Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 02:59 PM JST

PDB ID	:	5WYJ
EMDB ID	:	EMD-6695
Title	:	Cryo-EM structure of the 90S small subunit pre-ribosome (Dhr1-depleted, Enp1-TAP, state 1)
Authors	:	Ye, K.; Zhu, X.; Sun, Q.
Deposited on	:	2017-01-13
Resolution	:	8.70 Å(reported)

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

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

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

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

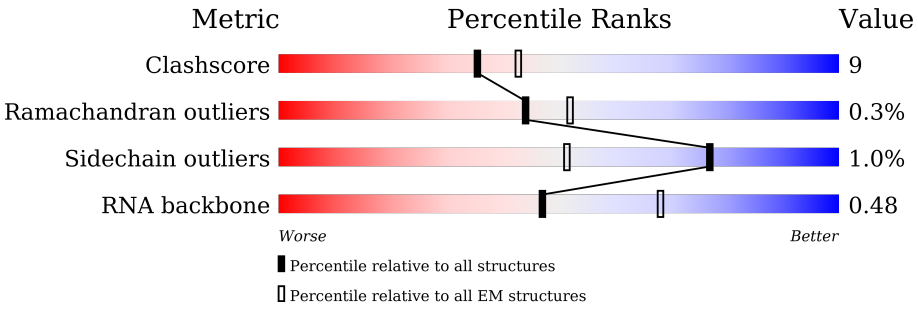
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 8.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	3A	333	5% 24% 21% · 53%
2	3B	327	20% 58% 15% 27%
2	3C	327	38% 63% 10% 27%
3	3D	504	13% 61% 12% 27%
4	3E	511	22% 61% 14% 25%
5	3F	573	18% 42% 22% 36%
6	3G	126	19% 75% 22% ·

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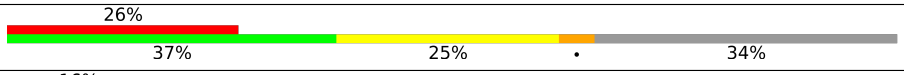
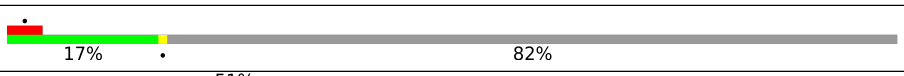
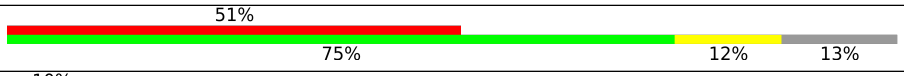
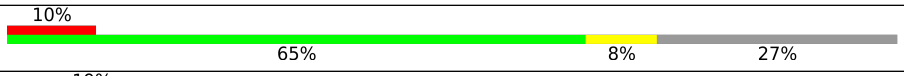
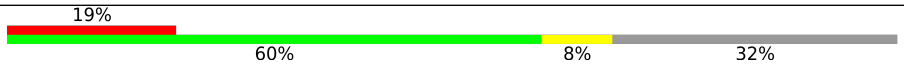
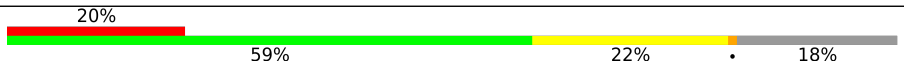
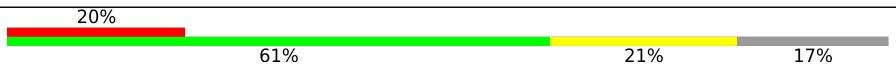
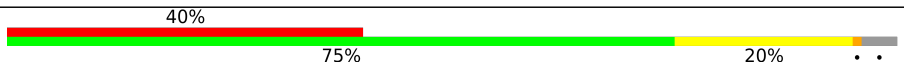
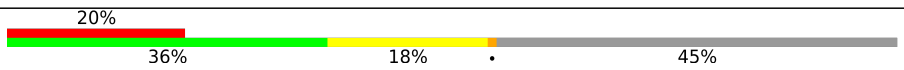
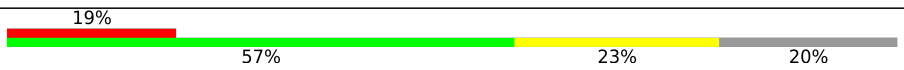
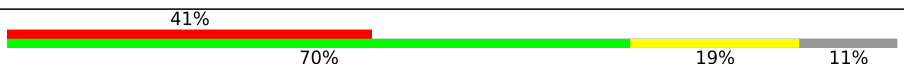
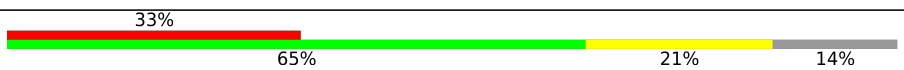
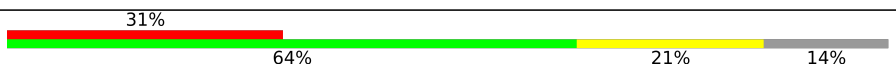
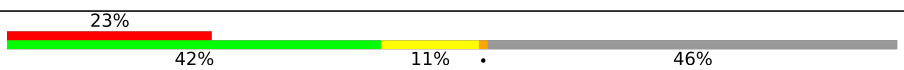
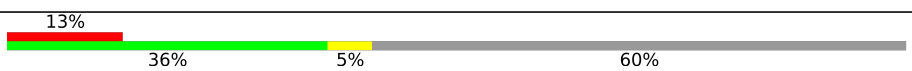
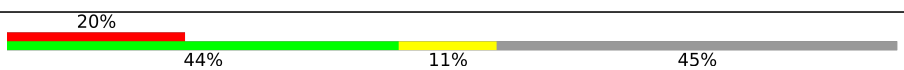
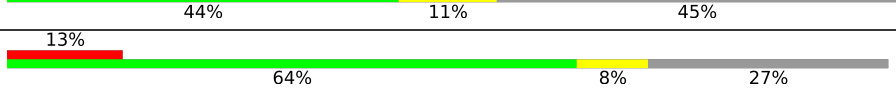
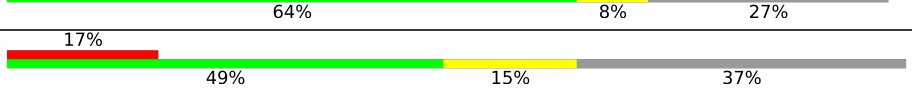
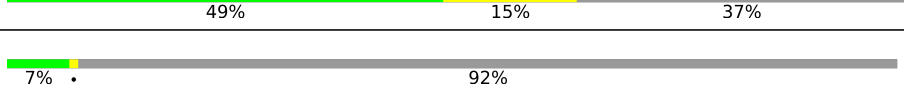
Mol	Chain	Length	Quality of chain
6	3H	126	
7	5A	700	
8	AA	776	
9	AB	643	
10	AC	713	
11	AD	575	
12	AE	1769	
13	AF	513	
14	AG	896	
15	B1	1183	
16	BA	923	
17	BB	943	
18	BC	817	
19	BD	594	
20	BE	939	
21	CA	297	
22	CB	1237	
23	E1	252	
23	E2	252	
24	E3	483	
25	E4	707	
26	K1	316	
27	MA	183	
28	MB	290	
29	MC	593	

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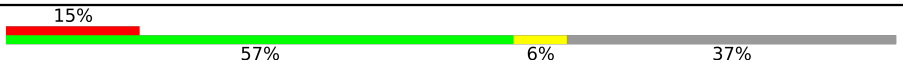
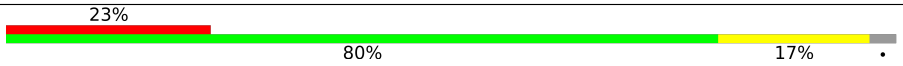
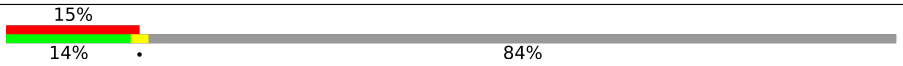
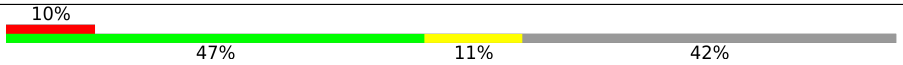
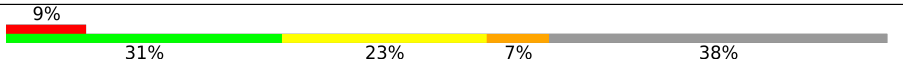
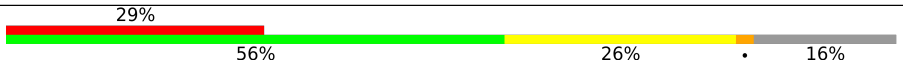
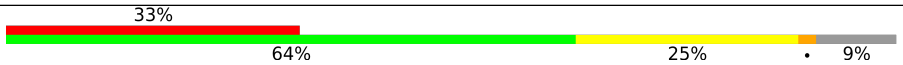
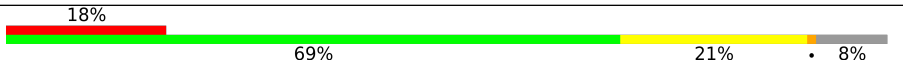
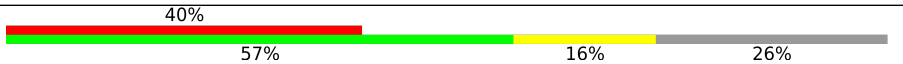
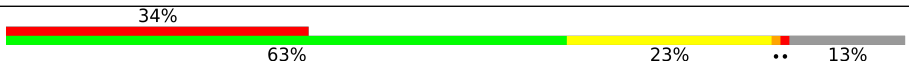
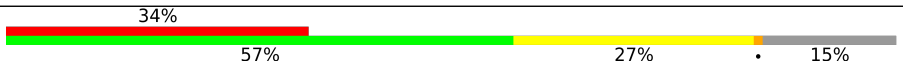
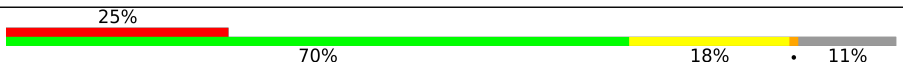
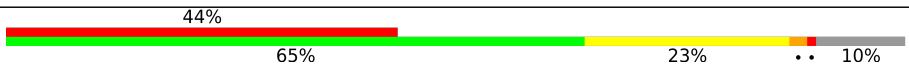
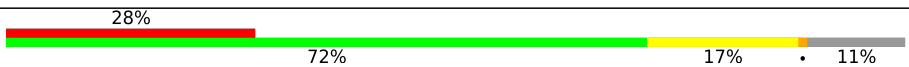
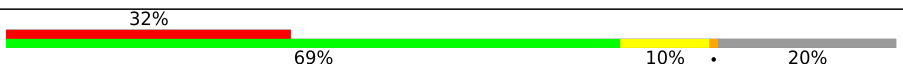
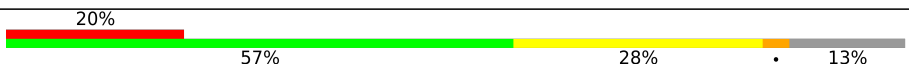
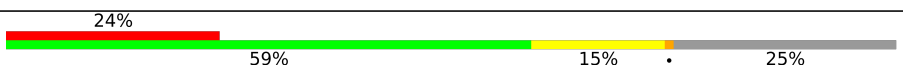
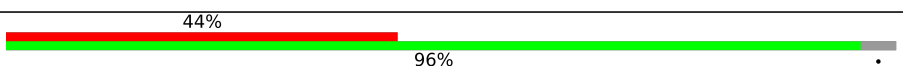
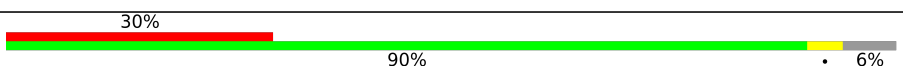
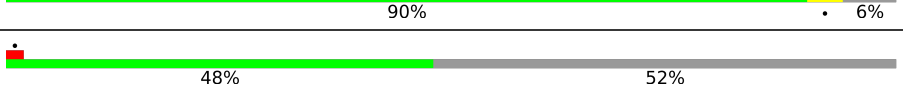
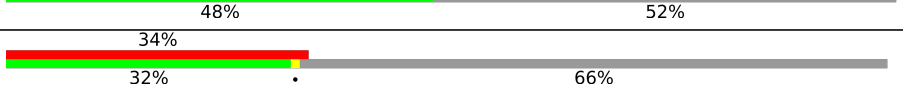
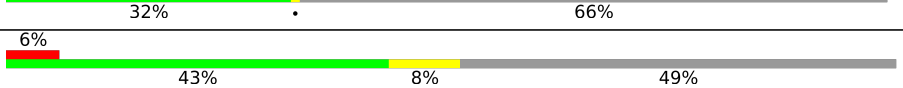
Mol	Chain	Length	Quality of chain
30	P1	274	
31	R1	367	
32	R2	1729	
33	S1	489	
34	SA	1812	
35	SC	255	
36	SF	261	
37	SG	225	
38	SH	236	
39	SI	190	
40	SJ	200	
41	SK	197	
42	SM	156	
43	SN	143	
44	SO	151	
45	SP	137	
46	SR	143	
47	SX	130	
48	SY	145	
49	SZ	135	
50	Sc	82	
51	Sd	67	
52	Sf	63	
53	Sg	152	
54	U1	554	

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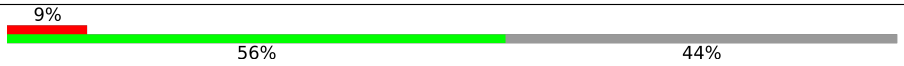
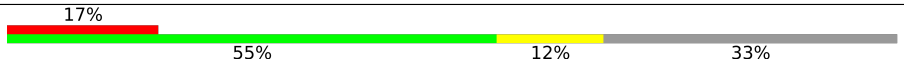
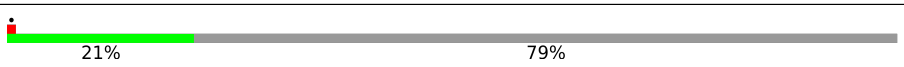
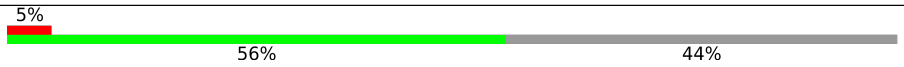
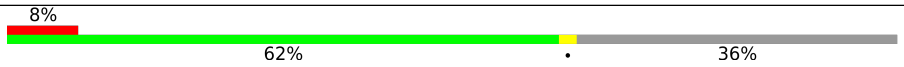
Mol	Chain	Length	Quality of chain
55	U2	250	
56	U3	2493	
57	U4	189	
58	U5	274	
59	UA	1615	
60	UB	987	
61	UC	1033	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 173863 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 U3 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3A	157	Total	C	N	O	P	0	0
			3327	1488	575	1107	157		

- Molecule 2 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3B	239	Total	C	N	O	S	0	0
			1866	1183	332	341	10		
2	3C	239	Total	C	N	O	S	0	0
			1866	1183	332	341	10		

- Molecule 3 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3D	370	Total	C	N	O	S	0	0
			2915	1843	503	560	9		

- Molecule 4 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3E	382	Total	C	N	O	S	0	0
			2935	1859	498	570	8		

- Molecule 5 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3F	365	Total	C	N	O	S	0	0
			2916	1871	506	529	10		

- Molecule 6 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3G	122	Total	C	N	O	S	0	0
			924	589	159	172	4		
6	3H	122	Total	C	N	O	S	0	0
			924	589	159	172	4		

- Molecule 7 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5A	462	Total	C	N	O	P	0	0
			9867	4406	1749	3250	462		

- Molecule 8 is a protein called Utp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AA	569	Total	C	N	O	0	0
			2845	1707	569	569		

- Molecule 9 is a protein called Utp5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AB	403	Total	C	N	O	0	0
			2015	1209	403	403		

- Molecule 10 is a protein called Utp8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AC	472	Total	C	N	O	0	0
			2360	1416	472	472		

- Molecule 11 is a protein called Utp9.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AD	101	Total	C	N	O	0	0
			505	303	101	101		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 10,Utp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AE	1536	Total	C	N	O	S	0	0
			9970	6261	1772	1918	19		

- Molecule 13 is a protein called Utp15.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AF	376	Total 1880	C 1128	N 376	O 376	0	0

- Molecule 14 is a protein called Utp17.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AG	612	Total 3060	C 1836	N 612	O 612	0	0

- Molecule 15 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B1	536	Total 4325	C 2801	N 758	O 746	S 20	0	0

- Molecule 16 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BA	755	Total 6026	C 3862	N 1025	O 1123	S 16	0	0

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BB	778	Total 6138	C 3931	N 1019	O 1161	S 27	0	0

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BC	783	Total 6117	C 3870	N 1033	O 1187	S 27	0	0

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	325	Total 2539	C 1606	N 458	O 466	S 9	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BE	753	Total	C	N	O	S	0	0
			5936	3769	1020	1126	21		

- Molecule 21 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CA	196	Total	C	N	O	S	0	0
			1582	1016	259	300	7		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CB	1098	Total	C	N	O	S	0	0
			8870	5763	1462	1621	24		

- Molecule 23 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E1	217	Total	C	N	O	S	0	0
			1689	1073	293	312	11		
23	E2	216	Total	C	N	O	S	0	0
			1695	1078	295	313	9		

- Molecule 24 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E3	260	Total	C	N	O	S	0	0
			2114	1378	359	374	3		

- Molecule 25 is a protein called Enp2.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	E4	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 26 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K1	175	Total	C	N	O	S	0	0
			1410	903	252	245	10		

- Molecule 27 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	MA	133	Total	C	N	O	S	0	0
			1097	692	204	194	7		

- Molecule 28 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	MB	184	Total	C	N	O	S	0	0
			1465	926	273	260	6		

- Molecule 29 is a protein called Mpp10,U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	MC	46	Total	C	N	O	0	0
			307	193	52	62		

- Molecule 30 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	P1	173	Total	C	N	O	S	0	0
			1368	876	245	243	4		

- Molecule 31 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R1	355	Total	C	N	O	S	0	0
			2742	1756	466	509	11		

- Molecule 32 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R2	272	Total	C	N	O	S	0	0
			2228	1433	374	416	5		

- Molecule 33 is a protein called Sof1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	S1	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SA	1115	Total	C	N	O	P	0	0
			23759	10623	4225	7796	1115		

- Molecule 35 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SC	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 36 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SF	237	Total	C	N	O	S	0	0
			1881	1205	345	328	3		

- Molecule 37 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SG	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 38 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SH	174	Total	C	N	O	S	0	0
			1369	856	262	248	3		

- Molecule 39 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	SI	165	Total	C	N	O	0	0
			1322	856	227	239		

- Molecule 40 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SJ	170	Total	C	N	O	S	0	0
			1350	839	268	241	2		

- Molecule 41 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SK	175	Total	C	N	O	S	0	0
			1412	892	272	247	1		

- Molecule 42 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SM	141	Total	C	N	O	S	0	0
			1143	733	216	191	3		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SN	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 44 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SO	134	Total	C	N	O	S	0	0
			1087	698	202	186	1		

- Molecule 45 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SP	109	Total	C	N	O	S	0	0
			750	462	147	140	1		

- Molecule 46 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	SR	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 47 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SX	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 48 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SY	103	Total	C	N	O	S	0	0
			785	501	144	138	2		

- Molecule 49 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	SZ	101	Total	C	N	O	0	0
			801	512	144	145		

- Molecule 50 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Sc	79	Total	C	N	O	S	0	0
			595	371	108	111	5		

- Molecule 51 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 52 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Sf	30	Total	C	N	O	0	0
			251	162	50	39		

- Molecule 53 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Sg	51	Total	C	N	O	S	0	0
			397	249	73	71	4		

- Molecule 54 is a protein called Utp7.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	U1	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 55 is a protein called Utp11.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	U2	73	Total 365	C 219	N 73	O 73	0	0

- Molecule 56 is a protein called Utp20.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	U3	1407	Total 7035	C 4221	N 1407	O 1407	0	0

- Molecule 57 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	U4	126	Total 990	C 633	N 179	O 168	S 10	0	0

- Molecule 58 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	U5	248	Total 2009	C 1285	N 357	O 359	S 8	0	0

- Molecule 59 is a protein called Helical domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UA	338	Total 1690	C 1014	N 338	O 338	0	0

- Molecule 60 is a protein called Helical domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	UB	555	Total 2775	C 1665	N 555	O 555	0	0

- Molecule 61 is a protein called Unassigned helices.

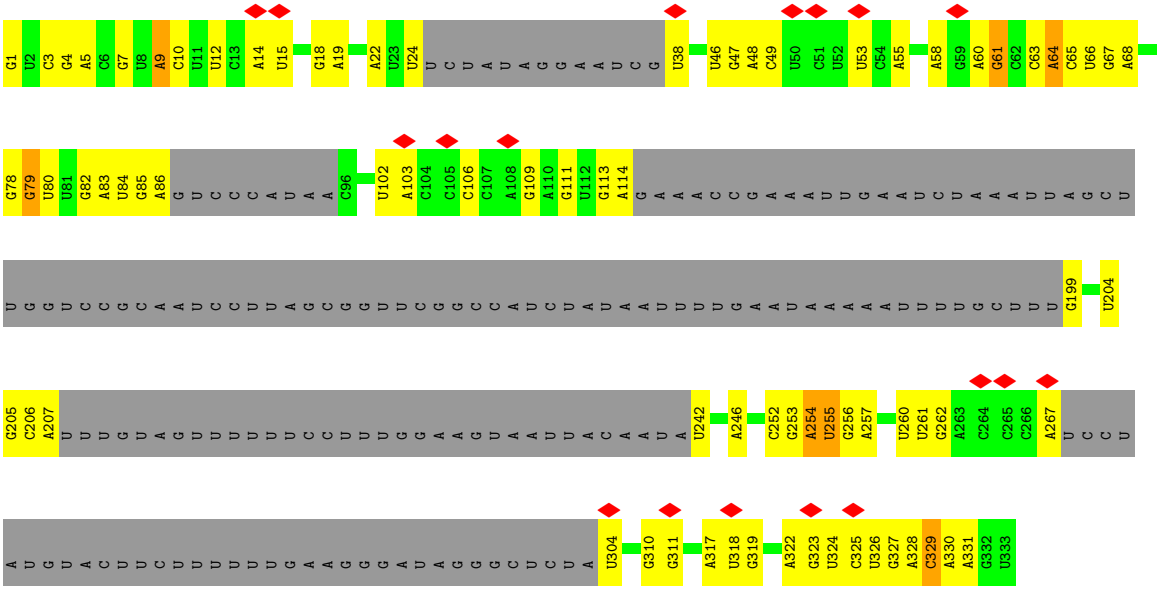
Mol	Chain	Residues	Atoms				AltConf	Trace
61	UC	660	Total 3300	C 1980	N 660	O 660	0	0

3 Residue-property plots (i)

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

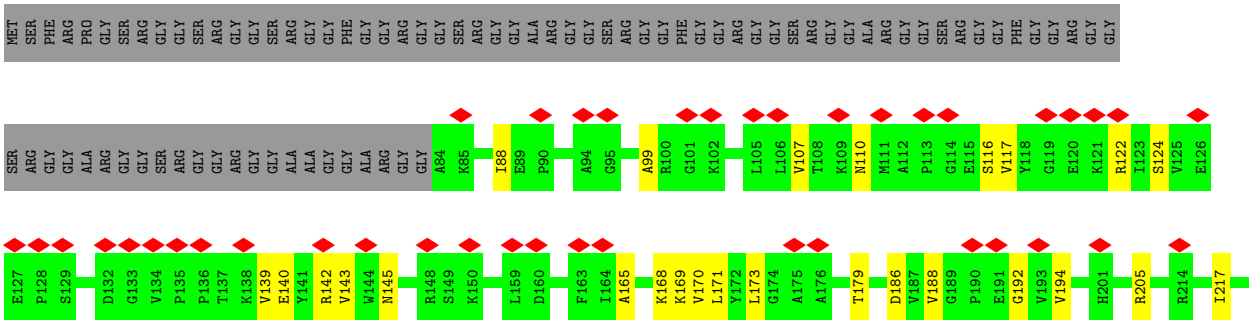
• Molecule 1: U3 RNA

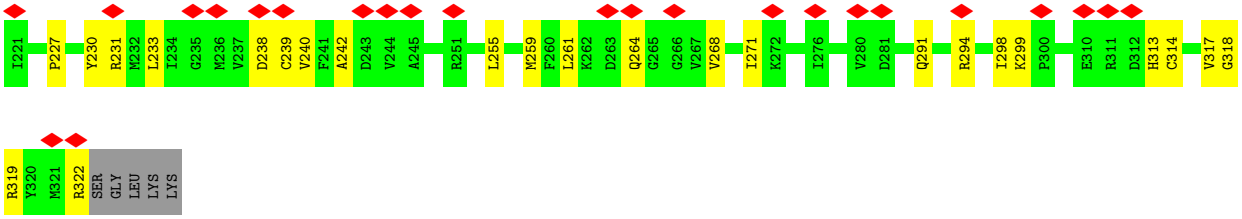
Chain 3A:



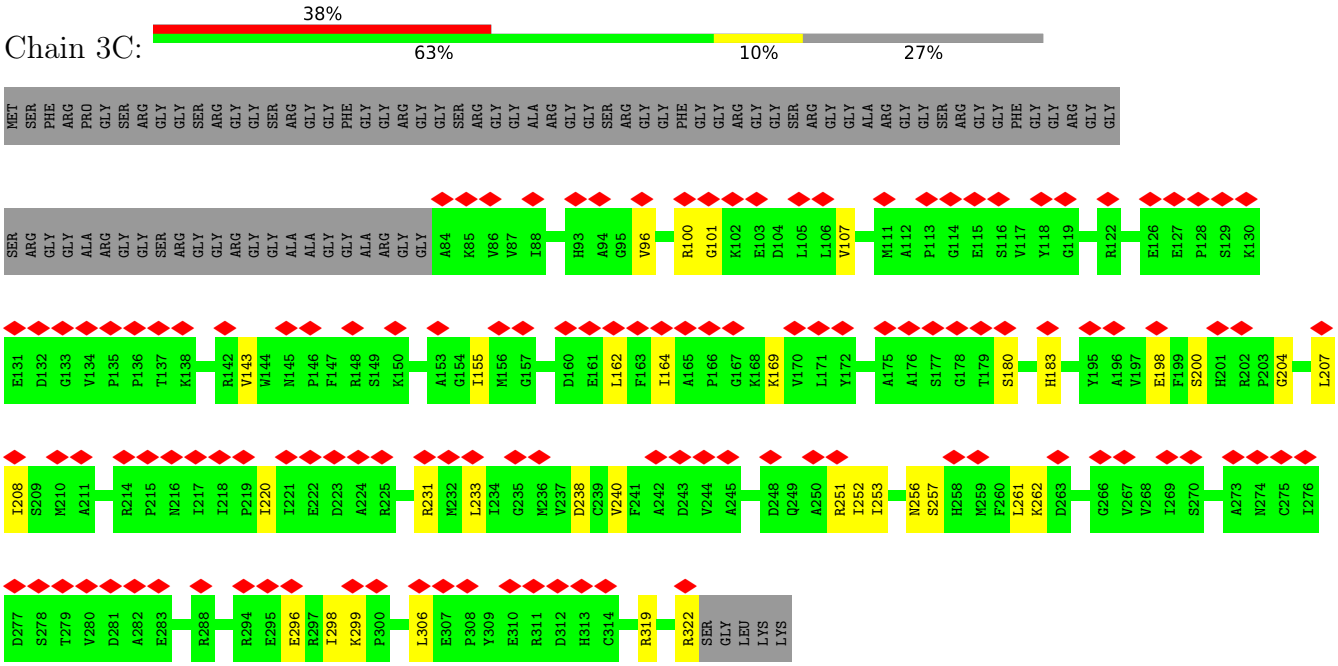
• Molecule 2: rRNA 2'-O-methyltransferase fibrillarin

Chain 3B:

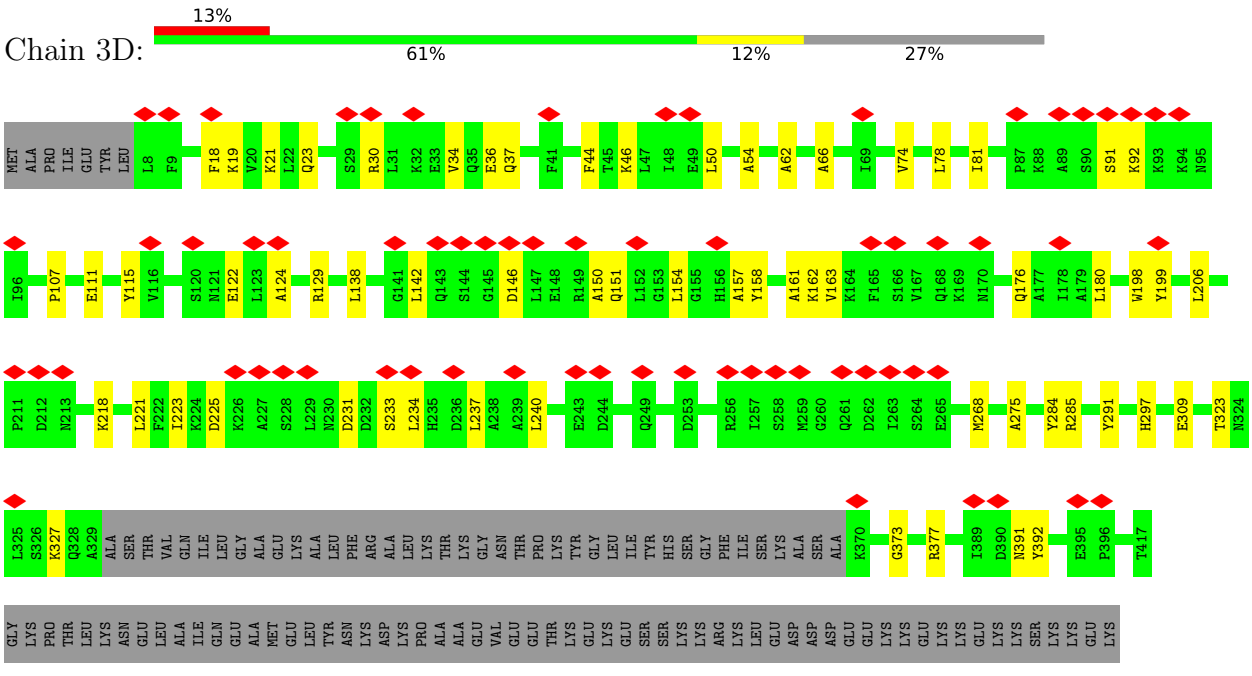




• Molecule 2: rRNA 2'-O-methyltransferase fibrillarin

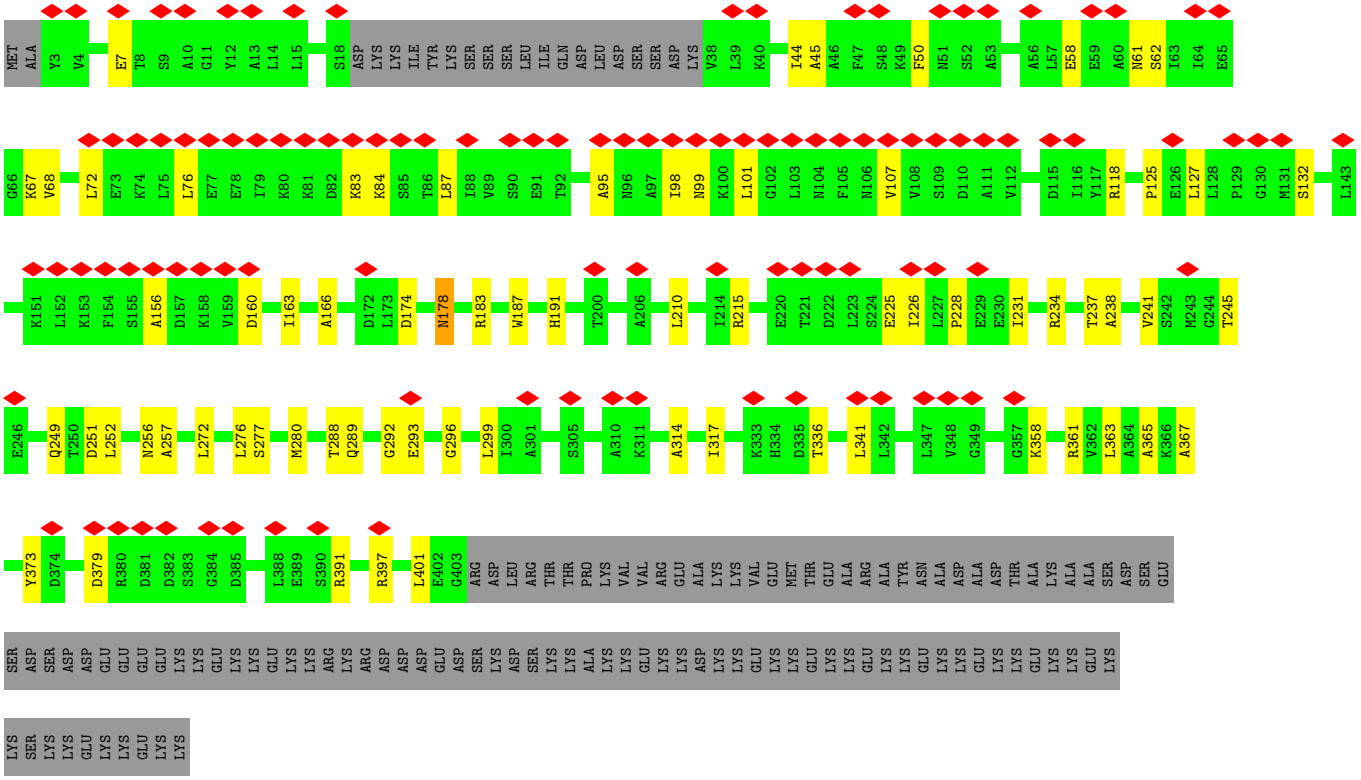


• Molecule 3: Nucleolar protein 56



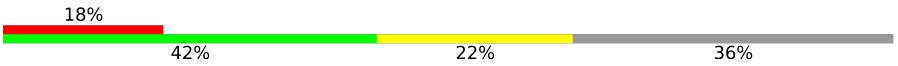
• Molecule 4: Nucleolar protein 58

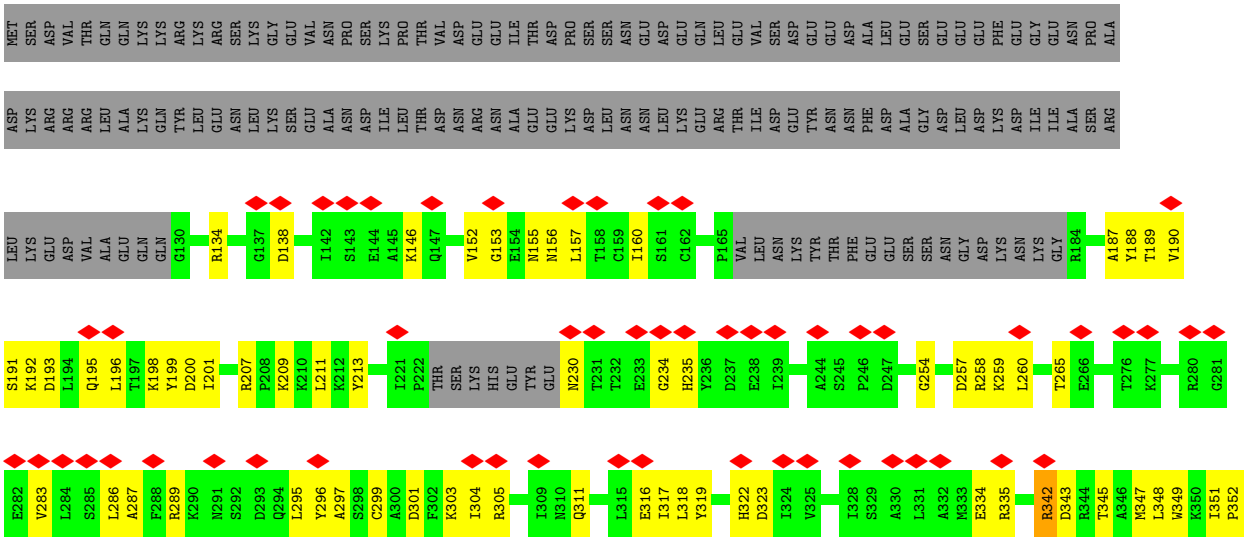
Chain 3E:

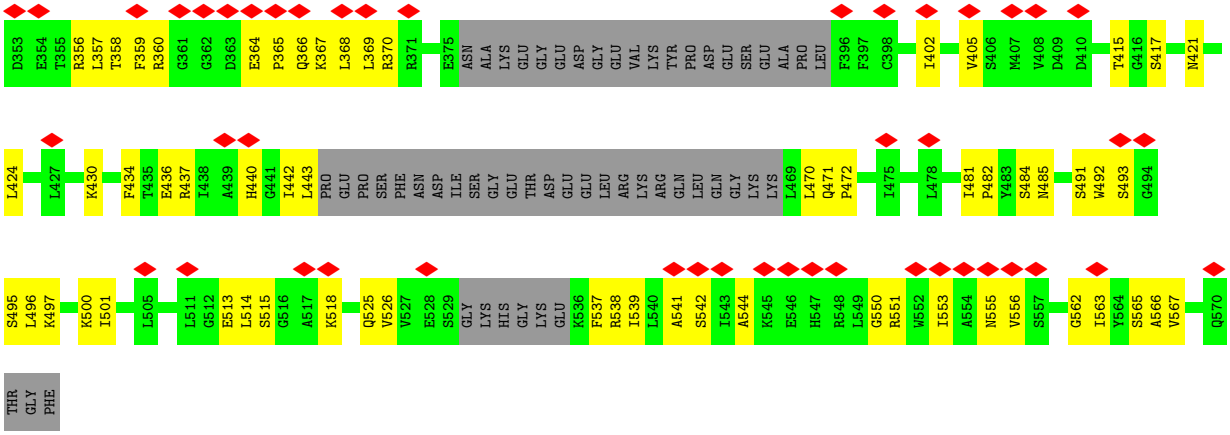


• Molecule 5: Ribosomal RNA-processing protein 9

Chain 3F:

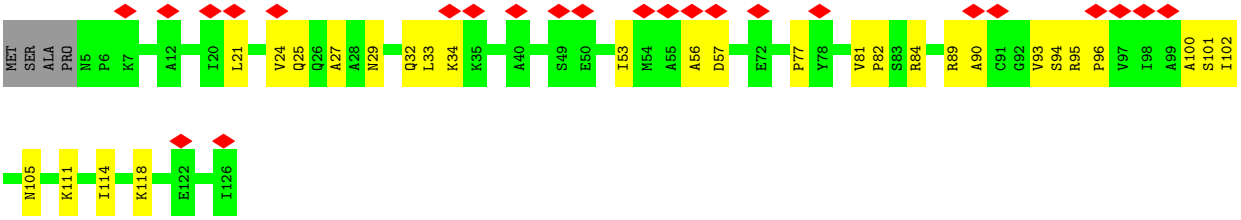






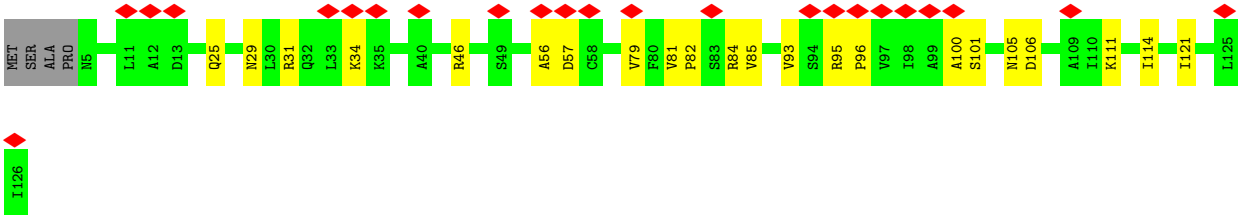
• Molecule 6: 13 kDa ribonucleoprotein-associated protein

Chain 3G:



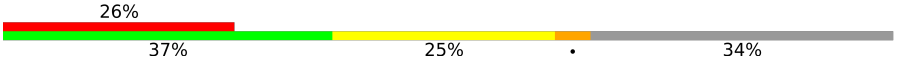
• Molecule 6: 13 kDa ribonucleoprotein-associated protein

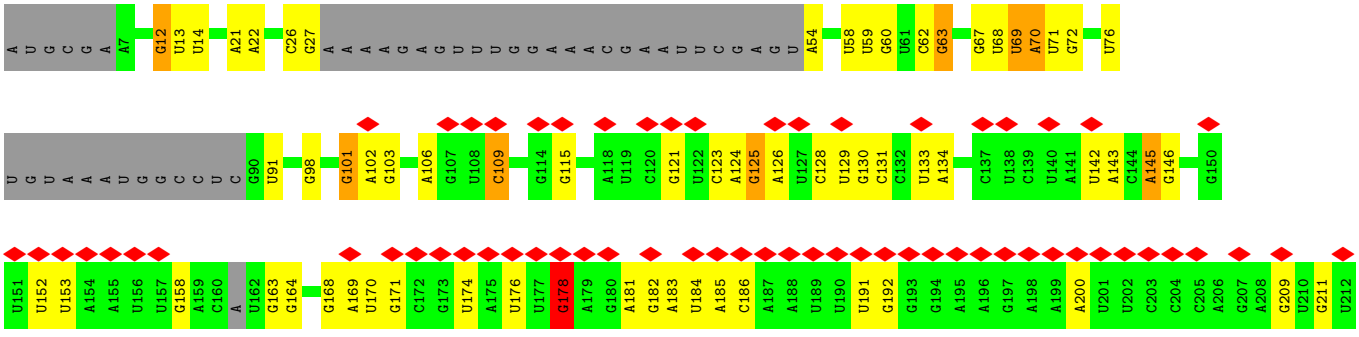
Chain 3H:

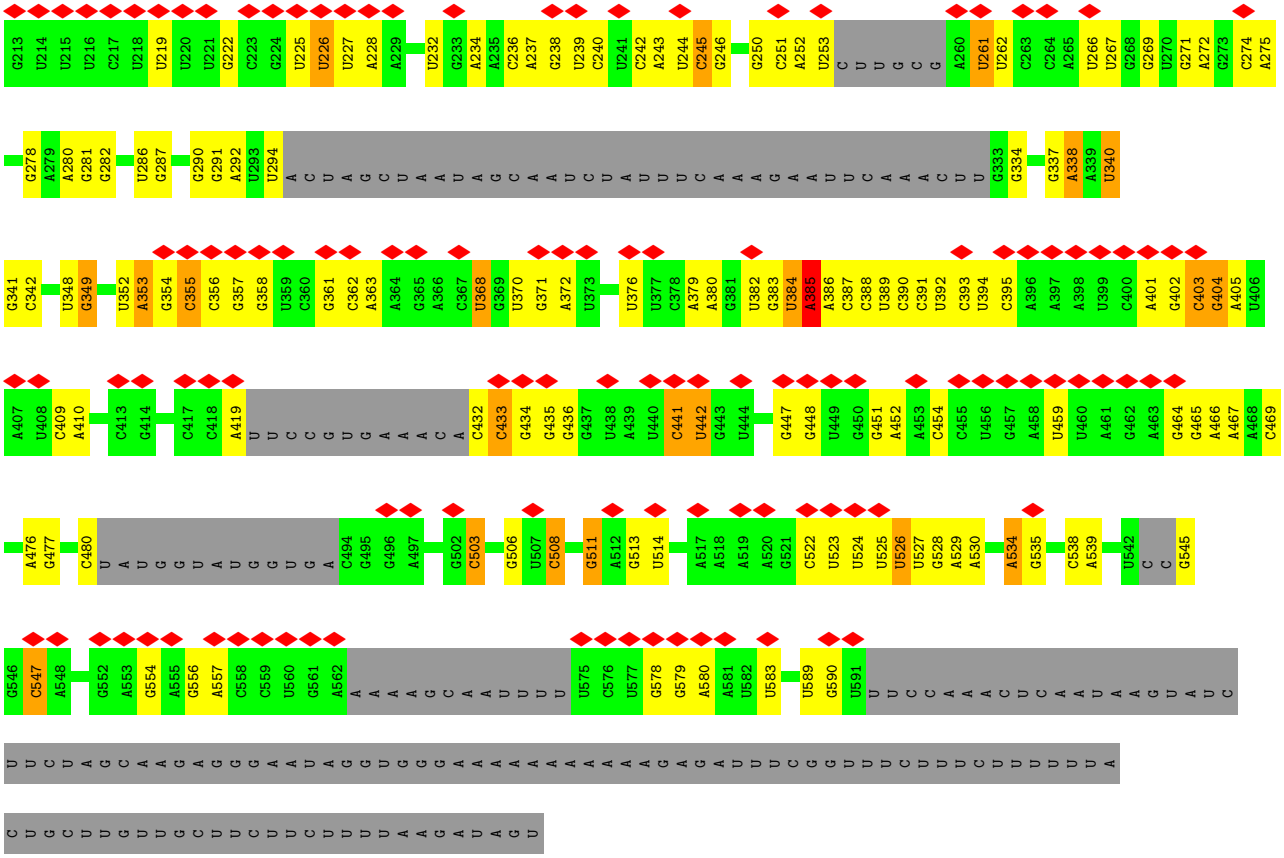


• Molecule 7: 5ETS RNA

Chain 5A:

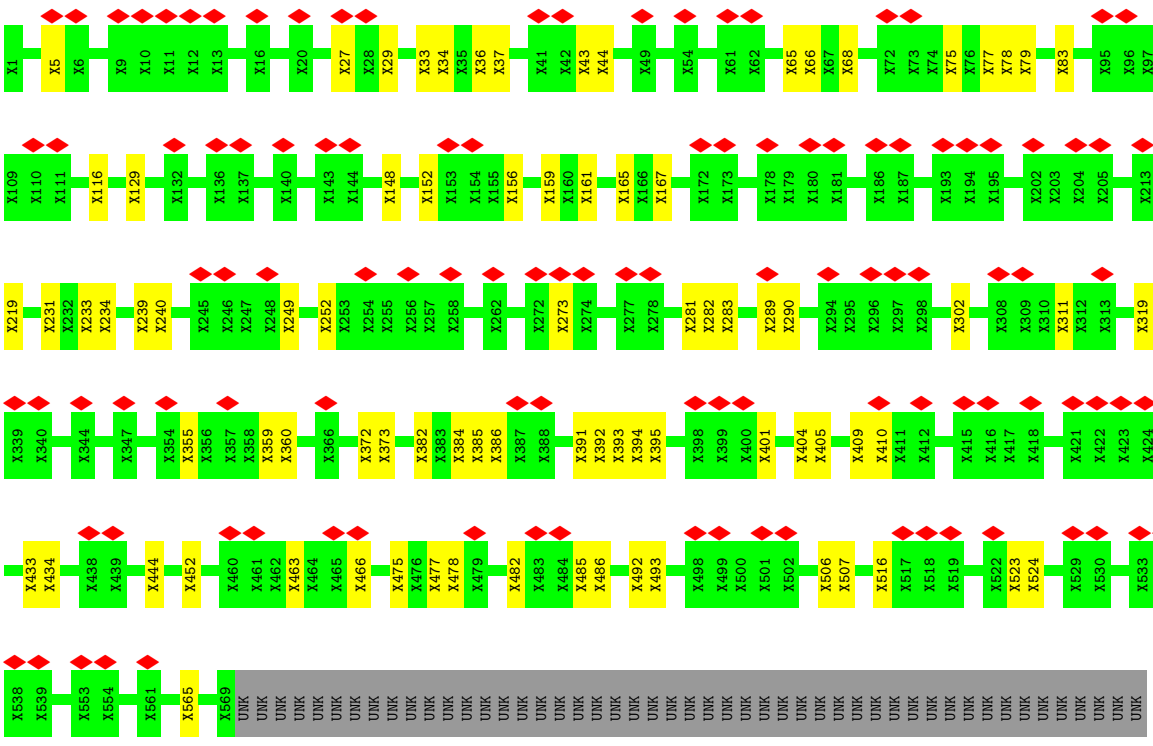


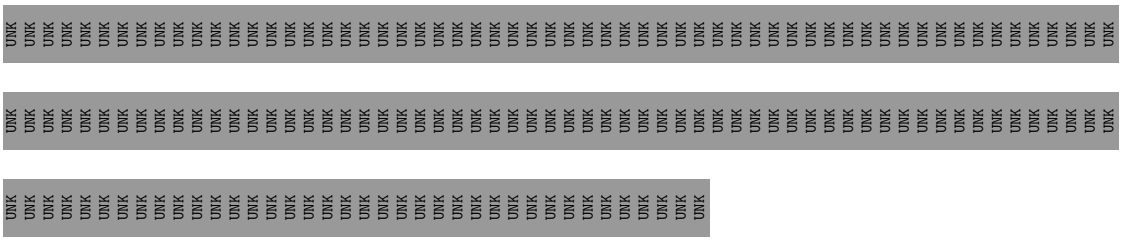




• Molecule 8: Utp4

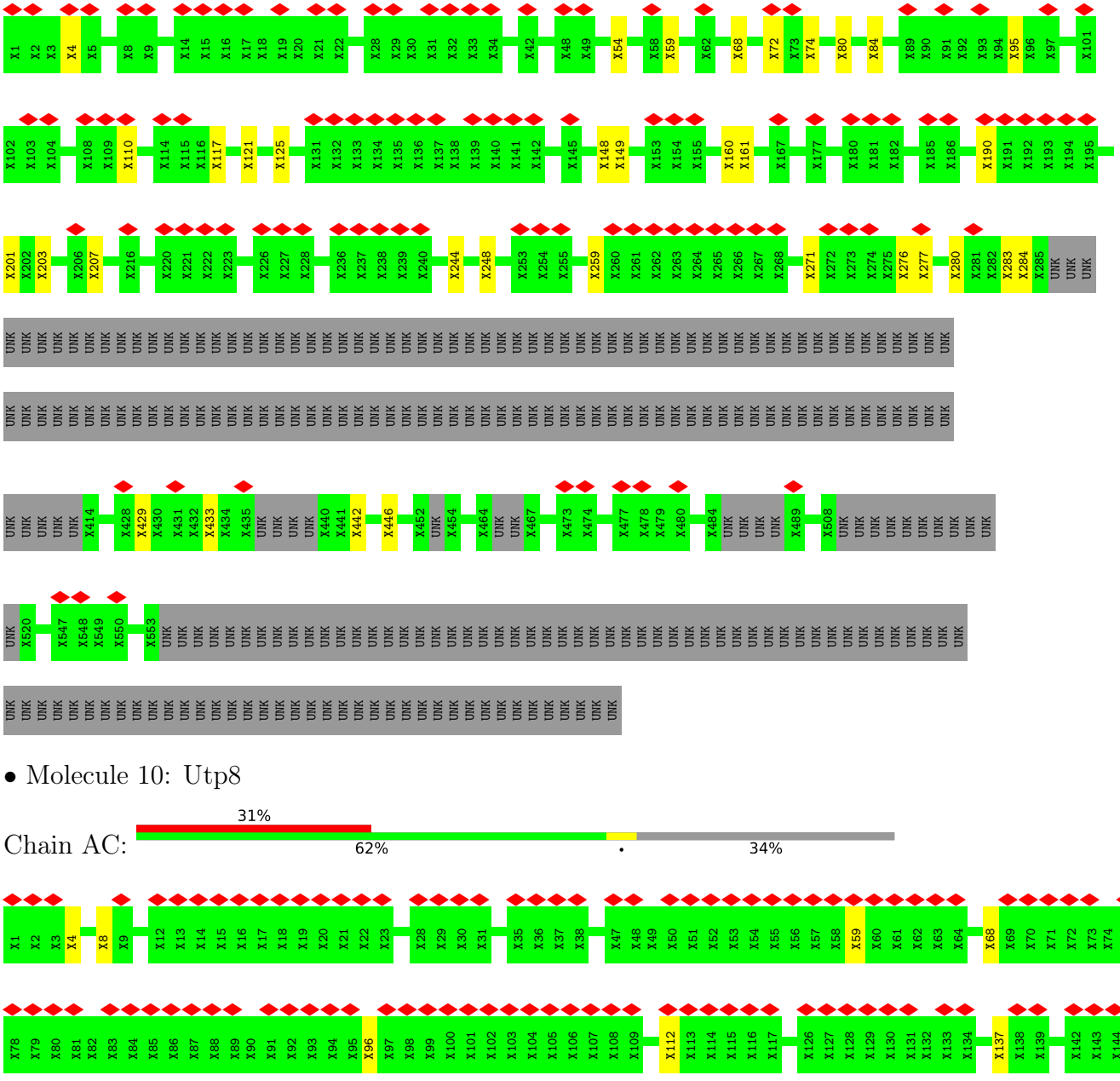
Chain AA:





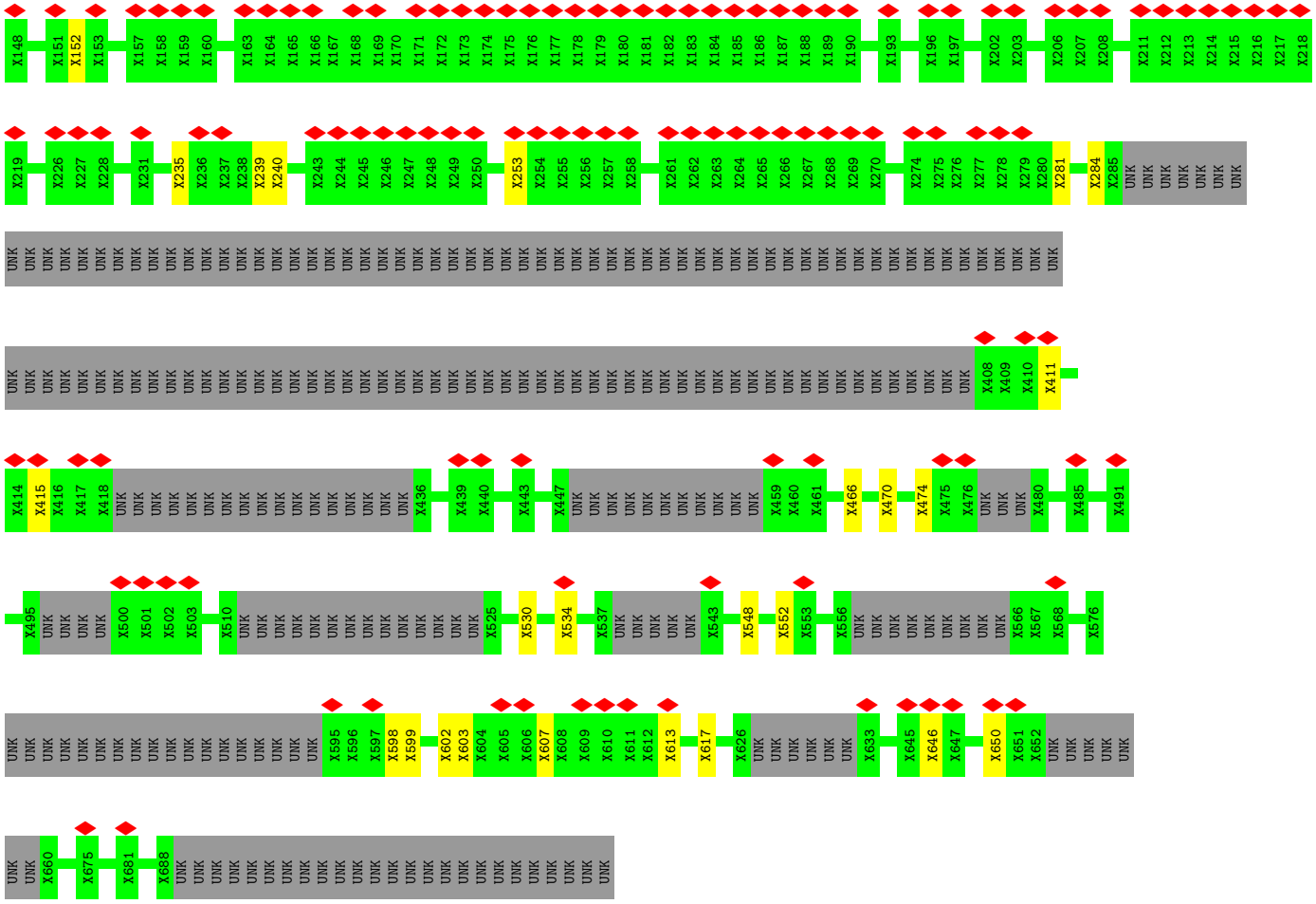
• Molecule 9: Utp5

Chain AB:



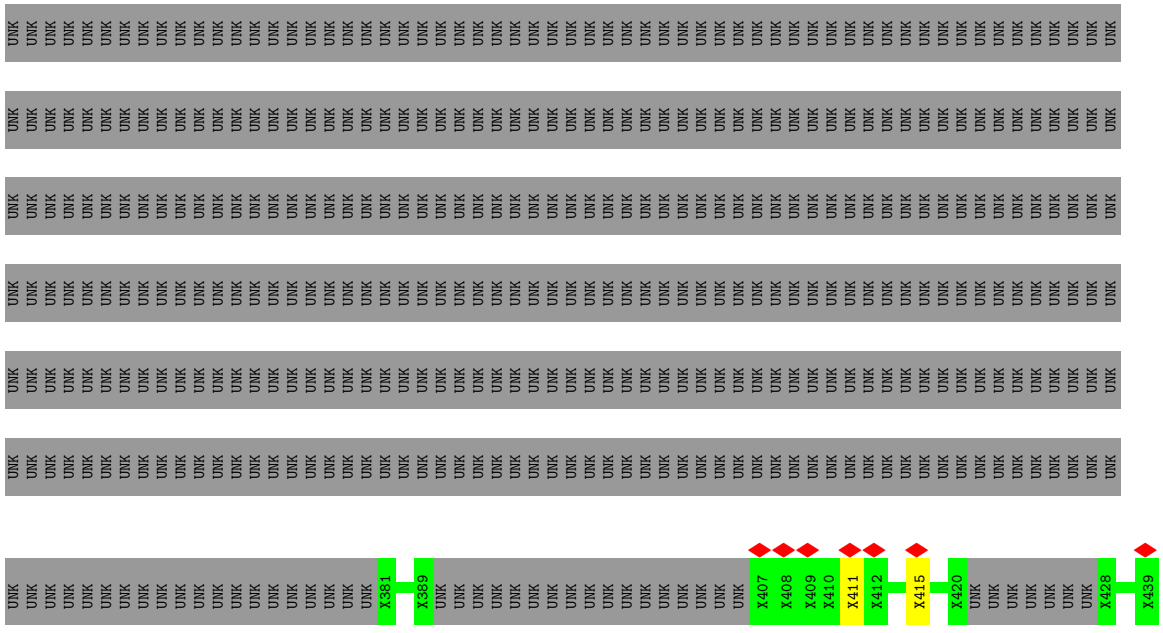
• Molecule 10: Utp8

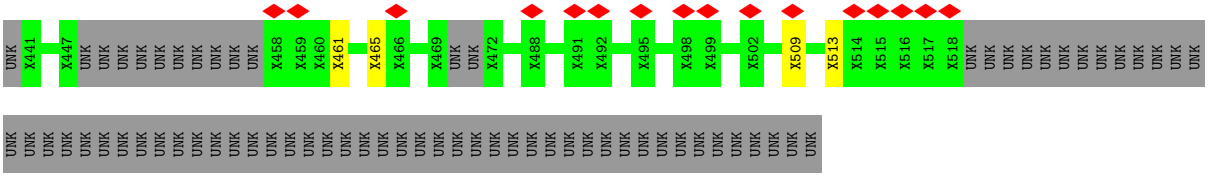
Chain AC:



• Molecule 11: Utp9

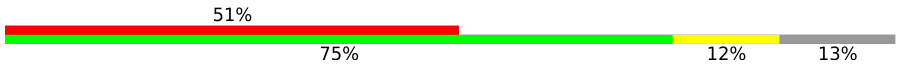
Chain AD:

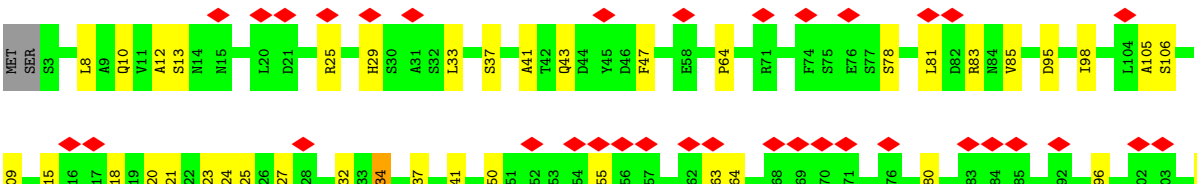


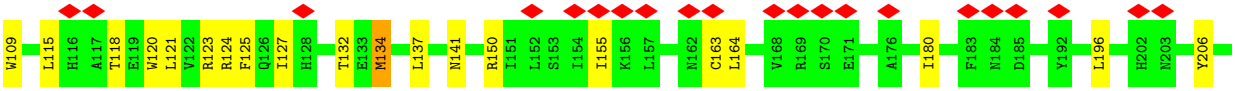


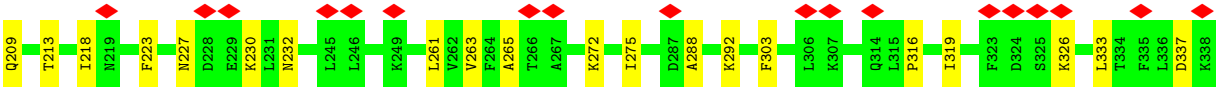
• Molecule 12: U3 small nucleolar RNA-associated protein 10,Utp10

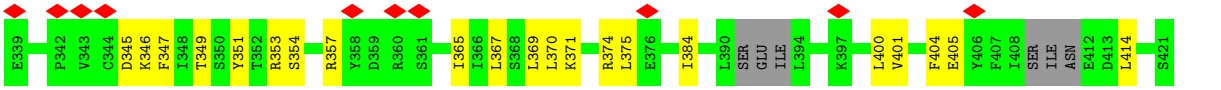
Chain AE:

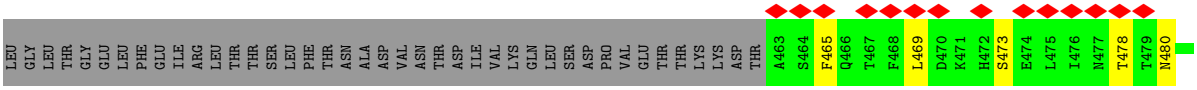


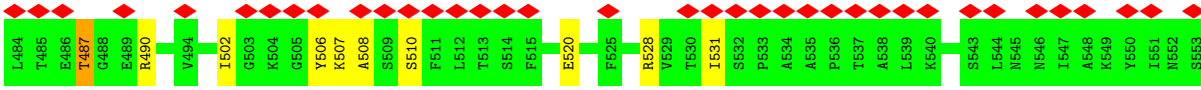


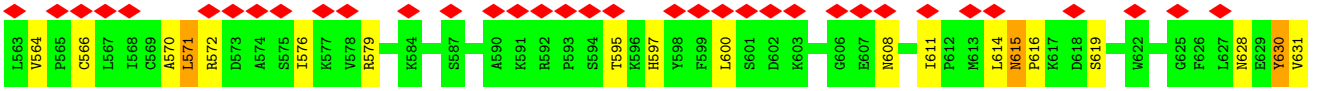


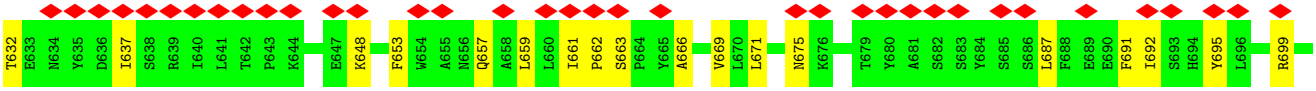


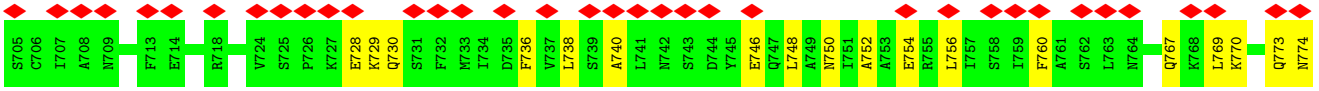


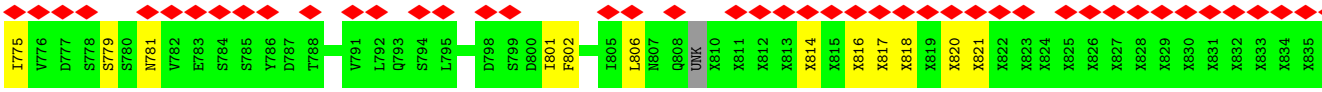


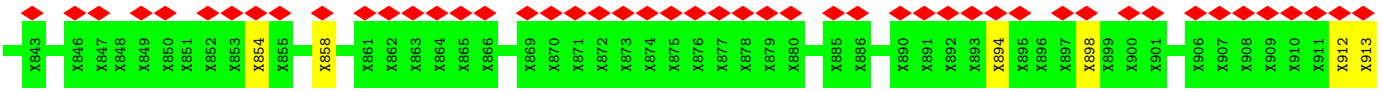


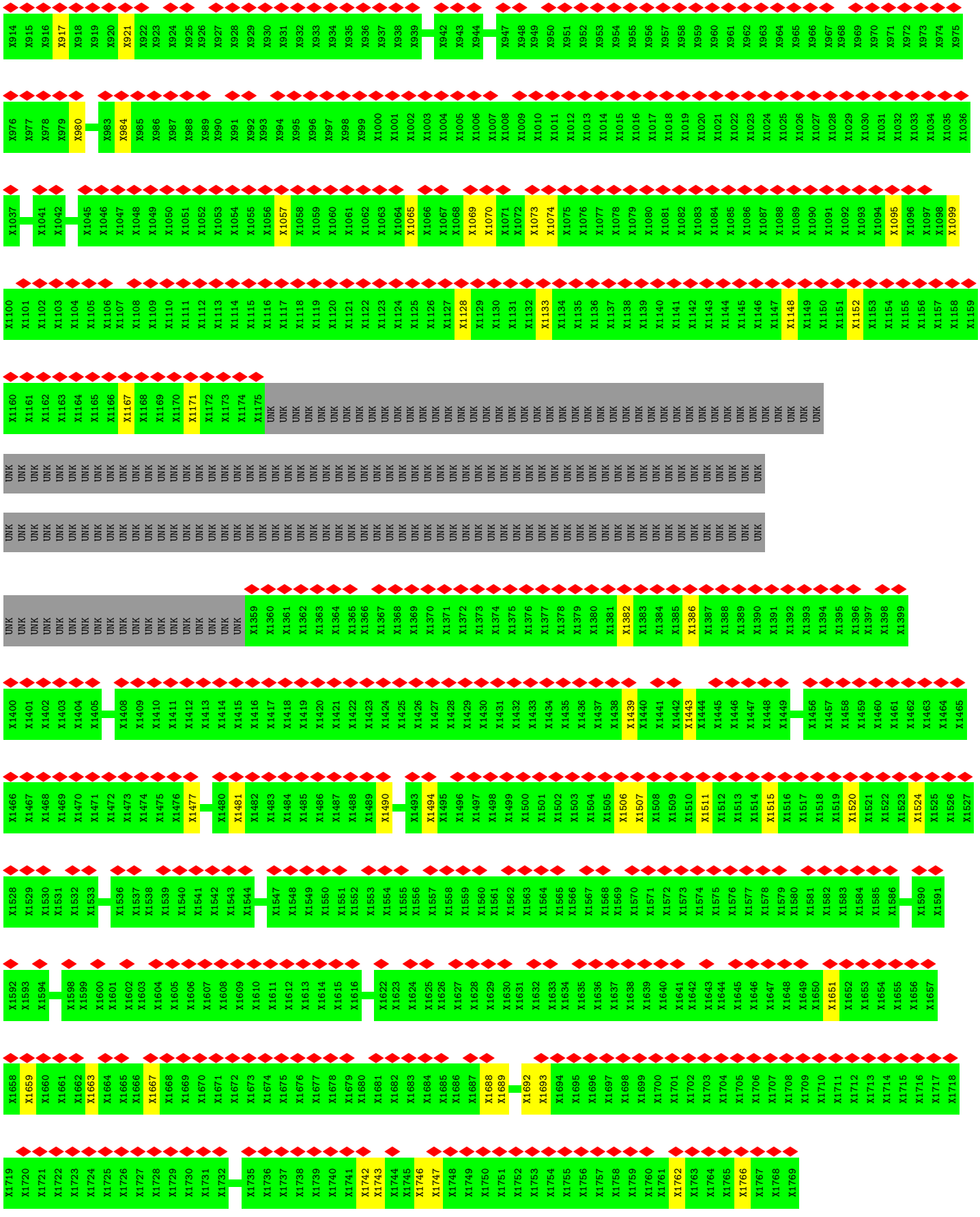








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UNK
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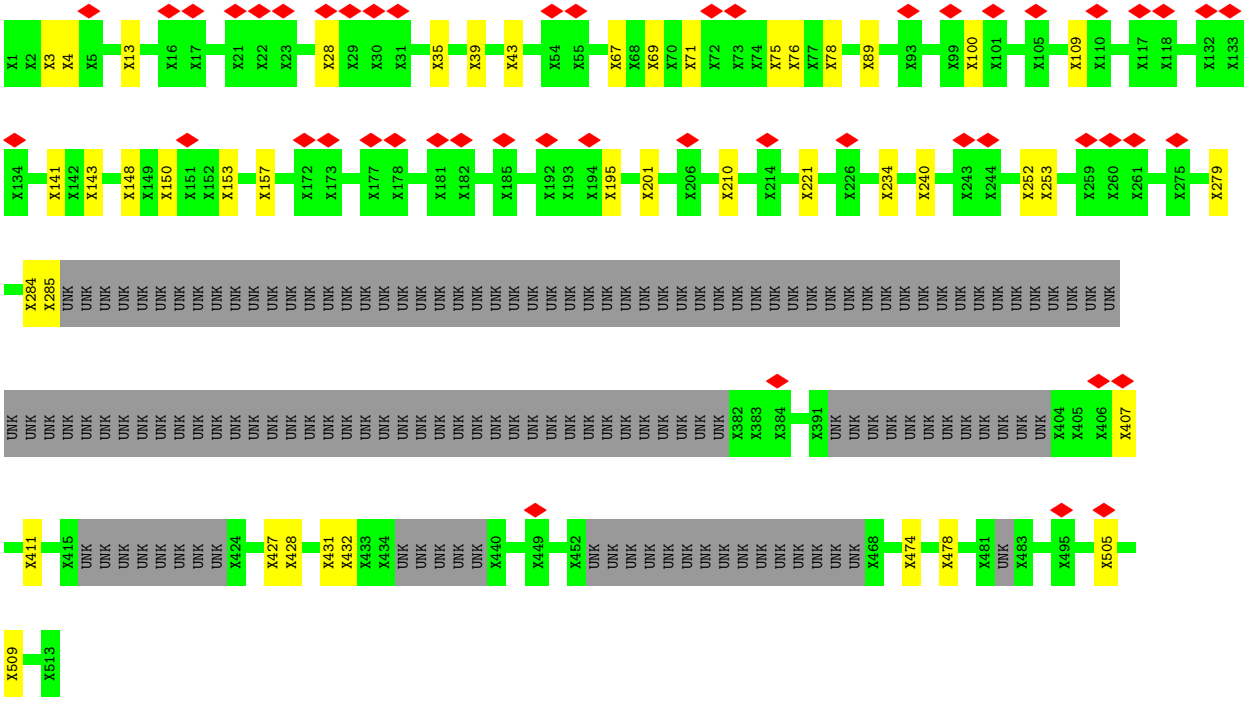
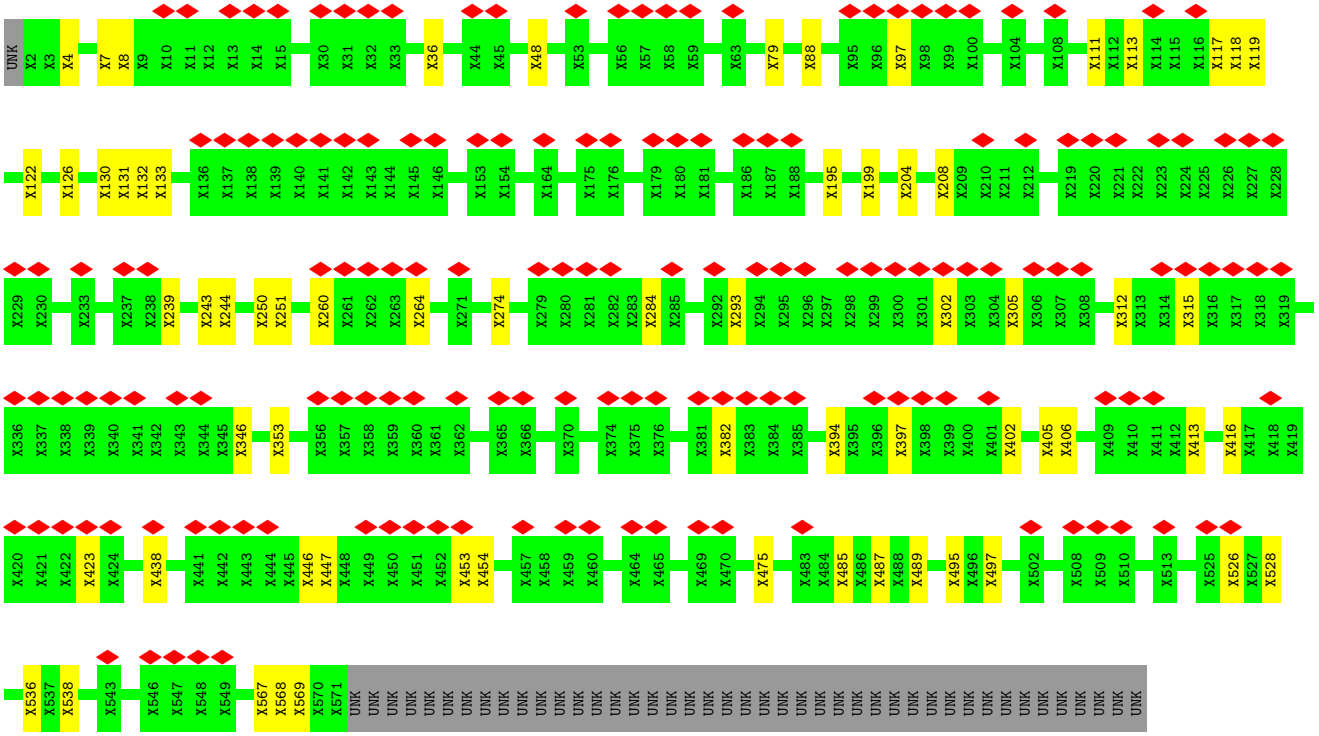
• Molecule 13: Utp15

