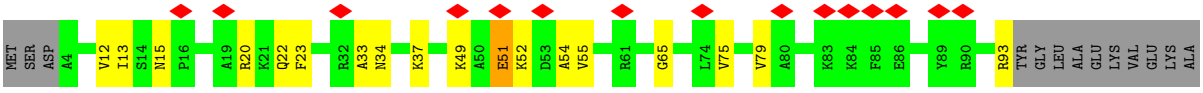
• Molecule 13: rpS22_uS8

Chain LE:



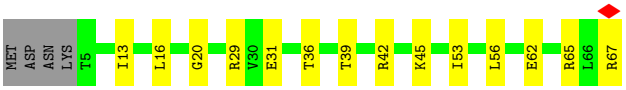
• Molecule 14: rpS24_eS24

Chain LF:



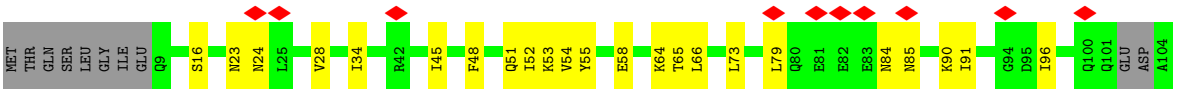
• Molecule 15: rpS28_eS28

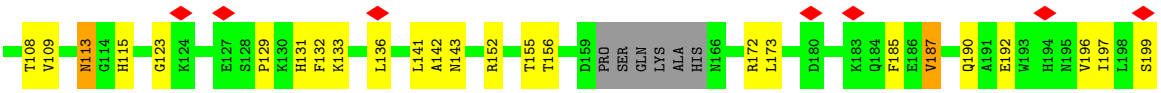
Chain LG:

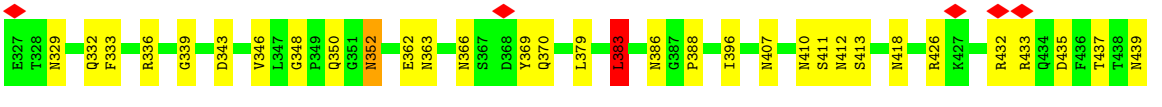


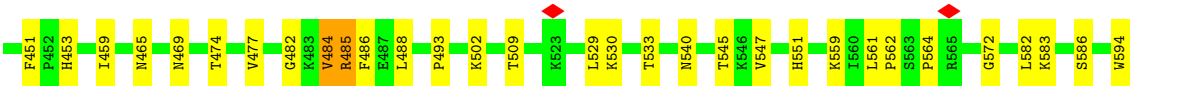
• Molecule 16: Utp17

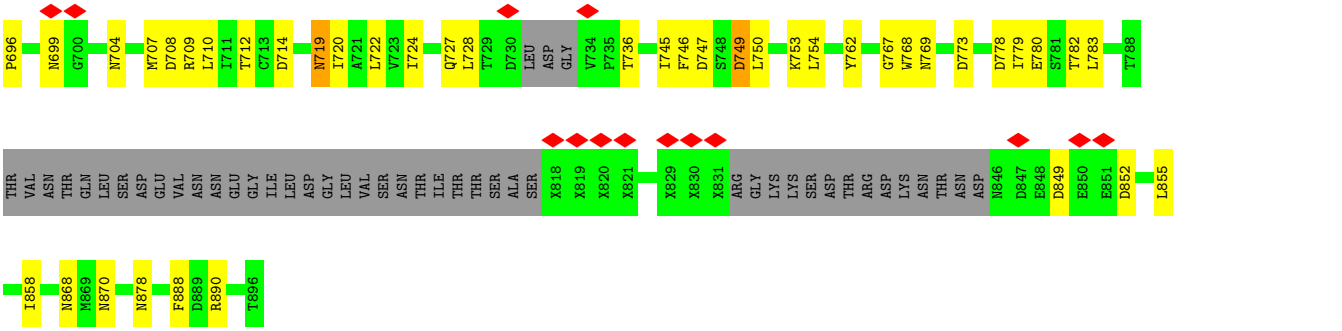
Chain LH:



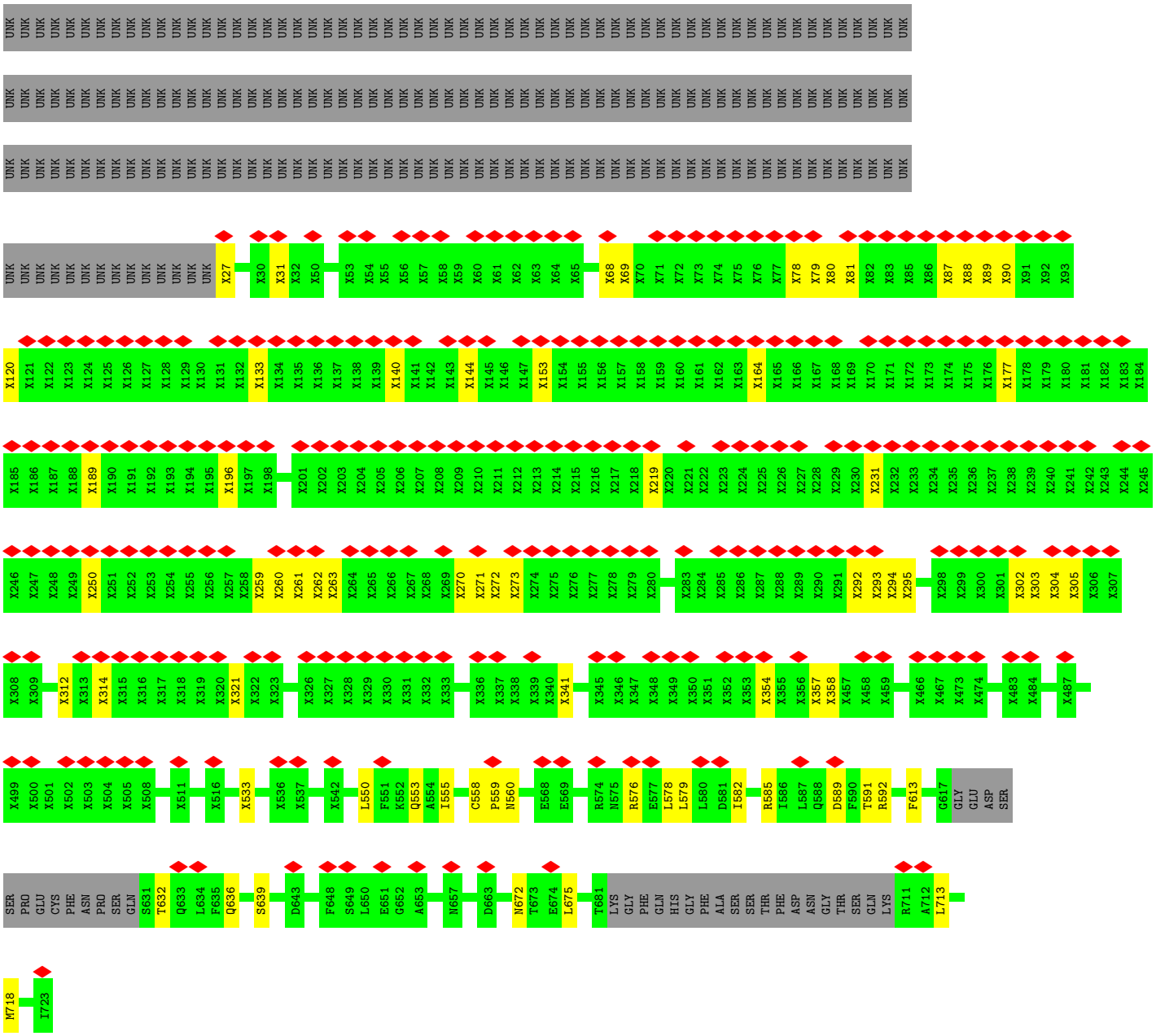






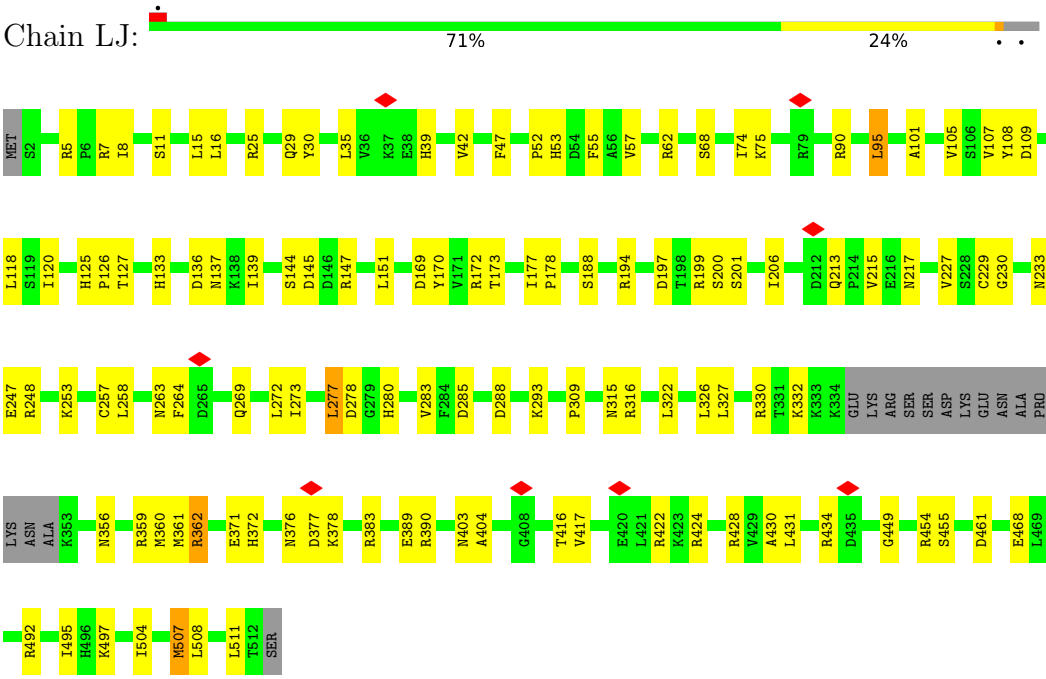


• Molecule 17: Utp8



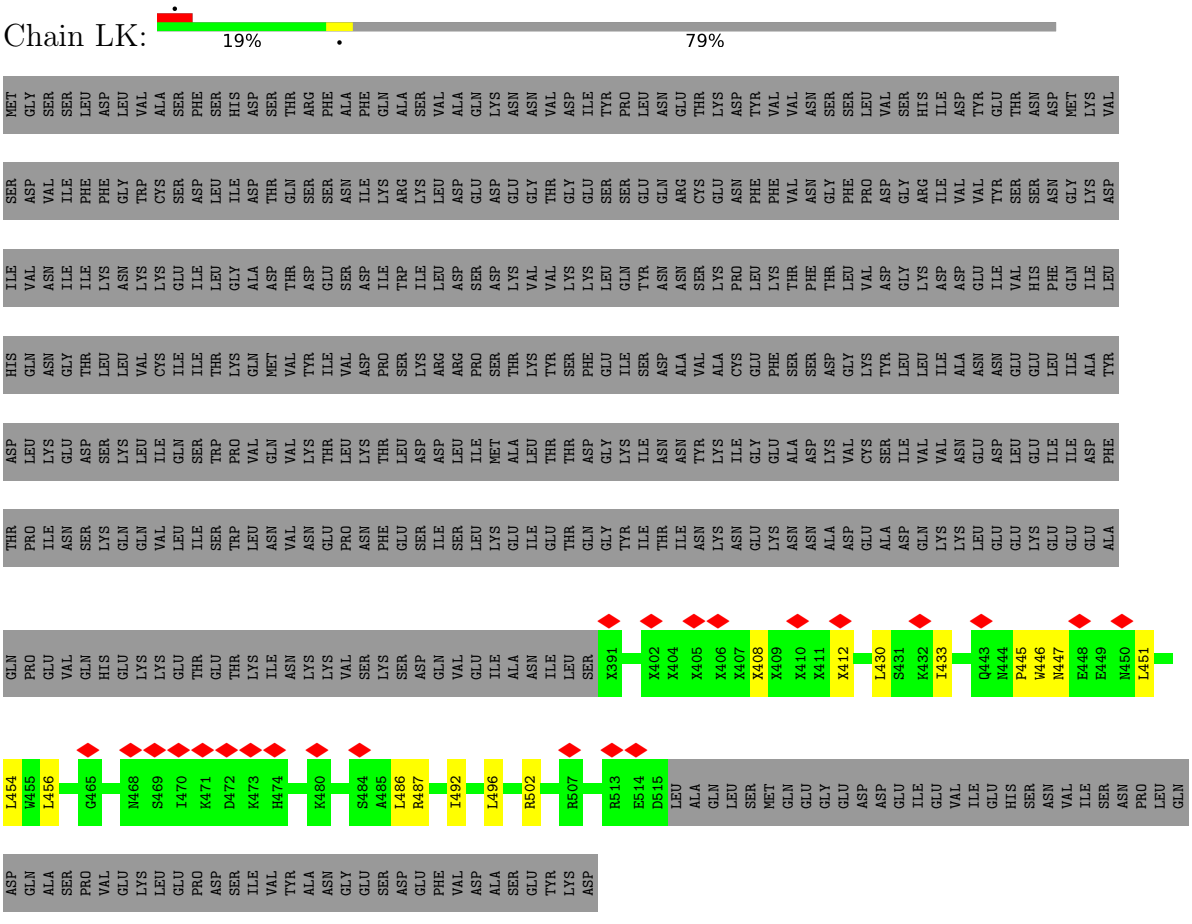
• Molecule 18: Utp15

Chain LJ:



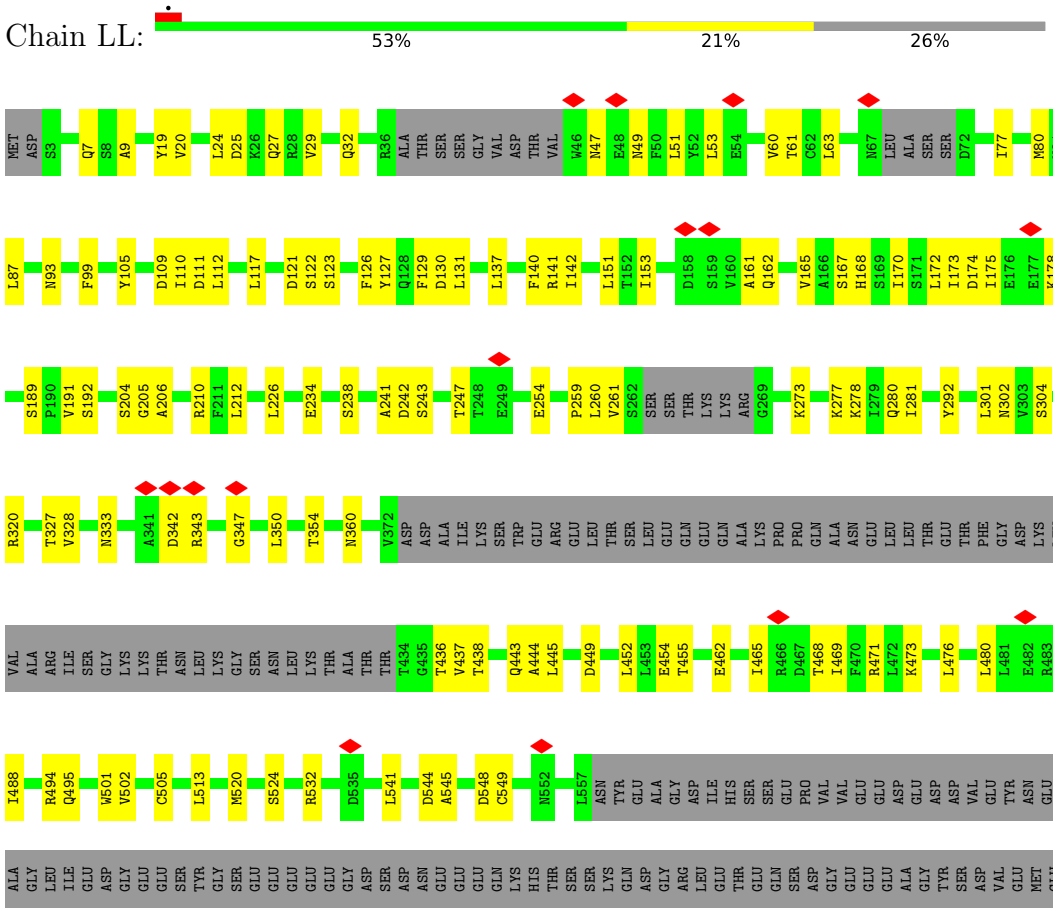
• Molecule 19: Utp9

Chain LK:



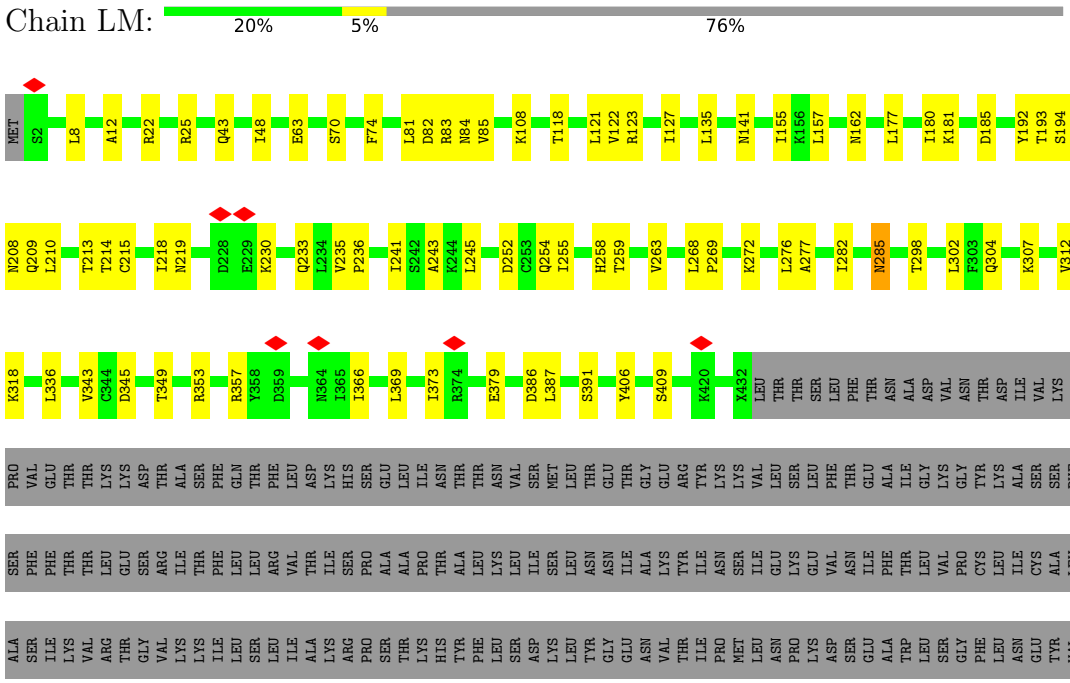
• Molecule 20: Utp5

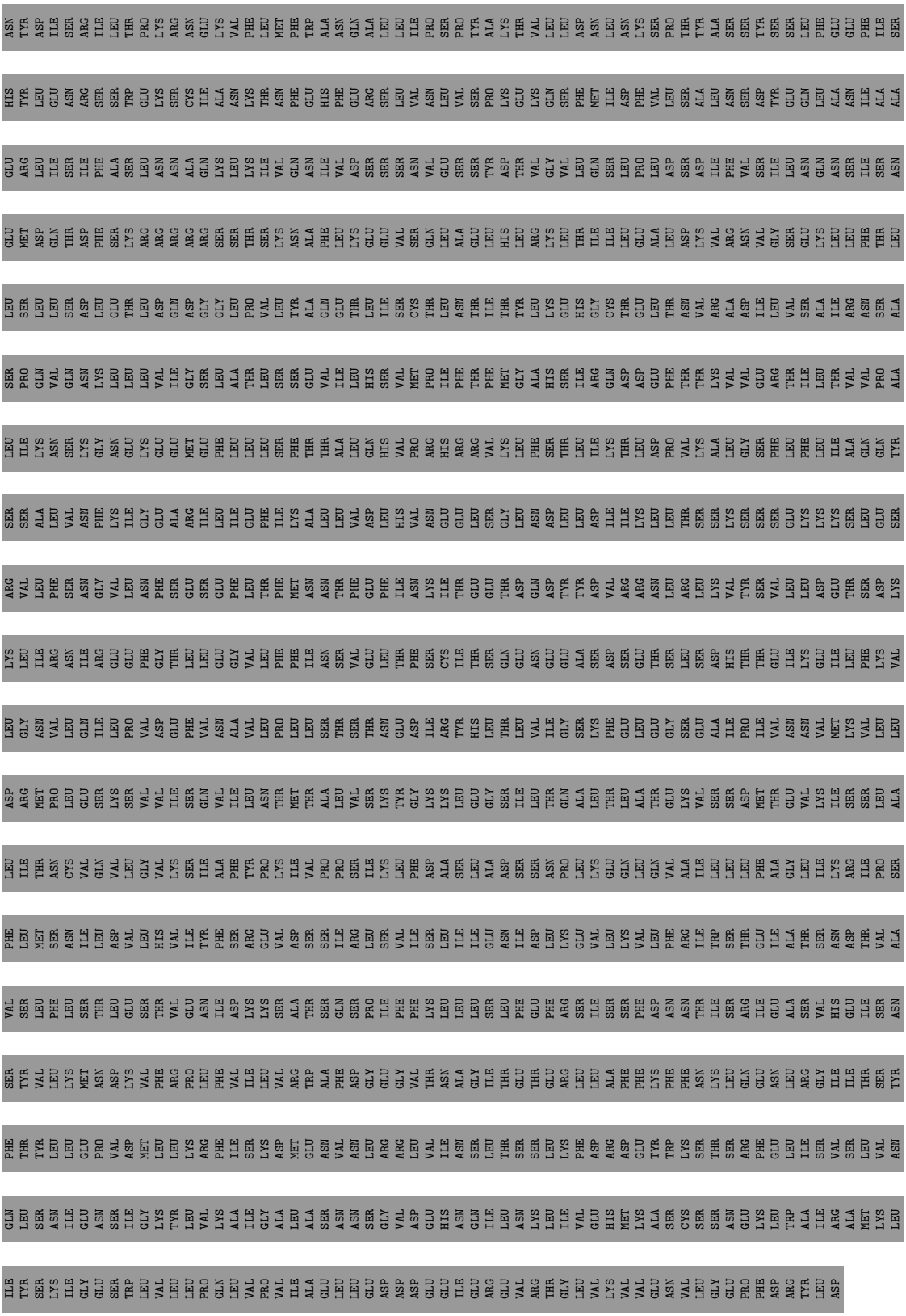
Chain LL:



• Molecule 21: Utp10

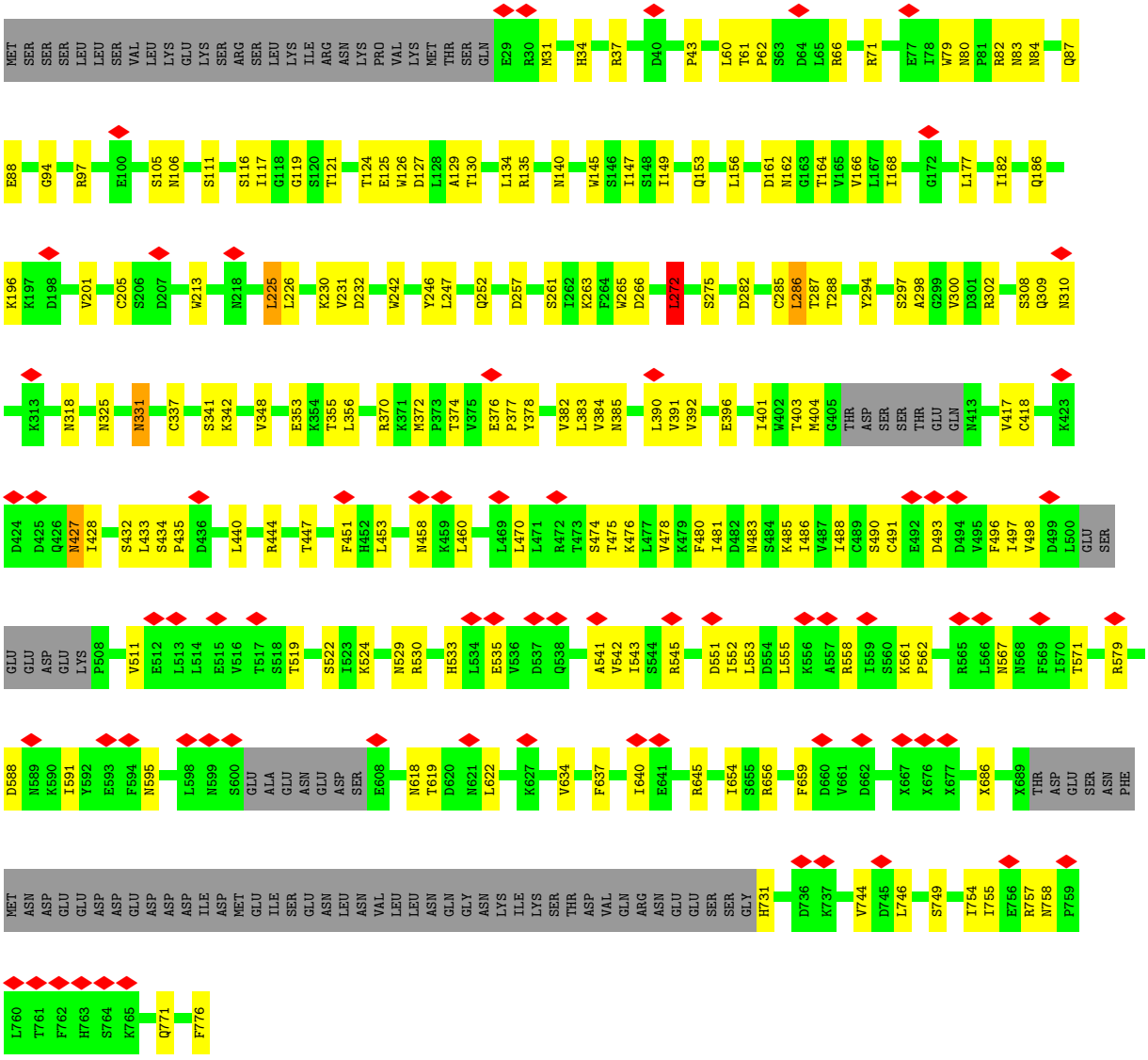
Chain LM:





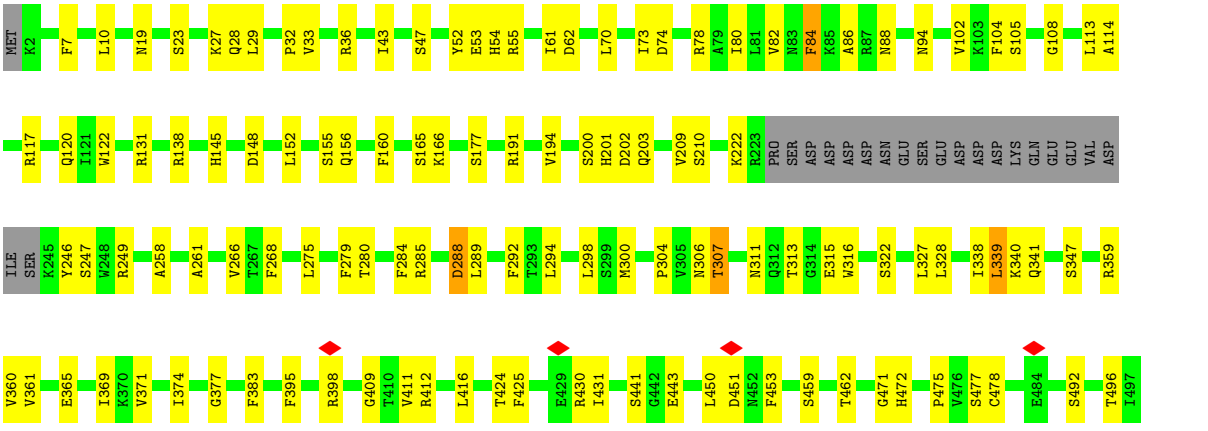
• Molecule 22: Utp4

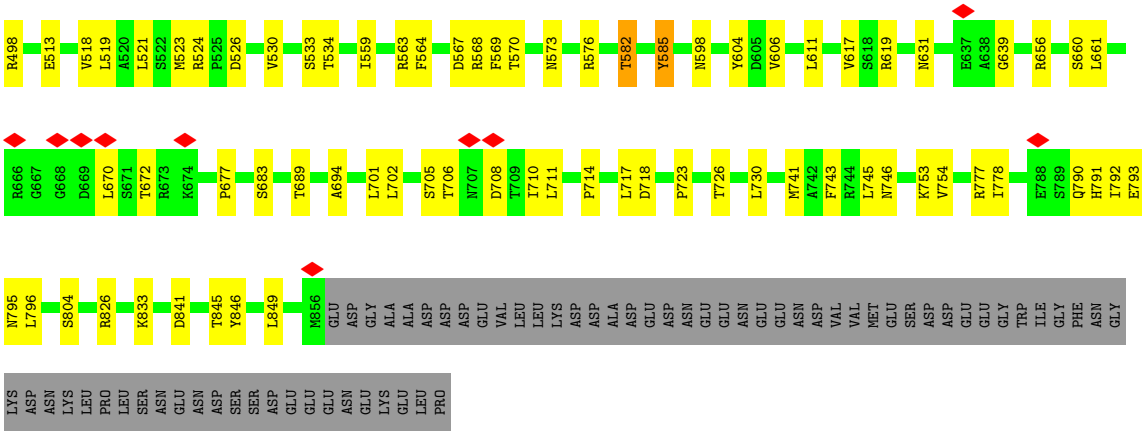
Chain LN:



• Molecule 23: Utp1

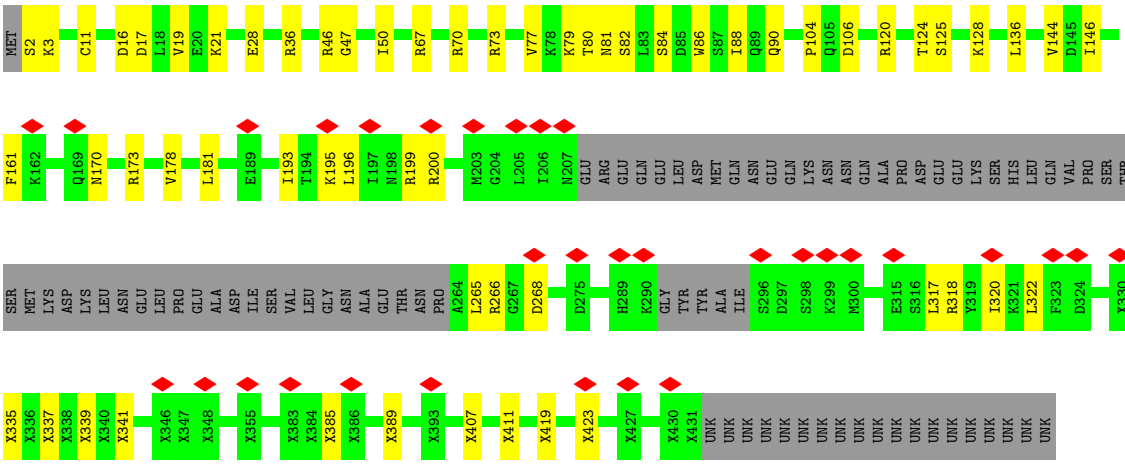
Chain LO:





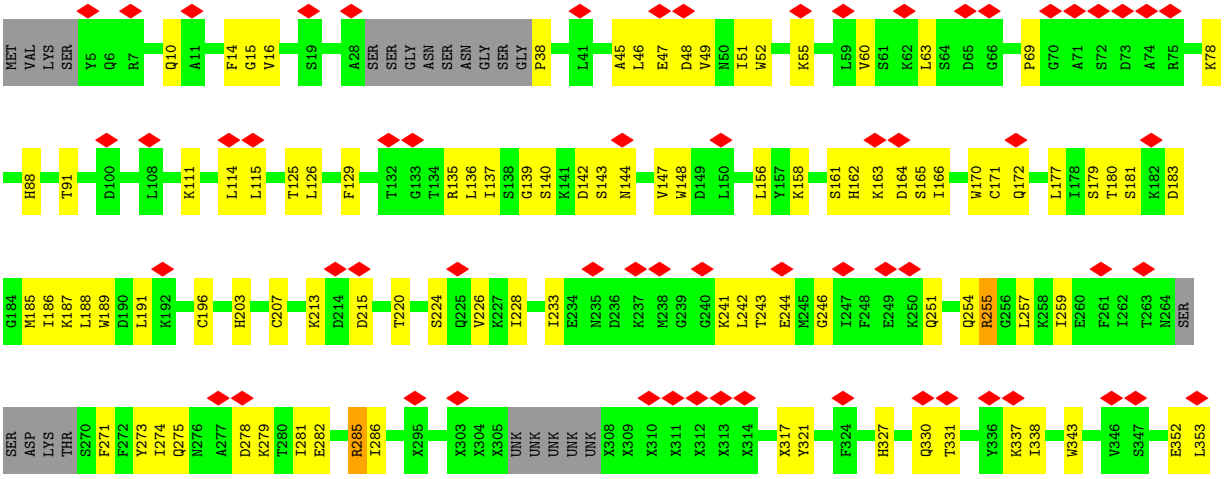
• Molecule 24: Utp6

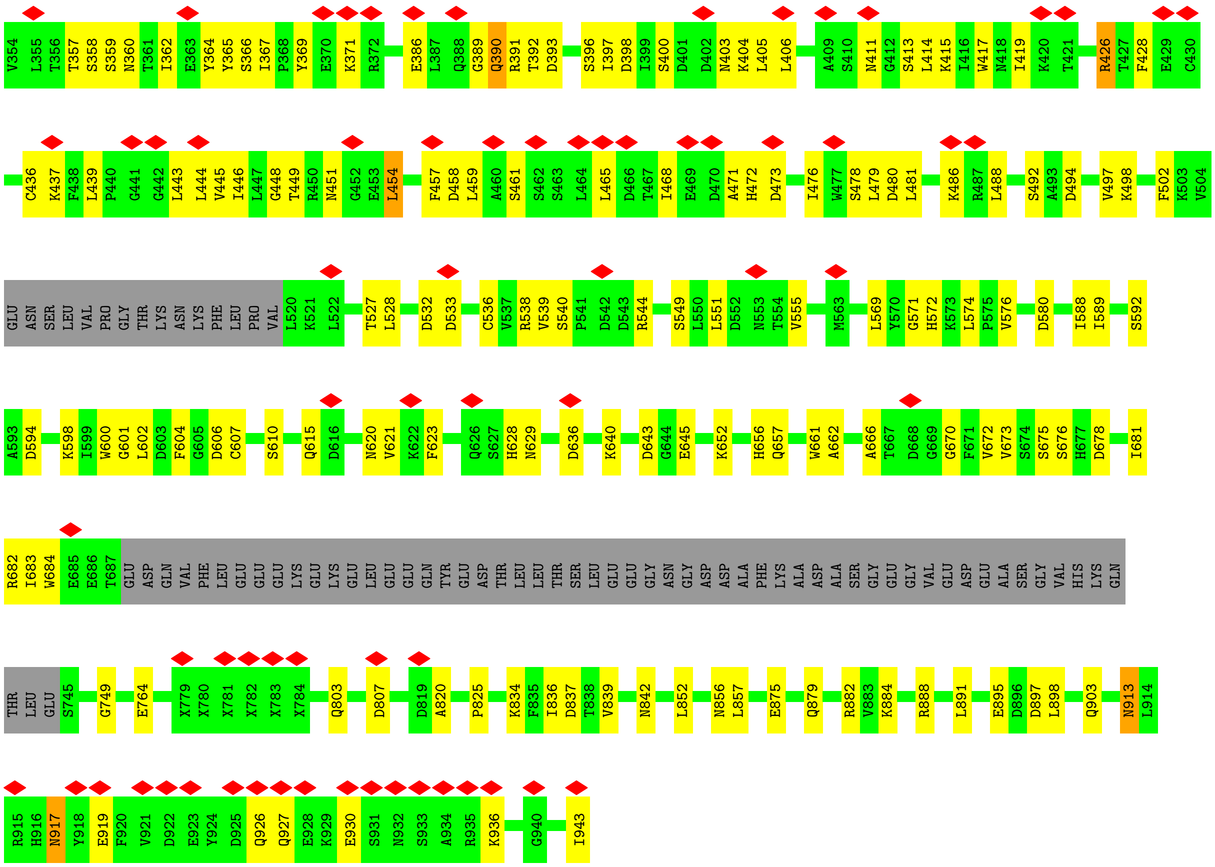
Chain LP:



• Molecule 25: Utp12

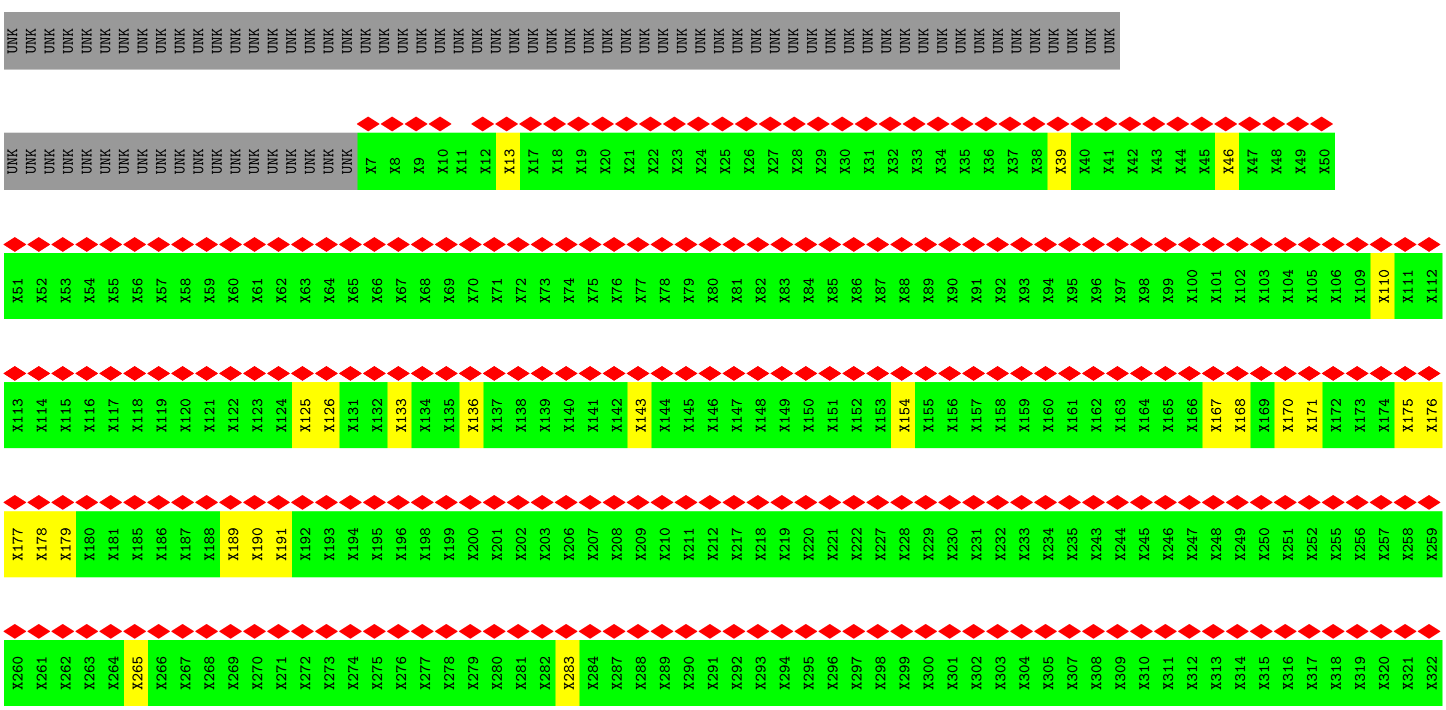
Chain LQ:

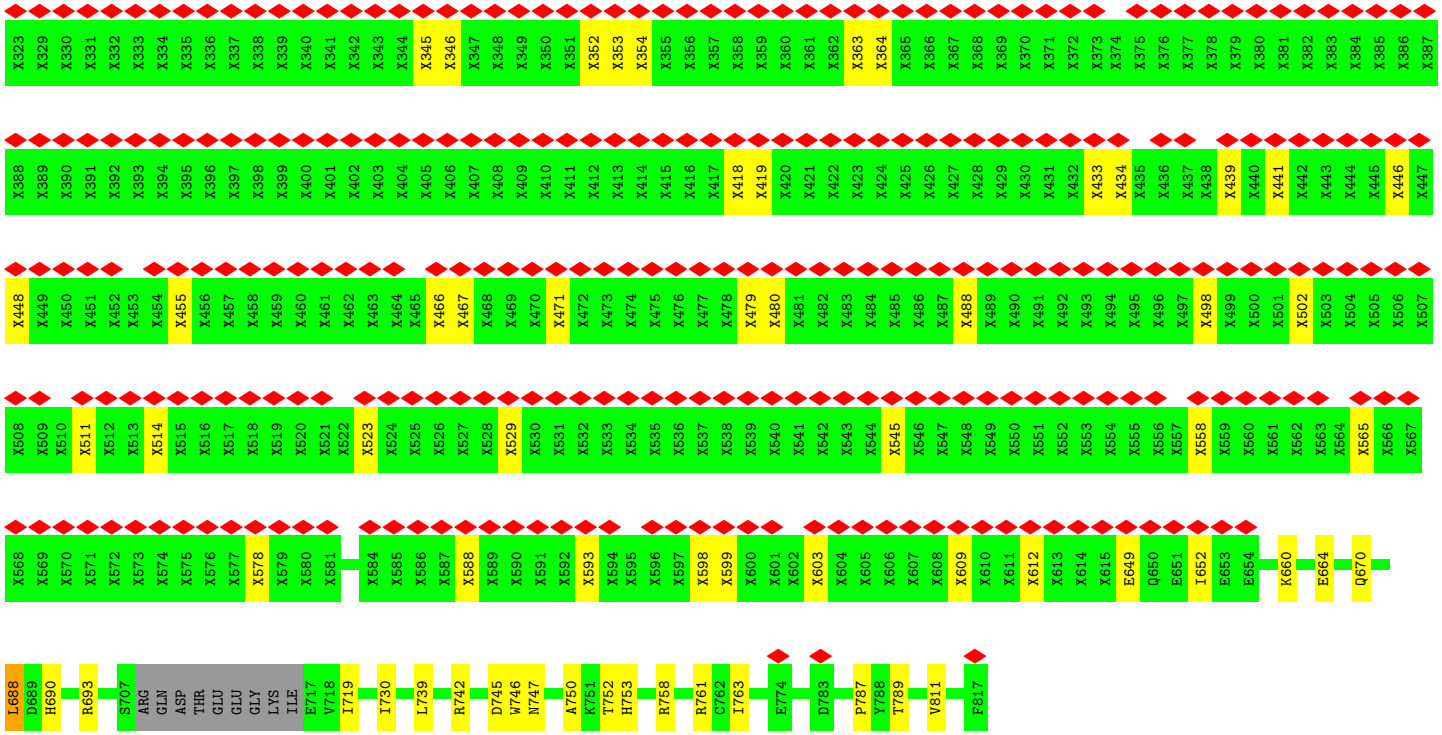




• Molecule 26: Utp13

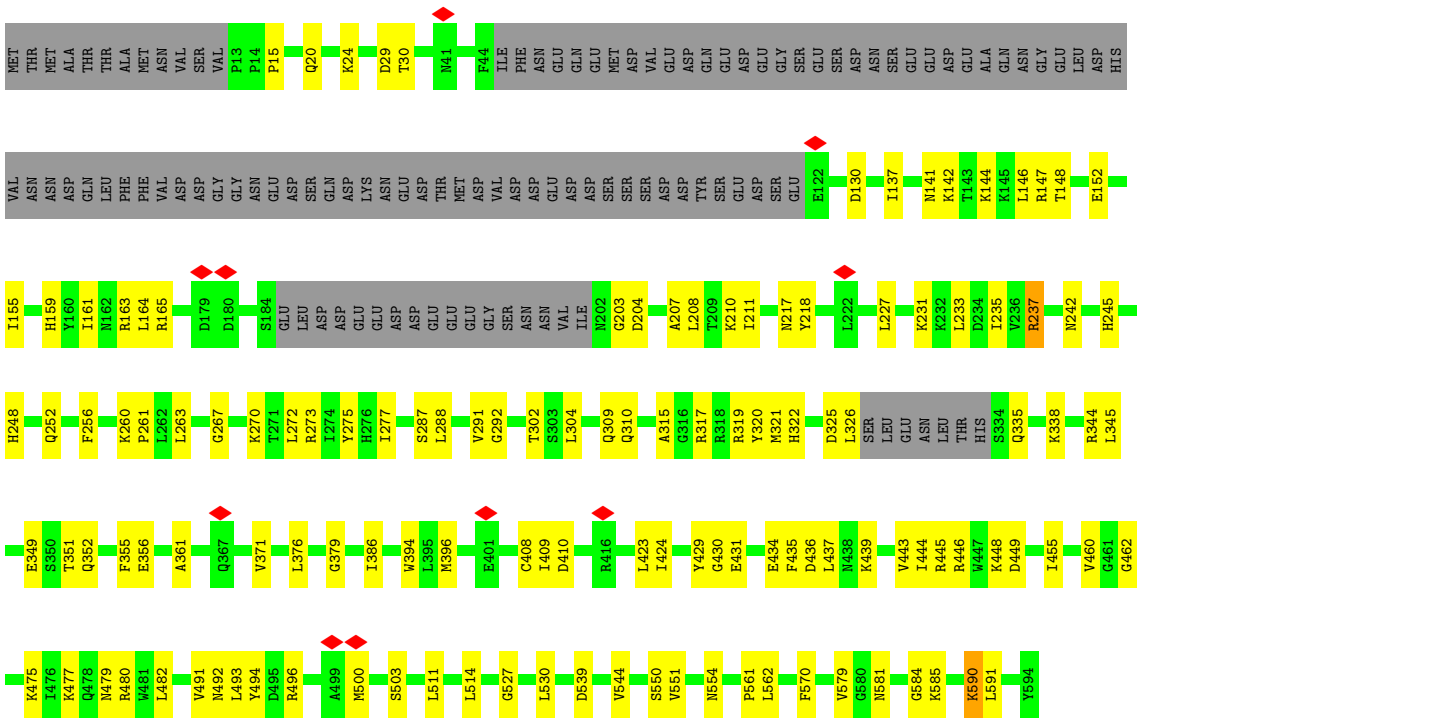
Chain LR:





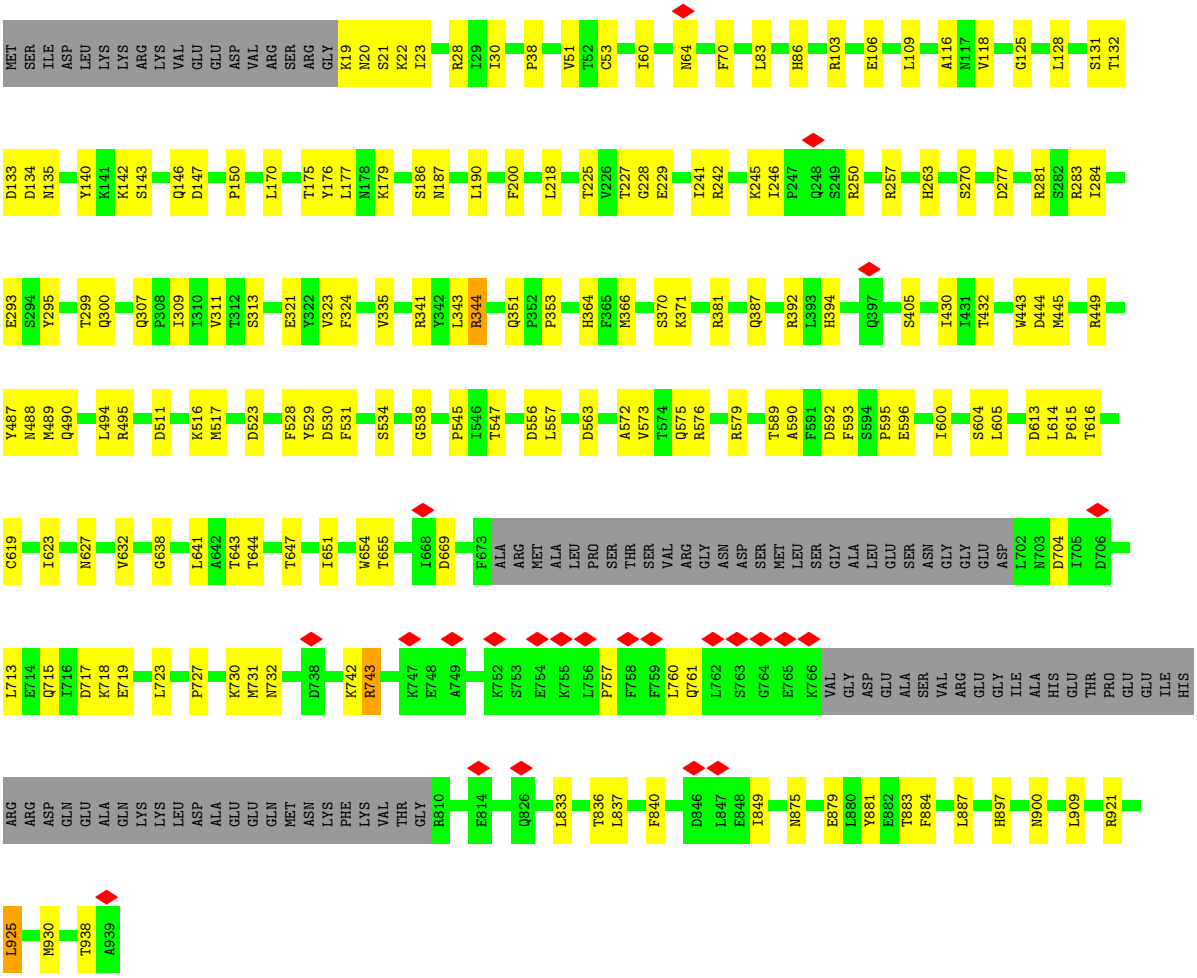
• Molecule 27: Utp18

Chain LS:



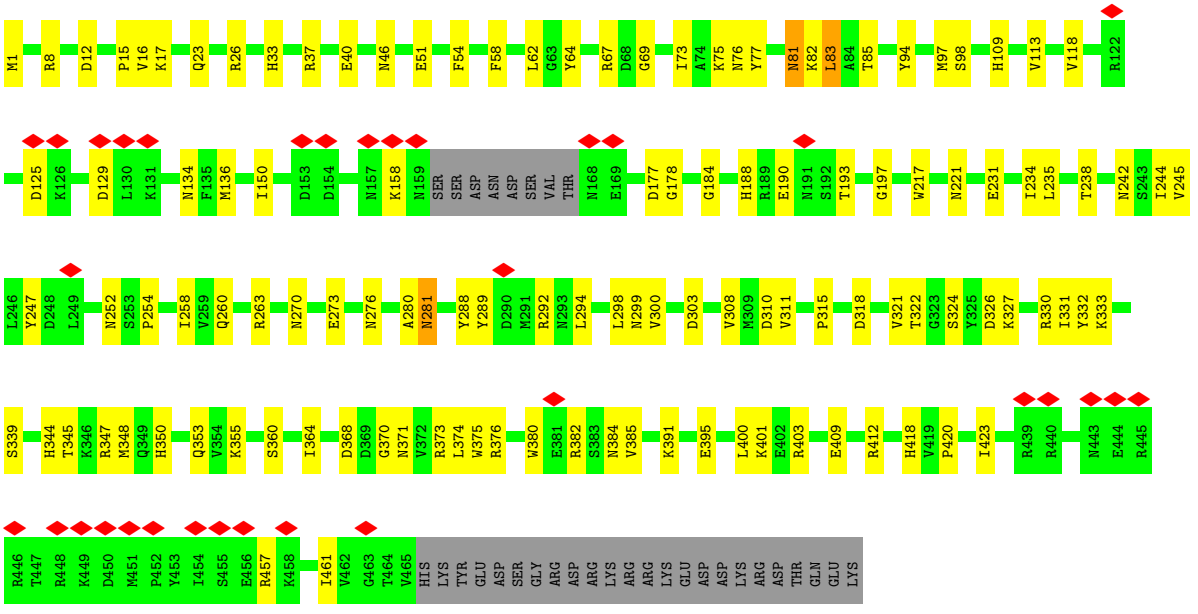
• Molecule 28: Utp21

Chain LT:



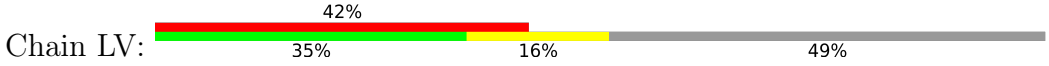
• Molecule 29: Sof1

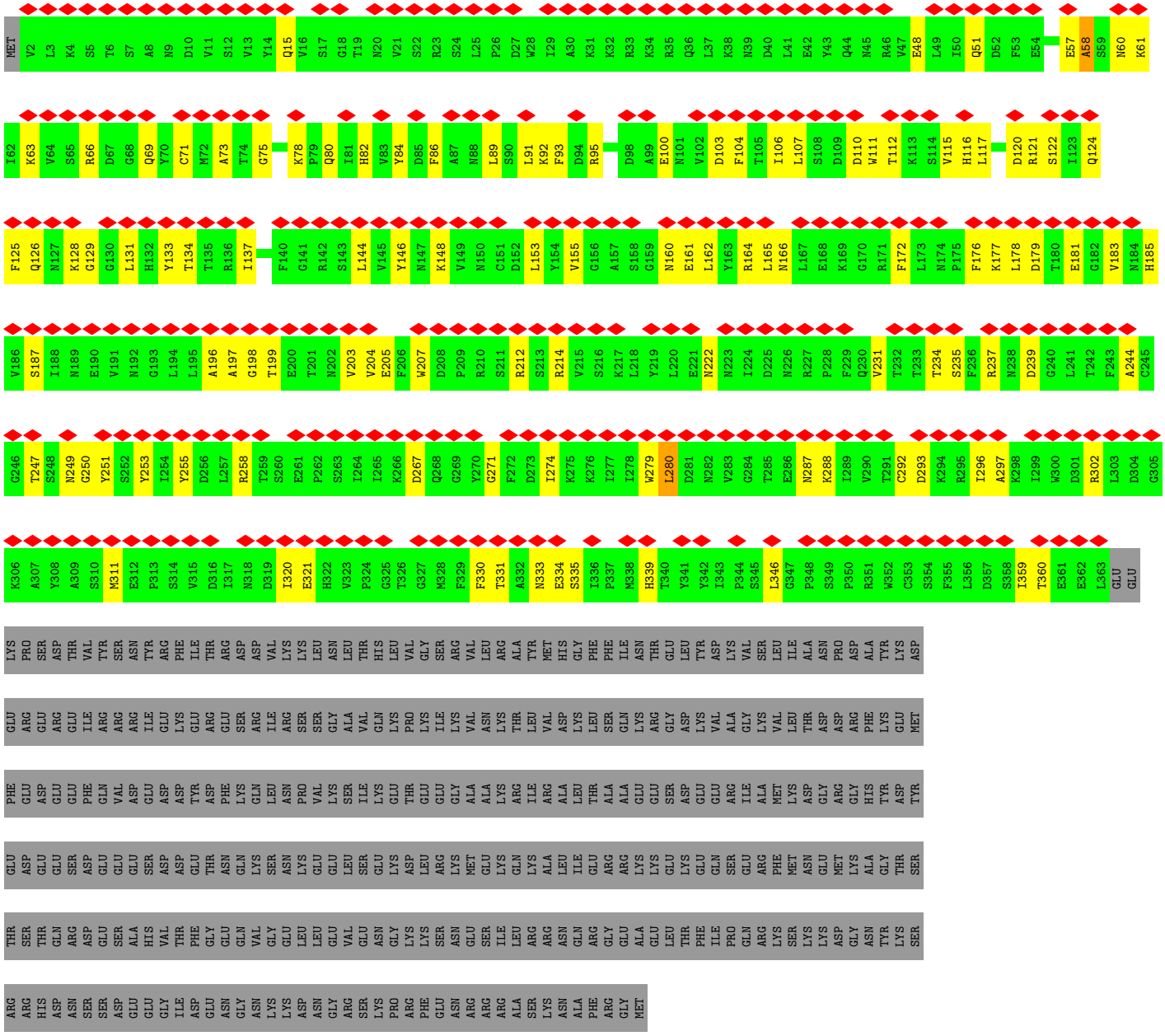
Chain LU:



• Molecule 30: Enp2

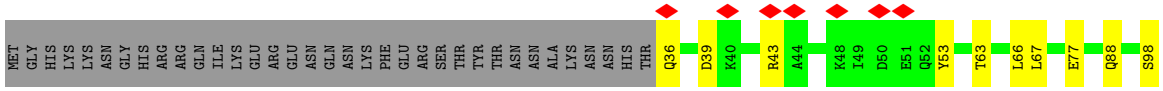
Chain LV:

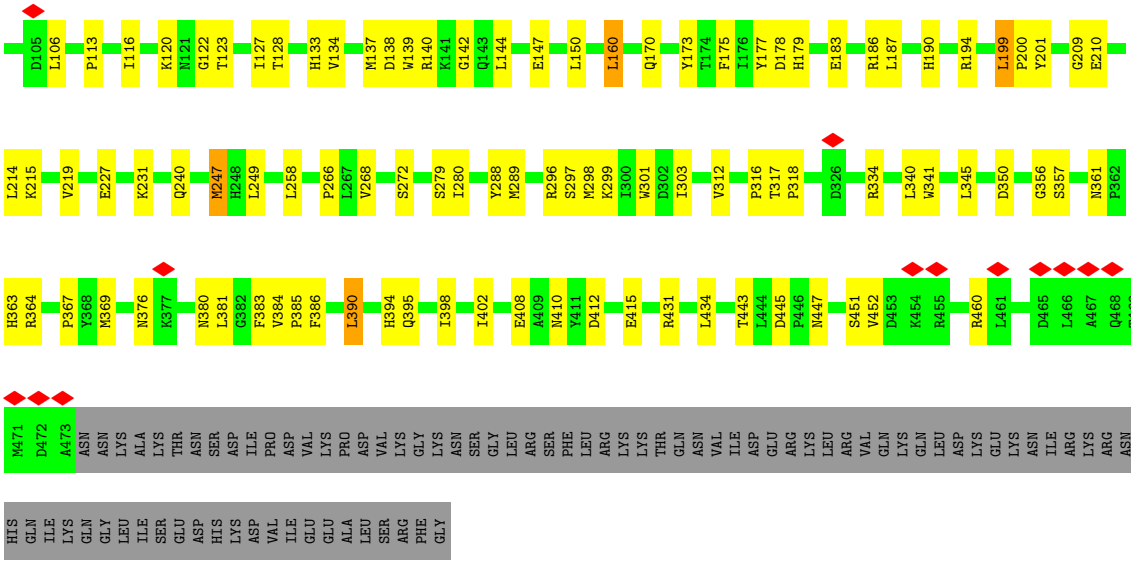




• Molecule 31: Utp7

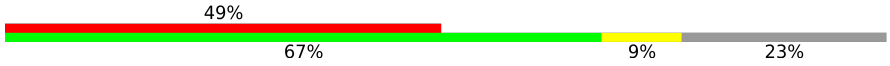
Chain LW:

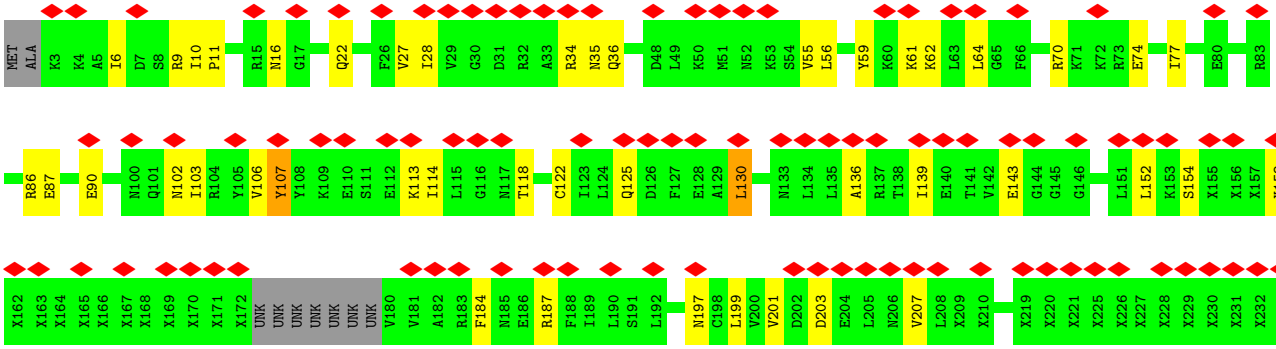


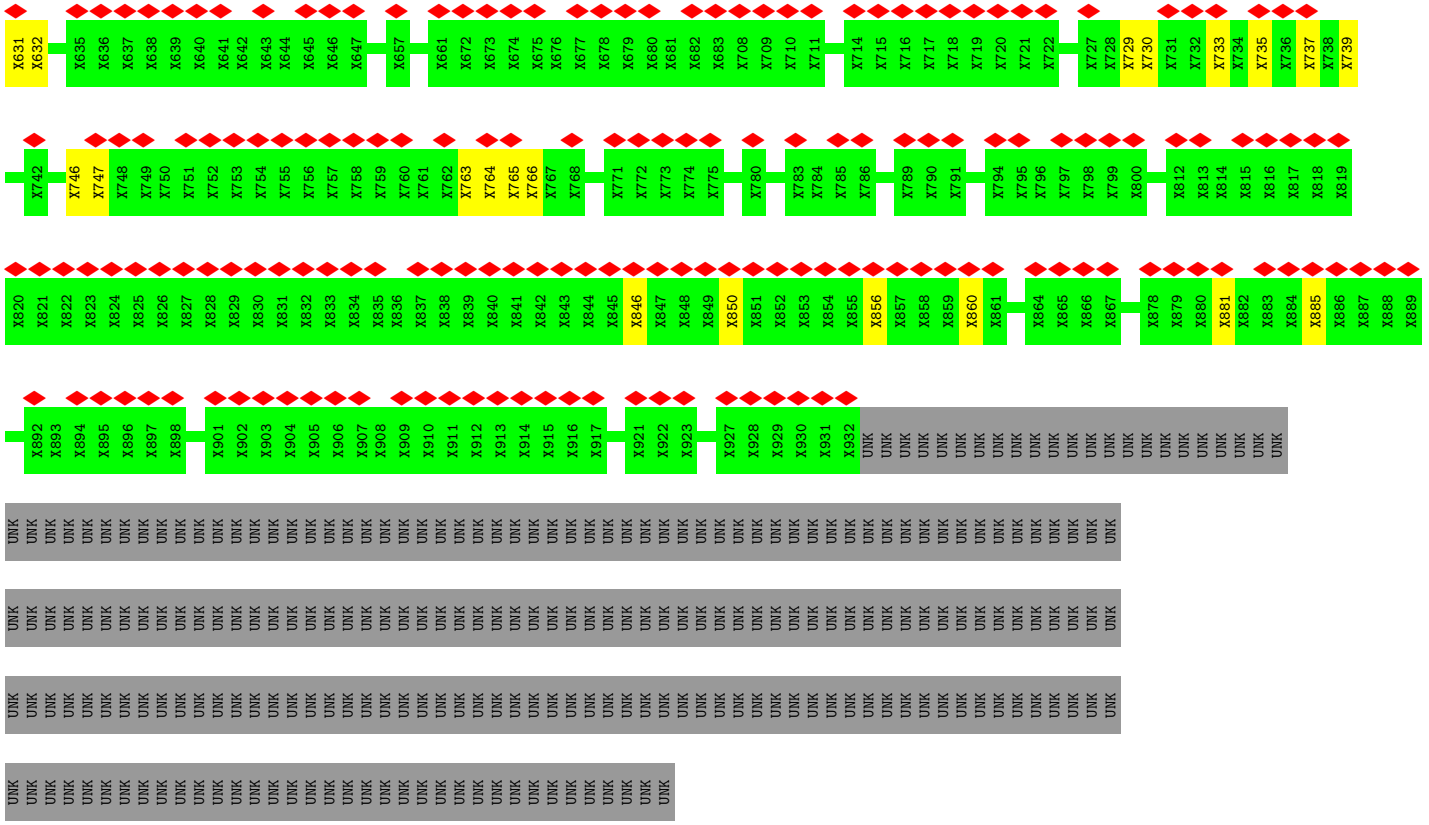


• Molecule 32: Kre33

Chain LX:

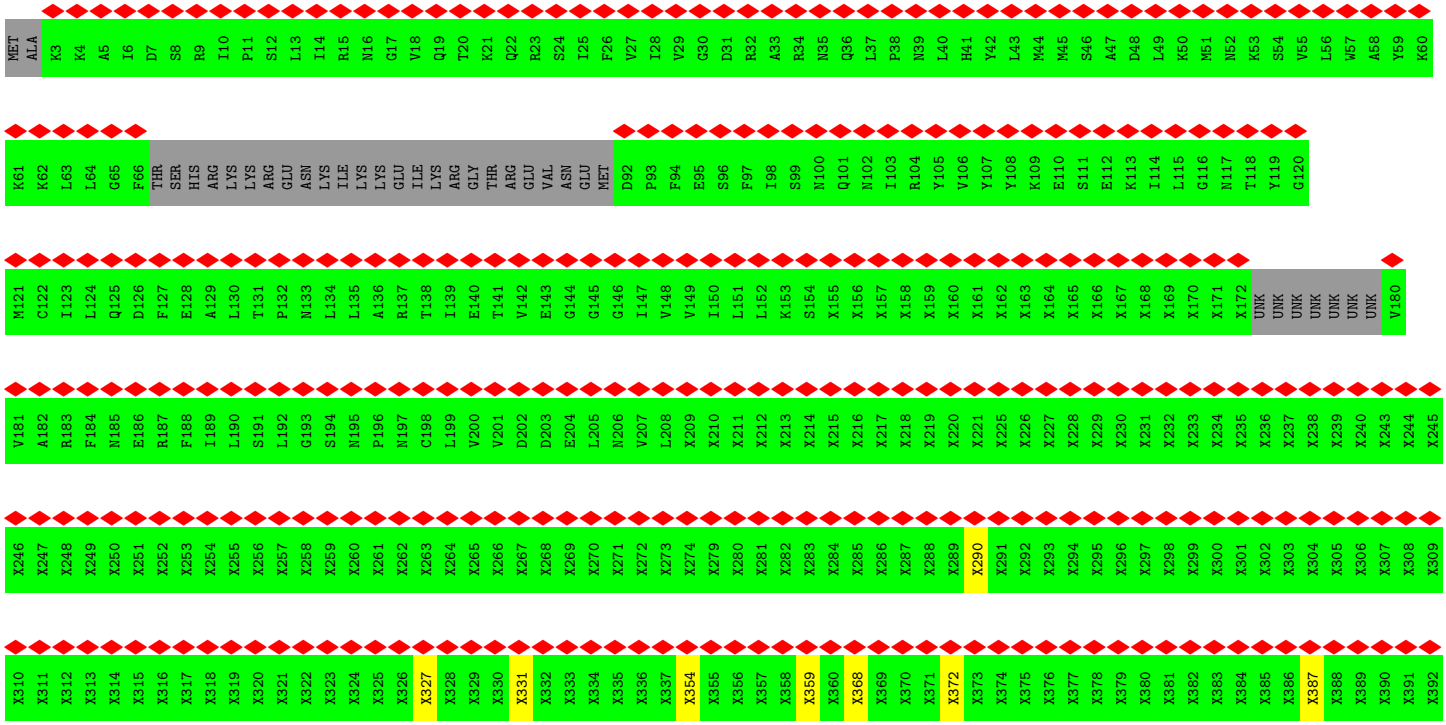


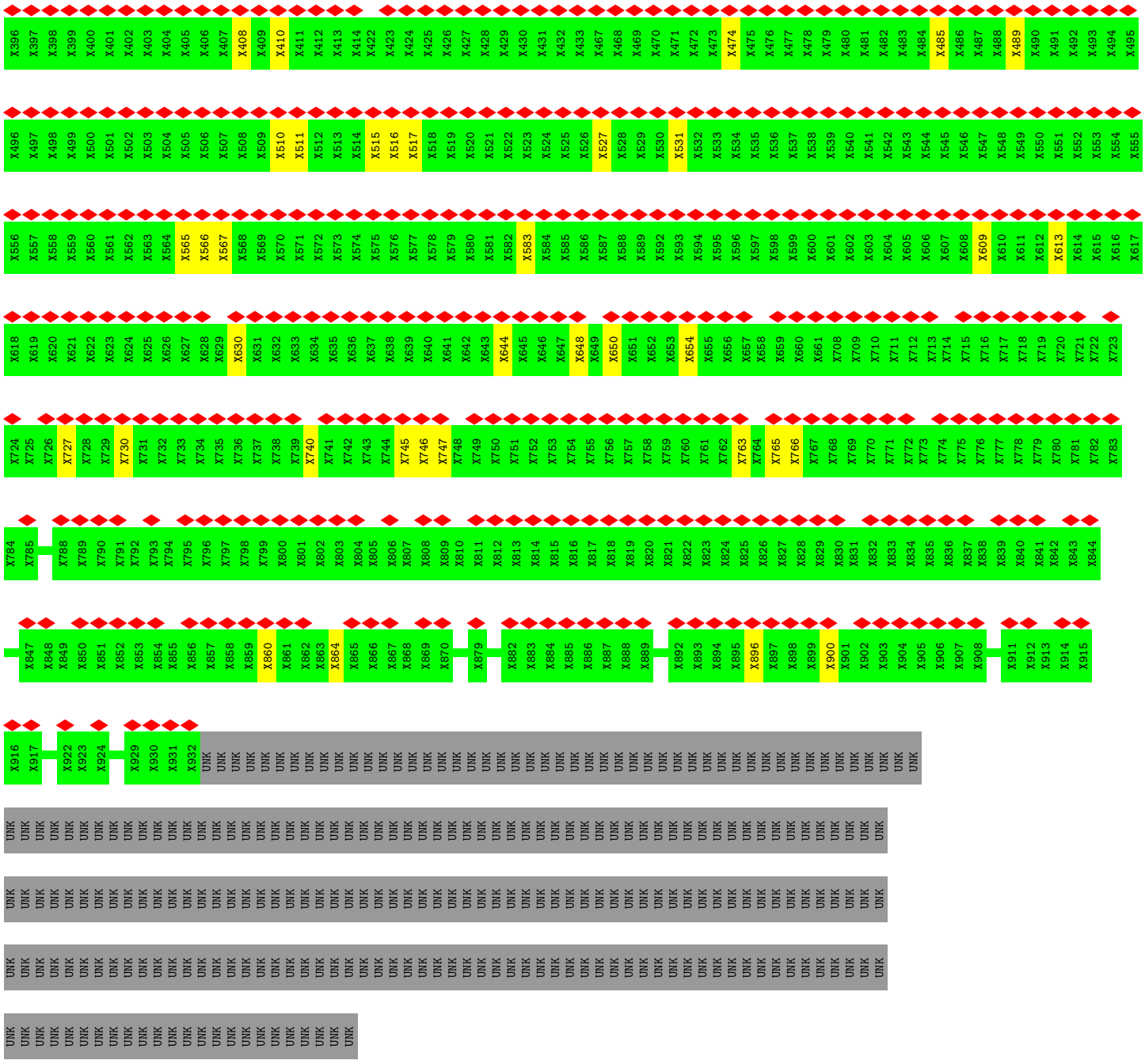




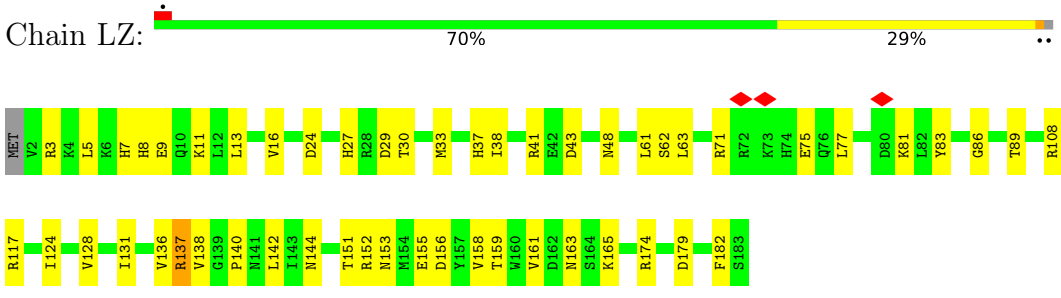
• Molecule 32: Kre33

Chain LY:



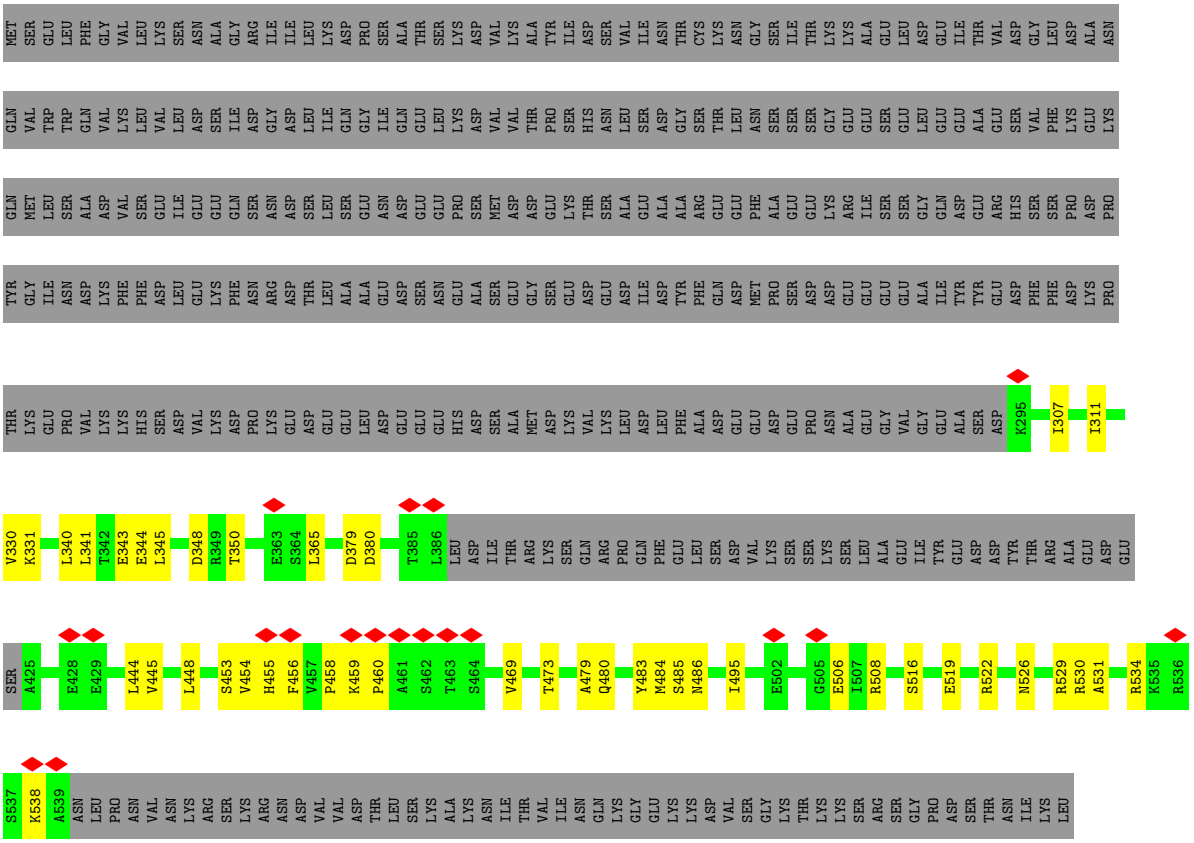


• Molecule 33: Imp3



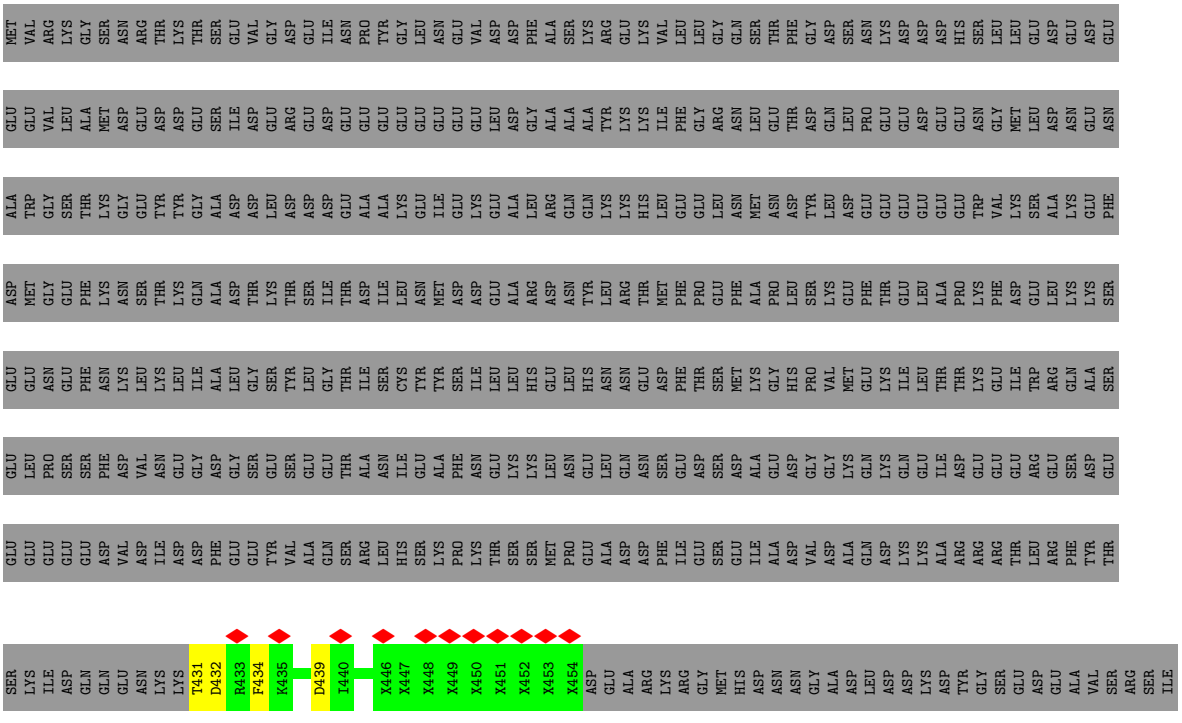
• Molecule 34: Mpp10

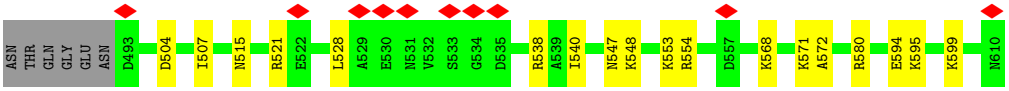
Chain NA:



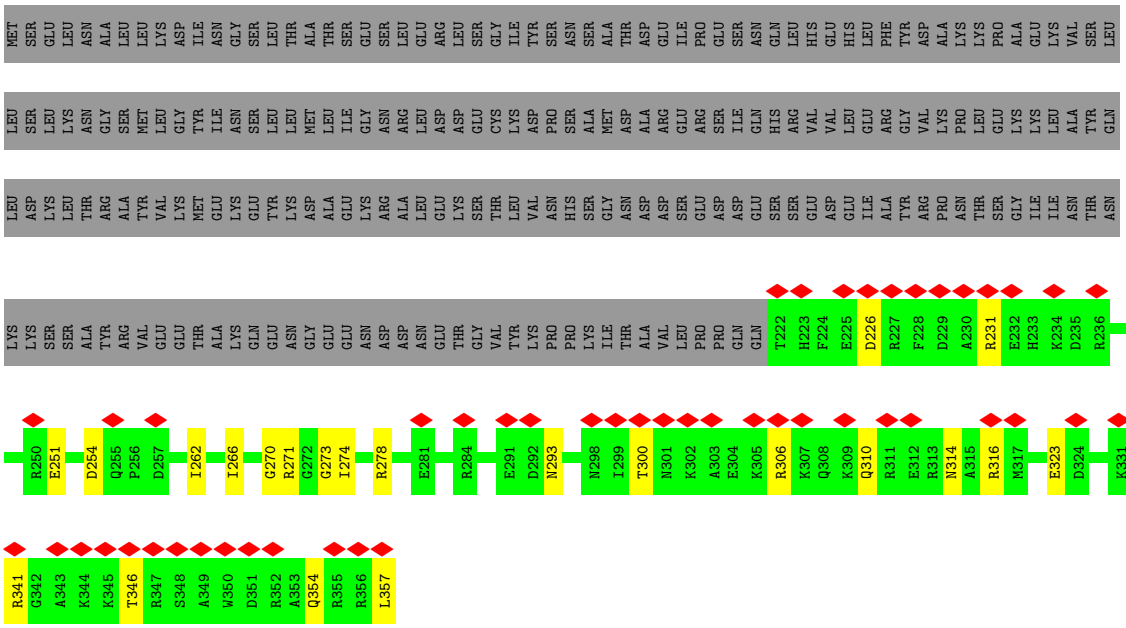
• Molecule 35: Sas10

Chain NB:

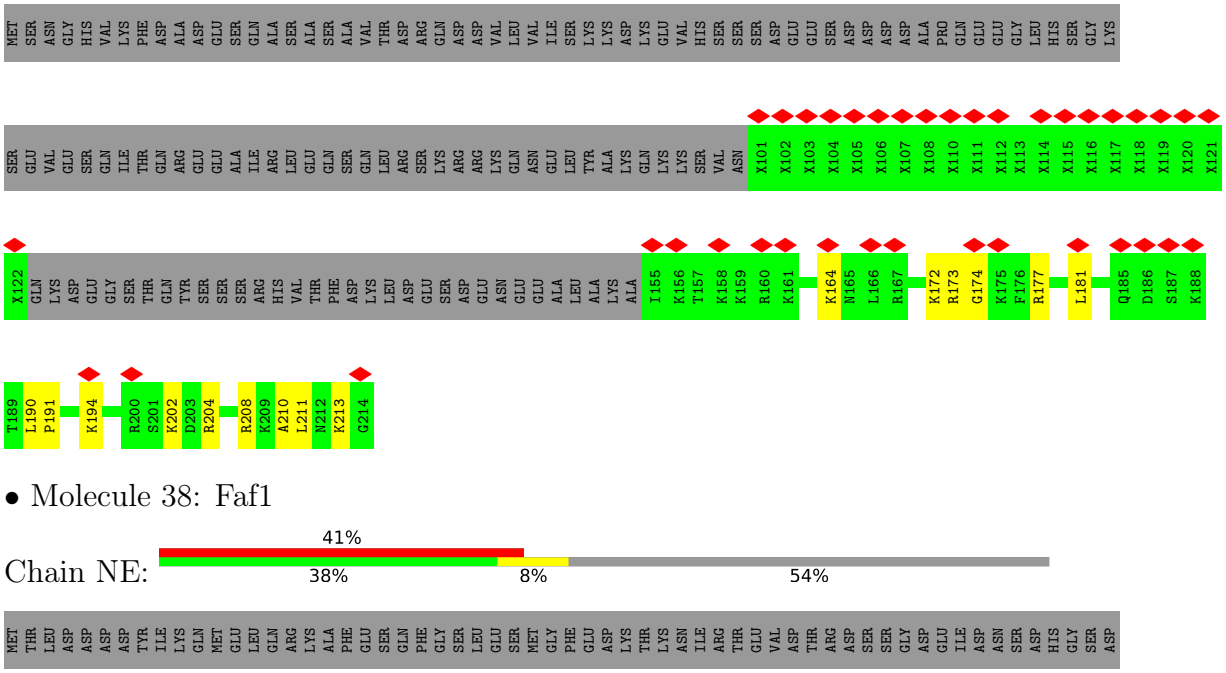




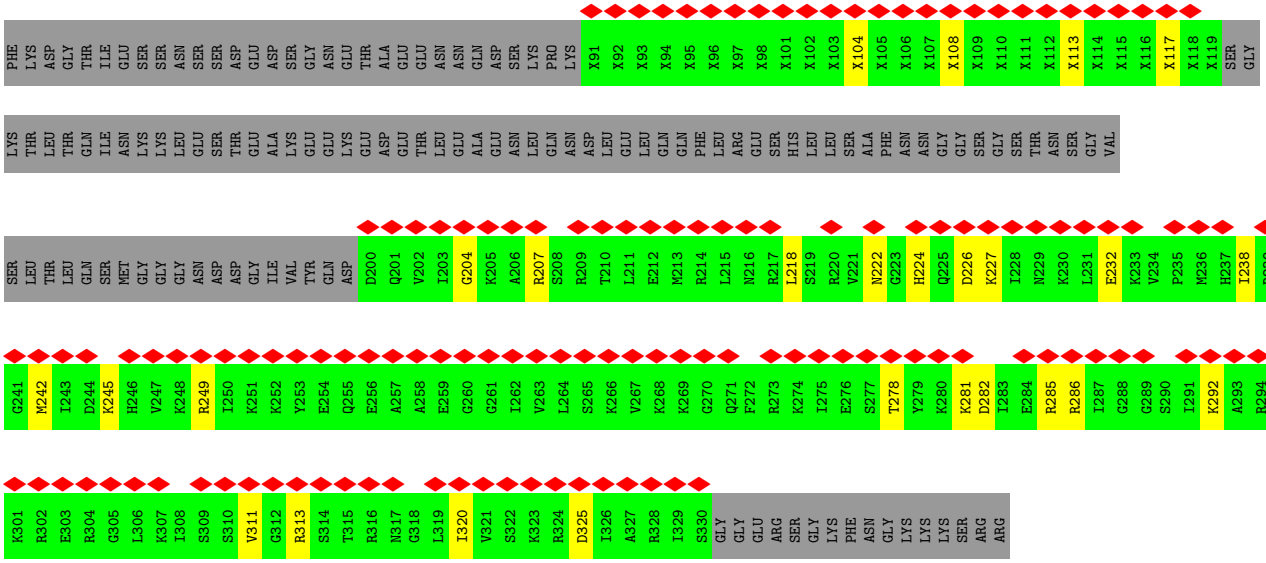
• Molecule 36: Lcp5



• Molecule 37: Bud21



• Molecule 38: Faf1

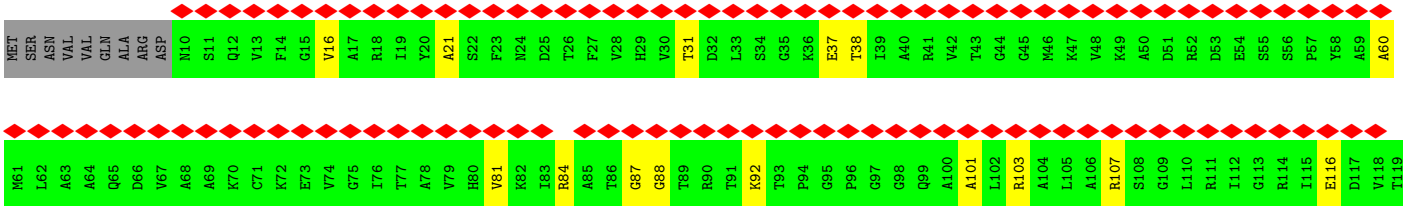


• Molecule 39: rpS13_uS15

Chain NF:

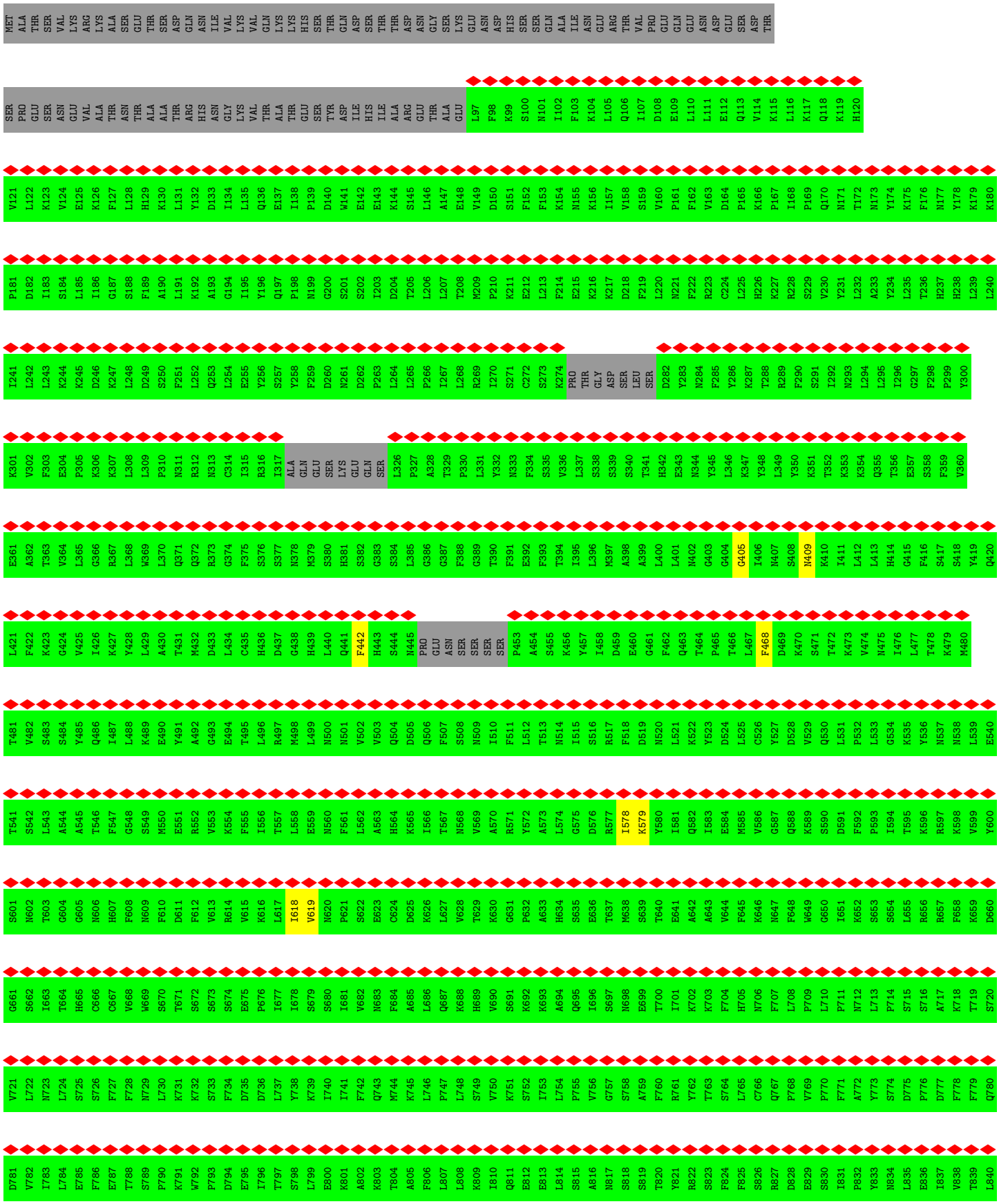
• Molecule 40: rpS14_uS11

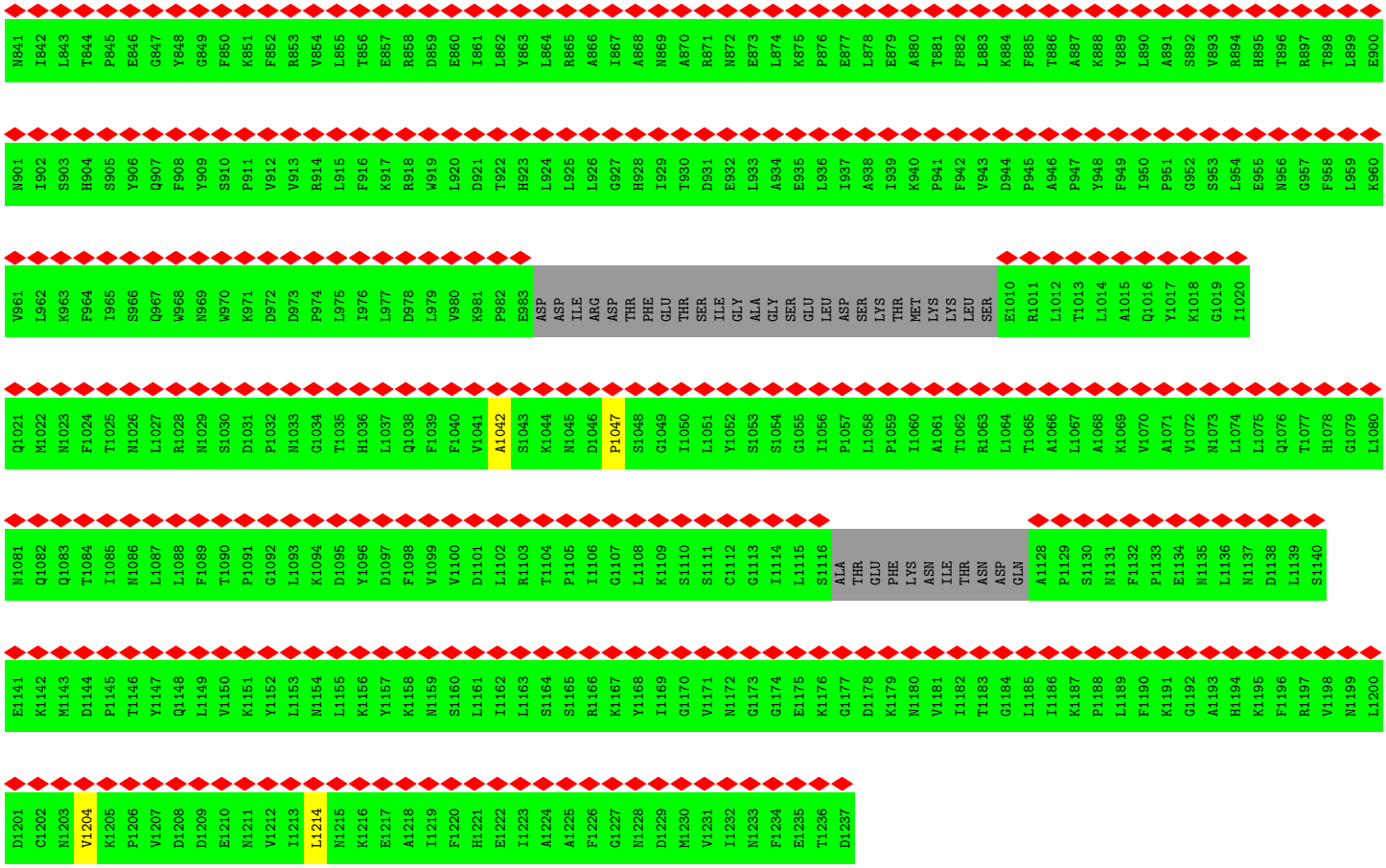
Chain NG:



• Molecule 41: Utp22

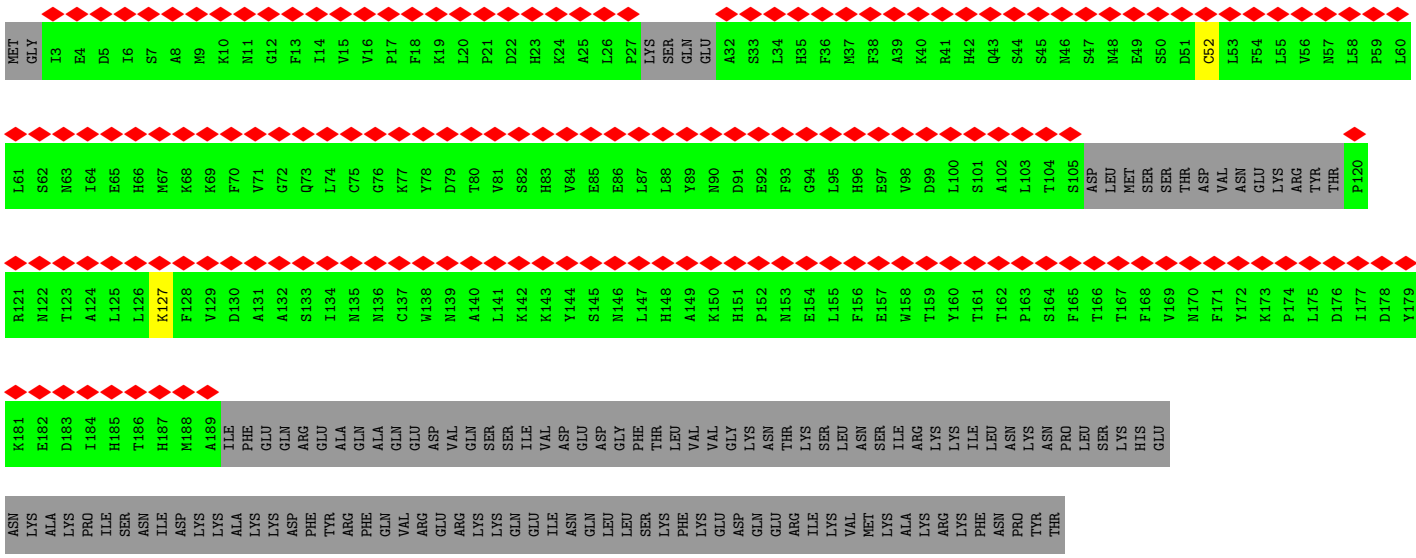
Chain NH:


MET ALA THR SER VAL LYS ARG LYS ALA SER GLU THR SER ASP GLN ASN ILE VAL LYS VAL GLN LYS LYS HIS SER THR GLN ASP SER THR THR ASP ASN GLY SER LYS GLU ASN ASP HIS SER SER GLN ALA ILE ASN GLU ARG THR VAL PRO GLU GLN GLU ASN ASP GLU SER ASP THR
SER PRO GLU SER ASN GLU VAL ALA THR ASN THR ALA ALA THR ARG HIS ASN GLY LYS VAL THR ALA THR GLU SER TYR ASP ILE HIS ILE ALA ARG GLU THR ALA GLU
L97 F98 K99 S100 N101 I102 F103 K104 L105 Q106 I107 D108 E109 L110 L111 E112 Q113 V114 K115 L116 K117 Q118 K119 H120
V121 L122 K123 V124 E125 K126 F127 L128 H129 K130 L131 Y132 D133 I134 L135 Q136 E137 I138 P139 D140 W141 E142 E143 K144 S145 L146 A147 E148 V149 D150 S151 F152 F153 K154 N155 K156 I157 V158 S159 V160 P161 F162 V163 D164 P165 K166 P167 I168 P169 Q170 N171 T172 N173 Y174 K175 F176 N177 Y178 K179 K180
P181 D182 I183 S184 L185 I186 G187 S188 F189 A190 L191 K192 A193 G194 I195 Y196 Q197 P198 N199 G200 S201 S202 I203 D204 T205 L206 L207 T208 M209 P210 K211 E212 L213 F214 E215 K216 K217 D218 F219 L220 N221 F222 R223 C224 L225 H226 K227 R228 S229 V230 Y231 L232 A233 Y234 L235 T236 H237 H238 L239 L240
I241 L242 L243 K244 K245 D246 K247 L248 D249 S250 F251 L252 Q253 L254 E255 Y256 S257 Y258 F259 D260 N261 D262 P263 L264 L265 P266 I267 L268 R269 I270 S271 C272 S273 K274 PRO THR GLY ASP SER LEU SER D282 Y283 N284 F285 Y286 K287 T288 R289 F290 S291 I292 N293 L294 L295 I296 G297 F298 P299 Y300
K301 V302 F303 E304 P305 K306 K307 L308 L309 P310 N311 R312 N313 C314 I315 R316 I317 ALA GLN GLU SER LYS GLU GLN SER L326 P327 A328 T329 P330 L331 Y332 N333 F334 S335 V336 L337 S338 S339 S340 T341 H342 E343 N344 Y345 L346 K347 Y348 L349 Y350 K351 T352 K353 K354 Q355 T356 E357 S358 F359 V360
E361 A362 T363 V364 L365 G366 R367 L368 W369 L370 Q371 Q372 R373 G374 F375 S376 S377 N378 M379 S380 H381 S382 G383 S384 L385 G386 G387 F388 G389 T390 F391 E392 F393 T394 I395 L396 M397 A398 A399 L400 L401 N402 G403 G404 G405 I406 N407 S408 N409 K410 I411 L412 L413 H414 G415 F416 S417 S418 Y419 Q420
L421 F422 K423 G424 V425 I426 K427 Y428 L429 A430 T431 M432 D433 L434 C435 H436 D437 G438 H439 L440 Q441 F442 H443 S444 N445 PRO GLU ASN SER SER SER SER P453 A454 S455 K456 Y457 I458 D459 E460 G461 F462 Q463 T464 P465 T466 L467 F468 D469 K470 S471 T472 K473 V474 N475 I476 L477 T478 K479 M480
T481 V482 S483 S484 Y485 Q486 I487 L488 K489 E490 Y491 A492 G493 E494 T495 L496 R497 M498 L499 N500 N501 V502 V503 Q504 D505 Q506 F507 S508 N509 I510 F511 L512 T513 N514 I515 S516 R517 F518 D519 N520 L521 K522 Y523 D524 L525 C526 Y527 D528 V529 Q530 L531 P532 L533 G534 K535 Y536 N537 N538 L539 E540
T541 S542 L543 A544 A545 T546 F547 G548 S549 M550 E551 R552 V553 K554 F555 I556 T557 L558 E559 N560 F561 L562 A563 H564 K565 I566 T567 N568 V569 A570 R571 Y572 A573 L574 G575 D576 R577 I578 K579 Y580 I581 Q582 I583 E584 M585 V586 G587 Q588 K589 S590 D591 F592 P593 I594 T595 K596 R597 K598 V599 Y600
S601 N602 T603 G604 G605 N606 H607 F608 N609 F610 D611 F612 V613 R614 V615 K616 L617 I618 V619 N620 P621 S622 E623 C624 D625 K626 L627 V628 T629 K630 G631 P632 A633 H634 S635 E636 T637 M638 S639 T640 E641 A642 A643 V644 F645 K646 N647 F648 W649 G650 I651 K652 S653 S654 L655 R656 R657 F658 K659 D660
G661 S662 I663 T664 H665 C666 C667 V668 W669 S670 T671 S672 S673 S674 E675 P676 I677 I678 S679 S680 I681 V682 N683 F684 A685 L686 Q687 K688 H689 V690 S691 K692 K693 A694 Q695 I696 S697 N698 E699 T700 I701 K702 K703 F704 H705 N706 F707 L708 P709 L710 P711 N712 L713 P714 S715 S716 A717 K718 T719 S720
V721 L722 N723 L724 S725 S726 F727 F728 N729 L730 K731 K732 S733 F734 D735 D736 L737 Y738 K739 I740 I741 F742 Q743 M744 K745 L746 P747 L748 S749 V750 K751 S752 I753 L754 P755 V756 G757 S758 A759 F760 R761 Y762 T763 S764 L765 C766 Q767 P768 V769 P770 F771 A772 Y773 S774 D775 P776 D777 F778 F779 Q780
D781 V782 I783 L784 E785 F786 E787 T788 S789 P790 K791 W792 P793 D794 E795 I796 T797 S798 L799 E800 K801 A802 K803 T804 A805 P806 L807 L808 K809 I810 Q811 E812 E813 L814 S815 A816 N817 S818 S819 T820 Y821 R822 S823 F824 F825 S826 R827 D828 E829 S830 I831 P832 Y833 N834 L835 E836 I837 V838 T839 L840



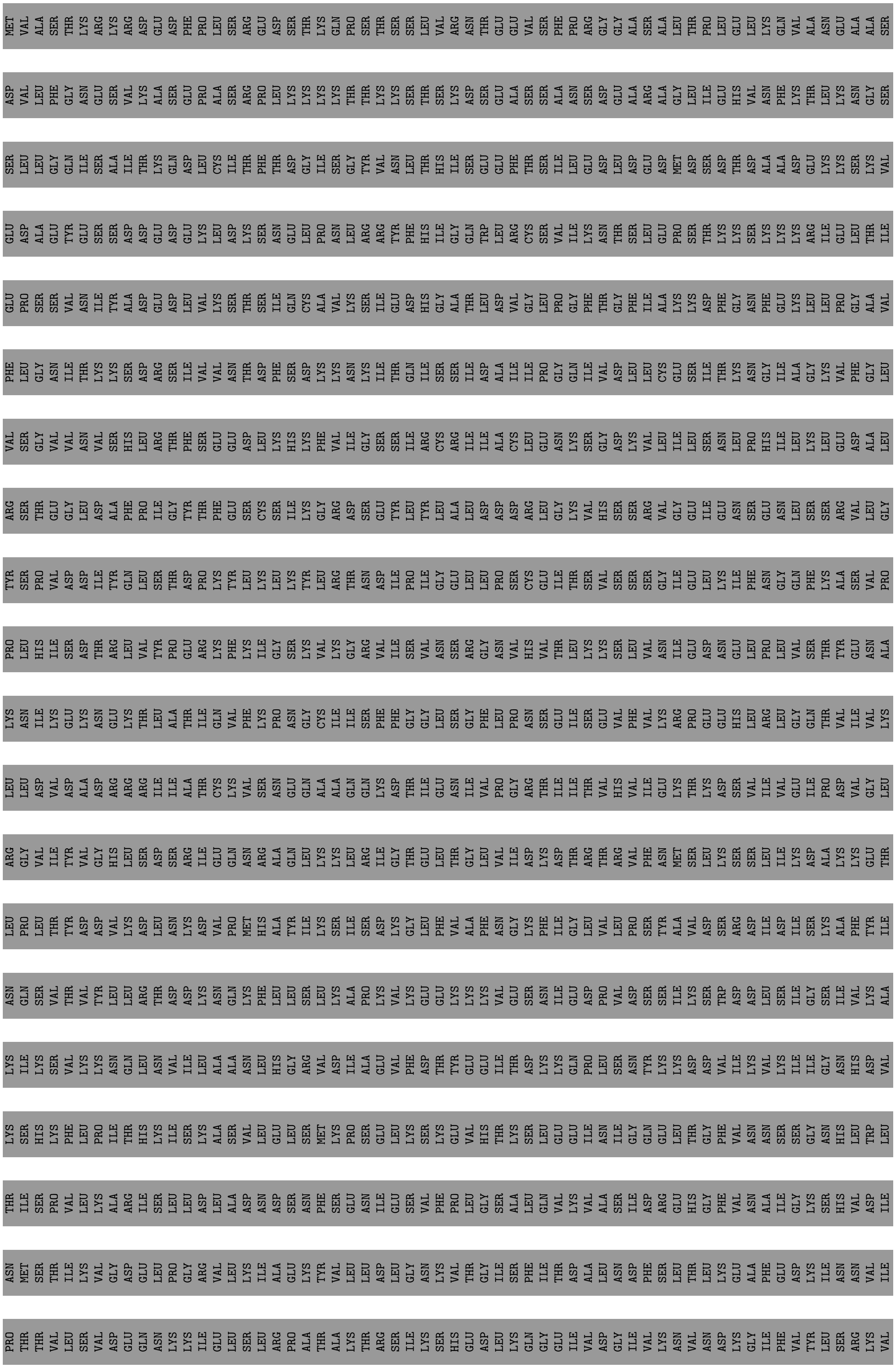
• Molecule 42: Rrp7

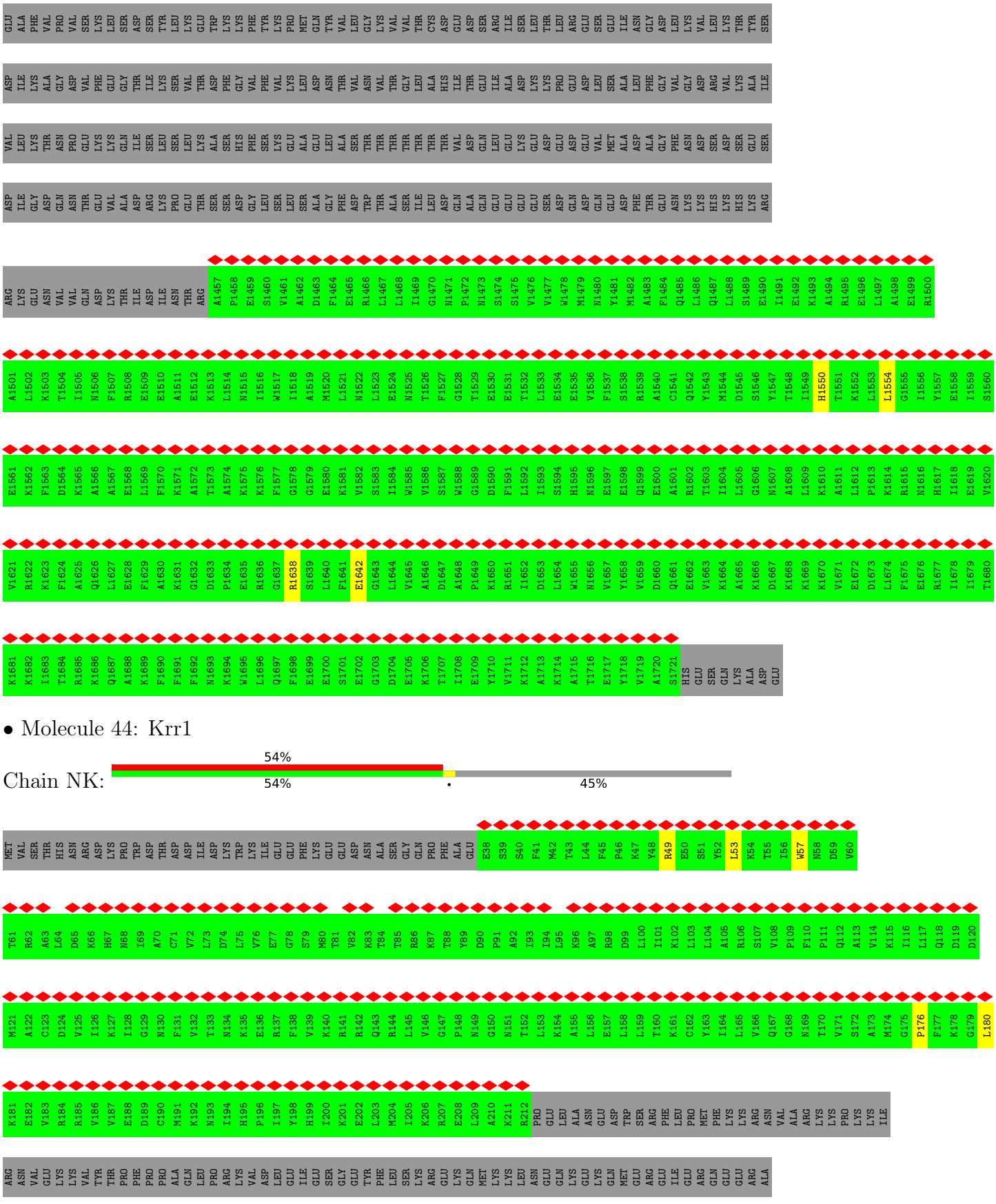
Chain NI:



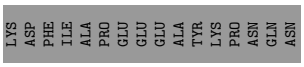
• Molecule 43: Rrp5

Chain NJ:


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

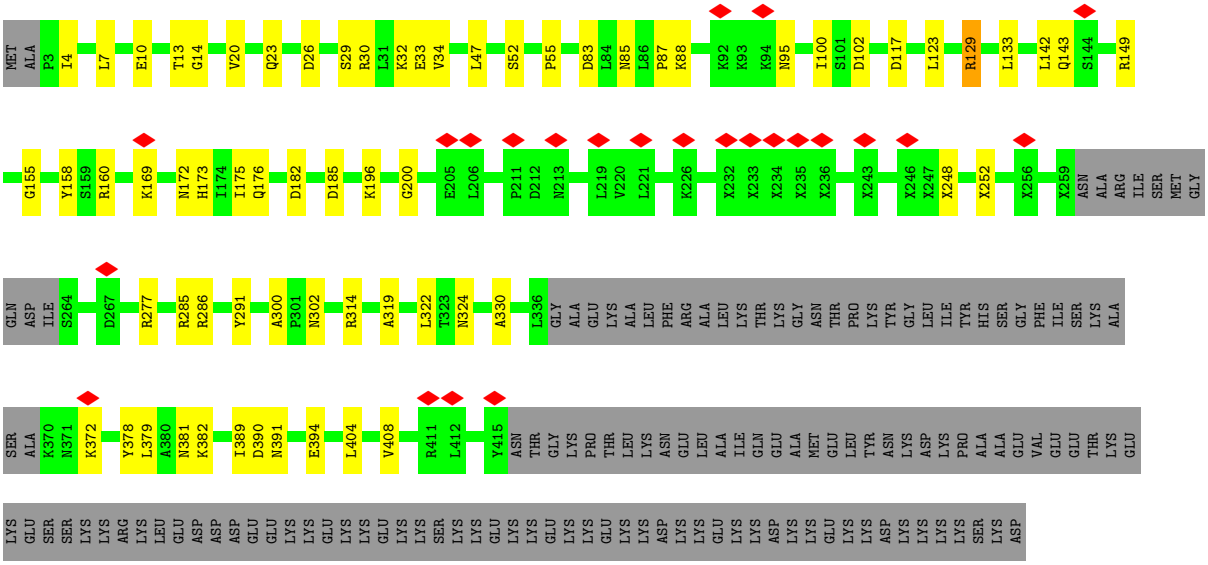


• Molecule 44: Krr1



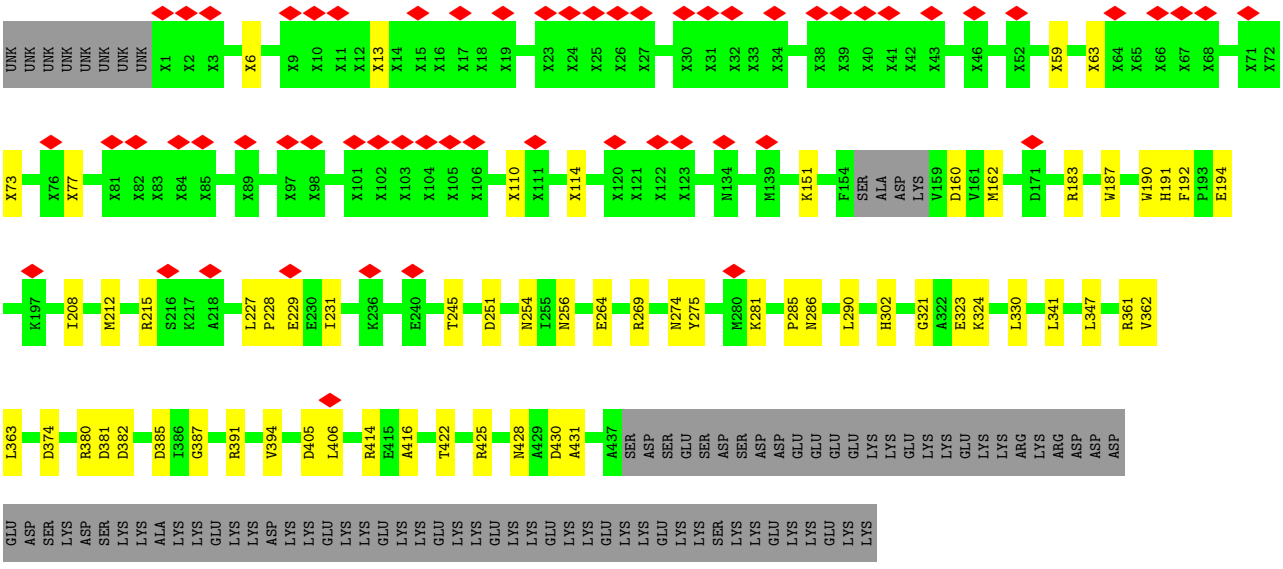
- Molecule 45: Nop56

Chain SA:



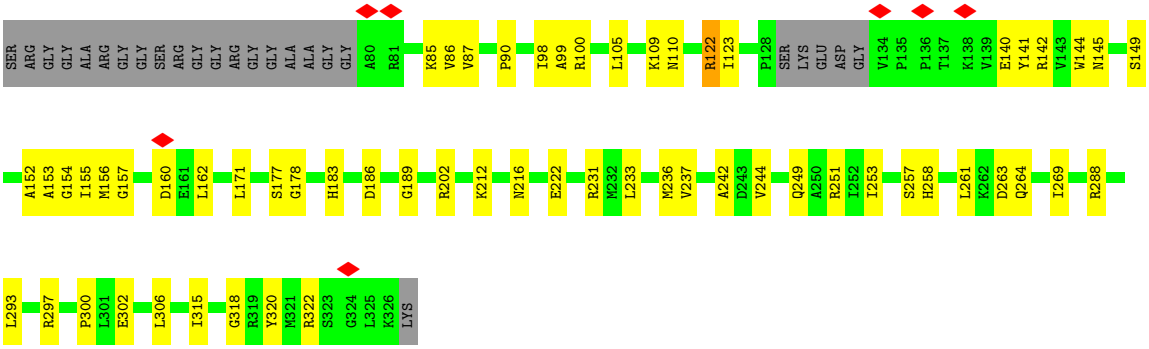
- Molecule 46: Nop58

Chain SB:



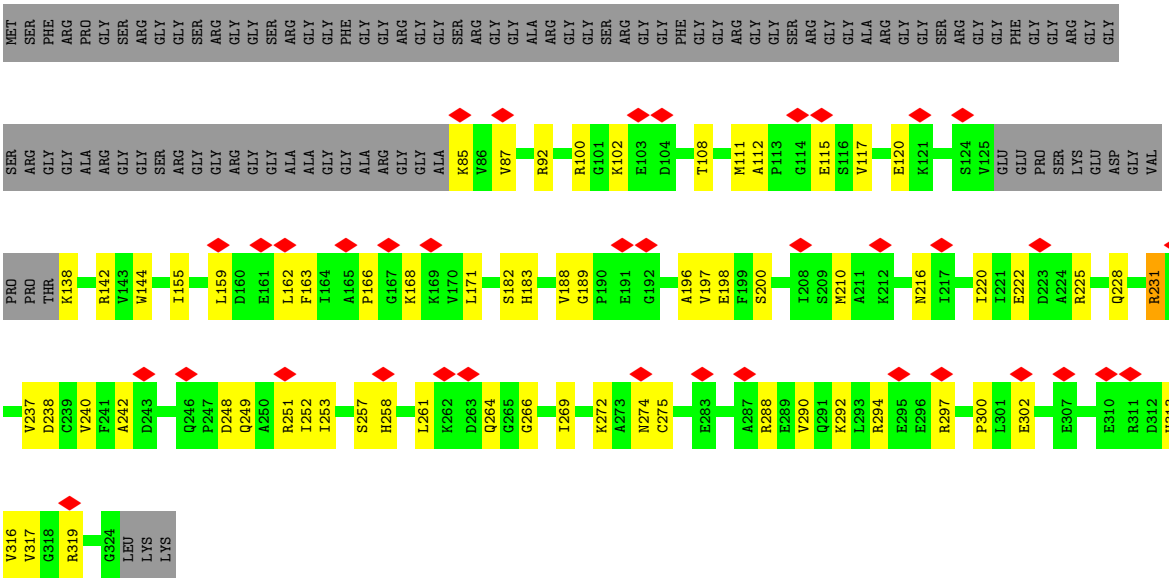
- Molecule 47: Nop1

Chain SC:



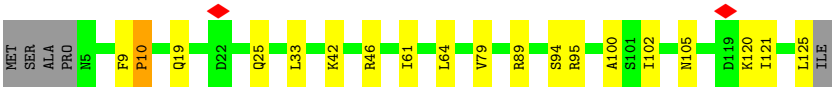
• Molecule 47: Nop1

Chain SD:



• Molecule 48: Snu13

Chain SE:

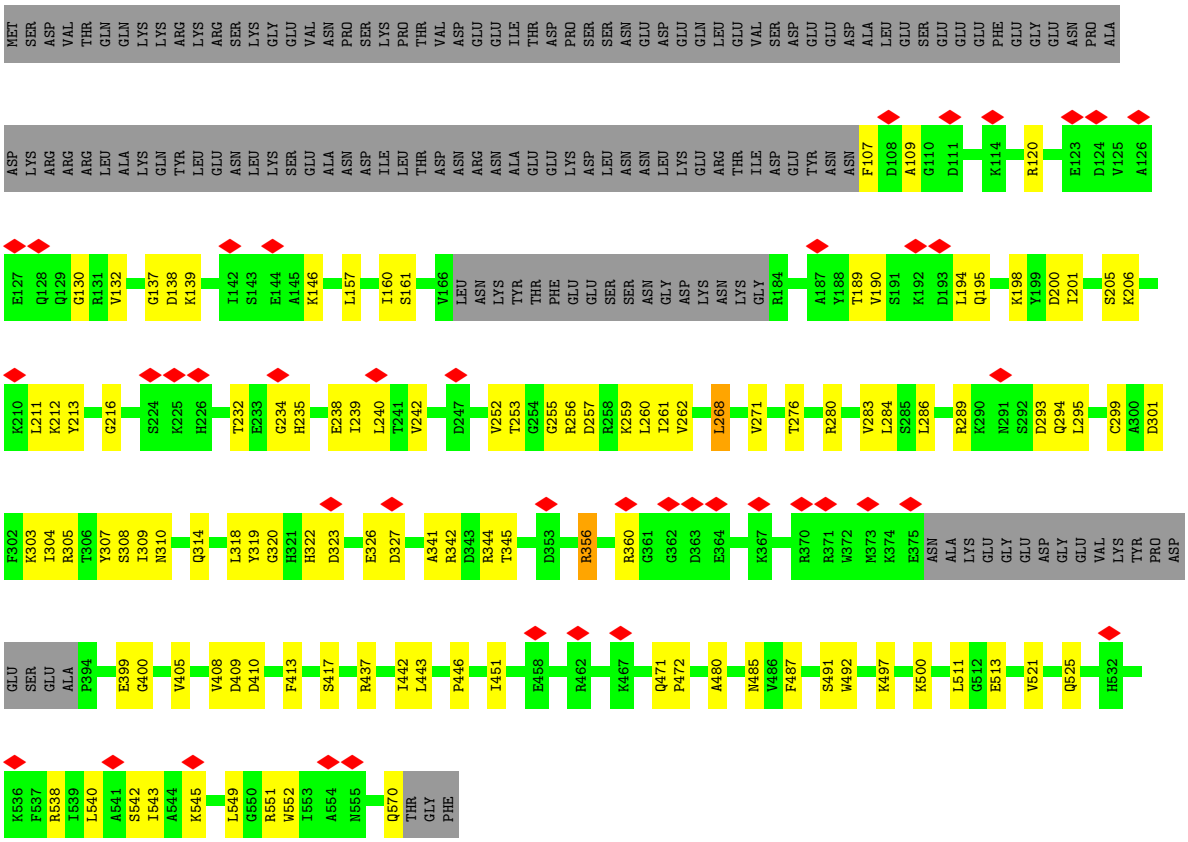


• Molecule 48: Snu13

Chain SF:

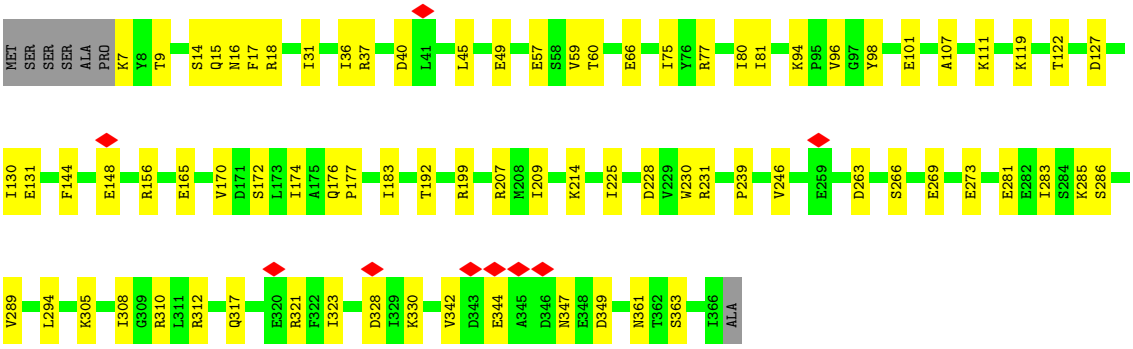
• Molecule 49: Rrp9

Chain SG:



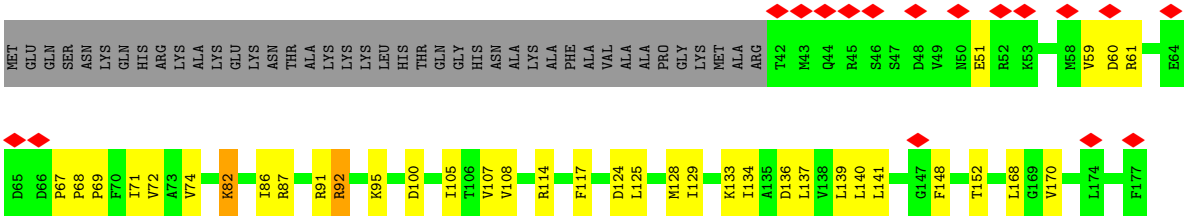
• Molecule 50: Rcl1

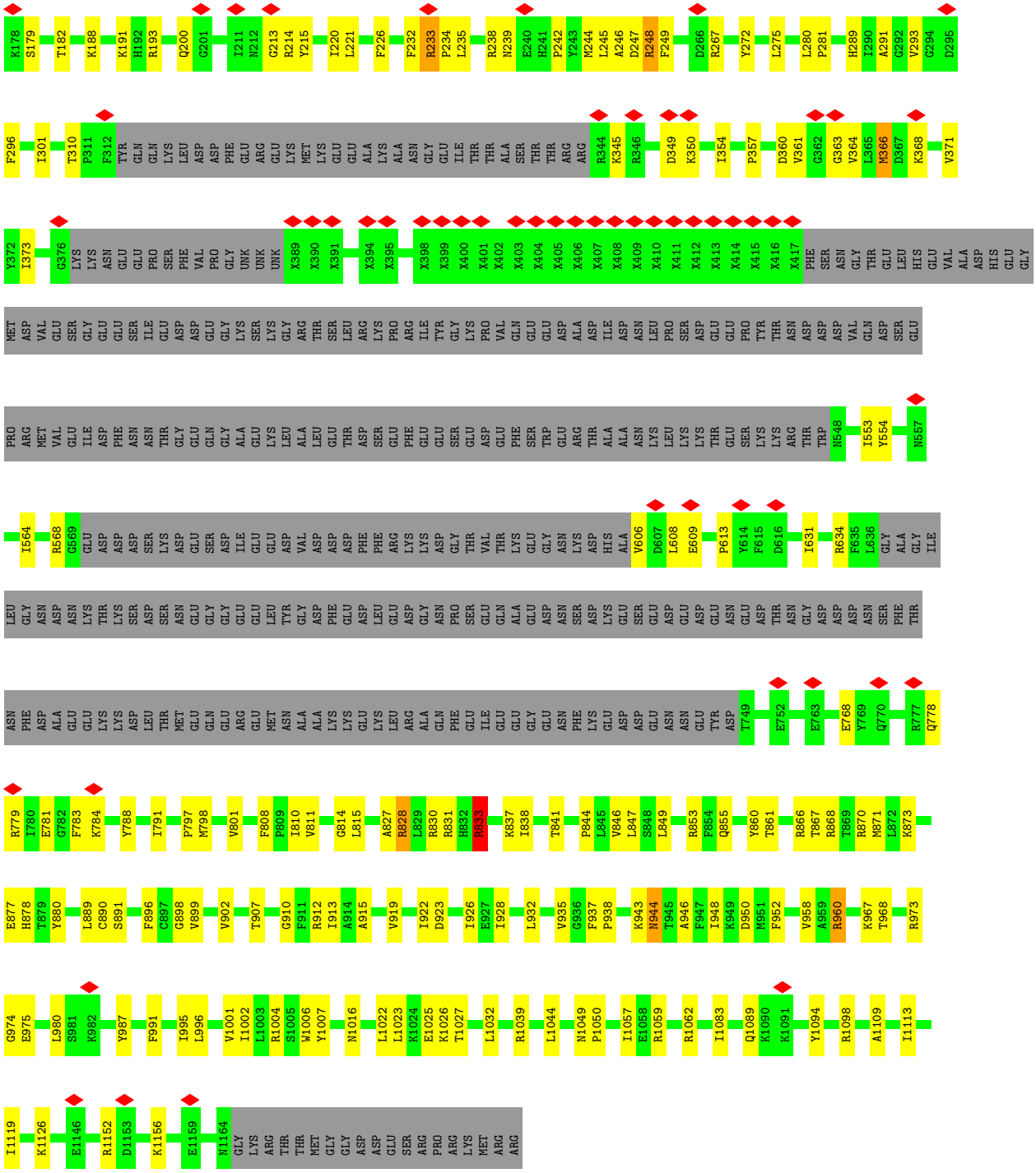
Chain SH:



• Molecule 51: Bms1

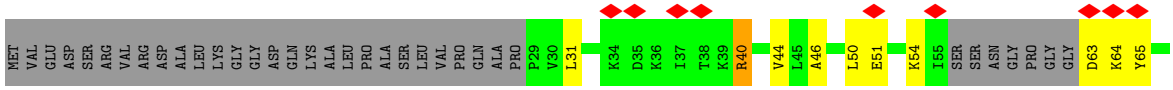
Chain SI:

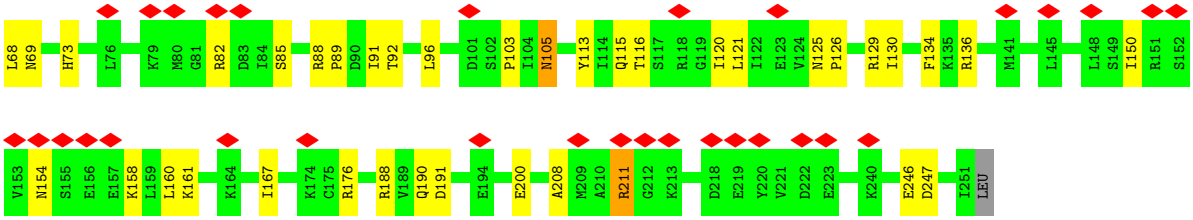




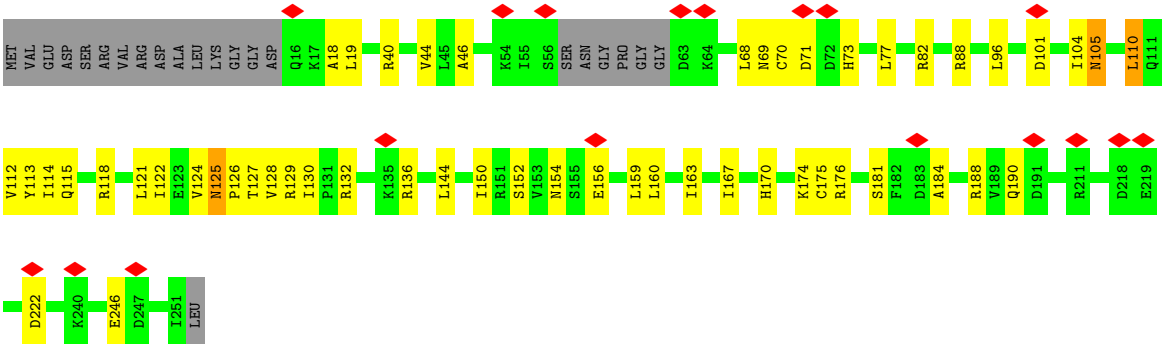
• Molecule 52: Emg1

Chain SJ:

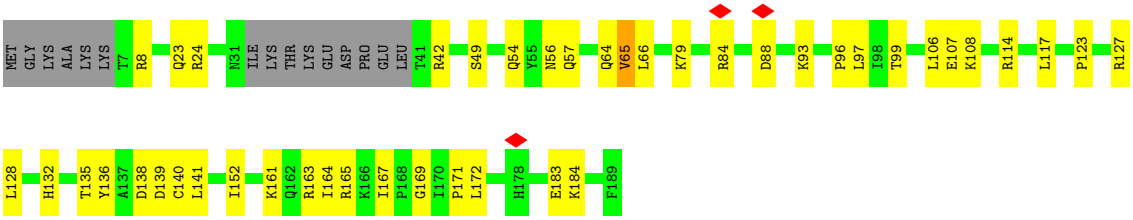




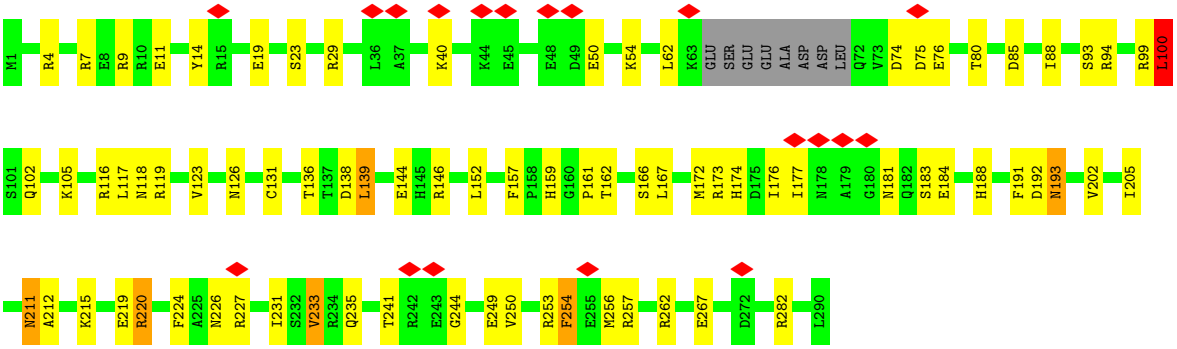
• Molecule 52: Emg1



• Molecule 53: Utp24

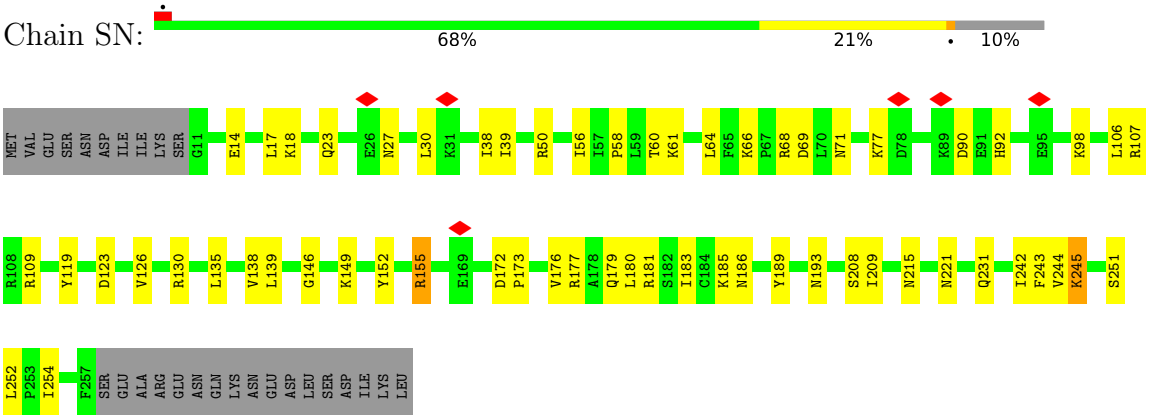


• Molecule 54: Imp4



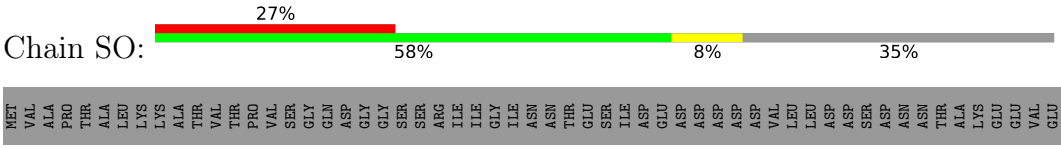
• Molecule 55: Utp30

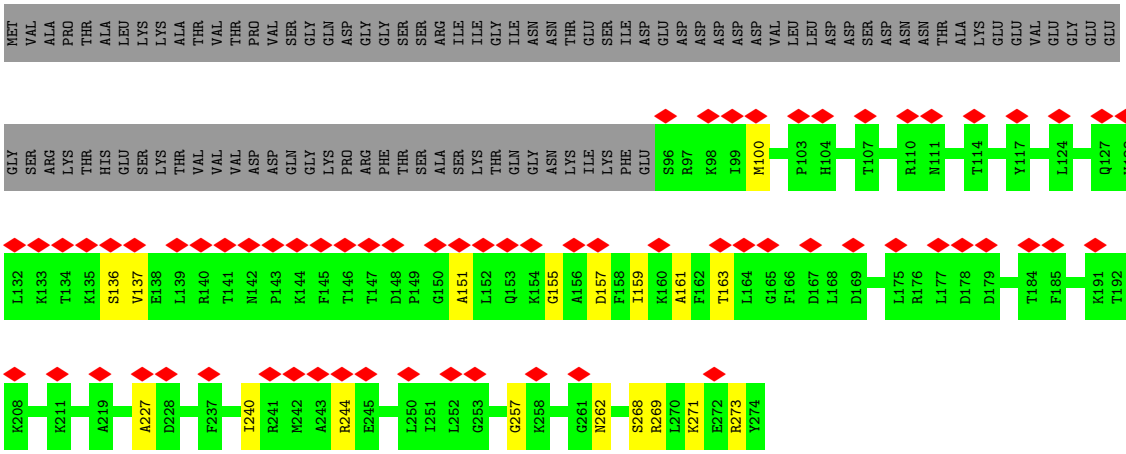
Chain SN:



• Molecule 56: Pno1

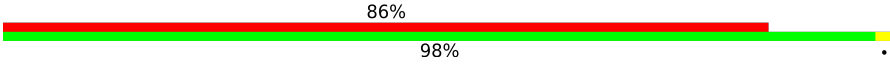
Chain SO:

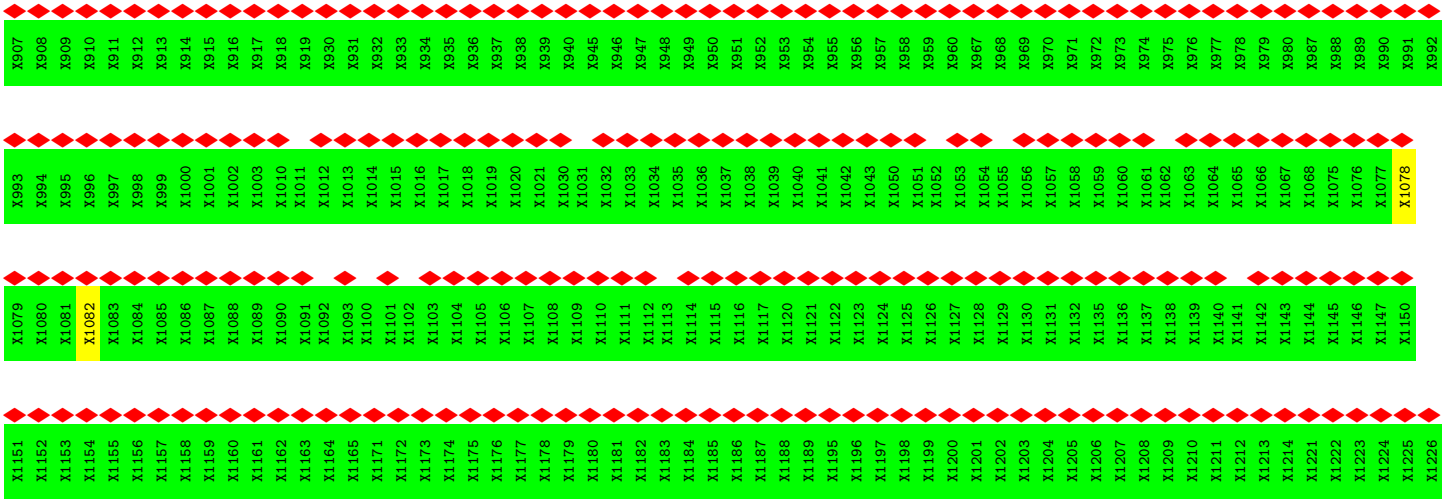


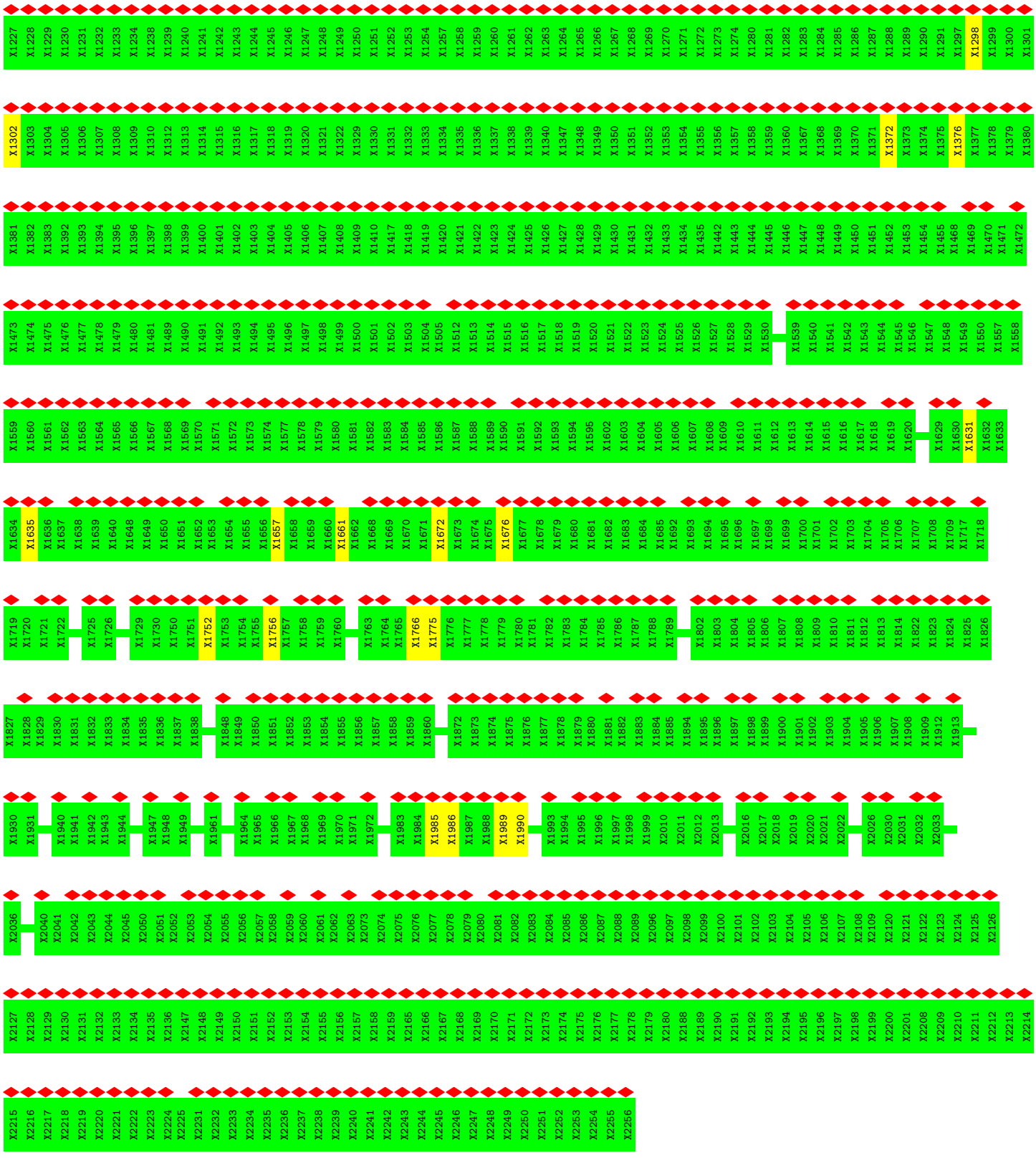


• Molecule 57: Utp20

Chain SP:

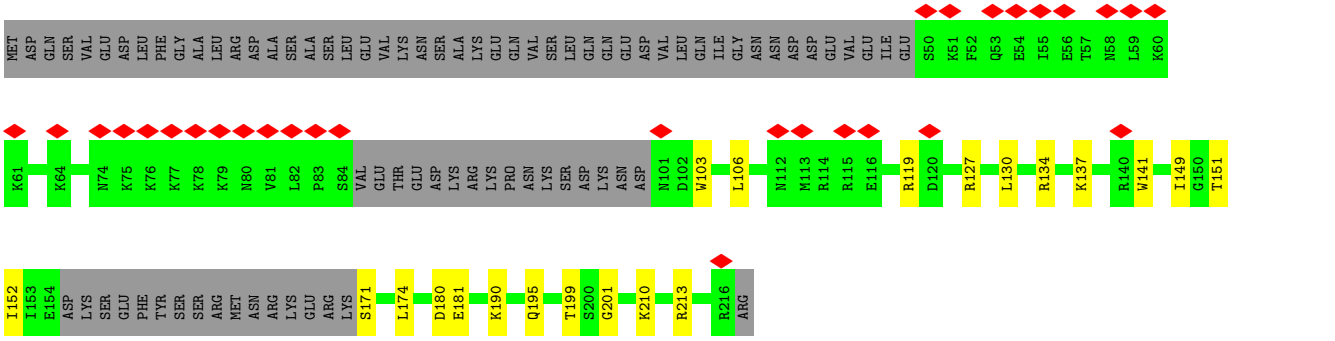






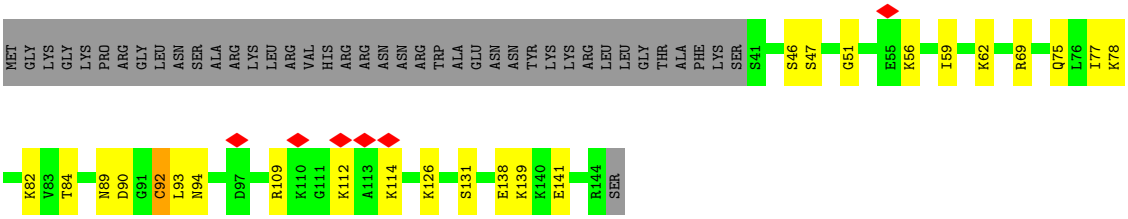
- Molecule 58: Fcf2

Chain SQ:



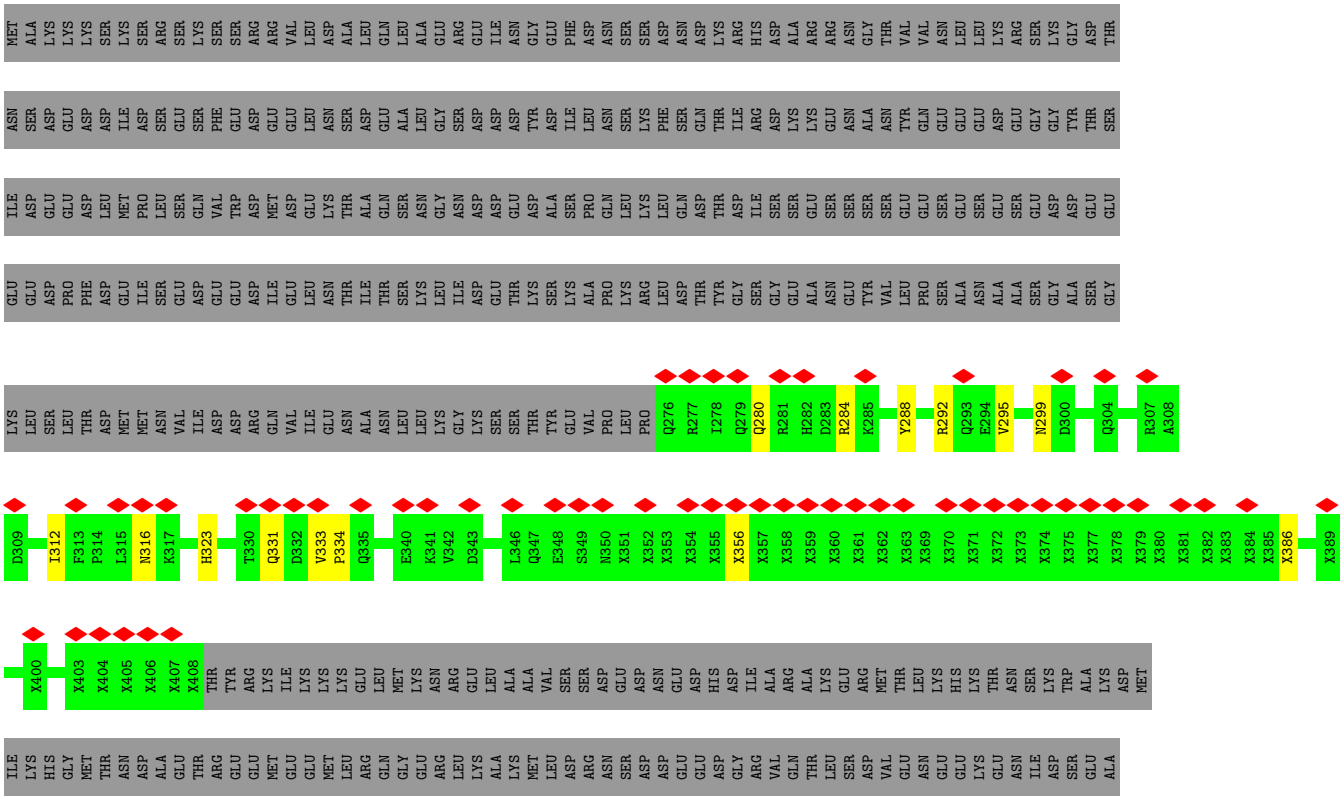
• Molecule 59: rpS23_uS12

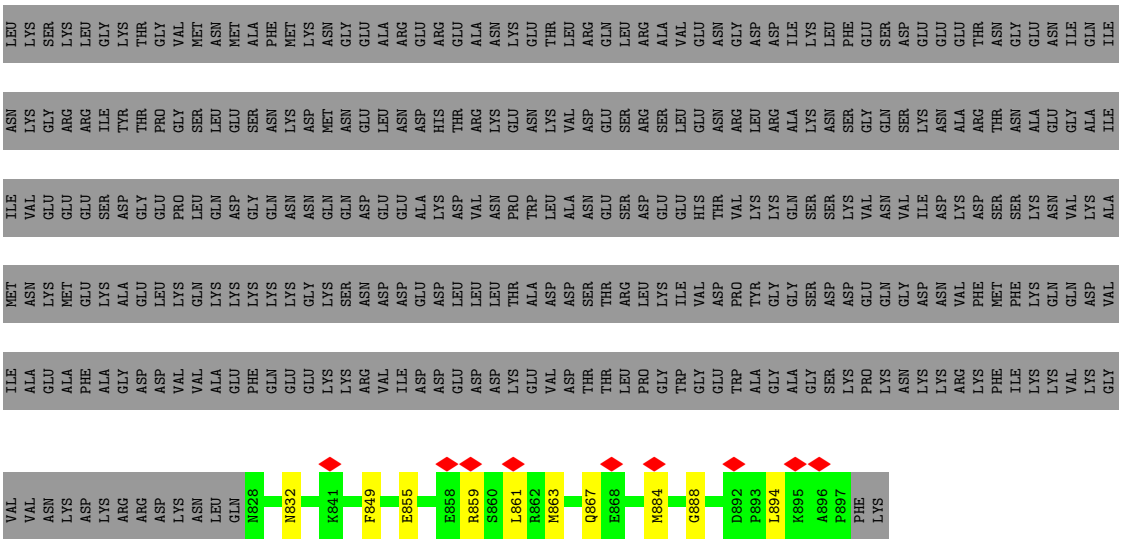
Chain SR:



• Molecule 60: Utp14

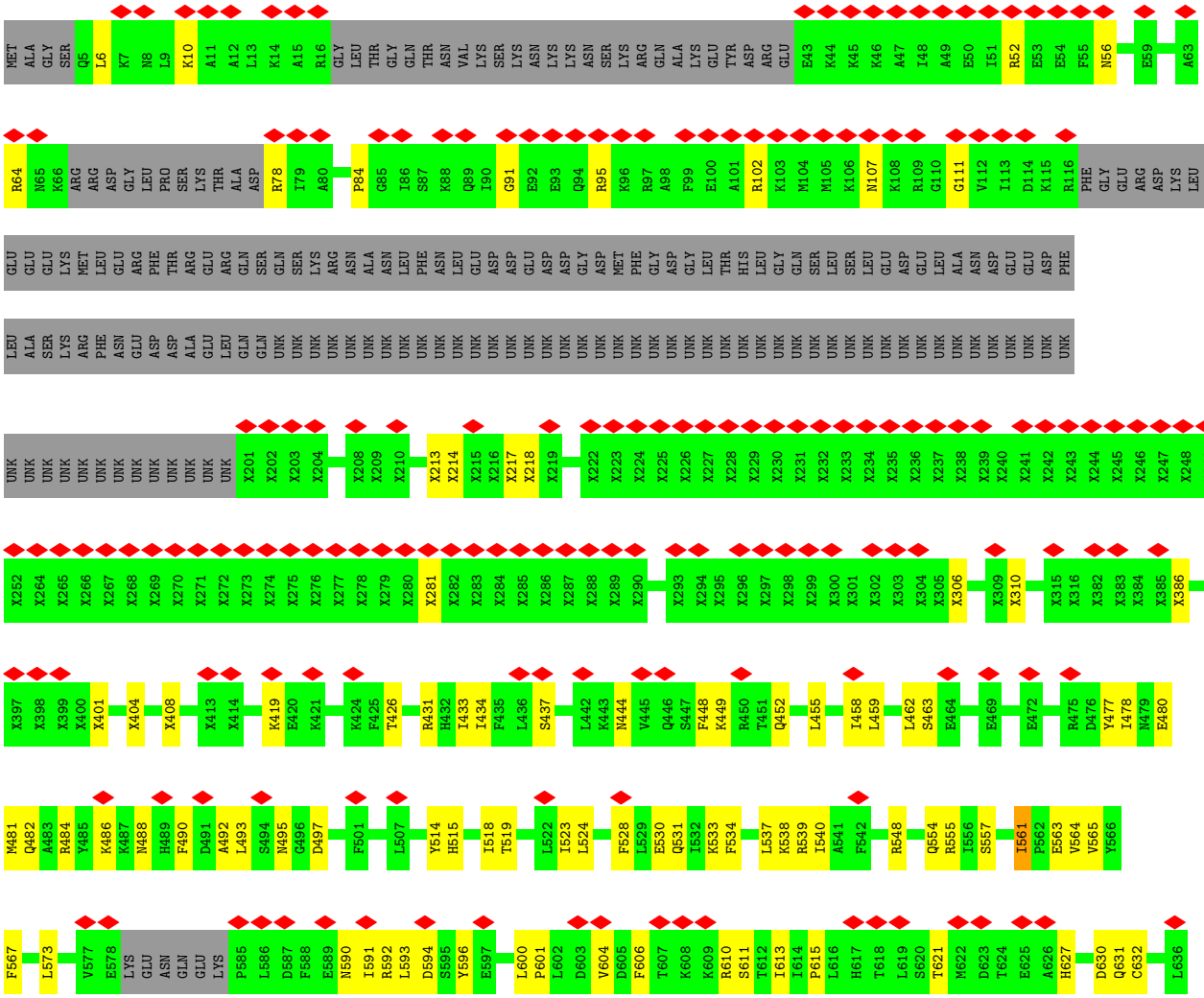
Chain SS:

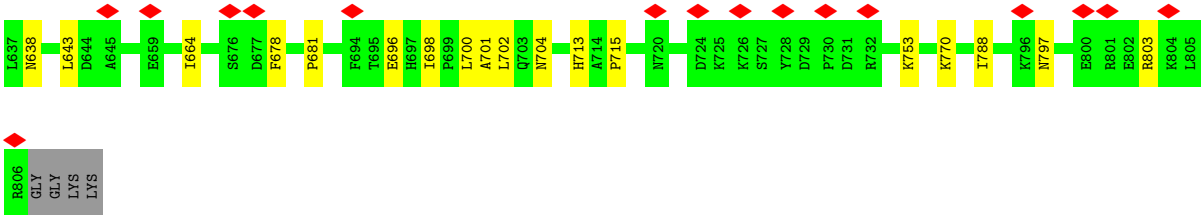




• Molecule 61: Nop14

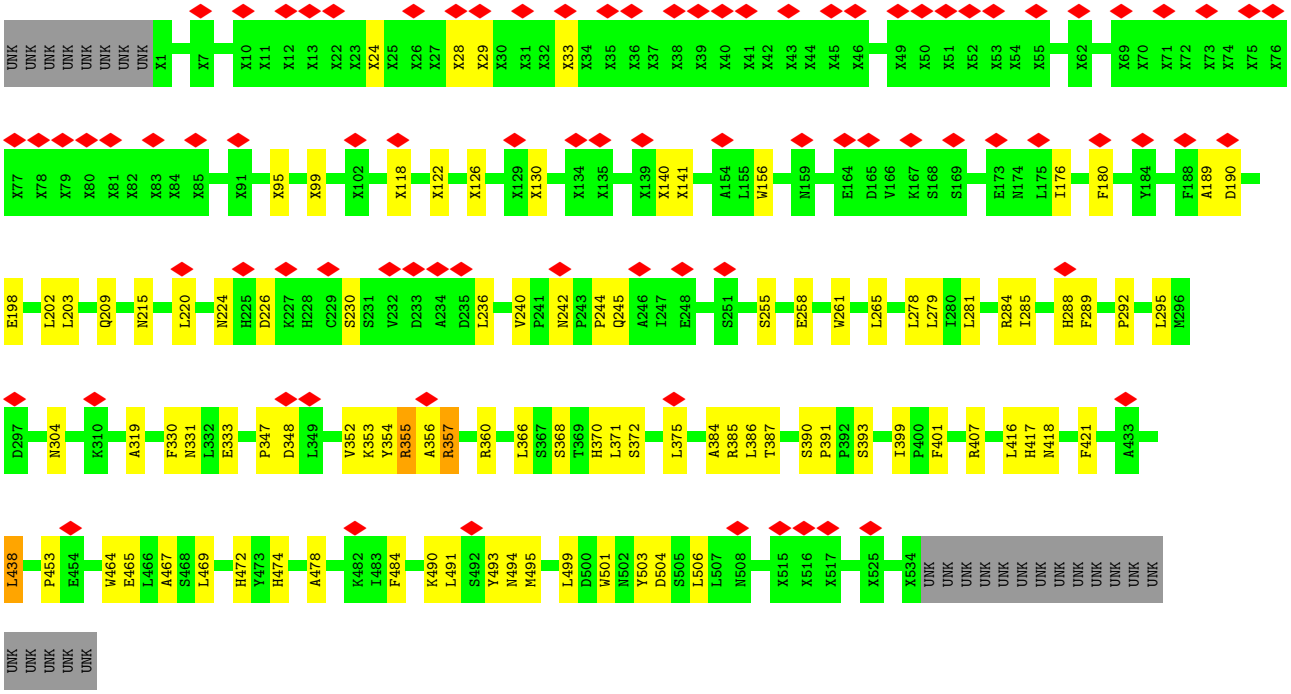
Chain ST:





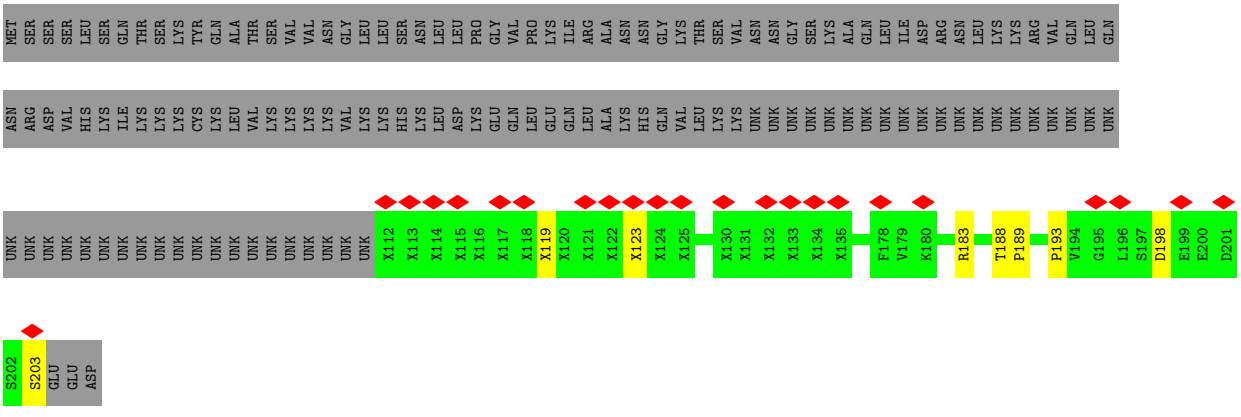
• Molecule 62: Noc4

Chain SU:



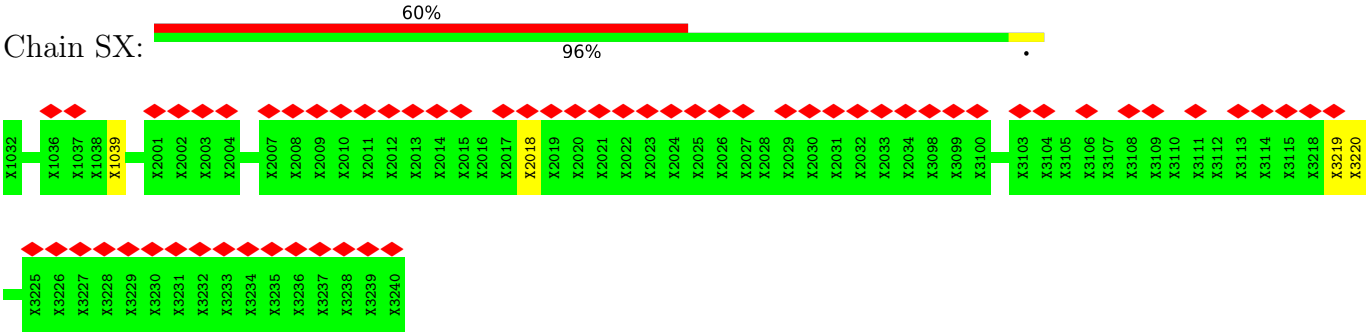
• Molecule 63: Rrt14

Chain SV:



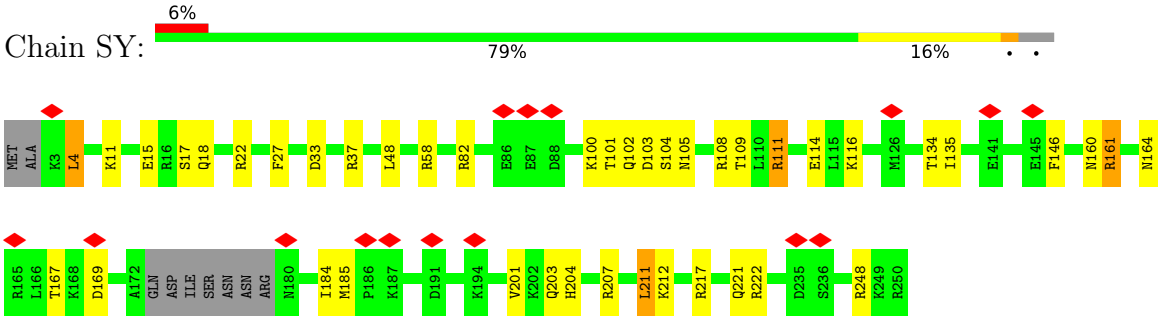
• Molecule 64: Unassigned peptides

Chain SX:



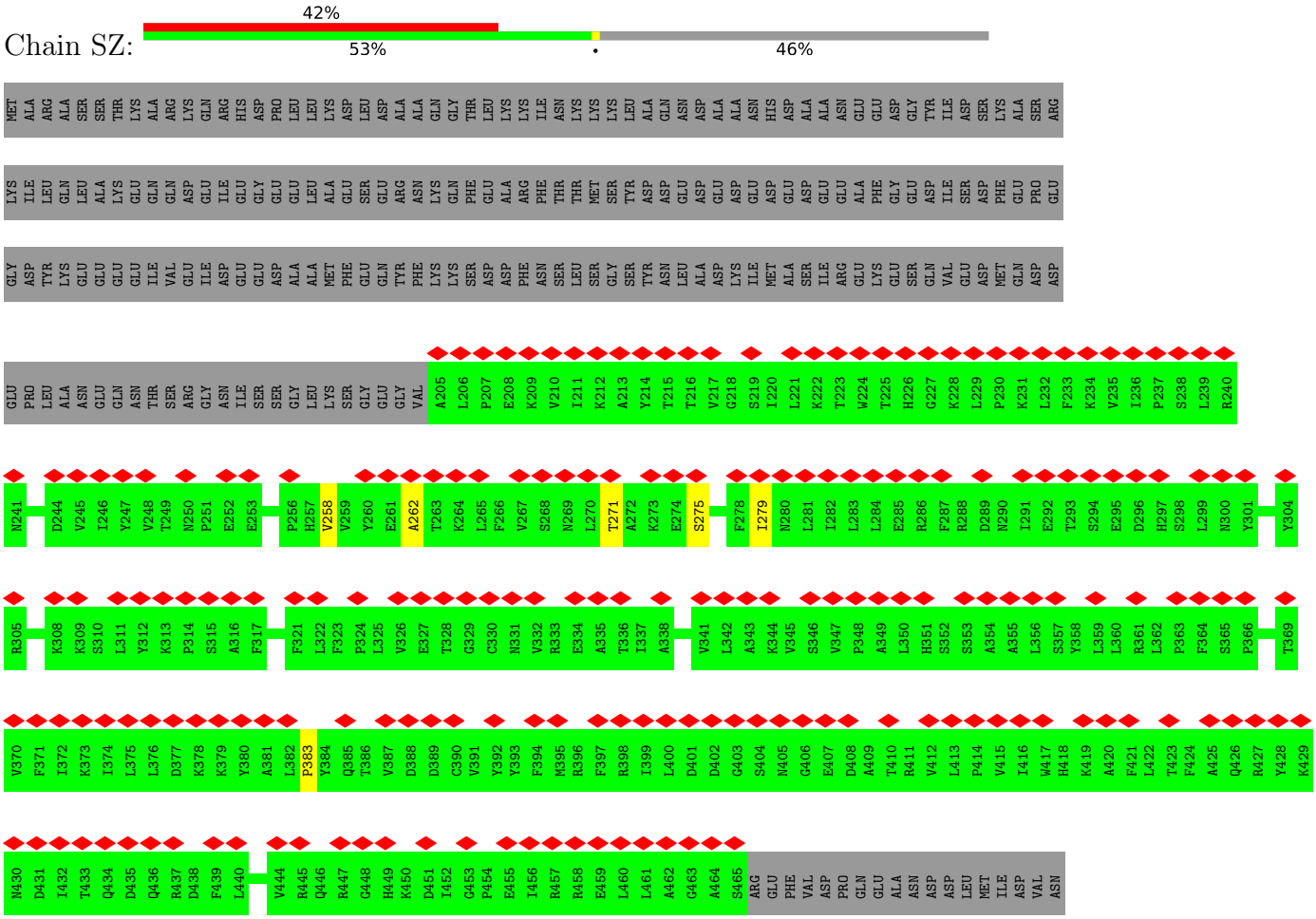
• Molecule 65: Utp11

Chain SY:



• Molecule 66: Enp1

Chain SZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	284213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.56	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	520.0, 520.0, 520.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	L0	0.72	0/11634	1.03	32/18120 (0.2%)
2	L1	0.54	0/24442	1.01	70/38042 (0.2%)
3	L2	0.74	0/4001	1.03	11/6215 (0.2%)
4	L3	0.30	0/871	0.53	0/1171
5	L4	0.31	0/1849	0.65	1/2497 (0.0%)
6	L5	0.44	0/1690	0.61	0/2285
7	L6	0.29	0/899	0.58	0/1201
8	L7	0.30	0/1342	0.62	0/1807
9	L8	0.28	0/1372	0.53	0/1834
10	L9	0.43	0/1437	0.63	0/1924
11	LC	0.60	0/990	0.72	1/1335 (0.1%)
12	LD	0.31	0/1050	0.57	0/1415
13	LE	0.31	0/1020	0.54	0/1371
14	LF	0.36	0/727	0.70	0/977
15	LG	0.44	0/499	0.62	0/670
16	LH	0.38	0/6694	0.63	5/9070 (0.1%)
17	LI	0.28	0/1105	0.53	0/1491
18	LJ	0.44	0/3993	0.63	2/5413 (0.0%)
19	LK	0.27	0/735	0.51	0/987
20	LL	0.40	0/3840	0.62	0/5208
21	LM	0.44	0/3470	0.61	2/4694 (0.0%)
22	LN	0.39	0/5369	0.63	4/7272 (0.1%)
23	LO	0.54	0/6780	0.68	3/9175 (0.0%)
24	LP	0.39	0/2281	0.53	0/3059
25	LQ	0.34	0/6574	0.61	2/8881 (0.0%)
26	LR	0.39	0/1336	0.55	1/1800 (0.1%)
27	LS	0.50	0/3875	0.64	1/5254 (0.0%)
28	LT	0.47	0/6834	0.60	0/9238
29	LU	0.48	0/3802	0.63	2/5118 (0.0%)
30	LV	0.33	0/2902	0.64	2/3941 (0.1%)
31	LW	0.55	0/3505	0.69	4/4748 (0.1%)
32	LX	0.32	0/1481	0.57	0/1987

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LY	0.22	0/768	0.40	0/1065
33	LZ	0.57	0/1559	0.71	0/2097
34	NA	0.39	0/1685	0.61	0/2261
35	NB	0.40	0/1042	0.53	0/1377
36	NC	0.33	0/1139	0.61	1/1512 (0.1%)
37	ND	0.31	0/499	0.58	0/659
38	NE	0.27	0/1063	0.56	0/1402
39	NF	0.23	0/614	0.42	0/855
40	NG	0.26	0/542	0.53	0/750
41	NH	0.23	0/5356	0.42	0/7460
42	NI	0.23	0/838	0.41	0/1166
43	NJ	0.23	0/1313	0.37	0/1830
44	NK	0.24	0/867	0.42	0/1208
45	SA	0.39	0/2769	0.54	1/3728 (0.0%)
46	SB	0.40	0/2344	0.59	0/3160
47	SC	0.54	0/1917	0.66	1/2588 (0.0%)
47	SD	0.35	0/1815	0.57	0/2448
48	SE	0.44	0/928	0.60	0/1262
48	SF	0.39	0/928	0.61	0/1262
49	SG	0.36	0/3498	0.58	0/4712
50	SH	0.36	0/2832	0.54	0/3825
51	SI	0.45	0/6403	0.63	1/8616 (0.0%)
52	SJ	0.30	0/1727	0.51	0/2329
52	SK	0.35	0/1828	0.55	0/2470
53	SL	0.49	0/1418	0.64	0/1906
54	SM	0.51	0/2337	0.72	5/3148 (0.2%)
55	SN	0.40	0/2041	0.64	0/2745
56	SO	0.28	0/1003	0.47	0/1381
58	SQ	0.39	0/1156	0.56	0/1536
59	SR	0.44	0/804	0.67	1/1074 (0.1%)
60	SS	0.34	0/1230	0.54	0/1660
61	ST	0.32	0/3826	0.52	1/5125 (0.0%)
62	SU	0.36	0/3064	0.57	0/4163
63	SV	0.36	0/201	0.56	0/273
65	SY	0.44	0/2042	0.62	0/2704
66	SZ	0.24	0/1294	0.39	0/1804
All	All	0.46	0/183089	0.72	154/255761 (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
4	L3	0	1
5	L4	0	2
8	L7	0	4
11	LC	0	1
12	LD	0	1
14	LF	0	1
16	LH	0	2
22	LN	0	2
23	LO	0	2
25	LQ	0	2
28	LT	0	1
29	LU	0	1
30	LV	0	3
31	LW	0	2
34	NA	0	1
36	NC	0	2
46	SB	0	1
48	SE	0	1
49	SG	0	1
54	SM	0	3
56	SO	0	1
58	SQ	0	2
All	All	0	37

There are no bond length outliers.

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	965	U	N1-C2-O2	11.23	130.66	122.80
1	L0	430	C	N1-C2-O2	11.16	125.59	118.90
2	L1	374	U	N1-C2-O2	11.06	130.54	122.80
2	L1	965	U	C2-N1-C1'	11.06	130.97	117.70
2	L1	374	U	C2-N1-C1'	10.92	130.80	117.70
1	L0	430	C	C2-N1-C1'	10.86	130.75	118.80
1	L0	524	U	OP1-P-O3'	-10.73	81.59	105.20
1	L0	430	C	C6-N1-C2	-10.58	116.07	120.30
2	L1	543	C	N1-C2-O2	10.25	125.05	118.90
2	L1	374	U	N3-C2-O2	-10.22	115.04	122.20
2	L1	965	U	N3-C2-O2	-9.95	115.23	122.20
1	L0	525	U	OP1-P-OP2	9.35	133.62	119.60
1	L0	430	C	C5-C6-N1	9.17	125.58	121.00
1	L0	430	C	N3-C2-O2	-8.99	115.60	121.90
1	L0	524	U	OP2-P-O3'	-8.86	85.72	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	543	C	N3-C2-O2	-8.58	115.90	121.90
47	SC	306	LEU	CA-CB-CG	8.20	134.17	115.30
31	LW	160	LEU	CA-CB-CG	8.07	133.87	115.30
2	L1	1175	U	N3-C2-O2	-7.91	116.66	122.20
54	SM	100	LEU	CB-CG-CD2	-7.90	97.57	111.00
2	L1	1175	U	N1-C2-O2	7.61	128.13	122.80
2	L1	965	U	C6-N1-C1'	-7.54	110.64	121.20
1	L0	151	U	N1-C2-O2	7.53	128.07	122.80
54	SM	152	LEU	CA-CB-CG	7.41	132.33	115.30
3	L2	252	C	N1-C2-O2	7.24	123.25	118.90
1	L0	394	U	N3-C2-O2	-7.18	117.17	122.20
22	LN	272	LEU	CB-CG-CD2	-7.09	98.95	111.00
16	LH	749	ASP	CB-CG-OD1	7.08	124.68	118.30
2	L1	374	U	C6-N1-C1'	-7.01	111.39	121.20
1	L0	311	C	P-O3'-C3'	6.97	128.06	119.70
5	L4	189	LEU	CA-CB-CG	6.95	131.29	115.30
1	L0	151	U	C2-N1-C1'	6.95	126.04	117.70
1	L0	151	U	N3-C2-O2	-6.83	117.42	122.20
11	LC	57	LEU	CA-CB-CG	6.83	131.01	115.30
1	L0	394	U	C2-N1-C1'	6.80	125.86	117.70
2	L1	411	C	N1-C2-O2	6.77	122.96	118.90
1	L0	432	C	N1-C2-O2	6.76	122.96	118.90
2	L1	453	U	N1-C2-O2	6.72	127.51	122.80
27	LS	376	LEU	CB-CG-CD2	-6.65	99.70	111.00
54	SM	117	LEU	CA-CB-CG	6.59	130.47	115.30
51	SI	833	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	L1	1465	C	C6-N1-C2	-6.43	117.73	120.30
1	L0	430	C	C6-N1-C1'	-6.42	113.09	120.80
22	LN	622	LEU	CA-CB-CG	6.37	129.94	115.30
2	L1	1132	A	C2-N3-C4	6.36	113.78	110.60
2	L1	542	A	P-O3'-C3'	6.27	127.22	119.70
1	L0	123	C	N1-C2-O2	6.23	122.64	118.90
2	L1	579	A	P-O3'-C3'	6.19	127.12	119.70
2	L1	20	G	P-O3'-C3'	6.18	127.12	119.70
2	L1	374	U	C5-C6-N1	6.14	125.77	122.70
16	LH	79	LEU	CA-CB-CG	6.14	129.42	115.30
3	L2	201	C	N1-C2-O2	6.13	122.58	118.90
2	L1	1000	C	C2-N1-C1'	6.13	125.54	118.80
2	L1	25	C	N1-C2-O2	6.05	122.53	118.90
2	L1	990	C	N1-C2-O2	6.03	122.52	118.90
2	L1	1594	G	P-O3'-C3'	6.03	126.93	119.70
2	L1	934	C	N1-C2-O2	6.02	122.51	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	1000	C	N1-C2-O2	6.01	122.50	118.90
2	L1	934	C	C2-N1-C1'	6.00	125.40	118.80
61	ST	643	LEU	CA-CB-CG	5.99	129.08	115.30
16	LH	383	LEU	CA-CB-CG	5.99	129.07	115.30
1	L0	492	G	P-O3'-C3'	5.98	126.88	119.70
2	L1	453	U	N3-C2-O2	-5.97	118.02	122.20
2	L1	1200	G	C4-N9-C1'	5.97	134.26	126.50
2	L1	0	U	P-O3'-C3'	5.96	126.85	119.70
2	L1	272	U	P-O3'-C3'	5.90	126.78	119.70
2	L1	25	C	C2-N1-C1'	5.89	125.28	118.80
1	L0	432	C	C2-N1-C1'	5.85	125.23	118.80
3	L2	252	C	N3-C2-O2	-5.83	117.82	121.90
2	L1	1200	G	N3-C4-C5	-5.83	125.69	128.60
3	L2	252	C	C2-N1-C1'	5.82	125.20	118.80
2	L1	965	U	C5-C6-N1	5.81	125.60	122.70
1	L0	394	U	N1-C2-O2	5.80	126.86	122.80
2	L1	1620	C	P-O3'-C3'	5.76	126.61	119.70
3	L2	91	C	N1-C2-O2	5.70	122.32	118.90
1	L0	90	G	O5'-P-OP2	5.68	117.52	110.70
3	L2	249	G	N3-C4-N9	5.63	129.38	126.00
2	L1	280	U	N1-C2-O2	5.62	126.74	122.80
2	L1	1492	A	C4-N9-C1'	5.62	136.41	126.30
1	L0	90	G	O5'-P-OP1	-5.61	100.65	105.70
22	LN	225	LEU	CA-CB-CG	5.60	128.18	115.30
29	LU	83	LEU	CB-CG-CD2	-5.59	101.50	111.00
2	L1	411	C	N3-C2-O2	-5.58	117.99	121.90
3	L2	55	A	O4'-C1'-N9	5.54	112.63	108.20
31	LW	390	LEU	CA-CB-CG	5.53	128.03	115.30
2	L1	990	C	C6-N1-C2	-5.53	118.09	120.30
31	LW	247	MET	CG-SD-CE	-5.52	91.37	100.20
2	L1	901	G	C4-N9-C1'	5.52	133.67	126.50
59	SR	92	CYS	CA-CB-SG	-5.52	104.07	114.00
2	L1	298	C	C6-N1-C2	-5.51	118.09	120.30
22	LN	286	LEU	CA-CB-CG	5.50	127.94	115.30
2	L1	280	U	C2-N1-C1'	5.48	124.28	117.70
1	L0	81	A	P-O3'-C3'	5.48	126.27	119.70
1	L0	123	C	C6-N1-C2	-5.47	118.11	120.30
2	L1	453	U	C2-N1-C1'	5.46	124.25	117.70
2	L1	1492	A	N7-C8-N9	5.46	116.53	113.80
2	L1	372	G	OP1-P-O3'	5.46	117.20	105.20
21	LM	81	LEU	CA-CB-CG	5.45	127.83	115.30
29	LU	83	LEU	CA-CB-CG	5.43	127.79	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	LW	381	LEU	CA-CB-CG	5.43	127.79	115.30
2	L1	1200	G	N3-C4-N9	5.43	129.26	126.00
23	LO	33	VAL	N-CA-C	-5.40	96.42	111.00
21	LM	210	LEU	CB-CG-CD2	-5.39	101.83	111.00
2	L1	1220	C	C6-N1-C2	-5.39	118.14	120.30
2	L1	1132	A	C4-N9-C1'	5.38	135.98	126.30
2	L1	1136	U	N3-C2-O2	-5.37	118.44	122.20
2	L1	1175	U	C2-N1-C1'	5.37	124.15	117.70
54	SM	139	LEU	CA-CB-CG	5.37	127.64	115.30
3	L2	54	C	C2-N1-C1'	5.35	124.68	118.80
2	L1	374	U	C6-N1-C2	-5.34	117.80	121.00
2	L1	111	U	C2-N1-C1'	5.33	124.10	117.70
16	LH	230	LEU	CB-CG-CD2	-5.32	101.96	111.00
36	NC	254	ASP	CB-CG-OD1	5.32	123.09	118.30
2	L1	1132	A	N1-C6-N6	-5.31	115.42	118.60
2	L1	354	C	C6-N1-C2	-5.30	118.18	120.30
30	LV	280	LEU	CA-CB-CG	5.30	127.49	115.30
25	LQ	454	LEU	CA-CB-CG	5.29	127.48	115.30
2	L1	990	C	N3-C2-O2	-5.28	118.20	121.90
2	L1	411	C	C2-N1-C1'	5.28	124.61	118.80
3	L2	51	C	C6-N1-C2	-5.28	118.19	120.30
2	L1	1135	U	P-O3'-C3'	5.27	126.03	119.70
2	L1	1573	A	P-O3'-C3'	5.25	126.00	119.70
45	SA	7	LEU	CA-CB-CG	5.24	127.36	115.30
3	L2	54	C	N1-C2-O2	5.24	122.05	118.90
1	L0	333	G	C4-N9-C1'	5.24	133.31	126.50
2	L1	194	U	C2-N1-C1'	5.24	123.98	117.70
2	L1	1620	C	C6-N1-C2	-5.21	118.21	120.30
54	SM	167	LEU	CA-CB-CG	5.20	127.26	115.30
18	LJ	277	LEU	CA-CB-CG	5.19	127.23	115.30
2	L1	484	C	C6-N1-C2	-5.17	118.23	120.30
18	LJ	15	LEU	CA-CB-CG	5.16	127.18	115.30
1	L0	432	C	N3-C2-O2	-5.16	118.29	121.90
2	L1	542	A	N7-C8-N9	5.13	116.37	113.80
2	L1	354	C	C5-C6-N1	5.13	123.56	121.00
1	L0	123	C	C2-N1-C1'	5.13	124.44	118.80
3	L2	80	U	N1-C2-O2	5.12	126.39	122.80
2	L1	1492	A	N3-C4-N9	5.11	131.49	127.40
2	L1	629	U	N1-C2-O2	5.11	126.38	122.80
30	LV	110	ASP	CB-CG-OD1	5.11	122.90	118.30
2	L1	1633	A	C2-N3-C4	5.09	113.15	110.60
1	L0	451	G	OP2-P-O3'	5.08	116.38	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	1136	U	N1-C2-O2	5.08	126.35	122.80
1	L0	395	C	C6-N1-C2	-5.07	118.27	120.30
25	LQ	406	LEU	CA-CB-CG	5.07	126.96	115.30
1	L0	333	G	C6-C5-N7	-5.07	127.36	130.40
1	L0	123	C	C5-C6-N1	5.06	123.53	121.00
2	L1	280	U	N3-C2-O2	-5.05	118.67	122.20
1	L0	108	U	OP1-P-O3'	5.04	116.28	105.20
23	LO	521	LEU	CB-CG-CD1	-5.04	102.43	111.00
26	LR	730	ILE	CG1-CB-CG2	-5.04	100.32	111.40
16	LH	678	LEU	CA-CB-CG	5.02	126.85	115.30
2	L1	1220	C	N1-C2-O2	5.01	121.91	118.90
23	LO	316	TRP	CA-CB-CG	5.01	123.21	113.70
2	L1	1599	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L3	13	HIS	Peptide
5	L4	193	GLY	Peptide
5	L4	194	THR	Peptide
8	L7	10	SER	Peptide
8	L7	12	ALA	Peptide
8	L7	130	VAL	Peptide
8	L7	64	VAL	Peptide
11	LC	13	LYS	Peptide
12	LD	129	ARG	Peptide
14	LF	51	GLU	Peptide
16	LH	187	VAL	Peptide
16	LH	484	VAL	Peptide
22	LN	427	ASN	Peptide
22	LN	84	ASN	Peptide
23	LO	288	ASP	Peptide
23	LO	689	THR	Peptide
25	LQ	16	VAL	Peptide
25	LQ	678	ASP	Peptide
28	LT	86	HIS	Peptide
29	LU	81	ASN	Peptide
30	LV	107	LEU	Peptide
30	LV	57	GLU	Peptide
30	LV	78	LYS	Peptide
31	LW	137	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
31	LW	199	LEU	Peptide
34	NA	453	SER	Peptide
36	NC	273	GLY	Peptide
36	NC	300	THR	Peptide
46	SB	254	ASN	Peptide
48	SE	9	PHE	Peptide
49	SG	437	ARG	Peptide
54	SM	254	PHE	Peptide
54	SM	267	GLU	Peptide
54	SM	80	THR	Peptide
56	SO	227	ALA	Peptide
58	SQ	199	THR	Peptide
58	SQ	201	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L0	10405	0	5231	112	0
2	L1	21866	0	11031	252	0
3	L2	3585	0	1819	43	0
4	L3	901	0	904	15	0
5	L4	1810	0	1865	52	0
6	L5	1669	0	1724	35	0
7	L6	888	0	928	20	0
8	L7	1321	0	1390	18	0
9	L8	1349	0	1372	38	0
10	L9	1415	0	1497	31	0
11	LC	973	0	1029	16	0
12	LD	1027	0	1084	24	0
13	LE	1003	0	1040	12	0
14	LF	715	0	744	11	0
15	LG	497	0	535	12	0
16	LH	6633	0	6509	125	0
17	LI	2857	0	1520	46	0
18	LJ	3911	0	3906	93	0
19	LK	898	0	809	11	0
20	LL	3772	0	3806	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	LM	3443	0	3558	56	0
22	LN	5344	0	5303	116	0
23	LO	6635	0	6525	136	0
24	LP	2709	0	2363	45	0
25	LQ	6640	0	6501	172	0
26	LR	4144	0	1952	53	0
27	LS	3791	0	3772	105	0
28	LT	6697	0	6676	136	0
29	LU	3725	0	3679	94	0
30	LV	2840	0	2685	78	0
31	LW	3428	0	3407	81	0
32	LX	4583	0	2198	62	0
32	LY	3823	0	983	25	0
33	LZ	1530	0	1572	40	0
34	NA	1667	0	1701	43	0
35	NB	1098	0	1100	23	0
36	NC	1125	0	1101	18	0
37	ND	600	0	586	18	0
38	NE	1192	0	1184	22	0
39	NF	615	0	280	0	0
40	NG	543	0	277	9	0
41	NH	5362	0	2295	6	0
42	NI	841	0	365	1	0
43	NJ	1314	0	610	2	0
44	NK	868	0	379	3	0
45	SA	2854	0	2787	50	0
46	SB	2937	0	2512	43	0
47	SC	1881	0	1928	42	0
47	SD	1782	0	1826	43	0
48	SE	916	0	964	15	0
48	SF	916	0	964	19	0
49	SG	3428	0	3446	76	0
50	SH	2781	0	2878	57	0
51	SI	6412	0	6497	160	0
52	SJ	1701	0	1767	25	0
52	SK	1799	0	1872	40	0
53	SL	1395	0	1473	35	0
54	SM	2296	0	2325	61	0
55	SN	2006	0	2118	45	0
56	SO	998	0	631	11	0
57	SP	4910	0	1107	10	0
58	SQ	1137	0	1188	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	SR	792	0	847	26	0
60	SS	1466	0	1253	24	0
61	ST	4473	0	4053	73	0
62	SU	3781	0	3106	62	0
63	SV	381	0	224	7	0
64	SX	515	0	118	4	0
65	SY	2016	0	2093	38	0
66	SZ	1295	0	571	4	0
67	SL	1	0	0	0	0
All	All	196921	0	158343	2804	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 8.

All (2804) 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)
2:L1:547:U:OP2	35:NB:554:ARG:NH1	1.81	1.12
1:L0:90:G:OP1	18:LJ:378:LYS:NZ	1.84	1.10
3:L2:253:G:OP2	48:SF:95:ARG:NH1	1.93	1.00
51:SI:1059:ARG:NH1	65:SY:33:ASP:OD2	1.95	0.99
29:LU:292:ARG:HH12	60:SS:299:ASN:HB2	1.28	0.98
2:L1:330:G:OP2	9:L8:172:ARG:NH1	1.99	0.95
16:LH:849:ASP:OD2	27:LS:475:LYS:NZ	2.00	0.95
27:LS:142:LYS:NZ	46:SB:430:ASP:OD1	2.01	0.94
51:SI:51:GLU:OE2	59:SR:78:LYS:NZ	2.01	0.94
2:L1:19:A:N1	53:SL:165:ARG:NH1	2.15	0.94
27:LS:514:LEU:O	65:SY:248:ARG:NH1	2.02	0.93
23:LO:471:GLY:O	23:LO:498:ARG:NH1	2.03	0.91
51:SI:830:ARG:NH1	59:SR:138:GLU:OE2	2.03	0.91
21:LM:43:GLN:HE21	21:LM:123:ARG:HH12	1.19	0.89
9:L8:42:ARG:HH12	30:LV:335:SER:HA	1.36	0.89
7:L6:31:ARG:NH2	30:LV:48:GLU:OE2	2.05	0.89
25:LQ:389:GLY:O	25:LQ:415:LYS:NZ	2.06	0.89
28:LT:579:ARG:NH1	28:LT:614:LEU:O	2.06	0.89
51:SI:267:ARG:HH12	51:SI:798:MET:HG2	1.36	0.89
16:LH:878:ASN:HD22	16:LH:890:ARG:HH12	1.21	0.88
27:LS:492:ASN:HD21	48:SE:89:ARG:HH12	1.21	0.88
2:L1:505:A:N1	35:NB:553:LYS:NZ	2.22	0.87
23:LO:36:ARG:NH2	23:LO:53:GLU:OE2	2.07	0.87
22:LN:374:THR:HB	22:LN:757:ARG:HH12	1.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SA:129:ARG:HD2	47:SC:322:ARG:HH12	1.40	0.86
1:L0:135:G:O2'	20:LL:494:ARG:NH1	2.07	0.86
29:LU:298:LEU:O	29:LU:457:ARG:NH1	2.08	0.86
1:L0:183:A:OP1	37:ND:172:LYS:NZ	2.09	0.85
29:LU:376:ARG:HH12	29:LU:382:ARG:HH11	1.24	0.85
47:SC:258:HIS:HD1	47:SC:320:TYR:HH	1.24	0.85
23:LO:62:ASP:OD2	23:LO:104:PHE:N	2.09	0.85
29:LU:303:ASP:OD2	29:LU:339:SER:N	2.07	0.85
2:L1:628:G:N1	2:L1:970:A:OP2	2.09	0.84
10:L9:149:ARG:NH2	36:NC:323:GLU:OE2	2.10	0.84
22:LN:476:LYS:NZ	22:LN:490:SER:O	2.10	0.84
2:L1:578:U:OP1	51:SI:1039:ARG:NH1	2.11	0.84
29:LU:33:HIS:NE2	31:LW:412:ASP:OD2	2.10	0.84
50:SH:228:ASP:OD2	50:SH:230:TRP:NE1	2.11	0.84
52:SK:101:ASP:OD2	52:SK:132:ARG:NH2	2.10	0.84
22:LN:97:ARG:HH12	37:ND:190:LEU:HB3	1.42	0.83
25:LQ:162:HIS:HE2	25:LQ:179:SER:HG	1.23	0.83
26:LR:742:ARG:NH1	34:NA:506:GLU:OE1	2.11	0.83
1:L0:220:U:OP1	37:ND:204:ARG:NH1	2.11	0.83
10:L9:53:ARG:NH1	10:L9:99:LEU:O	2.11	0.83
1:L0:89:C:OP1	27:LS:319:ARG:NH1	2.11	0.83
48:SF:106:ASP:OD1	48:SF:111:LYS:NZ	2.10	0.83
65:SY:114:GLU:OE2	65:SY:204:HIS:ND1	2.11	0.83
46:SB:290:LEU:O	46:SB:391:ARG:NH1	2.12	0.82
2:L1:540:G:O2'	2:L1:542:A:OP2	1.98	0.82
3:L2:112:U:OP1	48:SF:46:ARG:NH1	2.13	0.82
2:L1:1584:G:N2	2:L1:1611:A:OP2	2.13	0.81
2:L1:560:U:OP2	54:SM:282:ARG:NH2	2.11	0.81
2:L1:1464:G:O2'	54:SM:99:ARG:NH1	2.14	0.81
47:SC:109:LYS:NZ	58:SQ:103:TRP:O	2.13	0.81
18:LJ:356:ASN:OD1	18:LJ:359:ARG:NH1	2.13	0.80
2:L1:1192:C:OP2	52:SJ:129:ARG:NE	2.14	0.80
2:L1:104:A:OP2	2:L1:308:C:N4	2.15	0.80
16:LH:84:ASN:ND2	16:LH:780:GLU:OE2	2.14	0.80
3:L2:324:U:N3	46:SB:323:GLU:OE2	2.14	0.80
2:L1:349:U:OP2	12:LD:106:ASN:ND2	2.13	0.80
13:LE:92:ASN:O	53:SL:79:LYS:NZ	2.14	0.80
61:ST:548:ARG:NH1	61:ST:638:ASN:OD1	2.13	0.79
2:L1:1194:A:OP2	2:L1:1196:A:N6	2.15	0.79
16:LH:855:LEU:HD12	27:LS:477:LYS:HZ2	1.44	0.79
33:LZ:83:TYR:O	33:LZ:152:ARG:NH1	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:111:U:OP1	5:L4:221:ARG:NH1	2.16	0.79
2:L1:467:G:OP1	51:SI:191:LYS:NZ	2.14	0.79
13:LE:44:HIS:NE2	13:LE:112:ASP:OD2	2.16	0.79
46:SB:374:ASP:HA	46:SB:380:ARG:HH12	1.46	0.79
2:L1:103:A:OP2	2:L1:360:A:N6	2.13	0.79
31:LW:272:SER:O	31:LW:299:LYS:NZ	2.16	0.79
6:L5:95:ASN:OD1	6:L5:107:LYS:NZ	2.15	0.78
20:LL:109:ASP:OD2	20:LL:151:LEU:N	2.12	0.78
62:SU:279:LEU:HG	62:SU:357:ARG:HH12	1.47	0.78
22:LN:80:ASN:ND2	22:LN:88:GLU:OE2	2.16	0.78
9:L8:110:ARG:NH1	9:L8:160:PHE:O	2.15	0.78
49:SG:497:LYS:NZ	49:SG:513:GLU:OE2	2.16	0.78
1:L0:127:U:OP2	62:SU:245:GLN:NE2	2.16	0.78
20:LL:454:GLU:OE2	20:LL:487:ARG:NH1	2.17	0.78
29:LU:318:ASP:OD2	29:LU:333:LYS:NZ	2.16	0.77
5:L4:152:PRO:O	5:L4:155:LYS:NZ	2.17	0.77
27:LS:165:ARG:HH11	28:LT:218:LEU:HD23	1.48	0.77
24:LP:161:PHE:HZ	24:LP:195:LYS:HZ2	1.32	0.77
2:L1:1133:A:OP2	2:L1:1134:C:N4	2.18	0.77
2:L1:511:A:OP2	10:L9:176:ASN:ND2	2.16	0.76
3:L2:324:U:OP1	65:SY:116:LYS:NZ	2.18	0.76
12:LD:118:GLN:N	12:LD:121:ASP:OD2	2.12	0.76
1:L0:426:G:N2	1:L0:429:A:OP2	2.18	0.76
24:LP:173:ARG:NH2	45:SA:83:ASP:OD2	2.20	0.75
2:L1:20:G:O2'	2:L1:22:A:OP2	2.04	0.75
2:L1:368:U:H5	36:NC:231:ARG:HH12	1.35	0.75
21:LM:353:ARG:NE	21:LM:386:ASP:OD2	2.19	0.75
29:LU:403:ARG:HH11	60:SS:861:LEU:HA	1.50	0.75
16:LH:64:LYS:NZ	16:LH:123:GLY:O	2.16	0.75
20:LL:443:GLN:HE22	62:SU:333:GLU:H	1.34	0.75
1:L0:100:G:N7	18:LJ:25:ARG:NH2	2.36	0.74
50:SH:131:GLU:OE2	50:SH:156:ARG:NH2	2.20	0.74
17:LI:558:CYS:O	17:LI:585:ARG:NH1	2.21	0.74
22:LN:645:ARG:HH11	22:LN:656:ARG:CZ	2.01	0.74
29:LU:51:GLU:OE1	29:LU:401:LYS:NZ	2.21	0.74
61:ST:91:GLY:O	61:ST:95:ARG:NH1	2.21	0.73
10:L9:57:ARG:NH1	53:SL:84:ARG:O	2.22	0.73
2:L1:160:C:O2'	7:L6:95:LYS:NZ	2.21	0.73
65:SY:207:ARG:HH12	65:SY:211:LEU:HD23	1.52	0.73
2:L1:337:G:N2	2:L1:340:U:OP2	2.20	0.73
34:NA:365:LEU:HD13	54:SM:227:ARG:HH12	1.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:568:G:O3'	59:SR:114:LYS:NZ	2.22	0.73
16:LH:249:THR:O	16:LH:257:ARG:NH1	2.21	0.73
10:L9:82:ARG:NH2	36:NC:247:GLU:OE2	2.22	0.72
61:ST:563:GLU:OE2	62:SU:503:TYR:OH	2.07	0.72
9:L8:22:ARG:NH1	9:L8:28:GLU:OE1	2.23	0.72
25:LQ:480:ASP:OD2	25:LQ:539:VAL:N	2.13	0.72
51:SI:1059:ARG:NH2	65:SY:15:GLU:OE2	2.22	0.72
49:SG:190:VAL:HB	49:SG:239:ILE:HD13	1.72	0.72
2:L1:413:U:OP1	51:SI:345:LYS:NZ	2.23	0.72
24:LP:67:ARG:HH11	24:LP:80:THR:HG21	1.53	0.71
27:LS:159:HIS:HB3	27:LS:163:ARG:HH12	1.55	0.71
2:L1:487:G:OP1	51:SI:1126:LYS:NZ	2.20	0.71
23:LO:564:PHE:N	23:LO:567:ASP:OD2	2.23	0.71
50:SH:16:ASN:ND2	50:SH:328:ASP:OD2	2.23	0.71
2:L1:208:U:O2'	9:L8:180:ASP:OD2	2.07	0.71
16:LH:221:GLU:HG2	16:LH:242:GLY:HA3	1.70	0.71
51:SI:248:ARG:HB3	51:SI:357:PRO:HB2	1.71	0.71
1:L0:329:A:N6	31:LW:227:GLU:OE2	2.24	0.71
2:L1:498:G:OP1	53:SL:42:ARG:NH1	2.23	0.71
16:LH:551:HIS:H	16:LH:583:LYS:HZ2	1.35	0.71
20:LL:465:ILE:HG23	20:LL:501:TRP:HD1	1.56	0.71
5:L4:183:VAL:HB	5:L4:190:GLY:H	1.56	0.71
47:SC:155:ILE:HD11	47:SC:162:LEU:HD22	1.70	0.71
1:L0:307:C:H5'	27:LS:141:ASN:HD22	1.56	0.70
16:LH:852:ASP:OD1	27:LS:477:LYS:NZ	2.23	0.70
15:LG:31:GLU:OE2	15:LG:36:THR:OG1	2.06	0.70
5:L4:176:ASP:H	5:L4:179:LYS:NZ	1.90	0.70
21:LM:63:GLU:OE2	21:LM:108:LYS:NZ	2.24	0.70
28:LT:579:ARG:NH1	28:LT:615:PRO:O	2.24	0.70
48:SF:7:LYS:NZ	48:SF:62:GLU:OE2	2.24	0.70
20:LL:242:ASP:OD2	20:LL:320:ARG:NH1	2.25	0.70
29:LU:303:ASP:HB3	29:LU:330:ARG:NH1	2.05	0.70
61:ST:534:PHE:N	61:ST:594:ASP:OD2	2.21	0.70
3:L2:37:G:N3	31:LW:431:ARG:NH1	2.40	0.69
2:L1:472:U:O2'	36:NC:316:ARG:NH1	2.26	0.69
2:L1:318:U:O3'	9:L8:11:ARG:NH1	2.25	0.69
16:LH:296:HIS:ND1	16:LH:318:GLU:OE2	2.25	0.69
32:LX:34:ARG:HH11	32:LX:64:LEU:HG	1.57	0.69
49:SG:299:CYS:SG	49:SG:305:ARG:NH1	2.64	0.69
18:LJ:371:GLU:OE2	27:LS:273:ARG:NH2	2.24	0.69
61:ST:613:ILE:HG22	61:ST:615:PRO:HD3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:929:A:OP2	2:L1:931:C:N4	2.26	0.69
47:SD:264:GLN:HE21	47:SD:319:ARG:HE	1.41	0.69
54:SM:7:ARG:NH2	54:SM:11:GLU:OE2	2.26	0.69
25:LQ:144:ASN:HD22	25:LQ:158:LYS:HE3	1.58	0.69
62:SU:355:ARG:NH1	62:SU:393:SER:OG	2.26	0.68
18:LJ:430:ALA:O	18:LJ:434:ARG:NH1	2.27	0.68
50:SH:283:ILE:O	51:SI:634:ARG:NH1	2.27	0.68
29:LU:292:ARG:NH1	60:SS:299:ASN:HB2	2.07	0.68
52:SK:104:ILE:N	52:SK:246:GLU:OE2	2.27	0.68
29:LU:310:ASP:OD2	29:LU:353:GLN:NE2	2.27	0.68
36:NC:266:ILE:HG22	36:NC:274:ILE:HG23	1.75	0.68
22:LN:83:ASN:ND2	22:LN:588:ASP:OD1	2.26	0.68
2:L1:417:A:OP1	32:LX:113:LYS:NZ	2.27	0.67
29:LU:376:ARG:HH12	29:LU:382:ARG:NH1	1.92	0.67
45:SA:169:LYS:NZ	45:SA:394:GLU:OE1	2.28	0.67
1:L0:291:G:H21	28:LT:387:GLN:HE22	1.42	0.67
2:L1:440:U:H5’	2:L1:441:A:H5’	1.76	0.67
25:LQ:14:PHE:HB2	25:LQ:681:ILE:HB	1.75	0.67
2:L1:629:U:OP2	2:L1:969:C:N4	2.27	0.67
10:L9:29:LYS:NZ	53:SL:57:GLN:OE1	2.28	0.67
30:LV:66:ARG:HH12	30:LV:148:LYS:HZ1	1.40	0.67
47:SC:300:PRO:HA	47:SC:318:GLY:HA2	1.76	0.67
8:L7:139:ARG:HB2	8:L7:151:LYS:HB2	1.76	0.67
22:LN:145:TRP:HE1	22:LN:161:ASP:HB3	1.60	0.67
24:LP:21:LYS:NZ	24:LP:82:SER:OG	2.22	0.67
25:LQ:600:TRP:HA	25:LQ:607:CYS:HA	1.75	0.67
24:LP:195:LYS:NZ	60:SS:386:UNK:O	2.27	0.67
2:L1:158:U:O2’	2:L1:160:C:OP2	2.11	0.67
7:L6:2:LYS:HB2	7:L6:108:VAL:HG12	1.77	0.67
51:SI:291:ALA:HB1	51:SI:853:ARG:HH22	1.59	0.67
5:L4:104:ASP:OD2	49:SG:109:ALA:N	2.28	0.67
8:L7:17:GLU:OE2	8:L7:46:ILE:N	2.26	0.67
25:LQ:446:ILE:HD13	25:LQ:488:LEU:HD11	1.76	0.67
5:L4:79:ASP:HB3	5:L4:82:TYR:HB2	1.75	0.66
47:SC:99:ALA:HB3	47:SC:105:LEU:HB2	1.77	0.66
50:SH:17:PHE:N	51:SI:609:GLU:OE2	2.28	0.66
54:SM:100:LEU:HD22	54:SM:144:GLU:HG2	1.76	0.66
8:L7:85:PHE:HB3	8:L7:88:ARG:HD2	1.78	0.66
18:LJ:197:ASP:HB2	18:LJ:206:ILE:HD11	1.78	0.66
25:LQ:405:LEU:HB3	25:LQ:417:TRP:HB2	1.76	0.66
6:L5:166:ARG:HH12	15:LG:45:LYS:HE3	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:585:ARG:NE	17:LI:589:ASP:OD2	2.20	0.66
28:LT:51:VAL:HG12	28:LT:60:ILE:HG12	1.77	0.66
51:SI:368:LYS:NZ	51:SI:801:VAL:O	2.26	0.66
18:LJ:108:TYR:HB3	18:LJ:117:LEU:H	1.60	0.66
23:LO:53:GLU:HG3	23:LO:619:ARG:HE	1.61	0.66
5:L4:193:GLY:HA3	5:L4:210:ILE:HG23	1.78	0.66
52:SK:105:ASN:HD21	52:SK:126:PRO:HB3	1.61	0.66
1:L0:248:G:P	65:SY:82:ARG:HH12	2.18	0.66
2:L1:19:A:H5"	51:SI:1152:ARG:HE	1.61	0.66
2:L1:1601:G:O2'	54:SM:146:ARG:NH1	2.29	0.66
2:L1:5:U:O2	2:L1:7:G:N2	2.28	0.66
18:LJ:90:ARG:HH21	18:LJ:137:ASN:HB3	1.60	0.66
49:SG:446:PRO:HB2	49:SG:451:ILE:HD11	1.78	0.66
33:LZ:174:ARG:HH12	65:SY:58:ARG:HD2	1.61	0.66
45:SA:160:ARG:HD3	47:SC:212:LYS:HZ1	1.62	0.66
2:L1:1191:U:O2	52:SK:88:ARG:NH1	2.28	0.65
28:LT:632:VAL:HG12	28:LT:643:THR:HG22	1.78	0.65
1:L0:296:C:OP2	23:LO:94:ASN:ND2	2.29	0.65
20:LL:261:VAL:O	20:LL:273:LYS:NZ	2.27	0.65
25:LQ:473:ASP:N	25:LQ:494:ASP:OD2	2.22	0.65
51:SI:87:ARG:NH1	51:SI:213:GLY:O	2.25	0.65
2:L1:498:G:OP1	35:NB:599:LYS:NZ	2.29	0.65
49:SG:304:ILE:HB	49:SG:318:LEU:HB2	1.77	0.65
55:SN:60:THR:HG23	55:SN:61:LYS:HG2	1.79	0.65
22:LN:392:VAL:HG22	22:LN:401:ILE:HG12	1.79	0.65
27:LS:361:ALA:HB2	27:LS:409:ILE:HD13	1.79	0.65
52:SJ:54:LYS:NZ	52:SJ:63:ASP:OD2	2.23	0.65
16:LH:302:SER:OG	16:LH:343:ASP:OD1	2.14	0.65
45:SA:160:ARG:HD3	47:SC:212:LYS:NZ	2.11	0.65
46:SB:286:ASN:HD22	46:SB:387:GLY:H	1.45	0.65
27:LS:492:ASN:HD21	48:SE:89:ARG:NH1	1.94	0.65
6:L5:92:ARG:NH2	6:L5:169:ASN:OD1	2.30	0.65
31:LW:194:ARG:H	31:LW:209:GLY:HA2	1.62	0.65
55:SN:58:PRO:HA	55:SN:186:ASN:HD22	1.60	0.65
18:LJ:377:ASP:OD2	27:LS:322:HIS:NE2	2.29	0.64
51:SI:168:LEU:HD11	51:SI:226:PHE:HB3	1.79	0.64
51:SI:890:CYS:SG	51:SI:891:SER:N	2.69	0.64
2:L1:400:A:OP2	9:L8:25:ARG:NH2	2.30	0.64
30:LV:258:ARG:HH11	32:LY:511:UNK:HA	1.63	0.64
27:LS:148:THR:N	27:LS:152:GLU:OE2	2.21	0.64
29:LU:235:LEU:HB3	29:LU:247:TYR:HB2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1471:A:N1	6:L5:102:ARG:NH1	2.34	0.64
5:L4:176:ASP:H	5:L4:179:LYS:HZ3	1.45	0.64
29:LU:371:ASN:ND2	53:SL:107:GLU:OE2	2.29	0.64
31:LW:133:HIS:HE1	31:LW:147:GLU:OE2	1.79	0.64
52:SK:104:ILE:HG23	52:SK:110:LEU:HD22	1.80	0.64
60:SS:312:ILE:HA	60:SS:884:MET:HB2	1.79	0.64
27:LS:20:GLN:HG2	27:LS:24:LYS:NZ	2.13	0.64
30:LV:112:THR:HA	30:LV:128:LYS:NZ	2.13	0.64
51:SI:114:ARG:HH11	51:SI:310:THR:HG23	1.62	0.64
50:SH:66:GLU:HB2	50:SH:75:ILE:HB	1.78	0.64
31:LW:150:LEU:HD13	31:LW:170:GLN:HE22	1.62	0.64
31:LW:357:SER:HA	31:LW:364:ARG:HD3	1.80	0.64
51:SI:935:VAL:HG12	51:SI:1002:ILE:HG22	1.80	0.64
16:LH:545:THR:HG21	16:LH:594:TRP:H	1.63	0.63
45:SA:129:ARG:NH1	47:SC:261:LEU:O	2.31	0.63
61:ST:548:ARG:HH12	61:ST:613:ILE:HD13	1.63	0.63
8:L7:30:SER:HB2	8:L7:34:LEU:HB2	1.78	0.63
18:LJ:474:LEU:HD11	18:LJ:484:MET:HG3	1.79	0.63
18:LJ:492:ARG:NH2	20:LL:548:ASP:OD2	2.31	0.63
36:NC:341:ARG:HH22	36:NC:346:THR:H	1.45	0.63
51:SI:938:PRO:HD2	65:SY:22:ARG:HH12	1.64	0.63
18:LJ:127:THR:HA	18:LJ:144:SER:HA	1.81	0.63
23:LO:131:ARG:HB3	28:LT:655:THR:HG21	1.80	0.63
25:LQ:588:ILE:HB	25:LQ:600:TRP:HB2	1.79	0.63
28:LT:392:ARG:CZ	28:LT:449:ARG:HH12	2.11	0.63
1:L0:490:G:N7	24:LP:90:GLN:NE2	2.46	0.63
23:LO:430:ARG:HB3	34:NA:458:PRO:HB2	1.81	0.63
28:LT:143:SER:OG	28:LT:147:ASP:OD2	2.17	0.63
29:LU:254:PRO:HG3	60:SS:284:ARG:HH11	1.63	0.63
2:L1:122:U:H4'	5:L4:77:ARG:HH22	1.63	0.63
10:L9:108:ARG:HH21	10:L9:145:SER:HB2	1.63	0.63
52:SJ:190:GLN:NE2	52:SJ:247:ASP:OD2	2.31	0.63
52:SK:114:ILE:HB	52:SK:122:ILE:HB	1.81	0.63
58:SQ:127:ARG:HA	58:SQ:130:LEU:HD13	1.81	0.63
54:SM:100:LEU:HD13	54:SM:144:GLU:HB3	1.80	0.63
16:LH:680:ALA:HB1	16:LH:749:ASP:HB2	1.81	0.63
23:LO:359:ARG:HH12	34:NA:484:MET:HB2	1.63	0.63
23:LO:430:ARG:HG3	34:NA:460:PRO:HA	1.79	0.63
23:LO:717:LEU:O	28:LT:576:ARG:NH2	2.31	0.63
33:LZ:62:SER:HA	33:LZ:71:ARG:HH21	1.63	0.63
49:SG:157:LEU:HD11	49:SG:189:THR:HB	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SG:303:LYS:HG2	49:SG:319:TYR:HE1	1.62	0.63
62:SU:353:LYS:HE3	64:SX:3219:UNK:HA	1.80	0.63
2:L1:368:U:H3	2:L1:377:G:H1	1.45	0.63
2:L1:369:A:P	5:L4:22:LYS:HZ3	2.22	0.63
2:L1:122:U:H5"	5:L4:77:ARG:HH12	1.62	0.63
2:L1:514:G:O6	2:L1:543:C:N4	2.31	0.63
16:LH:322:SER:HA	16:LH:333:PHE:HB3	1.81	0.63
20:LL:254:GLU:OE2	20:LL:278:LYS:NZ	2.21	0.63
20:LL:438:THR:HG22	20:LL:468:THR:HA	1.80	0.63
31:LW:128:THR:HG22	31:LW:134:VAL:HG22	1.81	0.63
50:SH:321:ARG:HH12	51:SI:613:PRO:HB3	1.64	0.62
12:LD:71:LEU:HB3	12:LD:88:ARG:HH12	1.64	0.62
18:LJ:213:GLN:NE2	18:LJ:233:ASN:OD1	2.32	0.62
49:SG:146:LYS:NZ	49:SG:205:SER:HA	2.14	0.62
8:L7:62:VAL:HG12	8:L7:64:VAL:H	1.64	0.62
9:L8:7:SER:HA	9:L8:10:LYS:HZ3	1.64	0.62
25:LQ:538:ARG:NH1	25:LQ:580:ASP:OD1	2.32	0.62
27:LS:159:HIS:HB3	27:LS:163:ARG:NH1	2.14	0.62
52:SJ:85:SER:HB3	52:SJ:211:ARG:NH1	2.14	0.62
22:LN:434:SER:HB3	22:LN:483:ASN:HD22	1.64	0.62
26:LR:565:UNK:HA	26:LR:578:UNK:HA	1.81	0.62
31:LW:178:ASP:OD1	31:LW:179:HIS:ND1	2.32	0.62
51:SI:944:ASN:ND2	51:SI:991:PHE:O	2.33	0.62
2:L1:324:U:OP1	12:LD:133:LYS:NZ	2.30	0.62
22:LN:135:ARG:NH1	22:LN:177:LEU:H	1.98	0.62
30:LV:199:THR:HB	30:LV:203:VAL:H	1.65	0.62
31:LW:298:MET:HB3	31:LW:312:VAL:HB	1.80	0.62
2:L1:338:C:OP2	9:L8:10:LYS:HE3	1.99	0.62
13:LE:105:THR:HB	13:LE:124:LYS:HB2	1.82	0.62
3:L2:59:G:H5'	23:LO:570:THR:HG23	1.80	0.62
3:L2:100:U:O3'	47:SD:138:LYS:NZ	2.32	0.62
22:LN:497:ILE:HD12	22:LN:558:ARG:HH12	1.64	0.62
49:SG:232:THR:OG1	49:SG:259:LYS:NZ	2.26	0.62
53:SL:132:HIS:HE1	53:SL:140:CYS:SG	2.23	0.62
23:LO:656:ARG:NH1	31:LW:210:GLU:OE1	2.33	0.61
29:LU:76:ASN:ND2	29:LU:94:TYR:OH	2.33	0.61
31:LW:266:PRO:O	60:SS:832:ASN:ND2	2.33	0.61
47:SD:142:ARG:NH1	47:SD:182:SER:O	2.22	0.61
2:L1:992:A:OP2	2:L1:1011:G:N1	2.32	0.61
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.08	0.61
30:LV:179:ASP:HB2	30:LV:214:ARG:HH12	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LU:391:LYS:NZ	29:LU:395:GLU:OE2	2.32	0.61
31:LW:178:ASP:OD2	53:SL:24:ARG:NH1	2.23	0.61
41:NH:578:ILE:HA	41:NH:619:VAL:HA	1.81	0.61
7:L6:70:PRO:HB3	7:L6:101:ILE:HB	1.83	0.61
29:LU:83:LEU:HD21	29:LU:364:ILE:HG21	1.82	0.61
47:SD:257:SER:HA	47:SD:261:LEU:HD23	1.82	0.61
18:LJ:74:ILE:HG22	18:LJ:75:LYS:HG3	1.81	0.61
22:LN:263:LYS:NZ	22:LN:275:SER:OG	2.33	0.61
23:LO:247:SER:H	23:LO:249:ARG:NH1	1.99	0.61
24:LP:11:CYS:SG	24:LP:36:ARG:NH2	2.74	0.61
29:LU:299:ASN:OD1	29:LU:457:ARG:NH1	2.28	0.61
47:SD:155:ILE:HD11	47:SD:162:LEU:HD22	1.81	0.61
51:SI:867:THR:HG22	59:SR:62:LYS:NZ	2.15	0.61
13:LE:87:GLU:OE2	13:LE:97:ARG:NH2	2.33	0.61
18:LJ:233:ASN:ND2	18:LJ:247:GLU:OE2	2.31	0.61
22:LN:252:GLN:HA	22:LN:266:ASP:HA	1.82	0.61
25:LQ:88:HIS:HD2	25:LQ:91:THR:H	1.46	0.61
16:LH:141:LEU:HA	16:LH:155:THR:HG22	1.82	0.61
23:LO:472:HIS:ND1	23:LO:492:SER:OG	2.33	0.61
26:LR:110:UNK:HA	26:LR:126:UNK:HA	1.83	0.61
52:SK:46:ALA:HA	52:SK:115:GLN:HB3	1.81	0.61
26:LR:455:UNK:HA	26:LR:471:UNK:HA	1.83	0.61
55:SN:23:GLN:OE1	55:SN:27:ASN:ND2	2.34	0.61
1:L0:444:U:O2	58:SQ:195:GLN:NE2	2.33	0.61
22:LN:383:LEU:HD21	22:LN:432:SER:HA	1.83	0.61
1:L0:166:U:OP1	22:LN:230:LYS:NZ	2.29	0.61
6:L5:166:ARG:NH1	15:LG:45:LYS:HE3	2.16	0.61
29:LU:129:ASP:OD2	29:LU:158:LYS:NZ	2.33	0.61
25:LQ:10:GLN:HE22	25:LQ:682:ARG:NH1	1.98	0.60
26:LR:353:UNK:HA	26:LR:364:UNK:HA	1.83	0.60
2:L1:593:U:H4'	2:L1:595:G:H4'	1.82	0.60
6:L5:100:ASN:HD22	6:L5:180:ARG:HH11	1.49	0.60
23:LO:155:SER:OG	23:LO:203:GLN:NE2	2.33	0.60
23:LO:582:THR:HG21	23:LO:683:SER:HA	1.83	0.60
33:LZ:61:LEU:HB3	33:LZ:75:GLU:OE2	2.01	0.60
51:SI:1098:ARG:NH1	65:SY:102:GLN:OE1	2.34	0.60
12:LD:124:THR:HB	12:LD:141:LYS:HB3	1.84	0.60
20:LL:85:ILE:HB	20:LL:99:PHE:HB2	1.83	0.60
52:SK:68:LEU:HD21	52:SK:77:LEU:HD21	1.83	0.60
55:SN:242:ILE:HG13	55:SN:254:ILE:HG23	1.82	0.60
22:LN:265:TRP:HA	22:LN:272:LEU:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC:154:GLY:HA3	47:SC:315:ILE:HD11	1.84	0.60
5:L4:100:ARG:NH2	5:L4:118:GLU:O	2.34	0.60
30:LV:321:GLU:HB3	30:LV:330:PHE:HB2	1.82	0.60
51:SI:235:LEU:HD22	51:SI:238:ARG:NH1	2.16	0.60
52:SJ:46:ALA:HA	52:SJ:115:GLN:HB3	1.83	0.60
1:L0:207:G:H5"	37:ND:174:GLY:HA3	1.83	0.60
2:L1:325:G:H2'	2:L1:326:G:H8	1.66	0.60
5:L4:106:LYS:CB	5:L4:108:ARG:HH11	2.15	0.60
16:LH:58:GLU:OE2	27:LS:338:LYS:NZ	2.33	0.60
18:LJ:16:LEU:HD13	18:LJ:454:ARG:HH11	1.64	0.60
22:LN:401:ILE:HB	22:LN:418:CYS:HB2	1.83	0.60
25:LQ:359:SER:HB3	25:LQ:391:ARG:HG2	1.83	0.60
25:LQ:476:ILE:HA	25:LQ:492:SER:HA	1.82	0.60
51:SI:249:PHE:HZ	51:SI:801:VAL:HG22	1.65	0.60
55:SN:123:ASP:HA	55:SN:149:LYS:NZ	2.15	0.60
61:ST:482:GLN:NE2	62:SU:504:ASP:OD1	2.34	0.60
65:SY:167:THR:HG22	65:SY:169:ASP:H	1.67	0.60
18:LJ:428:ARG:NH2	18:LJ:468:GLU:OE2	2.35	0.60
23:LO:670:LEU:HD21	23:LO:677:PRO:HG3	1.83	0.60
29:LU:376:ARG:NH1	29:LU:382:ARG:HH11	1.95	0.60
50:SH:308:ILE:HG21	51:SI:768:GLU:HG2	1.84	0.60
51:SI:866:ARG:NH1	59:SR:69:ARG:NH1	2.50	0.60
51:SI:1094:TYR:OH	65:SY:103:ASP:OD2	2.18	0.60
16:LH:878:ASN:ND2	16:LH:890:ARG:HH12	1.97	0.60
25:LQ:15:GLY:O	25:LQ:360:ASN:ND2	2.35	0.60
35:NB:547:ASN:HB2	51:SI:193:ARG:HH22	1.65	0.60
2:L1:1159:C:H5'	54:SM:105:LYS:NZ	2.17	0.60
17:LI:261:UNK:HA	17:LI:271:UNK:HA	1.84	0.60
28:LT:22:LYS:HG3	28:LT:23:ILE:HD12	1.83	0.60
48:SF:57:ASP:O	48:SF:84:ARG:NH1	2.35	0.60
52:SJ:88:ARG:HH22	52:SK:132:ARG:HD3	1.66	0.60
5:L4:185:GLY:H	5:L4:189:LEU:HD13	1.67	0.59
20:LL:49:ASN:HB3	20:LL:93:ASN:HD21	1.67	0.59
2:L1:338:C:H5'	9:L8:10:LYS:NZ	2.17	0.59
2:L1:1642:G:OP2	34:NA:530:ARG:NH2	2.35	0.59
29:LU:73:ILE:HG12	29:LU:85:THR:HG22	1.83	0.59
29:LU:376:ARG:NH1	29:LU:382:ARG:NH1	2.50	0.59
50:SH:119:LYS:HG2	50:SH:165:GLU:HG2	1.84	0.59
2:L1:1262:U:H5"	61:ST:419:LYS:HE2	1.84	0.59
23:LO:156:GLN:HE22	23:LO:201:HIS:HA	1.67	0.59
27:LS:144:LYS:HG2	27:LS:147:ARG:HE	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SE:79:VAL:HG13	48:SE:121:ILE:HG23	1.84	0.59
20:LL:281:ILE:HG12	20:LL:328:VAL:HB	1.84	0.59
10:L9:143:ILE:HD13	36:NC:270:GLY:HA3	1.85	0.59
23:LO:617:VAL:HG23	23:LO:702:LEU:HD11	1.83	0.59
38:NE:108:UNK:O	38:NE:113:UNK:N	2.36	0.59
49:SG:206:LYS:O	49:SG:538:ARG:NH2	2.35	0.59
52:SJ:44:VAL:HG22	52:SJ:113:TYR:HB2	1.84	0.59
60:SS:855:GLU:OE2	60:SS:859:ARG:NE	2.35	0.59
2:L1:1177:C:H5	61:ST:753:LYS:HZ3	1.51	0.59
23:LO:796:LEU:HB3	28:LT:925:LEU:HD12	1.84	0.59
29:LU:1:MET:N	31:LW:77:GLU:OE1	2.35	0.59
46:SB:347:LEU:HD23	46:SB:363:LEU:HD21	1.83	0.59
1:L0:323:A:OP1	23:LO:191:ARG:NH1	2.36	0.59
2:L1:323:A:OP2	9:L8:11:ARG:N	2.22	0.59
6:L5:97:LEU:O	6:L5:180:ARG:NH2	2.35	0.59
4:L3:27:LYS:HE3	4:L3:55:HIS:HA	1.85	0.59
21:LM:25:ARG:HH11	29:LU:16:VAL:HA	1.68	0.59
21:LM:43:GLN:HE21	21:LM:123:ARG:NH1	1.96	0.59
23:LO:23:SER:HB3	23:LO:28:GLN:HB2	1.85	0.59
1:L0:311:C:N4	27:LS:141:ASN:OD1	2.36	0.59
2:L1:468:A:O4'	51:SI:188:LYS:NZ	2.28	0.59
16:LH:710:LEU:HD22	16:LH:722:LEU:HD12	1.85	0.59
28:LT:242:ARG:HH12	28:LT:281:ARG:HE	1.51	0.59
30:LV:66:ARG:HH12	30:LV:148:LYS:NZ	2.00	0.59
54:SM:224:PHE:HB3	54:SM:231:ILE:HD11	1.84	0.59
62:SU:141:UNK:HA	62:SU:244:PRO:HB3	1.85	0.59
29:LU:260:GLN:NE2	29:LU:289:TYR:OH	2.35	0.59
54:SM:123:VAL:HG23	54:SM:126:ASN:H	1.67	0.59
3:L2:326:U:OP1	65:SY:108:ARG:NH2	2.36	0.58
16:LH:630:LEU:HB2	16:LH:653:PHE:HB2	1.84	0.58
18:LJ:431:LEU:HD12	18:LJ:434:ARG:HG3	1.84	0.58
23:LO:453:PHE:HB3	23:LO:475:PRO:HA	1.83	0.58
24:LP:47:GLY:O	29:LU:17:LYS:NZ	2.36	0.58
52:SK:188:ARG:NH1	52:SK:190:GLN:HB2	2.17	0.58
62:SU:279:LEU:HG	62:SU:357:ARG:NH1	2.18	0.58
3:L2:256:G:OP1	45:SA:382:LYS:NZ	2.34	0.58
11:LC:99:GLU:H	28:LT:490:GLN:HG3	1.68	0.58
22:LN:488:ILE:HB	22:LN:496:PHE:HB2	1.83	0.58
27:LS:263:LEU:HB2	27:LS:277:ILE:HD11	1.84	0.58
47:SC:85:LYS:HZ3	58:SQ:171:SER:N	2.02	0.58
48:SE:46:ARG:HH12	65:SY:108:ARG:NH2	2.01	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:87:C:OP1	18:LJ:5:ARG:NH1	2.36	0.58
6:L5:76:ARG:NH2	11:LC:120:ASP:OD1	2.36	0.58
22:LN:162:ASN:HB2	22:LN:164:THR:HG22	1.85	0.58
27:LS:165:ARG:NH1	28:LT:218:LEU:HD23	2.17	0.58
28:LT:176:TYR:HB3	28:LT:179:LYS:HB2	1.84	0.58
33:LZ:24:ASP:OD2	33:LZ:27:HIS:NE2	2.37	0.58
38:NE:224:HIS:ND1	38:NE:226:ASP:OD1	2.35	0.58
1:L0:308:A:H5"	1:L0:309:A:H5"	1.85	0.58
1:L0:316:U:OP1	31:LW:364:ARG:NH2	2.36	0.58
11:LC:98:ASP:N	11:LC:98:ASP:OD1	2.33	0.58
12:LD:17:PRO:HG3	12:LD:63:LEU:HD11	1.85	0.58
16:LH:610:SER:HB3	16:LH:704:ASN:HB2	1.84	0.58
18:LJ:125:HIS:HB3	18:LJ:145:ASP:HB3	1.85	0.58
27:LS:237:ARG:HH12	27:LS:561:PRO:HG2	1.68	0.58
47:SC:142:ARG:NH1	47:SC:186:ASP:OD2	2.35	0.58
52:SK:44:VAL:HG22	52:SK:113:TYR:HB2	1.85	0.58
21:LM:318:LYS:HE2	27:LS:203:GLY:HA2	1.84	0.58
30:LV:162:LEU:HB3	30:LV:176:PHE:HB2	1.85	0.58
33:LZ:61:LEU:HD13	33:LZ:75:GLU:HG3	1.85	0.58
47:SD:111:MET:SD	47:SD:216:ASN:ND2	2.76	0.58
53:SL:56:ASN:ND2	53:SL:169:GLY:O	2.36	0.58
2:L1:1615:C:N4	6:L5:80:LYS:O	2.36	0.58
23:LO:841:ASP:OD1	25:LQ:903:GLN:NE2	2.37	0.58
28:LT:311:VAL:HG22	28:LT:321:GLU:HG2	1.86	0.58
28:LT:627:ASN:ND2	28:LT:647:THR:OG1	2.36	0.58
31:LW:240:GLN:HA	31:LW:247:MET:HG2	1.85	0.58
32:LX:22:GLN:HG2	32:LX:480:UNK:HA	1.85	0.58
49:SG:240:LEU:HD23	49:SG:284:LEU:HA	1.86	0.58
51:SI:889:LEU:HG	51:SI:922:ILE:HG21	1.84	0.58
2:L1:512:A:OP2	10:L9:173:ALA:N	2.35	0.58
15:LG:62:GLU:OE2	25:LQ:825:PRO:HB3	2.04	0.58
23:LO:411:VAL:HG13	23:LO:425:PHE:HB2	1.85	0.58
25:LQ:203:HIS:HD2	25:LQ:207:CYS:HB3	1.69	0.58
59:SR:56:LYS:HB3	59:SR:59:ILE:HD11	1.86	0.58
16:LH:437:THR:HB	16:LH:709:ARG:HD2	1.85	0.58
17:LI:140:UNK:HA	17:LI:164:UNK:HA	1.86	0.58
20:LL:123:SER:O	20:LL:141:ARG:NH2	2.37	0.58
21:LM:82:ASP:OD1	21:LM:83:ARG:N	2.37	0.58
25:LQ:666:ALA:HB3	25:LQ:670:GLY:H	1.68	0.58
8:L7:141:ARG:HH12	8:L7:151:LYS:NZ	2.02	0.58
52:SJ:150:ILE:HB	52:SJ:160:LEU:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:445:A:H62	2:L1:461:G:H21	1.52	0.58
2:L1:1529:C:OP2	6:L5:112:ARG:NH2	2.36	0.58
24:LP:170:ASN:HD22	24:LP:173:ARG:NH1	2.01	0.58
51:SI:140:LEU:HD11	51:SI:152:THR:HG23	1.85	0.58
2:L1:53:G:OP1	51:SI:92:ARG:NH2	2.36	0.57
4:L3:53:ASP:HB3	4:L3:56:LYS:HG3	1.86	0.57
5:L4:136:VAL:HG21	5:L4:148:ARG:NH1	2.19	0.57
22:LN:111:SER:HA	22:LN:524:LYS:HA	1.86	0.57
28:LT:242:ARG:HH12	28:LT:281:ARG:NE	2.01	0.57
54:SM:131:CYS:HG	54:SM:136:THR:HG1	1.48	0.57
2:L1:627:C:H42	2:L1:972:G:H1	1.51	0.57
18:LJ:213:GLN:NE2	18:LJ:230:GLY:O	2.37	0.57
27:LS:429:TYR:OH	27:LS:448:LYS:NZ	2.28	0.57
29:LU:26:ARG:NH1	60:SS:867:GLN:O	2.37	0.57
16:LH:45:ILE:HG12	16:LH:54:VAL:HG22	1.86	0.57
16:LH:289:GLN:NE2	22:LN:310:ASN:OD1	2.36	0.57
21:LM:243:ALA:HB2	27:LS:208:LEU:HD12	1.86	0.57
22:LN:186:GLN:NE2	22:LN:205:CYS:SG	2.78	0.57
27:LS:436:ASP:OD2	27:LS:439:LYS:HE2	2.03	0.57
3:L2:60:A:OP2	23:LO:563:ARG:NH2	2.36	0.57
18:LJ:11:SER:H	18:LJ:416:THR:HG22	1.67	0.57
19:LK:412:UNK:HA	19:LK:451:LEU:HD23	1.84	0.57
20:LL:454:GLU:OE1	20:LL:494:ARG:NH2	2.37	0.57
28:LT:241:ILE:HG22	28:LT:242:ARG:HG3	1.86	0.57
28:LT:849:ILE:HD12	28:LT:887:LEU:HD23	1.87	0.57
29:LU:347:ARG:O	29:LU:373:ARG:NH2	2.38	0.57
32:LX:6:ILE:HD12	51:SI:371:VAL:HG13	1.86	0.57
35:NB:548:LYS:HA	59:SR:139:LYS:NZ	2.18	0.57
40:NG:87:GLY:H	40:NG:92:LYS:HA	1.68	0.57
11:LC:39:VAL:O	11:LC:45:ARG:NH2	2.33	0.57
12:LD:71:LEU:HB3	12:LD:88:ARG:NH1	2.18	0.57
20:LL:167:SER:O	20:LL:168:HIS:ND1	2.37	0.57
20:LL:436:THR:OG1	20:LL:471:ARG:NH2	2.37	0.57
22:LN:149:ILE:HD13	22:LN:153:GLN:HG3	1.86	0.57
33:LZ:109:ARG:HH12	33:LZ:155:GLU:HG3	1.68	0.57
51:SI:74:VAL:HG12	51:SI:139:LEU:HB2	1.87	0.57
2:L1:1132:A:O3'	50:SH:231:ARG:NH2	2.37	0.57
18:LJ:188:SER:OG	18:LJ:194:ARG:NH2	2.37	0.57
22:LN:541:ALA:HB3	22:LN:553:LEU:HB2	1.86	0.57
25:LQ:255:ARG:NH1	25:LQ:257:LEU:HD11	2.19	0.57
25:LQ:604:PHE:HD2	50:SH:239:PRO:HG2	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SA:176:GLN:OE1	46:SB:183:ARG:NH1	2.37	0.57
58:SQ:180:ASP:OD1	58:SQ:181:GLU:N	2.38	0.57
2:L1:156:A:OP2	32:LX:107:TYR:OH	2.22	0.57
16:LH:551:HIS:H	16:LH:583:LYS:NZ	2.02	0.57
18:LJ:227:VAL:HG22	18:LJ:236:VAL:HG12	1.86	0.57
20:LL:437:VAL:H	20:LL:468:THR:HG22	1.70	0.57
22:LN:79:TRP:HH2	22:LN:376:GLU:HG3	1.69	0.57
22:LN:121:THR:HG21	47:SD:288:ARG:HE	1.68	0.57
25:LQ:177:LEU:HB2	25:LQ:189:TRP:HB2	1.86	0.57
51:SI:242:PRO:HG2	51:SI:814:GLY:HA3	1.86	0.57
2:L1:579:A:H62	35:NB:528:LEU:HD11	1.70	0.57
8:L7:81:LEU:HB3	8:L7:90:VAL:HG21	1.86	0.57
16:LH:559:LYS:HE2	16:LH:708:ASP:OD2	2.05	0.57
23:LO:275:LEU:HG	23:LO:289:LEU:HD21	1.87	0.57
23:LO:523:MET:HG2	23:LO:530:VAL:HG22	1.86	0.57
24:LP:199:ARG:NH1	60:SS:356:UNK:O	2.37	0.57
28:LT:723:LEU:HD22	28:LT:879:GLU:HB2	1.87	0.57
31:LW:88:GLN:HE22	31:LW:402:ILE:H	1.53	0.57
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.37	0.57
22:LN:645:ARG:HH12	22:LN:731:HIS:CE1	2.23	0.57
23:LO:790:GLN:NE2	28:LT:713:LEU:O	2.38	0.57
26:LR:787:PRO:HG3	34:NA:495:ILE:HD11	1.86	0.57
28:LT:53:CYS:HB3	28:LT:83:LEU:HD11	1.87	0.57
2:L1:372:G:N2	10:L9:72:GLU:OE2	2.32	0.57
2:L1:573:C:O2'	51:SI:870:ARG:NH2	2.38	0.57
15:LG:29:ARG:NH1	15:LG:39:THR:HG21	2.20	0.57
29:LU:420:PRO:HD2	29:LU:423:ILE:HD12	1.87	0.57
30:LV:116:HIS:NE2	30:LV:126:GLN:OE1	2.37	0.57
20:LL:241:ALA:HB1	20:LL:260:LEU:HD23	1.86	0.56
29:LU:315:PRO:HG2	29:LU:360:SER:HB3	1.86	0.56
2:L1:1579:U:O2'	54:SM:102:GLN:NE2	2.37	0.56
17:LI:262:UNK:O	17:LI:270:UNK:N	2.38	0.56
23:LO:10:LEU:HD13	23:LO:702:LEU:HD23	1.87	0.56
25:LQ:171:CYS:SG	25:LQ:172:GLN:N	2.79	0.56
26:LR:346:UNK:HA	26:LR:352:UNK:HA	1.87	0.56
32:LY:517:UNK:HA	32:LY:565:UNK:HA	1.85	0.56
2:L1:862:A:O2'	2:L1:963:A:N6	2.37	0.56
3:L2:84:U:OP2	46:SB:361:ARG:NH2	2.39	0.56
14:LF:13:ILE:HG23	14:LF:22:GLN:HB2	1.86	0.56
18:LJ:253:LYS:HE2	62:SU:333:GLU:HB3	1.86	0.56
20:LL:60:VAL:HG22	20:LL:80:MET:HE1	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:97:ARG:NH1	37:ND:190:LEU:HB3	2.17	0.56
25:LQ:656:HIS:ND1	25:LQ:676:SER:OG	2.38	0.56
27:LS:142:LYS:HE3	46:SB:431:ALA:HB2	1.85	0.56
28:LT:517:MET:HB3	28:LT:529:TYR:HB2	1.87	0.56
29:LU:46:ASN:ND2	31:LW:434:LEU:O	2.39	0.56
47:SC:87:VAL:HG22	58:SQ:149:ILE:HG12	1.88	0.56
52:SJ:158:LYS:HE3	52:SJ:161:LYS:HE2	1.86	0.56
2:L1:364:G:H1	2:L1:380:U:H3	1.52	0.56
2:L1:473:A:N3	36:NC:271:ARG:NH1	2.52	0.56
16:LH:614:ALA:HB1	16:LH:664:LEU:HD22	1.86	0.56
18:LJ:75:LYS:HD3	18:LJ:113:PRO:HD3	1.86	0.56
21:LM:194:SER:HB3	28:LT:335:VAL:HG11	1.87	0.56
47:SD:197:VAL:HA	47:SD:220:ILE:HB	1.86	0.56
2:L1:418:G:O2'	7:L6:72:ARG:NH2	2.39	0.56
6:L5:118:LEU:HD22	6:L5:129:PRO:HB2	1.87	0.56
49:SG:235:HIS:NE2	49:SG:253:THR:OG1	2.35	0.56
22:LN:744:VAL:HG22	22:LN:754:ILE:HA	1.87	0.56
23:LO:518:VAL:HG12	23:LO:534:THR:HG22	1.87	0.56
25:LQ:426:ARG:NH1	25:LQ:459:LEU:O	2.39	0.56
25:LQ:764:GLU:HG2	25:LQ:834:LYS:NZ	2.21	0.56
44:NK:53:LEU:O	44:NK:57:TRP:N	2.38	0.56
2:L1:332:U:OP1	9:L8:56:ARG:NH1	2.31	0.56
2:L1:1133:A:H4'	50:SH:199:ARG:HH11	1.71	0.56
23:LO:105:SER:HB2	23:LO:108:GLY:H	1.69	0.56
23:LO:804:SER:HB2	26:LR:811:VAL:HG11	1.87	0.56
30:LV:207:TRP:HA	30:LV:214:ARG:HA	1.86	0.56
51:SI:364:VAL:HG12	51:SI:373:ILE:HG12	1.88	0.56
51:SI:1109:ALA:O	58:SQ:119:ARG:NH2	2.38	0.56
52:SJ:121:LEU:HD11	52:SJ:167:ILE:HD13	1.88	0.56
55:SN:181:ARG:HH12	63:SV:203:SER:HB3	1.70	0.56
16:LH:73:LEU:HD13	16:LH:129:PRO:HD2	1.87	0.56
51:SI:855:GLN:HE22	51:SI:1032:LEU:H	1.52	0.56
2:L1:306:U:H2'	2:L1:307:G:H8	1.70	0.56
2:L1:1629:G:H1'	2:L1:1631:A:H62	1.71	0.56
17:LI:69:UNK:HA	17:LI:79:UNK:HA	1.87	0.56
18:LJ:107:VAL:HG13	18:LJ:118:LEU:HB3	1.87	0.56
23:LO:360:VAL:HG23	23:LO:374:ILE:HD11	1.88	0.56
25:LQ:629:ASN:ND2	25:LQ:643:ASP:OD1	2.39	0.56
51:SI:114:ARG:NH1	51:SI:310:THR:HG23	2.21	0.56
2:L1:332:U:OP2	9:L8:56:ARG:NH2	2.32	0.56
2:L1:576:G:OP2	51:SI:873:LYS:NZ	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L2:60:A:N7	23:LO:563:ARG:NH1	2.51	0.56
16:LH:509:THR:HB	16:LH:530:LYS:HB2	1.88	0.56
31:LW:178:ASP:OD1	31:LW:179:HIS:N	2.39	0.56
35:NB:521:ARG:NH2	51:SI:1044:LEU:O	2.36	0.56
47:SC:263:ASP:OD1	47:SC:264:GLN:N	2.39	0.56
49:SG:198:LYS:HD2	49:SG:268:LEU:HD23	1.88	0.56
51:SI:830:ARG:HH22	51:SI:833:ARG:HB3	1.71	0.56
51:SI:907:THR:HG21	51:SI:912:ARG:NH1	2.20	0.56
2:L1:1132:A:H62	25:LQ:598:LYS:NZ	2.04	0.55
22:LN:645:ARG:HH11	22:LN:656:ARG:NH1	2.04	0.55
25:LQ:282:GLU:HG2	25:LQ:331:THR:HG22	1.88	0.55
31:LW:460:ARG:NH2	60:SS:849:PHE:O	2.39	0.55
32:LY:747:UNK:HA	32:LY:765:UNK:HA	1.87	0.55
49:SG:139:LYS:HB3	49:SG:570:GLN:HG2	1.86	0.55
51:SI:134:ILE:HG12	51:SI:811:VAL:HG11	1.88	0.55
51:SI:1004:ARG:HH21	51:SI:1006:TRP:HZ2	1.52	0.55
55:SN:66:LYS:HE3	55:SN:68:ARG:HH21	1.71	0.55
2:L1:338:C:H5'	9:L8:10:LYS:HZ2	1.71	0.55
2:L1:1513:G:OP2	55:SN:119:TYR:OH	2.18	0.55
20:LL:161:ALA:HA	20:LL:175:ILE:HD13	1.88	0.55
20:LL:170:ILE:HB	20:LL:184:PHE:HB2	1.88	0.55
30:LV:95:ARG:NH2	30:LV:129:GLY:O	2.40	0.55
3:L2:105:C:H5"	45:SA:372:LYS:NZ	2.21	0.55
21:LM:230:LYS:HD3	21:LM:233:GLN:HE21	1.72	0.55
25:LQ:220:THR:HA	25:LQ:226:VAL:HG12	1.87	0.55
2:L1:328:A:OP2	12:LD:56:LYS:NZ	2.33	0.55
2:L1:1168:U:O2'	2:L1:1465:C:OP2	2.21	0.55
2:L1:1478:G:P	55:SN:109:ARG:HH12	2.29	0.55
10:L9:57:ARG:NE	53:SL:88:ASP:OD1	2.40	0.55
18:LJ:90:ARG:NH2	18:LJ:137:ASN:O	2.39	0.55
20:LL:191:VAL:HA	20:LL:206:ALA:HA	1.89	0.55
22:LN:476:LYS:HZ2	22:LN:491:CYS:HA	1.72	0.55
34:NA:531:ALA:HA	34:NA:534:ARG:NH1	2.20	0.55
47:SC:153:ALA:O	47:SC:157:GLY:N	2.38	0.55
51:SI:60:ASP:O	51:SI:239:ASN:ND2	2.39	0.55
52:SJ:136:ARG:NE	52:SK:71:ASP:OD1	2.39	0.55
54:SM:118:ASN:OD1	54:SM:118:ASN:N	2.37	0.55
5:L4:221:ARG:HG3	36:NC:226:ASP:OD2	2.07	0.55
12:LD:10:GLU:OE1	12:LD:14:GLN:NE2	2.40	0.55
23:LO:730:LEU:HD21	23:LO:754:VAL:HG23	1.89	0.55
23:LO:849:LEU:O	28:LT:900:ASN:ND2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SD:171:LEU:HB3	47:SD:240:VAL:HG12	1.88	0.55
51:SI:828:ARG:NH2	59:SR:94:ASN:O	2.39	0.55
9:L8:67:TRP:NE1	9:L8:69:SER:OG	2.39	0.55
16:LH:271:LEU:HB3	16:LH:283:VAL:HG13	1.89	0.55
18:LJ:39:HIS:HE1	18:LJ:62:ARG:HH12	1.55	0.55
25:LQ:46:LEU:HD22	25:LQ:657:GLN:HE22	1.71	0.55
31:LW:120:LYS:NZ	31:LW:200:PRO:HD3	2.22	0.55
47:SC:122:ARG:HG3	47:SC:140:GLU:OE2	2.07	0.55
51:SI:200:GLN:OE1	51:SI:233:ARG:NH1	2.40	0.55
54:SM:176:ILE:HG22	54:SM:177:ILE:HG12	1.89	0.55
2:L1:553:G:N2	2:L1:584:C:N3	2.54	0.55
6:L5:219:ARG:NH1	52:SK:222:ASP:OD2	2.40	0.55
17:LI:27:UNK:N	17:LI:357:UNK:O	2.39	0.55
22:LN:475:THR:HG22	22:LN:488:ILE:HG23	1.87	0.55
23:LO:409:GLY:O	23:LO:430:ARG:NH1	2.40	0.55
26:LR:177:UNK:HA	26:LR:189:UNK:HA	1.89	0.55
23:LO:791:HIS:O	23:LO:795:ASN:ND2	2.40	0.55
29:LU:109:HIS:HD2	29:LU:113:VAL:HG12	1.72	0.55
48:SE:19:GLN:OE1	48:SE:120:LYS:NZ	2.31	0.55
7:L6:77:LEU:HD12	7:L6:95:LYS:HB2	1.89	0.55
18:LJ:257:CYS:SG	18:LJ:258:LEU:N	2.80	0.55
28:LT:757:PRO:HD2	28:LT:760:LEU:HD12	1.88	0.55
29:LU:40:GLU:HB3	29:LU:400:LEU:HD11	1.88	0.55
49:SG:252:VAL:HG13	49:SG:286:LEU:HD13	1.89	0.55
50:SH:59:VAL:HG23	50:SH:60:THR:HG23	1.87	0.55
1:L0:146:G:H21	20:LL:360:ASN:HD21	1.54	0.55
13:LE:103:ILE:HA	13:LE:112:ASP:HA	1.89	0.55
15:LG:42:ARG:NH1	15:LG:56:LEU:HD22	2.21	0.55
21:LM:185:ASP:OD1	46:SB:414:ARG:NH2	2.36	0.55
25:LQ:837:ASP:OD1	25:LQ:882:ARG:NH1	2.40	0.55
2:L1:1532:U:OP2	18:LJ:114:ARG:NH2	2.40	0.54
22:LN:519:THR:N	22:LN:522:SER:OG	2.40	0.54
22:LN:43:PRO:HB2	22:LN:71:ARG:HH12	1.72	0.54
31:LW:122:GLY:HA2	31:LW:385:PRO:HD2	1.88	0.54
33:LZ:86:GLY:HA2	33:LZ:152:ARG:NH1	2.22	0.54
34:NA:350:THR:HG21	51:SI:975:GLU:HB3	1.90	0.54
46:SB:228:PRO:HB2	46:SB:229:GLU:HG3	1.88	0.54
50:SH:289:VAL:HG21	50:SH:294:LEU:HD13	1.88	0.54
55:SN:56:ILE:HD11	63:SV:193:PRO:HD2	1.89	0.54
1:L0:180:G:H5”	37:ND:164:LYS:NZ	2.22	0.54
16:LH:769:ASN:HB3	16:LH:773:ASP:OD1	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:542:VAL:HG22	22:LN:552:ILE:HG12	1.89	0.54
27:LS:304:LEU:HD23	27:LS:371:VAL:HG11	1.89	0.54
34:NA:348:ASP:OD2	61:ST:770:LYS:NZ	2.39	0.54
47:SC:242:ALA:HB3	47:SC:269:ILE:HA	1.88	0.54
3:L2:251:G:O6	49:SG:545:LYS:NZ	2.35	0.54
17:LI:675:LEU:HD21	19:LK:456:LEU:HD23	1.88	0.54
25:LQ:135:ARG:HH22	25:LQ:191:LEU:HD21	1.72	0.54
31:LW:289:MET:HB3	31:LW:301:TRP:HB2	1.88	0.54
32:LX:22:GLN:OE1	32:LX:197:ASN:ND2	2.41	0.54
2:L1:1510:U:OP1	55:SN:50:ARG:NH2	2.40	0.54
3:L2:326:U:OP2	48:SE:42:LYS:NZ	2.26	0.54
16:LH:690:ASN:ND2	16:LH:750:LEU:O	2.41	0.54
18:LJ:147:ARG:HH21	52:SK:18:ALA:HB2	1.71	0.54
21:LM:25:ARG:NH1	29:LU:16:VAL:HA	2.22	0.54
25:LQ:188:LEU:HD11	25:LQ:242:LEU:HB2	1.90	0.54
29:LU:409:GLU:OE2	29:LU:412:ARG:NH1	2.35	0.54
30:LV:197:ALA:HB3	30:LV:205:GLU:H	1.73	0.54
50:SH:14:SER:HB3	50:SH:36:ILE:HG23	1.88	0.54
51:SI:778:GLN:HG2	51:SI:779:ARG:HG3	1.89	0.54
55:SN:38:ILE:HD11	55:SN:242:ILE:HB	1.90	0.54
61:ST:455:LEU:HD23	61:ST:458:ILE:HD12	1.87	0.54
2:L1:938:G:N2	2:L1:941:A:OP2	2.35	0.54
4:L3:80:LYS:HA	55:SN:68:ARG:NH1	2.23	0.54
16:LH:48:PHE:HD2	16:LH:51:GLN:HE21	1.56	0.54
20:LL:292:TYR:O	20:LL:304:SER:OG	2.25	0.54
25:LQ:576:VAL:HA	25:LQ:592:SER:HB2	1.90	0.54
30:LV:297:ALA:HB3	30:LV:311:MET:HB2	1.90	0.54
32:LY:515:UNK:HA	32:LY:567:UNK:HA	1.88	0.54
33:LZ:156:ASP:OD2	54:SM:4:ARG:HB2	2.07	0.54
37:ND:177:ARG:HB3	65:SY:134:THR:HG22	1.89	0.54
51:SI:844:PRO:HG3	51:SI:1032:LEU:HD22	1.88	0.54
65:SY:111:ARG:NH1	65:SY:212:LYS:HD3	2.22	0.54
16:LH:200:ASN:HD22	16:LH:262:MET:HB2	1.73	0.54
22:LN:435:PRO:O	22:LN:483:ASN:ND2	2.37	0.54
23:LO:27:LYS:HG2	23:LO:43:ILE:HD12	1.89	0.54
23:LO:450:LEU:HA	23:LO:475:PRO:HB3	1.90	0.54
26:LR:588:UNK:HA	26:LR:603:UNK:HA	1.89	0.54
50:SH:18:ARG:HH12	50:SH:98:TYR:HA	1.73	0.54
52:SK:82:ARG:NH1	52:SK:118:ARG:NH1	2.56	0.54
62:SU:366:LEU:HD12	62:SU:401:PHE:HZ	1.73	0.54
1:L0:522:C:O2'	29:LU:125:ASP:O	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:22:HIS:HA	7:L6:25:ARG:NH1	2.22	0.54
15:LG:20:GLY:O	15:LG:65:ARG:NE	2.40	0.54
22:LN:62:PRO:O	22:LN:82:ARG:NH2	2.41	0.54
23:LO:19:ASN:HA	23:LO:307:THR:HG21	1.88	0.54
25:LQ:458:ASP:OD2	25:LQ:465:LEU:HD12	2.08	0.54
31:LW:113:PRO:HB3	31:LW:395:GLN:HG2	1.89	0.54
50:SH:183:ILE:HD13	50:SH:310:ARG:NH1	2.23	0.54
54:SM:183:SER:OG	54:SM:219:GLU:OE2	2.14	0.54
22:LN:331:ASN:H	22:LN:353:GLU:HB2	1.72	0.54
22:LN:640:ILE:HD11	22:LN:749:SER:HA	1.89	0.54
25:LQ:574:LEU:HB2	25:LQ:594:ASP:HB3	1.90	0.54
61:ST:52:ARG:O	61:ST:56:ASN:ND2	2.40	0.54
61:ST:702:LEU:HD11	62:SU:467:ALA:HB2	1.90	0.54
1:L0:585:C:H2'	1:L0:586:A:H8	1.73	0.54
2:L1:122:U:H5"	5:L4:77:ARG:NH1	2.23	0.54
5:L4:72:VAL:HB	5:L4:77:ARG:HG3	1.90	0.54
19:LK:451:LEU:HA	19:LK:454:LEU:HB2	1.89	0.54
23:LO:604:TYR:HA	23:LO:611:LEU:HA	1.89	0.54
31:LW:296:ARG:HH21	31:LW:316:PRO:HA	1.73	0.54
47:SC:160:ASP:N	47:SC:302:GLU:OE2	2.34	0.54
47:SD:198:GLU:OE2	47:SD:200:SER:OG	2.12	0.54
52:SK:96:LEU:HD23	52:SK:130:ILE:HD13	1.90	0.54
2:L1:329:G:H5"	9:L8:98:LYS:HB3	1.90	0.53
2:L1:1478:G:OP1	55:SN:109:ARG:NH1	2.34	0.53
2:L1:1491:U:OP2	58:SQ:213:ARG:NH1	2.40	0.53
18:LJ:105:VAL:HG13	18:LJ:120:ILE:HB	1.90	0.53
22:LN:529:ASN:O	22:LN:545:ARG:NH2	2.34	0.53
23:LO:78:ARG:HH11	23:LO:94:ASN:CG	2.12	0.53
45:SA:182:ASP:CG	45:SA:314:ARG:HH12	2.11	0.53
49:SG:262:VAL:HG13	49:SG:271:VAL:HG13	1.90	0.53
55:SN:126:VAL:HG22	55:SN:152:TYR:HB2	1.90	0.53
56:SO:151:ALA:O	56:SO:155:GLY:N	2.39	0.53
2:L1:569:C:P	59:SR:114:LYS:HZ3	2.30	0.53
2:L1:1628:U:H5"	34:NA:538:LYS:NZ	2.22	0.53
22:LN:533:HIS:NE2	22:LN:571:THR:O	2.41	0.53
25:LQ:398:ASP:OD2	25:LQ:437:LYS:HA	2.09	0.53
25:LQ:615:GLN:N	25:LQ:636:ASP:OD2	2.42	0.53
25:LQ:620:ASN:HD22	25:LQ:662:ALA:HA	1.73	0.53
31:LW:317:THR:HG23	31:LW:334:ARG:HB3	1.90	0.53
35:NB:595:LYS:HB3	58:SQ:134:ARG:HH11	1.74	0.53
51:SI:898:GLY:N	51:SI:915:ALA:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SN:17:LEU:HD23	55:SN:209:ILE:HG23	1.90	0.53
55:SN:135:LEU:HD21	55:SN:139:LEU:HD13	1.91	0.53
2:L1:332:U:P	9:L8:56:ARG:HH12	2.30	0.53
25:LQ:275:GLN:HA	25:LQ:281:ILE:HG12	1.90	0.53
25:LQ:279:LYS:HG3	25:LQ:338:ILE:HG23	1.90	0.53
28:LT:430:ILE:HB	28:LT:443:TRP:HB2	1.90	0.53
32:LX:9:ARG:NH1	32:LX:207:VAL:O	2.41	0.53
33:LZ:113:VAL:HG22	33:LZ:124:ILE:HD11	1.89	0.53
35:NB:540:ILE:HD11	51:SI:148:PHE:HB2	1.89	0.53
45:SA:23:GLN:HB2	60:SS:888:GLY:HA3	1.90	0.53
62:SU:285:ILE:O	62:SU:289:PHE:N	2.38	0.53
9:L8:27:PHE:HB2	9:L8:49:ARG:HH12	1.72	0.53
11:LC:7:VAL:HG23	33:LZ:179:ASP:HB2	1.90	0.53
16:LH:24:ASN:ND2	16:LH:369:TYR:OH	2.41	0.53
21:LM:215:CYS:O	21:LM:219:ASN:ND2	2.42	0.53
23:LO:209:VAL:HG11	23:LO:266:VAL:HG21	1.90	0.53
27:LS:242:ASN:ND2	27:LS:584:GLY:O	2.41	0.53
28:LT:761:GLN:HE22	56:SO:271:LYS:HG2	1.72	0.53
31:LW:177:TYR:HE1	31:LW:183:GLU:HG2	1.73	0.53
47:SD:258:HIS:HE1	47:SD:297:ARG:NH1	2.05	0.53
53:SL:106:LEU:HB3	53:SL:117:LEU:HD23	1.90	0.53
61:ST:678:PHE:HB3	61:ST:681:PRO:HD2	1.90	0.53
9:L8:42:ARG:NH1	30:LV:335:SER:HA	2.15	0.53
12:LD:57:LYS:O	12:LD:138:ASN:ND2	2.40	0.53
23:LO:568:ARG:HH22	53:SL:8:ARG:NE	2.07	0.53
31:LW:106:LEU:HB2	31:LW:398:ILE:HB	1.90	0.53
1:L0:97:G:O2'	1:L0:154:A:N3	2.35	0.53
10:L9:34:PHE:HD1	10:L9:111:THR:HG21	1.74	0.53
10:L9:172:VAL:O	10:L9:176:ASN:ND2	2.41	0.53
17:LI:68:UNK:O	17:LI:80:UNK:N	2.41	0.53
27:LS:492:ASN:ND2	48:SE:89:ARG:HH12	1.99	0.53
38:NE:313:ARG:HB3	38:NE:320:ILE:HB	1.89	0.53
51:SI:95:LYS:NZ	51:SI:349:ASP:OD2	2.41	0.53
52:SJ:91:ILE:HD13	52:SJ:208:ALA:HB1	1.91	0.53
52:SJ:105:ASN:HD21	52:SJ:126:PRO:HB3	1.73	0.53
52:SJ:188:ARG:HD3	52:SJ:191:ASP:OD2	2.09	0.53
1:L0:386:A:H5'	1:L0:387:C:OP2	2.08	0.53
2:L1:634:G:N2	2:L1:964:U:O2'	2.40	0.53
2:L1:999:U:O2	2:L1:1006:C:N4	2.42	0.53
17:LI:144:UNK:O	17:LI:153:UNK:N	2.42	0.53
17:LI:177:UNK:N	17:LI:189:UNK:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:349:THR:HG21	21:LM:379:GLU:HB3	1.91	0.53
23:LO:54:HIS:ND1	23:LO:74:ASP:OD1	2.38	0.53
23:LO:431:ILE:HG23	23:LO:451:ASP:HB3	1.90	0.53
25:LQ:673:VAL:HG22	25:LQ:683:ILE:HG12	1.91	0.53
26:LR:176:UNK:N	26:LR:190:UNK:O	2.41	0.53
26:LR:439:UNK:HA	26:LR:448:UNK:HA	1.89	0.53
30:LV:165:LEU:HG	30:LV:172:PHE:HB3	1.91	0.53
52:SJ:31:LEU:HD22	52:SJ:40:ARG:NH1	2.23	0.53
55:SN:185:LYS:NZ	63:SV:198:ASP:OD1	2.40	0.53
2:L1:318:U:H5"	9:L8:11:ARG:NH1	2.24	0.53
23:LO:793:GLU:OE2	28:LT:921:ARG:NH1	2.42	0.53
24:LP:67:ARG:NH2	24:LP:84:SER:O	2.42	0.53
51:SI:246:ALA:HB3	51:SI:810:ILE:HG13	1.90	0.53
1:L0:293:U:H2'	23:LO:631:ASN:HA	1.91	0.53
20:LL:343:ARG:NH1	20:LL:347:GLY:O	2.42	0.53
23:LO:138:ARG:HD3	28:LT:103:ARG:NH1	2.24	0.53
23:LO:155:SER:OG	23:LO:156:GLN:N	2.42	0.53
23:LO:315:GLU:HG3	56:SO:273:ARG:HD2	1.90	0.53
38:NE:104:UNK:CB	50:SH:231:ARG:HH11	2.22	0.53
52:SK:68:LEU:HD12	52:SK:73:HIS:HE1	1.72	0.53
1:L0:394:U:OP1	33:LZ:108:ARG:NH1	2.42	0.53
20:LL:488:ILE:HG23	20:LL:495:GLN:HB3	1.90	0.53
21:LM:22:ARG:HH12	29:LU:15:PRO:HG2	1.74	0.53
22:LN:61:THR:HG22	22:LN:341:SER:HB3	1.91	0.53
26:LR:418:UNK:HA	26:LR:434:UNK:HA	1.89	0.53
30:LV:359:ILE:HG13	30:LV:360:THR:HG23	1.91	0.53
51:SI:923:ASP:N	51:SI:923:ASP:OD1	2.40	0.53
52:SK:152:SER:HA	61:ST:715:PRO:HA	1.90	0.53
2:L1:1601:G:O3'	54:SM:146:ARG:NH1	2.42	0.52
3:L2:251:G:H5"	3:L2:252:C:H5'	1.91	0.52
16:LH:650:VAL:HG12	16:LH:652:GLU:H	1.74	0.52
17:LI:533:UNK:HA	17:LI:559:PRO:HG3	1.91	0.52
20:LL:541:LEU:HA	20:LL:544:ASP:OD2	2.09	0.52
26:LR:125:UNK:HA	26:LR:133:UNK:HA	1.91	0.52
27:LS:237:ARG:HH12	27:LS:561:PRO:CG	2.22	0.52
28:LT:511:ASP:OD2	28:LT:516:LYS:HG2	2.09	0.52
32:LX:61:LYS:HG2	32:LX:62:LYS:HG3	1.91	0.52
51:SI:92:ARG:HH21	51:SI:221:LEU:HD13	1.74	0.52
2:L1:327:U:H5'	12:LD:82:ARG:HH12	1.73	0.52
12:LD:97:TYR:HB3	12:LD:99:ARG:HD3	1.90	0.52
16:LH:720:ILE:HG12	16:LH:745:ILE:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:474:SER:OG	22:LN:491:CYS:SG	2.65	0.52
25:LQ:497:VAL:HB	25:LQ:528:LEU:HB2	1.91	0.52
27:LS:408:CYS:SG	27:LS:409:ILE:N	2.81	0.52
32:LX:567:UNK:N	32:LX:581:UNK:O	2.42	0.52
61:ST:604:VAL:HG13	61:ST:606:PHE:HD1	1.74	0.52
2:L1:895:G:H1'	40:NG:37:GLU:HA	1.91	0.52
6:L5:133:VAL:HG22	6:L5:198:LEU:HD13	1.90	0.52
21:LM:304:GLN:HE22	21:LM:343:VAL:HB	1.73	0.52
23:LO:200:SER:OG	23:LO:202:ASP:O	2.24	0.52
47:SC:144:TRP:HE1	47:SC:152:ALA:HA	1.74	0.52
50:SH:323:ILE:HG23	51:SI:553:ILE:HG23	1.90	0.52
52:SJ:103:PRO:HD2	52:SJ:246:GLU:OE2	2.10	0.52
52:SK:69:ASN:H	52:SK:73:HIS:CE1	2.27	0.52
59:SR:75:GLN:HA	59:SR:82:LYS:HA	1.92	0.52
1:L0:210:U:H2'	1:L0:211:G:H8	1.74	0.52
5:L4:85:GLY:N	5:L4:88:ASP:OD2	2.33	0.52
13:LE:75:ILE:HG12	13:LE:127:GLY:HA2	1.90	0.52
18:LJ:197:ASP:OD1	18:LJ:199:ARG:HG2	2.10	0.52
20:LL:444:ALA:HB2	20:LL:452:LEU:HD22	1.92	0.52
23:LO:412:ARG:NH2	25:LQ:943:ILE:O	2.42	0.52
25:LQ:163:LYS:HA	34:NA:522:ARG:NH1	2.24	0.52
25:LQ:414:LEU:N	25:LQ:428:PHE:O	2.40	0.52
31:LW:357:SER:OG	31:LW:361:ASN:N	2.42	0.52
32:LY:630:UNK:O	32:LY:727:UNK:N	2.42	0.52
49:SG:137:GLY:H	49:SG:485:ASN:HD21	1.58	0.52
49:SG:194:LEU:O	49:SG:216:GLY:N	2.37	0.52
49:SG:260:LEU:HD21	49:SG:283:VAL:HG11	1.91	0.52
16:LH:540:ASN:HD21	20:LL:354:THR:HG21	1.75	0.52
22:LN:66:ARG:NH1	22:LN:80:ASN:OD1	2.42	0.52
22:LN:82:ARG:NH1	22:LN:686:UNK:HA	2.25	0.52
22:LN:377:PRO:HB2	22:LN:634:VAL:HG11	1.91	0.52
25:LQ:927:GLN:NE2	28:LT:742:LYS:O	2.42	0.52
55:SN:208:SER:OG	55:SN:209:ILE:N	2.43	0.52
61:ST:565:VAL:HG23	61:ST:664:ILE:HD11	1.91	0.52
1:L0:413:C:H2'	1:L0:414:G:H8	1.74	0.52
22:LN:124:THR:HG21	37:ND:191:PRO:HB3	1.92	0.52
22:LN:370:ARG:NH2	22:LN:372:MET:SD	2.83	0.52
22:LN:444:ARG:HB2	22:LN:447:THR:H	1.75	0.52
25:LQ:620:ASN:ND2	25:LQ:661:TRP:O	2.42	0.52
25:LQ:936:LYS:HG2	34:NA:469:VAL:HG22	1.91	0.52
32:LX:199:LEU:HD13	32:LX:207:VAL:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SA:185:ASP:OD1	45:SA:285:ARG:NE	2.42	0.52
50:SH:263:ASP:HB2	50:SH:266:SER:HB3	1.91	0.52
51:SI:1059:ARG:NH1	65:SY:27:PHE:HZ	2.07	0.52
3:L2:93:U:OP1	46:SB:302:HIS:HD2	1.93	0.52
16:LH:115:HIS:CE1	16:LH:133:LYS:HZ3	2.27	0.52
18:LJ:173:THR:HG21	18:LJ:217:ASN:HA	1.91	0.52
22:LN:470:LEU:HD11	22:LN:498:VAL:HG21	1.91	0.52
25:LQ:836:ILE:HG21	25:LQ:857:LEU:HD11	1.90	0.52
30:LV:161:GLU:HA	30:LV:177:LYS:HA	1.91	0.52
31:LW:443:THR:OG1	31:LW:445:ASP:O	2.28	0.52
32:LY:609:UNK:O	32:LY:613:UNK:N	2.43	0.52
33:LZ:81:LYS:NZ	34:NA:445:VAL:HG13	2.25	0.52
45:SA:129:ARG:HD2	47:SC:322:ARG:NH1	2.18	0.52
54:SM:233:VAL:HG13	54:SM:254:PHE:HB2	1.91	0.52
18:LJ:139:ILE:HD11	18:LJ:151:LEU:HD23	1.92	0.52
20:LL:105:TYR:HB3	20:LL:122:SER:HB3	1.91	0.52
25:LQ:572:HIS:ND1	25:LQ:594:ASP:OD2	2.43	0.52
61:ST:213:UNK:O	61:ST:217:UNK:N	2.43	0.52
18:LJ:8:ILE:HD12	18:LJ:389:GLU:HG3	1.92	0.52
22:LN:166:VAL:HG22	22:LN:182:ILE:HG12	1.91	0.52
22:LN:453:LEU:HB3	22:LN:460:LEU:HD23	1.92	0.52
23:LO:306:ASN:HD22	23:LO:322:SER:H	1.56	0.52
27:LS:460:VAL:HG22	27:LS:482:LEU:HD13	1.92	0.52
30:LV:231:VAL:HA	30:LV:247:THR:HA	1.92	0.52
46:SB:321:GLY:HA3	46:SB:341:LEU:HB2	1.91	0.52
55:SN:71:ASN:HD22	55:SN:98:LYS:HD2	1.74	0.52
59:SR:84:THR:HG21	61:ST:788:ILE:HD12	1.91	0.52
3:L2:45:U:O2'	53:SL:23:GLN:NE2	2.42	0.52
16:LH:762:TYR:HB3	16:LH:779:ILE:HG12	1.92	0.52
16:LH:878:ASN:HD22	16:LH:890:ARG:NH1	2.01	0.52
17:LI:555:ILE:HG21	17:LI:582:ILE:HG13	1.91	0.52
17:LI:555:ILE:O	17:LI:585:ARG:NH2	2.43	0.52
20:LL:212:LEU:HB2	20:LL:226:LEU:HB2	1.91	0.52
21:LM:218:ILE:HG23	21:LM:263:VAL:HG11	1.91	0.52
21:LM:241:ILE:O	21:LM:245:LEU:N	2.41	0.52
22:LN:87:GLN:HB3	22:LN:378:TYR:HD2	1.75	0.52
24:LP:17:ASP:HB3	24:LP:84:SER:HB3	1.91	0.52
25:LQ:317:UNK:O	25:LQ:321:TYR:N	2.42	0.52
25:LQ:897:ASP:OD1	26:LR:761:ARG:NH2	2.43	0.52
32:LX:130:LEU:HD12	32:LX:184:PHE:HE2	1.75	0.52
32:LX:593:UNK:O	32:LX:597:UNK:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:746:UNK:N	32:LX:766:UNK:O	2.43	0.52
51:SI:846:VAL:HG22	51:SI:855:GLN:HB3	1.91	0.52
2:L1:539:G:H8	2:L1:539:G:OP2	1.93	0.51
10:L9:94:ASP:HB3	53:SL:93:LYS:HZ2	1.75	0.51
11:LC:67:VAL:HG11	11:LC:81:ILE:HG22	1.92	0.51
24:LP:144:VAL:HG13	24:LP:181:LEU:HD12	1.91	0.51
25:LQ:414:LEU:HD13	25:LQ:457:PHE:HD2	1.74	0.51
25:LQ:572:HIS:CD2	25:LQ:598:LYS:HD2	2.45	0.51
28:LT:392:ARG:HE	28:LT:449:ARG:HH22	1.58	0.51
32:LX:313:UNK:O	32:LX:373:UNK:N	2.43	0.51
35:NB:580:ARG:HH11	53:SL:49:SER:HA	1.75	0.51
48:SF:89:ARG:NH2	49:SG:326:GLU:OE2	2.43	0.51
51:SI:100:ASP:HB3	51:SI:360:ASP:OD2	2.10	0.51
51:SI:105:ILE:HG23	51:SI:117:PHE:HB2	1.91	0.51
54:SM:181:ASN:OD1	54:SM:181:ASN:N	2.44	0.51
56:SO:268:SER:OG	56:SO:269:ARG:NH1	2.40	0.51
61:ST:554:GLN:HG2	61:ST:557:SER:HB2	1.92	0.51
2:L1:332:U:H3'	9:L8:54:LYS:NZ	2.25	0.51
2:L1:537:G:H2'	10:L9:171:ARG:HH12	1.76	0.51
7:L6:70:PRO:HA	7:L6:98:ARG:HH22	1.75	0.51
16:LH:559:LYS:HG2	16:LH:612:SER:HA	1.92	0.51
20:LL:121:ASP:HB2	20:LL:127:TYR:HE2	1.75	0.51
21:LM:336:LEU:HD22	21:LM:373:ILE:HD11	1.91	0.51
31:LW:67:LEU:HB3	31:LW:410:ASN:HD22	1.75	0.51
45:SA:155:GLY:HA2	47:SC:233:LEU:HD23	1.90	0.51
47:SD:120:GLU:OE2	47:SD:142:ARG:HD2	2.10	0.51
51:SI:880:TYR:CD2	59:SR:94:ASN:HB3	2.45	0.51
55:SN:14:GLU:HG3	55:SN:209:ILE:HG21	1.92	0.51
55:SN:180:LEU:HA	55:SN:183:ILE:HG22	1.92	0.51
56:SO:130:MET:HA	56:SO:137:VAL:HA	1.92	0.51
1:L0:295:A:C6	28:LT:381:ARG:HD2	2.46	0.51
17:LI:80:UNK:HA	17:LI:88:UNK:HA	1.92	0.51
23:LO:300:MET:HG2	23:LO:328:LEU:HD13	1.90	0.51
23:LO:559:ILE:HG23	23:LO:598:ASN:HD22	1.74	0.51
28:LT:64:ASN:O	28:LT:344:ARG:NH1	2.22	0.51
33:LZ:33:MET:HG2	33:LZ:38:ILE:HD11	1.93	0.51
53:SL:165:ARG:NH2	53:SL:183:GLU:OE2	2.43	0.51
1:L0:152:U:O2'	1:L0:154:A:N7	2.44	0.51
13:LE:83:ILE:HG13	13:LE:86:ILE:HD12	1.93	0.51
18:LJ:280:HIS:NE2	20:LL:449:ASP:OD1	2.43	0.51
22:LN:637:PHE:HE2	22:LN:746:LEU:HG	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:403:ASN:HB3	25:LQ:419:ILE:HD13	1.92	0.51
29:LU:118:VAL:HG12	29:LU:136:MET:HA	1.93	0.51
50:SH:7:LYS:HE3	50:SH:77:ARG:NH1	2.25	0.51
50:SH:111:LYS:NZ	51:SI:923:ASP:HB3	2.26	0.51
62:SU:371:LEU:HD13	62:SU:375:LEU:HD12	1.91	0.51
14:LF:54:ALA:HB2	14:LF:79:VAL:HG22	1.91	0.51
23:LO:477:SER:OG	23:LO:478:CYS:N	2.43	0.51
25:LQ:259:ILE:HG12	25:LQ:274:ILE:HG12	1.92	0.51
28:LT:718:LYS:O	28:LT:875:ASN:ND2	2.37	0.51
32:LX:61:LYS:HE2	32:LX:62:LYS:HE3	1.93	0.51
38:NE:282:ASP:O	38:NE:286:ARG:NH1	2.44	0.51
62:SU:385:ARG:HG2	62:SU:465:GLU:OE2	2.11	0.51
2:L1:590:C:OP1	35:NB:571:LYS:NZ	2.43	0.51
9:L8:58:LEU:HD12	9:L8:59:ARG:HG2	1.93	0.51
16:LH:410:ASN:ND2	16:LH:488:LEU:O	2.42	0.51
18:LJ:125:HIS:NE2	52:SK:19:LEU:O	2.37	0.51
20:LL:142:ILE:HG21	20:LL:173:ILE:HD11	1.92	0.51
21:LM:122:VAL:HA	21:LM:127:ILE:HG12	1.91	0.51
23:LO:148:ASP:HB2	23:LO:166:LYS:HD3	1.93	0.51
23:LO:258:ALA:HB1	23:LO:261:ALA:HB3	1.92	0.51
25:LQ:764:GLU:HG2	25:LQ:834:LYS:HZ3	1.74	0.51
29:LU:332:TYR:HB3	29:LU:339:SER:HA	1.92	0.51
47:SC:90:PRO:HD3	58:SQ:106:LEU:HD12	1.93	0.51
1:L0:480:C:O2	24:LP:46:ARG:NH1	2.44	0.51
27:LS:20:GLN:HG2	27:LS:24:LYS:HZ3	1.75	0.51
27:LS:325:ASP:OD1	27:LS:326:LEU:N	2.42	0.51
32:LY:387:UNK:O	32:LY:410:UNK:N	2.44	0.51
46:SB:428:ASN:HB3	46:SB:430:ASP:OD1	2.11	0.51
49:SG:295:LEU:HB3	49:SG:307:TYR:HB2	1.92	0.51
59:SR:126:LYS:HG2	59:SR:131:SER:HA	1.92	0.51
1:L0:506:G:H1	1:L0:530:A:H61	1.57	0.51
2:L1:163:G:H4'	7:L6:53:SER:HB2	1.93	0.51
2:L1:1593:A:N6	2:L1:1594:G:O6	2.44	0.51
4:L3:13:HIS:HD2	4:L3:14:ILE:HG22	1.76	0.51
22:LN:116:SER:OG	22:LN:126:TRP:NE1	2.40	0.51
22:LN:129:ALA:O	22:LN:530:ARG:NH2	2.44	0.51
24:LP:73:ARG:NH1	27:LS:15:PRO:HB3	2.26	0.51
33:LZ:37:HIS:HD2	33:LZ:128:VAL:HG21	1.76	0.51
33:LZ:163:ASN:HD22	33:LZ:182:PHE:HE2	1.59	0.51
35:NB:439:ASP:OD1	52:SK:136:ARG:NH1	2.38	0.51
41:NH:1204:VAL:HA	41:NH:1214:LEU:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC:269:ILE:HG13	47:SC:293:LEU:HD11	1.91	0.51
59:SR:89:ASN:ND2	65:SY:4:LEU:O	2.44	0.51
2:L1:548:G:H2'	2:L1:549:G:H8	1.76	0.51
22:LN:106:ASN:H	22:LN:153:GLN:HG2	1.76	0.51
24:LP:385:UNK:O	24:LP:389:UNK:N	2.44	0.51
27:LS:410:ASP:OD1	27:LS:479:ASN:ND2	2.43	0.51
28:LT:277:ASP:HB2	28:LT:284:ILE:HD11	1.92	0.51
46:SB:110:UNK:O	46:SB:114:UNK:N	2.44	0.51
51:SI:69:PRO:HB3	51:SI:114:ARG:HG3	1.93	0.51
55:SN:123:ASP:HA	55:SN:149:LYS:HZ2	1.75	0.51
61:ST:478:ILE:HG23	61:ST:524:LEU:HD22	1.92	0.51
61:ST:481:MET:HA	61:ST:484:ARG:HE	1.76	0.51
2:L1:1490:C:OP1	51:SI:1062:ARG:NH2	2.44	0.51
8:L7:17:GLU:HG2	8:L7:46:ILE:HD12	1.92	0.51
16:LH:474:THR:HG21	16:LH:493:PRO:HB2	1.93	0.51
16:LH:615:TRP:HE1	16:LH:619:GLY:HA2	1.76	0.51
17:LI:292:UNK:O	17:LI:305:UNK:N	2.43	0.51
20:LL:259:PRO:HG2	20:LL:260:LEU:HD22	1.93	0.51
22:LN:497:ILE:HD11	22:LN:555:LEU:HD22	1.91	0.51
28:LT:719:GLU:O	28:LT:921:ARG:NH2	2.44	0.51
31:LW:215:LYS:HG2	31:LW:227:GLU:HG3	1.92	0.51
32:LX:747:UNK:HA	32:LX:765:UNK:HA	1.92	0.51
33:LZ:109:ARG:HH12	33:LZ:155:GLU:HB2	1.76	0.51
47:SC:123:ILE:N	47:SC:141:TYR:O	2.43	0.51
47:SD:225:ARG:HD2	47:SD:252:ILE:HD12	1.92	0.51
49:SG:320:GLY:HA3	49:SG:356:ARG:HH22	1.76	0.51
55:SN:173:PRO:HA	55:SN:176:VAL:HG22	1.93	0.51
2:L1:327:U:H5'	12:LD:82:ARG:NH1	2.26	0.50
2:L1:377:G:O2'	36:NC:306:ARG:NH2	2.44	0.50
2:L1:1628:U:H5"	34:NA:538:LYS:HZ2	1.76	0.50
23:LO:519:LEU:O	23:LO:533:SER:OG	2.29	0.50
25:LQ:532:ASP:HB3	25:LQ:551:LEU:H	1.75	0.50
25:LQ:749:GLY:HA3	25:LQ:820:ALA:HB1	1.93	0.50
25:LQ:913:ASN:ND2	25:LQ:917:ASN:OD1	2.45	0.50
26:LR:154:UNK:HA	26:LR:171:UNK:HA	1.93	0.50
28:LT:228:GLY:O	28:LT:246:ILE:N	2.40	0.50
28:LT:545:PRO:HB2	28:LT:563:ASP:OD2	2.12	0.50
29:LU:231:GLU:HB3	29:LU:234:ILE:HD13	1.92	0.50
29:LU:327:LYS:HG2	29:LU:350:HIS:H	1.76	0.50
32:LX:70:ARG:NH1	51:SI:350:LYS:HD3	2.26	0.50
34:NA:379:ASP:OD2	54:SM:191:PHE:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NE:226:ASP:OD1	38:NE:227:LYS:HG2	2.11	0.50
48:SE:94:SER:OG	65:SY:248:ARG:NH2	2.44	0.50
51:SI:125:LEU:HD23	51:SI:902:VAL:HG23	1.94	0.50
52:SK:125:ASN:HD22	52:SK:126:PRO:HD2	1.76	0.50
61:ST:592:ARG:NH1	64:SX:3220:UNK:HA	2.25	0.50
1:L0:234:A:H2'	18:LJ:360:MET:HE1	1.92	0.50
2:L1:1652:C:H5"	25:LQ:255:ARG:HH21	1.76	0.50
3:L2:100:U:H2'	3:L2:101:G:H8	1.75	0.50
10:L9:30:LEU:HD21	10:L9:102:GLU:OE2	2.10	0.50
16:LH:388:PRO:HB2	16:LH:451:PHE:HE2	1.75	0.50
16:LH:435:ASP:O	16:LH:762:TYR:OH	2.17	0.50
23:LO:285:ARG:HH11	23:LO:294:LEU:HD11	1.77	0.50
23:LO:361:VAL:HG22	23:LO:371:VAL:HG22	1.93	0.50
30:LV:69:GLN:HB3	30:LV:86:PHE:HD2	1.76	0.50
45:SA:100:ILE:HG22	45:SA:102:ASP:H	1.76	0.50
57:SP:1985:UNK:O	57:SP:1989:UNK:N	2.44	0.50
2:L1:388:G:OP2	2:L1:423:G:O2'	2.29	0.50
2:L1:987:G:N2	2:L1:1013:A:OP2	2.44	0.50
2:L1:1629:G:H22	2:L1:1637:C:H1'	1.77	0.50
16:LH:291:ARG:NH1	16:LH:326:LEU:O	2.37	0.50
18:LJ:7:ARG:HH12	18:LJ:383:ARG:HB3	1.76	0.50
18:LJ:360:MET:HG3	18:LJ:361:MET:HG3	1.93	0.50
21:LM:207:THR:HG22	21:LM:252:ASP:OD2	2.11	0.50
21:LM:312:VAL:O	21:LM:353:ARG:NH2	2.42	0.50
25:LQ:180:THR:HG22	25:LQ:186:ILE:HG12	1.94	0.50
25:LQ:273:TYR:HE1	25:LQ:343:TRP:HD1	1.59	0.50
25:LQ:478:SER:HB3	25:LQ:536:CYS:HA	1.93	0.50
25:LQ:533:ASP:H	25:LQ:551:LEU:HB2	1.75	0.50
28:LT:309:ILE:HG12	28:LT:323:VAL:HG12	1.93	0.50
28:LT:370:SER:OG	28:LT:371:LYS:N	2.43	0.50
29:LU:242:ASN:HA	29:LU:263:ARG:HA	1.93	0.50
31:LW:123:THR:HB	31:LW:140:ARG:HH12	1.76	0.50
45:SA:88:LYS:NZ	60:SS:331:GLN:HA	2.25	0.50
51:SI:124:ASP:OD1	51:SI:1027:THR:HG22	2.11	0.50
65:SY:184:ILE:HG22	65:SY:185:MET:HG2	1.92	0.50
4:L3:14:ILE:HD11	4:L3:21:ASN:HB3	1.94	0.50
18:LJ:322:LEU:HD12	18:LJ:326:LEU:HB2	1.92	0.50
25:LQ:640:LYS:HG2	25:LQ:652:LYS:HG3	1.94	0.50
26:LR:170:UNK:HA	26:LR:176:UNK:HA	1.93	0.50
28:LT:432:THR:OG1	28:LT:443:TRP:NE1	2.38	0.50
29:LU:254:PRO:HG3	60:SS:284:ARG:NH1	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LU:353:GLN:HE21	29:LU:355:LYS:NZ	2.08	0.50
32:LX:387:UNK:N	32:LX:408:UNK:O	2.44	0.50
32:LX:516:UNK:N	32:LX:566:UNK:O	2.44	0.50
45:SA:382:LYS:HD2	45:SA:404:LEU:HD11	1.92	0.50
2:L1:887:A:H2	2:L1:925:G:H22	1.58	0.50
6:L5:63:GLN:OE1	6:L5:66:GLN:NE2	2.45	0.50
11:LC:13:LYS:HG3	11:LC:14:LYS:H	1.75	0.50
16:LH:407:ASN:N	16:LH:413:SER:OG	2.45	0.50
17:LI:632:THR:HG22	19:LK:492:ILE:HD11	1.93	0.50
22:LN:543:ILE:O	22:LN:551:ASP:N	2.44	0.50
23:LO:29:LEU:HD21	23:LO:327:LEU:HD21	1.92	0.50
27:LS:352:GLN:HB3	27:LS:379:GLY:HA2	1.93	0.50
32:LX:484:UNK:O	32:LX:488:UNK:N	2.45	0.50
33:LZ:29:ASP:OD1	33:LZ:30:THR:N	2.45	0.50
47:SD:166:PRO:HA	47:SD:188:VAL:HA	1.92	0.50
47:SD:189:GLY:O	47:SD:216:ASN:ND2	2.45	0.50
48:SE:33:LEU:HD11	48:SE:100:ALA:HB1	1.93	0.50
48:SF:108:SER:HB2	48:SF:111:LYS:HB2	1.94	0.50
49:SG:198:LYS:HD3	49:SG:212:LYS:HB2	1.93	0.50
62:SU:176:ILE:O	62:SU:180:PHE:N	2.45	0.50
1:L0:248:G:OP1	65:SY:82:ARG:NH1	2.41	0.50
2:L1:153:G:N2	7:L6:56:ASN:OD1	2.45	0.50
2:L1:877:G:H1	2:L1:951:A:H2	1.59	0.50
2:L1:1512:G:OP2	55:SN:146:GLY:HA3	2.12	0.50
3:L2:16:A:H2'	3:L2:17:G:H8	1.76	0.50
5:L4:106:LYS:HB3	5:L4:108:ARG:HH11	1.76	0.50
8:L7:137:GLY:H	8:L7:153:LEU:HB2	1.76	0.50
9:L8:157:GLU:HA	9:L8:160:PHE:HD2	1.77	0.50
17:LI:250:UNK:O	17:LI:263:UNK:N	2.45	0.50
17:LI:304:UNK:N	17:LI:312:UNK:O	2.45	0.50
22:LN:247:LEU:HG	22:LN:288:THR:HG21	1.94	0.50
24:LP:17:ASP:OD2	24:LP:84:SER:N	2.41	0.50
31:LW:116:ILE:HD11	31:LW:398:ILE:HG12	1.94	0.50
31:LW:127:ILE:HG21	31:LW:398:ILE:HD11	1.93	0.50
31:LW:187:LEU:HB3	31:LW:190:HIS:HD2	1.77	0.50
32:LX:55:VAL:HB	32:LX:103:ILE:HG23	1.94	0.50
48:SE:33:LEU:HD13	48:SE:102:ILE:HD13	1.94	0.50
51:SI:781:GLU:OE2	51:SI:784:LYS:HG2	2.12	0.50
55:SN:64:LEU:HD11	55:SN:215:ASN:HD21	1.75	0.50
2:L1:360:A:O2'	2:L1:362:G:N2	2.45	0.50
2:L1:369:A:H5'	5:L4:22:LYS:NZ	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1274:C:H42	2:L1:1435:G:H1	1.60	0.50
6:L5:124:LEU:HD11	18:LJ:117:LEU:HD21	1.94	0.50
21:LM:314:GLN:OE1	21:LM:357:ARG:NE	2.41	0.50
23:LO:395:PHE:HE1	23:LO:416:LEU:HD11	1.77	0.50
29:LU:326:ASP:OD1	29:LU:327:LYS:N	2.45	0.50
32:LY:860:UNK:O	32:LY:864:UNK:N	2.45	0.50
44:NK:49:ARG:O	44:NK:53:LEU:N	2.44	0.50
53:SL:139:ASP:OD1	53:SL:163:ARG:NH1	2.45	0.50
1:L0:168:G:H22	1:L0:227:U:H3	1.58	0.50
1:L0:198:A:H8	1:L0:198:A:OP1	1.95	0.50
2:L1:548:G:H1	2:L1:590:C:H42	1.60	0.50
10:L9:78:ARG:HH12	36:NC:251:GLU:CD	2.14	0.50
13:LE:88:LYS:O	13:LE:92:ASN:ND2	2.45	0.50
18:LJ:147:ARG:HG2	18:LJ:170:TYR:H	1.77	0.50
25:LQ:137:ILE:HG23	25:LQ:147:VAL:HG22	1.94	0.50
26:LR:265:UNK:O	26:LR:283:UNK:N	2.44	0.50
26:LR:441:UNK:HA	26:LR:446:UNK:HA	1.92	0.50
28:LT:125:GLY:H	46:SB:430:ASP:HA	1.76	0.50
51:SI:831:ARG:NH1	51:SI:877:GLU:O	2.30	0.50
61:ST:426:THR:HG22	61:ST:462:LEU:HD13	1.94	0.50
2:L1:325:G:H4'	12:LD:83:THR:HG21	1.94	0.50
2:L1:1524:A:H2'	2:L1:1525:A:C8	2.46	0.50
16:LH:486:PHE:HB2	22:LN:776:PHE:HB3	1.93	0.50
25:LQ:63:LEU:HD11	25:LQ:111:LYS:HB2	1.92	0.50
25:LQ:140:SER:OG	25:LQ:142:ASP:OD1	2.27	0.50
25:LQ:837:ASP:OD2	25:LQ:879:GLN:HG2	2.12	0.50
28:LT:116:ALA:HB1	28:LT:133:ASP:OD1	2.11	0.50
29:LU:263:ARG:O	29:LU:281:ASN:ND2	2.44	0.50
30:LV:146:TYR:OH	64:SX:2018:UNK:O	2.29	0.50
30:LV:178:LEU:HD11	30:LV:183:VAL:HB	1.94	0.50
32:LX:481:UNK:O	32:LX:485:UNK:N	2.44	0.50
47:SD:290:VAL:HG13	47:SD:300:PRO:HG3	1.92	0.50
49:SG:500:LYS:HB2	49:SG:511:LEU:HG	1.93	0.50
61:ST:281:UNK:HA	66:SZ:383:PRO:HA	1.93	0.50
1:L0:254:C:H2'	63:SV:183:ARG:HH21	1.77	0.49
2:L1:1000:C:N4	2:L1:1003:A:OP2	2.44	0.49
5:L4:241:GLY:O	49:SG:107:PHE:N	2.45	0.49
20:LL:80:MET:HB3	20:LL:82:ASN:H	1.77	0.49
25:LQ:540:SER:OG	25:LQ:544:ARG:N	2.42	0.49
26:LR:168:UNK:HA	26:LR:178:UNK:HA	1.93	0.49
27:LS:511:LEU:HD13	27:LS:544:VAL:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:585:UNK:HA	32:LX:632:UNK:HA	1.92	0.49
45:SA:196:LYS:O	45:SA:200:GLY:N	2.45	0.49
65:SY:104:SER:HB3	65:SY:222:ARG:NH1	2.27	0.49
1:L0:90:G:OP1	27:LS:320:TYR:HE1	1.95	0.49
2:L1:350:U:H5"	2:L1:352:A:H5'	1.93	0.49
2:L1:540:G:H4'	2:L1:542:A:H5'	1.93	0.49
16:LH:28:VAL:HG12	16:LH:199:SER:H	1.78	0.49
28:LT:106:GLU:OE2	28:LT:109:LEU:HB2	2.12	0.49
47:SD:142:ARG:NH1	47:SD:183:HIS:HA	2.27	0.49
51:SI:841:THR:HG22	51:SI:860:TYR:H	1.77	0.49
5:L4:125:LYS:NZ	5:L4:223:ASN:O	2.45	0.49
6:L5:84:LYS:HG2	6:L5:92:ARG:HH12	1.77	0.49
16:LH:208:LEU:HD22	16:LH:230:LEU:HD13	1.94	0.49
25:LQ:125:THR:H	25:LQ:140:SER:HA	1.76	0.49
25:LQ:136:LEU:N	25:LQ:148:TRP:O	2.44	0.49
30:LV:280:LEU:HD22	30:LV:288:LYS:HB2	1.93	0.49
30:LV:331:THR:OG1	30:LV:339:HIS:O	2.30	0.49
31:LW:288:TYR:HB3	31:LW:345:LEU:HD12	1.95	0.49
50:SH:312:ARG:NH2	50:SH:344:GLU:OE1	2.45	0.49
51:SI:932:LEU:HD22	51:SI:1007:TYR:HB2	1.94	0.49
54:SM:93:SER:OG	54:SM:94:ARG:N	2.46	0.49
54:SM:139:LEU:HB2	54:SM:157:PHE:CE2	2.46	0.49
62:SU:356:ALA:O	62:SU:360:ARG:NH2	2.46	0.49
1:L0:306:G:O2'	27:LS:141:ASN:ND2	2.45	0.49
5:L4:180:LEU:HA	5:L4:194:THR:HA	1.94	0.49
5:L4:180:LEU:N	5:L4:229:GLY:O	2.45	0.49
17:LI:120:UNK:N	17:LI:133:UNK:O	2.39	0.49
23:LO:53:GLU:HB2	23:LO:619:ARG:HH11	1.76	0.49
23:LO:247:SER:H	23:LO:249:ARG:HH12	1.60	0.49
23:LO:833:LYS:NZ	28:LT:930:MET:HG3	2.27	0.49
27:LS:302:THR:HG22	27:LS:310:GLN:HG2	1.94	0.49
29:LU:258:ILE:HD12	29:LU:294:LEU:HB3	1.94	0.49
30:LV:66:ARG:HH22	30:LV:148:LYS:NZ	2.09	0.49
32:LX:77:ILE:HG23	32:LX:86:ARG:NH1	2.27	0.49
32:LY:644:UNK:O	32:LY:648:UNK:N	2.45	0.49
32:LY:746:UNK:O	32:LY:766:UNK:N	2.45	0.49
47:SC:171:LEU:HB2	47:SC:237:VAL:HG11	1.94	0.49
47:SD:302:GLU:HG2	65:SY:135:ILE:HG12	1.95	0.49
51:SI:827:ALA:HA	51:SI:919:VAL:HA	1.93	0.49
61:ST:523:ILE:HD11	62:SU:506:LEU:HD13	1.95	0.49
1:L0:86:C:N4	16:LH:482:GLY:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:290:G:H2'	1:L0:291:G:H8	1.77	0.49
16:LH:197:ILE:HD11	16:LH:213:LYS:HG3	1.94	0.49
23:LO:369:ILE:HB	23:LO:383:PHE:HB2	1.94	0.49
23:LO:694:ALA:HB1	23:LO:701:LEU:HD11	1.93	0.49
31:LW:175:PHE:CE1	31:LW:186:ARG:HG3	2.47	0.49
32:LY:387:UNK:N	32:LY:408:UNK:O	2.46	0.49
45:SA:133:LEU:HA	47:SC:236:MET:HG3	1.95	0.49
45:SA:158:TYR:OH	47:SC:222:GLU:OE1	2.24	0.49
49:SG:408:VAL:HG12	49:SG:413:PHE:HA	1.95	0.49
62:SU:203:LEU:HG	62:SU:209:GLN:HG3	1.93	0.49
2:L1:463:U:O2'	2:L1:527:A:N1	2.44	0.49
2:L1:579:A:OP2	51:SI:837:LYS:NZ	2.34	0.49
6:L5:16:VAL:HG21	28:LT:534:SER:HB3	1.93	0.49
20:LL:126:PHE:HB2	20:LL:140:PHE:HD2	1.77	0.49
23:LO:639:GLY:N	53:SL:8:ARG:HH11	2.11	0.49
24:LP:337:UNK:O	24:LP:341:UNK:N	2.46	0.49
25:LQ:285:ARG:HB3	25:LQ:327:HIS:HB3	1.94	0.49
27:LS:233:LEU:H	27:LS:554:ASN:HD21	1.59	0.49
30:LV:144:LEU:HB2	30:LV:155:VAL:HG12	1.94	0.49
46:SB:191:HIS:ND1	46:SB:245:THR:O	2.32	0.49
47:SD:182:SER:OG	47:SD:210:MET:SD	2.71	0.49
50:SH:209:ILE:HG23	50:SH:225:ILE:HD12	1.94	0.49
51:SI:867:THR:HG22	59:SR:62:LYS:HZ2	1.77	0.49
52:SK:129:ARG:NH1	52:SK:132:ARG:HD2	2.28	0.49
54:SM:74:ASP:OD1	54:SM:75:ASP:N	2.46	0.49
61:ST:495:ASN:ND2	61:ST:621:THR:OG1	2.46	0.49
61:ST:561:ILE:HD12	61:ST:564:VAL:HG21	1.93	0.49
2:L1:566:C:H2'	2:L1:567:A:H8	1.77	0.49
18:LJ:449:GLY:O	18:LJ:455:SER:OG	2.30	0.49
20:LL:20:VAL:HG22	20:LL:29:VAL:HG12	1.95	0.49
21:LM:193:THR:HG22	21:LM:241:ILE:HD11	1.95	0.49
23:LO:459:SER:OG	23:LO:462:THR:O	2.29	0.49
23:LO:708:ASP:HB3	23:LO:710:ILE:HG12	1.95	0.49
28:LT:60:ILE:HD12	28:LT:70:PHE:HB2	1.94	0.49
1:L0:423:C:H2'	1:L0:424:G:H8	1.77	0.49
4:L3:116:LEU:HD11	34:NA:341:LEU:HD22	1.94	0.49
6:L5:145:ASP:OD1	6:L5:146:THR:N	2.45	0.49
22:LN:294:TYR:HB3	22:LN:308:SER:HA	1.95	0.49
22:LN:440:LEU:HB2	22:LN:451:PHE:HB2	1.94	0.49
23:LO:849:LEU:HD22	28:LT:897:HIS:HB2	1.94	0.49
30:LV:73:ALA:HB3	30:LV:82:HIS:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SA:172:ASN:HA	45:SA:175:ILE:HD12	1.95	0.49
1:L0:238:G:N2	1:L0:274:C:O2	2.43	0.49
5:L4:196:VAL:HB	5:L4:209:HIS:HB2	1.95	0.49
9:L8:47:ARG:HH11	9:L8:50:GLY:H	1.61	0.49
12:LD:35:TYR:HA	12:LD:61:THR:HG22	1.94	0.49
16:LH:173:LEU:HG	16:LH:190:GLN:HB3	1.94	0.49
22:LN:353:GLU:OE1	22:LN:355:THR:OG1	2.29	0.49
25:LQ:391:ARG:NH1	25:LQ:411:ASN:HD21	2.11	0.49
25:LQ:580:ASP:OD2	25:LQ:621:VAL:HG12	2.13	0.49
45:SA:291:TYR:OH	46:SB:251:ASP:OD1	2.29	0.49
50:SH:281:GLU:OE2	50:SH:285:LYS:HE2	2.13	0.49
58:SQ:119:ARG:HB3	58:SQ:174:LEU:HD22	1.95	0.49
61:ST:700:LEU:HD11	62:SU:464:TRP:HA	1.94	0.49
2:L1:1154:G:H2'	2:L1:1155:G:H8	1.78	0.49
13:LE:81:VAL:O	13:LE:122:SER:OG	2.28	0.49
18:LJ:29:GLN:HG3	18:LJ:332:LYS:NZ	2.27	0.49
22:LN:156:LEU:HB2	22:LN:168:ILE:HB	1.95	0.49
27:LS:204:ASP:OD1	27:LS:207:ALA:HB2	2.13	0.49
29:LU:308:VAL:HA	29:LU:324:SER:HA	1.93	0.49
34:NA:344:GLU:HG3	51:SI:960:ARG:HH21	1.78	0.49
49:SG:234:GLY:O	49:SG:259:LYS:NZ	2.45	0.49
50:SH:96:VAL:HG22	50:SH:122:THR:HA	1.95	0.49
52:SJ:51:GLU:OE1	52:SJ:82:ARG:NH2	2.46	0.49
65:SY:101:THR:HA	65:SY:222:ARG:HH11	1.78	0.49
16:LH:311:TYR:OH	27:LS:394:TRP:O	2.28	0.48
17:LI:576:ARG:HB2	17:LI:578:LEU:HD13	1.93	0.48
18:LJ:35:LEU:HD23	18:LJ:326:LEU:HD13	1.94	0.48
21:LM:406:TYR:O	21:LM:409:SER:OG	2.28	0.48
23:LO:279:PHE:HE2	23:LO:285:ARG:HE	1.59	0.48
23:LO:753:LYS:HD3	28:LT:704:ASP:OD2	2.12	0.48
25:LQ:498:LYS:HG2	25:LQ:527:THR:HG22	1.95	0.48
32:LY:650:UNK:O	32:LY:654:UNK:N	2.46	0.48
38:NE:292:LYS:O	38:NE:296:LYS:N	2.45	0.48
47:SD:171:LEU:HB2	47:SD:237:VAL:HG11	1.95	0.48
49:SG:242:VAL:HG23	49:SG:253:THR:HG22	1.95	0.48
51:SI:861:THR:HA	51:SI:871:MET:HA	1.95	0.48
2:L1:325:G:OP1	12:LD:134:THR:OG1	2.27	0.48
6:L5:222:LYS:HA	6:L5:225:ARG:HH11	1.79	0.48
22:LN:302:ARG:HH11	22:LN:771:GLN:HB2	1.77	0.48
23:LO:846:TYR:HE1	28:LT:909:LEU:HB3	1.77	0.48
25:LQ:426:ARG:HH11	25:LQ:459:LEU:HA	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:926:GLN:NE2	25:LQ:930:GLU:OE2	2.46	0.48
26:LR:39:UNK:N	26:LR:46:UNK:O	2.47	0.48
26:LR:167:UNK:N	26:LR:179:UNK:O	2.46	0.48
26:LR:466:UNK:HA	26:LR:480:UNK:HA	1.95	0.48
33:LZ:137:ARG:NE	33:LZ:159:THR:OG1	2.45	0.48
41:NH:442:PHE:N	41:NH:468:PHE:O	2.45	0.48
16:LH:746:PHE:HE1	16:LH:753:LYS:HG2	1.79	0.48
18:LJ:39:HIS:HE1	18:LJ:62:ARG:NH1	2.10	0.48
18:LJ:172:ARG:HH12	62:SU:370:HIS:HA	1.78	0.48
18:LJ:422:ARG:NH1	18:LJ:461:ASP:OD2	2.45	0.48
20:LL:111:ASP:OD2	20:LL:153:ILE:HG12	2.13	0.48
21:LM:118:THR:O	21:LM:122:VAL:N	2.45	0.48
25:LQ:337:LYS:O	25:LQ:358:SER:N	2.37	0.48
28:LT:641:LEU:HB3	28:LT:654:TRP:HB2	1.94	0.48
29:LU:345:THR:HG22	29:LU:348:MET:HG2	1.93	0.48
45:SA:330:ALA:HB1	45:SA:381:ASN:HA	1.94	0.48
1:L0:295:A:C5	28:LT:381:ARG:NH1	2.80	0.48
1:L0:295:A:N7	28:LT:381:ARG:NH1	2.61	0.48
2:L1:569:C:H5'	59:SR:114:LYS:HZ1	1.79	0.48
6:L5:72:HIS:O	11:LC:79:TYR:OH	2.31	0.48
23:LO:268:PHE:HB2	23:LO:275:LEU:HD23	1.95	0.48
23:LO:570:THR:OG1	23:LO:573:ASN:OD1	2.31	0.48
25:LQ:45:ALA:HB3	25:LQ:48:ASP:HB3	1.95	0.48
28:LT:353:PRO:HG2	28:LT:644:THR:HB	1.96	0.48
29:LU:348:MET:HE3	29:LU:373:ARG:HD2	1.93	0.48
30:LV:51:GLN:HA	30:LV:89:LEU:HB3	1.96	0.48
51:SI:301:ILE:HG22	51:SI:791:ILE:HG22	1.96	0.48
52:SJ:176:ARG:HB2	52:SJ:200:GLU:OE2	2.13	0.48
53:SL:136:TYR:CZ	53:SL:138:ASP:HB3	2.48	0.48
57:SP:1672:UNK:O	57:SP:1676:UNK:N	2.47	0.48
61:ST:431:ARG:NH1	61:ST:477:TYR:HD1	2.11	0.48
63:SV:119:UNK:O	63:SV:123:UNK:N	2.46	0.48
1:L0:306:G:OP1	28:LT:146:GLN:NE2	2.43	0.48
1:L0:308:A:OP2	27:LS:142:LYS:HD3	2.13	0.48
2:L1:113:U:H3	2:L1:301:A:H61	1.62	0.48
2:L1:894:U:O4	2:L1:919:A:N6	2.46	0.48
9:L8:27:PHE:CB	9:L8:49:ARG:HH12	2.26	0.48
16:LH:16:SER:HB3	16:LH:783:LEU:HB2	1.96	0.48
16:LH:53:LYS:HG2	16:LH:65:THR:HG22	1.95	0.48
16:LH:312:LEU:HB2	16:LH:326:LEU:HD11	1.95	0.48
16:LH:348:GLY:HA3	16:LH:352:ASN:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:192:SER:N	20:LL:205:GLY:O	2.46	0.48
23:LO:705:SER:OG	23:LO:706:THR:N	2.47	0.48
26:LR:739:LEU:HD23	26:LR:763:ILE:HD11	1.95	0.48
28:LT:344:ARG:HD3	28:LT:344:ARG:H	1.78	0.48
28:LT:530:ASP:OD1	28:LT:531:PHE:N	2.47	0.48
30:LV:197:ALA:H	30:LV:204:VAL:HG13	1.77	0.48
35:NB:431:THR:OG1	35:NB:432:ASP:N	2.46	0.48
45:SA:389:ILE:HG22	48:SF:62:GLU:HB2	1.94	0.48
52:SK:144:LEU:HB2	52:SK:150:ILE:HD11	1.95	0.48
54:SM:29:ARG:NH1	54:SM:62:LEU:HD12	2.28	0.48
55:SN:39:ILE:HG13	55:SN:243:PHE:HB2	1.96	0.48
2:L1:332:U:H3'	9:L8:54:LYS:HZ2	1.78	0.48
2:L1:1511:U:OP2	55:SN:146:GLY:HA2	2.14	0.48
16:LH:132:PHE:HB3	16:LH:185:PHE:HE2	1.77	0.48
18:LJ:217:ASN:HB3	18:LJ:229:CYS:HB3	1.96	0.48
25:LQ:390:GLN:OE1	25:LQ:413:SER:OG	2.30	0.48
27:LS:462:GLY:HA2	27:LS:527:GLY:HA3	1.96	0.48
30:LV:124:GLN:HG2	30:LV:134:THR:HG22	1.95	0.48
32:LX:9:ARG:HH11	32:LX:207:VAL:HB	1.78	0.48
38:NE:113:UNK:O	38:NE:117:UNK:N	2.46	0.48
49:SG:146:LYS:HZ2	49:SG:205:SER:HA	1.78	0.48
61:ST:573:LEU:HD12	61:ST:591:ILE:HG13	1.94	0.48
4:L3:105:VAL:HA	4:L3:108:LYS:HD3	1.95	0.48
5:L4:77:ARG:NH2	5:L4:82:TYR:OH	2.43	0.48
12:LD:89:ALA:HA	12:LD:104:HIS:HA	1.94	0.48
14:LF:12:VAL:HA	14:LF:23:PHE:HB3	1.96	0.48
16:LH:113:ASN:O	16:LH:115:HIS:ND1	2.47	0.48
22:LN:384:VAL:HG12	22:LN:391:VAL:HG22	1.95	0.48
26:LR:479:UNK:HA	26:LR:488:UNK:HA	1.94	0.48
27:LS:482:LEU:HB2	27:LS:496:ARG:HD3	1.95	0.48
29:LU:82:LYS:NZ	29:LU:134:ASN:OD1	2.45	0.48
32:LX:554:UNK:O	32:LX:558:UNK:N	2.46	0.48
32:LY:740:UNK:O	32:LY:745:UNK:N	2.47	0.48
33:LZ:61:LEU:O	33:LZ:71:ARG:NE	2.46	0.48
37:ND:208:ARG:HH11	37:ND:211:LEU:HD22	1.79	0.48
37:ND:208:ARG:NH1	37:ND:211:LEU:HD22	2.29	0.48
49:SG:280:ARG:HB2	49:SG:301:ASP:HB3	1.95	0.48
49:SG:442:ILE:HA	49:SG:472:PRO:HA	1.96	0.48
52:SK:128:VAL:HB	52:SK:159:LEU:HD12	1.95	0.48
62:SU:189:ALA:HB2	62:SU:236:LEU:HB2	1.95	0.48
62:SU:352:VAL:HG13	62:SU:354:TYR:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SU:393:SER:OG	62:SU:501:TRP:O	2.26	0.48
8:L7:71:HIS:HA	8:L7:74:GLN:HB2	1.96	0.48
18:LJ:133:HIS:HD2	18:LJ:136:ASP:H	1.62	0.48
21:LM:12:ALA:HB2	31:LW:142:GLY:HA3	1.96	0.48
21:LM:206:TYR:CZ	21:LM:209:GLN:HB2	2.49	0.48
25:LQ:254:GLN:HB2	25:LQ:278:ASP:OD2	2.13	0.48
25:LQ:588:ILE:HD11	25:LQ:602:LEU:HD23	1.95	0.48
28:LT:270:SER:HA	28:LT:293:GLU:HG3	1.96	0.48
28:LT:600:ILE:HG13	28:LT:614:LEU:HD11	1.96	0.48
29:LU:258:ILE:HD11	29:LU:461:ILE:HG12	1.96	0.48
29:LU:382:ARG:HD2	45:SA:33:GLU:OE2	2.14	0.48
36:NC:310:GLN:OE1	36:NC:314:ASN:ND2	2.42	0.48
47:SD:168:LYS:HD3	47:SD:238:ASP:OD2	2.14	0.48
50:SH:36:ILE:HG21	50:SH:45:LEU:HD23	1.95	0.48
52:SK:121:LEU:HD11	52:SK:167:ILE:HD13	1.95	0.48
52:SK:175:CYS:SG	52:SK:176:ARG:N	2.86	0.48
54:SM:231:ILE:HG23	54:SM:256:MET:HB3	1.96	0.48
2:L1:1163:A:N3	2:L1:1613:U:O2'	2.44	0.48
8:L7:9:LEU:HD11	8:L7:21:ALA:HB2	1.95	0.48
16:LH:152:ARG:NH1	16:LH:190:GLN:HG2	2.29	0.48
20:LL:9:ALA:HB3	20:LL:63:LEU:HD12	1.96	0.48
21:LM:48:ILE:HD11	21:LM:123:ARG:NH1	2.29	0.48
25:LQ:143:SER:HB3	34:NA:522:ARG:HH12	1.79	0.48
25:LQ:369:TYR:HD2	25:LQ:371:LYS:H	1.61	0.48
25:LQ:803:GLN:O	25:LQ:807:ASP:N	2.42	0.48
25:LQ:884:LYS:HD3	25:LQ:888:ARG:HH22	1.78	0.48
29:LU:376:ARG:HH12	29:LU:382:ARG:HD3	1.79	0.48
30:LV:61:LYS:HG3	30:LV:103:ASP:HA	1.96	0.48
30:LV:237:ARG:HG2	30:LV:239:ASP:H	1.78	0.48
48:SF:51:PHE:HE1	48:SF:114:ILE:HG23	1.79	0.48
51:SI:943:LYS:HD3	51:SI:944:ASN:HB2	1.95	0.48
62:SU:281:LEU:HD21	62:SU:295:LEU:HD21	1.95	0.48
2:L1:9:U:OP1	38:NE:292:LYS:N	2.38	0.48
2:L1:1267:G:N2	2:L1:1442:U:O2	2.43	0.48
9:L8:89:GLU:HA	9:L8:92:ARG:HH11	1.78	0.48
12:LD:125:VAL:HG12	12:LD:139:VAL:HA	1.94	0.48
16:LH:669:ASN:HB3	16:LH:749:ASP:HB3	1.94	0.48
20:LL:259:PRO:O	20:LL:273:LYS:NZ	2.37	0.48
22:LN:140:ASN:HA	47:SD:292:LYS:HZ1	1.79	0.48
22:LN:654:ILE:HD11	22:LN:744:VAL:HG21	1.95	0.48
23:LO:660:SER:HA	23:LO:672:THR:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:628:HIS:HB2	25:LQ:645:GLU:OE2	2.14	0.48
26:LR:670:GLN:HE21	26:LR:693:ARG:NH1	2.12	0.48
32:LX:184:PHE:HD1	32:LX:187:ARG:HE	1.62	0.48
47:SD:253:ILE:O	47:SD:257:SER:N	2.47	0.48
50:SH:119:LYS:HE2	50:SH:165:GLU:OE2	2.14	0.48
51:SI:952:PHE:HD2	51:SI:958:VAL:HG22	1.79	0.48
52:SJ:96:LEU:HD23	52:SJ:130:ILE:HD13	1.96	0.48
52:SK:127:THR:HB	61:ST:713:HIS:HD2	1.79	0.48
2:L1:416:A:N1	32:LX:59:TYR:OH	2.43	0.47
2:L1:903:U:H2'	2:L1:905:A:OP2	2.14	0.47
18:LJ:273:ILE:HG22	18:LJ:283:VAL:HG22	1.96	0.47
20:LL:170:ILE:HD11	20:LL:204:SER:HB3	1.96	0.47
23:LO:70:LEU:HB3	23:LO:82:VAL:HB	1.96	0.47
25:LQ:48:ASP:OD1	25:LQ:63:LEU:N	2.44	0.47
25:LQ:330:GLN:HE22	25:LQ:367:ILE:HG21	1.79	0.47
26:LR:746:TRP:O	26:LR:752:THR:OG1	2.32	0.47