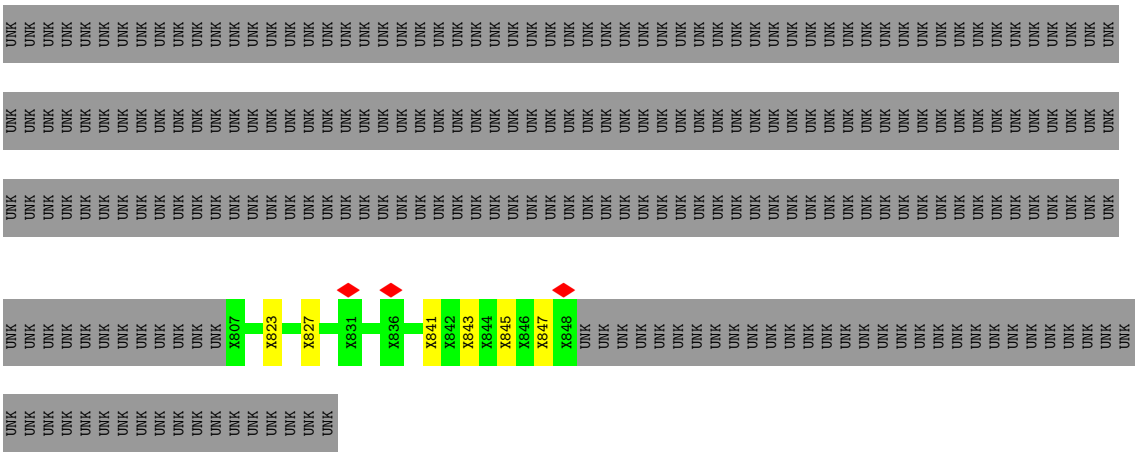
Chain AF:



• Molecule 14: Utp17

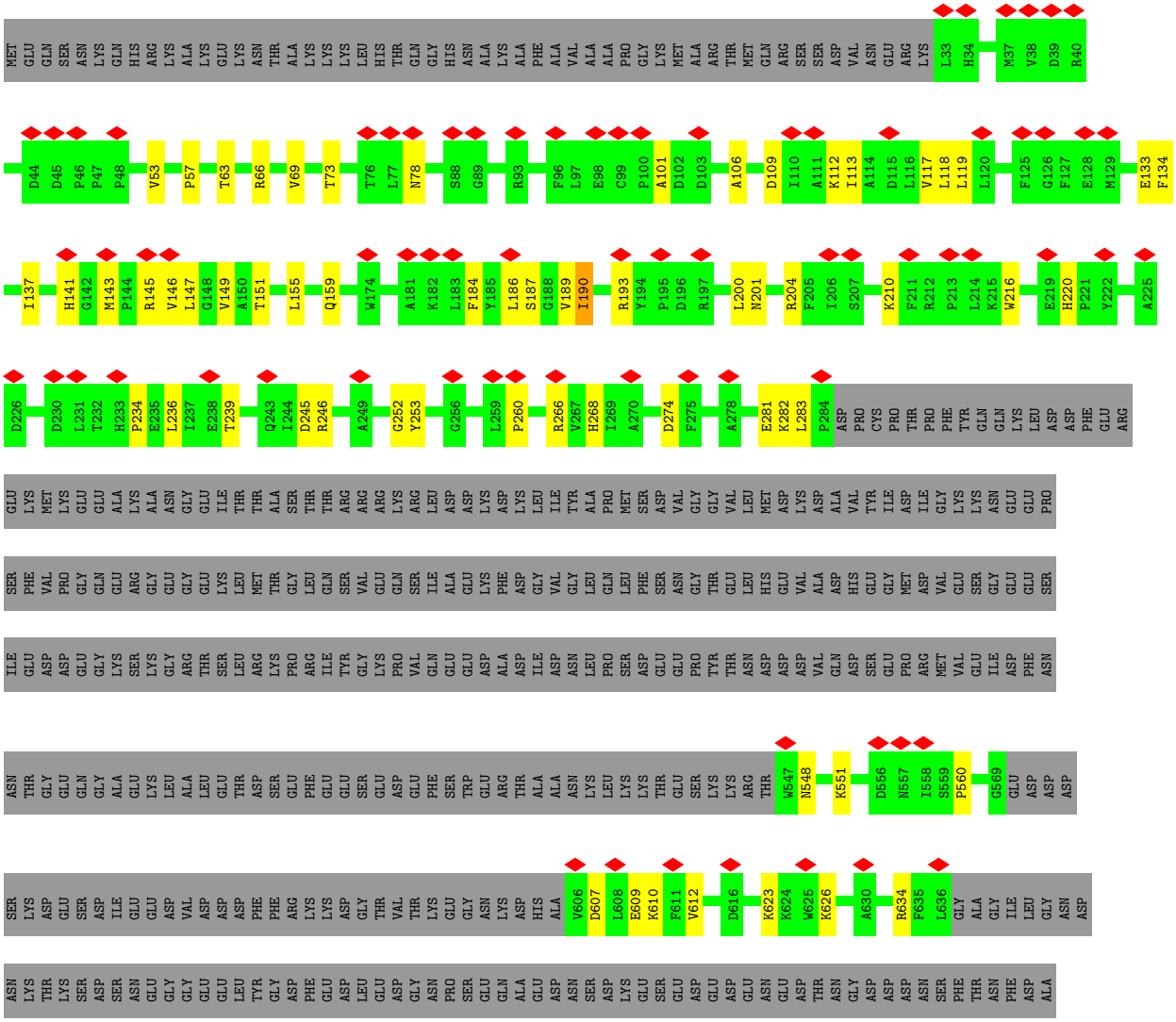
Chain AG:

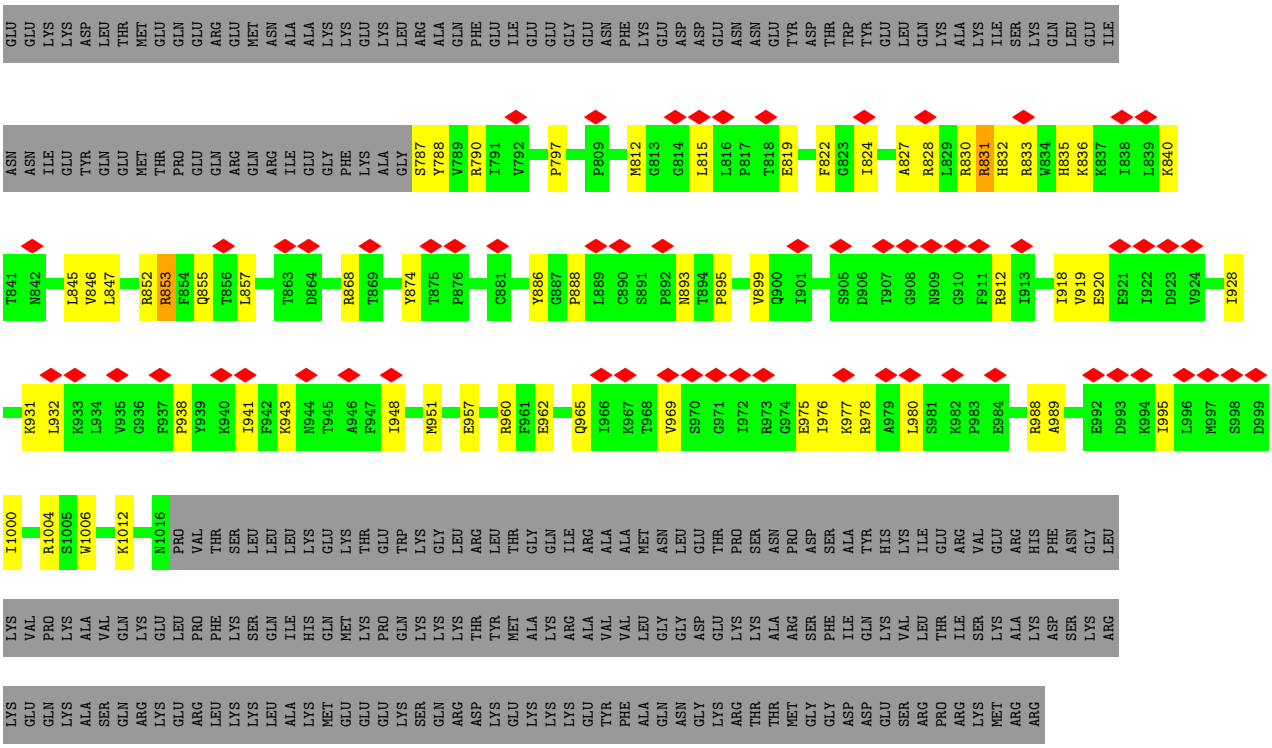




• Molecule 15: Ribosome biogenesis protein BMS1

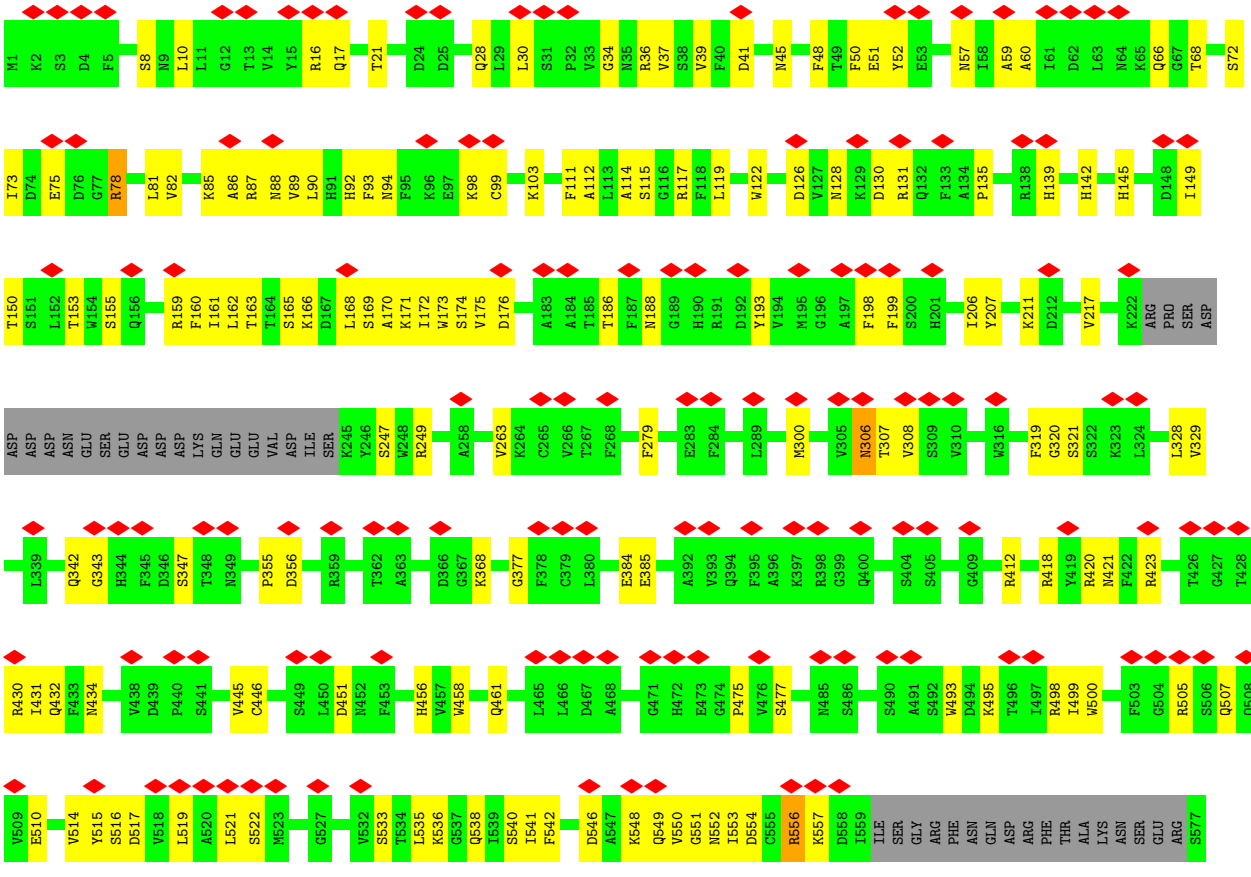
Chain B1:

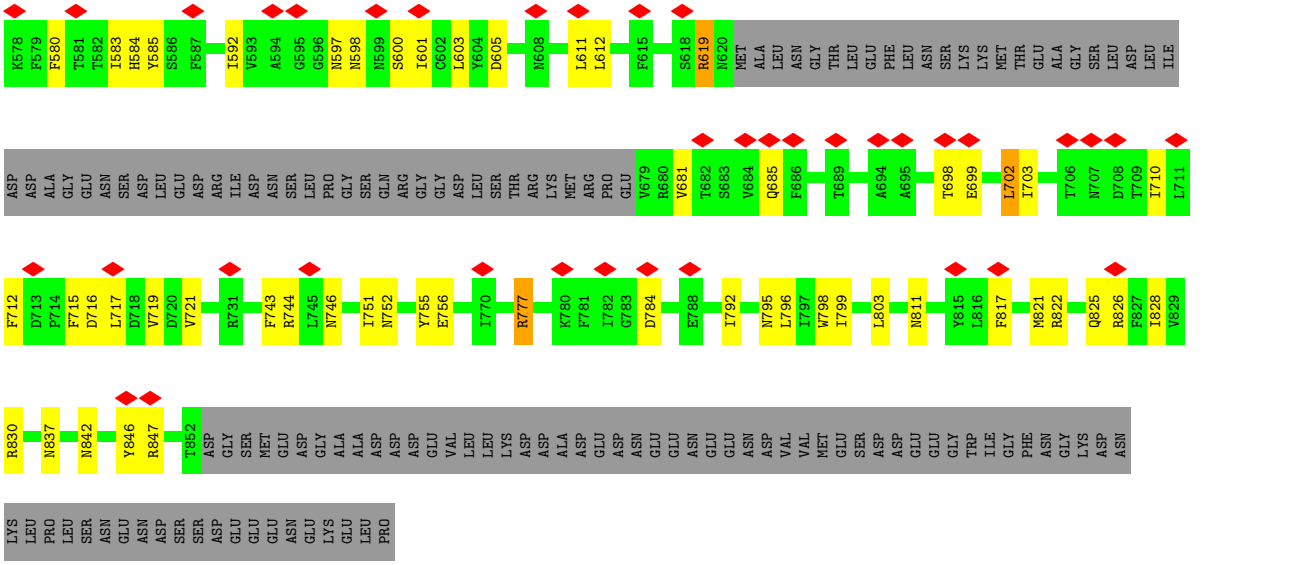




• Molecule 16: Periodic tryptophan protein 2

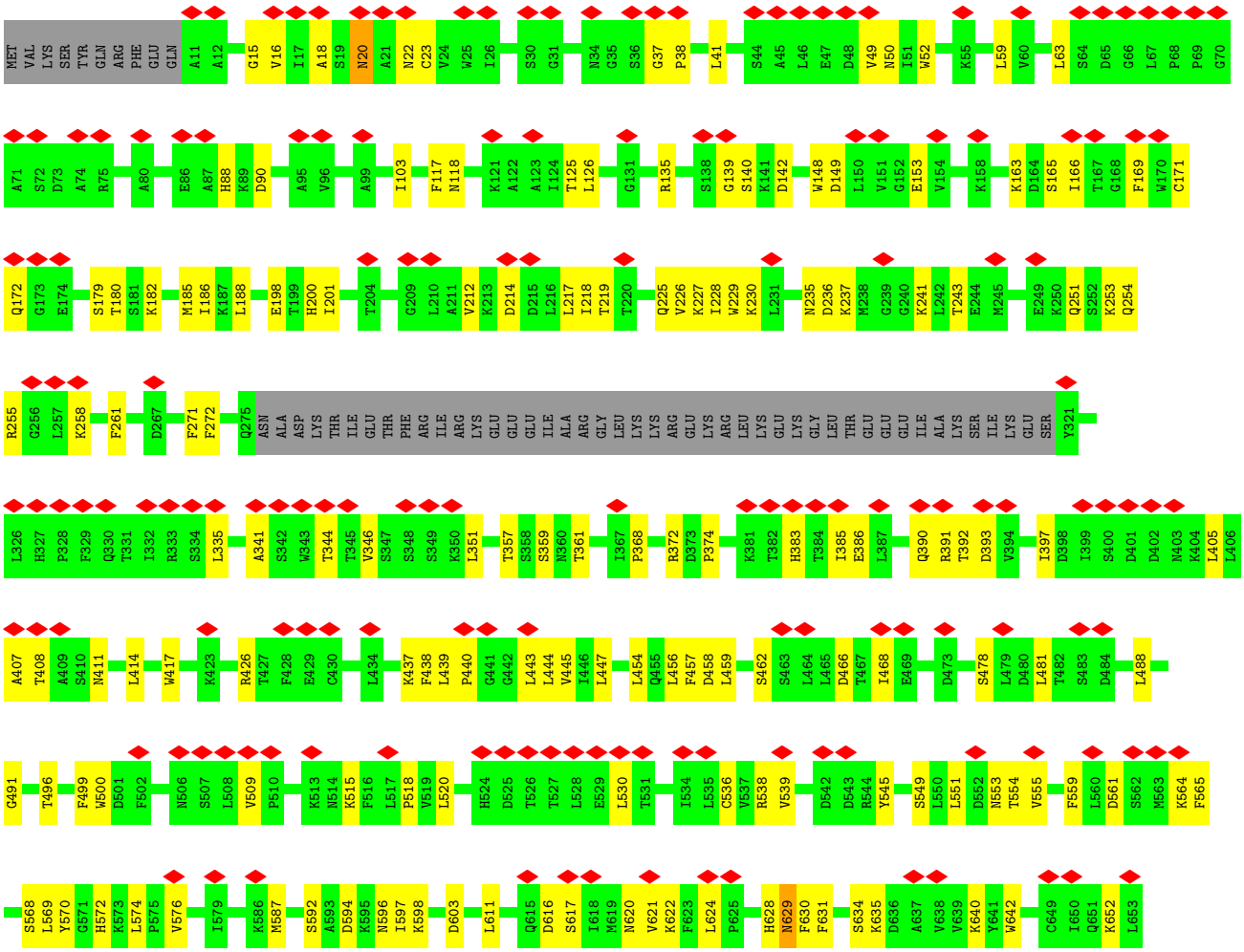
Chain BA:

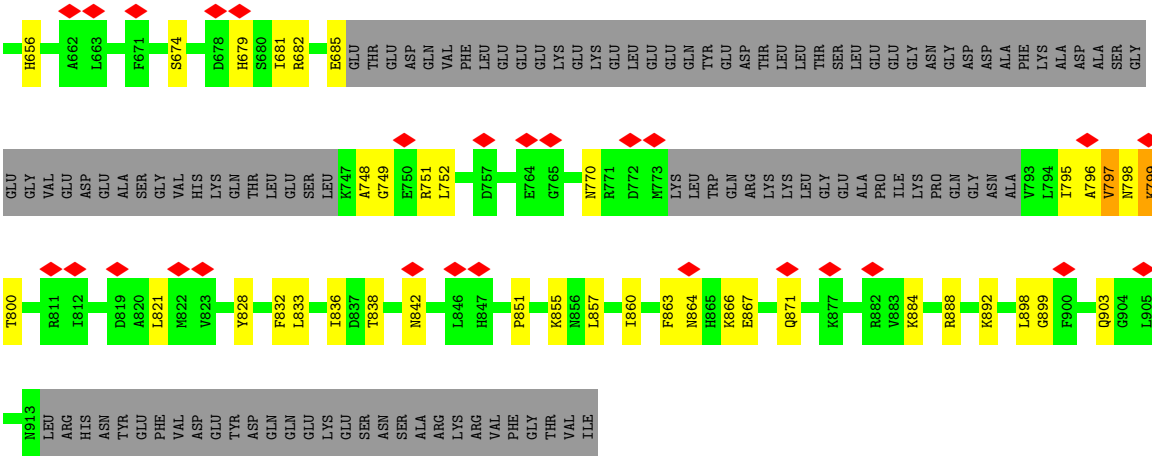




• Molecule 17: U3 small nucleolar RNA-associated protein 12

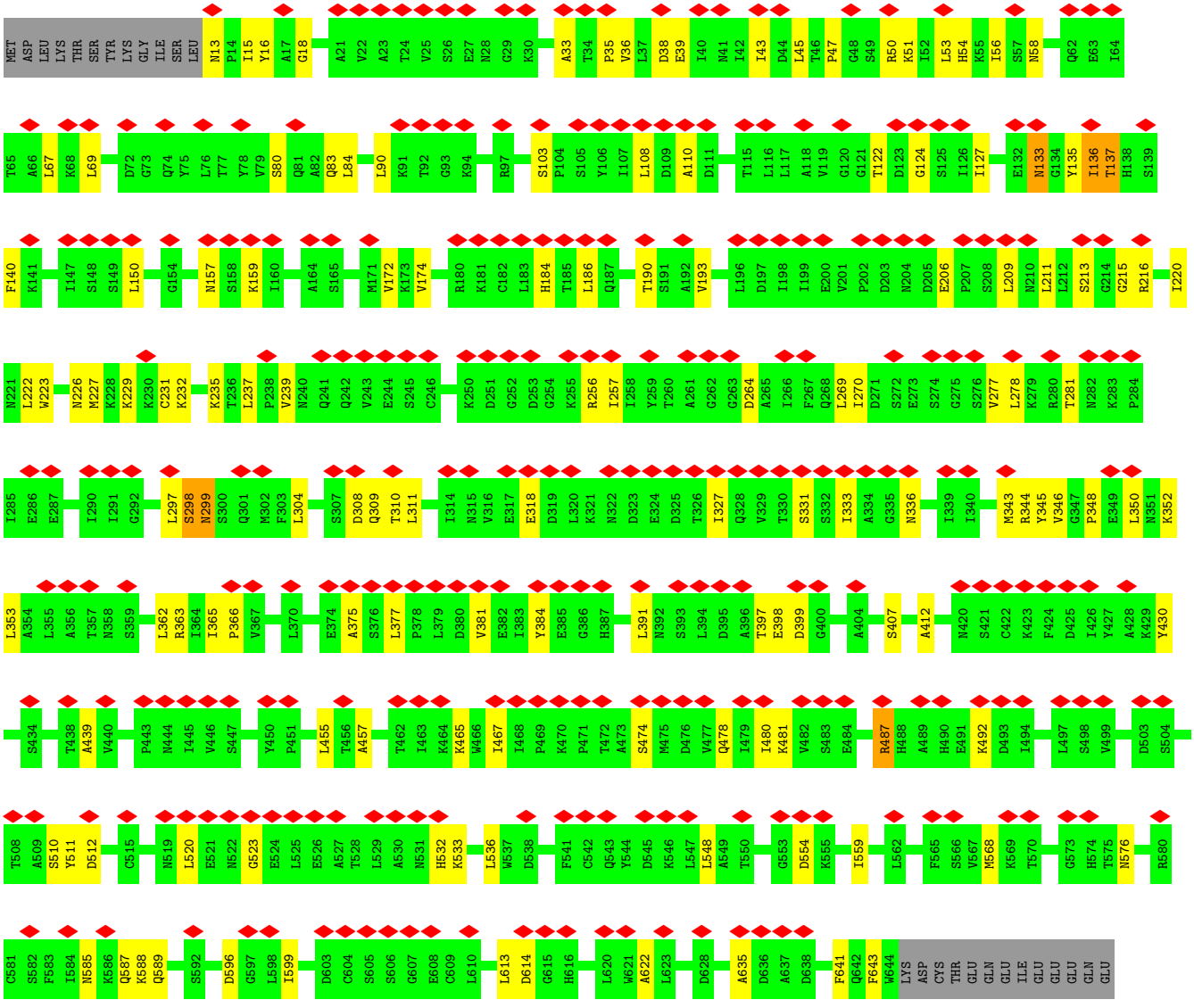
Chain BB:

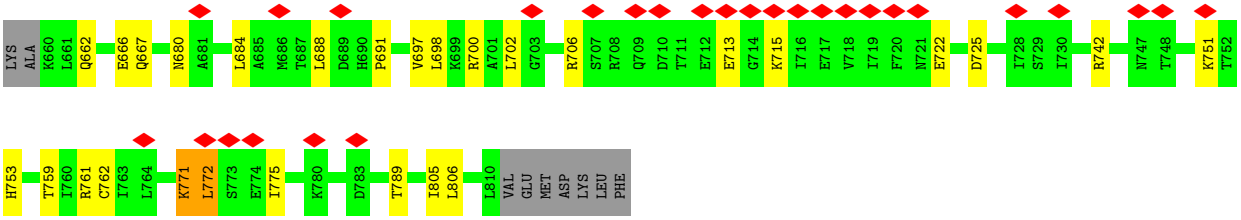




• Molecule 18: U3 small nucleolar RNA-associated protein 13

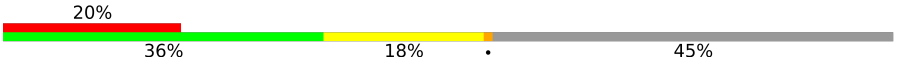
Chain BC:

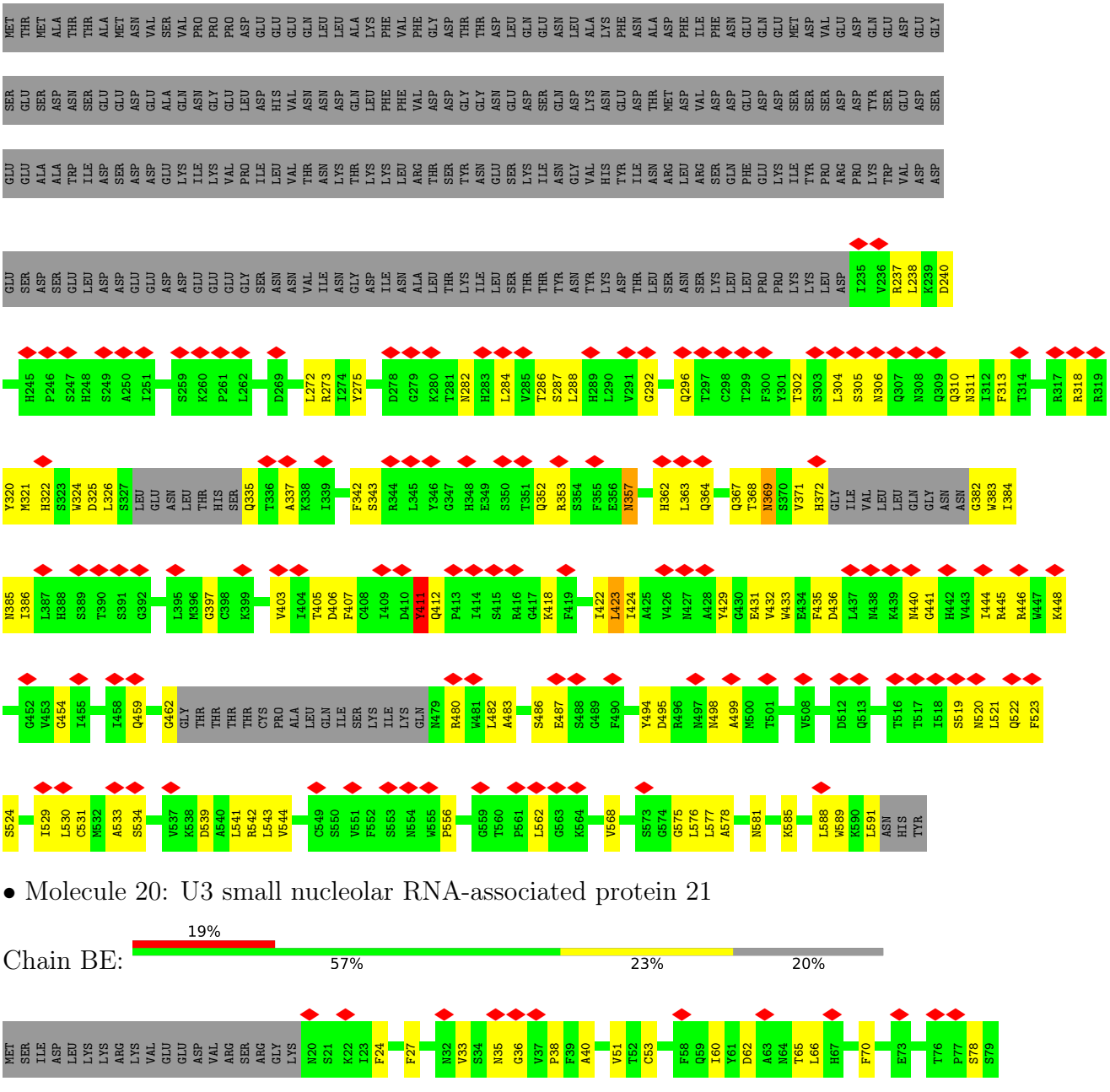




• Molecule 19: U3 small nucleolar RNA-associated protein 18

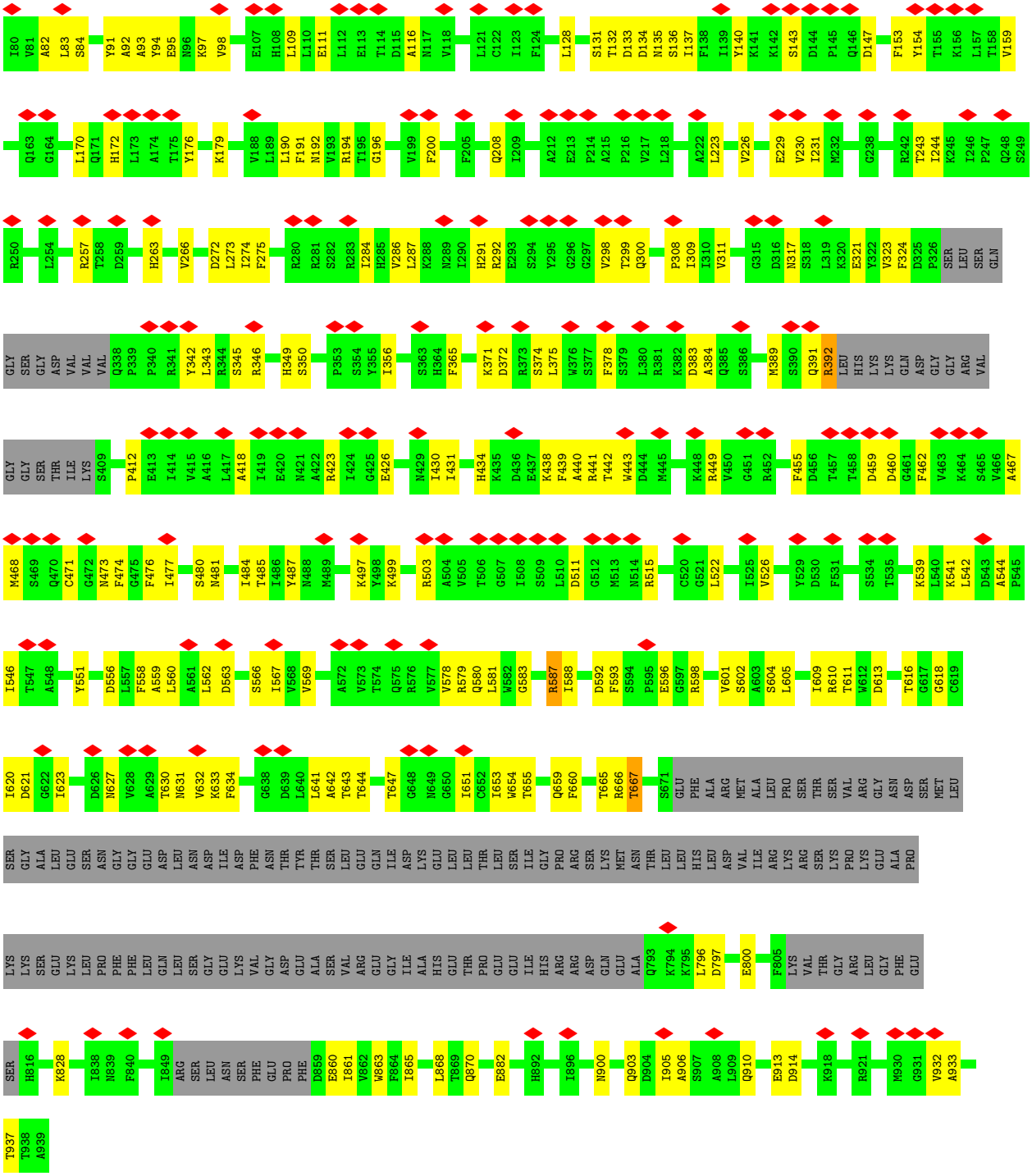
Chain BD:





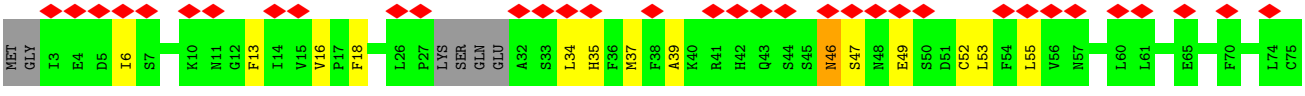
• Molecule 20: U3 small nucleolar RNA-associated protein 21

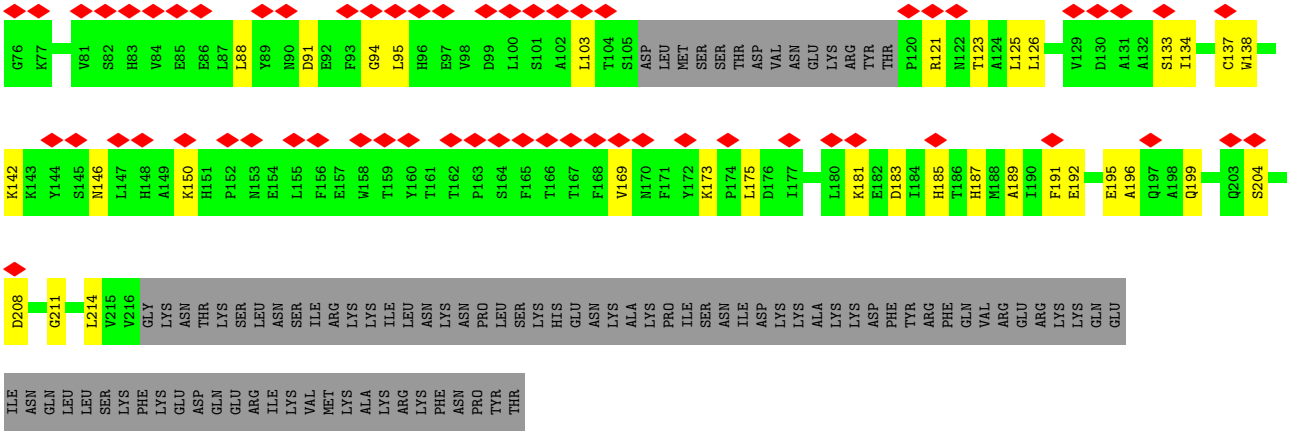
Chain BE:



• Molecule 21: Ribosomal RNA-processing protein 7

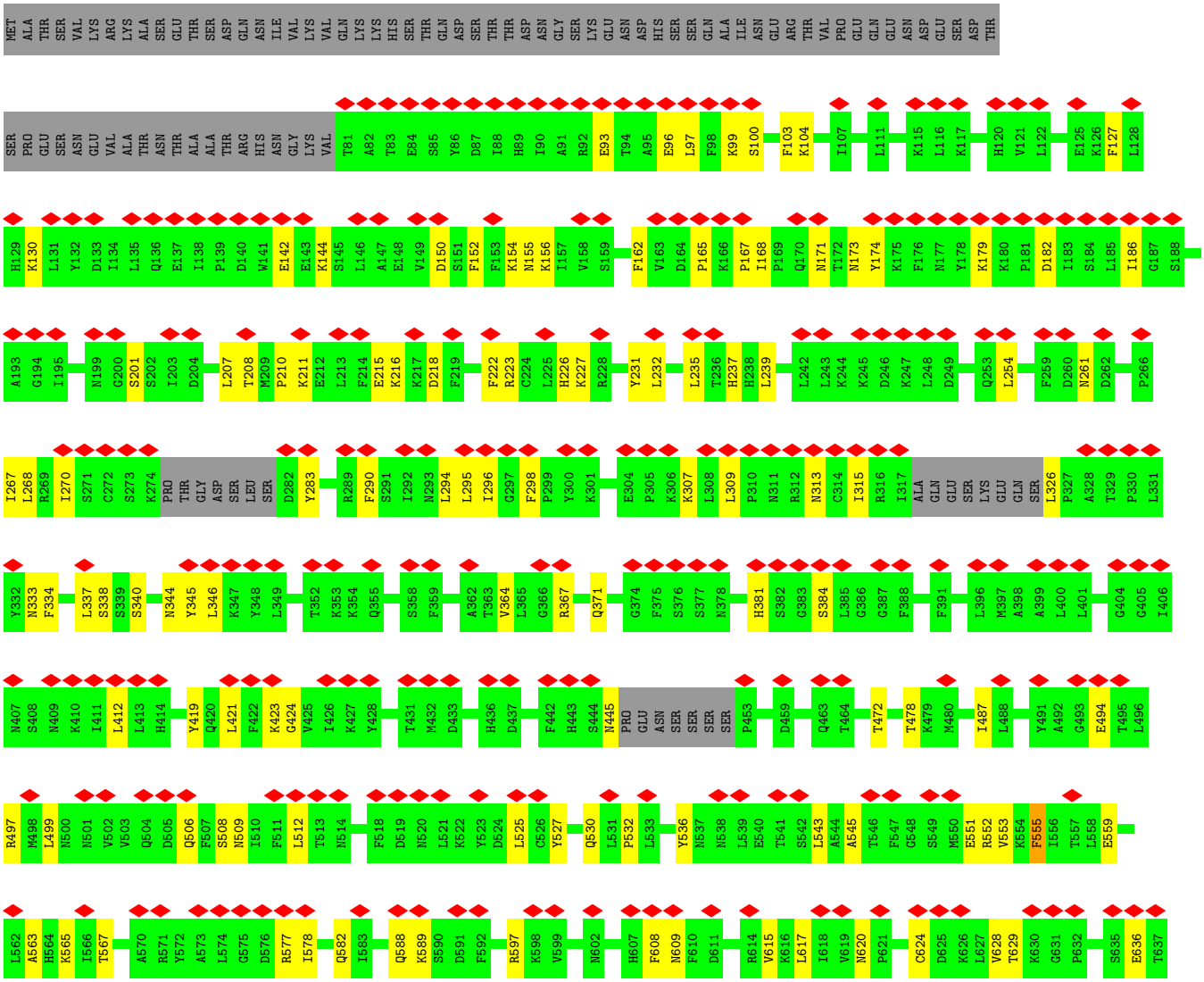
Chain CA:

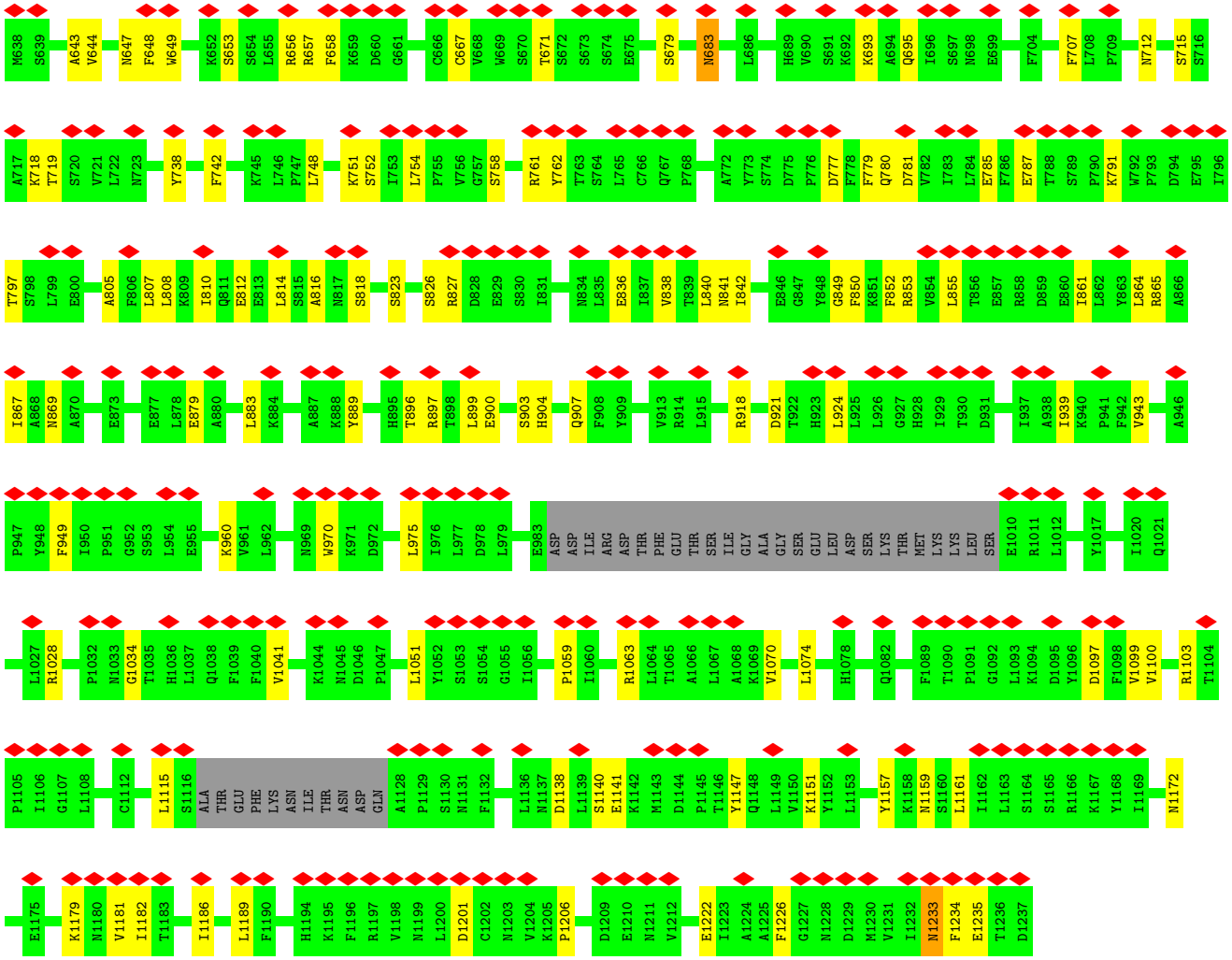




• Molecule 22: U3 small nucleolar RNA-associated protein 22

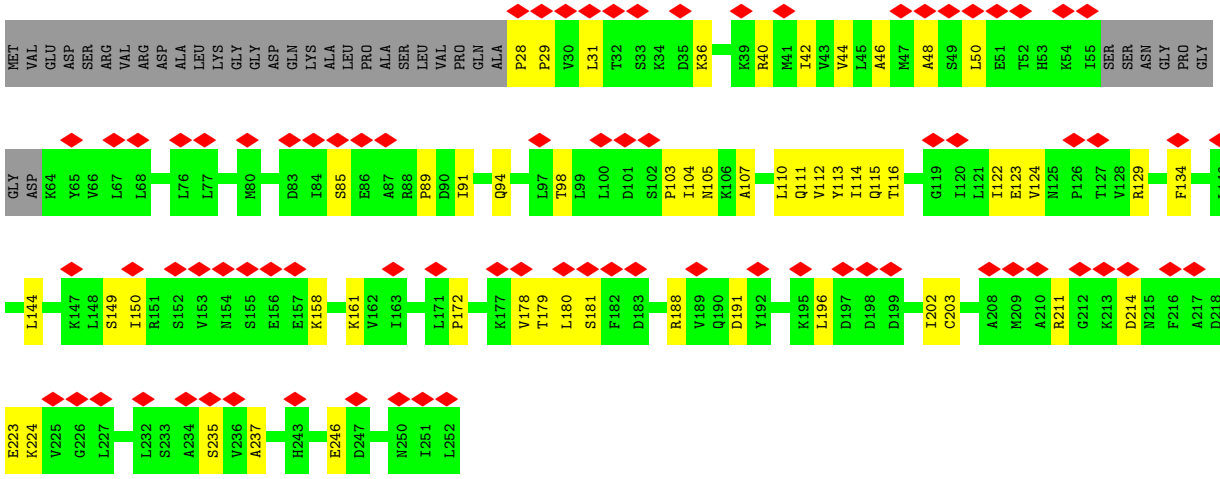
Chain CB:





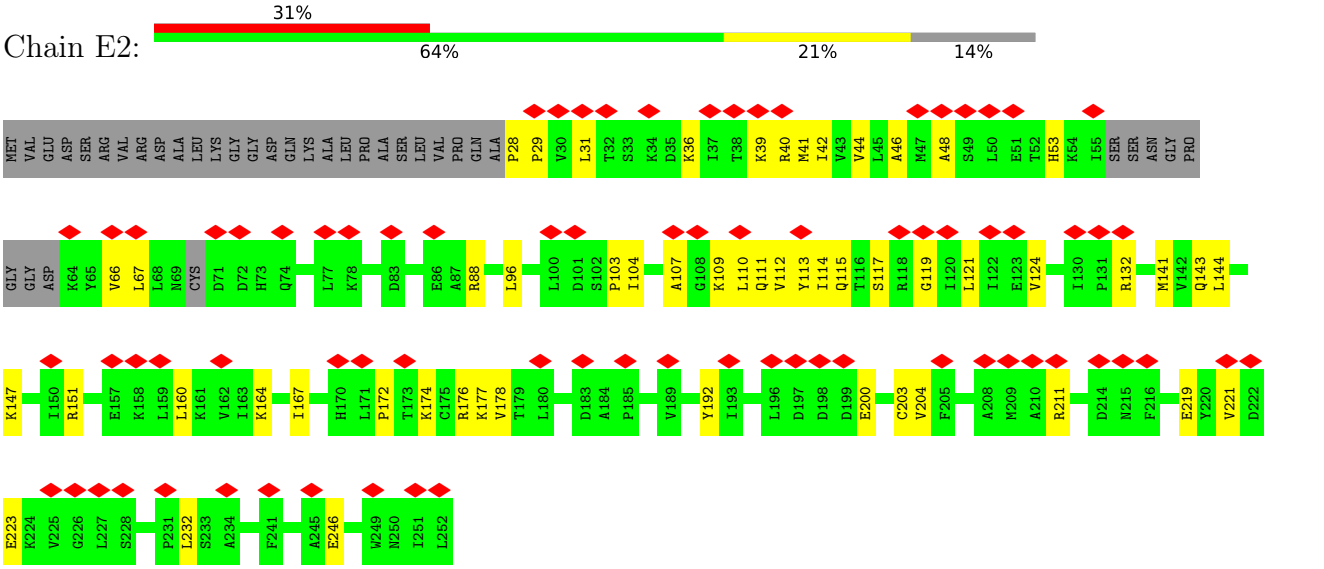
• Molecule 23: Ribosomal RNA small subunit methyltransferase NEP1

Chain E1:



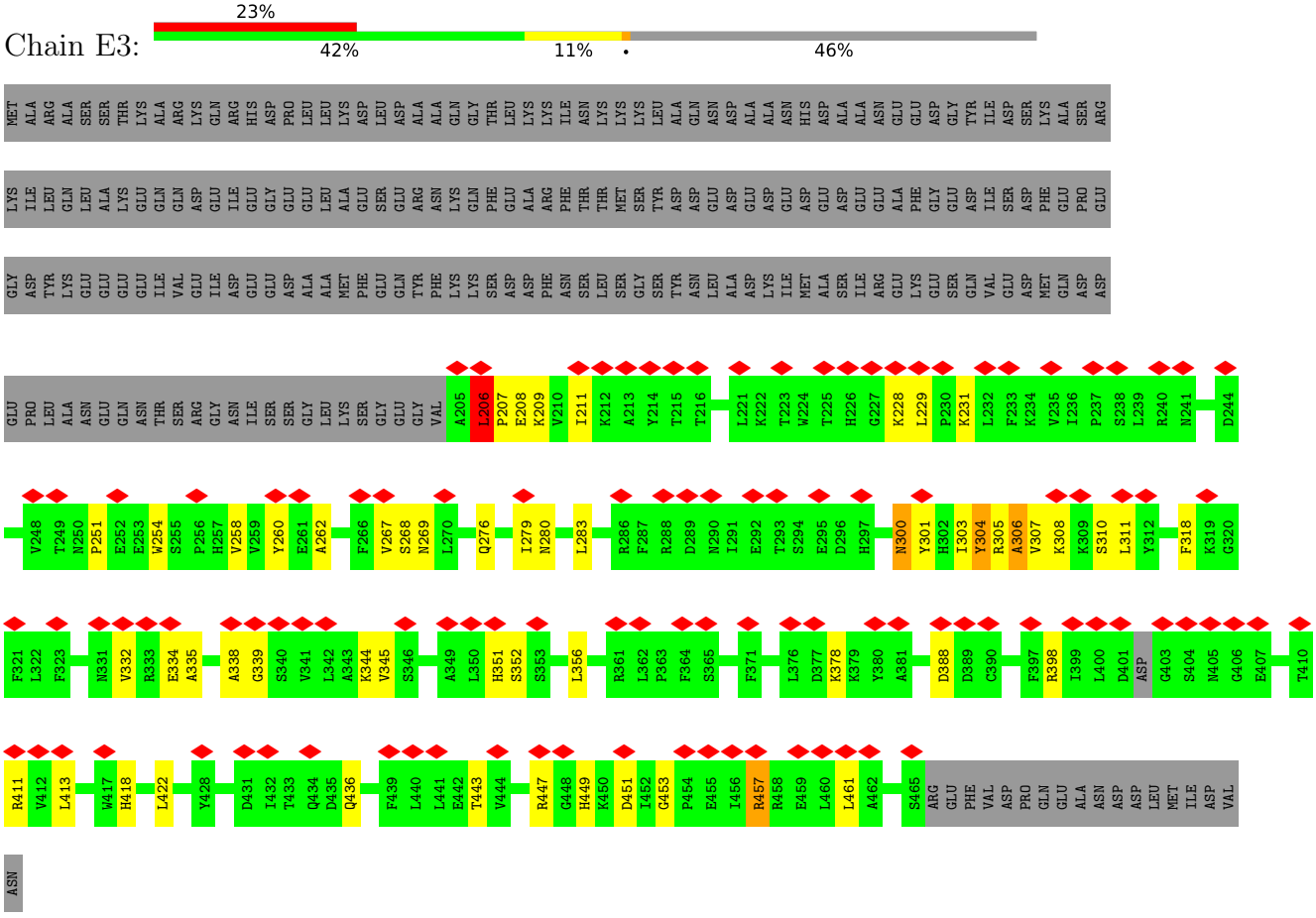
• Molecule 23: Ribosomal RNA small subunit methyltransferase NEP1

Chain E2:



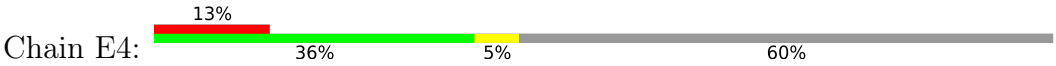
• Molecule 24: Essential nuclear protein 1

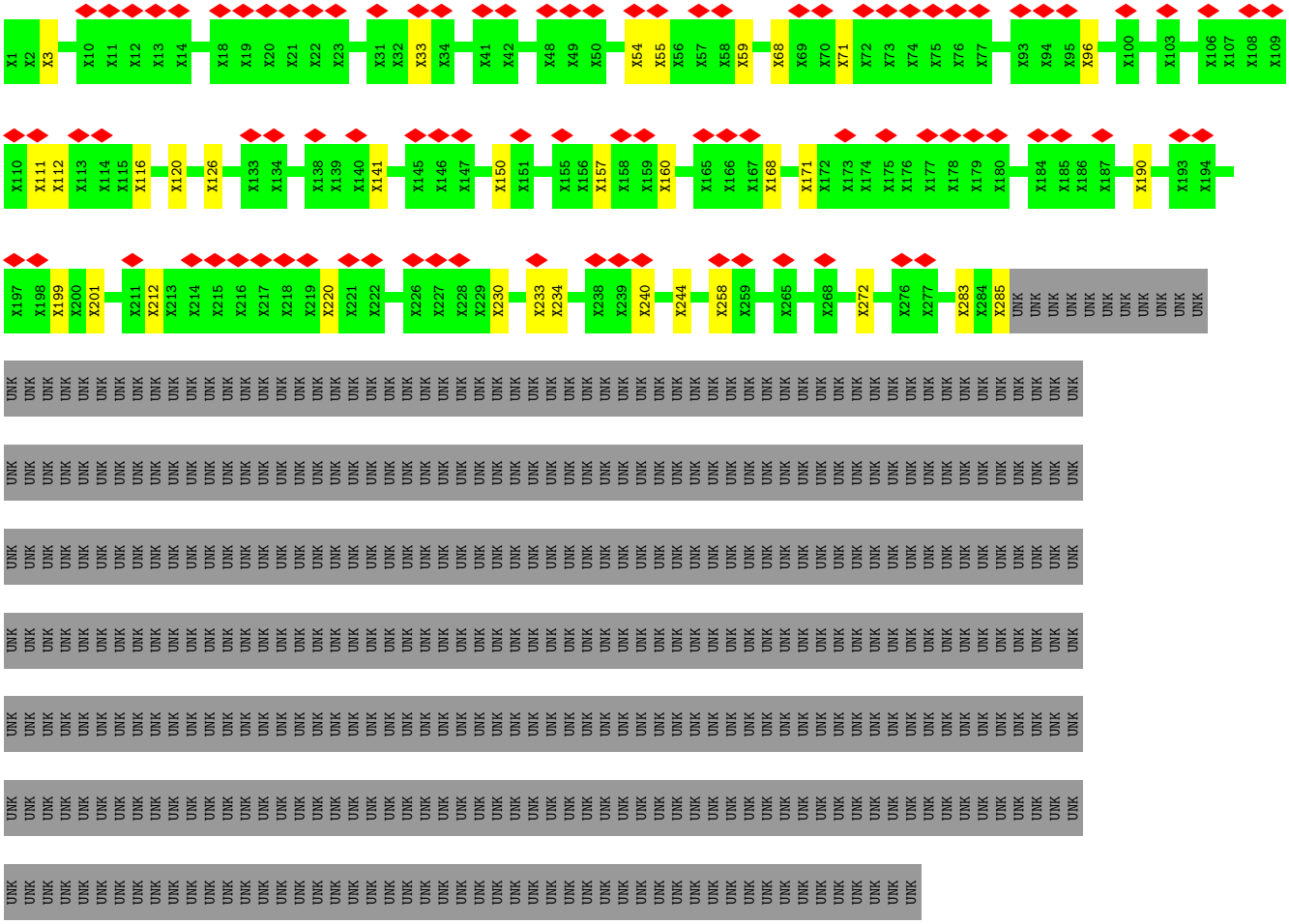
Chain E3:



• Molecule 25: Enp2

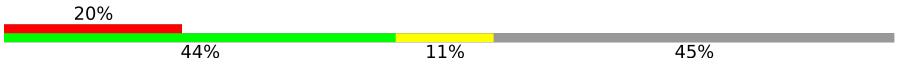
Chain E4:

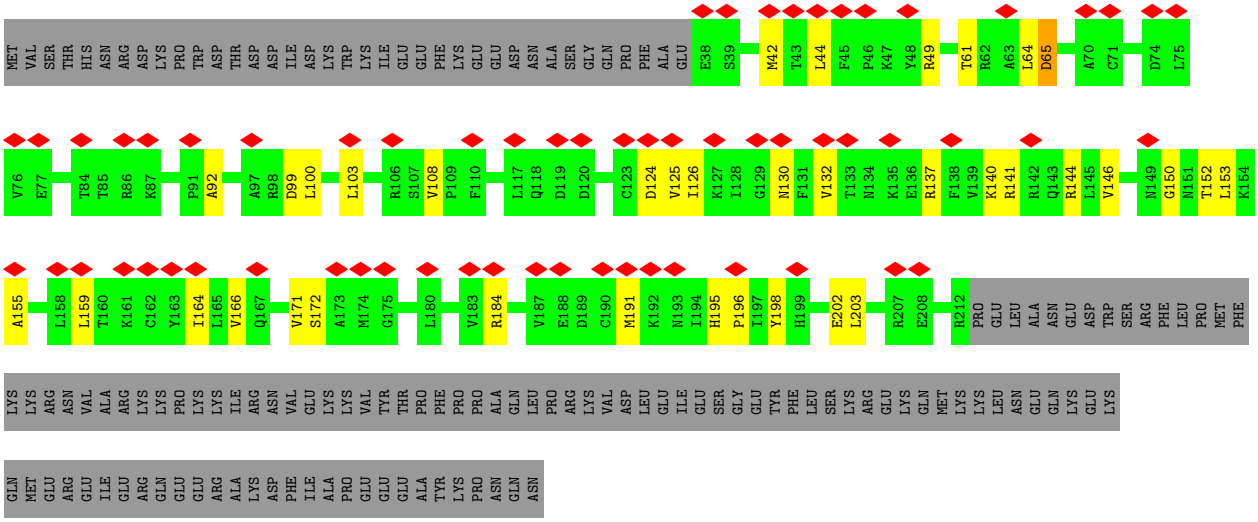




• Molecule 26: KRR1 small subunit processome component

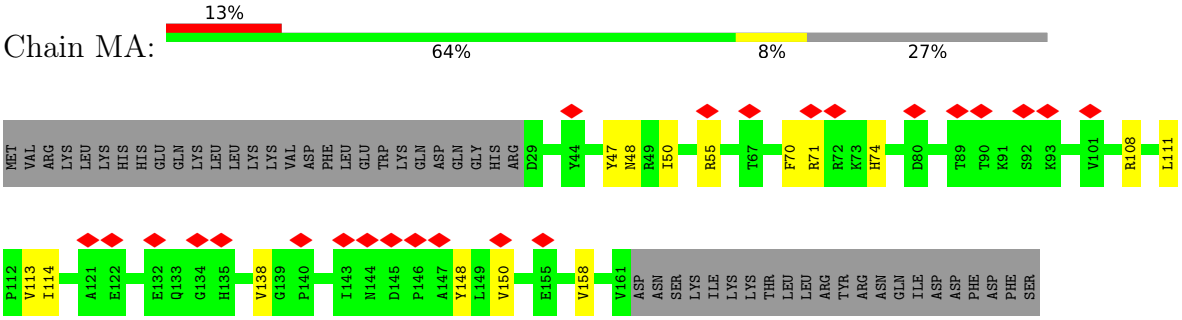
Chain K1:





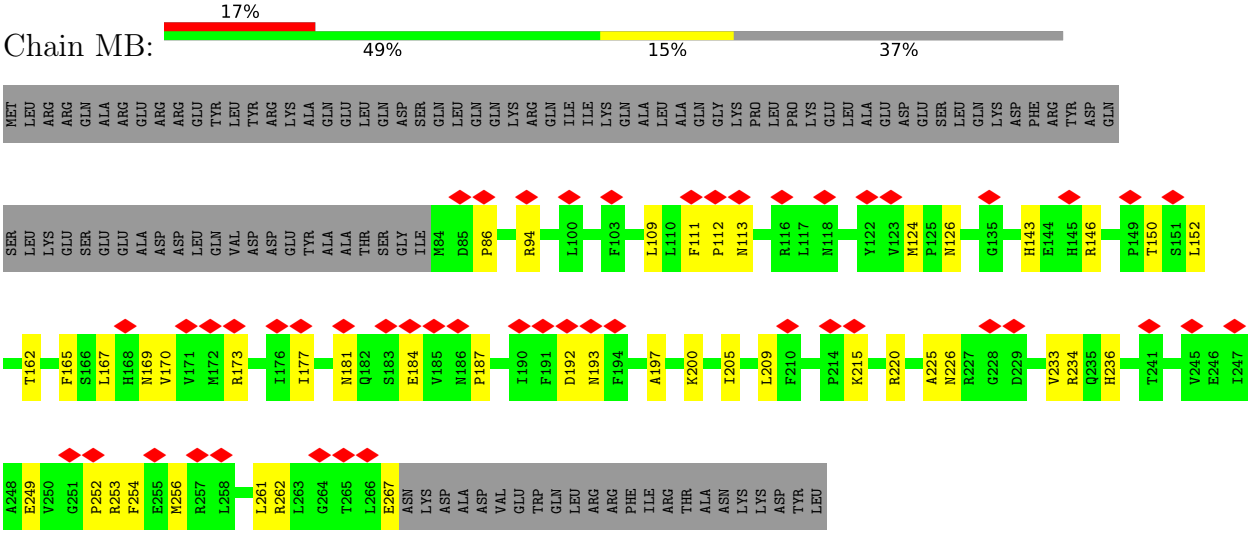
• Molecule 27: U3 small nucleolar ribonucleoprotein protein IMP3

Chain MA:



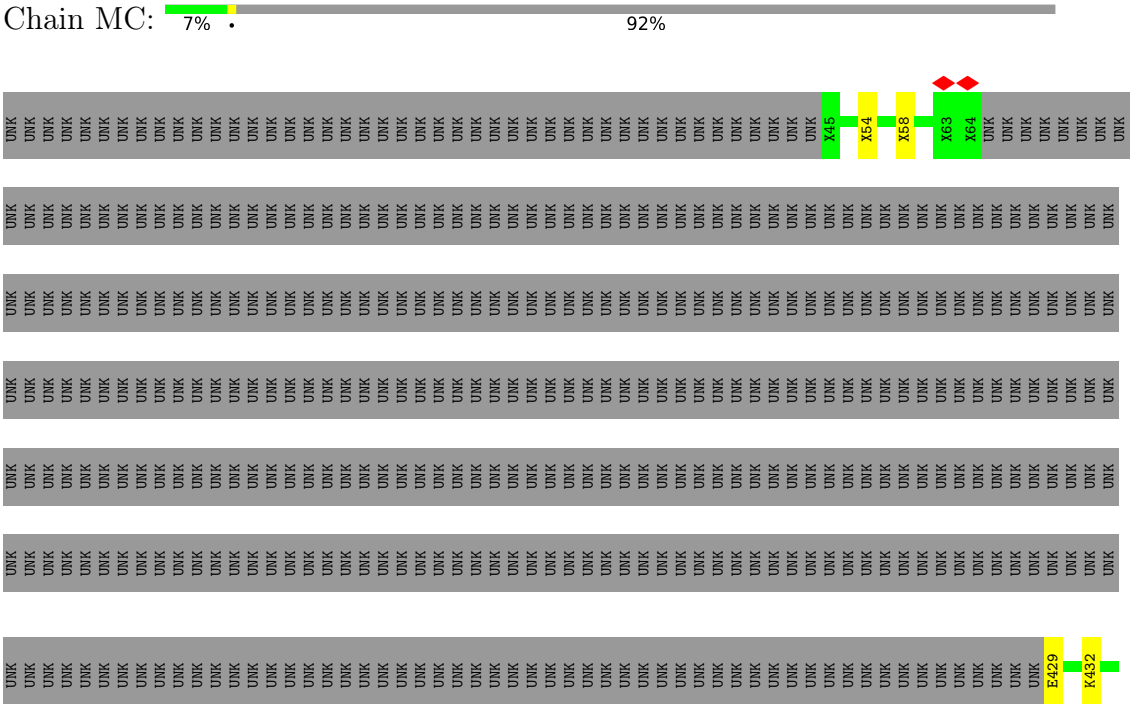
• Molecule 28: U3 small nucleolar ribonucleoprotein protein IMP4

Chain MB:



• Molecule 29: Mpp10,U3 small nucleolar RNA-associated protein MPP10

Chain MC:



V454 HIS PHE VAL PRO LYS PRO ALA SER THR SER LEU GLU ILE ARG VAL GLU THR PRO THR ILE SER MET GLU ASP ALA GLN PRO LEU TYR MET SER ASN ALA SER SER LEU ALA PRO GLN GLU ILE TYR ASN VAL GLY LYS ALA GLU LYS ASP GLY GLU ILE ARG LEU LYS ASN GLY VAL

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

ASP VAL SER GLY LYS THR LYS LYS SER ARG SER GLY PRO ASP SER THR ASN ILE LYS LEU

- Molecule 30: Pre-rRNA-processing protein PNO1

Chain P1: 15% | 57% | 6% | 37%

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

GLY SER ARG LYS THR HIS GLU SER LYS THR VAL VAL VAL ASP ASP GLN GLY LYS PRO ARG PHE THR SER ALA SER LYS THR GLN GLY ASN LYS ILE LYS F94 P103 H104 R105 M106 L109 W113 H123 L126 T134 K135 S136 N142 P143 K144 F145 T146 T147 D148 P149

L152 F158 A161 F162 T163 L164 G165 F166 D170 L174 L175 R176 L177 D178 D179 F185 E186 V187 K188 K191 T192 L193 T194 G195 D196 H197 L198 A201 I202 G203 R204 I205 A219 T220 R221 T222 H232 F237 I240 V248 I251 S254 P255 P256

V266 ALA SER ARG LEU LYS GLU ARG TYR

- Molecule 31: RNA 3'-terminal phosphate cyclase-like protein

Chain R1: 23% | 80% | 17% | •

MET SER SER SER ALA PRO K7 Y8 T9 T10 F11 S14 F17 R18 L19 R20 L23 L26 K29 P30 I31 K32 I33 G39 D40 L41 F52 E66 I67 V74 I75 Y76 R77 I81 A85 H88 I89 C90 V96 G97 Y98 E101 P102 Y105 L106

A107 P108 F109 S110 K111 F114 K119 G120 I121 T122 D127 A128 W135 G136 L137 V140 K143 E148 C149 A150 T153 L154 K155 R156 P159 P160 E165 V166 V169 V170 D171 S172 L173 I174 A175 Q176 P177 I178 T179 R185 P186 I187 I188 T192 T198 R199

V200 S201 P202 S203 L204 V205 N206 R207 M208 L216 L219 E222 A227 D228 V229 W230 R231 N234 S235 G236 Q248 K252 Y256 F257 A258 E259 D260 I261 G262 D263 A264 G265 L271 Q278 E281 K285 S286 A287 A288 V289 G290 R291 M301 G304 K305 E306

D307 I308 G309 R310 L311 R312 I313 E316 E320 R321 I332 F333 N334 T335 D343 E344 A345 D346 N347 E348 D349 M350 I351 A352 T353 I354 K355 G358 F359 T360 N361 THR SER LYS LYS ILE ALA

- Molecule 32: rRNA biogenesis protein RRP5

Chain R2: 15% | 14% | • | 84%

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 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 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

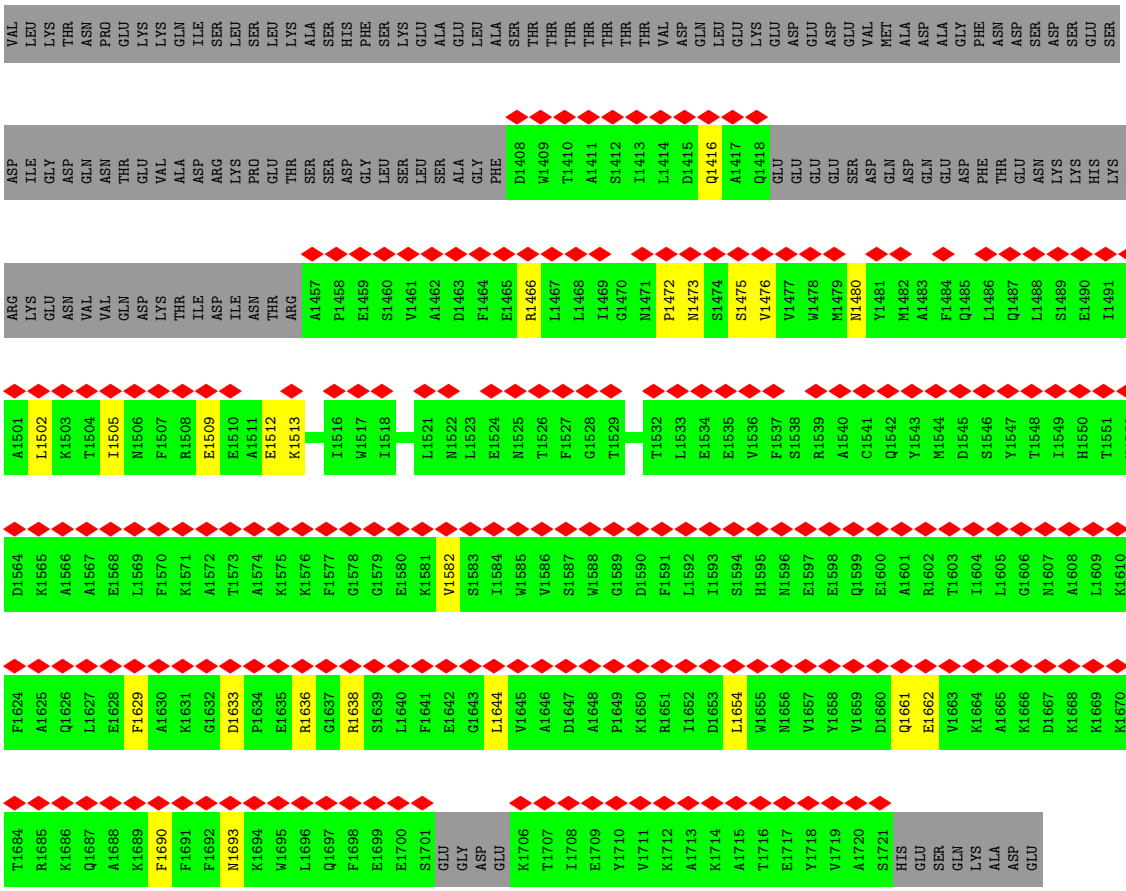
THR ILE SER PRO VAL LEU LYS ALA ARG ILE SER LEU LEU ASP LEU ALA ASP ASN ASP SER ASN PHE SER GLU ASN ILE GLU SER VAL PHE PRO LEU GLY SER ALA LEU GLN VAL LYS VAL ALA SER ILE ASP ARG GLU HIS GLY PHE VAL ASN ALA ILE GLY LYS SER HIS VAL ASP ILE

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

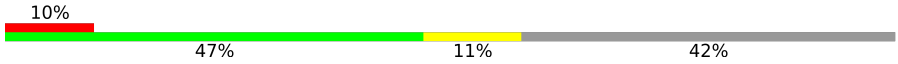
GLU ALA PHE VAL PRO VAL SER LYS LEU SER ASP SER TYR LEU LYS GLU TRP LYS LYS PHE TYR LYS PRO MET GLN TYR VAL LEU GLY LYS VAL VAL THR CYS ASP GLU ASP SER ARG ILE SER LEU THR LEU ARG GLU SER GLU ILE ASN GLY ASP LEU LYS VAL LEU LYS THR TYR SER

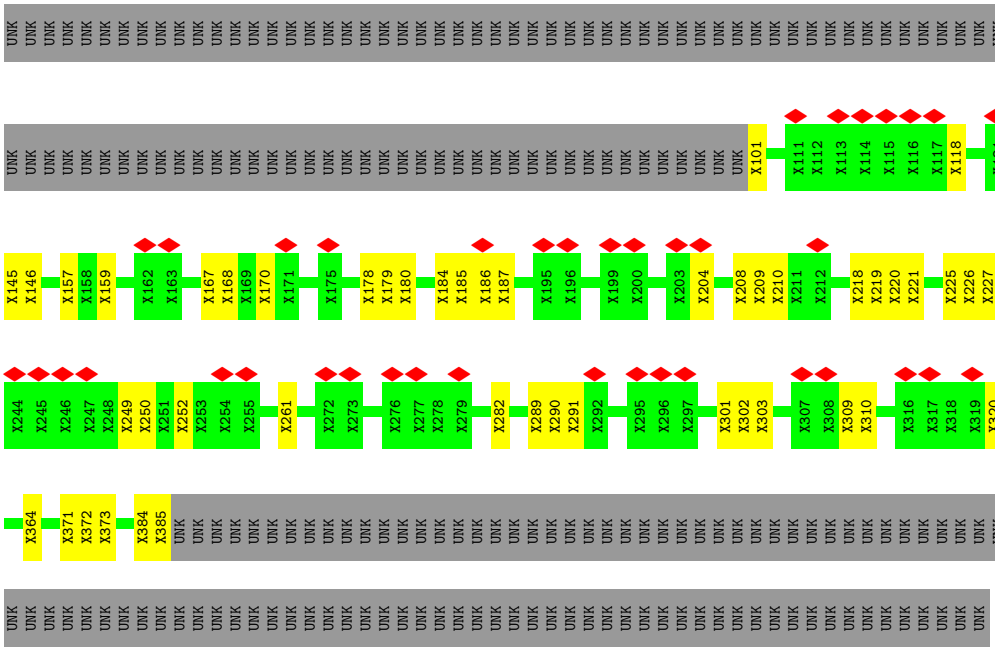
ASP ILE LYS ALA GLY ASP VAL PHE GLU GLY THR ILE LYS SER VAL THR ASP PHE GLY VAL PHE VAL LYS LEU ASP ASN THR VAL ASN VAL THR GLY LEU ALA HIS ILE THR GLU ILE ALA ASP LYS LYS PRO GLU ASP LEU SER ALA LEU PHE GLY VAL GLY ASP ARG VAL LYS ALA ILE



• Molecule 33: Sof1

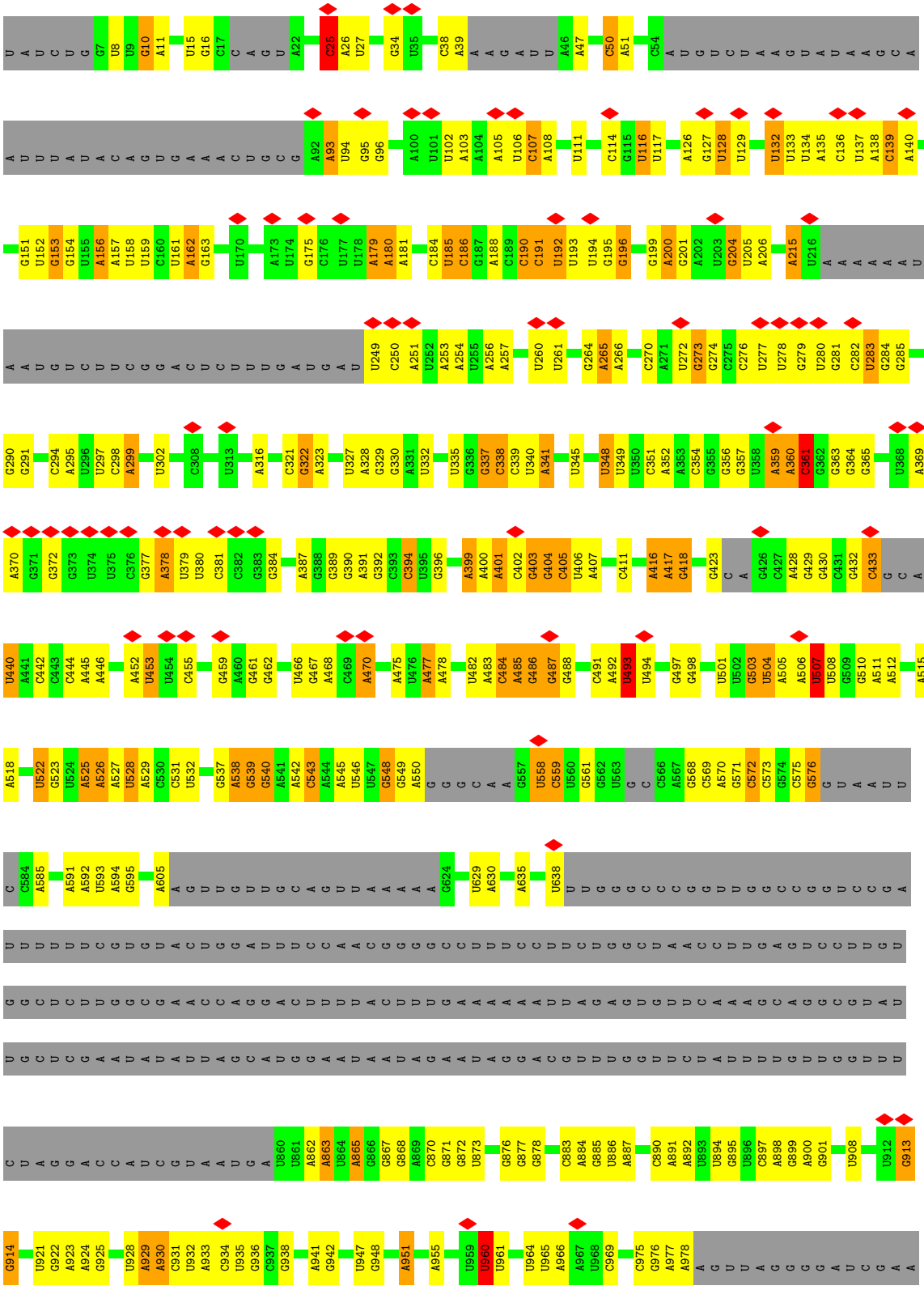
Chain S1:

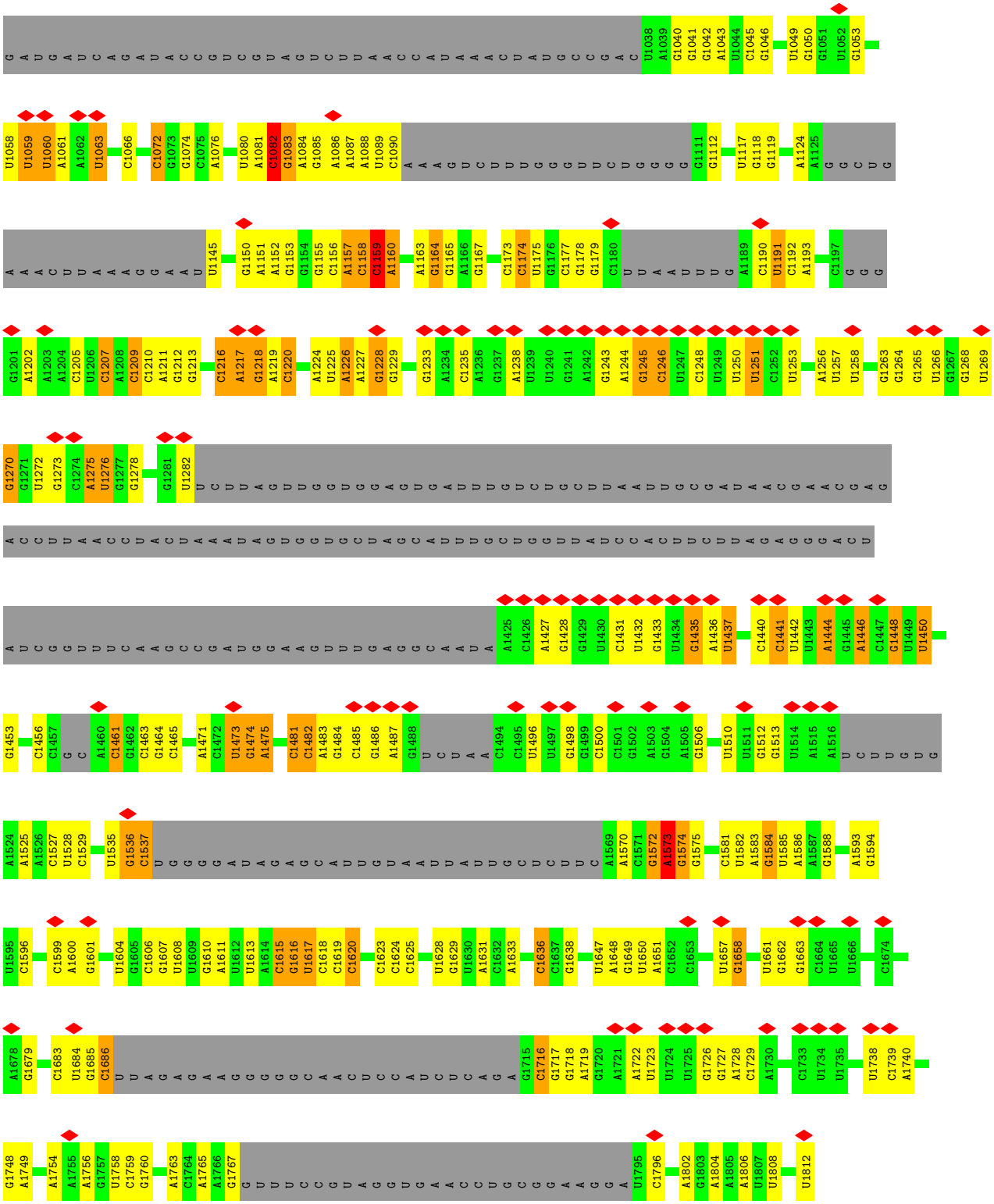




• Molecule 34: 18S ribosomal RNA

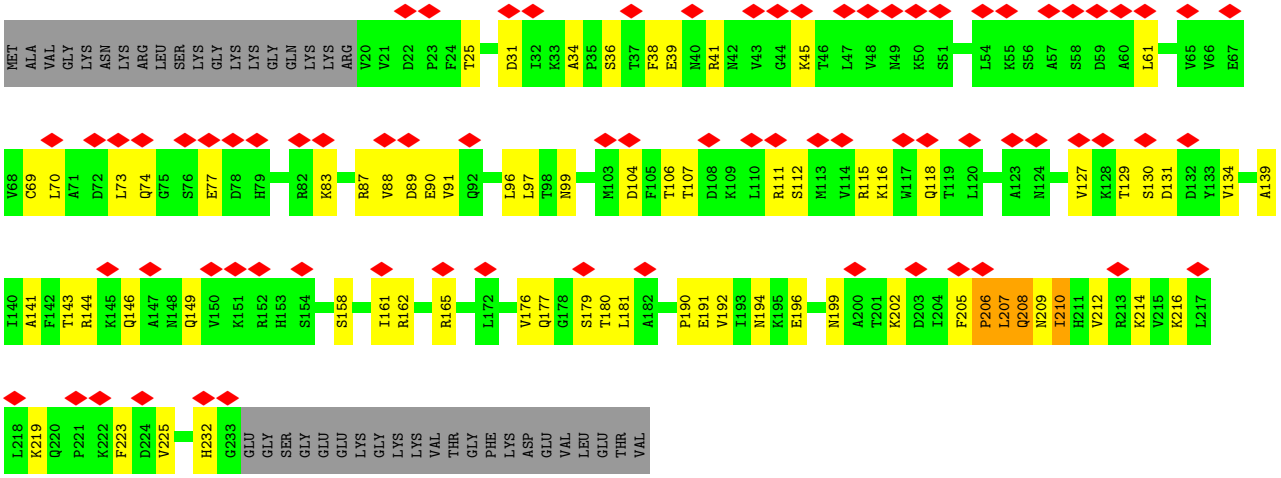
Chain SA:





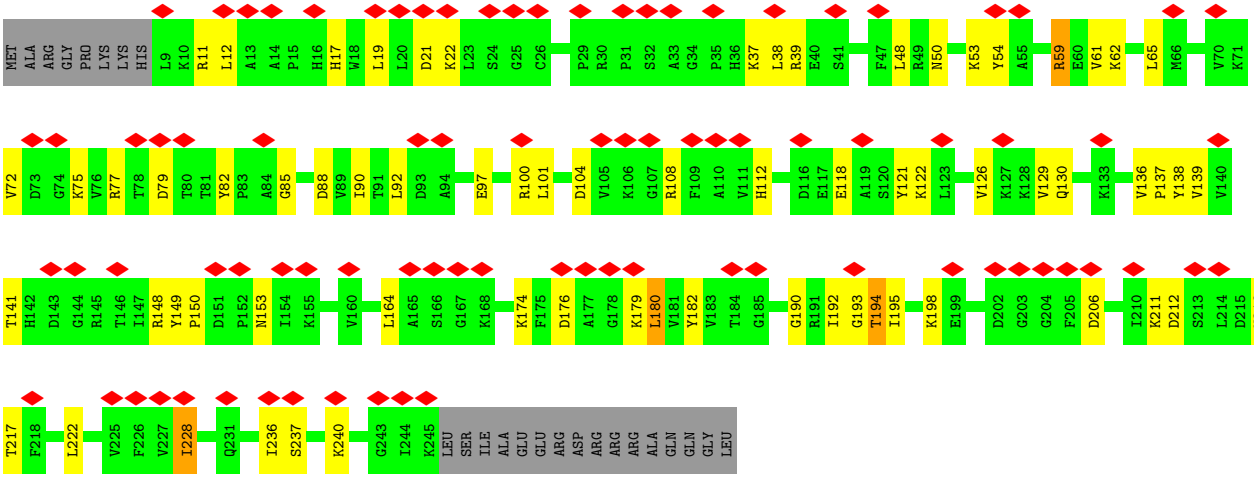
• Molecule 35: 40S ribosomal protein S1-A

Chain SC:



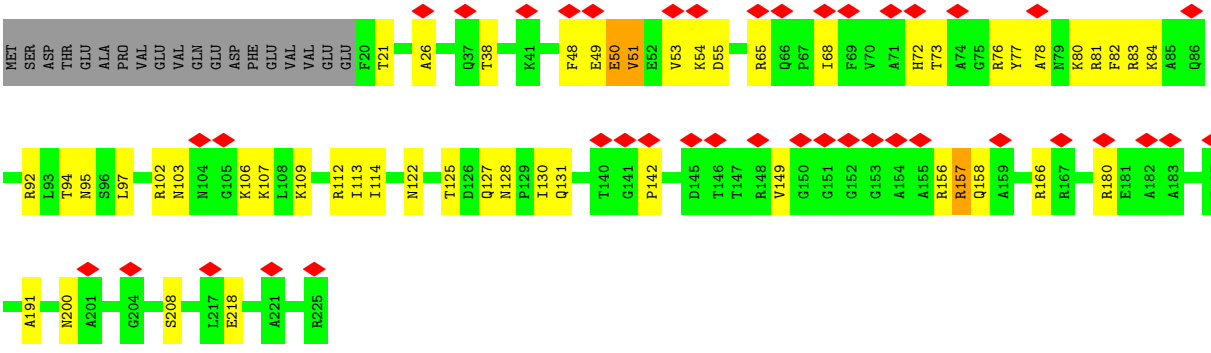
• Molecule 36: 40S ribosomal protein S4-A

Chain SF:



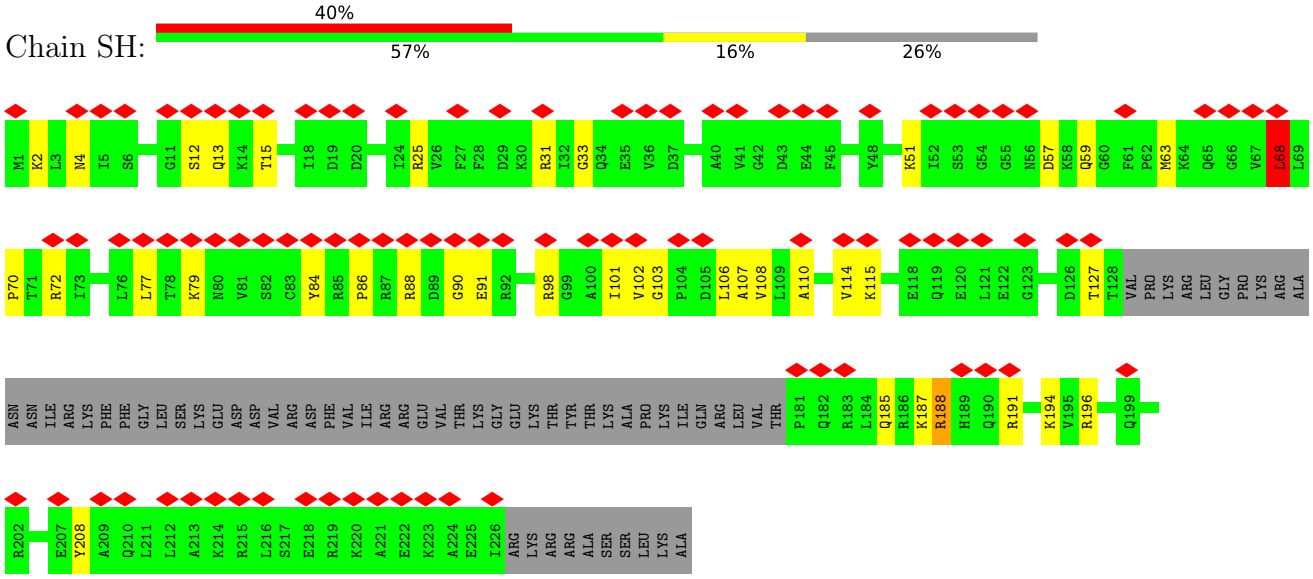
• Molecule 37: 40S ribosomal protein S5

Chain SG:



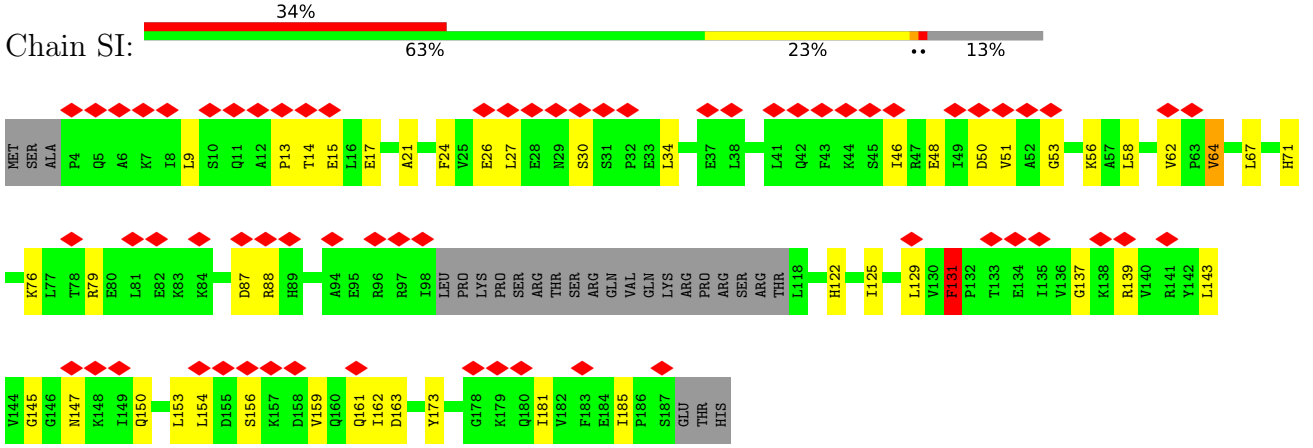
• Molecule 38: 40S ribosomal protein S6-A

Chain SH:



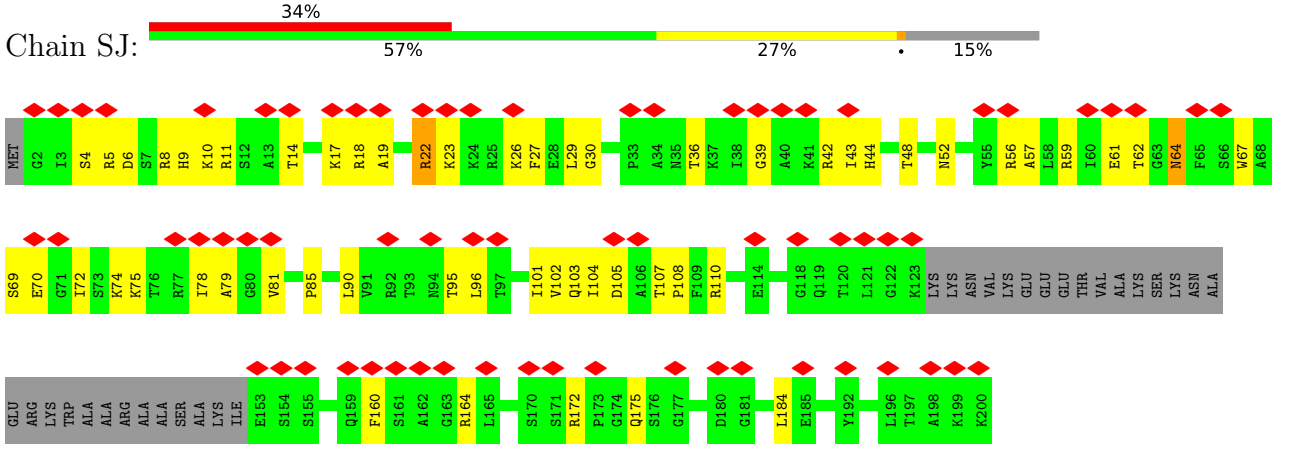
• Molecule 39: 40S ribosomal protein S7-A

Chain SI:



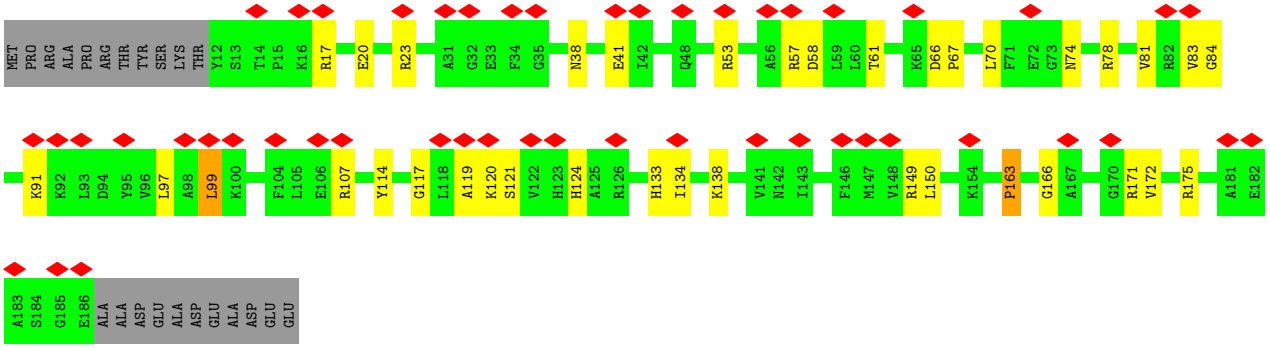
• Molecule 40: 40S ribosomal protein S8-A

Chain SJ:

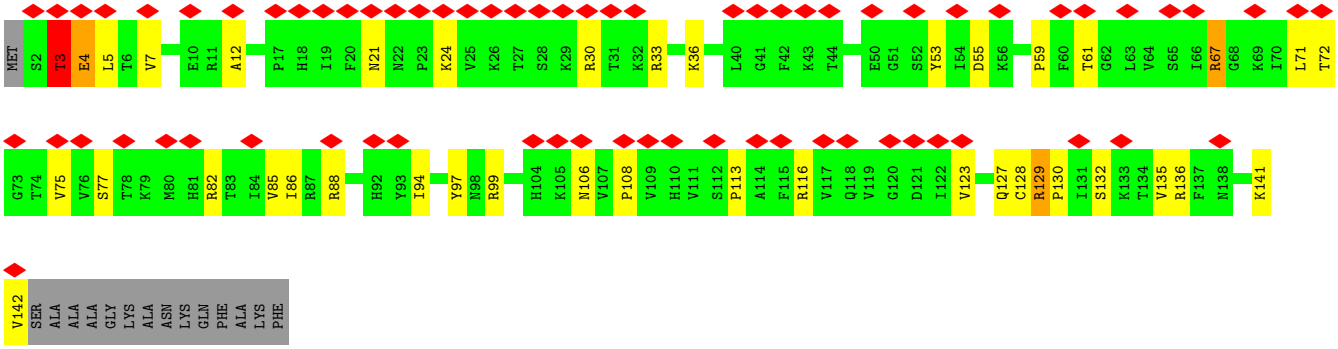


• Molecule 41: 40S ribosomal protein S9-A

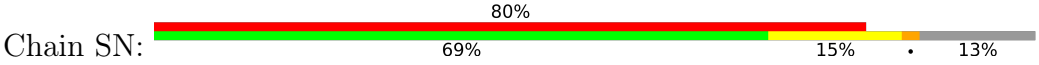
Chain SK:

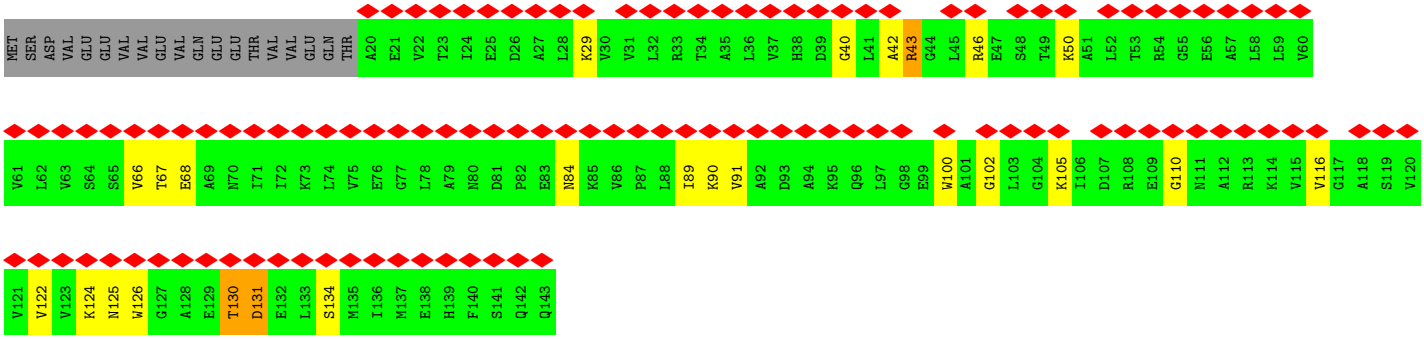


• Molecule 42: 40S ribosomal protein S11-A

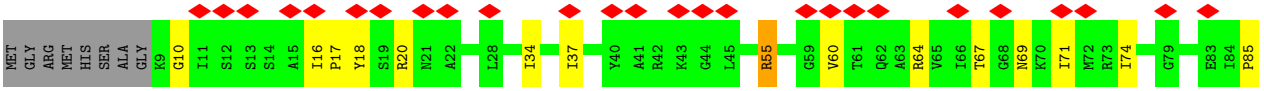


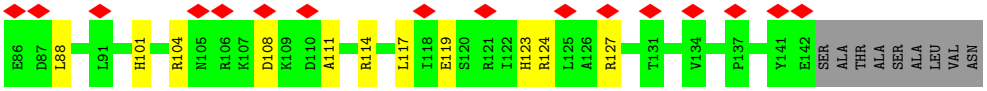
• Molecule 43: 40S ribosomal protein S12





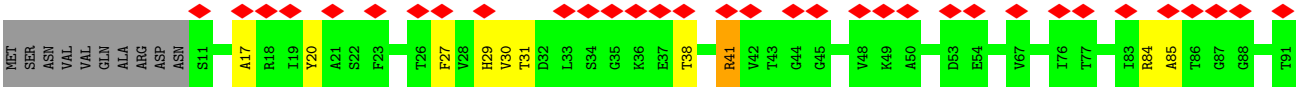
• Molecule 44: 40S ribosomal protein S13

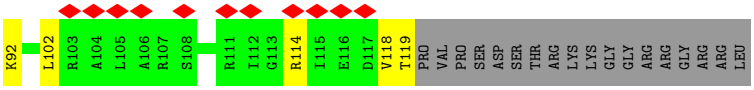




• Molecule 45: 40S ribosomal protein S14-A

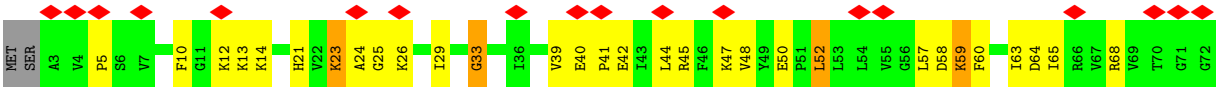
Chain SP:





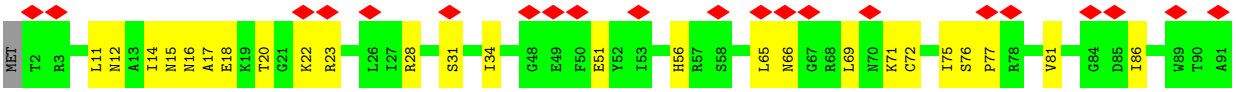
• Molecule 46: 40S ribosomal protein S16-A

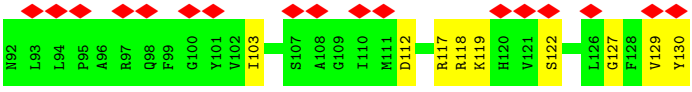
Chain SR:



• Molecule 47: 40S ribosomal protein S22-A

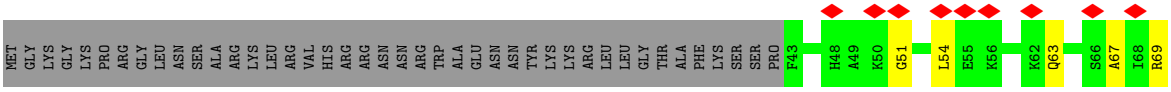
Chain SX:

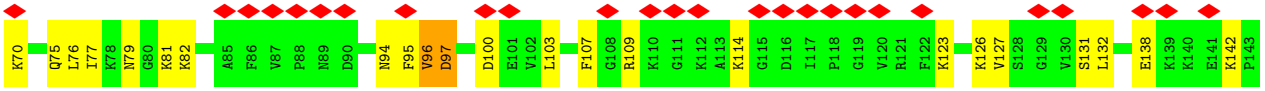




• Molecule 48: 40S ribosomal protein S23-A

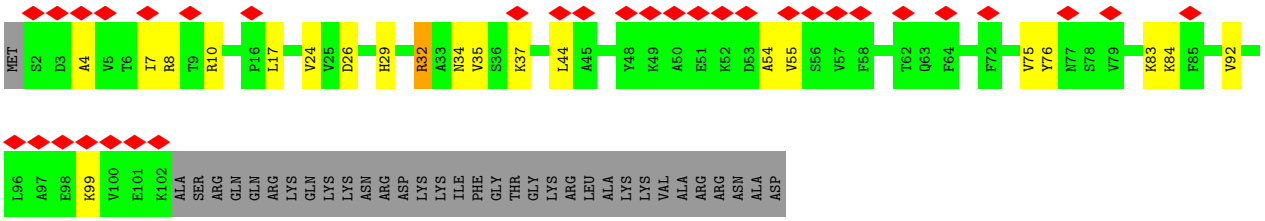
Chain SY:





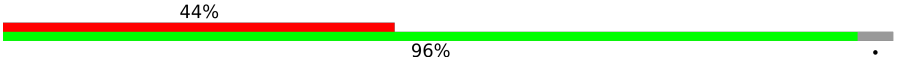
• Molecule 49: 40S ribosomal protein S24-A

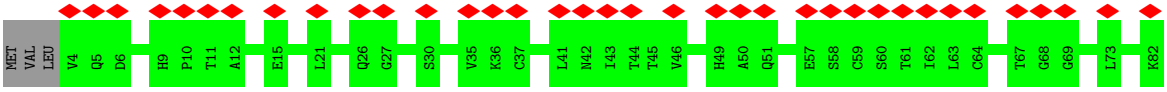
Chain SZ:



• Molecule 50: 40S ribosomal protein S27-A

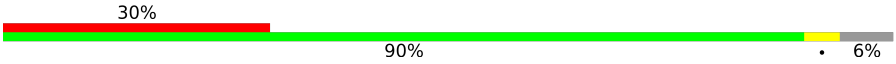
Chain Sc:

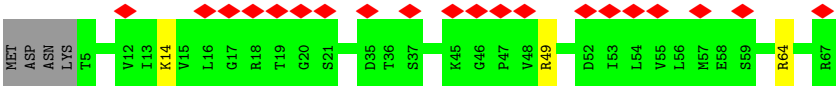




• Molecule 51: 40S ribosomal protein S28-A

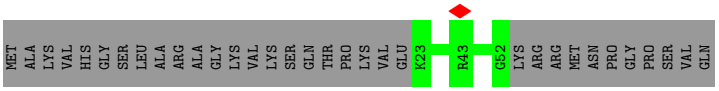
Chain Sd:





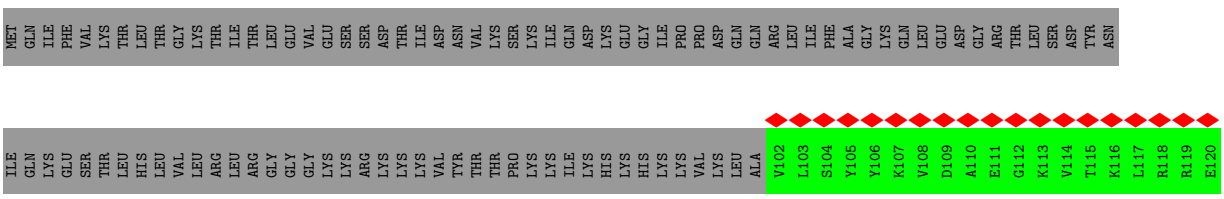
• Molecule 52: 40S ribosomal protein S30-A

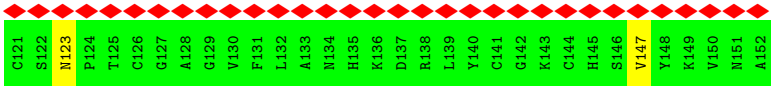
Chain Sf:



• Molecule 53: Ubiquitin-40S ribosomal protein S31

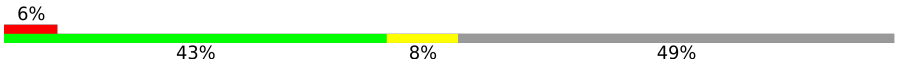
Chain Sg:

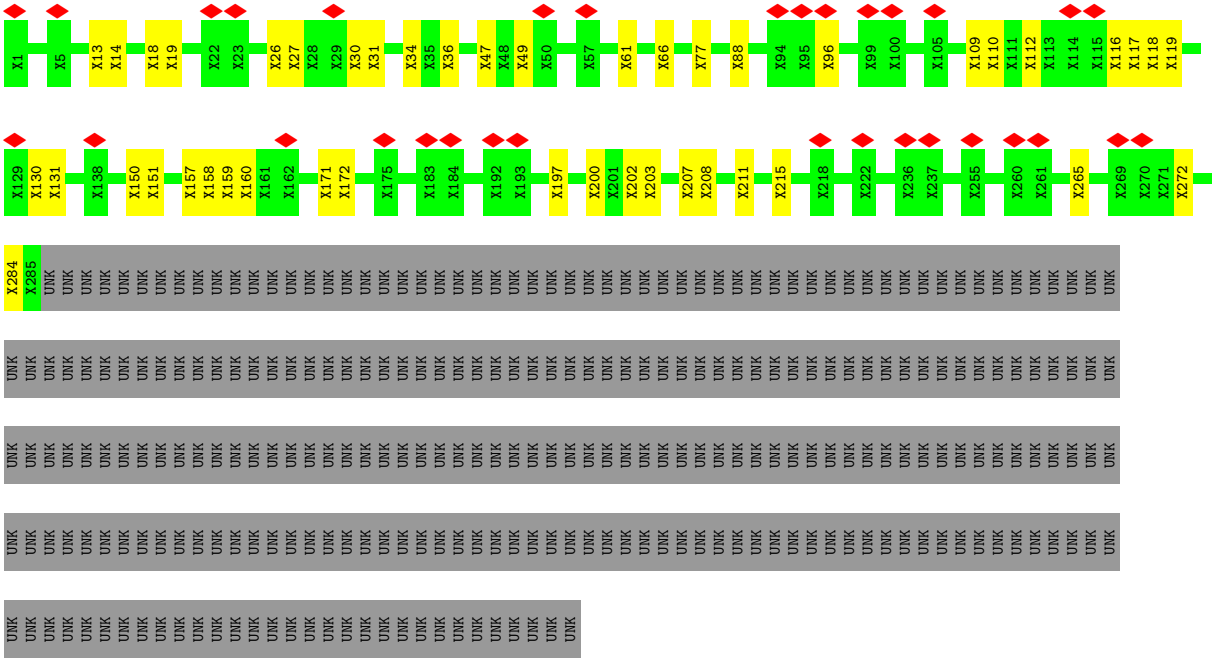




• Molecule 54: Utp7

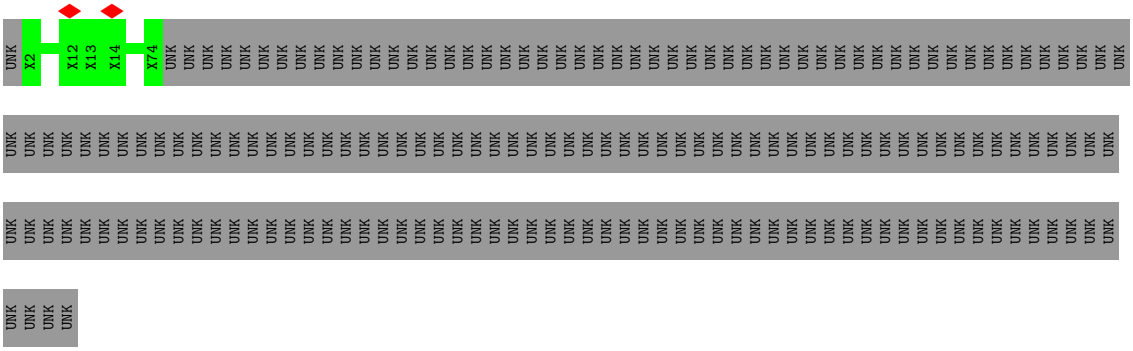
Chain U1:





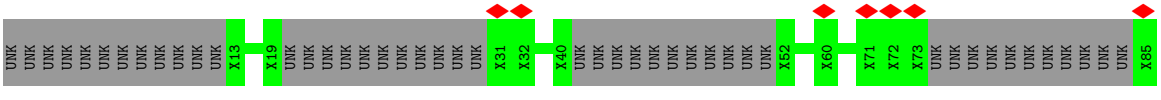
• Molecule 55: Utp11

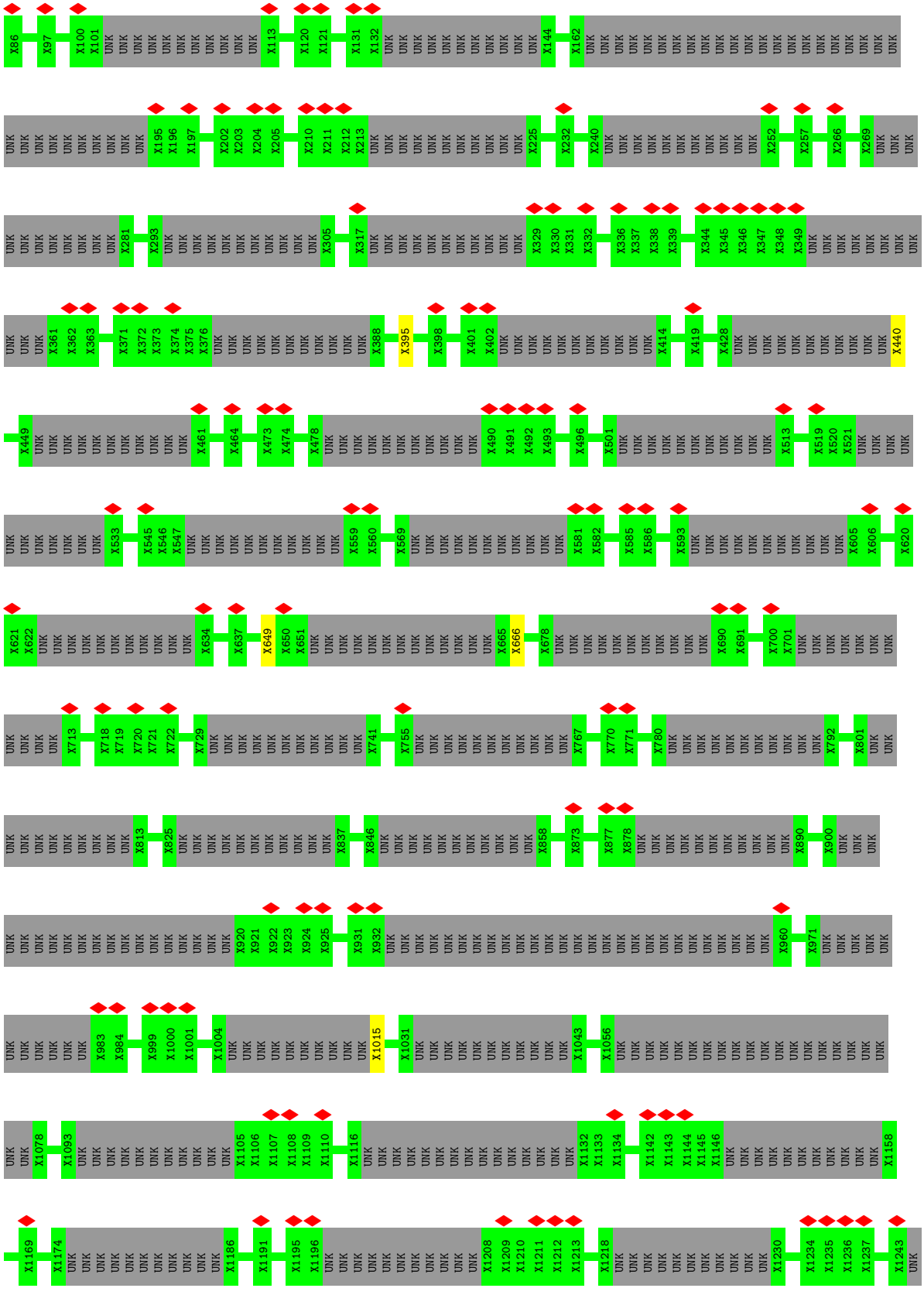
Chain U2:

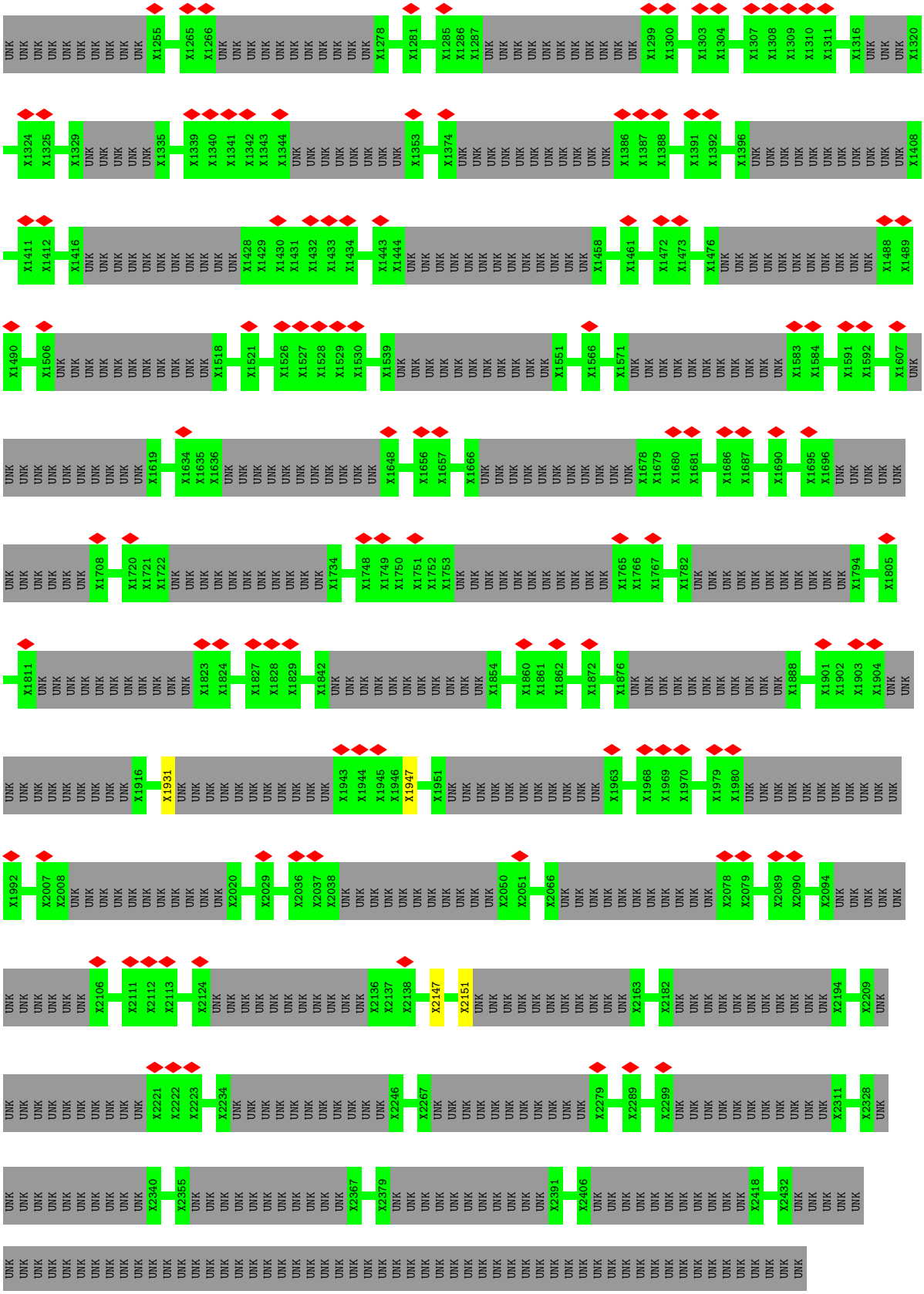


• Molecule 56: Utp20

Chain U3:

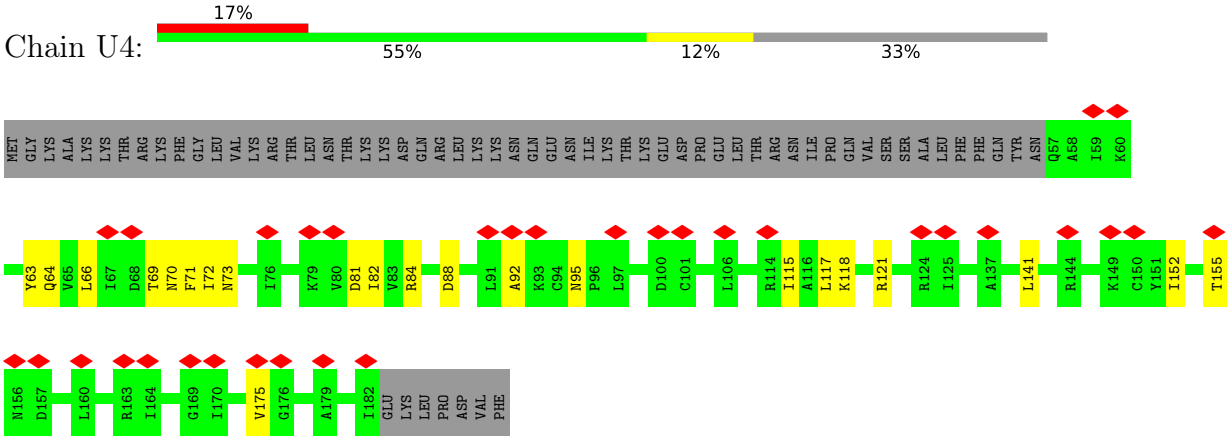






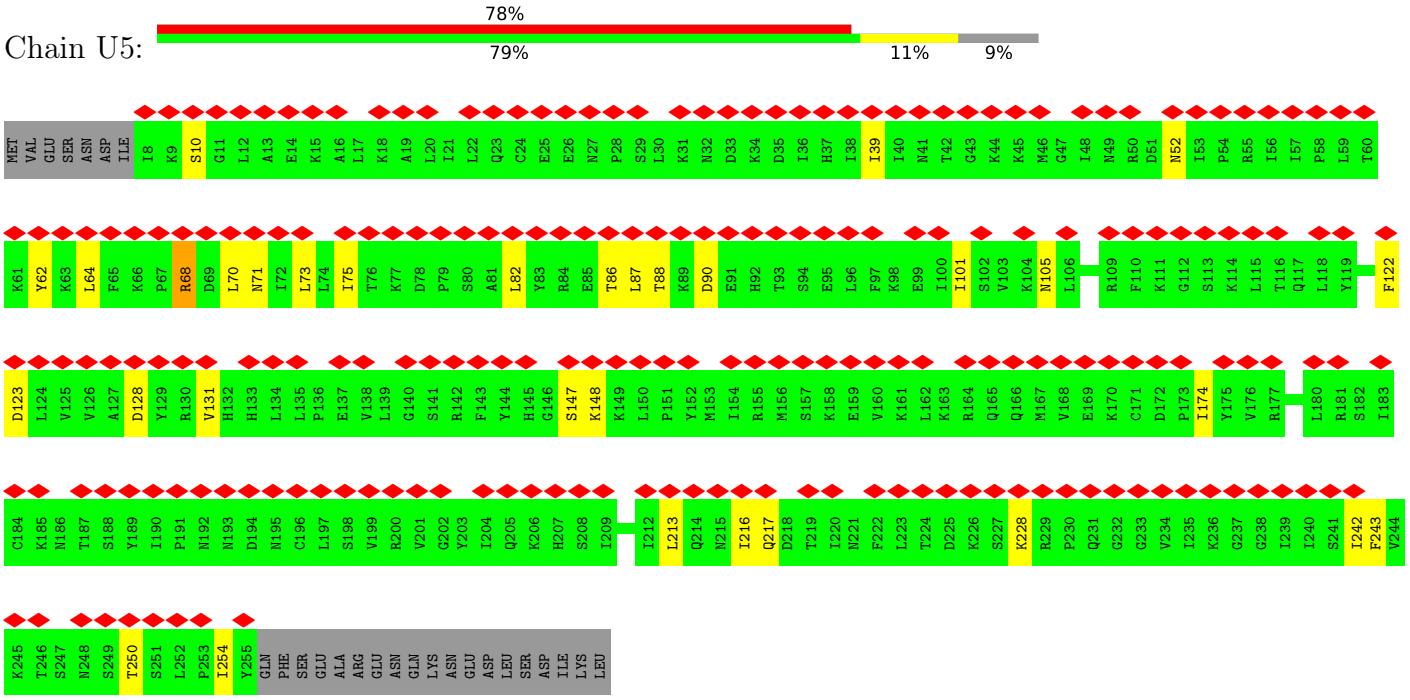
• Molecule 57: rRNA-processing protein FCF1

Chain U4:

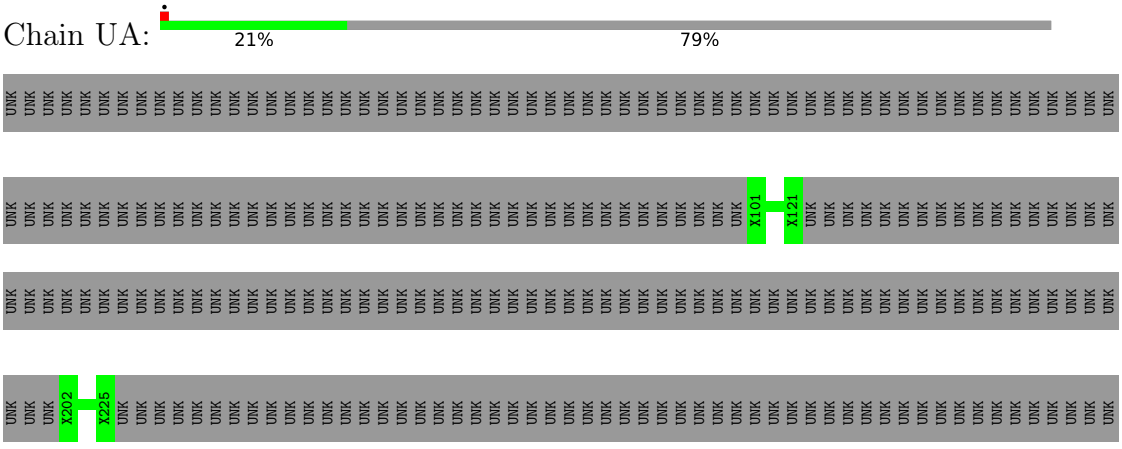


• Molecule 58: Ribosome biogenesis protein UTP30

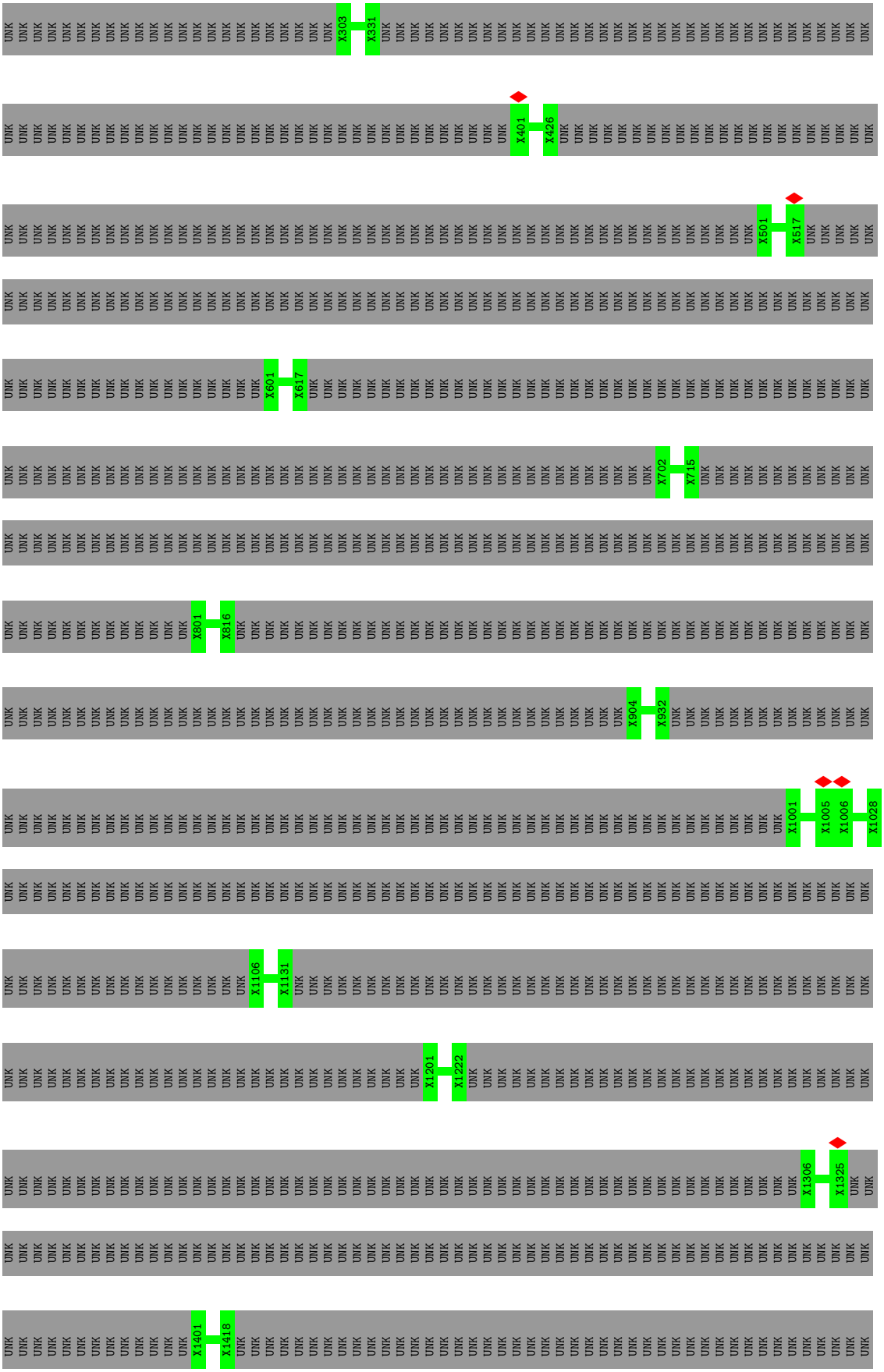
Chain U5:



Chain UA:



• Molecule 59: Helical domain protein


X303
X331
X401
X426
X501
X517
X601
X617
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X715
X801
X816
X904
X932
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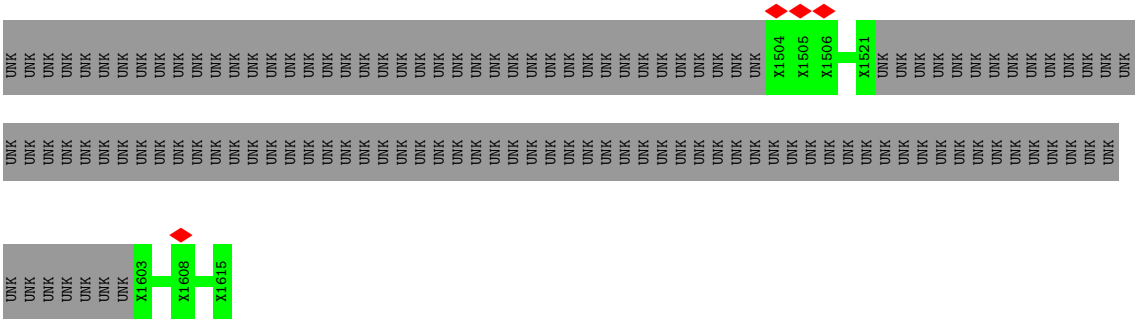
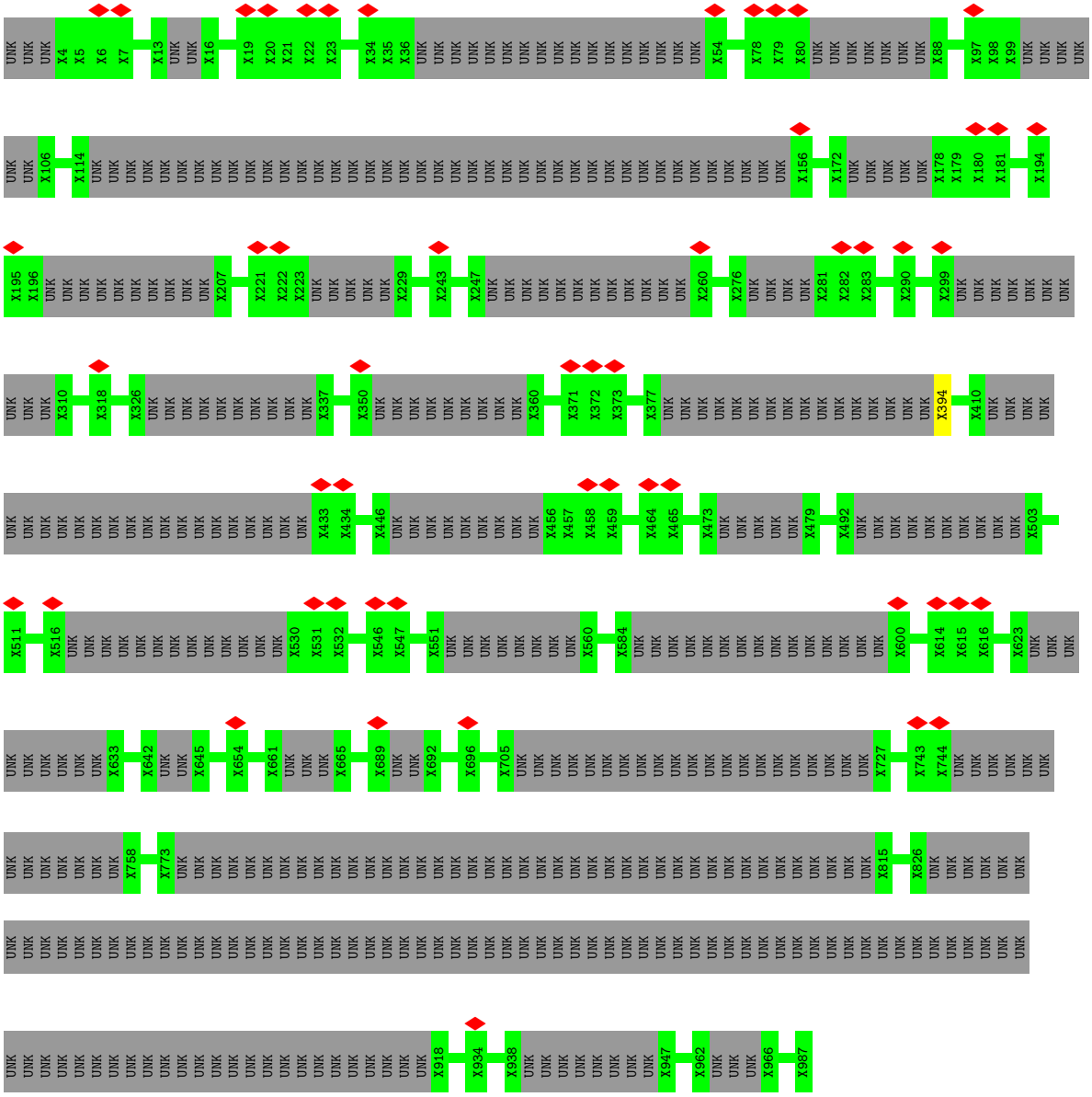
X1005
X1006
X1028
X1106
X1131
X1201
X1222
X1306
X1325
X1401
X1418



• Molecule 60: Helical domain protein

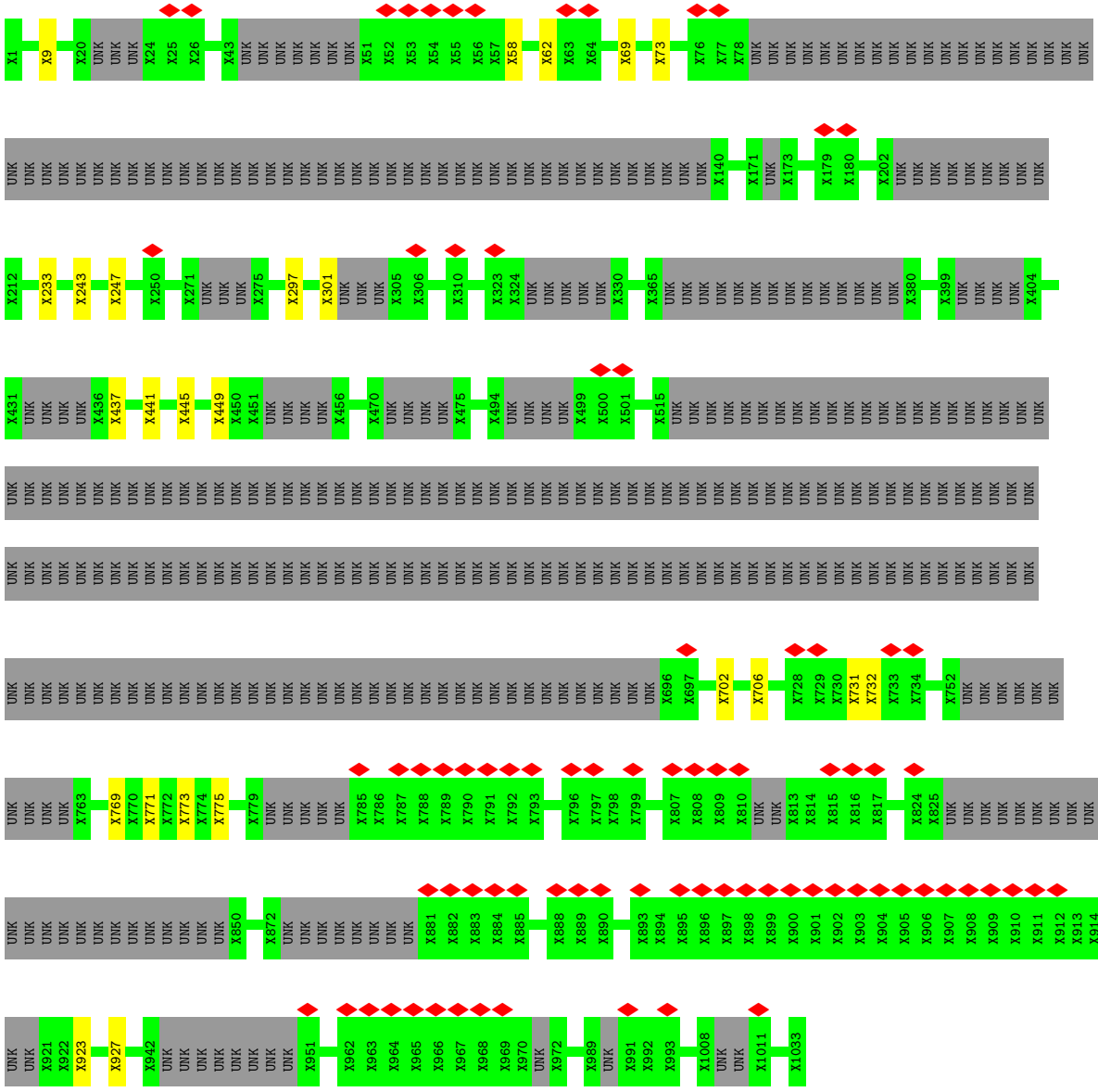
Chain UB:



• Molecule 61: Unassigned helices

Chain UC:


8%
62%
36%


X1 X9 X20 X24 X25 X26 X43 X51 X52 X53 X54 X55 X56 X57 X58 X62 X63 X64 X69 X73 X76 X77 X78
X140 X171 X173 X179 X180 X202
X212 X233 X243 X247 X250 X271 X275 X297 X301 X305 X306 X310 X323 X324 X330 X365 X380 X399 X404
X431 X436 X437 X441 X445 X449 X450 X451 X456 X470 X475 X494 X499 X500 X501 X515
X696 X697 X702 X706 X728 X729 X730 X731 X732 X733 X734 X752
X763 X769 X770 X771 X772 X773 X774 X775 X779 X785 X786 X787 X788 X789 X790 X791 X792 X793 X796 X797 X798 X799 X807 X808 X809 X810 X813 X814 X815 X816 X817 X824 X825
X850 X872 X881 X882 X883 X884 X885 X888 X889 X890 X893 X894 X895 X896 X897 X898 X899 X900 X901 X902 X903 X904 X905 X906 X907 X908 X909 X910 X911 X912 X913 X914
X921 X922 X923 X927 X942 X951 X962 X963 X964 X965 X966 X967 X968 X969 X970 X972 X989 X991 X992 X993 X1008 X1011 X1033

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30995	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	79545	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.265	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	704.0, 704.0, 704.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.76, 1.76, 1.76	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	3A	0.34	0/3710	1.04	6/5763 (0.1%)
2	3B	0.31	0/1903	0.53	0/2572
2	3C	0.28	0/1903	0.52	1/2572 (0.0%)
3	3D	0.30	0/2960	0.52	0/3987
4	3E	0.27	0/2970	0.46	0/4004
5	3F	0.30	0/2975	0.56	0/4008
6	3G	0.28	0/936	0.51	0/1273
6	3H	0.27	0/936	0.50	0/1273
7	5A	0.31	0/11029	1.07	51/17170 (0.3%)
12	AE	0.41	1/6194 (0.0%)	0.58	5/8384 (0.1%)
15	B1	0.30	0/4431	0.56	0/5988
16	BA	0.31	0/6164	0.58	4/8349 (0.0%)
17	BB	0.29	0/6264	0.59	0/8473
18	BC	0.29	0/6226	0.60	2/8442 (0.0%)
19	BD	0.46	4/2597 (0.2%)	0.64	4/3520 (0.1%)
20	BE	0.30	0/6056	0.56	0/8189
21	CA	0.27	0/1621	0.45	0/2196
22	CB	0.28	0/9081	0.47	0/12283
23	E1	0.25	0/1716	0.47	0/2319
23	E2	0.26	0/1721	0.48	0/2323
24	E3	0.29	0/2168	0.51	1/2942 (0.0%)
26	K1	0.29	0/1432	0.53	1/1926 (0.1%)
27	MA	0.27	0/1117	0.47	0/1509
28	MB	0.30	0/1496	0.53	0/2025
29	MC	0.26	0/209	0.50	0/282
30	P1	0.27	0/1394	0.51	0/1881
31	R1	0.28	0/2793	0.49	0/3774
32	R2	0.26	0/2271	0.44	0/3054
34	SA	0.70	9/26553 (0.0%)	1.17	165/41320 (0.4%)
35	SC	0.31	0/1735	0.72	1/2335 (0.0%)
36	SF	0.30	0/1920	0.64	3/2589 (0.1%)
37	SG	0.34	0/1629	0.62	0/2202
38	SH	0.28	0/1385	0.58	1/1851 (0.1%)
39	SI	0.33	0/1343	0.64	1/1808 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
40	SJ	0.28	0/1373	0.60	1/1834 (0.1%)
41	SK	0.29	0/1434	0.62	1/1920 (0.1%)
42	SM	0.35	0/1169	0.57	0/1576
43	SN	0.31	0/898	0.79	1/1220 (0.1%)
44	SO	0.28	0/1109	0.54	0/1495
45	SP	0.28	0/758	0.58	0/1028
46	SR	0.31	0/990	0.66	0/1335
47	SX	0.28	0/1038	0.58	0/1395
48	SY	0.30	0/796	0.67	0/1062
49	SZ	0.31	0/814	0.53	0/1093
50	Sc	0.28	0/605	0.56	0/817
51	Sd	0.26	0/499	0.55	0/670
52	Sf	0.29	0/255	0.54	0/339
53	Sg	0.29	0/404	0.56	0/542
57	U4	0.28	0/1007	0.54	0/1357
58	U5	0.27	0/2043	0.52	0/2747
All	All	0.41	14/144030 (0.0%)	0.78	249/203016 (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
3	3D	0	2
5	3F	0	2
12	AE	0	1
15	B1	0	3
16	BA	0	2
17	BB	0	7
18	BC	0	6
19	BD	0	3
20	BE	0	4
21	CA	0	1
22	CB	0	1
34	SA	0	1
35	SC	0	2
36	SF	0	2
37	SG	0	7
38	SH	0	1
39	SI	0	3
41	SK	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	SM	0	1
43	SN	0	4
45	SP	0	1
46	SR	0	3
48	SY	0	1
53	Sg	0	1
58	U5	0	1
61	UC	0	2
All	All	0	65

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SA	283	U	C2-N3	53.18	1.75	1.37
34	SA	283	U	N3-C4	40.53	1.75	1.38
34	SA	283	U	N1-C2	39.84	1.74	1.38
34	SA	283	U	N1-C6	36.49	1.70	1.38
34	SA	283	U	C4-C5	32.43	1.72	1.43
34	SA	283	U	C5-C6	29.26	1.60	1.34
12	AE	571	LEU	CA-C	22.36	2.11	1.52
34	SA	493	U	C2-N3	-14.56	1.27	1.37
19	BD	411	TYR	CB-CG	-10.84	1.35	1.51
19	BD	411	TYR	CE1-CZ	8.68	1.49	1.38
34	SA	487	G	C5-C6	7.07	1.49	1.42
19	BD	411	TYR	CD1-CE1	-6.50	1.29	1.39
34	SA	487	G	C5-C4	6.39	1.42	1.38
19	BD	411	TYR	CD2-CE2	-5.22	1.31	1.39

All (249) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SA	487	G	C5-C6-O6	38.33	151.60	128.60
34	SA	487	G	N1-C6-O6	-33.63	99.72	119.90
34	SA	493	U	C5-C4-O4	25.11	140.96	125.90
34	SA	493	U	N3-C4-O4	-20.41	105.11	119.40
34	SA	487	G	C4-C5-N7	-19.97	102.81	110.80
34	SA	493	U	C2-N3-C4	16.32	136.79	127.00
12	AE	571	LEU	O-C-N	-15.12	98.51	122.70
34	SA	493	U	N1-C2-N3	-14.92	105.95	114.90
34	SA	487	G	C5-N7-C8	13.80	111.20	104.30
12	AE	571	LEU	CB-CA-C	13.02	134.94	110.20
34	SA	487	G	C5-C6-N1	-11.74	105.63	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SA	283	U	C6-N1-C2	11.51	127.91	121.00
34	SA	487	G	C6-C5-N7	10.96	136.98	130.40
34	SA	283	U	N1-C2-N3	-10.37	108.68	114.90
34	SA	1082	C	C2-N1-C1'	10.24	130.07	118.80
7	5A	522	C	N3-C2-O2	-9.81	115.03	121.90
34	SA	1537	C	N1-C2-O2	9.78	124.77	118.90
34	SA	487	G	C6-N1-C2	9.59	130.85	125.10
12	AE	571	LEU	N-CA-CB	-9.52	91.37	110.40
34	SA	493	U	C4-C5-C6	-9.50	114.00	119.70
34	SA	558	U	N3-C2-O2	-9.19	115.77	122.20
34	SA	1537	C	C2-N1-C1'	9.02	128.72	118.80
34	SA	1456	C	N1-C2-O2	8.96	124.28	118.90
7	5A	356	C	N1-C2-O2	8.94	124.26	118.90
34	SA	1456	C	C2-N1-C1'	8.84	128.52	118.80
7	5A	355	C	N1-C2-O2	8.62	124.07	118.90
39	SI	87	ASP	CB-CG-OD1	8.56	126.00	118.30
34	SA	1159	C	C2-N1-C1'	8.48	128.13	118.80
7	5A	522	C	N1-C2-O2	8.29	123.88	118.90
34	SA	1537	C	N3-C2-O2	-8.20	116.16	121.90
12	AE	571	LEU	CA-C-N	8.12	135.06	117.20
7	5A	356	C	C6-N1-C2	-7.95	117.12	120.30
12	AE	571	LEU	CA-CB-CG	7.93	133.55	115.30
34	SA	1082	C	C6-N1-C1'	-7.93	111.28	120.80
34	SA	1456	C	N3-C2-O2	-7.89	116.37	121.90
34	SA	1159	C	N1-C2-O2	7.83	123.60	118.90
34	SA	487	G	N9-C4-C5	7.80	108.52	105.40
34	SA	1624	C	N1-C2-O2	7.76	123.56	118.90
34	SA	184	C	N1-C2-O2	7.63	123.48	118.90
34	SA	107	C	N1-C2-O2	7.50	123.40	118.90
34	SA	1246	C	C2-N1-C1'	7.49	127.04	118.80
34	SA	394	C	N1-C2-O2	7.40	123.34	118.90
7	5A	356	C	N3-C2-O2	-7.37	116.74	121.90
34	SA	1082	C	N1-C2-O2	7.34	123.30	118.90
34	SA	1258	U	C2-N1-C1'	7.24	126.39	117.70
19	BD	411	TYR	CB-CG-CD1	-7.17	116.70	121.00
34	SA	1596	C	N1-C2-O2	7.14	123.19	118.90
7	5A	355	C	N3-C2-O2	-7.12	116.91	121.90
34	SA	1537	C	C6-N1-C2	-7.11	117.46	120.30
19	BD	423	LEU	CA-CB-CG	7.08	131.59	115.30
7	5A	432	C	N1-C2-O2	7.07	123.14	118.90
34	SA	1246	C	N1-C2-O2	7.02	123.11	118.90
7	5A	469	C	N1-C2-O2	7.02	123.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SA	1258	U	N1-C2-O2	7.01	127.71	122.80
34	SA	934	C	N1-C2-O2	6.95	123.07	118.90
34	SA	1159	C	N3-C2-O2	-6.86	117.09	121.90
34	SA	1220	C	C2-N1-C1'	6.86	126.35	118.80
19	BD	411	TYR	CA-CB-CG	-6.82	100.44	113.40
34	SA	1258	U	N3-C2-O2	-6.82	117.43	122.20
34	SA	283	U	N3-C4-C5	6.79	118.68	114.60
34	SA	186	C	C2-N1-C1'	6.76	126.24	118.80
34	SA	185	U	C2-N1-C1'	6.75	125.80	117.70
34	SA	531	C	N1-C2-O2	6.75	122.95	118.90
7	5A	69	U	N1-C2-O2	6.72	127.51	122.80
34	SA	107	C	N3-C2-O2	-6.67	117.23	121.90
7	5A	69	U	C2-N1-C1'	6.67	125.70	117.70
34	SA	1596	C	C2-N1-C1'	6.64	126.11	118.80
7	5A	432	C	C2-N1-C1'	6.63	126.09	118.80
34	SA	394	C	N3-C2-O2	-6.61	117.28	121.90
34	SA	1220	C	C6-N1-C2	-6.59	117.66	120.30
34	SA	185	U	N1-C2-O2	6.53	127.37	122.80
34	SA	1456	C	C6-N1-C2	-6.50	117.70	120.30
7	5A	522	C	C6-N1-C2	-6.50	117.70	120.30
1	3A	38	U	C2-N1-C1'	6.49	125.48	117.70
34	SA	405	C	C5-C6-N1	6.49	124.25	121.00
34	SA	1473	U	N3-C2-O2	-6.48	117.66	122.20
34	SA	1072	C	C5-C6-N1	6.46	124.23	121.00
34	SA	1251	U	O5'-P-OP1	-6.43	99.91	105.70
7	5A	356	C	C5-C6-N1	6.43	124.21	121.00
34	SA	1624	C	C2-N1-C1'	6.41	125.85	118.80
34	SA	934	C	C2-N1-C1'	6.40	125.84	118.80
34	SA	1063	U	N1-C2-O2	6.39	127.27	122.80
35	SC	61	LEU	CA-CB-CG	6.38	129.97	115.30
34	SA	1220	C	C5-C6-N1	6.33	124.16	121.00
34	SA	1063	U	N3-C2-O2	-6.25	117.82	122.20
7	5A	342	C	N1-C2-O2	6.25	122.65	118.90
1	3A	38	U	N1-C2-O2	6.24	127.17	122.80
7	5A	433	C	N1-C2-O2	6.22	122.63	118.90
34	SA	1658	G	N3-C4-N9	6.21	129.73	126.00
34	SA	136	C	C2-N1-C1'	6.20	125.62	118.80
7	5A	508	C	C2-N1-C1'	6.18	125.60	118.80
34	SA	184	C	C2-N1-C1'	6.18	125.60	118.80
34	SA	185	U	N3-C2-O2	-6.17	117.89	122.20
34	SA	908	U	N1-C2-O2	6.16	127.11	122.80
1	3A	38	U	N3-C2-O2	-6.16	117.89	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SA	1624	C	N3-C2-O2	-6.16	117.59	121.90
34	SA	1159	C	C6-N1-C2	-6.15	117.84	120.30
18	BC	133	ASN	C-N-CA	6.13	135.18	122.30
7	5A	69	U	N3-C2-O2	-6.12	117.92	122.20
7	5A	547	C	N1-C2-O2	6.11	122.56	118.90
7	5A	441	C	C2-N1-C1'	6.10	125.51	118.80
34	SA	1473	U	N1-C2-O2	6.09	127.06	122.80
34	SA	531	C	C6-N1-C2	-6.08	117.87	120.30
34	SA	192	U	P-O3'-C3'	6.06	126.97	119.70
7	5A	433	C	C2-N1-C1'	6.06	125.46	118.80
34	SA	25	C	P-O3'-C3'	6.04	126.95	119.70
34	SA	250	C	C2-N1-C1'	6.03	125.43	118.80
7	5A	441	C	N1-C2-O2	6.00	122.50	118.90
34	SA	1624	C	C6-N1-C2	-5.97	117.91	120.30
34	SA	1191	U	C2-N1-C1'	5.94	124.82	117.70
34	SA	1248	C	C2-N1-C1'	5.90	125.29	118.80
34	SA	1082	C	O4'-C1'-N1	5.89	112.91	108.20
1	3A	304	U	C2-N1-C1'	5.88	124.76	117.70
34	SA	440	U	C2-N1-C1'	5.87	124.75	117.70
34	SA	908	U	N3-C2-O2	-5.86	118.10	122.20
34	SA	1456	C	C6-N1-C1'	-5.86	113.77	120.80
34	SA	487	G	N3-C4-N9	-5.86	122.48	126.00
34	SA	1536	G	N3-C4-C5	-5.85	125.67	128.60
36	SF	192	ILE	CG1-CB-CG2	-5.85	98.53	111.40
34	SA	531	C	C2-N1-C1'	5.84	125.23	118.80
34	SA	1537	C	C6-N1-C1'	-5.82	113.82	120.80
34	SA	1248	C	C6-N1-C2	-5.80	117.98	120.30
34	SA	1174	C	C5-C6-N1	5.79	123.90	121.00
34	SA	184	C	N3-C2-O2	-5.78	117.85	121.90
34	SA	249	U	C2-N1-C1'	5.78	124.64	117.70
34	SA	1620	C	N1-C2-O2	5.78	122.37	118.90
34	SA	531	C	C5-C6-N1	5.78	123.89	121.00
34	SA	1246	C	N3-C2-O2	-5.78	117.86	121.90
34	SA	1536	G	C4-N9-C1'	5.78	134.01	126.50
34	SA	283	U	N1-C2-O2	5.77	126.84	122.80
7	5A	115	G	N1-C6-O6	-5.77	116.44	119.90
18	BC	136	ILE	C-N-CA	5.77	136.12	121.70
34	SA	934	C	N3-C2-O2	-5.76	117.87	121.90
7	5A	480	C	C2-N1-C1'	5.75	125.12	118.80
34	SA	1573	A	P-O3'-C3'	5.74	126.59	119.70
34	SA	405	C	C6-N1-C2	-5.73	118.01	120.30
2	3C	306	LEU	C-N-CA	5.70	135.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SA	1072	C	C2-N1-C1'	5.70	125.07	118.80
34	SA	965	U	N1-C2-O2	5.70	126.79	122.80
34	SA	260	U	C2-N1-C1'	5.69	124.53	117.70
1	3A	49	C	N1-C2-O2	5.67	122.30	118.90
7	5A	442	U	C2-N1-C1'	5.67	124.50	117.70
34	SA	1573	A	OP2-P-O3'	5.67	117.66	105.20
41	SK	99	LEU	CA-CB-CG	5.66	128.31	115.30
7	5A	508	C	C5-C6-N1	5.65	123.82	121.00
34	SA	1159	C	C6-N1-C1'	-5.64	114.03	120.80
34	SA	558	U	N1-C2-N3	5.64	118.28	114.90
34	SA	1615	C	N1-C2-O2	5.63	122.28	118.90
34	SA	440	U	N1-C2-O2	5.63	126.74	122.80
7	5A	355	C	C6-N1-C2	-5.62	118.05	120.30
34	SA	107	C	C6-N1-C2	-5.62	118.05	120.30
34	SA	1246	C	C6-N1-C2	-5.61	118.06	120.30
7	5A	356	C	C2-N1-C1'	5.61	124.97	118.80
38	SH	68	LEU	CB-CG-CD2	5.61	120.54	111.00
34	SA	543	C	N1-C2-O2	5.61	122.27	118.90
34	SA	1473	U	C2-N1-C1'	5.61	124.43	117.70
7	5A	432	C	N3-C2-O2	-5.61	117.98	121.90
34	SA	507	U	C2-N1-C1'	5.59	124.41	117.70
34	SA	111	U	N1-C2-O2	5.59	126.71	122.80
7	5A	109	C	C2-N1-C1'	5.58	124.94	118.80
34	SA	274	G	C8-N9-C1'	-5.57	119.76	127.00
34	SA	1596	C	N3-C2-O2	-5.56	118.01	121.90
34	SA	1248	C	N1-C2-O2	5.55	122.23	118.90
7	5A	128	C	N1-C2-O2	5.53	122.22	118.90
34	SA	1617	U	C2-N1-C1'	5.53	124.33	117.70
7	5A	508	C	N1-C2-O2	5.52	122.21	118.90
34	SA	282	C	N1-C2-O2	5.51	122.21	118.90
34	SA	1536	G	N3-C4-N9	5.51	129.31	126.00
34	SA	1658	G	C4-N9-C1'	5.51	133.66	126.50
34	SA	507	U	N1-C2-O2	5.48	126.64	122.80
34	SA	1624	C	C5-C6-N1	5.47	123.73	121.00
36	SF	228	ILE	CG1-CB-CG2	-5.46	99.38	111.40
34	SA	283	U	C5-C6-N1	-5.46	119.97	122.70
34	SA	1257	U	C2-N1-C1'	5.46	124.25	117.70
7	5A	547	C	C6-N1-C2	-5.44	118.12	120.30
34	SA	274	G	N3-C4-N9	5.43	129.26	126.00
7	5A	186	C	C5-C6-N1	5.42	123.71	121.00
34	SA	960	U	N1-C2-O2	5.41	126.59	122.80
34	SA	1481	C	P-O3'-C3'	5.41	126.20	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	BA	721	VAL	C-N-CA	-5.39	108.22	121.70
34	SA	250	C	N1-C2-O2	5.39	122.14	118.90
34	SA	507	U	N3-C2-O2	-5.39	118.43	122.20
7	5A	385	A	P-O3'-C3'	5.38	126.16	119.70
34	SA	274	G	C4-N9-C1'	5.38	133.50	126.50
34	SA	1510	U	N1-C2-O2	5.38	126.56	122.80
34	SA	559	C	C2-N1-C1'	5.38	124.71	118.80
7	5A	245	C	C5-C6-N1	5.37	123.69	121.00
34	SA	1066	C	N3-C2-O2	-5.37	118.14	121.90
34	SA	965	U	N3-C2-O2	-5.36	118.45	122.20
34	SA	1617	U	N1-C2-O2	5.34	126.54	122.80
34	SA	1072	C	N1-C2-O2	5.33	122.10	118.90
34	SA	285	G	C4-N9-C1'	5.33	133.43	126.50
34	SA	960	U	N3-C2-O2	-5.33	118.47	122.20
26	K1	65	ASP	CB-CG-OD1	5.31	123.08	118.30
34	SA	1537	C	C5-C6-N1	5.31	123.65	121.00
7	5A	261	U	N3-C2-O2	-5.30	118.49	122.20
16	BA	546	ASP	CB-CG-OD1	5.30	123.07	118.30
34	SA	440	U	N3-C2-O2	-5.30	118.49	122.20
16	BA	717	LEU	CA-CB-CG	5.29	127.47	115.30
34	SA	531	C	N3-C2-O2	-5.27	118.21	121.90
34	SA	1072	C	C6-N1-C2	-5.27	118.19	120.30
7	5A	442	U	N1-C2-O2	5.26	126.48	122.80
7	5A	442	U	N3-C2-O2	-5.26	118.52	122.20
16	BA	521	LEU	CA-CB-CG	5.26	127.39	115.30
34	SA	1636	C	N1-C2-O2	5.25	122.05	118.90
34	SA	106	U	N1-C2-O2	5.25	126.47	122.80
34	SA	1191	U	N1-C2-O2	5.25	126.47	122.80
43	SN	89	ILE	C-N-CA	5.24	134.80	121.70
7	5A	454	C	C2-N1-C1'	5.22	124.54	118.80
40	SJ	22	ARG	CA-CB-CG	5.22	124.88	113.40
34	SA	1527	C	C2-N1-C1'	5.21	124.53	118.80
7	5A	342	C	N3-C2-O2	-5.20	118.26	121.90
7	5A	355	C	C2-N1-C1'	5.19	124.51	118.80
34	SA	453	U	C2-N1-C1'	5.19	123.93	117.70
7	5A	186	C	C6-N1-C2	-5.19	118.23	120.30
7	5A	261	U	N1-C2-O2	5.18	126.43	122.80
19	BD	411	TYR	CB-CA-C	5.18	120.75	110.40
34	SA	1596	C	C6-N1-C2	-5.17	118.23	120.30
7	5A	469	C	N3-C2-O2	-5.16	118.29	121.90
34	SA	1063	U	C2-N1-C1'	5.16	123.89	117.70
34	SA	249	U	N1-C2-O2	5.15	126.41	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SA	965	U	C2-N1-C1'	5.14	123.87	117.70
24	E3	211	ILE	C-N-CA	5.13	134.53	121.70
34	SA	136	C	N1-C2-O2	5.12	121.97	118.90
34	SA	638	U	C2-N1-C1'	5.11	123.83	117.70
7	5A	178	G	N3-C4-N9	5.08	129.05	126.00
7	5A	469	C	C2-N1-C1'	5.08	124.39	118.80
7	5A	131	C	N1-C2-O2	5.07	121.94	118.90
34	SA	260	U	N3-C2-O2	-5.07	118.65	122.20
36	SF	180	LEU	CA-CB-CG	5.06	126.93	115.30
34	SA	50	C	N1-C2-O2	5.05	121.93	118.90
34	SA	1441	C	P-O3'-C3'	5.04	125.75	119.70
7	5A	524	U	C5-C6-N1	5.04	125.22	122.70
34	SA	1619	C	N1-C2-O2	5.04	121.92	118.90
34	SA	111	U	C2-N1-C1'	5.04	123.75	117.70
7	5A	547	C	N3-C2-O2	-5.04	118.37	121.90
34	SA	1082	C	N3-C2-O2	-5.03	118.38	121.90
34	SA	1275	A	P-O3'-C3'	5.03	125.73	119.70
34	SA	1510	U	N3-C2-O2	-5.03	118.68	122.20
1	3A	304	U	N1-C2-O2	5.03	126.32	122.80
34	SA	186	C	C5-C6-N1	5.02	123.51	121.00
34	SA	638	U	N1-C2-O2	5.02	126.32	122.80
34	SA	1082	C	C5-C6-N1	5.02	123.51	121.00
34	SA	107	C	C2-N1-C1'	5.02	124.32	118.80
34	SA	285	G	N3-C4-N9	5.01	129.01	126.00
34	SA	1729	C	N1-C2-O2	5.01	121.91	118.90
7	5A	547	C	C5-C6-N1	5.01	123.51	121.00
34	SA	361	C	C6-N1-C2	-5.01	118.30	120.30
34	SA	1209	C	C5-C6-N1	5.01	123.50	121.00