27:LS:321:MET:HB2	27:LS:355:PHE:HD2	1.78	0.47
32:LX:729:UNK:HA	32:LX:764:UNK:HA	1.95	0.47
47:SD:87:VAL:HB	47:SD:100:ARG:HB2	1.96	0.47
49:SG:200:ASP:HB2	49:SG:211:LEU:HD11	1.96	0.47
50:SH:286:SER:OG	51:SI:634:ARG:NH1	2.36	0.47
1:L0:184:U:H2'	1:L0:185:A:H8	1.78	0.47
1:L0:278:G:N2	27:LS:539:ASP:OD2	2.47	0.47
2:L1:341:A:P	30:LV:121:ARG:HH12	2.37	0.47
2:L1:1272:U:H2'	2:L1:1273:G:H8	1.78	0.47
2:L1:1754:A:N7	34:NA:529:ARG:NH2	2.62	0.47
4:L3:4:VAL:H	62:SU:368:SER:HB2	1.79	0.47
5:L4:100:ARG:NH2	5:L4:121:TYR:O	2.47	0.47
18:LJ:213:GLN:HE22	18:LJ:233:ASN:H	1.61	0.47
21:LM:135:LEU:HD12	21:LM:155:ILE:HD11	1.94	0.47
23:LO:86:ALA:O	23:LO:88:ASN:ND2	2.47	0.47
24:LP:50:ILE:HD13	24:LP:106:ASP:OD2	2.14	0.47
24:LP:136:LEU:HD22	24:LP:146:ILE:HD13	1.96	0.47
26:LR:467:UNK:N	26:LR:479:UNK:O	2.47	0.47
26:LR:498:UNK:HA	26:LR:514:UNK:HA	1.96	0.47
30:LV:60:ASN:HD21	30:LV:100:GLU:HB3	1.79	0.47
30:LV:250:GLY:HA3	30:LV:271:GLY:HA2	1.96	0.47
34:NA:365:LEU:HD13	54:SM:227:ARG:NH1	2.26	0.47
54:SM:157:PHE:O	54:SM:159:HIS:N	2.46	0.47
2:L1:332:U:H1'	9:L8:5:ARG:HH12	1.78	0.47
2:L1:1003:A:O2'	2:L1:1005:A:N7	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LR:649:GLU:HA	26:LR:652:ILE:HD12	1.95	0.47
28:LT:131:SER:HB3	28:LT:170:LEU:HD11	1.95	0.47
32:LY:354:UNK:N	32:LY:372:UNK:O	2.47	0.47
49:SG:130:GLY:N	49:SG:410:ASP:OD2	2.41	0.47
50:SH:16:ASN:HB3	51:SI:608:LEU:HB3	1.96	0.47
54:SM:211:ASN:HD22	54:SM:212:ALA:H	1.61	0.47
62:SU:386:LEU:O	62:SU:390:SER:OG	2.33	0.47
1:L0:536:A:H2'	1:L0:537:G:H8	1.78	0.47
2:L1:1622:G:O2'	54:SM:181:ASN:ND2	2.47	0.47
18:LJ:169:ASP:OD2	62:SU:372:SER:HB2	2.14	0.47
18:LJ:362:ARG:NE	27:LS:248:HIS:O	2.39	0.47
18:LJ:495:ILE:HD11	20:LL:544:ASP:OD2	2.14	0.47
21:LM:272:LYS:HE2	21:LM:276:LEU:HD11	1.97	0.47
26:LR:136:UNK:HA	26:LR:143:UNK:HA	1.95	0.47
30:LV:15:GLN:HB2	30:LV:339:HIS:CE1	2.50	0.47
32:LX:534:UNK:O	32:LX:538:UNK:N	2.47	0.47
38:NE:218:LEU:HD22	54:SM:40:LYS:HA	1.96	0.47
45:SA:378:TYR:HE2	45:SA:408:VAL:HA	1.79	0.47
49:SG:327:ASP:OD2	49:SG:405:VAL:N	2.34	0.47
52:SK:150:ILE:HD12	52:SK:160:LEU:HD12	1.97	0.47
54:SM:162:THR:HG22	54:SM:262:ARG:HB2	1.96	0.47
2:L1:1512:G:H2'	2:L1:1513:G:H8	1.79	0.47
17:LI:81:UNK:N	17:LI:87:UNK:O	2.47	0.47
22:LN:478:VAL:HG13	22:LN:486:ILE:HD13	1.97	0.47
22:LN:493:ASP:OD2	22:LN:530:ARG:HG3	2.14	0.47
23:LO:585:TYR:HE1	23:LO:606:VAL:HG21	1.78	0.47
24:LP:67:ARG:NH1	24:LP:84:SER:OG	2.38	0.47
28:LT:307:GLN:NE2	46:SB:422:THR:O	2.38	0.47
28:LT:731:MET:HG3	28:LT:883:THR:HG21	1.96	0.47
32:LX:27:VAL:HG13	32:LX:152:LEU:HD13	1.95	0.47
45:SA:30:ARG:NH2	47:SC:297:ARG:HH12	2.11	0.47
55:SN:172:ASP:OD1	55:SN:172:ASP:N	2.47	0.47
22:LN:201:VAL:O	22:LN:213:TRP:N	2.48	0.47
23:LO:73:ILE:HD12	23:LO:102:VAL:HG21	1.97	0.47
30:LV:82:HIS:HD2	30:LV:91:LEU:HD21	1.79	0.47
30:LV:164:ARG:HH12	30:LV:212:ARG:HG2	1.78	0.47
50:SH:330:LYS:NZ	51:SI:554:TYR:HB3	2.29	0.47
51:SI:968:THR:HG21	51:SI:995:ILE:HD11	1.96	0.47
1:L0:187:A:H2'	1:L0:188:A:H8	1.79	0.47
1:L0:312:U:H1'	1:L0:313:A:H5'	1.97	0.47
1:L0:452:A:H1'	51:SI:1083:ILE:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:115:G:OP2	12:LD:129:ARG:HD2	2.15	0.47
2:L1:312:A:N6	2:L1:352:A:N3	2.63	0.47
7:L6:114:VAL:HG12	7:L6:115:LYS:HD3	1.95	0.47
9:L8:8:ARG:NH1	9:L8:21:PHE:H	2.13	0.47
14:LF:55:VAL:HG12	14:LF:75:VAL:HG22	1.97	0.47
16:LH:34:ILE:HG23	16:LH:90:LYS:HA	1.97	0.47
20:LL:112:LEU:HD21	20:LL:131:LEU:HD11	1.97	0.47
20:LL:545:ALA:O	20:LL:549:CYS:N	2.44	0.47
22:LN:390:LEU:HD23	22:LN:403:THR:HG22	1.97	0.47
25:LQ:672:VAL:HB	25:LQ:684:TRP:HB2	1.95	0.47
27:LS:29:ASP:OD1	27:LS:30:THR:N	2.48	0.47
27:LS:161:ILE:HD13	28:LT:177:LEU:HG	1.97	0.47
27:LS:570:PHE:HE1	27:LS:591:LEU:HD11	1.80	0.47
29:LU:348:MET:HB3	29:LU:373:ARG:NH1	2.30	0.47
29:LU:368:ASP:OD2	53:SL:114:ARG:NH2	2.48	0.47
30:LV:75:GLY:N	30:LV:80:GLN:O	2.47	0.47
31:LW:410:ASN:N	31:LW:410:ASN:OD1	2.47	0.47
31:LW:451:SER:OG	31:LW:452:VAL:N	2.47	0.47
49:SG:235:HIS:ND1	49:SG:257:ASP:OD2	2.32	0.47
49:SG:257:ASP:OD1	49:SG:257:ASP:N	2.48	0.47
50:SH:80:ILE:HD11	51:SI:923:ASP:HA	1.97	0.47
61:ST:592:ARG:HD2	62:SU:348:ASP:OD1	2.14	0.47
62:SU:118:UNK:O	62:SU:122:UNK:N	2.47	0.47
62:SU:190:ASP:OD2	62:SU:240:VAL:HG22	2.15	0.47
65:SY:203:GLN:O	65:SY:207:ARG:N	2.47	0.47
2:L1:334:G:OP2	9:L8:54:LYS:NZ	2.37	0.47
2:L1:569:C:H5'	59:SR:114:LYS:NZ	2.30	0.47
4:L3:82:PRO:HA	55:SN:68:ARG:HB2	1.97	0.47
11:LC:98:ASP:OD2	28:LT:495:ARG:NH1	2.33	0.47
16:LH:855:LEU:HD23	16:LH:858:ILE:HD12	1.95	0.47
21:LM:177:LEU:HD23	21:LM:180:ILE:HD12	1.96	0.47
22:LN:129:ALA:HA	22:LN:530:ARG:HH22	1.79	0.47
22:LN:257:ASP:OD2	22:LN:261:SER:HB2	2.15	0.47
25:LQ:114:LEU:HG	25:LQ:115:LEU:HG	1.97	0.47
28:LT:523:ASP:OD1	28:LT:523:ASP:N	2.48	0.47
28:LT:613:ASP:OD2	28:LT:616:THR:HG22	2.15	0.47
32:LX:184:PHE:HB2	32:LX:187:ARG:HH11	1.80	0.47
49:SG:160:ILE:HG13	49:SG:542:SER:HB3	1.96	0.47
52:SJ:69:ASN:H	52:SJ:73:HIS:CE1	2.33	0.47
56:SO:157:ASP:O	56:SO:161:ALA:N	2.45	0.47
1:L0:83:U:H5'	16:LH:294:LYS:HZ2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:529:LEU:HB3	16:LH:547:VAL:HB	1.97	0.47
16:LH:645:GLU:HB3	16:LH:647:THR:HG23	1.97	0.47
18:LJ:95:LEU:HA	18:LJ:109:ASP:HA	1.96	0.47
23:LO:78:ARG:HH11	23:LO:94:ASN:ND2	2.12	0.47
25:LQ:836:ILE:HA	25:LQ:839:VAL:HG12	1.97	0.47
26:LR:688:LEU:HD12	26:LR:690:HIS:CE1	2.50	0.47
33:LZ:7:HIS:CE1	33:LZ:11:LYS:HZ3	2.32	0.47
45:SA:149:ARG:NH2	46:SB:194:GLU:OE1	2.48	0.47
50:SH:207:ARG:HD2	50:SH:269:GLU:OE2	2.15	0.47
51:SI:938:PRO:HA	51:SI:948:ILE:HA	1.97	0.47
2:L1:6:G:H5"	38:NE:240:ARG:NH1	2.29	0.47
2:L1:1210:C:H2'	2:L1:1211:A:H8	1.79	0.47
3:L2:33:A:H1'	45:SA:32:LYS:NZ	2.30	0.47
18:LJ:492:ARG:HA	18:LJ:495:ILE:HD12	1.97	0.47
23:LO:792:ILE:HD12	28:LT:723:LEU:HD21	1.97	0.47
25:LQ:448:GLY:HA3	25:LQ:476:ILE:HD11	1.97	0.47
25:LQ:601:GLY:N	25:LQ:606:ASP:O	2.48	0.47
26:LR:719:ILE:O	26:LR:758:ARG:NH2	2.48	0.47
27:LS:431:GLU:OE1	27:LS:446:ARG:NH1	2.48	0.47
29:LU:58:PHE:HA	29:LU:375:TRP:HD1	1.80	0.47
49:SG:342:ARG:O	49:SG:344:ARG:NH1	2.47	0.47
51:SI:125:LEU:HD12	51:SI:128:MET:HB3	1.97	0.47
51:SI:244:MET:HB3	51:SI:275:LEU:HD23	1.96	0.47
51:SI:907:THR:HG21	51:SI:912:ARG:HH11	1.80	0.47
53:SL:65:VAL:HG13	53:SL:96:PRO:HA	1.97	0.47
53:SL:164:ILE:HA	53:SL:167:ILE:HD12	1.97	0.47
61:ST:306:UNK:O	61:ST:310:UNK:N	2.48	0.47
61:ST:490:PHE:HZ	61:ST:538:LYS:HZ2	1.60	0.47
1:L0:288:G:O2'	46:SB:416:ALA:O	2.33	0.46
2:L1:6:G:H5"	38:NE:240:ARG:HH12	1.80	0.46
18:LJ:511:LEU:HD13	20:LL:513:LEU:HD23	1.96	0.46
22:LN:196:LYS:HG3	22:LN:246:TYR:CZ	2.50	0.46
24:LP:67:ARG:HH11	24:LP:80:THR:CG2	2.27	0.46
27:LS:581:ASN:HD21	27:LS:585:LYS:H	1.63	0.46
28:LT:589:THR:OG1	28:LT:590:ALA:N	2.47	0.46
28:LT:592:ASP:OD1	28:LT:593:PHE:N	2.48	0.46
29:LU:238:THR:HA	29:LU:244:ILE:HD13	1.98	0.46
31:LW:383:PHE:HA	31:LW:390:LEU:HA	1.96	0.46
32:LX:187:ARG:HH12	32:LX:557:UNK:CB	2.28	0.46
33:LZ:131:ILE:HG12	33:LZ:136:VAL:HG11	1.96	0.46
34:NA:343:GLU:OE2	51:SI:1007:TYR:HE1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SI:926:ILE:HD12	51:SI:928:ILE:HB	1.96	0.46
51:SI:968:THR:HG23	51:SI:1001:VAL:HG12	1.98	0.46
52:SJ:64:LYS:NZ	52:SJ:65:TYR:O	2.34	0.46
54:SM:29:ARG:HH12	54:SM:62:LEU:HD12	1.80	0.46
61:ST:590:ASN:HB3	62:SU:347:PRO:HG3	1.96	0.46
1:L0:489:G:N7	24:LP:128:LYS:NZ	2.58	0.46
2:L1:190:C:N4	2:L1:196:G:O6	2.48	0.46
2:L1:532:U:O2'	14:LF:33:ALA:O	2.33	0.46
3:L2:266:C:O2	3:L2:305:G:N1	2.43	0.46
16:LH:778:ASP:OD1	16:LH:779:ILE:N	2.45	0.46
21:LM:307:LYS:HB2	27:LS:227:LEU:HD12	1.97	0.46
23:LO:416:LEU:O	34:NA:485:SER:OG	2.33	0.46
25:LQ:285:ARG:N	25:LQ:327:HIS:O	2.42	0.46
27:LS:449:ASP:OD1	27:LS:494:TYR:OH	2.30	0.46
28:LT:257:ARG:NH1	28:LT:324:PHE:HD2	2.13	0.46
32:LX:87:GLU:OE1	51:SI:91:ARG:NH2	2.47	0.46
32:LY:359:UNK:O	32:LY:368:UNK:N	2.48	0.46
41:NH:1042:ALA:HB1	41:NH:1047:PRO:HA	1.98	0.46
45:SA:4:ILE:HG23	45:SA:20:VAL:HG21	1.97	0.46
53:SL:161:LYS:HA	53:SL:172:LEU:HD11	1.97	0.46
59:SR:92:CYS:SG	59:SR:93:LEU:N	2.87	0.46
61:ST:563:GLU:O	61:ST:567:PHE:N	2.48	0.46
62:SU:198:GLU:O	62:SU:202:LEU:N	2.30	0.46
1:L0:114:G:H2'	1:L0:115:G:H8	1.80	0.46
1:L0:279:A:H2'	28:LT:405:SER:HA	1.96	0.46
2:L1:123:G:H21	5:L4:146:THR:HG21	1.81	0.46
3:L2:306:G:H2'	3:L2:307:G:C8	2.50	0.46
12:LD:123:VAL:HG23	12:LD:142:VAL:HG22	1.98	0.46
16:LH:172:ARG:HG2	16:LH:192:GLU:HG3	1.96	0.46
22:LN:82:ARG:HH11	22:LN:686:UNK:HA	1.80	0.46
46:SB:73:UNK:O	46:SB:77:UNK:N	2.49	0.46
61:ST:490:PHE:HA	61:ST:493:LEU:HD12	1.97	0.46
62:SU:472:HIS:HB3	62:SU:478:ALA:HB2	1.97	0.46
2:L1:391:A:H2'	2:L1:392:G:H8	1.81	0.46
11:LC:98:ASP:OD2	28:LT:488:ASN:ND2	2.49	0.46
24:LP:67:ARG:HH21	24:LP:88:ILE:HD12	1.81	0.46
25:LQ:352:GLU:HA	25:LQ:366:SER:HA	1.98	0.46
25:LQ:875:GLU:O	25:LQ:879:GLN:N	2.49	0.46
25:LQ:919:GLU:HG3	56:SO:257:GLY:HA2	1.98	0.46
27:LS:245:HIS:O	27:LS:275:TYR:OH	2.28	0.46
30:LV:258:ARG:NH1	32:LY:511:UNK:HA	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SH:7:LYS:HE3	50:SH:77:ARG:HH11	1.79	0.46
50:SH:122:THR:HB	50:SH:130:ILE:HD11	1.98	0.46
51:SI:361:VAL:HG13	51:SI:363:GLY:H	1.80	0.46
54:SM:184:GLU:N	54:SM:220:ARG:HH12	2.13	0.46
54:SM:202:VAL:HA	54:SM:205:ILE:HG22	1.98	0.46
54:SM:220:ARG:HE	54:SM:235:GLN:HE22	1.63	0.46
2:L1:1463:C:H5"	2:L1:1464:G:OP2	2.15	0.46
2:L1:1587:A:H2'	2:L1:1588:G:H8	1.81	0.46
9:L8:110:ARG:HG3	9:L8:121:LEU:HD23	1.97	0.46
16:LH:604:PHE:HE1	17:LI:591:THR:HA	1.80	0.46
20:LL:452:LEU:O	20:LL:455:THR:OG1	2.31	0.46
22:LN:591:ILE:HG23	22:LN:619:THR:HG22	1.97	0.46
25:LQ:189:TRP:CD1	25:LQ:196:CYS:HA	2.49	0.46
26:LR:354:UNK:N	26:LR:363:UNK:O	2.49	0.46
30:LV:187:SER:HB3	30:LV:196:ALA:HB3	1.97	0.46
32:LX:881:UNK:O	32:LX:885:UNK:N	2.48	0.46
32:LY:565:UNK:O	32:LY:583:UNK:N	2.49	0.46
35:NB:434:PHE:HA	52:SK:129:ARG:NH1	2.29	0.46
48:SF:33:LEU:HD11	48:SF:100:ALA:HB1	1.97	0.46
51:SI:137:LEU:HD22	51:SI:232:PHE:HZ	1.80	0.46
54:SM:173:ARG:HE	54:SM:250:VAL:HG22	1.80	0.46
56:SO:100:MET:HA	56:SO:136:SER:HA	1.97	0.46
62:SU:220:LEU:O	62:SU:224:ASN:ND2	2.48	0.46
2:L1:1198:G:H4'	2:L1:1199:G:H8	1.81	0.46
2:L1:1588:G:H1	2:L1:1608:U:H3	1.63	0.46
6:L5:196:GLU:O	6:L5:200:ASN:ND2	2.48	0.46
7:L6:20:ASP:OD2	7:L6:22:HIS:HB2	2.15	0.46
10:L9:79:ARG:HD2	36:NC:323:GLU:HB3	1.98	0.46
17:LI:31:UNK:HA	17:LI:354:UNK:HA	1.97	0.46
23:LO:32:PRO:HG3	23:LO:61:ILE:HD12	1.98	0.46
23:LO:155:SER:HB2	23:LO:160:PHE:HB2	1.96	0.46
24:LP:335:UNK:O	24:LP:339:UNK:N	2.49	0.46
25:LQ:353:LEU:HB3	25:LQ:365:TYR:HB2	1.97	0.46
29:LU:75:LYS:HE3	29:LU:77:TYR:HE1	1.80	0.46
30:LV:237:ARG:HH12	30:LV:287:ASN:ND2	2.13	0.46
31:LW:138:ASP:OD1	31:LW:139:TRP:N	2.49	0.46
45:SA:300:ALA:HB2	45:SA:322:LEU:HD11	1.98	0.46
51:SI:861:THR:O	51:SI:861:THR:OG1	2.33	0.46
54:SM:116:ARG:NH1	54:SM:118:ASN:HB3	2.31	0.46
2:L1:1178:G:H5"	61:ST:84:PRO:HB3	1.97	0.46
3:L2:76:U:O2'	16:LH:868:ASN:ND2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:27:LYS:O	4:L3:31:ALA:N	2.45	0.46
16:LH:769:ASN:N	16:LH:773:ASP:O	2.49	0.46
20:LL:172:LEU:HB3	20:LL:182:MET:HB2	1.96	0.46
22:LN:396:GLU:HA	22:LN:428:ILE:HG12	1.98	0.46
22:LN:427:ASN:HD21	37:ND:190:LEU:HD21	1.81	0.46
26:LR:345:UNK:O	26:LR:353:UNK:N	2.49	0.46
28:LT:128:LEU:HB3	28:LT:140:TYR:HB2	1.98	0.46
29:LU:62:LEU:HD21	29:LU:97:MET:HG2	1.98	0.46
29:LU:67:ARG:HH11	53:SL:123:PRO:HD3	1.81	0.46
29:LU:217:TRP:HB2	29:LU:245:VAL:HG11	1.98	0.46
30:LV:198:GLY:HA2	30:LV:231:VAL:HG13	1.97	0.46
32:LX:118:THR:HB	32:LX:143:GLU:OE2	2.15	0.46
32:LY:290:UNK:HA	32:LY:474:UNK:HA	1.98	0.46
38:NE:204:GLY:HA2	38:NE:207:ARG:HB3	1.96	0.46
47:SC:253:ILE:HG21	47:SC:269:ILE:HD11	1.97	0.46
47:SD:108:THR:O	47:SD:142:ARG:N	2.44	0.46
53:SL:66:LEU:HB3	53:SL:141:LEU:HD11	1.97	0.46
55:SN:77:LYS:HD2	55:SN:130:ARG:HD2	1.97	0.46
57:SP:1766:UNK:O	57:SP:1775:UNK:N	2.49	0.46
65:SY:17:SER:OG	65:SY:18:GLN:N	2.49	0.46
3:L2:37:G:C2	31:LW:431:ARG:NH1	2.84	0.46
16:LH:73:LEU:HD11	16:LH:131:HIS:HB2	1.97	0.46
25:LQ:228:ILE:HB	25:LQ:246:GLY:HA3	1.98	0.46
27:LS:493:LEU:HD21	27:LS:530:LEU:HD22	1.97	0.46
30:LV:333:ASN:OD1	30:LV:333:ASN:N	2.49	0.46
48:SE:10:PRO:HG3	48:SE:125:LEU:HD21	1.97	0.46
48:SF:95:ARG:HD3	48:SF:96:PRO:HD2	1.98	0.46
50:SH:214:LYS:HD3	50:SH:273:GLU:OE2	2.16	0.46
51:SI:289:HIS:HB2	51:SI:815:LEU:HD11	1.97	0.46
62:SU:226:ASP:HB2	62:SU:284:ARG:HH21	1.80	0.46
62:SU:230:SER:HB2	62:SU:288:HIS:CD2	2.51	0.46
2:L1:1605:G:OP1	54:SM:119:ARG:NH1	2.45	0.46
16:LH:271:LEU:HB2	16:LH:285:LEU:HD21	1.97	0.46
16:LH:727:GLN:O	16:LH:736:THR:OG1	2.30	0.46
21:LM:70:SER:HA	21:LM:74:PHE:HB2	1.98	0.46
22:LN:285:CYS:H	22:LN:298:ALA:HB3	1.81	0.46
22:LN:286:LEU:HD23	22:LN:297:SER:HA	1.98	0.46
25:LQ:338:ILE:HA	25:LQ:357:THR:HA	1.97	0.46
26:LR:742:ARG:HH11	34:NA:506:GLU:CD	2.18	0.46
28:LT:299:THR:OG1	28:LT:313:SER:O	2.34	0.46
31:LW:160:LEU:HD13	31:LW:219:VAL:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SA:319:ALA:HB1	45:SA:324:ASN:HB2	1.98	0.46
51:SI:247:ASP:OD2	51:SI:788:TYR:HE1	1.98	0.46
51:SI:366:MET:HA	51:SI:371:VAL:HA	1.97	0.46
55:SN:107:ARG:HE	55:SN:138:VAL:HG22	1.80	0.46
2:L1:388:G:H2'	2:L1:389:G:H8	1.81	0.46
6:L5:42:LEU:HD21	6:L5:90:ILE:HG21	1.98	0.46
10:L9:39:LYS:HG2	10:L9:43:TYR:HE2	1.81	0.46
14:LF:15:ASN:OD1	49:SG:120:ARG:NH2	2.49	0.46
18:LJ:16:LEU:HG	20:LL:532:ARG:NH1	2.30	0.46
22:LN:481:ILE:HB	22:LN:485:LYS:HG3	1.97	0.46
23:LO:743:PHE:HZ	23:LO:778:ILE:HD13	1.79	0.46
25:LQ:405:LEU:HD11	25:LQ:673:VAL:HG11	1.97	0.46
25:LQ:437:LYS:HZ3	25:LQ:481:LEU:N	2.14	0.46
28:LT:516:LYS:NZ	28:LT:573:VAL:HG22	2.31	0.46
30:LV:115:VAL:HG11	30:LV:153:LEU:HD11	1.98	0.46
30:LV:121:ARG:O	30:LV:137:ILE:N	2.40	0.46
47:SD:269:ILE:HB	47:SD:316:VAL:HB	1.98	0.46
49:SG:480:ALA:HB2	49:SG:487:PHE:HB3	1.98	0.46
49:SG:491:SER:OG	49:SG:492:TRP:N	2.48	0.46
54:SM:9:ARG:HD3	54:SM:159:HIS:HB2	1.97	0.46
54:SM:184:GLU:H	54:SM:220:ARG:HH12	1.64	0.46
61:ST:459:LEU:O	61:ST:463:SER:N	2.49	0.46
61:ST:514:TYR:HA	61:ST:519:THR:HG21	1.97	0.46
62:SU:140:UNK:HA	62:SU:242:ASN:HB3	1.97	0.46
2:L1:259:U:OP1	9:L8:75:LYS:NZ	2.49	0.45
2:L1:883:C:H2'	2:L1:884:A:H8	1.81	0.45
8:L7:46:ILE:HG12	8:L7:60:ILE:HG23	1.98	0.45
16:LH:693:ASP:OD2	16:LH:696:PRO:HD3	2.16	0.45
16:LH:719:ASN:HB3	16:LH:746:PHE:HB2	1.98	0.45
20:LL:438:THR:HG21	20:LL:471:ARG:HB3	1.98	0.45
27:LS:315:ALA:HB2	27:LS:321:MET:HG3	1.97	0.45
30:LV:58:ALA:HB2	30:LV:334:GLU:HA	1.97	0.45
30:LV:247:THR:H	30:LV:274:ILE:HD12	1.81	0.45
47:SD:248:ASP:HB2	47:SD:251:ARG:HB3	1.99	0.45
48:SF:18:GLN:NE2	49:SG:399:GLU:O	2.49	0.45
61:ST:630:ASP:OD1	61:ST:631:GLN:N	2.49	0.45
1:L0:170:U:H4'	37:ND:204:ARG:HH21	1.80	0.45
1:L0:184:U:H3	1:L0:213:G:H1	1.63	0.45
2:L1:360:A:H4'	2:L1:362:G:H1'	1.98	0.45
27:LS:260:LYS:HE3	27:LS:310:GLN:HE22	1.82	0.45
29:LU:58:PHE:HD1	29:LU:375:TRP:HE1	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:746:UNK:O	32:LX:766:UNK:N	2.49	0.45
50:SH:37:ARG:HB3	50:SH:40:ASP:OD2	2.16	0.45
56:SO:159:ILE:O	56:SO:163:THR:N	2.46	0.45
1:L0:260:A:C8	65:SY:217:ARG:NH1	2.84	0.45
1:L0:338:A:O2'	1:L0:340:U:O4	2.28	0.45
2:L1:628:G:H21	2:L1:971:A:H62	1.64	0.45
2:L1:1602:C:H5'	54:SM:146:ARG:NH1	2.31	0.45
16:LH:136:LEU:HD12	16:LH:187:VAL:HB	1.98	0.45
16:LH:780:GLU:O	16:LH:782:THR:N	2.49	0.45
20:LL:238:SER:HB3	20:LL:243:SER:HB2	1.98	0.45
21:LM:268:LEU:HD12	21:LM:269:PRO:HD2	1.97	0.45
23:LO:524:ARG:NE	23:LO:526:ASP:OD2	2.49	0.45
23:LO:726:THR:HG22	23:LO:741:MET:HB3	1.98	0.45
25:LQ:38:PRO:HD2	25:LQ:55:LYS:HE3	1.98	0.45
25:LQ:426:ARG:NH1	25:LQ:461:SER:O	2.43	0.45
26:LR:660:LYS:HE2	26:LR:664:GLU:OE2	2.17	0.45
34:NA:380:ASP:N	34:NA:380:ASP:OD1	2.49	0.45
45:SA:13:THR:HG21	45:SA:143:GLN:HG3	1.98	0.45
46:SB:330:LEU:HD22	65:SY:105:ASN:HB3	1.98	0.45
61:ST:515:HIS:HB3	61:ST:518:ILE:HB	1.98	0.45
2:L1:-1:G:C6	29:LU:300:VAL:HG22	2.50	0.45
10:L9:78:ARG:NH2	36:NC:251:GLU:OE1	2.43	0.45
10:L9:112:GLN:NE2	10:L9:153:GLU:OE2	2.49	0.45
11:LC:7:VAL:HG13	11:LC:22:VAL:HB	1.97	0.45
17:LI:260:UNK:O	17:LI:272:UNK:N	2.49	0.45
22:LN:348:VAL:HG13	22:LN:356:LEU:HD21	1.98	0.45
22:LN:535:GLU:O	22:LN:542:VAL:N	2.44	0.45
28:LT:242:ARG:HH22	28:LT:281:ARG:HG2	1.81	0.45
28:LT:556:ASP:HB3	28:LT:572:ALA:HB3	1.97	0.45
30:LV:160:ASN:HA	30:LV:181:GLU:HG2	1.99	0.45
31:LW:53:TYR:HD1	60:SS:863:MET:HB2	1.80	0.45
32:LX:730:UNK:O	32:LX:763:UNK:N	2.50	0.45
45:SA:88:LYS:HZ2	60:SS:331:GLN:HA	1.82	0.45
61:ST:64:ARG:HB3	61:ST:78:ARG:NH1	2.31	0.45
61:ST:404:UNK:O	61:ST:408:UNK:N	2.49	0.45
62:SU:29:UNK:O	62:SU:33:UNK:N	2.49	0.45
1:L0:86:C:H5"	16:LH:295:TRP:HZ2	1.82	0.45
2:L1:233:C:O2	2:L1:234:G:N2	2.49	0.45
6:L5:84:LYS:HG2	6:L5:92:ARG:NH1	2.31	0.45
17:LI:293:UNK:HA	17:LI:304:UNK:HA	1.97	0.45
21:LM:141:ASN:HD22	21:LM:209:GLN:HA	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:579:ARG:HH12	22:LN:659:PHE:C	2.20	0.45
26:LR:745:ASP:OD1	34:NA:508:ARG:NH2	2.50	0.45
28:LT:118:VAL:HA	28:LT:132:THR:HA	1.97	0.45
28:LT:593:PHE:HE1	28:LT:614:LEU:HD21	1.82	0.45
28:LT:833:LEU:O	28:LT:836:THR:OG1	2.29	0.45
30:LV:92:LYS:HD3	30:LV:111:TRP:HZ2	1.81	0.45
34:NA:506:GLU:HA	34:NA:516:SER:HA	1.98	0.45
47:SD:85:LYS:NZ	47:SD:102:LYS:NZ	2.64	0.45
49:SG:138:ASP:OD1	49:SG:500:LYS:NZ	2.35	0.45
53:SL:65:VAL:HB	53:SL:152:ILE:HG23	1.98	0.45
61:ST:493:LEU:HD22	61:ST:528:PHE:HE1	1.81	0.45
2:L1:382:C:H3'	2:L1:383:G:H8	1.81	0.45
10:L9:21:SER:HB3	53:SL:54:GLN:HG3	1.99	0.45
16:LH:660:GLN:HB3	16:LH:707:MET:HB3	1.98	0.45
20:LL:117:LEU:HB3	20:LL:129:PHE:HB2	1.97	0.45
23:LO:47:SER:HB2	23:LO:377:GLY:H	1.82	0.45
23:LO:339:LEU:HB2	23:LO:341:GLN:HG2	1.97	0.45
24:LP:77:VAL:HG12	24:LP:79:LYS:H	1.82	0.45
29:LU:188:HIS:HB3	29:LU:193:THR:HB	1.97	0.45
31:LW:36:GLN:HE21	31:LW:43:ARG:HH21	1.65	0.45
35:NB:504:ASP:HA	35:NB:507:ILE:HG12	1.98	0.45
35:NB:548:LYS:HA	59:SR:139:LYS:HZ3	1.82	0.45
36:NC:262:ILE:HD11	49:SG:320:GLY:HA2	1.97	0.45
46:SB:59:UNK:O	46:SB:63:UNK:N	2.48	0.45
52:SK:181:SER:HB3	52:SK:184:ALA:HB2	1.98	0.45
56:SO:240:ILE:O	56:SO:244:ARG:N	2.44	0.45
61:ST:701:ALA:HA	62:SU:417:HIS:HB2	1.99	0.45
2:L1:538:A:OP2	10:L9:175:ARG:NH1	2.50	0.45
2:L1:910:C:O2	2:L1:915:A:O2'	2.34	0.45
22:LN:561:LYS:HA	22:LN:562:PRO:HD3	1.79	0.45
25:LQ:400:SER:OG	25:LQ:404:LYS:N	2.41	0.45
25:LQ:443:LEU:HB3	25:LQ:459:LEU:HD12	1.98	0.45
28:LT:21:SER:HB2	28:LT:623:ILE:HG12	1.99	0.45
29:LU:273:GLU:OE1	29:LU:276:ASN:ND2	2.44	0.45
30:LV:237:ARG:NE	30:LV:239:ASP:OD2	2.42	0.45
33:LZ:13:LEU:HB3	33:LZ:16:VAL:HG22	1.99	0.45
47:SD:272:LYS:HG3	47:SD:275:CYS:H	1.80	0.45
51:SI:60:ASP:OD1	51:SI:234:PRO:HG3	2.17	0.45
61:ST:537:LEU:HA	61:ST:540:ILE:HD12	1.99	0.45
2:L1:1472:C:N4	2:L1:1534:G:O2'	2.37	0.45
15:LG:65:ARG:HG2	15:LG:67:ARG:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:259:UNK:HA	17:LI:273:UNK:HA	1.99	0.45
18:LJ:234:PHE:CE1	18:LJ:248:ARG:HB2	2.52	0.45
18:LJ:285:ASP:OD1	18:LJ:285:ASP:N	2.50	0.45
21:LM:22:ARG:NH1	29:LU:15:PRO:HG2	2.32	0.45
22:LN:60:LEU:HD23	22:LN:342:LYS:HD3	1.98	0.45
25:LQ:213:LYS:HD3	25:LQ:215:ASP:HB2	1.99	0.45
27:LS:20:GLN:HG2	27:LS:24:LYS:HZ2	1.79	0.45
27:LS:270:LYS:HD2	27:LS:292:GLY:H	1.82	0.45
27:LS:386:ILE:HD13	27:LS:396:MET:HG3	1.98	0.45
29:LU:12:ASP:O	29:LU:23:GLN:NE2	2.50	0.45
29:LU:81:ASN:ND2	29:LU:98:SER:OG	2.49	0.45
29:LU:292:ARG:O	60:SS:288:TYR:OH	2.34	0.45
29:LU:376:ARG:NH1	29:LU:382:ARG:HD3	2.32	0.45
45:SA:87:PRO:HB3	60:SS:323:HIS:HA	1.97	0.45
46:SB:405:ASP:OD1	46:SB:406:LEU:N	2.50	0.45
47:SD:112:ALA:HB3	47:SD:115:GLU:OE2	2.16	0.45
48:SF:18:GLN:HE22	49:SG:400:GLY:HA2	1.81	0.45
50:SH:176:GLN:HE21	50:SH:305:LYS:HD3	1.81	0.45
55:SN:27:ASN:HB2	55:SN:30:LEU:HB2	1.98	0.45
5:L4:21:ASP:OD2	5:L4:23:LEU:HB2	2.16	0.45
6:L5:57:SER:HA	15:LG:53:ILE:HB	1.98	0.45
20:LL:280:GLN:HB2	20:LL:327:THR:HG22	1.99	0.45
22:LN:282:ASP:N	22:LN:282:ASP:OD1	2.50	0.45
22:LN:385:ASN:HB3	22:LN:390:LEU:HB2	1.98	0.45
25:LQ:589:ILE:HD12	25:LQ:623:PHE:HE1	1.81	0.45
28:LT:343:LEU:HG	28:LT:344:ARG:HD3	1.98	0.45
45:SA:95:ASN:ND2	45:SA:117:ASP:OD2	2.49	0.45
45:SA:379:LEU:HD13	45:SA:408:VAL:HG11	1.98	0.45
50:SH:37:ARG:HH12	50:SH:49:GLU:CD	2.19	0.45
54:SM:188:HIS:NE2	54:SM:215:LYS:O	2.47	0.45
1:L0:509:A:H2'	1:L0:510:A:C8	2.52	0.45
3:L2:315:A:H2'	3:L2:316:A:H8	1.82	0.45
7:L6:49:VAL:HB	7:L6:115:LYS:H	1.80	0.45
12:LD:72:THR:O	12:LD:88:ARG:NH1	2.49	0.45
17:LI:304:UNK:O	17:LI:312:UNK:N	2.50	0.45
18:LJ:497:LYS:HD3	20:LL:495:GLN:HE21	1.81	0.45
23:LO:145:HIS:CG	23:LO:165:SER:HG	2.34	0.45
27:LS:436:ASP:HB3	27:LS:444:ILE:HD11	1.98	0.45
28:LT:28:ARG:NH1	28:LT:30:ILE:HD13	2.31	0.45
28:LT:715:GLN:NE2	28:LT:717:ASP:O	2.50	0.45
30:LV:235:SER:HG	30:LV:279:TRP:HD1	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LY:896:UNK:O	32:LY:900:UNK:N	2.49	0.45
33:LZ:89:THR:HB	54:SM:14:TYR:HE2	1.82	0.45
50:SH:18:ARG:NH2	50:SH:101:GLU:OE1	2.50	0.45
50:SH:107:ALA:HB1	50:SH:170:VAL:HG11	1.99	0.45
51:SI:899:VAL:HG12	51:SI:913:ILE:HA	1.98	0.45
62:SU:292:PRO:HG2	62:SU:330:PHE:HE2	1.83	0.45
2:L1:537:G:C4	10:L9:171:ARG:NH1	2.85	0.44
16:LH:714:ASP:HA	16:LH:768:TRP:CE2	2.52	0.44
19:LK:408:UNK:O	19:LK:412:UNK:N	2.50	0.44
21:LM:298:THR:O	21:LM:302:LEU:N	2.38	0.44
23:LO:430:ARG:NE	34:NA:459:LYS:O	2.43	0.44
25:LQ:279:LYS:HD2	25:LQ:337:LYS:HA	1.99	0.44
25:LQ:555:VAL:HB	25:LQ:569:LEU:HD12	1.97	0.44
26:LR:175:UNK:HA	26:LR:191:UNK:HA	1.99	0.44
28:LT:743:ARG:NH1	34:NA:480:GLN:O	2.50	0.44
29:LU:270:ASN:HD21	29:LU:276:ASN:HB2	1.82	0.44
45:SA:248:UNK:O	45:SA:252:UNK:N	2.50	0.44
61:ST:449:LYS:HA	61:ST:452:GLN:HB3	1.99	0.44
2:L1:165:G:H5'	7:L6:8:PRO:HB3	1.98	0.44
5:L4:179:LYS:H	5:L4:195:ILE:HD12	1.82	0.44
6:L5:114:ILE:HD13	6:L5:114:ILE:HA	1.86	0.44
7:L6:113:ILE:HD11	7:L6:124:LEU:HD21	1.99	0.44
13:LE:113:HIS:O	13:LE:117:ARG:N	2.48	0.44
16:LH:712:THR:HG21	16:LH:767:GLY:HA2	1.99	0.44
17:LI:341:UNK:O	17:LI:358:UNK:N	2.50	0.44
23:LO:55:ARG:NH1	23:LO:619:ARG:HB3	2.32	0.44
24:LP:2:SER:OG	24:LP:3:LYS:N	2.50	0.44
25:LQ:391:ARG:HH11	25:LQ:411:ASN:HD21	1.65	0.44
25:LQ:405:LEU:N	25:LQ:417:TRP:O	2.51	0.44
26:LR:13:UNK:HA	26:LR:609:UNK:HA	1.99	0.44
27:LS:482:LEU:HB3	27:LS:494:TYR:HB2	1.99	0.44
30:LV:95:ARG:NH1	30:LV:131:LEU:H	2.14	0.44
40:NG:16:VAL:O	40:NG:31:THR:N	2.50	0.44
46:SB:190:TRP:O	46:SB:245:THR:N	2.46	0.44
46:SB:374:ASP:CA	46:SB:380:ARG:HH12	2.25	0.44
10:L9:151:ASP:HA	49:SG:322:HIS:HE1	1.82	0.44
17:LI:639:SER:HB2	19:LK:502:ARG:NH1	2.32	0.44
18:LJ:504:ILE:O	18:LJ:508:LEU:N	2.49	0.44
21:LM:366:ILE:HD12	21:LM:369:LEU:HD12	1.99	0.44
24:LP:86:TRP:O	24:LP:90:GLN:N	2.49	0.44
28:LT:190:LEU:HD12	28:LT:200:PHE:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LV:66:ARG:HH22	30:LV:148:LYS:HZ3	1.64	0.44
30:LV:293:ASP:HB3	30:LV:296:ILE:H	1.82	0.44
31:LW:258:LEU:HD13	31:LW:268:VAL:HG13	1.99	0.44
48:SF:32:GLN:NE2	48:SF:108:SER:OG	2.41	0.44
62:SU:490:LYS:NZ	62:SU:493:TYR:HE1	2.14	0.44
1:L0:298:A:OP2	28:LT:103:ARG:NH1	2.51	0.44
2:L1:-5:G:N1	31:LW:39:ASP:OD1	2.44	0.44
2:L1:1169:G:N1	2:L1:1575:G:OP2	2.44	0.44
16:LH:215:VAL:O	16:LH:219:ASP:N	2.50	0.44
25:LQ:88:HIS:CD2	25:LQ:91:THR:H	2.32	0.44
26:LR:167:UNK:O	26:LR:179:UNK:N	2.51	0.44
50:SH:148:GLU:N	50:SH:172:SER:OG	2.43	0.44
51:SI:247:ASP:N	51:SI:272:TYR:O	2.44	0.44
61:ST:444:ASN:O	61:ST:448:PHE:N	2.45	0.44
3:L2:78:G:N2	3:L2:83:A:O2'	2.50	0.44
6:L5:58:LEU:HD13	6:L5:167:ARG:NH1	2.33	0.44
6:L5:84:LYS:CG	6:L5:92:ARG:HH12	2.29	0.44
16:LH:656:ASP:OD1	16:LH:657:SER:N	2.51	0.44
18:LJ:30:TYR:HB3	18:LJ:330:ARG:HB3	1.98	0.44
20:LL:277:LYS:HZ1	20:LL:320:ARG:HA	1.82	0.44
25:LQ:386:GLU:O	25:LQ:415:LYS:NZ	2.38	0.44
27:LS:204:ASP:OD2	27:LS:210:LYS:NZ	2.30	0.44
28:LT:538:GLY:HA3	28:LT:575:GLN:NE2	2.32	0.44
32:LY:730:UNK:O	32:LY:763:UNK:N	2.50	0.44
40:NG:81:VAL:O	40:NG:116:GLU:N	2.47	0.44
46:SB:363:LEU:HD23	46:SB:363:LEU:HA	1.79	0.44
48:SF:85:VAL:HG13	49:SG:552:TRP:HB3	2.00	0.44
49:SG:259:LYS:HE2	49:SG:261:ILE:HD11	1.99	0.44
51:SI:71:ILE:HG23	51:SI:136:ASP:H	1.83	0.44
51:SI:108:VAL:HG23	51:SI:114:ARG:HB3	2.00	0.44
51:SI:296:PHE:HZ	51:SI:797:PRO:HD3	1.82	0.44
51:SI:849:LEU:HD23	51:SI:896:PHE:HB3	1.99	0.44
59:SR:46:SER:OG	59:SR:47:SER:N	2.51	0.44
1:L0:462:G:O6	3:L2:55:A:N6	2.50	0.44
2:L1:153:G:H2'	2:L1:154:G:H8	1.83	0.44
11:LC:16:ALA:HB2	11:LC:72:GLY:HA3	2.00	0.44
16:LH:196:VAL:HG11	16:LH:199:SER:HB3	2.00	0.44
21:LM:254:GLN:NE2	21:LM:285:ASN:O	2.50	0.44
23:LO:155:SER:HG	23:LO:203:GLN:NE2	2.15	0.44
23:LO:790:GLN:O	28:LT:723:LEU:N	2.51	0.44
23:LO:833:LYS:HZ1	28:LT:930:MET:HG3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:352:GLU:OE1	25:LQ:364:TYR:OH	2.34	0.44
27:LS:445:ARG:NH2	27:LS:500:MET:O	2.42	0.44
29:LU:311:VAL:HG12	29:LU:322:THR:HB	2.00	0.44
30:LV:258:ARG:NH1	32:LY:510:UNK:O	2.51	0.44
31:LW:350:ASP:OD1	31:LW:363:HIS:HB3	2.18	0.44
33:LZ:63:LEU:HA	38:NE:204:GLY:HA3	1.98	0.44
47:SD:144:TRP:CE2	47:SD:183:HIS:HB3	2.53	0.44
47:SD:228:GLN:HA	47:SD:231:ARG:HB2	2.00	0.44
50:SH:283:ILE:HG22	51:SI:631:ILE:HD11	1.99	0.44
52:SJ:50:LEU:HD11	52:SJ:92:THR:HG21	1.99	0.44
54:SM:192:ASP:OD1	54:SM:193:ASN:N	2.51	0.44
55:SN:92:HIS:HB3	55:SN:177:ARG:HD2	1.99	0.44
62:SU:126:UNK:O	62:SU:130:UNK:N	2.51	0.44
1:L0:435:G:H2'	1:L0:436:G:H8	1.83	0.44
2:L1:591:A:OP1	35:NB:568:LYS:NZ	2.45	0.44
2:L1:1178:G:H2'	2:L1:1179:G:H8	1.83	0.44
5:L4:52:LEU:HD21	5:L4:111:VAL:HG11	1.99	0.44
5:L4:207:LEU:HB3	5:L4:219:VAL:HG13	1.99	0.44
16:LH:51:GLN:HE22	16:LH:465:ASN:HD21	1.66	0.44
22:LN:34:HIS:HB3	22:LN:404:MET:HE1	1.99	0.44
24:LP:407:UNK:O	24:LP:411:UNK:N	2.51	0.44
25:LQ:52:TRP:HZ2	25:LQ:362:ILE:HG13	1.83	0.44
28:LT:394:HIS:CE1	28:LT:449:ARG:HE	2.36	0.44
32:LX:10:ILE:HG23	32:LX:11:PRO:HD3	1.99	0.44
33:LZ:7:HIS:CE1	33:LZ:11:LYS:NZ	2.85	0.44
35:NB:568:LYS:O	35:NB:572:ALA:N	2.46	0.44
51:SI:301:ILE:HD13	51:SI:783:PHE:HE2	1.83	0.44
51:SI:830:ARG:HB3	51:SI:880:TYR:HD1	1.81	0.44
52:SK:82:ARG:HH12	52:SK:118:ARG:CZ	2.31	0.44
52:SK:112:VAL:HG13	52:SK:124:VAL:HB	1.98	0.44
62:SU:255:SER:HA	62:SU:258:GLU:HG2	1.99	0.44
62:SU:279:LEU:HA	62:SU:357:ARG:HH22	1.83	0.44
1:L0:192:G:H2'	1:L0:193:G:H8	1.81	0.44
2:L1:19:A:H5'	51:SI:1156:LYS:NZ	2.33	0.44
2:L1:327:U:H2'	2:L1:328:A:C8	2.52	0.44
5:L4:54:TYR:O	14:LF:15:ASN:ND2	2.50	0.44
21:LM:218:ILE:HD12	21:LM:263:VAL:HG21	1.99	0.44
22:LN:302:ARG:NH1	22:LN:771:GLN:HB2	2.32	0.44
25:LQ:147:VAL:HG12	25:LQ:156:LEU:HD12	1.99	0.44
49:SG:308:SER:OG	49:SG:310:ASN:OD1	2.35	0.44
51:SI:71:ILE:HD12	51:SI:245:LEU:HD22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:248:G:OP2	65:SY:82:ARG:NH2	2.38	0.44
1:L0:307:C:H5'	27:LS:141:ASN:HB2	2.00	0.44
3:L2:91:C:OP1	46:SB:324:LYS:NZ	2.39	0.44
16:LH:411:SER:OG	16:LH:412:ASN:N	2.50	0.44
18:LJ:315:ASN:N	18:LJ:315:ASN:OD1	2.51	0.44
22:LN:119:GLY:HA3	37:ND:194:LYS:HG3	1.99	0.44
24:LP:200:ARG:HH12	24:LP:266:ARG:NH2	2.16	0.44
25:LQ:165:SER:OG	25:LQ:166:ILE:N	2.51	0.44
25:LQ:891:LEU:O	25:LQ:895:GLU:N	2.51	0.44
27:LS:423:LEU:HD13	27:LS:437:LEU:HD21	2.00	0.44
30:LV:185:HIS:HE1	30:LV:187:SER:HB2	1.81	0.44
31:LW:88:GLN:NE2	31:LW:402:ILE:H	2.16	0.44
37:ND:208:ARG:HG2	37:ND:210:ALA:H	1.81	0.44
51:SI:948:ILE:HD13	51:SI:1001:VAL:HG21	2.00	0.44
54:SM:9:ARG:HH21	54:SM:159:HIS:HD2	1.66	0.44
62:SU:375:LEU:HD22	62:SU:453:PRO:HB2	1.99	0.44
63:SV:188:THR:HG23	63:SV:189:PRO:HD3	1.98	0.44
1:L0:178:G:H1	1:L0:219:U:H3	1.66	0.43
1:L0:295:A:C5	28:LT:381:ARG:HD2	2.52	0.43
2:L1:939:A:N6	2:L1:975:C:O2'	2.37	0.43
14:LF:20:ARG:HH11	14:LF:22:GLN:NE2	2.16	0.43
15:LG:65:ARG:HD3	15:LG:67:ARG:NH1	2.33	0.43
16:LH:379:LEU:HB2	27:LS:344:ARG:NH1	2.32	0.43
16:LH:502:LYS:HG3	16:LH:564:PRO:HA	2.00	0.43
16:LH:673:ALA:HB2	16:LH:678:LEU:HD23	1.99	0.43
19:LK:492:ILE:HG22	19:LK:496:LEU:HG	1.98	0.43
25:LQ:10:GLN:HE22	25:LQ:682:ARG:HH11	1.63	0.43
27:LS:435:PHE:HE1	27:LS:443:VAL:HG22	1.83	0.43
29:LU:184:GLY:O	29:LU:197:GLY:N	2.40	0.43
30:LV:179:ASP:HB2	30:LV:214:ARG:NH1	2.33	0.43
33:LZ:81:LYS:NZ	34:NA:445:VAL:HG22	2.33	0.43
33:LZ:138:VAL:HG22	33:LZ:158:VAL:HG12	1.99	0.43
41:NH:405:GLY:N	41:NH:409:ASN:O	2.47	0.43
49:SG:201:ILE:HG21	49:SG:540:LEU:HD11	2.00	0.43
49:SG:256:ARG:NH1	49:SG:549:LEU:O	2.50	0.43
57:SP:1986:UNK:O	57:SP:1990:UNK:N	2.50	0.43
60:SS:280:GLN:HG2	60:SS:284:ARG:HG3	1.99	0.43
1:L0:83:U:H5'	16:LH:294:LYS:NZ	2.33	0.43
1:L0:84:G:OP1	22:LN:325:ASN:ND2	2.38	0.43
1:L0:345:U:H2'	1:L0:346:G:H8	1.83	0.43
6:L5:89:ILE:HA	6:L5:92:ARG:HB3	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:250:GLN:HA	16:LH:257:ARG:NH1	2.33	0.43
18:LJ:258:LEU:HD21	18:LJ:272:LEU:HD11	2.00	0.43
21:LM:255:ILE:HA	21:LM:258:HIS:HD2	1.83	0.43
24:LP:144:VAL:HG21	24:LP:178:VAL:HG11	2.00	0.43
25:LQ:136:LEU:HB3	25:LQ:148:TRP:HB2	1.99	0.43
25:LQ:161:SER:O	25:LQ:187:LYS:NZ	2.51	0.43
25:LQ:536:CYS:H	25:LQ:549:SER:HG	1.63	0.43
28:LT:528:PHE:HE2	28:LT:575:GLN:HA	1.83	0.43
29:LU:288:TYR:O	29:LU:298:LEU:N	2.50	0.43
31:LW:116:ILE:HG12	31:LW:127:ILE:HG22	2.00	0.43
32:LY:485:UNK:O	32:LY:489:UNK:N	2.51	0.43
35:NB:580:ARG:NH1	53:SL:49:SER:HA	2.33	0.43
38:NE:311:VAL:HG23	38:NE:325:ASP:OD2	2.17	0.43
47:SC:149:SER:HB2	47:SC:152:ALA:HB2	2.00	0.43
47:SD:272:LYS:HB3	47:SD:313:HIS:CD2	2.53	0.43
50:SH:192:THR:N	50:SH:246:VAL:O	2.47	0.43
1:L0:295:A:OP1	28:LT:364:HIS:NE2	2.51	0.43
2:L1:29:U:H2'	2:L1:30:G:H8	1.83	0.43
3:L2:79:G:H2'	48:SE:95:ARG:HG3	1.98	0.43
5:L4:125:LYS:HB2	5:L4:226:PHE:HD1	1.83	0.43
17:LI:219:UNK:N	17:LI:231:UNK:O	2.51	0.43
20:LL:126:PHE:N	20:LL:140:PHE:O	2.50	0.43
20:LL:277:LYS:NZ	20:LL:320:ARG:HA	2.32	0.43
21:LM:277:ALA:HB2	27:LS:211:ILE:HD12	2.00	0.43
24:LP:120:ARG:NH1	24:LP:124:THR:HG22	2.33	0.43
25:LQ:51:ILE:HG23	25:LQ:60:VAL:HB	1.99	0.43
25:LQ:224:SER:OG	25:LQ:251:GLN:N	2.32	0.43
27:LS:317:ARG:NH1	27:LS:356:GLU:OE1	2.46	0.43
27:LS:424:ILE:HG12	27:LS:434:GLU:OE2	2.18	0.43
28:LT:257:ARG:HD3	28:LT:263:HIS:CD2	2.54	0.43
28:LT:516:LYS:HZ2	28:LT:573:VAL:HA	1.83	0.43
29:LU:54:PHE:HB3	29:LU:382:ARG:HH21	1.83	0.43
31:LW:177:TYR:CE1	31:LW:183:GLU:HG2	2.53	0.43
38:NE:245:LYS:HG3	38:NE:249:ARG:HH21	1.83	0.43
46:SB:380:ARG:HG2	46:SB:382:ASP:H	1.83	0.43
47:SD:117:VAL:HG12	47:SD:120:GLU:OE2	2.19	0.43
47:SD:253:ILE:HG21	47:SD:269:ILE:HD11	2.01	0.43
48:SF:11:LEU:HA	48:SF:80:PHE:HB2	2.00	0.43
50:SH:60:THR:HG22	50:SH:81:ILE:HA	2.01	0.43
55:SN:90:ASP:OD2	55:SN:173:PRO:HG2	2.18	0.43
2:L1:325:G:H2'	2:L1:326:G:C8	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:24:GLY:O	4:L3:59:GLY:N	2.51	0.43
4:L3:26:ILE:HG13	4:L3:31:ALA:HB2	2.00	0.43
4:L3:83:ALA:HB3	55:SN:69:ASP:HA	2.00	0.43
10:L9:105:LEU:HA	10:L9:108:ARG:HG3	2.01	0.43
16:LH:265:ASP:HB2	16:LH:270:GLN:HB2	2.00	0.43
17:LI:68:UNK:N	17:LI:80:UNK:O	2.52	0.43
18:LJ:263:ASN:OD1	18:LJ:269:GLN:NE2	2.43	0.43
18:LJ:264:PHE:HB2	18:LJ:316:ARG:HH21	1.84	0.43
18:LJ:434:ARG:HB2	18:LJ:470:TYR:HE2	1.82	0.43
21:LM:82:ASP:HB3	21:LM:85:VAL:HG23	2.00	0.43
23:LO:412:ARG:NH1	23:LO:424:THR:HG21	2.34	0.43
24:LP:16:ASP:HA	24:LP:19:VAL:HG12	2.01	0.43
24:LP:196:LEU:HD12	24:LP:199:ARG:HD3	2.00	0.43
28:LT:392:ARG:NE	28:LT:449:ARG:HH12	2.15	0.43
28:LT:595:PRO:HG2	28:LT:638:GLY:HA2	1.98	0.43
31:LW:120:LYS:HZ2	31:LW:200:PRO:HD3	1.82	0.43
31:LW:460:ARG:HH12	60:SS:849:PHE:HD1	1.66	0.43
33:LZ:137:ARG:HG2	33:LZ:161:VAL:HA	2.01	0.43
38:NE:232:GLU:OE2	38:NE:286:ARG:NE	2.52	0.43
45:SA:302:ASN:HB2	45:SA:390:ASP:OD1	2.19	0.43
1:L0:20:C:H2'	1:L0:21:A:H8	1.83	0.43
2:L1:1007:C:H2'	2:L1:1008:G:H8	1.83	0.43
3:L2:31:G:C6	29:LU:347:ARG:HD2	2.54	0.43
5:L4:47:PHE:HD2	5:L4:48:LEU:HD12	1.83	0.43
5:L4:125:LYS:HB2	5:L4:226:PHE:CD1	2.54	0.43
5:L4:180:LEU:HG	5:L4:194:THR:HG22	1.99	0.43
6:L5:216:GLU:OE2	52:SK:174:LYS:HA	2.17	0.43
21:LM:255:ILE:HA	21:LM:258:HIS:CD2	2.54	0.43
23:LO:311:ASN:HB3	23:LO:313:THR:H	1.83	0.43
25:LQ:188:LEU:HD13	25:LQ:241:LYS:HG3	2.00	0.43
25:LQ:439:LEU:HB2	25:LQ:444:LEU:HB2	2.00	0.43
35:NB:439:ASP:CG	52:SK:136:ARG:HH11	2.21	0.43
49:SG:293:ASP:OD2	49:SG:310:ASN:N	2.48	0.43
61:ST:482:GLN:HE22	61:ST:486:LYS:HE3	1.81	0.43
2:L1:900:A:H3'	2:L1:901:G:H21	1.84	0.43
6:L5:84:LYS:HE3	6:L5:92:ARG:HH22	1.83	0.43
6:L5:94:THR:HG22	6:L5:114:ILE:HG13	1.99	0.43
20:LL:29:VAL:HG22	20:LL:51:LEU:HB3	1.99	0.43
20:LL:445:LEU:HD11	20:LL:480:LEU:HD13	2.00	0.43
20:LL:465:ILE:HD12	20:LL:501:TRP:CD1	2.54	0.43
23:LO:347:SER:HB2	23:LO:365:GLU:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LT:488:ASN:OD1	28:LT:489:MET:N	2.51	0.43
28:LT:516:LYS:HZ2	28:LT:573:VAL:HG22	1.84	0.43
30:LV:71:CYS:HB2	30:LV:84:TYR:HB2	2.00	0.43
31:LW:289:MET:HB2	31:LW:303:ILE:HD11	2.01	0.43
31:LW:297:SER:OG	31:LW:298:MET:N	2.52	0.43
33:LZ:81:LYS:HZ3	34:NA:456:PHE:HE1	1.65	0.43
34:NA:330:VAL:HG21	51:SI:932:LEU:HD12	2.01	0.43
35:NB:548:LYS:HA	59:SR:139:LYS:HZ1	1.82	0.43
45:SA:10:GLU:CD	47:SC:231:ARG:HH11	2.22	0.43
49:SG:160:ILE:HG12	49:SG:189:THR:HG22	2.00	0.43
49:SG:399:GLU:OE2	49:SG:417:SER:OG	2.28	0.43
50:SH:94:LYS:HE3	50:SH:127:ASP:OD2	2.18	0.43
51:SI:129:ILE:HG22	51:SI:133:LYS:NZ	2.33	0.43
51:SI:808:PHE:HE2	51:SI:1026:LYS:HB3	1.82	0.43
54:SM:76:GLU:HG2	54:SM:161:PRO:HD3	2.00	0.43
62:SU:156:TRP:O	62:SU:215:ASN:ND2	2.51	0.43
62:SU:261:TRP:O	62:SU:265:LEU:N	2.40	0.43
66:SZ:271:THR:O	66:SZ:275:SER:N	2.49	0.43
2:L1:-3:U:H4'	2:L1:-2:A:OP2	2.18	0.43
2:L1:623:A:H61	2:L1:969:C:H5"	1.84	0.43
2:L1:1134:C:O2'	25:LQ:610:SER:N	2.39	0.43
15:LG:13:ILE:HD11	15:LG:31:GLU:HB2	2.00	0.43
18:LJ:376:ASN:HB3	27:LS:291:VAL:HB	2.01	0.43
21:LM:192:TYR:HE2	21:LM:213:THR:HG22	1.83	0.43
23:LO:398:ARG:HH11	28:LT:938:THR:HG22	1.82	0.43
27:LS:231:LYS:HE3	27:LS:550:SER:HB2	2.00	0.43
28:LT:444:ASP:OD1	28:LT:445:MET:N	2.52	0.43
45:SA:277:ARG:NH2	46:SB:264:GLU:OE1	2.52	0.43
49:SG:443:LEU:N	49:SG:471:GLN:O	2.45	0.43
51:SI:86:ILE:HD11	51:SI:117:PHE:CG	2.54	0.43
51:SI:866:ARG:NH1	59:SR:69:ARG:HH12	2.15	0.43
53:SL:99:THR:HA	53:SL:128:LEU:HD23	2.01	0.43
1:L0:338:A:H5"	1:L0:339:A:OP1	2.19	0.43
18:LJ:117:LEU:HD23	18:LJ:118:LEU:HB2	2.01	0.43
18:LJ:177:ILE:HA	18:LJ:178:PRO:HD3	1.92	0.43
21:LM:8:LEU:HD12	31:LW:144:LEU:HB2	2.01	0.43
24:LP:125:SER:HB3	24:LP:128:LYS:HB2	2.01	0.43
29:LU:177:ASP:OD1	29:LU:178:GLY:N	2.51	0.43
42:NI:52:CYS:HA	42:NI:127:LYS:HA	2.00	0.43
43:NJ:1638:ARG:O	43:NJ:1642:GLU:N	2.43	0.43
49:SG:132:VAL:HG23	49:SG:409:ASP:OD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SG:146:LYS:HZ1	49:SG:205:SER:HA	1.81	0.43
57:SP:1631:UNK:O	57:SP:1635:UNK:N	2.51	0.43
61:ST:386:UNK:O	61:ST:390:UNK:N	2.52	0.43
61:ST:488:ASN:HB2	61:ST:492:ALA:H	1.84	0.43
1:L0:20:C:H2'	1:L0:21:A:C8	2.54	0.43
2:L1:623:A:N6	2:L1:970:A:OP1	2.50	0.43
7:L6:77:LEU:N	7:L6:93:LYS:O	2.51	0.43
10:L9:65:LYS:HG2	64:SX:1039:UNK:HA	2.01	0.43
10:L9:110:GLN:NE2	10:L9:126:ARG:HH11	2.17	0.43
17:LI:189:UNK:HA	17:LI:196:UNK:HA	2.00	0.43
20:LL:140:PHE:HZ	20:LL:178:LYS:HB2	1.84	0.43
20:LL:333:ASN:OD1	20:LL:333:ASN:N	2.52	0.43
21:LM:84:ASN:HB3	31:LW:98:SER:HB3	2.01	0.43
23:LO:288:ASP:O	23:LO:292:PHE:N	2.44	0.43
24:LP:317:LEU:HD23	24:LP:320:ILE:HD12	2.01	0.43
28:LT:487:TYR:CE1	28:LT:494:LEU:HG	2.54	0.43
32:LX:34:ARG:NH1	32:LX:64:LEU:HG	2.30	0.43
32:LY:527:UNK:O	32:LY:531:UNK:N	2.52	0.43
46:SB:162:MET:SD	46:SB:275:TYR:OH	2.70	0.43
46:SB:208:ILE:O	46:SB:212:MET:N	2.32	0.43
48:SF:20:ILE:HD13	48:SF:79:VAL:HG21	2.01	0.43
50:SH:15:GLN:NE2	51:SI:606:VAL:O	2.52	0.43
1:L0:315:U:H5'	31:LW:356:GLY:HA3	2.00	0.43
1:L0:433:C:H2'	1:L0:434:G:C8	2.54	0.43
2:L1:602:U:OP1	61:ST:803:ARG:NH2	2.47	0.43
4:L3:56:LYS:HE2	18:LJ:39:HIS:HD2	1.84	0.43
7:L6:102:VAL:HG13	7:L6:106:LEU:HD12	2.01	0.43
16:LH:370:GLN:HG3	16:LH:386:ASN:HB2	2.00	0.43
22:LN:242:TRP:HZ3	37:ND:202:LYS:HZ2	1.66	0.43
22:LN:432:SER:HB2	22:LN:480:PHE:HE2	1.82	0.43
26:LR:670:GLN:HE21	26:LR:693:ARG:HH12	1.67	0.43
28:LT:186:SER:HG	28:LT:187:ASN:N	2.16	0.43
28:LT:516:LYS:NZ	28:LT:573:VAL:HA	2.33	0.43
29:LU:8:ARG:NH2	31:LW:386:PHE:O	2.37	0.43
29:LU:321:VAL:HG22	29:LU:331:ILE:HG12	2.01	0.43
32:LX:56:LEU:HB3	32:LX:122:CYS:HA	2.00	0.43
45:SA:182:ASP:OD2	45:SA:314:ARG:NH1	2.51	0.43
47:SC:98:ILE:HG21	47:SC:100:ARG:HE	1.83	0.43
61:ST:401:UNK:HA	61:ST:455:LEU:HD21	2.00	0.43
2:L1:397:A:H5"	9:L8:50:GLY:HA3	1.99	0.42
2:L1:1159:C:H5'	54:SM:105:LYS:HZ3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:403:THR:HG23	22:LN:417:VAL:HG21	1.99	0.42
23:LO:114:ALA:HB2	23:LO:152:LEU:HD12	2.01	0.42
23:LO:711:LEU:HA	28:LT:596:GLU:HB2	2.00	0.42
26:LR:545:UNK:O	26:LR:558:UNK:N	2.52	0.42
27:LS:345:LEU:HD12	27:LS:349:GLU:HA	2.01	0.42
30:LV:207:TRP:CE2	30:LV:214:ARG:HB3	2.54	0.42
36:NC:354:GLN:HG2	36:NC:357:LEU:HD12	2.00	0.42
47:SC:144:TRP:CZ3	47:SC:183:HIS:HB3	2.54	0.42
50:SH:174:ILE:O	50:SH:361:ASN:ND2	2.44	0.42
51:SI:833:ARG:NH2	59:SR:141:GLU:OE2	2.51	0.42
52:SK:124:VAL:HG22	52:SK:160:LEU:HD22	2.00	0.42
57:SP:1078:UNK:O	57:SP:1082:UNK:N	2.52	0.42
57:SP:1657:UNK:O	57:SP:1661:UNK:N	2.52	0.42
61:ST:563:GLU:OE2	62:SU:391:PRO:HA	2.18	0.42
61:ST:610:ARG:HE	61:ST:611:SER:H	1.65	0.42
65:SY:100:LYS:HZ1	65:SY:221:GLN:NE2	2.17	0.42
2:L1:445:A:H61	2:L1:462:G:H1'	1.85	0.42
2:L1:598:U:H2'	2:L1:599:A:H8	1.84	0.42
2:L1:1015:U:H5"	2:L1:1016:C:OP2	2.19	0.42
5:L4:71:LYS:HG3	5:L4:91:THR:HB	1.99	0.42
8:L7:138:LYS:HG3	8:L7:152:VAL:HG22	2.01	0.42
11:LC:97:VAL:HG12	11:LC:98:ASP:H	1.83	0.42
18:LJ:215:VAL:HA	18:LJ:230:GLY:HA3	2.00	0.42
20:LL:110:ILE:HD11	20:LL:117:LEU:HD21	2.01	0.42
20:LL:342:ASP:O	20:LL:350:LEU:N	2.46	0.42
26:LR:593:UNK:HA	26:LR:599:UNK:HA	2.01	0.42
27:LS:233:LEU:HD13	27:LS:235:ILE:HB	2.00	0.42
27:LS:272:LEU:HD23	27:LS:272:LEU:HA	1.88	0.42
29:LU:69:GLY:HA2	29:LU:370:GLY:HA2	2.00	0.42
29:LU:385:VAL:HG11	45:SA:47:LEU:HD21	2.01	0.42
30:LV:93:PHE:HE2	30:LV:126:GLN:HE21	1.67	0.42
30:LV:117:LEU:HB2	30:LV:144:LEU:HD22	2.01	0.42
30:LV:247:THR:HG23	30:LV:249:ASN:H	1.85	0.42
30:LV:253:TYR:HB3	30:LV:255:TYR:HE2	1.84	0.42
31:LW:116:ILE:O	31:LW:380:ASN:ND2	2.51	0.42
32:LX:36:GLN:NE2	32:LX:203:ASP:O	2.53	0.42
32:LX:856:UNK:O	32:LX:860:UNK:N	2.52	0.42
49:SG:327:ASP:HB3	49:SG:405:VAL:HG12	2.00	0.42
51:SI:867:THR:HG22	59:SR:62:LYS:HZ1	1.83	0.42
61:ST:214:UNK:O	61:ST:218:UNK:N	2.52	0.42
2:L1:552:G:N1	2:L1:587:C:O2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L2:14:A:H5'	3:L2:15:U:OP2	2.19	0.42
18:LJ:372:HIS:N	27:LS:287:SER:OG	2.44	0.42
20:LL:333:ASN:HD22	27:LS:335:GLN:HA	1.84	0.42
22:LN:382:VAL:HG11	22:LN:755:ILE:HD13	2.00	0.42
23:LO:441:SER:O	23:LO:443:GLU:N	2.52	0.42
25:LQ:414:LEU:HD11	25:LQ:445:VAL:HG11	2.00	0.42
37:ND:211:LEU:HG	37:ND:213:LYS:HG3	2.01	0.42
48:SF:50:GLU:OE2	48:SF:104:THR:OG1	2.32	0.42
51:SI:354:ILE:H	51:SI:354:ILE:HG13	1.73	0.42
51:SI:948:ILE:HB	51:SI:987:TYR:CZ	2.54	0.42
57:SP:1752:UNK:O	57:SP:1756:UNK:N	2.53	0.42
62:SU:384:ALA:O	62:SU:387:THR:OG1	2.36	0.42
1:L0:400:C:H2'	1:L0:401:A:H8	1.83	0.42
2:L1:549:G:H2'	2:L1:550:A:C8	2.55	0.42
3:L2:15:U:OP2	38:NE:224:HIS:NE2	2.52	0.42
5:L4:53:LYS:HZ3	36:NC:293:ASN:HD21	1.67	0.42
6:L5:113:ILE:O	6:L5:117:THR:N	2.50	0.42
7:L6:4:ASN:HA	7:L6:15:THR:HG22	1.99	0.42
7:L6:94:ARG:NH2	30:LV:91:LEU:O	2.52	0.42
11:LC:50:GLU:OE1	11:LC:82:ARG:NH2	2.41	0.42
16:LH:747:ASP:OD2	16:LH:754:LEU:HD21	2.19	0.42
22:LN:385:ASN:HB2	22:LN:433:LEU:HD13	2.01	0.42
25:LQ:137:ILE:HG12	25:LQ:147:VAL:HG22	2.00	0.42
25:LQ:162:HIS:NE2	25:LQ:179:SER:OG	2.35	0.42
25:LQ:479:LEU:HD11	25:LQ:488:LEU:HD13	2.00	0.42
26:LR:688:LEU:HD22	26:LR:688:LEU:HA	1.79	0.42
30:LV:95:ARG:NH1	30:LV:126:GLN:HG3	2.34	0.42
30:LV:104:PHE:HE2	30:LV:106:ILE:HG12	1.84	0.42
32:LX:106:VAL:HG21	32:LX:114:ILE:HD13	2.01	0.42
32:LX:256:UNK:O	32:LX:260:UNK:N	2.52	0.42
32:LX:733:UNK:O	32:LX:737:UNK:N	2.53	0.42
34:NA:340:LEU:HD11	34:NA:345:LEU:HD21	2.02	0.42
49:SG:201:ILE:HD13	49:SG:540:LEU:HD11	2.02	0.42
60:SS:316:ASN:HD21	60:SS:894:LEU:HA	1.84	0.42
65:SY:201:VAL:HA	65:SY:204:HIS:HD2	1.85	0.42
2:L1:1511:U:H2'	2:L1:1512:G:C8	2.55	0.42
16:LH:582:LEU:HD21	16:LH:624:HIS:CD2	2.54	0.42
20:LL:19:TYR:HE1	20:LL:32:GLN:HG2	1.83	0.42
22:LN:127:ASP:HB3	22:LN:130:THR:H	1.84	0.42
23:LO:194:VAL:HA	23:LO:210:SER:HA	2.02	0.42
23:LO:714:PRO:HG3	28:LT:557:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LP:28:GLU:OE2	24:LP:70:ARG:NH1	2.36	0.42
25:LQ:162:HIS:O	34:NA:522:ARG:NH2	2.52	0.42
27:LS:436:ASP:OD1	27:LS:436:ASP:N	2.51	0.42
29:LU:270:ASN:ND2	29:LU:273:GLU:HB2	2.35	0.42
31:LW:63:THR:HG22	31:LW:66:LEU:HD12	2.02	0.42
33:LZ:8:HIS:NE2	33:LZ:9:GLU:OE2	2.53	0.42
37:ND:173:ARG:HH12	65:SY:146:PHE:C	2.20	0.42
46:SB:281:LYS:HA	46:SB:285:PRO:HB3	2.01	0.42
51:SI:996:LEU:HD21	65:SY:37:ARG:HH12	1.85	0.42
52:SK:163:ILE:HD12	52:SK:170:HIS:CD2	2.54	0.42
55:SN:155:ARG:HB3	55:SN:179:GLN:HE22	1.84	0.42
65:SY:105:ASN:HD22	65:SY:108:ARG:NH1	2.17	0.42
2:L1:898:A:N1	2:L1:911:U:O2'	2.46	0.42
3:L2:89:C:O2'	3:L2:91:C:O2'	2.36	0.42
5:L4:103:TYR:CZ	5:L4:189:LEU:HG	2.54	0.42
9:L8:7:SER:HA	9:L8:10:LYS:NZ	2.33	0.42
16:LH:91:ILE:HG12	16:LH:109:VAL:HG22	2.02	0.42
16:LH:319:LYS:HD3	16:LH:339:GLY:H	1.84	0.42
20:LL:151:LEU:HB2	20:LL:165:VAL:HG13	2.02	0.42
22:LN:511:VAL:HG11	22:LN:553:LEU:HD22	2.02	0.42
26:LR:502:UNK:N	26:LR:511:UNK:O	2.52	0.42
28:LT:837:LEU:HA	28:LT:840:PHE:HD2	1.84	0.42
33:LZ:38:ILE:HD13	33:LZ:43:ASP:HB3	2.00	0.42
47:SC:253:ILE:O	47:SC:257:SER:N	2.52	0.42
49:SG:276:THR:O	49:SG:305:ARG:NH2	2.53	0.42
51:SI:67:PRO:HA	51:SI:68:PRO:HD3	1.90	0.42
54:SM:19:GLU:O	54:SM:23:SER:N	2.52	0.42
54:SM:138:ASP:N	54:SM:138:ASP:OD1	2.51	0.42
55:SN:14:GLU:O	55:SN:18:LYS:N	2.36	0.42
55:SN:244:VAL:HG23	55:SN:252:LEU:HB2	2.01	0.42
62:SU:24:UNK:O	62:SU:28:UNK:N	2.53	0.42
9:L8:56:ARG:NH2	9:L8:174:GLY:O	2.52	0.42
16:LH:306:SER:HA	16:LH:346:VAL:HG11	2.00	0.42
16:LH:888:PHE:HD1	21:LM:259:THR:HG22	1.83	0.42
18:LJ:29:GLN:HG3	18:LJ:332:LYS:HZ2	1.85	0.42
19:LK:430:LEU:HA	19:LK:433:ILE:HD12	2.01	0.42
20:LL:130:ASP:OD2	20:LL:137:LEU:HD21	2.20	0.42
23:LO:222:LYS:HA	23:LO:246:TYR:HB2	2.01	0.42
25:LQ:47:GLU:OE2	25:LQ:69:PRO:HG3	2.19	0.42
25:LQ:78:LYS:HD3	25:LQ:657:GLN:HB2	2.02	0.42
27:LS:445:ARG:HH11	27:LS:503:SER:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LT:28:ARG:HH11	28:LT:30:ILE:HD13	1.85	0.42
28:LT:619:CYS:HB3	28:LT:669:ASP:OD2	2.20	0.42
32:LX:531:UNK:O	32:LX:535:UNK:N	2.52	0.42
47:SC:202:ARG:HH11	48:SF:65:LEU:HD13	1.84	0.42
49:SG:289:ARG:HH11	49:SG:294:GLN:CD	2.23	0.42
49:SG:293:ASP:HB2	49:SG:309:ILE:HB	2.02	0.42
49:SG:323:ASP:OD2	49:SG:341:ALA:HB3	2.19	0.42
51:SI:1089:GLN:HB3	65:SY:82:ARG:NE	2.34	0.42
54:SM:249:GLU:OE1	54:SM:253:ARG:NH1	2.53	0.42
1:L0:192:G:H2'	1:L0:193:G:C8	2.54	0.42
1:L0:237:A:H8	1:L0:237:A:H2'	1.76	0.42
1:L0:336:G:O2'	38:NE:285:ARG:NH1	2.52	0.42
2:L1:924:A:H2'	2:L1:925:G:C8	2.55	0.42
5:L4:106:LYS:HB2	5:L4:108:ARG:HH11	1.81	0.42
7:L6:5:ILE:HG12	7:L6:111:LEU:HD11	2.01	0.42
8:L7:82:GLU:OE2	8:L7:89:HIS:HA	2.20	0.42
9:L8:90:LEU:HB3	9:L8:95:THR:HB	2.02	0.42
17:LI:78:UNK:HA	17:LI:90:UNK:HA	2.02	0.42
17:LI:120:UNK:O	17:LI:133:UNK:N	2.53	0.42
20:LL:210:ARG:HH11	28:LT:547:THR:HG22	1.84	0.42
21:LM:236:PRO:HD3	27:LS:218:TYR:HE2	1.85	0.42
21:LM:387:LEU:O	21:LM:391:SER:N	2.53	0.42
23:LO:338:ILE:HG21	23:LO:338:ILE:HD13	1.84	0.42
23:LO:845:THR:OG1	25:LQ:903:GLN:NE2	2.47	0.42
25:LQ:48:ASP:OD1	25:LQ:49:VAL:N	2.49	0.42
25:LQ:454:LEU:HB3	25:LQ:468:ILE:HD12	2.01	0.42
28:LT:257:ARG:HB3	28:LT:263:HIS:HB2	2.02	0.42
28:LT:295:TYR:OH	28:LT:351:GLN:NE2	2.30	0.42
31:LW:201:TYR:OH	31:LW:415:GLU:OE2	2.26	0.42
32:LX:589:UNK:O	32:LX:593:UNK:N	2.52	0.42
34:NA:516:SER:HB3	34:NA:519:GLU:HG3	2.01	0.42
38:NE:278:THR:HA	38:NE:281:LYS:HB3	2.02	0.42
47:SC:177:SER:OG	47:SC:178:GLY:N	2.50	0.42
49:SG:307:TYR:HD1	49:SG:314:GLN:HA	1.85	0.42
50:SH:144:PHE:HB3	50:SH:177:PRO:HB3	2.02	0.42
51:SI:974:GLY:HA3	51:SI:991:PHE:HD1	1.85	0.42
54:SM:85:ASP:OD1	54:SM:85:ASP:N	2.51	0.42
61:ST:696:GLU:HB3	61:ST:698:ILE:HG13	2.01	0.42
66:SZ:258:VAL:O	66:SZ:262:ALA:N	2.51	0.42
1:L0:517:A:H8	1:L0:517:A:OP1	2.03	0.42
2:L1:1503:A:H8	2:L1:1503:A:OP1	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LD:16:GLN:HE22	12:LD:61:THR:HB	1.84	0.42
16:LH:396:ILE:HD12	16:LH:779:ILE:HG23	2.02	0.42
17:LI:550:LEU:HD22	17:LI:553:GLN:HB3	2.02	0.42
17:LI:636:GLN:O	17:LI:639:SER:OG	2.32	0.42
20:LL:25:ASP:OD2	27:LS:590:LYS:HG3	2.20	0.42
20:LL:541:LEU:HD23	20:LL:544:ASP:OD2	2.19	0.42
21:LM:304:GLN:HE21	21:LM:345:ASP:H	1.67	0.42
23:LO:496:THR:HG22	23:LO:513:GLU:HG2	2.01	0.42
24:LP:21:LYS:NZ	24:LP:80:THR:O	2.53	0.42
25:LQ:164:ASP:OD2	25:LQ:183:ASP:HB3	2.20	0.42
25:LQ:243:THR:OG1	25:LQ:244:GLU:N	2.48	0.42
28:LT:133:ASP:OD1	28:LT:134:ASP:N	2.53	0.42
28:LT:604:SER:OG	28:LT:605:LEU:N	2.53	0.42
29:LU:344:HIS:NE2	29:LU:418:HIS:O	2.46	0.42
32:LX:6:ILE:HD11	51:SI:373:ILE:HG13	2.01	0.42
46:SB:227:LEU:HD12	46:SB:231:ILE:HD13	2.02	0.42
47:SC:86:VAL:HG11	47:SC:99:ALA:HB1	2.01	0.42
47:SD:242:ALA:HB3	47:SD:269:ILE:HA	2.02	0.42
48:SE:61:ILE:HD12	48:SE:64:LEU:HD21	2.02	0.42
50:SH:57:GLU:OE2	61:ST:111:GLY:HA2	2.20	0.42
51:SI:107:VAL:HG12	51:SI:354:ILE:HG22	2.01	0.42
52:SJ:116:THR:HB	52:SJ:120:ILE:H	1.85	0.42
60:SS:333:VAL:HA	60:SS:334:PRO:HD3	1.84	0.42
61:ST:490:PHE:CG	61:ST:539:ARG:NH1	2.88	0.42
2:L1:358:U:H2'	2:L1:360:A:C8	2.55	0.42
16:LH:724:ILE:HD13	16:LH:762:TYR:CE1	2.54	0.42
17:LI:260:UNK:N	17:LI:272:UNK:O	2.53	0.42
17:LI:294:UNK:O	17:LI:303:UNK:N	2.53	0.42
17:LI:295:UNK:HA	17:LI:302:UNK:HA	2.02	0.42
18:LJ:57:VAL:HG21	18:LJ:327:LEU:HD11	2.02	0.42
18:LJ:90:ARG:HH11	18:LJ:95:LEU:HD22	1.84	0.42
20:LL:473:LYS:HB2	20:LL:476:LEU:HD23	2.00	0.42
22:LN:156:LEU:N	22:LN:168:ILE:O	2.48	0.42
25:LQ:589:ILE:HD12	25:LQ:623:PHE:CE1	2.55	0.42
26:LR:719:ILE:HG23	26:LR:758:ARG:HE	1.85	0.42
28:LT:142:LYS:HA	28:LT:150:PRO:HA	2.02	0.42
28:LT:229:GLU:HG2	28:LT:245:LYS:HG2	2.02	0.42
29:LU:292:ARG:HE	60:SS:295:VAL:HG12	1.85	0.42
32:LX:59:TYR:HA	32:LX:125:GLN:HB3	2.01	0.42
32:LX:90:GLU:HB2	51:SI:91:ARG:HH21	1.84	0.42
33:LZ:81:LYS:HZ3	34:NA:445:VAL:HG13	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SB:6:UNK:N	46:SB:13:UNK:O	2.53	0.42
46:SB:362:VAL:HG12	46:SB:394:VAL:HG22	2.02	0.42
46:SB:374:ASP:OD1	46:SB:380:ARG:NH1	2.53	0.42
47:SC:189:GLY:O	47:SC:216:ASN:ND2	2.52	0.42
51:SI:247:ASP:HB3	51:SI:357:PRO:HG3	2.00	0.42
55:SN:245:LYS:HB3	55:SN:251:SER:HA	2.01	0.42
1:L0:395:C:H6	33:LZ:117:ARG:NH1	2.17	0.41
2:L1:452:A:H3'	2:L1:453:U:H6	1.85	0.41
3:L2:46:U:H2'	3:L2:47:G:H8	1.84	0.41
8:L7:143:LEU:HD11	29:LU:221:ASN:HD22	1.84	0.41
8:L7:152:VAL:HB	8:L7:183:PHE:HE1	1.85	0.41
13:LE:6:VAL:HG12	13:LE:34:ILE:HD11	2.00	0.41
16:LH:477:VAL:HG12	18:LJ:424:ARG:HG2	2.02	0.41
20:LL:80:MET:HG3	20:LL:86:TRP:HE3	1.85	0.41
20:LL:167:SER:O	20:LL:167:SER:OG	2.37	0.41
23:LO:284:PHE:CE2	23:LO:298:LEU:HD12	2.54	0.41
25:LQ:396:SER:OG	25:LQ:436:CYS:SG	2.68	0.41
25:LQ:852:LEU:O	25:LQ:856:ASN:ND2	2.53	0.41
45:SA:14:GLY:HA3	45:SA:55:PRO:HA	2.02	0.41
49:SG:161:SER:HA	49:SG:525:GLN:HG3	2.02	0.41
49:SG:521:VAL:HG22	49:SG:543:ILE:HG13	2.01	0.41
50:SH:111:LYS:HB2	50:SH:363:SER:HB2	2.01	0.41
51:SI:215:TYR:HB2	51:SI:220:ILE:HD11	2.02	0.41
51:SI:847:LEU:HA	51:SI:898:GLY:HA2	2.02	0.41
52:SK:70:CYS:SG	52:SK:71:ASP:N	2.93	0.41
57:SP:1298:UNK:O	57:SP:1302:UNK:N	2.53	0.41
60:SS:288:TYR:CE2	60:SS:292:ARG:HD2	2.55	0.41
62:SU:278:LEU:HD21	62:SU:319:ALA:HB2	2.01	0.41
62:SU:407:ARG:HE	62:SU:491:LEU:HB3	1.85	0.41
1:L0:233:G:H22	27:LS:317:ARG:NH1	2.18	0.41
2:L1:226:A:H1'	2:L1:227:U:H2'	2.03	0.41
2:L1:368:U:O3'	5:L4:22:LYS:NZ	2.51	0.41
2:L1:1606:C:H2'	2:L1:1607:G:C8	2.55	0.41
5:L4:103:TYR:O	5:L4:182:TYR:OH	2.37	0.41
10:L9:49:LEU:HD13	10:L9:101:VAL:HG12	2.01	0.41
11:LC:55:VAL:HG21	11:LC:105:LEU:HG	2.02	0.41
16:LH:96:ILE:HG12	16:LH:108:THR:HG21	2.02	0.41
17:LI:672:ASN:HD21	19:LK:486:LEU:HD12	1.84	0.41
18:LJ:507:MET:HA	19:LK:502:ARG:HG2	2.01	0.41
21:LM:258:HIS:HE1	21:LM:282:ILE:HG23	1.85	0.41
22:LN:66:ARG:NE	22:LN:88:GLU:OE1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:105:SER:HA	22:LN:153:GLN:HG2	2.01	0.41
22:LN:231:VAL:HG22	22:LN:265:TRP:HH2	1.86	0.41
24:LP:67:ARG:HH22	24:LP:84:SER:HB2	1.85	0.41
24:LP:193:ILE:HG21	24:LP:266:ARG:HB3	2.02	0.41
30:LV:235:SER:HB3	30:LV:244:ALA:HB3	2.02	0.41
32:LX:28:ILE:HG12	32:LX:201:VAL:HB	2.01	0.41
49:SG:195:GLN:HE21	49:SG:213:TYR:HB2	1.85	0.41
50:SH:9:THR:HB	50:SH:31:ILE:HG22	2.02	0.41
51:SI:1049:ASN:HA	51:SI:1050:PRO:HD3	1.83	0.41
2:L1:993:A:H5"	2:L1:994:G:OP2	2.20	0.41
3:L2:37:G:O4'	31:LW:431:ARG:NH2	2.53	0.41
16:LH:362:GLU:HB2	16:LH:453:HIS:HE1	1.85	0.41
18:LJ:101:ALA:HA	18:LJ:126:PRO:HB3	2.02	0.41
23:LO:7:PHE:HZ	23:LO:10:LEU:HB2	1.84	0.41
23:LO:746:ASN:OD1	23:LO:777:ARG:NE	2.42	0.41
24:LP:265:LEU:HA	24:LP:268:ASP:OD2	2.20	0.41
24:LP:419:UNK:O	24:LP:423:UNK:N	2.54	0.41
25:LQ:271:PHE:HD1	25:LQ:286:ILE:H	1.68	0.41
25:LQ:414:LEU:HB3	25:LQ:428:PHE:HB2	2.01	0.41
25:LQ:446:ILE:HG22	25:LQ:479:LEU:HD21	2.01	0.41
25:LQ:594:ASP:N	25:LQ:594:ASP:OD1	2.43	0.41
29:LU:37:ARG:HG3	31:LW:447:ASN:HA	2.02	0.41
35:NB:538:ARG:NH2	51:SI:910:GLY:O	2.53	0.41
38:NE:226:ASP:OD1	38:NE:227:LYS:N	2.53	0.41
41:NH:579:LYS:N	41:NH:618:ILE:O	2.52	0.41
47:SD:159:LEU:HD11	47:SD:317:VAL:HG21	2.03	0.41
47:SD:258:HIS:HE1	47:SD:297:ARG:HH11	1.68	0.41
51:SI:141:LEU:HB3	51:SI:170:VAL:HG23	2.02	0.41
51:SI:293:VAL:HG13	51:SI:1022:LEU:HD21	2.02	0.41
55:SN:71:ASN:HB2	55:SN:123:ASP:H	1.84	0.41
59:SR:51:GLY:HA2	59:SR:77:ILE:HG13	2.02	0.41
61:ST:530:GLU:OE1	61:ST:531:GLN:NE2	2.53	0.41
62:SU:472:HIS:CD2	62:SU:474:HIS:H	2.38	0.41
1:L0:69:U:H5	16:LH:426:ARG:HH11	1.68	0.41
1:L0:96:C:O2	1:L0:155:A:O2'	2.31	0.41
1:L0:181:A:H2'	1:L0:182:G:H8	1.85	0.41
2:L1:354:C:OP1	9:L8:14:THR:OG1	2.31	0.41
2:L1:454:U:OP1	2:L1:455:C:N4	2.53	0.41
2:L1:1482:C:O2'	11:LC:72:GLY:O	2.39	0.41
3:L2:105:C:H5"	45:SA:372:LYS:HZ3	1.85	0.41
5:L4:179:LYS:HZ2	5:L4:179:LYS:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:674:THR:N	16:LH:677:THR:O	2.53	0.41
17:LI:314:UNK:HA	17:LI:321:UNK:HA	2.02	0.41
21:LM:157:LEU:HD23	21:LM:157:LEU:HA	1.88	0.41
25:LQ:397:ILE:HD11	25:LQ:675:SER:HB3	2.02	0.41
26:LR:419:UNK:N	26:LR:433:UNK:O	2.53	0.41
26:LR:523:UNK:N	26:LR:529:UNK:O	2.53	0.41
27:LS:351:THR:OG1	27:LS:352:GLN:N	2.53	0.41
27:LS:562:LEU:HD22	27:LS:579:VAL:HG11	2.02	0.41
28:LT:225:THR:OG1	28:LT:227:THR:O	2.32	0.41
28:LT:366:MET:HE2	28:LT:651:ILE:HD13	2.02	0.41
29:LU:188:HIS:CE1	29:LU:190:GLU:HB2	2.55	0.41
30:LV:185:HIS:CE1	30:LV:234:THR:H	2.38	0.41
32:LX:154:SER:O	32:LX:158:UNK:N	2.53	0.41
32:LX:586:UNK:N	32:LX:631:UNK:O	2.53	0.41
32:LY:516:UNK:N	32:LY:566:UNK:O	2.54	0.41
34:NA:307:ILE:O	34:NA:311:ILE:N	2.48	0.41
34:NA:331:LYS:HE3	51:SI:937:PHE:HE2	1.86	0.41
40:NG:21:ALA:N	40:NG:84:ARG:O	2.53	0.41
47:SC:244:VAL:HG23	47:SC:249:GLN:HG3	2.00	0.41
47:SD:249:GLN:HA	47:SD:252:ILE:HG22	2.02	0.41
48:SE:46:ARG:CZ	65:SY:108:ARG:HD3	2.51	0.41
54:SM:131:CYS:SG	54:SM:136:THR:OG1	2.62	0.41
54:SM:241:THR:OG1	54:SM:244:GLY:O	2.32	0.41
55:SN:30:LEU:HD13	55:SN:30:LEU:HA	1.91	0.41
61:ST:477:TYR:OH	61:ST:497:ASP:OD1	2.30	0.41
1:L0:433:C:H2'	1:L0:434:G:H8	1.85	0.41
2:L1:-2:A:OP2	2:L1:-2:A:H4'	2.20	0.41
3:L2:37:G:C4	31:LW:431:ARG:NH1	2.88	0.41
4:L3:82:PRO:HG2	4:L3:85:PHE:HB2	2.01	0.41
6:L5:100:ASN:ND2	6:L5:180:ARG:HH11	2.15	0.41
6:L5:207:THR:HA	6:L5:212:LYS:NZ	2.35	0.41
9:L8:12:SER:OG	9:L8:16:ALA:N	2.53	0.41
16:LH:350:GLN:HE22	27:LS:309:GLN:HE22	1.67	0.41
17:LI:579:LEU:HD11	17:LI:613:PHE:HE2	1.86	0.41
18:LJ:52:PRO:HB3	18:LJ:309:PRO:HD2	2.02	0.41
18:LJ:172:ARG:NH1	62:SU:370:HIS:HA	2.35	0.41
18:LJ:404:ALA:HB2	18:LJ:417:VAL:HG11	2.02	0.41
20:LL:301:LEU:HD12	20:LL:317:LEU:HD11	2.02	0.41
20:LL:520:MET:O	20:LL:524:SER:OG	2.27	0.41
25:LQ:126:LEU:O	25:LQ:139:GLY:N	2.41	0.41
28:LT:881:TYR:HA	28:LT:884:PHE:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LV:120:ASP:O	30:LV:122:SER:N	2.54	0.41
30:LV:125:PHE:HB2	30:LV:133:TYR:HB3	2.02	0.41
30:LV:125:PHE:N	30:LV:133:TYR:O	2.46	0.41
31:LW:317:THR:HA	31:LW:318:PRO:HD3	1.90	0.41
34:NA:344:GLU:OE1	61:ST:102:ARG:NH2	2.52	0.41
34:NA:444:LEU:HG	34:NA:448:LEU:HD23	2.03	0.41
35:NB:594:GLU:HB2	47:SC:156:MET:HE2	2.02	0.41
46:SB:151:LYS:HZ2	47:SD:222:GLU:CD	2.24	0.41
51:SI:833:ARG:HH12	59:SR:141:GLU:CG	2.34	0.41
56:SO:196:ASP:O	56:SO:200:ARG:N	2.54	0.41
61:ST:533:LYS:O	61:ST:539:ARG:NE	2.54	0.41
62:SU:495:MET:O	62:SU:499:LEU:N	2.53	0.41
1:L0:114:G:H2'	1:L0:115:G:C8	2.56	0.41
2:L1:1437:U:H2'	2:L1:1438:G:H8	1.86	0.41
6:L5:62:VAL:HG13	6:L5:89:ILE:HG21	2.02	0.41
10:L9:78:ARG:HH12	36:NC:251:GLU:CG	2.33	0.41
16:LH:459:ILE:HB	16:LH:469:ASN:HB2	2.03	0.41
20:LL:77:ILE:HG12	20:LL:87:LEU:HD23	2.01	0.41
22:LN:213:TRP:NE1	22:LN:225:LEU:HB3	2.36	0.41
23:LO:661:LEU:HD13	23:LO:661:LEU:HA	1.85	0.41
25:LQ:162:HIS:CG	25:LQ:181:SER:HG	2.38	0.41
25:LQ:449:THR:OG1	25:LQ:451:ASN:O	2.33	0.41
25:LQ:606:ASP:OD2	50:SH:239:PRO:HG3	2.19	0.41
26:LR:598:UNK:HA	26:LR:612:UNK:HA	2.03	0.41
31:LW:279:SER:OG	31:LW:280:ILE:N	2.54	0.41
31:LW:386:PHE:HE1	31:LW:408:GLU:OE2	2.03	0.41
32:LX:294:UNK:O	32:LX:298:UNK:N	2.54	0.41
38:NE:238:ILE:O	38:NE:242:MET:N	2.53	0.41
40:NG:31:THR:HA	40:NG:38:THR:HA	2.03	0.41
49:SG:295:LEU:O	49:SG:307:TYR:N	2.52	0.41
49:SG:345:THR:HG22	49:SG:360:ARG:HG2	2.02	0.41
52:SJ:68:LEU:HD12	52:SJ:73:HIS:HE1	1.85	0.41
61:ST:593:LEU:HD11	61:ST:596:TYR:HD1	1.86	0.41
1:L0:313:A:OP1	31:LW:357:SER:N	2.43	0.41
2:L1:10:G:H1	3:L2:21:C:H42	1.69	0.41
2:L1:557:G:OP1	51:SI:967:LYS:NZ	2.34	0.41
2:L1:894:U:H2'	2:L1:895:G:C8	2.55	0.41
3:L2:64:A:OP2	28:LT:392:ARG:NH2	2.53	0.41
3:L2:80:U:OP2	48:SE:95:ARG:NE	2.42	0.41
5:L4:163:ASP:OD2	5:L4:165:ALA:HB3	2.20	0.41
5:L4:183:VAL:HG11	5:L4:220:THR:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L7:12:ALA:O	8:L7:14:THR:N	2.54	0.41
16:LH:484:VAL:HG12	16:LH:485:ARG:H	1.86	0.41
16:LH:572:GLY:HA2	16:LH:586:SER:HA	2.03	0.41
20:LL:189:SER:HB3	20:LL:206:ALA:HB1	2.03	0.41
23:LO:52:TYR:HE2	23:LO:54:HIS:HD2	1.67	0.41
23:LO:120:GLN:HB3	23:LO:122:TRP:HE1	1.85	0.41
23:LO:472:HIS:HE1	23:LO:498:ARG:HB3	1.84	0.41
24:LP:104:PRO:HG2	45:SA:142:LEU:HD11	2.02	0.41
24:LP:318:ARG:O	24:LP:322:LEU:N	2.50	0.41
25:LQ:472:HIS:HB3	25:LQ:494:ASP:OD2	2.21	0.41
25:LQ:898:LEU:HD23	25:LQ:898:LEU:HA	1.82	0.41
27:LS:544:VAL:HG22	27:LS:551:VAL:HG22	2.03	0.41
28:LT:38:PRO:HB3	28:LT:300:GLN:HE21	1.85	0.41
28:LT:323:VAL:HG21	28:LT:341:ARG:NH1	2.35	0.41
28:LT:727:PRO:HG2	28:LT:730:LYS:HG3	2.03	0.41
28:LT:732:ASN:HB3	34:NA:483:TYR:HE1	1.85	0.41
30:LV:63:LYS:HB3	30:LV:106:ILE:HD11	2.02	0.41
40:NG:60:ALA:HB1	40:NG:101:ALA:HB2	2.03	0.41
47:SC:288:ARG:HH11	53:SL:64:GLN:HE22	1.69	0.41
47:SD:196:ALA:O	47:SD:220:ILE:N	2.53	0.41
54:SM:50:GLU:OE2	54:SM:54:LYS:HE3	2.20	0.41
54:SM:102:GLN:HB3	54:SM:174:HIS:CD2	2.55	0.41
57:SP:1372:UNK:O	57:SP:1376:UNK:N	2.54	0.41
65:SY:161:ARG:NE	65:SY:164:ASN:O	2.47	0.41
66:SZ:275:SER:O	66:SZ:279:ILE:N	2.54	0.41
1:L0:205:C:H2'	1:L0:206:A:C8	2.56	0.41
1:L0:232:U:H2'	1:L0:233:G:C8	2.56	0.41
1:L0:395:C:H6	33:LZ:117:ARG:HH12	1.68	0.41
2:L1:1132:A:H62	25:LQ:598:LYS:HZ2	1.67	0.41
10:L9:139:GLN:HE22	14:LF:65:GLY:HA3	1.85	0.41
16:LH:712:THR:O	16:LH:719:ASN:ND2	2.52	0.41
17:LI:713:LEU:HB2	22:LN:37:ARG:HH12	1.85	0.41
18:LJ:229:CYS:HB2	18:LJ:258:LEU:HD13	2.03	0.41
20:LL:24:LEU:HG	27:LS:261:PRO:HB3	2.02	0.41
20:LL:162:GLN:HA	20:LL:174:ASP:HA	2.03	0.41
25:LQ:233:ILE:HA	25:LQ:241:LYS:HZ2	1.86	0.41
25:LQ:898:LEU:HD21	26:LR:753:HIS:CE1	2.55	0.41
27:LS:130:ASP:OD1	28:LT:177:LEU:HD12	2.21	0.41
27:LS:491:VAL:HB	27:LS:511:LEU:HB2	2.03	0.41
28:LT:579:ARG:HA	28:LT:579:ARG:HD3	1.95	0.41
29:LU:64:TYR:HB3	53:SL:127:ARG:CZ	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LU:299:ASN:HA	29:LU:457:ARG:NH1	2.36	0.41
31:LW:173:TYR:CE2	31:LW:186:ARG:NH1	2.89	0.41
31:LW:186:ARG:HD3	33:LZ:41:ARG:HE	1.85	0.41
33:LZ:151:THR:HG22	33:LZ:153:ASN:H	1.85	0.41
40:NG:103:ARG:O	40:NG:107:ARG:N	2.50	0.41
50:SH:347:ASN:ND2	50:SH:349:ASP:OD2	2.54	0.41
51:SI:1119:ILE:HD12	58:SQ:190:LYS:HG3	2.03	0.41
52:SJ:89:PRO:HG2	52:SJ:134:PHE:HZ	1.86	0.41
52:SK:156:GLU:OE2	61:ST:713:HIS:NE2	2.54	0.41
55:SN:106:LEU:HD12	55:SN:106:LEU:HA	1.93	0.41
55:SN:231:GLN:NE2	63:SV:189:PRO:O	2.54	0.41
61:ST:627:HIS:CE1	61:ST:632:CYS:HB2	2.56	0.41
65:SY:105:ASN:O	65:SY:109:THR:N	2.46	0.41
1:L0:105:G:H2'	1:L0:106:A:H8	1.86	0.41
1:L0:546:G:OP2	1:L0:547:C:OP2	2.38	0.41
2:L1:19:A:H61	53:SL:165:ARG:HH12	1.68	0.41
2:L1:526:A:P	14:LF:93:ARG:HH21	2.44	0.41
2:L1:1132:A:O5'	2:L1:1134:C:N4	2.52	0.41
2:L1:1202:A:H2	2:L1:1210:C:H4'	1.86	0.41
3:L2:253:G:N7	49:SG:551:ARG:NE	2.68	0.41
5:L4:122:LYS:HG2	5:L4:164:LEU:HD21	2.03	0.41
8:L7:94:ALA:HB3	8:L7:128:ASP:OD2	2.21	0.41
13:LE:122:SER:OG	13:LE:123:GLY:N	2.53	0.41
14:LF:20:ARG:NH1	14:LF:22:GLN:HE21	2.19	0.41
16:LH:55:TYR:HB3	16:LH:383:LEU:HD21	2.01	0.41
16:LH:603:ASN:HD22	17:LI:592:ARG:HH21	1.69	0.41
18:LJ:278:ASP:O	62:SU:331:ASN:ND2	2.53	0.41
22:LN:37:ARG:HH11	22:LN:758:ASN:HD21	1.68	0.41
22:LN:125:GLU:O	22:LN:134:LEU:N	2.52	0.41
22:LN:287:THR:HG21	22:LN:337:CYS:HA	2.03	0.41
22:LN:309:GLN:HE21	22:LN:318:ASN:HA	1.86	0.41
23:LO:54:HIS:CD2	23:LO:80:ILE:HD12	2.55	0.41
23:LO:340:LYS:H	34:NA:479:ALA:HB3	1.85	0.41
23:LO:723:PRO:HG3	23:LO:745:LEU:HD21	2.03	0.41
25:LQ:471:ALA:O	25:LQ:498:LYS:NZ	2.37	0.41
27:LS:137:ILE:HD11	27:LS:155:ILE:HD12	2.03	0.41
29:LU:75:LYS:HE2	29:LU:355:LYS:HD2	2.02	0.41
29:LU:280:ALA:HB2	29:LU:311:VAL:HG13	2.03	0.41
30:LV:251:TYR:CD1	30:LV:267:ASP:HB3	2.56	0.41
31:LW:214:LEU:HD13	31:LW:249:LEU:HD21	2.02	0.41
32:LX:735:UNK:O	32:LX:739:UNK:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:NK:176:PRO:O	44:NK:180:LEU:N	2.42	0.41
45:SA:26:ASP:OD2	45:SA:123:LEU:HD22	2.21	0.41
45:SA:29:SER:HA	45:SA:34:VAL:HG11	2.03	0.41
46:SB:191:HIS:NE2	46:SB:215:ARG:HG3	2.36	0.41
49:SG:260:LEU:HD23	49:SG:260:LEU:HA	1.79	0.41
49:SG:549:LEU:HB2	49:SG:552:TRP:HZ3	1.86	0.41
50:SH:312:ARG:NH1	50:SH:342:VAL:HG11	2.36	0.41
51:SI:82:LYS:HD2	51:SI:82:LYS:H	1.85	0.41
51:SI:179:SER:OG	51:SI:182:THR:OG1	2.32	0.41
51:SI:631:ILE:HD12	51:SI:631:ILE:HA	1.95	0.41
51:SI:831:ARG:HD3	51:SI:838:ILE:HA	2.03	0.41
52:SK:77:LEU:HA	52:SK:77:LEU:HD23	1.87	0.41
53:SL:108:LYS:NZ	53:SL:135:THR:HG21	2.36	0.41
53:SL:171:PRO:HA	53:SL:184:LYS:HB2	2.02	0.41
54:SM:166:SER:O	54:SM:257:ARG:N	2.53	0.41
55:SN:189:TYR:OH	55:SN:231:GLN:O	2.31	0.41
62:SU:399:ILE:HG23	62:SU:484:PHE:HE2	1.86	0.41
62:SU:421:PHE:HE1	62:SU:438:LEU:HD12	1.85	0.41
1:L0:423:C:H2'	1:L0:424:G:C8	2.55	0.41
1:L0:527:U:H2'	1:L0:528:G:C8	2.56	0.41
2:L1:482:U:H2'	2:L1:483:A:H8	1.86	0.41
2:L1:1132:A:C8	25:LQ:571:GLY:HA3	2.55	0.41
2:L1:1788:G:H2'	2:L1:1789:G:H8	1.86	0.41
16:LH:303:LEU:HD22	16:LH:312:LEU:HD11	2.03	0.41
16:LH:561:LEU:HD12	16:LH:562:PRO:HD2	2.02	0.41
17:LI:79:UNK:N	17:LI:89:UNK:O	2.54	0.41
18:LJ:200:SER:OG	18:LJ:201:SER:N	2.53	0.41
18:LJ:288:ASP:OD2	18:LJ:293:LYS:NZ	2.35	0.41
22:LN:427:ASN:O	22:LN:444:ARG:NH1	2.54	0.41
23:LO:102:VAL:HG22	23:LO:113:LEU:HD13	2.03	0.41
25:LQ:129:PHE:HB2	25:LQ:136:LEU:HA	2.03	0.41
25:LQ:392:THR:OG1	25:LQ:393:ASP:N	2.54	0.41
33:LZ:29:ASP:OD2	33:LZ:41:ARG:NH1	2.54	0.41
49:SG:239:ILE:HA	49:SG:255:GLY:HA3	2.01	0.41
51:SI:59:VAL:HG12	51:SI:61:ARG:HG3	2.03	0.41
51:SI:564:ILE:O	51:SI:568:ARG:N	2.48	0.41
61:ST:6:LEU:HD21	61:ST:10:LYS:HE3	2.03	0.41
1:L0:121:G:H1'	1:L0:124:A:H61	1.86	0.40
1:L0:328:A:OP2	31:LW:231:LYS:HE3	2.21	0.40
1:L0:545:G:H2'	24:LP:79:LYS:NZ	2.36	0.40
2:L1:29:U:H2'	2:L1:30:G:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:115:G:H5'	12:LD:129:ARG:HE	1.86	0.40
2:L1:306:U:H2'	2:L1:307:G:C8	2.54	0.40
2:L1:499:U:OP2	58:SQ:137:LYS:HD3	2.22	0.40
2:L1:1164:G:H2'	2:L1:1165:G:H8	1.86	0.40
2:L1:1210:C:H2'	2:L1:1211:A:C8	2.55	0.40
20:LL:234:GLU:HB3	20:LL:247:THR:HB	2.02	0.40
20:LL:469:ILE:HG21	20:LL:505:CYS:HA	2.03	0.40
22:LN:94:GLY:HA2	22:LN:396:GLU:OE2	2.21	0.40
23:LO:563:ARG:NE	23:LO:569:PHE:O	2.55	0.40
25:LQ:486:LYS:HA	25:LQ:502:PHE:HB3	2.03	0.40
25:LQ:538:ARG:HH11	25:LQ:580:ASP:HA	1.86	0.40
26:LR:747:ASN:HD21	26:LR:789:THR:HG23	1.86	0.40
27:LS:493:LEU:HD23	27:LS:493:LEU:HA	1.86	0.40
30:LV:280:LEU:HD21	30:LV:346:LEU:HD11	2.03	0.40
31:LW:214:LEU:HD22	31:LW:249:LEU:HD11	2.04	0.40
31:LW:376:ASN:HB3	31:LW:394:HIS:HB2	2.02	0.40
32:LX:136:ALA:HA	32:LX:139:ILE:HD12	2.03	0.40
45:SA:52:SER:HB2	45:SA:85:ASN:HD21	1.86	0.40
46:SB:160:ASP:OD1	46:SB:160:ASP:N	2.48	0.40
51:SI:280:LEU:HD12	51:SI:281:PRO:HD2	2.02	0.40
51:SI:877:GLU:HG3	51:SI:878:HIS:CD2	2.57	0.40
51:SI:1113:ILE:HD13	51:SI:1113:ILE:HA	1.92	0.40
61:ST:431:ARG:NH1	61:ST:480:GLU:OE1	2.52	0.40
1:L0:329:A:N6	1:L0:385:A:O2'	2.55	0.40
2:L1:347:G:H5"	2:L1:348:U:OP2	2.21	0.40
2:L1:1602:C:H5'	54:SM:146:ARG:HH11	1.85	0.40
5:L4:178:GLY:H	5:L4:195:ILE:HB	1.85	0.40
12:LD:47:THR:HG22	12:LD:53:TYR:HE1	1.87	0.40
16:LH:362:GLU:HB2	16:LH:453:HIS:CE1	2.56	0.40
18:LJ:53:HIS:O	18:LJ:68:SER:N	2.54	0.40
19:LK:445:PRO:HG2	19:LK:446:TRP:CD1	2.57	0.40
20:LL:462:GLU:HA	20:LL:465:ILE:HB	2.03	0.40
20:LL:484:LEU:HD13	20:LL:502:VAL:HG22	2.04	0.40
23:LO:138:ARG:HD3	28:LT:103:ARG:CZ	2.52	0.40
27:LS:256:PHE:CE1	27:LS:263:LEU:HD13	2.56	0.40
27:LS:272:LEU:O	27:LS:288:LEU:N	2.54	0.40
29:LU:94:TYR:CD2	29:LU:150:ILE:HG21	2.57	0.40
30:LV:292:CYS:HB2	30:LV:320:ILE:HD11	2.02	0.40
32:LX:846:UNK:O	32:LX:850:UNK:N	2.55	0.40
37:ND:181:LEU:HD23	47:SD:294:ARG:HE	1.87	0.40
46:SB:381:ASP:OD2	46:SB:385:ASP:OD2	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SG:194:LEU:HD11	49:SG:238:GLU:H	1.87	0.40
50:SH:18:ARG:NH1	50:SH:98:TYR:O	2.51	0.40
51:SI:946:ALA:HB2	51:SI:995:ILE:HG21	2.02	0.40
62:SU:281:LEU:HA	62:SU:285:ILE:HD12	2.01	0.40
62:SU:416:LEU:HD23	62:SU:416:LEU:HA	1.89	0.40
1:L0:234:A:N1	27:LS:252:GLN:NE2	2.62	0.40
1:L0:304:U:O2'	23:LO:177:SER:OG	2.38	0.40
2:L1:340:U:H2'	2:L1:341:A:H8	1.87	0.40
2:L1:368:U:H2'	2:L1:369:A:O4'	2.21	0.40
2:L1:1115:U:H2'	2:L1:1116:A:H8	1.86	0.40
2:L1:1574:G:H5"	2:L1:1575:G:OP1	2.22	0.40
5:L4:131:LEU:HD11	5:L4:135:GLY:HA2	2.04	0.40
5:L4:185:GLY:N	5:L4:189:LEU:HD13	2.32	0.40
15:LG:16:LEU:HD21	15:LG:29:ARG:HG3	2.03	0.40
16:LH:728:LEU:HA	16:LH:736:THR:HG23	2.04	0.40
20:LL:301:LEU:HB2	20:LL:319:TRP:CD1	2.57	0.40
21:LM:121:LEU:HD23	21:LM:127:ILE:HD13	2.03	0.40
23:LO:280:THR:HA	23:LO:304:PRO:HB3	2.02	0.40
25:LQ:353:LEU:N	25:LQ:365:TYR:O	2.37	0.40
26:LR:750:ALA:HA	26:LR:753:HIS:HB2	2.03	0.40
31:LW:384:VAL:HA	31:LW:385:PRO:HD3	1.91	0.40
54:SM:172:MET:N	54:SM:172:MET:SD	2.94	0.40
61:ST:434:ILE:O	61:ST:437:SER:OG	2.29	0.40
61:ST:600:LEU:HD12	61:ST:601:PRO:HD2	2.02	0.40
62:SU:95:UNK:O	62:SU:99:UNK:N	2.54	0.40
2:L1:1152:A:H2'	2:L1:1153:G:H8	1.86	0.40
2:L1:1260:U:H2'	2:L1:1261:G:C8	2.57	0.40
2:L1:1491:U:H3'	58:SQ:210:LYS:NZ	2.36	0.40
3:L2:58:A:OP2	33:LZ:165:LYS:HD2	2.21	0.40
16:LH:296:HIS:HA	16:LH:318:GLU:OE2	2.21	0.40
20:LL:27:GLN:HB2	20:LL:53:LEU:HD12	2.03	0.40
21:LM:214:THR:O	21:LM:218:ILE:HG12	2.21	0.40
22:LN:117:ILE:HD11	22:LN:147:ILE:HB	2.02	0.40
23:LO:576:ARG:HH12	33:LZ:144:ASN:HB2	1.85	0.40
27:LS:164:LEU:HG	28:LT:175:THR:HG22	2.03	0.40
28:LT:229:GLU:OE2	28:LT:245:LYS:HE2	2.22	0.40
30:LV:287:ASN:HD22	30:LV:302:ARG:HE	1.69	0.40
31:LW:340:LEU:HD12	31:LW:369:MET:HB3	2.04	0.40
31:LW:341:TRP:CD1	31:LW:367:PRO:HA	2.56	0.40
32:LX:320:UNK:O	32:LX:324:UNK:N	2.55	0.40
32:LX:391:UNK:N	32:LX:412:UNK:O	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:NJ:1550:HIS:O	43:NJ:1554:LEU:N	2.52	0.40
45:SA:173:HIS:CD2	46:SB:187:TRP:HE1	2.39	0.40
47:SC:100:ARG:NH1	58:SQ:141:TRP:CD1	2.89	0.40
51:SI:1023:LEU:HD13	51:SI:1025:GLU:H	1.86	0.40
51:SI:1057:ILE:H	51:SI:1057:ILE:HG13	1.68	0.40
54:SM:211:ASN:HD22	54:SM:212:ALA:N	2.18	0.40
58:SQ:151:THR:OG1	58:SQ:152:ILE:N	2.55	0.40
61:ST:433:ILE:HG23	61:ST:452:GLN:NE2	2.36	0.40
2:L1:887:A:H4'	40:NG:88:GLY:HA2	2.04	0.40
2:L1:1606:C:H5	54:SM:94:ARG:NH1	2.20	0.40
16:LH:52:ILE:O	16:LH:66:LEU:N	2.53	0.40
16:LH:142:ALA:HB2	16:LH:156:THR:HG23	2.03	0.40
18:LJ:47:PHE:CD1	18:LJ:55:PHE:HB3	2.57	0.40
20:LL:7:GLN:NE2	20:LL:61:THR:O	2.51	0.40
20:LL:484:LEU:HD23	20:LL:484:LEU:HA	1.82	0.40
22:LN:232:ASP:N	22:LN:232:ASP:OD1	2.55	0.40
22:LN:252:GLN:H	22:LN:252:GLN:HG2	1.75	0.40
23:LO:84:PHE:HD1	23:LO:84:PHE:HA	1.70	0.40
23:LO:398:ARG:NH1	28:LT:938:THR:HG22	2.37	0.40
23:LO:718:ASP:OD1	28:LT:576:ARG:NH2	2.54	0.40
25:LQ:170:TRP:CH2	25:LQ:172:GLN:HB2	2.56	0.40
27:LS:146:LEU:HD21	27:LS:164:LEU:HD13	2.04	0.40
27:LS:252:GLN:HB2	27:LS:267:GLY:HA2	2.04	0.40
27:LS:430:GLY:HA2	27:LS:455:ILE:HD12	2.03	0.40
32:LX:74:GLU:HA	32:LX:77:ILE:HD12	2.02	0.40
32:LX:566:UNK:HA	32:LX:582:UNK:HA	2.02	0.40
32:LY:327:UNK:O	32:LY:331:UNK:N	2.55	0.40
34:NA:365:LEU:HB2	54:SM:227:ARG:HH12	1.87	0.40
47:SD:163:PHE:CG	47:SD:266:GLY:HA3	2.57	0.40
50:SH:286:SER:HA	50:SH:317:GLN:HE21	1.86	0.40
51:SI:889:LEU:HG	51:SI:922:ILE:HD13	2.04	0.40
51:SI:980:LEU:H	51:SI:987:TYR:HA	1.86	0.40
53:SL:152:ILE:HB	53:SL:171:PRO:HG2	2.02	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
4	L3	100/146 (68%)	93 (93%)	6 (6%)	1 (1%)	15 52
5	L4	226/261 (87%)	206 (91%)	19 (8%)	1 (0%)	34 70
6	L5	211/225 (94%)	198 (94%)	13 (6%)	0	100 100
7	L6	109/236 (46%)	100 (92%)	8 (7%)	1 (1%)	17 54
8	L7	161/190 (85%)	149 (92%)	10 (6%)	2 (1%)	13 50
9	L8	166/200 (83%)	155 (93%)	11 (7%)	0	100 100
10	L9	173/197 (88%)	165 (95%)	8 (5%)	0	100 100
11	LC	123/143 (86%)	111 (90%)	12 (10%)	0	100 100
12	LD	123/156 (79%)	109 (89%)	13 (11%)	1 (1%)	19 57
13	LE	125/130 (96%)	119 (95%)	6 (5%)	0	100 100
14	LF	88/135 (65%)	73 (83%)	12 (14%)	3 (3%)	3 31
15	LG	61/67 (91%)	57 (93%)	4 (7%)	0	100 100
16	LH	810/896 (90%)	760 (94%)	50 (6%)	0	100 100
17	LI	128/713 (18%)	121 (94%)	7 (6%)	0	100 100
18	LJ	489/513 (95%)	459 (94%)	30 (6%)	0	100 100
19	LK	86/575 (15%)	83 (96%)	3 (4%)	0	100 100
20	LL	465/643 (72%)	437 (94%)	28 (6%)	0	100 100
21	LM	424/1769 (24%)	407 (96%)	17 (4%)	0	100 100
22	LN	654/776 (84%)	600 (92%)	54 (8%)	0	100 100
23	LO	830/923 (90%)	762 (92%)	68 (8%)	0	100 100
24	LP	259/440 (59%)	253 (98%)	6 (2%)	0	100 100
25	LQ	798/943 (85%)	747 (94%)	51 (6%)	0	100 100
26	LR	156/817 (19%)	152 (97%)	4 (3%)	0	100 100
27	LS	473/594 (80%)	442 (93%)	31 (7%)	0	100 100
28	LT	844/939 (90%)	800 (95%)	44 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LU	453/489 (93%)	431 (95%)	22 (5%)	0	100	100
30	LV	360/707 (51%)	319 (89%)	40 (11%)	1 (0%)	41	74
31	LW	436/554 (79%)	405 (93%)	31 (7%)	0	100	100
32	LX	179/1056 (17%)	170 (95%)	9 (5%)	0	100	100
32	LY	152/1056 (14%)	139 (91%)	13 (9%)	0	100	100
33	LZ	180/183 (98%)	168 (93%)	11 (6%)	1 (1%)	25	62
34	NA	203/593 (34%)	188 (93%)	13 (6%)	2 (1%)	15	52
35	NB	126/610 (21%)	119 (94%)	7 (6%)	0	100	100
36	NC	134/357 (38%)	118 (88%)	16 (12%)	0	100	100
37	ND	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
38	NE	129/346 (37%)	124 (96%)	5 (4%)	0	100	100
39	NF	122/151 (81%)	116 (95%)	6 (5%)	0	100	100
40	NG	109/137 (80%)	94 (86%)	15 (14%)	0	100	100
41	NH	1070/1237 (86%)	1019 (95%)	51 (5%)	0	100	100
42	NI	163/297 (55%)	159 (98%)	4 (2%)	0	100	100
43	NJ	263/1729 (15%)	256 (97%)	7 (3%)	0	100	100
44	NK	173/316 (55%)	164 (95%)	9 (5%)	0	100	100
45	SA	338/504 (67%)	326 (96%)	12 (4%)	0	100	100
46	SB	297/511 (58%)	283 (95%)	14 (5%)	0	100	100
47	SC	238/327 (73%)	220 (92%)	18 (8%)	0	100	100
47	SD	224/327 (68%)	216 (96%)	8 (4%)	0	100	100
48	SE	119/126 (94%)	114 (96%)	4 (3%)	1 (1%)	19	57
48	SF	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
49	SG	423/573 (74%)	395 (93%)	28 (7%)	0	100	100
50	SH	358/367 (98%)	343 (96%)	15 (4%)	0	100	100
51	SI	763/1184 (64%)	721 (94%)	41 (5%)	1 (0%)	51	83
52	SJ	212/252 (84%)	208 (98%)	4 (2%)	0	100	100
52	SK	226/252 (90%)	219 (97%)	7 (3%)	0	100	100
53	SL	170/189 (90%)	157 (92%)	13 (8%)	0	100	100
54	SM	278/290 (96%)	252 (91%)	26 (9%)	0	100	100
55	SN	245/274 (89%)	230 (94%)	15 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
56	SO	177/274 (65%)	167 (94%)	10 (6%)	0	100 100
58	SQ	129/217 (59%)	121 (94%)	8 (6%)	0	100 100
59	SR	102/145 (70%)	88 (86%)	13 (13%)	1 (1%)	15 52
60	SS	142/898 (16%)	134 (94%)	8 (6%)	0	100 100
61	ST	448/792 (57%)	432 (96%)	16 (4%)	0	100 100
62	SU	366/552 (66%)	349 (95%)	17 (5%)	0	100 100
63	SV	24/206 (12%)	20 (83%)	4 (17%)	0	100 100
65	SY	237/250 (95%)	218 (92%)	18 (8%)	1 (0%)	34 70
66	SZ	259/483 (54%)	245 (95%)	14 (5%)	0	100 100
All	All	18286/31778 (58%)	17177 (94%)	1092 (6%)	17 (0%)	54 83

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L4	195	ILE
34	NA	454	VAL
59	SR	90	ASP
14	LF	52	LYS
30	LV	58	ALA
14	LF	37	LYS
7	L6	68	LEU
34	NA	455	HIS
14	LF	51	GLU
51	SI	950	ASP
65	SY	11	LYS
8	L7	11	GLN
8	L7	65	PRO
33	LZ	140	PRO
48	SE	10	PRO
4	L3	14	ILE
12	LD	130	PRO

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	
4	L3	96/123 (78%)	95 (99%)	1 (1%)	76	86
5	L4	196/222 (88%)	194 (99%)	2 (1%)	76	86
6	L5	180/191 (94%)	180 (100%)	0	100	100
7	L6	96/201 (48%)	94 (98%)	2 (2%)	53	74
8	L7	146/170 (86%)	145 (99%)	1 (1%)	84	91
9	L8	138/161 (86%)	137 (99%)	1 (1%)	84	91
10	L9	150/166 (90%)	149 (99%)	1 (1%)	84	91
11	LC	105/119 (88%)	105 (100%)	0	100	100
12	LD	114/137 (83%)	112 (98%)	2 (2%)	59	77
13	LE	108/111 (97%)	107 (99%)	1 (1%)	78	88
14	LF	76/113 (67%)	74 (97%)	2 (3%)	46	69
15	LG	56/60 (93%)	56 (100%)	0	100	100
16	LH	758/813 (93%)	737 (97%)	21 (3%)	43	68
17	LI	126/153 (82%)	124 (98%)	2 (2%)	62	79
18	LJ	437/454 (96%)	430 (98%)	7 (2%)	62	79
19	LK	83/500 (17%)	81 (98%)	2 (2%)	49	71
20	LL	428/574 (75%)	426 (100%)	2 (0%)	88	94
21	LM	391/1627 (24%)	386 (99%)	5 (1%)	69	82
22	LN	604/699 (86%)	595 (98%)	9 (2%)	65	81
23	LO	730/812 (90%)	723 (99%)	7 (1%)	76	86
24	LP	248/303 (82%)	247 (100%)	1 (0%)	91	95
25	LQ	717/794 (90%)	709 (99%)	8 (1%)	73	85
26	LR	147/155 (95%)	146 (99%)	1 (1%)	84	91
27	LS	424/529 (80%)	420 (99%)	4 (1%)	78	88
28	LT	745/819 (91%)	737 (99%)	8 (1%)	73	85
29	LU	412/443 (93%)	407 (99%)	5 (1%)	71	84
30	LV	307/636 (48%)	305 (99%)	2 (1%)	84	91
31	LW	373/480 (78%)	372 (100%)	1 (0%)	92	96
32	LX	164/165 (99%)	159 (97%)	5 (3%)	41	66
33	LZ	171/172 (99%)	165 (96%)	6 (4%)	36	64
34	NA	187/535 (35%)	184 (98%)	3 (2%)	62	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	NB	108/525 (21%)	107 (99%)	1 (1%)	78 88
36	NC	119/315 (38%)	118 (99%)	1 (1%)	81 89
37	ND	57/176 (32%)	57 (100%)	0	100 100
38	NE	114/278 (41%)	113 (99%)	1 (1%)	78 88
45	SA	296/413 (72%)	293 (99%)	3 (1%)	76 86
46	SB	243/319 (76%)	238 (98%)	5 (2%)	53 74
47	SC	202/240 (84%)	198 (98%)	4 (2%)	55 75
47	SD	192/240 (80%)	189 (98%)	3 (2%)	62 79
48	SE	100/104 (96%)	98 (98%)	2 (2%)	55 75
48	SF	100/104 (96%)	100 (100%)	0	100 100
49	SG	373/503 (74%)	371 (100%)	2 (0%)	88 94
50	SH	307/312 (98%)	307 (100%)	0	100 100
51	SI	684/1014 (68%)	670 (98%)	14 (2%)	55 75
52	SJ	195/222 (88%)	190 (97%)	5 (3%)	46 69
52	SK	206/222 (93%)	201 (98%)	5 (2%)	49 71
53	SL	156/169 (92%)	154 (99%)	2 (1%)	69 82
54	SM	251/258 (97%)	244 (97%)	7 (3%)	43 68
55	SN	230/256 (90%)	226 (98%)	4 (2%)	60 78
56	SO	33/238 (14%)	32 (97%)	1 (3%)	41 66
58	SQ	124/200 (62%)	124 (100%)	0	100 100
59	SR	86/120 (72%)	84 (98%)	2 (2%)	50 72
60	SS	135/758 (18%)	135 (100%)	0	100 100
61	ST	417/534 (78%)	412 (99%)	5 (1%)	71 84
62	SU	330/338 (98%)	323 (98%)	7 (2%)	53 74
63	SV	22/117 (19%)	22 (100%)	0	100 100
65	SY	226/234 (97%)	220 (97%)	6 (3%)	44 69
All	All	14219/20646 (69%)	14027 (99%)	192 (1%)	68 81