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3D	392	TYR	Peptide
3	3D	91	SER	Peptide
5	3F	342	ARG	Peptide
5	3F	437	ARG	Peptide
12	AE	64	PRO	Peptide
15	B1	190	ILE	Peptide
15	B1	234	PRO	Peptide
15	B1	73	THR	Peptide
16	BA	515	TYR	Peptide

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Mol	Chain	Res	Type	Group
16	BA	702	LEU	Peptide
17	BB	169	PHE	Peptide
17	BB	235	ASN	Peptide
17	BB	335	LEU	Peptide
17	BB	795	ILE	Peptide
17	BB	796	ALA	Peptide
17	BB	797	VAL	Peptide
17	BB	864	ASN	Peptide
18	BC	133	ASN	Peptide
18	BC	136	ILE	Peptide
18	BC	299	ASN	Peptide
18	BC	365	ILE	Peptide
18	BC	771	LYS	Peptide
18	BC	772	LEU	Peptide
19	BD	304	LEU	Peptide
19	BD	411	TYR	Peptide,Sidechain
20	BE	660	PHE	Peptide
20	BE	665	THR	Peptide
20	BE	667	THR	Peptide
20	BE	94	TYR	Peptide
21	CA	199	GLN	Peptide
22	CB	555	PHE	Peptide
34	SA	493	U	Sidechain
35	SC	206	PRO	Peptide
35	SC	208	GLN	Peptide
36	SF	193	GLY	Peptide
36	SF	194	THR	Peptide
37	SG	125	THR	Peptide
37	SG	127	GLN	Peptide
37	SG	128	ASN	Peptide
37	SG	48	PHE	Peptide
37	SG	49	GLU	Peptide
37	SG	50	GLU	Peptide
37	SG	65	ARG	Peptide
38	SH	68	LEU	Peptide
39	SI	131	PHE	Peptide
39	SI	156	SER	Peptide
39	SI	64	VAL	Peptide
41	SK	117	GLY	Peptide
41	SK	133	HIS	Peptide
41	SK	163	PRO	Peptide
42	SM	3	THR	Peptide

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Mol	Chain	Res	Type	Group
43	SN	105	LYS	Peptide
43	SN	110	GLY	Peptide
43	SN	130	THR	Peptide
43	SN	84	ASN	Peptide
45	SP	41	ARG	Peptide
46	SR	33	GLY	Peptide
46	SR	40	GLU	Peptide
46	SR	52	LEU	Peptide
48	SY	96	VAL	Peptide
53	Sg	147	VAL	Peptide
58	U5	62	TYR	Peptide
61	UC	233	UNK	Peptide,Mainchain

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	3A	3327	0	1687	58	0
2	3B	1866	0	1904	30	0
2	3C	1866	0	1904	20	0
3	3D	2915	0	2930	43	0
4	3E	2935	0	3033	48	0
5	3F	2916	0	2947	82	0
6	3G	924	0	975	20	0
6	3H	924	0	975	17	0
7	5A	9867	0	4954	82	0
8	AA	2845	0	658	47	0
9	AB	2015	0	454	19	0
10	AC	2360	0	534	17	0
11	AD	505	0	116	3	0
12	AE	9970	0	7056	161	0
13	AF	1880	0	425	23	0
14	AG	3060	0	707	36	0
15	B1	4325	0	4434	83	0
16	BA	6026	0	5940	129	0
17	BB	6138	0	6163	116	0
18	BC	6117	0	6141	98	0
19	BD	2539	0	2520	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	BE	5936	0	5882	137	0
21	CA	1582	0	1528	35	0
22	CB	8870	0	8975	149	0
23	E1	1689	0	1738	34	0
23	E2	1695	0	1757	38	0
24	E3	2114	0	2154	55	0
25	E4	1425	0	322	18	0
26	K1	1410	0	1503	27	0
27	MA	1097	0	1130	7	0
28	MB	1465	0	1486	31	0
29	MC	307	0	231	2	0
30	P1	1368	0	1436	9	0
31	R1	2742	0	2829	40	0
32	R2	2228	0	2228	15	0
33	S1	1425	0	334	35	0
34	SA	23759	0	11991	338	0
35	SC	1709	0	1784	47	0
36	SF	1881	0	1958	50	0
37	SG	1609	0	1675	41	0
38	SH	1369	0	1414	69	0
39	SI	1322	0	1394	29	0
40	SJ	1350	0	1374	41	0
41	SK	1412	0	1486	22	0
42	SM	1143	0	1210	26	0
43	SN	890	0	887	12	0
44	SO	1087	0	1152	16	0
45	SP	750	0	728	9	0
46	SR	973	0	1029	37	0
47	SX	1021	0	1060	27	0
48	SY	785	0	840	20	0
49	SZ	801	0	828	13	0
50	Sc	595	0	613	0	0
51	Sd	497	0	535	0	0
52	Sf	251	0	277	0	0
53	Sg	397	0	399	0	0
54	U1	1425	0	329	23	0
55	U2	365	0	75	0	0
56	U3	7035	0	1590	5	0
57	U4	990	0	1054	13	0
58	U5	2009	0	2130	16	0
59	UA	1690	0	370	0	0
60	UB	2775	0	620	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	UC	3300	0	727	12	0
All	All	173863	0	129519	2467	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 9.