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L3	103	ASN
5	L4	59	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L4	113	ARG
7	L6	68	LEU
7	L6	98	ARG
8	L7	174	ASN
9	L8	64	ASN
10	L9	57	ARG
12	LD	67	ARG
12	LD	98	ASN
13	LE	15	ASN
14	LF	34	ASN
14	LF	49	LYS
16	LH	23	ASN
16	LH	85	ASN
16	LH	113	ASN
16	LH	143	ASN
16	LH	223	LYS
16	LH	329	ASN
16	LH	336	ARG
16	LH	352	ASN
16	LH	363	ASN
16	LH	366	ASN
16	LH	383	LEU
16	LH	418	ASN
16	LH	432	ARG
16	LH	433	ARG
16	LH	439	ASN
16	LH	485	ARG
16	LH	533	THR
16	LH	609	ASN
16	LH	699	ASN
16	LH	719	ASN
16	LH	870	ASN
17	LI	560	ASN
17	LI	718	MET
18	LJ	42	VAL
18	LJ	95	LEU
18	LJ	277	LEU
18	LJ	362	ARG
18	LJ	390	ARG
18	LJ	403	ASN
18	LJ	507	MET
19	LK	447	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	LK	487	ARG
20	LL	47	ASN
20	LL	302	ASN
21	LM	162	ASN
21	LM	181	LYS
21	LM	208	ASN
21	LM	235	VAL
21	LM	285	ASN
22	LN	31	MET
22	LN	226	LEU
22	LN	272	LEU
22	LN	300	VAL
22	LN	331	ASN
22	LN	458	ASN
22	LN	567	ASN
22	LN	595	ASN
22	LN	618	ASN
23	LO	84	PHE
23	LO	117	ARG
23	LO	307	THR
23	LO	339	LEU
23	LO	582	THR
23	LO	585	TYR
23	LO	826	ARG
24	LP	81	ASN
25	LQ	185	MET
25	LQ	255	ARG
25	LQ	285	ARG
25	LQ	390	GLN
25	LQ	426	ARG
25	LQ	842	ASN
25	LQ	913	ASN
25	LQ	917	ASN
26	LR	688	LEU
27	LS	217	ASN
27	LS	237	ARG
27	LS	480	ARG
27	LS	590	LYS
28	LT	19	LYS
28	LT	20	ASN
28	LT	135	ASN
28	LT	250	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	LT	283	ARG
28	LT	344	ARG
28	LT	743	ARG
28	LT	925	LEU
29	LU	252	ASN
29	LU	281	ASN
29	LU	374	LEU
29	LU	380	TRP
29	LU	384	ASN
30	LV	166	ASN
30	LV	222	ASN
31	LW	199	LEU
32	LX	16	ASN
32	LX	35	ASN
32	LX	102	ASN
32	LX	107	TYR
32	LX	130	LEU
33	LZ	3	ARG
33	LZ	5	LEU
33	LZ	48	ASN
33	LZ	77	LEU
33	LZ	137	ARG
33	LZ	142	LEU
34	NA	473	THR
34	NA	486	ASN
34	NA	526	ASN
35	NB	515	ASN
36	NC	278	ARG
38	NE	222	ASN
45	SA	129	ARG
45	SA	286	ARG
45	SA	391	ASN
46	SB	192	PHE
46	SB	256	ASN
46	SB	269	ARG
46	SB	274	ASN
46	SB	425	ARG
47	SC	110	ASN
47	SC	122	ARG
47	SC	145	ASN
47	SC	251	ARG
47	SD	92	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	SD	231	ARG
47	SD	274	ASN
48	SE	25	GLN
48	SE	105	ASN
49	SG	268	LEU
49	SG	356	ARG
51	SI	72	VAL
51	SI	82	LYS
51	SI	92	ARG
51	SI	214	ARG
51	SI	233	ARG
51	SI	248	ARG
51	SI	366	MET
51	SI	828	ARG
51	SI	833	ARG
51	SI	868	ARG
51	SI	944	ASN
51	SI	960	ARG
51	SI	973	ARG
51	SI	1016	ASN
52	SJ	40	ARG
52	SJ	105	ASN
52	SJ	125	ASN
52	SJ	154	ASN
52	SJ	211	ARG
52	SK	40	ARG
52	SK	105	ASN
52	SK	110	LEU
52	SK	125	ASN
52	SK	154	ASN
53	SL	65	VAL
53	SL	97	LEU
54	SM	88	ILE
54	SM	100	LEU
54	SM	193	ASN
54	SM	211	ASN
54	SM	220	ARG
54	SM	226	ASN
54	SM	233	VAL
55	SN	155	ARG
55	SN	193	ASN
55	SN	221	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	SN	245	LYS
56	SO	262	ASN
59	SR	109	ARG
59	SR	112	LYS
61	ST	107	ASN
61	ST	555	ARG
61	ST	561	ILE
61	ST	704	ASN
61	ST	797	ASN
62	SU	304	ASN
62	SU	355	ARG
62	SU	357	ARG
62	SU	418	ASN
62	SU	438	LEU
62	SU	469	LEU
62	SU	494	ASN
65	SY	4	LEU
65	SY	48	LEU
65	SY	111	ARG
65	SY	160	ASN
65	SY	161	ARG
65	SY	211	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (259) such sidechains are listed below:

Mol	Chain	Res	Type
4	L3	13	HIS
4	L3	55	HIS
4	L3	103	ASN
5	L4	216	ASN
5	L4	224	ASN
6	L5	66	GLN
6	L5	100	ASN
6	L5	103	ASN
8	L7	89	HIS
9	L8	64	ASN
9	L8	116	HIS
10	L9	133	HIS
10	L9	139	GLN
12	LD	14	GLN
12	LD	16	GLN
12	LD	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	LD	110	HIS
13	LE	70	ASN
13	LE	92	ASN
14	LF	22	GLN
14	LF	29	HIS
14	LF	34	ASN
16	LH	23	ASN
16	LH	51	GLN
16	LH	85	ASN
16	LH	113	ASN
16	LH	143	ASN
16	LH	189	HIS
16	LH	329	ASN
16	LH	350	GLN
16	LH	352	ASN
16	LH	363	ASN
16	LH	366	ASN
16	LH	407	ASN
16	LH	418	ASN
16	LH	439	ASN
16	LH	453	HIS
16	LH	491	GLN
16	LH	540	ASN
16	LH	551	HIS
16	LH	603	ASN
16	LH	606	HIS
16	LH	609	ASN
16	LH	624	HIS
16	LH	690	ASN
16	LH	699	ASN
16	LH	719	ASN
16	LH	868	ASN
16	LH	870	ASN
16	LH	878	ASN
17	LI	560	ASN
17	LI	636	GLN
18	LJ	44	HIS
18	LJ	135	GLN
18	LJ	213	GLN
18	LJ	391	ASN
18	LJ	403	ASN
18	LJ	502	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	LK	447	ASN
19	LK	509	GLN
20	LL	47	ASN
20	LL	67	ASN
20	LL	213	ASN
20	LL	302	ASN
20	LL	360	ASN
20	LL	371	HIS
20	LL	443	GLN
20	LL	495	GLN
20	LL	509	HIS
21	LM	15	ASN
21	LM	43	GLN
21	LM	162	ASN
21	LM	202	HIS
21	LM	208	ASN
21	LM	226	ASN
21	LM	233	GLN
21	LM	258	HIS
21	LM	285	ASN
21	LM	304	GLN
22	LN	73	ASN
22	LN	140	ASN
22	LN	186	GLN
22	LN	274	GLN
22	LN	279	HIS
22	LN	292	ASN
22	LN	329	HIS
22	LN	331	ASN
22	LN	427	ASN
22	LN	483	ASN
22	LN	567	ASN
22	LN	595	ASN
22	LN	618	ASN
22	LN	731	HIS
23	LO	88	ASN
23	LO	156	GLN
23	LO	203	GLN
23	LO	296	GLN
23	LO	306	ASN
23	LO	565	ASN
23	LO	791	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	LP	81	ASN
24	LP	143	ASN
24	LP	169	GLN
24	LP	170	ASN
24	LP	284	HIS
24	LP	301	ASN
25	LQ	88	HIS
25	LQ	200	HIS
25	LQ	254	GLN
25	LQ	383	HIS
25	LQ	388	GLN
25	LQ	411	ASN
25	LQ	620	ASN
25	LQ	842	ASN
25	LQ	849	HIS
25	LQ	864	ASN
25	LQ	913	ASN
25	LQ	916	HIS
25	LQ	917	ASN
26	LR	670	GLN
26	LR	690	HIS
26	LR	767	HIS
27	LS	141	ASN
27	LS	159	HIS
27	LS	217	ASN
27	LS	242	ASN
27	LS	440	ASN
27	LS	472	GLN
27	LS	492	ASN
28	LT	20	ASN
28	LT	67	HIS
28	LT	135	ASN
28	LT	172	HIS
28	LT	263	HIS
28	LT	300	GLN
28	LT	387	GLN
28	LT	394	HIS
28	LT	490	GLN
28	LT	514	ASN
28	LT	627	ASN
28	LT	736	HIS
28	LT	761	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	LU	76	ASN
29	LU	81	ASN
29	LU	252	ASN
29	LU	260	GLN
29	LU	304	HIS
29	LU	353	GLN
29	LU	384	ASN
29	LU	460	GLN
30	LV	9	ASN
30	LV	60	ASN
30	LV	82	HIS
30	LV	166	ASN
30	LV	222	ASN
30	LV	287	ASN
31	LW	36	GLN
31	LW	88	GLN
31	LW	124	HIS
31	LW	133	HIS
31	LW	170	GLN
31	LW	190	HIS
31	LW	251	HIS
32	LX	16	ASN
32	LX	35	ASN
32	LX	36	GLN
32	LX	102	ASN
32	LX	117	ASN
32	LX	125	GLN
33	LZ	48	ASN
34	NA	486	ASN
34	NA	526	ASN
35	NB	513	HIS
35	NB	515	ASN
35	NB	531	ASN
36	NC	269	HIS
38	NE	222	ASN
45	SA	85	ASN
45	SA	95	ASN
45	SA	121	ASN
45	SA	143	GLN
45	SA	151	GLN
45	SA	173	HIS
46	SB	274	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	SB	286	ASN
46	SB	302	HIS
46	SB	334	HIS
46	SB	428	ASN
47	SC	110	ASN
47	SC	145	ASN
47	SD	93	HIS
47	SD	264	GLN
47	SD	274	ASN
48	SE	105	ASN
48	SF	18	GLN
48	SF	38	ASN
49	SG	226	HIS
49	SG	322	HIS
50	SH	15	GLN
50	SH	125	HIS
51	SI	50	ASN
51	SI	145	ASN
51	SI	754	GLN
51	SI	761	GLN
51	SI	855	GLN
51	SI	878	HIS
51	SI	900	GLN
51	SI	1016	ASN
51	SI	1114	GLN
52	SJ	73	HIS
52	SJ	105	ASN
52	SJ	111	GLN
52	SJ	125	ASN
52	SJ	154	ASN
52	SK	73	HIS
52	SK	125	ASN
52	SK	154	ASN
52	SK	170	HIS
53	SL	23	GLN
53	SL	46	GLN
53	SL	70	ASN
54	SM	102	GLN
54	SM	159	HIS
54	SM	174	HIS
54	SM	181	ASN
54	SM	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	SM	193	ASN
54	SM	211	ASN
55	SN	37	HIS
55	SN	71	ASN
55	SN	193	ASN
55	SN	221	ASN
56	SO	239	HIS
56	SO	262	ASN
58	SQ	58	ASN
58	SQ	126	HIS
59	SR	89	ASN
61	ST	107	ASN
61	ST	438	ASN
61	ST	482	GLN
61	ST	495	ASN
61	ST	627	HIS
61	ST	697	HIS
61	ST	704	ASN
61	ST	713	HIS
61	ST	797	ASN
62	SU	174	ASN
62	SU	288	HIS
62	SU	304	ASN
62	SU	418	ASN
62	SU	472	HIS
62	SU	494	ASN
65	SY	12	GLN
65	SY	59	ASN
65	SY	65	HIS
65	SY	68	HIS
65	SY	105	ASN
65	SY	160	ASN
65	SY	221	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	484/700 (69%)	122 (25%)	7 (1%)
2	L1	1004/1807 (55%)	282 (28%)	19 (1%)
3	L2	163/333 (48%)	45 (27%)	0
All	All	1651/2840 (58%)	449 (27%)	26 (1%)

All (449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	63	G
1	L0	64	U
1	L0	82	A
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	87	C
1	L0	90	G
1	L0	98	G
1	L0	100	G
1	L0	101	G
1	L0	102	A
1	L0	103	G
1	L0	109	C
1	L0	110	G
1	L0	124	A
1	L0	125	G
1	L0	126	A
1	L0	129	U
1	L0	130	G
1	L0	133	U
1	L0	142	U
1	L0	143	A
1	L0	144	C
1	L0	150	G
1	L0	151	U
1	L0	152	U
1	L0	153	U
1	L0	161	A
1	L0	162	U
1	L0	163	G
1	L0	169	A
1	L0	171	G
1	L0	176	U
1	L0	177	U
1	L0	190	U
1	L0	197	G
1	L0	200	A
1	L0	226	U
1	L0	227	U
1	L0	234	A
1	L0	236	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L0	238	G
1	L0	239	U
1	L0	240	C
1	L0	252	A
1	L0	253	U
1	L0	254	C
1	L0	256	U
1	L0	258	C
1	L0	259	G
1	L0	261	U
1	L0	267	U
1	L0	268	G
1	L0	273	G
1	L0	278	G
1	L0	279	A
1	L0	280	A
1	L0	281	G
1	L0	298	A
1	L0	299	G
1	L0	303	A
1	L0	304	U
1	L0	305	A
1	L0	307	C
1	L0	309	A
1	L0	310	U
1	L0	311	C
1	L0	312	U
1	L0	313	A
1	L0	314	U
1	L0	315	U
1	L0	316	U
1	L0	320	A
1	L0	322	A
1	L0	323	A
1	L0	324	U
1	L0	325	U
1	L0	326	C
1	L0	327	A
1	L0	330	C
1	L0	331	U
1	L0	332	U
1	L0	336	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L0	339	A
1	L0	352	U
1	L0	373	U
1	L0	381	G
1	L0	382	U
1	L0	385	A
1	L0	386	A
1	L0	397	A
1	L0	399	U
1	L0	407	A
1	L0	418	C
1	L0	427	A
1	L0	430	C
1	L0	431	A
1	L0	432	C
1	L0	440	U
1	L0	442	U
1	L0	461	A
1	L0	462	G
1	L0	468	A
1	L0	469	C
1	L0	470	U
1	L0	481	U
1	L0	482	A
1	L0	483	U
1	L0	485	G
1	L0	487	A
1	L0	488	U
1	L0	491	U
1	L0	492	G
1	L0	493	A
1	L0	526	U
1	L0	535	G
1	L0	536	A
1	L0	540	U
1	L0	541	U
1	L0	545	G
1	L0	546	G
2	L1	-4	A
2	L1	-3	U
2	L1	-2	A
2	L1	-1	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	0	U
2	L1	1	U
2	L1	2	A
2	L1	5	U
2	L1	6	G
2	L1	8	U
2	L1	17	C
2	L1	18	C
2	L1	20	G
2	L1	21	U
2	L1	23	G
2	L1	25	C
2	L1	26	A
2	L1	35	U
2	L1	49	C
2	L1	100	A
2	L1	102	U
2	L1	104	A
2	L1	113	U
2	L1	114	C
2	L1	116	U
2	L1	127	G
2	L1	128	U
2	L1	140	A
2	L1	141	U
2	L1	144	U
2	L1	145	A
2	L1	146	U
2	L1	147	A
2	L1	153	G
2	L1	158	U
2	L1	166	C
2	L1	185	U
2	L1	188	A
2	L1	189	C
2	L1	190	C
2	L1	191	C
2	L1	192	U
2	L1	193	U
2	L1	195	G
2	L1	196	G
2	L1	198	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	200	A
2	L1	201	G
2	L1	204	G
2	L1	223	U
2	L1	227	U
2	L1	233	C
2	L1	243	G
2	L1	261	U
2	L1	265	A
2	L1	266	A
2	L1	271	A
2	L1	272	U
2	L1	273	G
2	L1	275	C
2	L1	277	U
2	L1	278	U
2	L1	280	U
2	L1	287	G
2	L1	299	A
2	L1	302	U
2	L1	308	C
2	L1	314	C
2	L1	316	A
2	L1	319	U
2	L1	320	U
2	L1	321	C
2	L1	322	G
2	L1	337	G
2	L1	338	C
2	L1	350	U
2	L1	351	C
2	L1	352	A
2	L1	359	A
2	L1	360	A
2	L1	361	C
2	L1	366	A
2	L1	368	U
2	L1	370	A
2	L1	371	G
2	L1	372	G
2	L1	373	G
2	L1	374	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	375	U
2	L1	376	C
2	L1	377	G
2	L1	382	C
2	L1	383	G
2	L1	388	G
2	L1	390	G
2	L1	400	A
2	L1	401	A
2	L1	402	C
2	L1	404	G
2	L1	407	A
2	L1	416	A
2	L1	418	G
2	L1	419	G
2	L1	423	G
2	L1	428	A
2	L1	440	U
2	L1	444	C
2	L1	445	A
2	L1	451	A
2	L1	454	U
2	L1	468	A
2	L1	469	C
2	L1	470	A
2	L1	477	A
2	L1	478	A
2	L1	487	G
2	L1	496	G
2	L1	497	G
2	L1	500	C
2	L1	501	U
2	L1	502	U
2	L1	505	A
2	L1	506	A
2	L1	510	G
2	L1	512	A
2	L1	514	G
2	L1	515	A
2	L1	525	A
2	L1	534	A
2	L1	536	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	538	A
2	L1	539	G
2	L1	540	G
2	L1	541	A
2	L1	542	A
2	L1	543	C
2	L1	544	A
2	L1	545	A
2	L1	552	G
2	L1	555	A
2	L1	557	G
2	L1	564	G
2	L1	565	C
2	L1	570	A
2	L1	572	C
2	L1	573	C
2	L1	574	G
2	L1	576	G
2	L1	579	A
2	L1	580	A
2	L1	582	U
2	L1	583	C
2	L1	584	C
2	L1	585	A
2	L1	586	G
2	L1	587	C
2	L1	594	A
2	L1	595	G
2	L1	624	G
2	L1	862	A
2	L1	863	A
2	L1	873	U
2	L1	876	G
2	L1	886	U
2	L1	897	C
2	L1	898	A
2	L1	906	A
2	L1	912	U
2	L1	913	G
2	L1	914	G
2	L1	928	U
2	L1	933	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	934	C
2	L1	935	U
2	L1	942	G
2	L1	944	A
2	L1	959	U
2	L1	960	U
2	L1	966	A
2	L1	969	C
2	L1	970	A
2	L1	971	A
2	L1	973	A
2	L1	980	G
2	L1	981	U
2	L1	983	A
2	L1	988	A
2	L1	992	A
2	L1	994	G
2	L1	996	U
2	L1	1003	A
2	L1	1004	U
2	L1	1005	A
2	L1	1019	A
2	L1	1118	G
2	L1	1119	G
2	L1	1128	C
2	L1	1129	U
2	L1	1131	A
2	L1	1132	A
2	L1	1134	C
2	L1	1135	U
2	L1	1136	U
2	L1	1144	U
2	L1	1146	G
2	L1	1158	C
2	L1	1160	A
2	L1	1191	U
2	L1	1192	C
2	L1	1193	A
2	L1	1194	A
2	L1	1195	C
2	L1	1196	A
2	L1	1197	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	1198	G
2	L1	1199	G
2	L1	1200	G
2	L1	1202	A
2	L1	1205	C
2	L1	1206	U
2	L1	1207	C
2	L1	1217	A
2	L1	1218	G
2	L1	1219	A
2	L1	1259	U
2	L1	1263	G
2	L1	1266	U
2	L1	1268	G
2	L1	1269	U
2	L1	1270	G
2	L1	1272	U
2	L1	1434	U
2	L1	1436	A
2	L1	1437	U
2	L1	1440	C
2	L1	1463	C
2	L1	1464	G
2	L1	1468	U
2	L1	1471	A
2	L1	1472	C
2	L1	1473	U
2	L1	1474	G
2	L1	1478	G
2	L1	1483	A
2	L1	1488	G
2	L1	1489	U
2	L1	1490	C
2	L1	1492	A
2	L1	1504	G
2	L1	1506	G
2	L1	1516	A
2	L1	1526	A
2	L1	1534	G
2	L1	1542	G
2	L1	1571	C
2	L1	1572	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	1573	A
2	L1	1574	G
2	L1	1582	U
2	L1	1583	A
2	L1	1584	G
2	L1	1590	G
2	L1	1592	A
2	L1	1595	U
2	L1	1601	G
2	L1	1602	C
2	L1	1614	A
2	L1	1618	C
2	L1	1619	C
2	L1	1621	U
2	L1	1628	U
2	L1	1629	G
2	L1	1630	U
2	L1	1631	A
2	L1	1632	C
2	L1	1633	A
2	L1	1639	C
2	L1	1640	C
2	L1	1645	G
2	L1	1780	G
2	L1	1783	C
2	L1	1791	A
3	L2	14	A
3	L2	15	U
3	L2	18	G
3	L2	22	A
3	L2	23	U
3	L2	24	U
3	L2	25	U
3	L2	28	A
3	L2	30	A
3	L2	31	G
3	L2	32	G
3	L2	33	A
3	L2	34	A
3	L2	35	U
3	L2	37	G
3	L2	38	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L2	39	C
3	L2	48	A
3	L2	51	C
3	L2	55	A
3	L2	56	A
3	L2	60	A
3	L2	61	G
3	L2	72	C
3	L2	82	G
3	L2	83	A
3	L2	87	G
3	L2	88	U
3	L2	89	C
3	L2	90	C
3	L2	91	C
3	L2	93	U
3	L2	94	A
3	L2	114	A
3	L2	115	G
3	L2	117	A
3	L2	118	A
3	L2	248	G
3	L2	250	C
3	L2	251	G
3	L2	254	A
3	L2	319	G
3	L2	324	U
3	L2	325	C
3	L2	329	C

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L0	81	A
1	L0	237	A
1	L0	311	C
1	L0	314	U
1	L0	325	U
1	L0	487	A
1	L0	492	G
2	L1	0	U
2	L1	1	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	20	G
2	L1	34	G
2	L1	103	A
2	L1	139	C
2	L1	187	G
2	L1	272	U
2	L1	372	G
2	L1	417	A
2	L1	542	A
2	L1	579	A
2	L1	1135	U
2	L1	1218	G
2	L1	1489	U
2	L1	1573	A
2	L1	1594	G
2	L1	1620	C
2	L1	1632	C

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
57	SP	61
26	LR	14
32	LY	11
32	LX	11
17	LI	9
64	SX	3
61	ST	2
24	LP	2
19	LK	2
45	SA	2
46	SB	2
63	SV	1
22	LN	1
60	SS	1
38	NE	1
62	SU	1
37	ND	1
25	LQ	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SX	2034:UNK	C	3098:UNK	N	257.52
1	SX	1058:UNK	C	2000:UNK	N	68.50
1	SX	3115:UNK	C	3218:UNK	N	49.43
1	LI	358:UNK	C	457:UNK	N	41.95
1	LR	323:UNK	C	329:UNK	N	40.86
1	ST	316:UNK	C	382:UNK	N	38.56
1	LR	13:UNK	C	17:UNK	N	38.37
1	SV	148:UNK	C	178:PHE	N	33.34
1	LY	661:UNK	C	708:UNK	N	28.07
1	LI	487:UNK	C	496:UNK	N	26.76
1	LR	615:UNK	C	649:GLU	N	25.81
1	LX	683:UNK	C	708:UNK	N	24.78
1	SP	940:UNK	C	945:UNK	N	23.12

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LI	467:UNK	C	473:UNK	N	21.18
1	LN	667:UNK	C	676:UNK	N	19.72
1	SP	919:UNK	C	930:UNK	N	17.73
1	LY	337:UNK	C	354:UNK	N	17.50
1	LI	93:UNK	C	120:UNK	N	16.70
1	SP	2089:UNK	C	2096:UNK	N	16.70
1	LX	337:UNK	C	354:UNK	N	16.20
1	SP	1254:UNK	C	1257:UNK	N	16.16
1	SP	1709:UNK	C	1717:UNK	N	16.05
1	SP	1068:UNK	C	1075:UNK	N	16.04
1	SP	1814:UNK	C	1822:UNK	N	15.99
1	SP	1132:UNK	C	1135:UNK	N	15.91
1	SP	1214:UNK	C	1221:UNK	N	15.88
1	SP	2201:UNK	C	2208:UNK	N	15.87
1	LX	661:UNK	C	672:UNK	N	15.86
1	SP	1953:UNK	C	1961:UNK	N	15.73
1	SP	1234:UNK	C	1238:UNK	N	15.33
1	SP	1340:UNK	C	1347:UNK	N	15.15
1	SP	1909:UNK	C	1912:UNK	N	15.11
1	SP	1003:UNK	C	1010:UNK	N	14.93
1	SP	2241:UNK	C	2242:UNK	N	14.81
1	ST	252:UNK	C	264:UNK	N	14.79
1	SP	1117:UNK	C	1120:UNK	N	14.29
1	LP	416:UNK	C	418:UNK	N	14.17
1	SP	1838:UNK	C	1843:UNK	N	13.92
1	SS	363:UNK	C	369:UNK	N	13.73
1	SP	1093:UNK	C	1100:UNK	N	13.68
1	SP	1574:UNK	C	1577:UNK	N	13.36
1	SP	1291:UNK	C	1297:UNK	N	13.13
1	SP	2225:UNK	C	2231:UNK	N	13.09
1	SP	1189:UNK	C	1195:UNK	N	13.07
1	SP	1730:UNK	C	1750:UNK	N	12.91
1	SP	1165:UNK	C	1171:UNK	N	12.88
1	SP	1862:UNK	C	1871:UNK	N	12.60
1	SP	2045:UNK	C	2050:UNK	N	12.56
1	SP	1595:UNK	C	1602:UNK	N	12.38
1	SP	1435:UNK	C	1442:UNK	N	12.34
1	SP	2180:UNK	C	2188:UNK	N	12.11
1	NE	98:UNK	C	101:UNK	N	11.83
1	LY	240:UNK	C	243:UNK	N	11.82
1	SP	1274:UNK	C	1280:UNK	N	11.54
1	LI	147:UNK	C	153:UNK	N	11.19

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LI	517:UNK	C	524:UNK	N	11.15
1	LP	369:UNK	C	379:UNK	N	11.14
1	SP	1791:UNK	C	1800:UNK	N	11.11
1	LX	240:UNK	C	243:UNK	N	11.06
1	SP	1410:UNK	C	1417:UNK	N	10.97
1	SP	1505:UNK	C	1512:UNK	N	10.96
1	SP	1043:UNK	C	1050:UNK	N	10.89
1	SP	1383:UNK	C	1392:UNK	N	10.89
1	SP	1662:UNK	C	1668:UNK	N	10.74
1	LR	235:UNK	C	243:UNK	N	10.49
1	LX	221:UNK	C	225:UNK	N	10.30
1	SP	2026:UNK	C	2030:UNK	N	10.29
1	SP	1974:UNK	C	1982:UNK	N	10.19
1	SP	1481:UNK	C	1489:UNK	N	9.84
1	SP	1685:UNK	C	1692:UNK	N	9.83
1	SP	1360:UNK	C	1367:UNK	N	9.79
1	SP	1310:UNK	C	1312:UNK	N	9.77
1	SP	1885:UNK	C	1894:UNK	N	9.71
1	SP	1620:UNK	C	1627:UNK	N	9.59
1	SP	1147:UNK	C	1150:UNK	N	9.46
1	SP	1999:UNK	C	2010:UNK	N	9.46
1	LY	221:UNK	C	225:UNK	N	9.42
1	LX	414:UNK	C	422:UNK	N	9.18
1	SP	1640:UNK	C	1648:UNK	N	9.00
1	LI	505:UNK	C	508:UNK	N	8.68
1	SP	2063:UNK	C	2073:UNK	N	8.65
1	SP	2109:UNK	C	2120:UNK	N	8.46
1	SP	1550:UNK	C	1557:UNK	N	8.39
1	SP	1931:UNK	C	1937:UNK	N	8.09
1	LK	426:UNK	C	428:ASP	N	8.04
1	SU	13:UNK	C	22:UNK	N	7.86
1	LY	414:UNK	C	422:UNK	N	7.82
1	LR	126:UNK	C	131:UNK	N	7.75
1	LX	433:UNK	C	467:UNK	N	7.71
1	LR	284:UNK	C	287:UNK	N	7.66
1	SP	1455:UNK	C	1468:UNK	N	7.64
1	LY	433:UNK	C	467:UNK	N	7.63
1	LR	106:UNK	C	109:UNK	N	7.53
1	SP	2136:UNK	C	2147:UNK	N	7.47
1	SP	980:UNK	C	987:UNK	N	7.24
1	LK	402:UNK	C	404:UNK	N	6.97
1	SP	1530:UNK	C	1537:UNK	N	6.94

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SA	238:UNK	C	242:UNK	N	6.66
1	SP	2159:UNK	C	2165:UNK	N	6.61
1	SP	1322:UNK	C	1329:UNK	N	6.60
1	SP	960:UNK	C	967:UNK	N	6.58
1	LY	871:UNK	C	878:UNK	N	6.51
1	LI	32:UNK	C	50:UNK	N	6.36
1	LX	392:UNK	C	396:UNK	N	6.09
1	LY	392:UNK	C	396:UNK	N	6.06
1	ND	108:UNK	C	110:UNK	N	5.85
1	LR	181:UNK	C	185:UNK	N	5.84
1	LX	871:UNK	C	878:UNK	N	5.60
1	LR	212:UNK	C	217:UNK	N	5.59
1	LX	360:UNK	C	368:UNK	N	5.38
1	LY	360:UNK	C	368:UNK	N	5.23
1	LX	274:UNK	C	279:UNK	N	5.13
1	SP	1021:UNK	C	1030:UNK	N	4.97
1	LR	196:UNK	C	198:UNK	N	4.94
1	SB	19:UNK	C	21:UNK	N	4.89
1	LR	222:UNK	C	227:UNK	N	4.78
1	LR	203:UNK	C	206:UNK	N	4.54
1	LR	252:UNK	C	255:UNK	N	4.24
1	SA	227:ALA	C	231:UNK	N	4.22
1	LR	305:UNK	C	307:UNK	N	3.93
1	LY	274:UNK	C	279:UNK	N	3.90
1	LI	83:UNK	C	85:UNK	N	3.76
1	LY	589:UNK	C	592:UNK	N	3.75
1	SP	1766:UNK	C	1775:UNK	N	3.66
1	SB	125:UNK	C	133:ASP	N	3.36
1	LQ	317:UNK	C	321:TYR	N	3.24

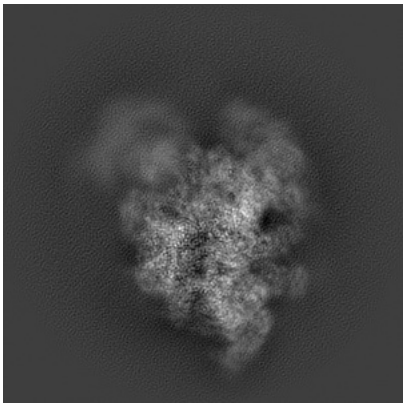
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8859. These allow visual inspection of the internal detail of the map and identification of artifacts.

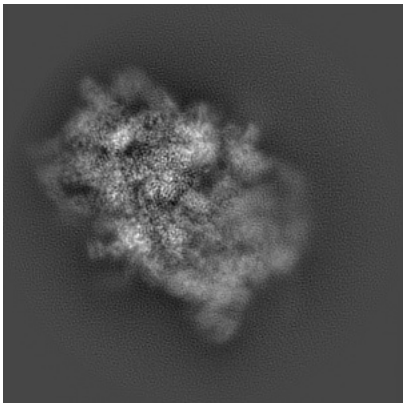
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

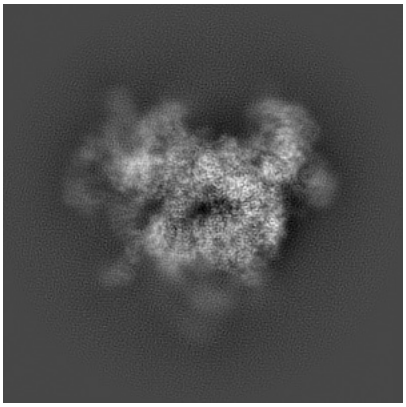
6.1.1 Primary map



X



Y

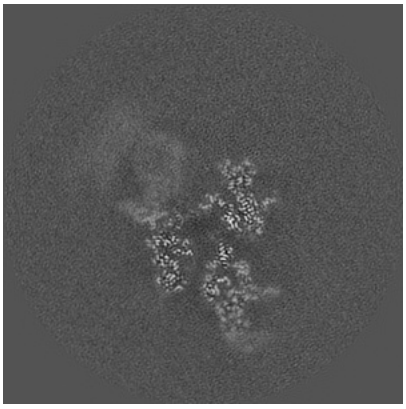


Z

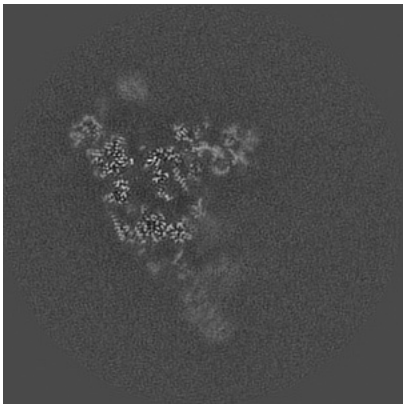
The images above show the map projected in three orthogonal directions.

6.2 Central slices

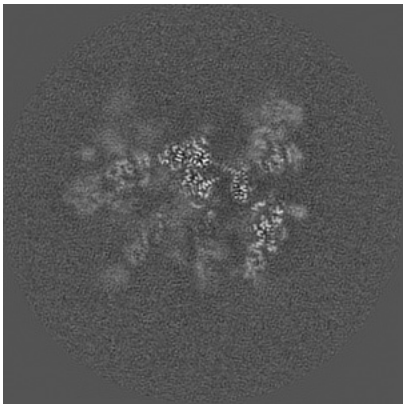
6.2.1 Primary map



X Index: 200



Y Index: 200

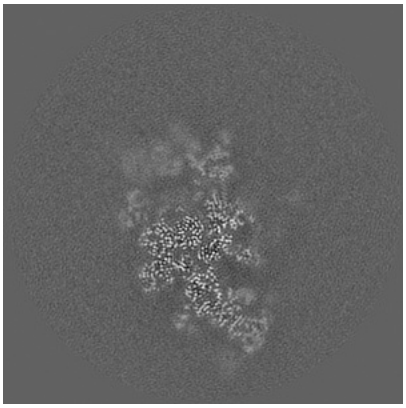


Z Index: 200

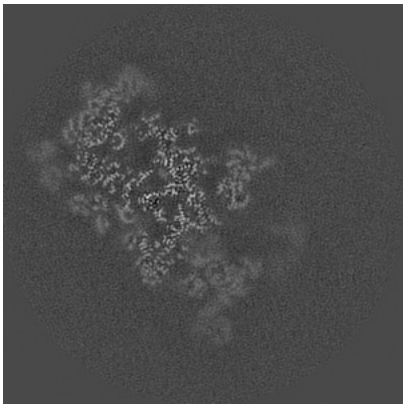
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

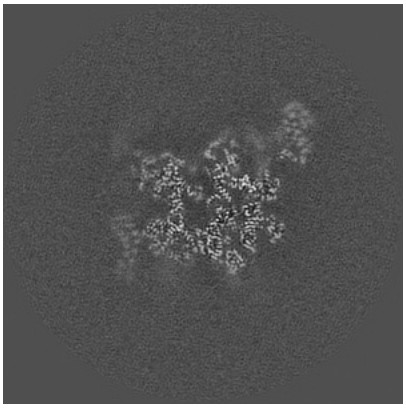
6.3.1 Primary map



X Index: 242



Y Index: 223

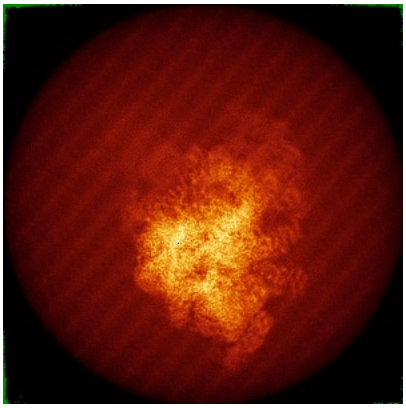


Z Index: 167

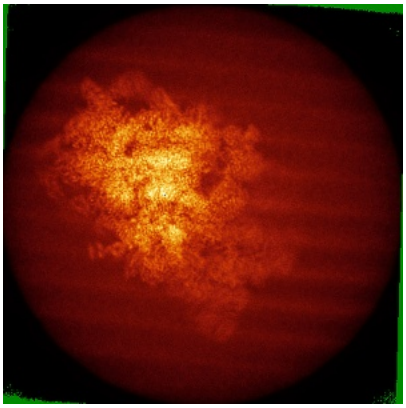
The images above show the largest variance slices of the map in three orthogonal directions.

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

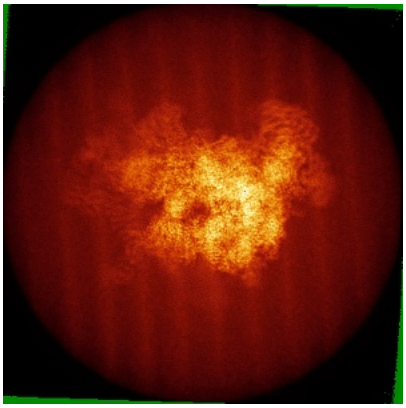
6.4.1 Primary map



X



Y

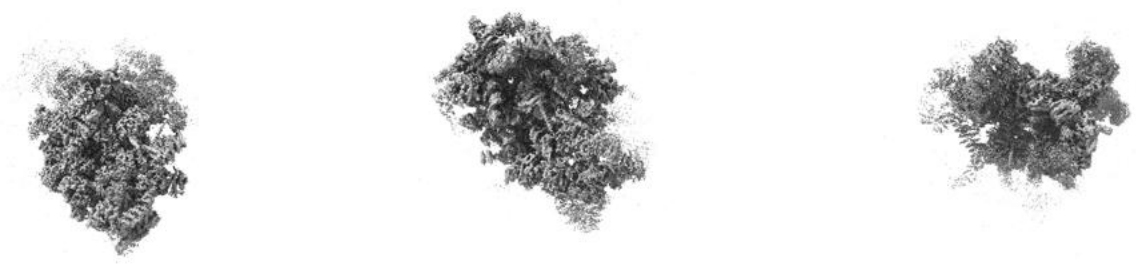


Z

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 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

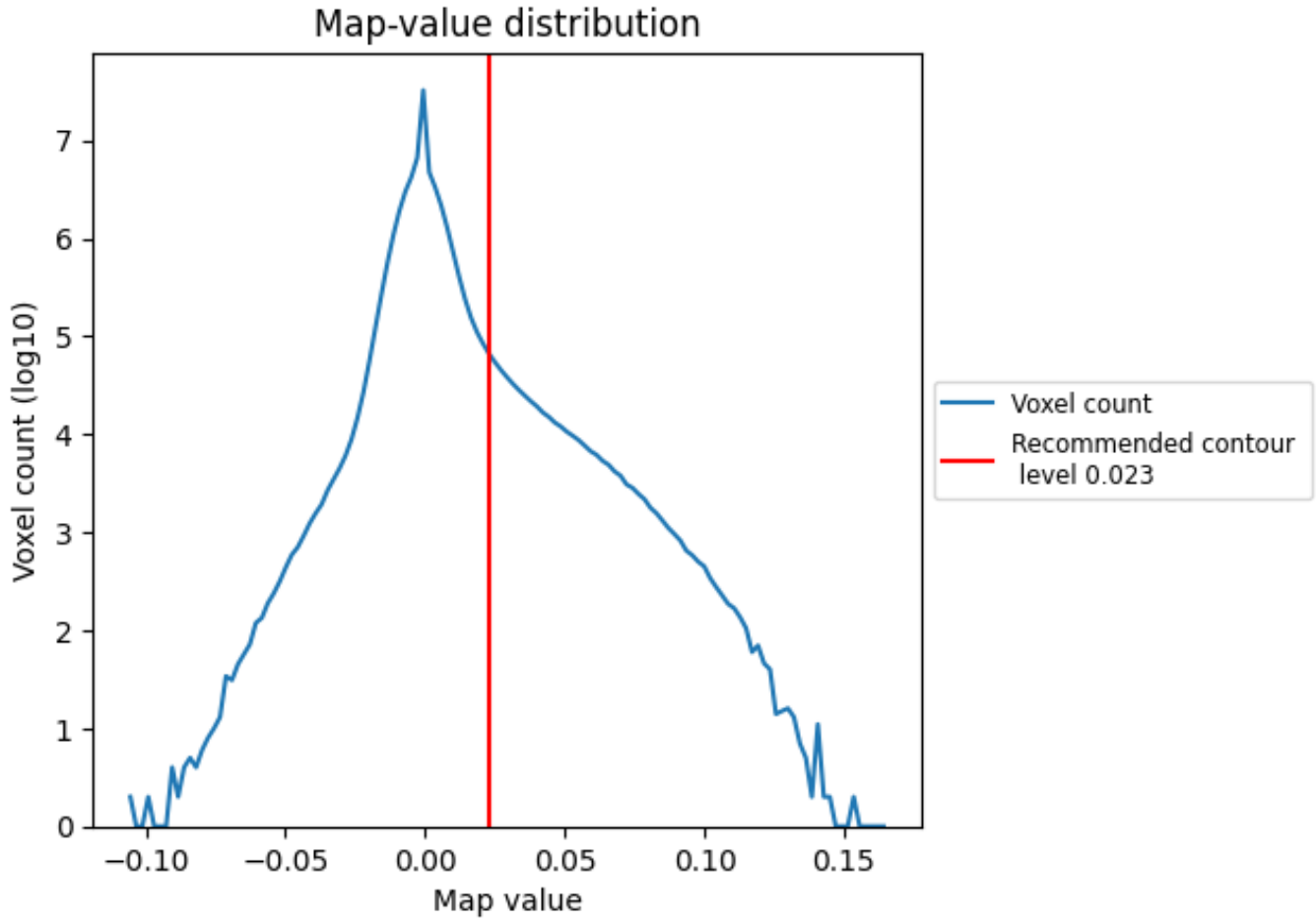
6.6 Mask visualisation (i)

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

7 Map analysis

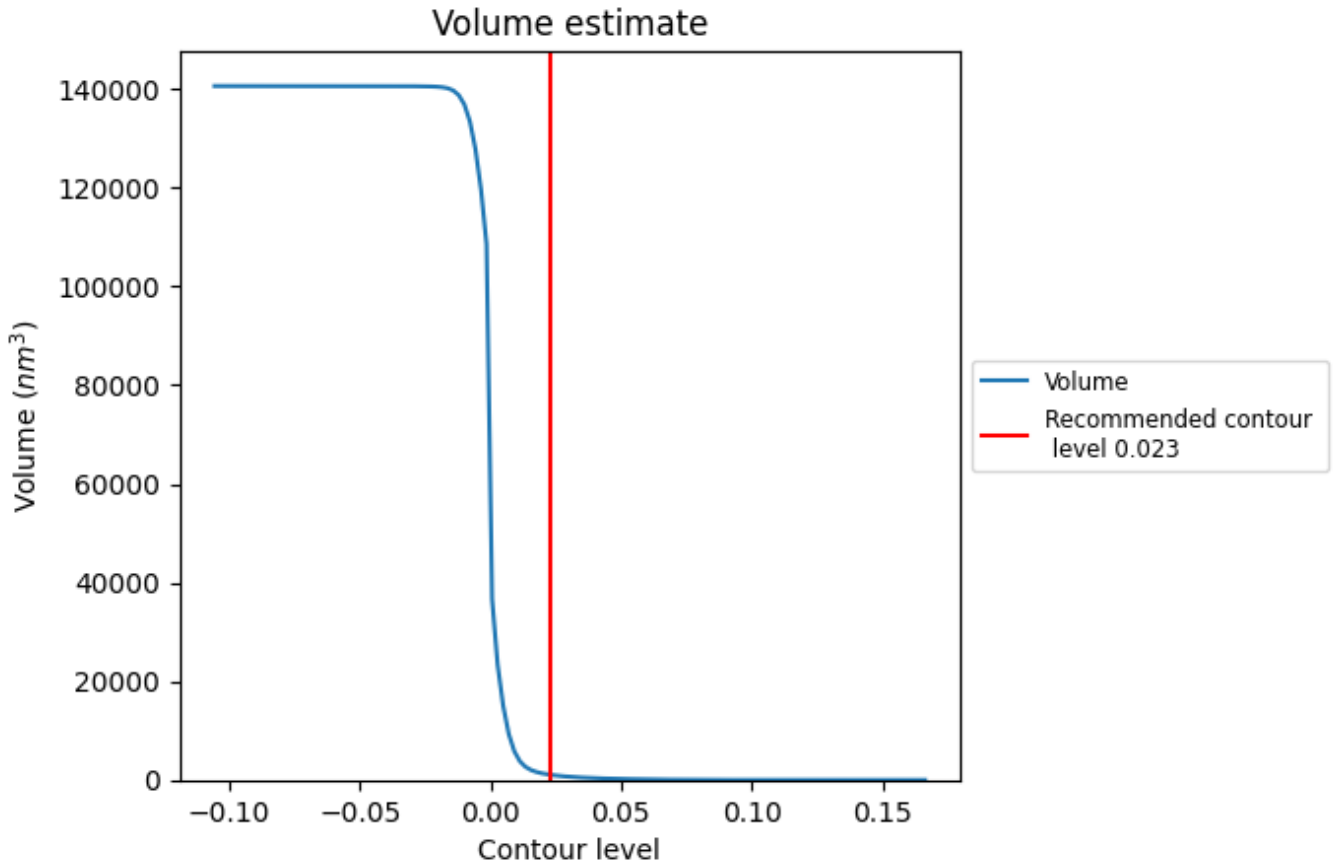
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

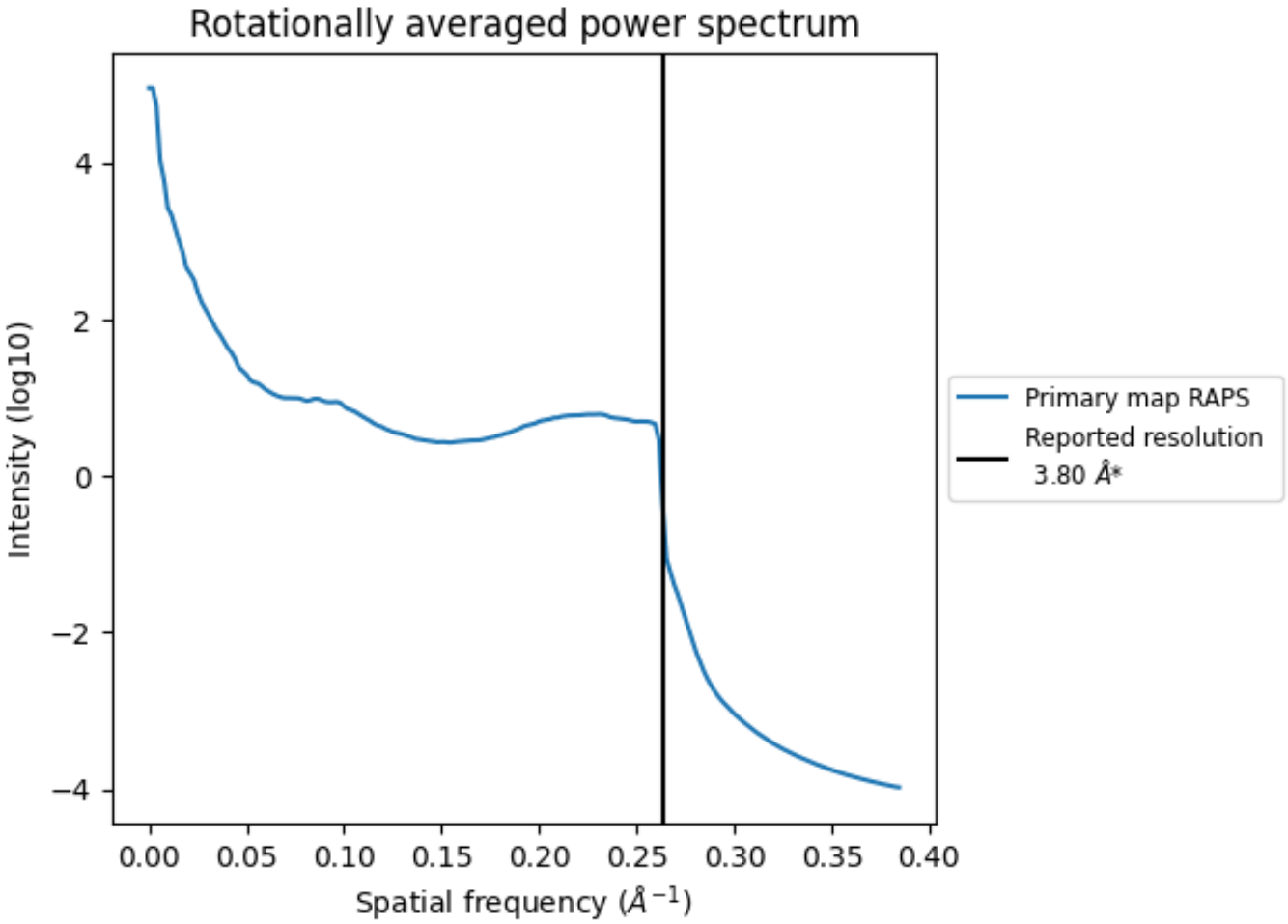
7.2 Volume estimate



The volume at the recommended contour level is 1051 nm^3; this corresponds to an approximate mass of 950 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 0.263 Å^{-1}

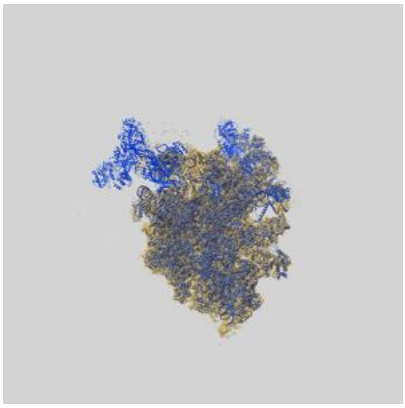
8 Fourier-Shell correlation (i)

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

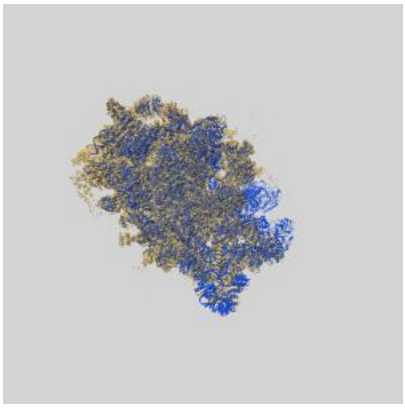
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8859 and PDB model 5WLC. Per-residue inclusion information can be found in section 3 on page 16.

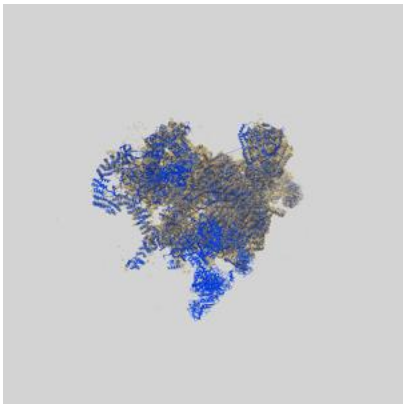
9.1 Map-model overlay



X



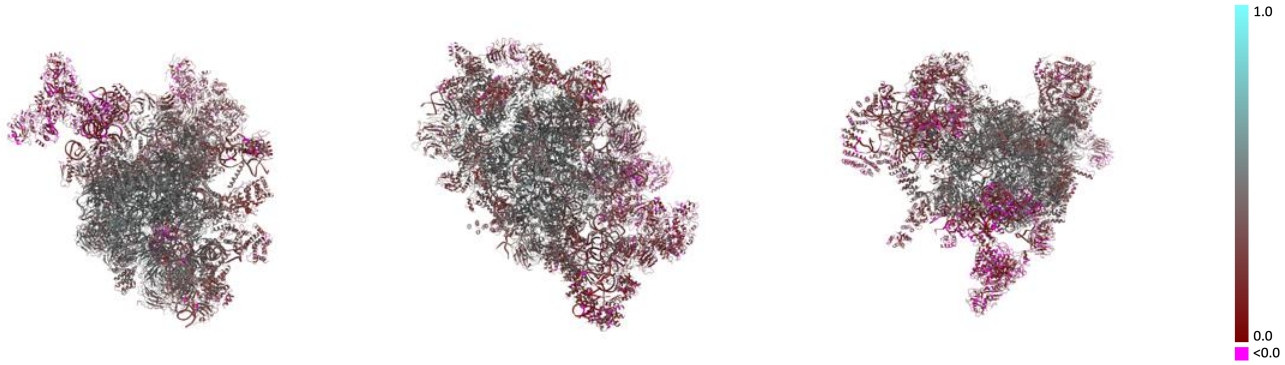
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

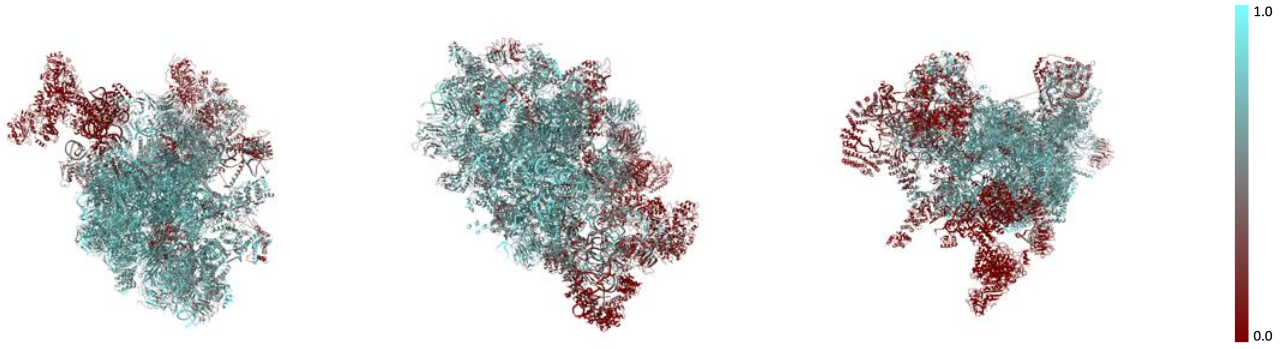
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

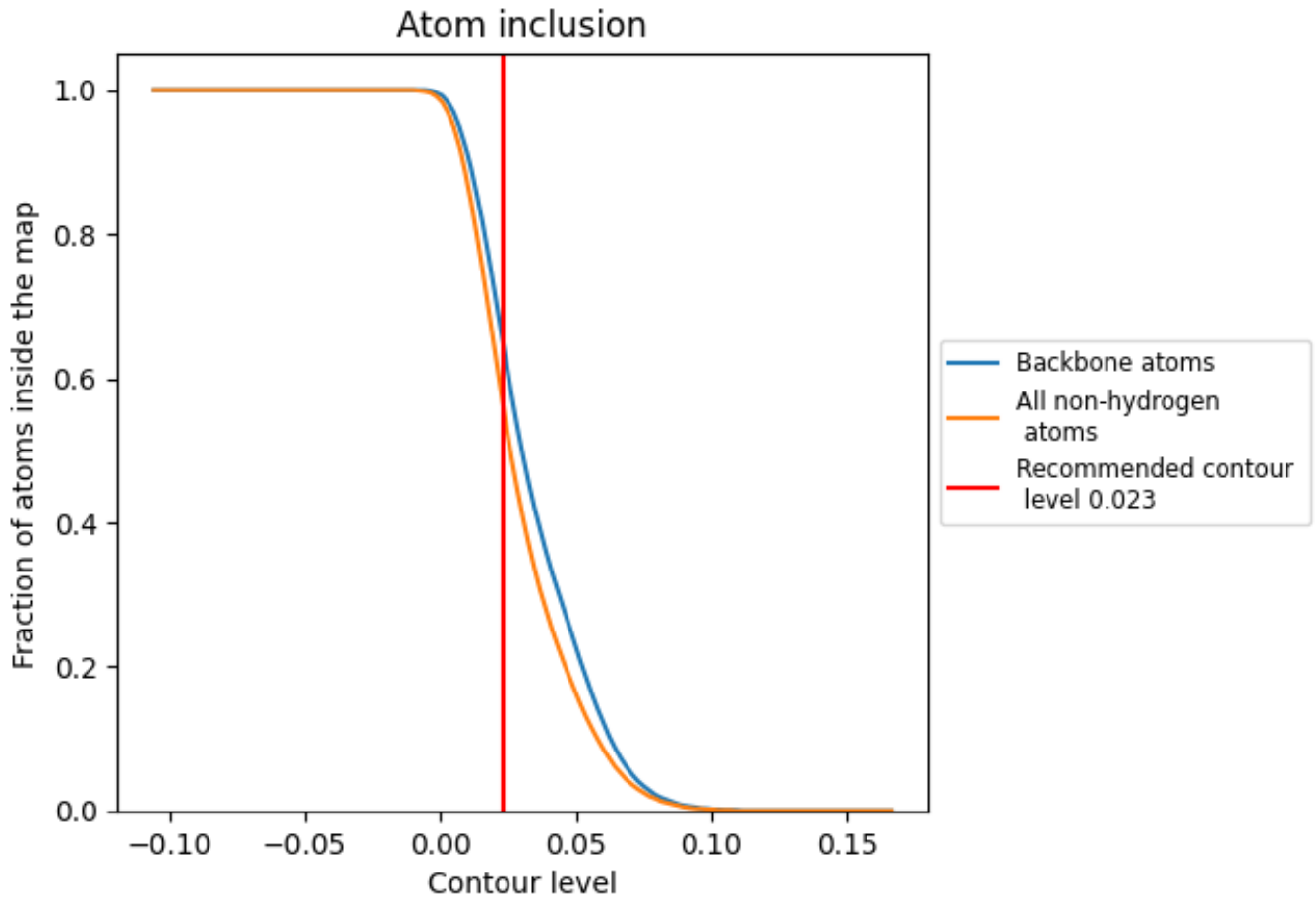
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5650	0.3730
L0	0.8090	0.4030
L1	0.5150	0.2950
L2	0.8300	0.4230
L3	0.3460	0.3430
L4	0.4540	0.3550
L5	0.7190	0.4610
L6	0.2410	0.2740
L7	0.1010	0.2740
L8	0.2820	0.2460
L9	0.6940	0.4630
LC	0.7830	0.5000
LD	0.1950	0.2040
LE	0.3400	0.3730
LF	0.5690	0.3810
LG	0.7150	0.4880
LH	0.6650	0.4140
LI	0.4180	0.2590
LJ	0.7440	0.4610
LK	0.5910	0.3190
LL	0.7170	0.4470
LM	0.7370	0.4510
LN	0.6410	0.3930
LO	0.7680	0.4850
LP	0.7110	0.3720
LQ	0.6090	0.3670
LR	0.2600	0.2480
LS	0.7660	0.4780
LT	0.7600	0.4740
LU	0.7010	0.4550
LV	0.2140	0.2370
LW	0.7590	0.4840
LX	0.3660	0.3050
LY	0.0880	0.2160
LZ	0.7750	0.4920

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NA	0.6390	0.4320
NB	0.6630	0.4450
NC	0.4820	0.3750
ND	0.4500	0.3620
NE	0.1180	0.3550
NF	0.0110	0.1620
NG	0.0350	0.1830
NH	0.0020	0.1540
NI	0.0000	0.1450
NJ	0.0090	0.1660
NK	0.0590	0.2090
SA	0.6830	0.4210
SB	0.6800	0.4140
SC	0.7530	0.4900
SD	0.5960	0.4080
SE	0.7460	0.4860
SF	0.6960	0.4560
SG	0.6520	0.3940
SH	0.6970	0.4420
SI	0.6950	0.4410
SJ	0.5630	0.3460
SK	0.6560	0.4430
SL	0.7730	0.4890
SM	0.7210	0.4730
SN	0.7190	0.4400
SO	0.5020	0.3520
SP	0.1840	0.2730
SQ	0.6440	0.4410
SR	0.7030	0.4700
SS	0.5080	0.3900
ST	0.5060	0.3310
SU	0.6330	0.3490
SV	0.5000	0.4130
SX	0.3690	0.3230
SY	0.7330	0.4650
SZ	0.2670	0.2490