All (2467) 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)
12:AE:630:TYR:CE1	12:AE:637:ILE:CD1	1.86	1.56
34:SA:283:U:N3	34:SA:283:U:C2	1.75	1.54
34:SA:283:U:N1	34:SA:283:U:C6	1.70	1.54
34:SA:283:U:N3	34:SA:283:U:C4	1.74	1.53
34:SA:283:U:C2	34:SA:283:U:N1	1.74	1.52
34:SA:283:U:N1	38:SH:188:ARG:CG	1.79	1.44
34:SA:283:U:N1	38:SH:188:ARG:HG3	1.04	1.37
12:AE:630:TYR:CZ	12:AE:637:ILE:HD13	1.63	1.33
12:AE:630:TYR:CE1	12:AE:637:ILE:HD12	1.52	1.32
38:SH:188:ARG:NH1	38:SH:191:ARG:CD	2.05	1.20
12:AE:571:LEU:CA	12:AE:571:LEU:C	2.11	1.19
38:SH:188:ARG:NH1	38:SH:191:ARG:HD2	1.57	1.19
24:E3:206:LEU:H	24:E3:207:PRO:CD	1.54	1.17
34:SA:283:U:H5"	38:SH:188:ARG:HD2	1.23	1.17
12:AE:630:TYR:OH	12:AE:637:ILE:HD13	1.43	1.17
12:AE:630:TYR:CE1	12:AE:637:ILE:HD13	1.66	1.16
34:SA:283:U:OP2	38:SH:188:ARG:CZ	1.95	1.12
12:AE:571:LEU:HB3	12:AE:630:TYR:CD2	1.83	1.12
38:SH:188:ARG:NH2	38:SH:191:ARG:HH21	1.53	1.07
12:AE:630:TYR:HE1	12:AE:637:ILE:CB	1.68	1.07
12:AE:630:TYR:HE1	12:AE:637:ILE:CG1	1.67	1.06
24:E3:206:LEU:H	24:E3:207:PRO:HD3	1.08	1.05
16:BA:538:GLN:HA	16:BA:552:ASN:O	1.57	1.03
34:SA:283:U:C1'	38:SH:188:ARG:HG3	1.88	1.03
12:AE:630:TYR:HE1	12:AE:637:ILE:CD1	1.37	1.02
34:SA:126:A:H62	34:SA:291:G:N2	1.57	1.02
34:SA:126:A:N6	34:SA:291:G:H21	1.57	1.02
1:3A:254:A:OP2	6:3G:95:ARG:NH1	1.91	1.02
12:AE:630:TYR:CZ	12:AE:637:ILE:CD1	2.31	1.01
38:SH:188:ARG:CZ	38:SH:191:ARG:HD2	1.94	0.98
34:SA:283:U:C5'	38:SH:188:ARG:HD2	1.93	0.98
34:SA:877:G:H1	34:SA:951:A:H61	1.03	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B1:283:LEU:O	15:B1:788:TYR:HB3	1.64	0.97
12:AE:630:TYR:CE1	12:AE:637:ILE:CB	2.47	0.97
34:SA:1175:U:H3	34:SA:1464:G:H1	1.03	0.97
12:AE:630:TYR:CE1	12:AE:637:ILE:HG21	2.00	0.97
34:SA:330:G:OP2	40:SJ:172:ARG:NH1	1.99	0.96
38:SH:188:ARG:HH12	38:SH:191:ARG:HD3	1.32	0.95
8:AA:66:UNK:O	8:AA:77:UNK:HA	1.67	0.95
15:B1:847:LEU:O	15:B1:853:ARG:HA	1.67	0.94
34:SA:1213:G:H1	34:SA:1450:U:H3	1.10	0.94
1:3A:7:G:H1	34:SA:1117:U:H3	1.08	0.94
5:3F:421:ASN:HA	5:3F:436:GLU:O	1.68	0.93
20:BE:27:PHE:HB3	20:BE:653:ILE:O	1.68	0.93
7:5A:506:G:H1	7:5A:530:A:H61	1.04	0.92
5:3F:539:ILE:O	5:3F:565:SER:HA	1.70	0.92
17:BB:597:ILE:O	17:BB:611:LEU:HB2	1.69	0.92
7:5A:506:G:H1	7:5A:530:A:N6	1.67	0.92
34:SA:1663:G:H1	34:SA:1738:U:H3	0.92	0.91
34:SA:283:U:H5"	38:SH:188:ARG:CD	2.00	0.91
28:MB:197:ALA:O	28:MB:200:LYS:NZ	2.04	0.91
20:BE:631:ASN:O	20:BE:643:THR:HA	1.71	0.90
24:E3:206:LEU:N	24:E3:207:PRO:CD	2.27	0.90
7:5A:250:G:H1	7:5A:262:U:H3	0.95	0.90
34:SA:283:U:C4	38:SH:188:ARG:HB2	2.06	0.90
47:SX:23:ARG:HH12	47:SX:66:ASN:HA	1.35	0.89
19:BD:367:GLN:O	19:BD:386:ILE:HA	1.70	0.89
5:3F:497:LYS:NZ	5:3F:513:GLU:OE2	2.05	0.89
38:SH:188:ARG:NH1	38:SH:191:ARG:HD3	1.88	0.89
8:AA:359:UNK:HA	8:AA:373:UNK:O	1.72	0.89
6:3G:57:ASP:O	6:3G:84:ARG:NH1	2.06	0.89
34:SA:1219:A:H62	34:SA:1264:G:N2	1.71	0.88
12:AE:571:LEU:CB	12:AE:630:TYR:CD2	2.56	0.88
17:BB:555:VAL:O	17:BB:568:SER:HA	1.72	0.88
12:AE:630:TYR:CE1	12:AE:637:ILE:HB	2.08	0.88
15:B1:281:GLU:HB2	15:B1:790:ARG:O	1.73	0.87
12:AE:571:LEU:CA	12:AE:630:TYR:CD2	2.57	0.87
37:SG:84:LYS:HG2	37:SG:92:ARG:HH12	1.40	0.87
1:3A:326:U:OP1	6:3H:46:ARG:NH1	2.09	0.86
12:AE:630:TYR:CE1	12:AE:637:ILE:CG2	2.58	0.86
5:3F:235:HIS:ND1	5:3F:257:ASP:OD2	2.09	0.86
5:3F:347:MET:HA	5:3F:357:LEU:O	1.75	0.86
34:SA:877:G:H1	34:SA:951:A:N6	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:482:LEU:HB2	19:BD:494:TYR:O	1.76	0.85
12:AE:571:LEU:C	12:AE:630:TYR:CD2	2.49	0.85
36:SF:153:ASN:O	36:SF:174:LYS:NZ	2.10	0.84
22:CB:150:ASP:O	22:CB:154:LYS:HB2	1.77	0.84
13:AF:75:UNK:HA	13:AF:89:UNK:O	1.77	0.84
34:SA:1529:C:OP1	37:SG:112:ARG:NH1	2.10	0.84
34:SA:523:G:N2	34:SA:529:A:OP2	2.10	0.84
39:SI:76:LYS:HG2	39:SI:79:ARG:HH12	1.42	0.84
5:3F:146:LYS:O	5:3F:566:ALA:HA	1.77	0.84
7:5A:513:G:H1	7:5A:523:U:H3	1.25	0.84
31:R1:29:LYS:NZ	31:R1:332:ILE:O	2.10	0.84
40:SJ:110:ARG:NH1	40:SJ:160:PHE:O	2.10	0.84
1:3A:84:U:OP2	4:3E:361:ARG:NH2	2.11	0.83
26:K1:124:ASP:OD1	26:K1:184:ARG:NH1	2.11	0.83
36:SF:75:LYS:NZ	36:SF:77:ARG:HH12	1.76	0.83
34:SA:1482:C:N4	34:SA:1525:A:OP2	2.10	0.83
22:CB:536:TYR:OH	22:CB:552:ARG:NH1	2.12	0.83
8:AA:360:UNK:O	8:AA:372:UNK:HA	1.77	0.82
34:SA:283:U:N3	38:SH:188:ARG:HB2	1.92	0.82
42:SM:72:THR:O	42:SM:88:ARG:NH1	2.12	0.82
5:3F:551:ARG:NH1	6:3G:93:VAL:O	2.12	0.82
17:BB:554:THR:HA	17:BB:569:LEU:O	1.80	0.82
34:SA:1588:G:H1	34:SA:1608:U:H3	0.85	0.82
22:CB:152:PHE:O	22:CB:156:LYS:NZ	2.13	0.82
22:CB:307:LYS:NZ	34:SA:1683:C:OP1	2.13	0.81
20:BE:423:ARG:NH1	20:BE:426:GLU:OE1	2.13	0.81
12:AE:571:LEU:C	12:AE:571:LEU:HA	1.98	0.81
34:SA:322:G:O2'	40:SJ:10:LYS:NZ	2.13	0.81
1:3A:5:A:H2	34:SA:1119:G:H1	1.22	0.81
34:SA:396:G:N1	34:SA:399:A:OP2	2.13	0.81
1:3A:5:A:C2	34:SA:1119:G:N1	2.48	0.81
5:3F:495:SER:HA	5:3F:514:LEU:O	1.80	0.81
22:CB:779:PHE:HA	22:CB:849:GLY:O	1.80	0.81
20:BE:24:PHE:HA	20:BE:655:THR:O	1.81	0.80
47:SX:20:THR:OG1	47:SX:22:LYS:NZ	2.13	0.80
20:BE:66:LEU:O	20:BE:346:ARG:NH1	2.12	0.80
22:CB:707:PHE:O	22:CB:918:ARG:NH1	2.14	0.80
34:SA:283:U:OP2	38:SH:188:ARG:NH2	2.14	0.80
34:SA:1216:C:O2'	34:SA:1217:A:O5'	1.97	0.80
14:AG:118:UNK:O	14:AG:130:UNK:HA	1.81	0.80
22:CB:367:ARG:O	22:CB:371:GLN:HB2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:SM:132:SER:O	42:SM:136:ARG:NH1	2.14	0.80
15:B1:988:ARG:HH12	28:MB:146:ARG:HH11	1.29	0.80
34:SA:1636:C:H42	34:SA:1765:A:H61	1.28	0.79
12:AE:571:LEU:CB	12:AE:630:TYR:CE2	2.66	0.79
15:B1:845:LEU:O	15:B1:855:GLN:HA	1.81	0.79
20:BE:796:LEU:O	20:BE:800:GLU:HB2	1.83	0.79
23:E1:178:VAL:HA	23:E1:223:GLU:O	1.83	0.79
34:SA:163:G:N2	34:SA:163:G:OP2	2.14	0.79
3:3D:158:TYR:O	3:3D:162:LYS:HB2	1.82	0.79
24:E3:334:GLU:O	24:E3:338:ALA:HB3	1.83	0.78
34:SA:1085:G:N2	34:SA:1088:A:OP2	2.16	0.78
20:BE:356:ILE:O	20:BE:633:LYS:NZ	2.16	0.78
34:SA:1584:G:N2	34:SA:1611:A:OP2	2.17	0.78
36:SF:75:LYS:HZ2	36:SF:77:ARG:NH1	1.80	0.78
19:BD:382:GLY:N	19:BD:405:THR:HG1	1.81	0.78
23:E2:44:VAL:HA	23:E2:113:TYR:O	1.83	0.78
34:SA:522:U:OP1	49:SZ:37:LYS:NZ	2.16	0.78
8:AA:524:UNK:O	8:AA:536:UNK:HA	1.84	0.77
1:3A:80:U:OP2	6:3H:95:ARG:NH1	2.17	0.77
23:E2:88:ARG:NH1	34:SA:1191:U:OP1	2.17	0.77
26:K1:141:ARG:NH1	26:K1:191:MET:O	2.16	0.77
38:SH:188:ARG:NH2	38:SH:191:ARG:NH2	2.32	0.77
36:SF:50:ASN:O	36:SF:53:LYS:NZ	2.18	0.77
6:3H:57:ASP:O	6:3H:84:ARG:NH1	2.18	0.77
12:AE:571:LEU:HB3	12:AE:630:TYR:CE2	2.19	0.77
36:SF:11:ARG:NH1	36:SF:21:ASP:OD1	2.18	0.76
38:SH:188:ARG:HH22	38:SH:191:ARG:HH21	1.34	0.76
34:SA:1253:U:OP1	43:SN:50:LYS:NZ	2.18	0.76
14:AG:382:UNK:HA	14:AG:397:UNK:O	1.86	0.76
23:E1:42:ILE:O	23:E1:203:CYS:HA	1.86	0.76
35:SC:158:SER:O	35:SC:162:ARG:NH1	2.19	0.76
1:3A:206:C:N4	1:3A:242:U:OP2	2.18	0.76
20:BE:439:PHE:HA	20:BE:455:PHE:O	1.86	0.76
22:CB:921:ASP:OD2	22:CB:1172:ASN:ND2	2.19	0.76
12:AE:571:LEU:C	12:AE:630:TYR:HD2	1.89	0.75
34:SA:364:G:OP2	34:SA:377:G:N2	2.18	0.75
34:SA:1216:C:O2'	34:SA:1217:A:P	2.44	0.75
24:E3:206:LEU:N	24:E3:207:PRO:HD3	1.85	0.75
34:SA:335:U:O2'	42:SM:129:ARG:NH1	2.19	0.75
9:AB:190:UNK:O	9:AB:201:UNK:HA	1.87	0.75
6:3H:29:ASN:O	6:3H:31:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:E3:301:TYR:O	24:E3:304:TYR:N	2.20	0.74
16:BA:21:THR:O	16:BA:30:LEU:HB2	1.87	0.74
26:K1:164:ILE:HA	26:K1:172:SER:O	1.88	0.74
2:3B:170:VAL:HA	2:3B:239:CYS:O	1.88	0.74
9:AB:110:UNK:O	9:AB:117:UNK:HA	1.87	0.73
1:3A:67:G:H1	7:5A:286:U:H3	1.37	0.73
14:AG:4:UNK:HA	14:AG:569:UNK:O	1.87	0.73
15:B1:607:ASP:O	31:R1:321:ARG:NH1	2.19	0.73
12:AE:571:LEU:CA	12:AE:630:TYR:CE2	2.71	0.72
34:SA:432:G:OP2	34:SA:433:C:N4	2.22	0.72
15:B1:610:LYS:NZ	15:B1:612:VAL:O	2.21	0.72
26:K1:198:TYR:O	26:K1:202:GLU:HB2	1.90	0.72
20:BE:132:THR:OG1	20:BE:134:ASP:OD1	2.06	0.72
12:AE:756:LEU:O	12:AE:760:PHE:HB2	1.89	0.72
22:CB:100:SER:O	22:CB:104:LYS:HB2	1.88	0.72
22:CB:899:LEU:O	22:CB:903:SER:HB3	1.89	0.72
22:CB:1097:ASP:OD2	22:CB:1186:ILE:N	2.16	0.72
23:E2:41:MET:O	23:E2:110:LEU:HA	1.89	0.72
1:3A:83:A:OP2	4:3E:361:ARG:NE	2.23	0.72
36:SF:75:LYS:HZ2	36:SF:77:ARG:HH12	1.33	0.72
24:E3:301:TYR:CE2	34:SA:1217:A:N6	2.57	0.72
38:SH:188:ARG:HH12	38:SH:191:ARG:CD	1.88	0.72
34:SA:283:U:C2	34:SA:283:U:C1'	2.73	0.72
34:SA:405:C:O4'	38:SH:88:ARG:NH1	2.22	0.71
46:SR:42:GLU:HG3	46:SR:45:ARG:HH12	1.55	0.71
36:SF:118:GLU:OE2	36:SF:237:SER:N	2.23	0.71
41:SK:163:PRO:HA	41:SK:166:GLY:H	1.55	0.71
12:AE:120:TRP:O	12:AE:124:ARG:HB3	1.91	0.71
9:AB:271:UNK:HA	9:AB:284:UNK:O	1.90	0.71
17:BB:186:ILE:HB	17:BB:200:HIS:O	1.90	0.71
7:5A:337:G:H21	7:5A:338:A:H62	1.39	0.71
28:MB:234:ARG:NH1	28:MB:254:PHE:O	2.22	0.71
34:SA:538:A:H1'	34:SA:540:G:H1	1.56	0.71
16:BA:60:ALA:O	16:BA:72:SER:HA	1.91	0.70
19:BD:577:LEU:O	19:BD:588:LEU:HA	1.91	0.70
24:E3:206:LEU:H	24:E3:207:PRO:HD2	1.52	0.70
34:SA:337:G:OP2	34:SA:338:C:N4	2.24	0.70
12:AE:746:GLU:O	12:AE:750:ASN:HB2	1.91	0.70
15:B1:943:LYS:NZ	34:SA:572:C:OP2	2.14	0.70
16:BA:198:PHE:O	16:BA:207:TYR:HB3	1.91	0.70
34:SA:1174:C:H42	34:SA:1465:C:H42	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BE:273:LEU:O	20:BE:286:VAL:HA	1.91	0.70
37:SG:76:ARG:NH1	46:SR:120:ASP:OD1	2.23	0.70
2:3C:299:LYS:HD2	2:3C:322:ARG:HB3	1.73	0.70
17:BB:447:LEU:O	17:BB:454:LEU:HA	1.90	0.70
20:BE:84:SER:HB2	20:BE:91:TYR:HB2	1.72	0.69
5:3F:198:LYS:NZ	5:3F:265:THR:O	2.25	0.69
19:BD:313:PHE:HA	19:BD:322:HIS:O	1.92	0.69
1:3A:1:G:C6	34:SA:1124:A:N1	2.60	0.69
18:BC:662:GLN:O	18:BC:666:GLU:HB2	1.93	0.69
18:BC:722:GLU:O	18:BC:725:ASP:HB2	1.92	0.69
19:BD:369:ASN:O	19:BD:384:ILE:HA	1.91	0.69
18:BC:698:LEU:O	18:BC:702:LEU:HB2	1.92	0.69
15:B1:200:LEU:O	15:B1:204:ARG:HB2	1.92	0.69
5:3F:155:ASN:N	5:3F:193:ASP:OD2	2.22	0.69
21:CA:134:ILE:O	21:CA:138:TRP:HB2	1.93	0.69
48:SY:67:ALA:HB3	48:SY:69:ARG:HH12	1.58	0.69
19:BD:311:ASN:HA	19:BD:324:TRP:O	1.92	0.69
18:BC:190:THR:OG1	22:CB:657:ARG:NH1	2.25	0.68
34:SA:938:G:N2	34:SA:941:A:OP2	2.19	0.68
34:SA:1217:A:H2	34:SA:1448:G:H21	1.41	0.68
5:3F:299:CYS:HB2	5:3F:303:LYS:O	1.92	0.68
21:CA:18:PHE:O	21:CA:34:LEU:HA	1.94	0.68
34:SA:867:G:H1	34:SA:961:U:H3	1.38	0.68
38:SH:187:LYS:HZ1	38:SH:191:ARG:HH12	1.39	0.68
19:BD:325:ASP:HB2	19:BD:337:ALA:H	1.57	0.68
12:AE:571:LEU:CA	12:AE:630:TYR:HD2	2.06	0.68
36:SF:59:ARG:HA	36:SF:62:LYS:HZ3	1.59	0.68
12:AE:630:TYR:CD1	12:AE:637:ILE:HB	2.28	0.68
34:SA:1219:A:N6	34:SA:1264:G:N2	2.40	0.68
7:5A:511:G:H1	7:5A:525:U:H3	1.42	0.67
16:BA:103:LYS:O	16:BA:112:ALA:HB3	1.94	0.67
19:BD:424:ILE:HB	19:BD:433:TRP:HB3	1.75	0.67
12:AE:367:LEU:O	12:AE:371:LYS:HB2	1.95	0.67
14:AG:423:UNK:HA	14:AG:438:UNK:O	1.94	0.67
36:SF:11:ARG:NH1	36:SF:21:ASP:O	2.26	0.67
40:SJ:105:ASP:OD2	40:SJ:107:THR:OG1	2.11	0.67
42:SM:36:LYS:NZ	42:SM:59:PRO:O	2.24	0.67
17:BB:488:LEU:HB2	17:BB:500:TRP:HB2	1.77	0.67
17:BB:851:PRO:O	17:BB:855:LYS:HB2	1.94	0.67
14:AG:402:UNK:HA	14:AG:416:UNK:O	1.95	0.67
34:SA:283:U:C6	34:SA:283:U:C1'	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BB:393:ASP:HA	17:BB:679:HIS:HB3	1.77	0.67
20:BE:309:ILE:HG12	20:BE:323:VAL:HG12	1.75	0.67
12:AE:597:HIS:HB3	12:AE:615:ASN:HB3	1.77	0.66
5:3F:189:THR:O	5:3F:196:LEU:HA	1.94	0.66
34:SA:323:A:H61	34:SA:345:U:H3	1.43	0.66
34:SA:394:C:O2	34:SA:401:A:N6	2.29	0.66
2:3B:298:ILE:HA	2:3B:319:ARG:O	1.96	0.66
22:CB:182:ASP:HB2	22:CB:208:THR:HB	1.78	0.66
34:SA:283:U:C5	38:SH:188:ARG:NE	2.50	0.66
20:BE:477:ILE:O	20:BE:484:ILE:HA	1.96	0.66
38:SH:188:ARG:HH11	38:SH:191:ARG:HB2	1.61	0.66
7:5A:348:U:H3	7:5A:376:U:H3	1.42	0.66
16:BA:59:ALA:HA	16:BA:73:ILE:O	1.96	0.66
35:SC:144:ARG:HB3	35:SC:208:GLN:HB3	1.76	0.66
19:BD:411:TYR:OH	19:BD:423:LEU:N	2.29	0.66
20:BE:567:ILE:O	20:BE:580:GLN:HA	1.96	0.66
23:E2:44:VAL:HG22	23:E2:113:TYR:HB2	1.76	0.66
26:K1:140:LYS:O	26:K1:144:ARG:HB2	1.96	0.66
38:SH:79:LYS:HG3	38:SH:86:PRO:HG2	1.77	0.66
7:5A:538:C:H2'	7:5A:539:A:H8	1.60	0.66
15:B1:827:ALA:HA	15:B1:920:GLU:H	1.61	0.66
20:BE:97:LYS:HZ2	20:BE:111:GLU:HB2	1.60	0.66
34:SA:629:U:OP2	34:SA:969:C:N4	2.28	0.66
39:SI:143:LEU:HD23	39:SI:145:GLY:H	1.60	0.66
7:5A:557:A:H61	7:5A:580:A:H61	1.43	0.66
5:3F:322:HIS:HB2	5:3F:343:ASP:HB3	1.78	0.65
12:AE:559:ASN:HB2	12:AE:616:PRO:HD3	1.77	0.65
34:SA:283:U:N1	38:SH:188:ARG:CB	2.58	0.65
22:CB:412:LEU:HD21	22:CB:424:GLY:HA3	1.78	0.65
34:SA:1163:A:H4'	37:SG:166:ARG:HH12	1.60	0.65
5:3F:335:ARG:HA	5:3F:349:TRP:O	1.96	0.65
20:BE:481:ASN:O	20:BE:499:LYS:NZ	2.30	0.65
28:MB:152:LEU:HB3	28:MB:165:PHE:HB2	1.78	0.65
39:SI:51:VAL:HG13	39:SI:53:GLY:H	1.61	0.65
18:BC:697:VAL:HG12	18:BC:700:ARG:HH21	1.61	0.65
28:MB:94:ARG:NH1	34:SA:1588:G:N7	2.45	0.65
7:5A:334:G:H1'	27:MA:55:ARG:HE	1.62	0.65
20:BE:630:THR:N	20:BE:644:THR:O	2.30	0.65
7:5A:503:C:H1'	7:5A:535:G:H1	1.61	0.65
8:AA:68:UNK:O	8:AA:75:UNK:HA	1.96	0.65
3:3D:23:GLN:HG2	3:3D:50:LEU:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:SF:180:LEU:HA	36:SF:194:THR:HG22	1.77	0.65
2:3B:194:VAL:HB	2:3B:217:ILE:HA	1.78	0.65
15:B1:988:ARG:HH12	28:MB:146:ARG:NH1	1.94	0.65
17:BB:838:THR:O	17:BB:842:ASN:HB2	1.97	0.65
34:SA:1219:A:N6	34:SA:1264:G:H21	1.95	0.65
12:AE:579:ARG:HD2	12:AE:631:VAL:HG22	1.80	0.64
23:E2:39:LYS:O	23:E2:109:LYS:NZ	2.22	0.64
34:SA:537:G:OP2	41:SK:175:ARG:NH2	2.27	0.64
5:3F:496:LEU:HB2	5:3F:514:LEU:HB2	1.79	0.64
20:BE:223:LEU:HB2	20:BE:231:ILE:HB	1.79	0.64
24:E3:305:ARG:O	24:E3:307:VAL:N	2.30	0.64
8:AA:218:UNK:HA	8:AA:234:UNK:HA	1.79	0.64
20:BE:609:ILE:HB	20:BE:623:ILE:HB	1.78	0.64
19:BD:483:ALA:H	19:BD:523:PHE:HZ	1.44	0.64
12:AE:37:SER:O	12:AE:41:ALA:HB2	1.98	0.64
23:E2:164:LYS:HZ1	34:SA:1575:G:P	2.19	0.64
31:R1:18:ARG:NH1	31:R1:98:TYR:O	2.29	0.64
37:SG:53:VAL:HG22	37:SG:55:ASP:H	1.62	0.64
5:3F:551:ARG:HH11	6:3G:94:SER:HA	1.63	0.64
8:AA:486:UNK:HA	8:AA:492:UNK:HA	1.78	0.64
16:BA:712:PHE:H	16:BA:746:ASN:HD21	1.43	0.64
20:BE:467:ALA:HB3	20:BE:476:PHE:HB2	1.80	0.64
24:E3:301:TYR:HA	24:E3:304:TYR:HB2	1.80	0.64
14:AG:485:UNK:O	14:AG:497:UNK:HA	1.98	0.63
16:BA:715:PHE:HB2	16:BA:744:ARG:HG2	1.80	0.63
20:BE:179:LYS:HA	20:BE:191:PHE:O	1.98	0.63
20:BE:430:ILE:HB	20:BE:443:TRP:HB2	1.79	0.63
20:BE:350:SER:N	20:BE:372:ASP:OD2	2.30	0.63
22:CB:99:LYS:O	22:CB:103:PHE:HB3	1.98	0.63
24:E3:301:TYR:CE2	34:SA:1217:A:C6	2.86	0.63
37:SG:68:ILE:HG22	46:SR:114:ARG:HH12	1.64	0.63
12:AE:465:PHE:HB2	12:AE:507:LYS:HG2	1.81	0.63
34:SA:283:U:C2	38:SH:188:ARG:CB	2.82	0.63
3:3D:122:GLU:HG2	3:3D:124:ALA:H	1.63	0.63
22:CB:840:LEU:HB3	22:CB:852:PHE:HB2	1.79	0.63
35:SC:130:SER:HG	35:SC:180:THR:HG1	1.44	0.63
38:SH:31:ARG:HG2	38:SH:101:ILE:HG12	1.80	0.63
42:SM:71:LEU:HB3	42:SM:88:ARG:NH1	2.13	0.63
7:5A:174:U:H3	7:5A:222:G:H1	1.47	0.63
15:B1:143:MET:N	48:SY:144:ARG:HH11	1.97	0.63
21:CA:192:GLU:O	21:CA:196:ALA:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AE:465:PHE:H	12:AE:507:LYS:HE2	1.63	0.63
1:3A:5:A:N1	34:SA:1119:G:O6	2.31	0.63
20:BE:551:TYR:HD1	20:BE:558:PHE:HB3	1.64	0.63
22:CB:861:ILE:O	22:CB:865:ARG:HB2	1.99	0.63
24:E3:418:HIS:O	24:E3:422:LEU:HB2	1.99	0.63
7:5A:506:G:N2	7:5A:530:A:N1	2.47	0.62
16:BA:842:ASN:ND2	20:BE:882:GLU:OE1	2.32	0.62
18:BC:771:LYS:HB3	18:BC:775:ILE:HD12	1.80	0.62
21:CA:55:LEU:O	21:CA:123:THR:HA	1.98	0.62
34:SA:929:A:H4'	34:SA:930:A:OP2	1.98	0.62
5:3F:138:ASP:OD1	5:3F:500:LYS:NZ	2.31	0.62
15:B1:159:GLN:NE2	34:SA:518:A:OP2	2.32	0.62
16:BA:817:PHE:O	16:BA:821:MET:HB2	1.99	0.62
20:BE:266:VAL:HB	20:BE:274:ILE:HB	1.81	0.62
24:E3:301:TYR:CZ	34:SA:1217:A:C6	2.88	0.62
1:3A:5:A:H2	34:SA:1119:G:N1	1.92	0.62
1:3A:12:U:H3	34:SA:1112:G:H1	1.46	0.62
20:BE:596:GLU:HG3	20:BE:598:ARG:NH1	2.14	0.62
22:CB:525:LEU:HB2	22:CB:617:LEU:HB2	1.80	0.62
22:CB:530:GLN:HB2	22:CB:695:GLN:HB2	1.81	0.62
34:SA:51:A:H62	34:SA:429:G:H21	1.47	0.62
40:SJ:172:ARG:HE	40:SJ:175:GLN:HG3	1.65	0.62
8:AA:523:UNK:HA	8:AA:537:UNK:O	2.00	0.62
12:AE:365:ILE:O	12:AE:369:LEU:HB3	1.99	0.62
18:BC:318:GLU:HB3	18:BC:327:ILE:HG22	1.82	0.62
40:SJ:5:ARG:NH2	40:SJ:27:PHE:O	2.33	0.62
12:AE:571:LEU:C	12:AE:630:TYR:CE2	2.73	0.62
20:BE:861:ILE:HD11	20:BE:905:ILE:HD12	1.82	0.62
21:CA:16:VAL:HB	21:CA:37:MET:O	1.99	0.62
40:SJ:103:GLN:HB3	40:SJ:164:ARG:NH1	2.15	0.62
34:SA:411:C:H1'	34:SA:423:G:H22	1.65	0.61
46:SR:73:GLY:H	46:SR:76:SER:HB3	1.63	0.61
48:SY:107:PHE:HB3	48:SY:114:LYS:HD3	1.81	0.61
17:BB:426:ARG:HG2	17:BB:462:SER:HA	1.82	0.61
22:CB:1070:VAL:O	22:CB:1074:LEU:HB2	2.00	0.61
35:SC:199:ASN:HA	35:SC:202:LYS:HE3	1.81	0.61
36:SF:88:ASP:HB2	36:SF:101:LEU:HD12	1.82	0.61
42:SM:7:VAL:HG11	42:SM:53:TYR:HA	1.82	0.61
47:SX:118:ARG:NH1	47:SX:119:LYS:NZ	2.47	0.61
34:SA:1219:A:N6	34:SA:1264:G:C2	2.68	0.61
34:SA:273:G:N7	38:SH:185:GLN:NE2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:53:U:H3	7:5A:465:G:H1	1.49	0.61
18:BC:108:LEU:HD13	18:BC:150:LEU:HD22	1.82	0.61
20:BE:900:ASN:OD1	20:BE:903:GLN:NE2	2.34	0.61
32:R2:1416:GLN:HE21	32:R2:1559:ILE:HD12	1.66	0.61
5:3F:234:GLY:O	5:3F:259:LYS:NZ	2.31	0.61
26:K1:92:ALA:HB2	45:SP:102:LEU:HD12	1.81	0.61
36:SF:17:HIS:HA	36:SF:108:ARG:HG2	1.81	0.61
40:SJ:70:GLU:OE1	42:SM:24:LYS:NZ	2.33	0.61
4:3E:76:LEU:HD23	4:3E:84:LYS:NZ	2.15	0.61
30:P1:188:LYS:HA	30:P1:191:LYS:HZ3	1.65	0.61
38:SH:79:LYS:HE2	38:SH:90:GLY:H	1.64	0.61
2:3C:162:LEU:HG	2:3C:164:ILE:H	1.65	0.61
15:B1:112:LYS:HG3	15:B1:113:ILE:HG23	1.82	0.61
17:BB:251:GLN:HE21	17:BB:344:THR:HG23	1.66	0.61
17:BB:888:ARG:O	17:BB:892:LYS:HB2	2.00	0.61
24:E3:301:TYR:O	24:E3:304:TYR:CB	2.49	0.61
31:R1:143:LYS:HZ1	31:R1:252:LYS:HB3	1.66	0.61
1:3A:5:A:N1	34:SA:1119:G:C6	2.68	0.61
15:B1:988:ARG:HH22	28:MB:146:ARG:HE	1.49	0.61
17:BB:218:ILE:HA	17:BB:227:LYS:O	2.01	0.61
20:BE:229:GLU:HA	20:BE:244:ILE:O	2.00	0.61
22:CB:679:SER:O	22:CB:683:ASN:HB2	2.01	0.61
23:E1:46:ALA:HA	23:E1:115:GLN:HB3	1.82	0.61
34:SA:102:U:O2'	34:SA:105:A:N6	2.34	0.61
42:SM:21:ASN:ND2	42:SM:30:ARG:O	2.34	0.61
5:3F:311:GLN:HB3	49:SZ:4:ALA:HB1	1.83	0.60
16:BA:82:VAL:HG12	16:BA:88:ASN:H	1.65	0.60
19:BD:462:GLY:HA2	19:BD:480:ARG:H	1.64	0.60
20:BE:569:VAL:HB	20:BE:579:ARG:HB2	1.84	0.60
26:K1:49:ARG:NH2	26:K1:108:VAL:O	2.34	0.60
40:SJ:74:LYS:HD3	40:SJ:108:PRO:HB2	1.83	0.60
5:3F:424:LEU:HB3	5:3F:434:PHE:HB3	1.82	0.60
20:BE:308:PRO:HB2	20:BE:324:PHE:HB2	1.82	0.60
23:E1:94:GLN:OE1	23:E2:132:ARG:NH1	2.34	0.60
3:3D:34:VAL:HG23	3:3D:36:GLU:H	1.67	0.60
34:SA:51:A:H62	34:SA:429:G:N2	1.98	0.60
38:SH:70:PRO:HB3	38:SH:101:ILE:HB	1.83	0.60
5:3F:497:LYS:HG2	5:3F:513:GLU:HG2	1.84	0.60
13:AF:28:UNK:O	13:AF:35:UNK:HA	2.01	0.60
18:BC:45:LEU:HD12	18:BC:54:HIS:HB3	1.82	0.60
21:CA:204:SER:O	21:CA:208:ASP:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:900:A:H3'	34:SA:901:G:H21	1.65	0.60
16:BA:541:ILE:HG22	16:BA:550:VAL:HG22	1.84	0.60
47:SX:31:SER:H	47:SX:34:ILE:HD12	1.67	0.60
16:BA:533:SER:HB3	16:BA:580:PHE:HB2	1.83	0.60
17:BB:799:LYS:HD2	17:BB:800:THR:HG23	1.83	0.60
18:BC:83:GLN:NE2	18:BC:103:SER:O	2.35	0.60
20:BE:230:VAL:O	20:BE:243:THR:HA	2.02	0.60
28:MB:162:THR:HB	28:MB:262:ARG:HB3	1.83	0.60
34:SA:364:G:H3'	34:SA:365:G:H8	1.67	0.60
34:SA:1216:C:HO2'	34:SA:1217:A:P	2.23	0.60
17:BB:135:ARG:NH1	17:BB:149:ASP:OD1	2.35	0.60
20:BE:587:ARG:HB3	20:BE:605:LEU:HD13	1.83	0.60
38:SH:188:ARG:HH11	38:SH:191:ARG:CB	2.15	0.60
1:3A:64:A:H4'	20:BE:392:ARG:HH12	1.66	0.60
5:3F:304:ILE:HB	5:3F:318:LEU:HB2	1.83	0.60
8:AA:282:UNK:O	8:AA:290:UNK:N	2.35	0.60
13:AF:67:UNK:O	13:AF:78:UNK:HA	2.01	0.60
16:BA:169:SER:HB2	16:BA:186:THR:HB	1.84	0.60
17:BB:397:ILE:HG22	17:BB:408:THR:HG22	1.84	0.60
22:CB:812:GLU:O	22:CB:816:ALA:HB2	2.01	0.60
5:3F:187:ALA:HB3	5:3F:199:TYR:HB2	1.84	0.60
22:CB:268:LEU:HD23	22:CB:294:LEU:HD12	1.84	0.60
34:SA:477:A:N6	34:SA:540:G:O6	2.34	0.60
15:B1:609:GLU:OE2	31:R1:17:PHE:N	2.35	0.59
17:BB:828:TYR:O	17:BB:832:PHE:HB2	2.02	0.59
20:BE:641:LEU:O	20:BE:653:ILE:HA	2.02	0.59
43:SN:43:ARG:HH12	43:SN:102:GLY:HA3	1.66	0.59
4:3E:87:LEU:HB3	4:3E:107:VAL:HG22	1.83	0.59
3:3D:297:HIS:NE2	3:3D:309:GLU:OE2	2.33	0.59
15:B1:830:ARG:NH2	48:SY:138:GLU:OE2	2.35	0.59
20:BE:434:HIS:CD2	20:BE:441:ARG:HH11	2.21	0.59
23:E1:144:LEU:HD13	23:E1:150:ILE:HG12	1.85	0.59
34:SA:1160:A:H1'	34:SA:1620:C:H42	1.66	0.59
34:SA:1216:C:O2	34:SA:1446:A:N6	2.35	0.59
12:AE:469:LEU:O	12:AE:473:SER:HB3	2.03	0.59
15:B1:932:LEU:H	15:B1:1006:TRP:HD1	1.49	0.59
16:BA:431:ILE:HG23	16:BA:432:GLN:HG3	1.85	0.59
16:BA:719:VAL:HB	16:BA:744:ARG:HH22	1.68	0.59
23:E1:44:VAL:HG22	23:E1:113:TYR:HB2	1.84	0.59
7:5A:209:G:N2	7:5A:209:G:OP2	2.33	0.59
34:SA:593:U:H4'	34:SA:595:G:H4'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:SI:150:GLN:HB3	39:SI:181:ILE:HG22	1.84	0.59
47:SX:17:ALA:HA	47:SX:22:LYS:NZ	2.18	0.59
17:BB:867:GLU:O	17:BB:871:GLN:NE2	2.35	0.59
6:3G:34:LYS:HB2	6:3G:101:SER:HB3	1.84	0.59
22:CB:254:LEU:HG	22:CB:270:ILE:HG12	1.84	0.59
22:CB:313:ASN:HD22	22:CB:326:LEU:HB3	1.67	0.59
24:E3:305:ARG:CG	24:E3:306:ALA:N	2.66	0.59
34:SA:484:C:H42	34:SA:504:U:H3	1.48	0.59
3:3D:176:GLN:HG3	4:3E:187:TRP:HB3	1.85	0.59
6:3G:25:GLN:OE1	6:3G:29:ASN:ND2	2.36	0.59
7:5A:163:G:H1	7:5A:232:U:H3	1.50	0.59
13:AF:240:UNK:O	13:AF:252:UNK:HA	2.02	0.59
16:BA:846:TYR:HB3	20:BE:913:GLU:HG2	1.85	0.59
17:BB:359:SER:O	17:BB:391:ARG:NH2	2.36	0.59
19:BD:272:LEU:HD22	19:BD:288:LEU:HD23	1.85	0.59
34:SA:204:G:O6	34:SA:264:G:N2	2.36	0.59
14:AG:526:UNK:O	14:AG:538:UNK:HA	2.02	0.58
16:BA:554:ASP:O	16:BA:556:ARG:NH1	2.36	0.58
24:E3:279:ILE:HG12	24:E3:283:LEU:HD12	1.84	0.58
36:SF:126:VAL:HA	36:SF:141:THR:HA	1.85	0.58
38:SH:188:ARG:NH1	38:SH:191:ARG:CB	2.65	0.58
2:3B:142:ARG:NH2	2:3B:186:ASP:OD2	2.36	0.58
3:3D:36:GLU:OE1	3:3D:37:GLN:NE2	2.36	0.58
23:E2:178:VAL:HA	23:E2:223:GLU:O	2.03	0.58
20:BE:644:THR:HG22	20:BE:651:ILE:HG12	1.85	0.58
21:CA:52:CYS:HA	21:CA:126:LEU:O	2.04	0.58
25:E4:258:UNK:HA	40:SJ:42:ARG:NH1	2.18	0.58
31:R1:143:LYS:NZ	31:R1:252:LYS:HB3	2.17	0.58
16:BA:477:SER:HB2	16:BA:519:LEU:HD12	1.85	0.58
20:BE:78:SER:OG	20:BE:95:GLU:OE2	2.11	0.58
28:MB:124:MET:HG2	28:MB:126:ASN:H	1.67	0.58
28:MB:193:ASN:HB3	28:MB:226:ASN:HB2	1.84	0.58
39:SI:67:LEU:O	39:SI:71:HIS:ND1	2.37	0.58
16:BA:430:ARG:HH12	16:BA:451:ASP:HB2	1.67	0.58
16:BA:540:SER:HA	16:BA:550:VAL:O	2.03	0.58
34:SA:1163:A:N3	34:SA:1613:U:O2'	2.35	0.58
40:SJ:61:GLU:HG3	40:SJ:62:THR:HG23	1.85	0.58
5:3F:442:ILE:HA	5:3F:472:PRO:HA	1.85	0.58
12:AE:349:THR:O	12:AE:353:ARG:HB2	2.04	0.58
13:AF:69:UNK:O	13:AF:76:UNK:HA	2.03	0.58
15:B1:253:TYR:HA	15:B1:787:SER:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BA:306:ASN:H	16:BA:321:SER:HA	1.69	0.58
17:BB:565:PHE:O	31:R1:207:ARG:NH2	2.37	0.58
19:BD:272:LEU:HB2	19:BD:288:LEU:HB3	1.85	0.58
38:SH:187:LYS:NZ	38:SH:191:ARG:NH1	2.52	0.58
12:AE:365:ILE:O	12:AE:369:LEU:CB	2.52	0.58
16:BA:247:SER:O	16:BA:249:ARG:NH1	2.37	0.58
18:BC:412:ALA:HB3	18:BC:430:TYR:HB2	1.85	0.58
23:E1:85:SER:OG	23:E1:211:ARG:NH2	2.37	0.58
26:K1:44:LEU:HD22	35:SC:115:ARG:HH11	1.69	0.58
26:K1:146:VAL:HA	26:K1:153:LEU:HB2	1.84	0.58
54:U1:96:UNK:HA	54:U1:112:UNK:HA	1.85	0.58
16:BA:542:PHE:HB3	16:BA:548:LYS:HA	1.86	0.58
19:BD:568:VAL:HA	19:BD:578:ALA:O	2.03	0.58
22:CB:487:ILE:HD12	22:CB:582:GLN:HE21	1.68	0.58
37:SG:51:VAL:HG21	37:SG:131:GLN:HB2	1.85	0.58
48:SY:76:LEU:HD13	48:SY:79:ASN:HD22	1.67	0.58
6:3G:27:ALA:HB1	6:3G:32:GLN:HB3	1.86	0.58
12:AE:333:LEU:O	12:AE:337:ASP:HB2	2.04	0.58
17:BB:454:LEU:O	17:BB:468:ILE:HB	2.03	0.58
31:R1:156:ARG:NH2	31:R1:228:ASP:OD2	2.37	0.58
54:U1:202:UNK:HA	54:U1:208:UNK:HA	1.86	0.58
8:AA:485:UNK:O	8:AA:493:UNK:N	2.37	0.58
12:AE:480:ASN:ND2	12:AE:520:GLU:O	2.36	0.58
15:B1:117:VAL:HB	15:B1:146:VAL:HG12	1.86	0.58
15:B1:119:LEU:HB3	15:B1:147:LEU:O	2.03	0.58
24:E3:231:LYS:NZ	34:SA:1235:C:OP1	2.37	0.58
34:SA:897:C:O2'	34:SA:914:G:N2	2.37	0.58
2:3B:261:LEU:O	3:3D:129:ARG:NH2	2.37	0.57
2:3C:261:LEU:O	4:3E:118:ARG:NH2	2.37	0.57
5:3F:286:LEU:HB3	5:3F:295:LEU:HD11	1.84	0.57
12:AE:371:LYS:O	12:AE:374:ARG:NH2	2.36	0.57
16:BA:507:GLN:HB2	46:SR:127:LYS:HD3	1.85	0.57
17:BB:341:ALA:HA	17:BB:357:THR:HA	1.86	0.57
17:BB:439:LEU:HD23	17:BB:443:LEU:HB2	1.86	0.57
18:BC:759:THR:O	18:BC:762:CYS:HB3	2.03	0.57
21:CA:183:ASP:O	21:CA:187:HIS:HB2	2.04	0.57
26:K1:42:MET:SD	35:SC:112:SER:OG	2.61	0.57
34:SA:1253:U:H3'	43:SN:46:ARG:HH22	1.69	0.57
4:3E:289:GLN:O	4:3E:391:ARG:NH2	2.37	0.57
5:3F:537:PHE:O	5:3F:567:VAL:HA	2.04	0.57
6:3G:21:LEU:O	6:3G:25:GLN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AA:444:UNK:O	8:AA:452:UNK:N	2.37	0.57
17:BB:866:LYS:NZ	18:BC:806:LEU:O	2.36	0.57
18:BC:666:GLU:HG2	18:BC:688:LEU:HD11	1.85	0.57
20:BE:546:ILE:HD13	20:BE:560:LEU:HD13	1.85	0.57
22:CB:532:PRO:HG2	22:CB:693:LYS:HE2	1.85	0.57
23:E2:46:ALA:HA	23:E2:115:GLN:HB3	1.86	0.57
28:MB:181:ASN:HA	34:SA:1623:C:H4'	1.86	0.57
34:SA:1118:G:H2'	34:SA:1119:G:H8	1.69	0.57
57:U4:69:THR:HG22	57:U4:73:ASN:HD21	1.70	0.57
7:5A:466:A:H2'	7:5A:467:A:H8	1.69	0.57
8:AA:433:UNK:O	8:AA:444:UNK:HA	2.05	0.57
20:BE:616:THR:HG23	20:BE:618:GLY:H	1.69	0.57
54:U1:36:UNK:HA	54:U1:47:UNK:HA	1.85	0.57
19:BD:320:TYR:HB3	19:BD:343:SER:HB2	1.87	0.57
3:3D:157:ALA:O	3:3D:161:ALA:HB3	2.04	0.57
12:AE:630:TYR:CZ	12:AE:637:ILE:HG21	2.38	0.57
15:B1:283:LEU:HB3	15:B1:788:TYR:HD2	1.68	0.57
16:BA:126:ASP:OD1	16:BA:128:ASN:ND2	2.38	0.57
16:BA:505:ARG:HD3	34:SA:1616:G:H5'	1.86	0.57
37:SG:84:LYS:O	37:SG:92:ARG:NH1	2.38	0.57
4:3E:228:PRO:HD2	4:3E:231:ILE:HD12	1.86	0.57
16:BA:153:THR:HG21	16:BA:198:PHE:HA	1.85	0.57
17:BB:554:THR:HG22	17:BB:570:TYR:HB2	1.87	0.57
23:E1:114:ILE:HB	23:E1:122:ILE:HB	1.87	0.57
37:SG:73:THR:OG1	46:SR:114:ARG:NH2	2.37	0.57
39:SI:154:LEU:HD21	39:SI:185:ILE:HG13	1.86	0.57
34:SA:297:U:H5"	36:SF:37:LYS:HG2	1.85	0.57
34:SA:1213:G:N2	34:SA:1450:U:O2	2.35	0.57
5:3F:496:LEU:O	5:3F:513:GLU:HA	2.05	0.57
6:3H:25:GLN:OE1	6:3H:29:ASN:ND2	2.37	0.57
14:AG:7:UNK:HA	14:AG:568:UNK:HA	1.87	0.57
17:BB:230:LYS:HD3	17:BB:237:LYS:HB3	1.87	0.57
19:BD:429:TYR:OH	20:BE:563:ASP:OD1	2.22	0.57
23:E2:42:ILE:O	23:E2:203:CYS:HA	2.05	0.57
25:E4:233:UNK:O	25:E4:240:UNK:HA	2.04	0.57
42:SM:128:CYS:SG	42:SM:129:ARG:N	2.76	0.57
1:3A:3:C:H2'	1:3A:4:G:H8	1.69	0.57
20:BE:172:HIS:NE2	20:BE:176:TYR:O	2.36	0.57
21:CA:88:LEU:HB2	21:CA:125:LEU:HB2	1.87	0.57
22:CB:527:TYR:HB2	22:CB:615:VAL:HB	1.87	0.57
34:SA:1486:G:OP2	34:SA:1486:G:N2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:SG:68:ILE:HG22	46:SR:114:ARG:NH1	2.18	0.57
5:3F:305:ARG:HG2	5:3F:317:ILE:HG12	1.87	0.57
16:BA:585:TYR:HA	16:BA:592:ILE:HG22	1.87	0.56
18:BC:713:GLU:HB3	18:BC:762:CYS:HB2	1.86	0.56
21:CA:185:HIS:O	21:CA:189:ALA:HB2	2.05	0.56
24:E3:344:LYS:NZ	34:SA:1266:U:O2	2.37	0.56
17:BB:499:PHE:HB2	17:BB:518:PRO:HG2	1.87	0.56
3:3D:218:LYS:NZ	3:3D:240:LEU:HD22	2.19	0.56
5:3F:201:ILE:O	5:3F:538:ARG:NH1	2.38	0.56
5:3F:551:ARG:NH1	6:3G:94:SER:HA	2.21	0.56
12:AE:370:LEU:HD23	12:AE:400:LEU:HD13	1.88	0.56
15:B1:634:ARG:NH1	31:R1:185:ARG:HG2	2.20	0.56
16:BA:430:ARG:HE	16:BA:432:GLN:H	1.53	0.56
16:BA:553:ILE:HD13	46:SR:99:GLU:HG2	1.86	0.56
19:BD:541:LEU:O	19:BD:542:ARG:NH1	2.36	0.56
20:BE:92:ALA:O	20:BE:98:VAL:HA	2.04	0.56
22:CB:344:ASN:HD21	22:CB:445:ASN:HD21	1.51	0.56
23:E2:96:LEU:HD21	23:E2:114:ILE:HD11	1.86	0.56
34:SA:1080:U:O4	34:SA:1081:A:N6	2.38	0.56
34:SA:1583:A:H61	34:SA:1611:A:H5"	1.70	0.56
34:SA:1585:U:H3	34:SA:1611:A:H2	1.53	0.56
12:AE:25:ARG:O	12:AE:29:HIS:HB2	2.05	0.56
17:BB:171:CYS:SG	17:BB:172:GLN:N	2.79	0.56
18:BC:548:LEU:O	18:BC:559:ILE:HA	2.04	0.56
20:BE:311:VAL:HG22	20:BE:321:GLU:HG2	1.86	0.56
23:E1:104:ILE:N	23:E1:246:GLU:OE2	2.39	0.56
34:SA:349:U:OP2	42:SM:106:ASN:ND2	2.39	0.56
37:SG:54:LYS:HZ2	37:SG:131:GLN:HE22	1.54	0.56
38:SH:4:ASN:HB3	38:SH:110:ALA:HA	1.88	0.56
40:SJ:9:HIS:O	40:SJ:18:ARG:NH2	2.39	0.56
42:SM:67:ARG:NH1	42:SM:127:GLN:OE1	2.38	0.56
47:SX:75:ILE:HG12	47:SX:127:GLY:HA2	1.86	0.56
5:3F:304:ILE:O	5:3F:317:ILE:HA	2.05	0.56
12:AE:653:PHE:O	12:AE:657:GLN:HB2	2.06	0.56
16:BA:847:ARG:HH22	18:BC:761:ARG:HH11	1.54	0.56
20:BE:601:VAL:HA	20:BE:610:ARG:O	2.06	0.56
28:MB:261:LEU:H	34:SA:571:G:H21	1.54	0.56
7:5A:556:G:H2'	7:5A:557:A:H8	1.70	0.56
16:BA:799:ILE:O	16:BA:803:LEU:HB3	2.05	0.56
16:BA:799:ILE:O	16:BA:803:LEU:CB	2.54	0.56
20:BE:190:LEU:HB3	20:BE:200:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AE:33:LEU:HD22	12:AE:150:ARG:HB3	1.86	0.56
24:E3:311:LEU:HD22	24:E3:345:VAL:HB	1.87	0.56
5:3F:289:ARG:NH1	5:3F:334:GLU:HB2	2.21	0.56
16:BA:541:ILE:HG23	16:BA:549:GLN:HB2	1.88	0.56
18:BC:465:LYS:H	18:BC:481:LYS:HD2	1.70	0.56
2:3B:227:PRO:HB2	2:3B:259:MET:HG2	1.87	0.56
19:BD:292:GLY:O	19:BD:318:ARG:NH1	2.39	0.56
23:E2:176:ARG:NH2	23:E2:192:TYR:OH	2.39	0.56
34:SA:337:G:H1'	34:SA:339:C:OP2	2.05	0.56
15:B1:268:HIS:ND1	15:B1:274:ASP:OD1	2.37	0.55
17:BB:616:ASP:HB3	17:BB:635:LYS:HB3	1.88	0.55
20:BE:128:LEU:HB3	20:BE:140:TYR:HB2	1.87	0.55
35:SC:69:CYS:HA	35:SC:83:LYS:HA	1.88	0.55
58:U5:39:ILE:HB	58:U5:243:PHE:HB2	1.88	0.55
1:3A:82:G:N2	1:3A:327:G:O2'	2.35	0.55
4:3E:95:ALA:O	4:3E:99:ASN:HB2	2.06	0.55
4:3E:191:HIS:ND1	4:3E:245:THR:O	2.38	0.55
12:AE:671:LEU:O	12:AE:675:ASN:ND2	2.39	0.55
22:CB:970:TRP:O	22:CB:1028:ARG:NH2	2.39	0.55
34:SA:132:U:O4	56:U3:1015:UNK:N	2.39	0.55
34:SA:283:U:C2	38:SH:188:ARG:CG	2.89	0.55
17:BB:899:GLY:O	17:BB:903:GLN:NE2	2.40	0.55
19:BD:576:LEU:HA	19:BD:589:TRP:O	2.06	0.55
21:CA:53:LEU:HB2	21:CA:126:LEU:HB3	1.89	0.55
26:K1:146:VAL:HG22	26:K1:150:GLY:HA2	1.87	0.55
34:SA:446:A:N1	34:SA:461:G:O2'	2.35	0.55
34:SA:1085:G:N1	34:SA:1089:U:O4	2.40	0.55
46:SR:48:VAL:HG23	46:SR:82:ARG:HB3	1.88	0.55
46:SR:52:LEU:O	46:SR:59:LYS:NZ	2.38	0.55
12:AE:333:LEU:O	12:AE:337:ASP:CB	2.54	0.55
18:BC:216:ARG:NH1	35:SC:25:THR:O	2.39	0.55
19:BD:520:ASN:HD22	19:BD:533:ALA:HB3	1.72	0.55
23:E1:89:PRO:HG2	23:E1:134:PHE:HZ	1.71	0.55
31:R1:311:LEU:HB3	31:R1:352:ALA:HB3	1.87	0.55
36:SF:59:ARG:HG3	36:SF:62:LYS:NZ	2.22	0.55
6:3H:34:LYS:O	6:3H:100:ALA:HA	2.07	0.55
12:AE:141:ASN:ND2	12:AE:209:GLN:OE1	2.40	0.55
16:BA:17:GLN:NE2	16:BA:306:ASN:OD1	2.40	0.55
17:BB:509:VAL:HG13	17:BB:515:LYS:HE2	1.88	0.55
5:3F:440:HIS:HD1	5:3F:493:SER:HG	1.55	0.55
17:BB:16:VAL:HG13	17:BB:18:ALA:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CB:494:GLU:OE1	22:CB:497:ARG:NH2	2.38	0.55
25:E4:55:UNK:HA	25:E4:71:UNK:HA	1.88	0.55
36:SF:59:ARG:HA	36:SF:62:LYS:NZ	2.21	0.55
16:BA:603:LEU:HB3	16:BA:611:LEU:HB2	1.88	0.55
34:SA:1498:G:H4'	58:U5:250:THR:HA	1.89	0.55
16:BA:117:ARG:NH2	16:BA:145:HIS:O	2.40	0.55
17:BB:640:LYS:HG2	17:BB:652:LYS:HG3	1.89	0.55
18:BC:270:ILE:HG22	18:BC:277:VAL:HG12	1.86	0.55
19:BD:524:SER:HB3	19:BD:529:ILE:HB	1.89	0.55
34:SA:483:A:N6	34:SA:504:U:O4	2.40	0.55
48:SY:97:ASP:HB2	48:SY:100:ASP:OD2	2.06	0.55
49:SZ:32:ARG:NH1	49:SZ:35:VAL:HG23	2.22	0.55
57:U4:115:ILE:HA	57:U4:118:LYS:HE2	1.87	0.55
3:3D:323:THR:HG22	3:3D:327:LYS:NZ	2.22	0.55
8:AA:79:UNK:N	8:AA:83:UNK:O	2.40	0.55
12:AE:661:ILE:HG12	12:AE:663:SER:H	1.71	0.55
22:CB:1100:VAL:HB	22:CB:1182:ILE:HB	1.88	0.55
26:K1:198:TYR:O	26:K1:202:GLU:CB	2.54	0.55
31:R1:66:GLU:HB2	31:R1:75:ILE:HB	1.89	0.55
39:SI:137:GLY:H	39:SI:153:LEU:HB2	1.71	0.55
46:SR:25:GLY:HA3	46:SR:64:ASP:OD2	2.07	0.55
16:BA:10:LEU:HA	16:BA:702:LEU:H	1.70	0.54
17:BB:391:ARG:HG3	17:BB:392:THR:HG23	1.89	0.54
34:SA:151:G:N3	38:SH:13:GLN:NE2	2.55	0.54
36:SF:176:ASP:HB3	36:SF:179:LYS:NZ	2.23	0.54
23:E2:31:LEU:HD13	23:E2:40:ARG:HE	1.72	0.54
46:SR:10:PHE:HB2	46:SR:12:LYS:NZ	2.23	0.54
47:SX:118:ARG:HH12	47:SX:119:LYS:NZ	2.05	0.54
1:3A:86:A:N3	4:3E:336:THR:OG1	2.38	0.54
2:3C:198:GLU:HG3	2:3C:200:SER:H	1.73	0.54
24:E3:378:LYS:HD2	34:SA:1220:C:H4'	1.89	0.54
34:SA:442:C:O2'	34:SA:526:A:N6	2.41	0.54
15:B1:149:VAL:HG22	15:B1:184:PHE:HB2	1.90	0.54
20:BE:272:ASP:HA	20:BE:287:LEU:O	2.06	0.54
21:CA:18:PHE:HB2	21:CA:35:HIS:HB3	1.90	0.54
23:E1:31:LEU:HD22	23:E1:40:ARG:HE	1.72	0.54
31:R1:11:PHE:HB3	31:R1:20:ARG:NH1	2.22	0.54
34:SA:1610:G:H5"	37:SG:107:LYS:HE3	1.88	0.54
44:SO:20:ARG:HH21	47:SX:56:HIS:HB3	1.71	0.54
2:3C:319:ARG:HD2	2:3C:322:ARG:HD3	1.90	0.54
12:AE:802:PHE:O	12:AE:806:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B1:857:LEU:HD13	15:B1:1012:LYS:HD3	1.88	0.54
18:BC:310:THR:HB	18:BC:363:ARG:HH12	1.70	0.54
33:S1:209:UNK:HA	33:S1:219:UNK:HA	1.88	0.54
34:SA:955:A:H5"	44:SO:10:GLY:HA3	1.88	0.54
54:U1:109:UNK:HA	54:U1:119:UNK:HA	1.89	0.54
12:AE:367:LEU:HA	12:AE:400:LEU:HD11	1.88	0.54
18:BC:467:ILE:H	18:BC:480:ILE:HG21	1.71	0.54
28:MB:192:ASP:HB2	28:MB:225:ALA:HA	1.89	0.54
34:SA:1685:G:N2	34:SA:1716:C:N3	2.56	0.54
36:SF:104:ASP:N	36:SF:108:ARG:O	2.40	0.54
19:BD:237:ARG:NH1	19:BD:238:LEU:O	2.40	0.54
19:BD:576:LEU:HB3	19:BD:588:LEU:HD12	1.90	0.54
20:BE:131:SER:HB3	20:BE:170:LEU:HD11	1.89	0.54
23:E1:150:ILE:O	23:E1:158:LYS:HA	2.08	0.54
27:MA:138:VAL:HG22	27:MA:158:VAL:HG22	1.88	0.54
40:SJ:72:ILE:HD12	40:SJ:74:LYS:NZ	2.22	0.54
13:AF:195:UNK:O	60:UB:394:UNK:N	2.41	0.54
14:AG:346:UNK:HA	14:AG:353:UNK:HA	1.89	0.54
23:E1:179:THR:HB	23:E1:224:LYS:HG2	1.88	0.54
34:SA:1218:G:OP1	34:SA:1444:A:N6	2.40	0.54
35:SC:87:ARG:HH11	35:SC:99:ASN:HD22	1.53	0.54
38:SH:188:ARG:CZ	38:SH:191:ARG:CD	2.70	0.54
58:U5:128:ASP:HB3	58:U5:131:VAL:HG22	1.88	0.54
15:B1:931:LYS:HD3	15:B1:1004:ARG:HB3	1.90	0.54
16:BA:792:ILE:O	16:BA:796:LEU:HB2	2.08	0.54
19:BD:237:ARG:NH2	19:BD:240:ASP:OD1	2.41	0.54
24:E3:413:LEU:HG	24:E3:447:ARG:HH21	1.73	0.54
34:SA:273:G:O6	34:SA:283:U:O2	2.24	0.54
38:SH:187:LYS:NZ	38:SH:191:ARG:HH12	2.05	0.54
58:U5:71:ASN:HB2	58:U5:122:PHE:HA	1.90	0.54
14:AG:487:UNK:O	14:AG:495:UNK:N	2.41	0.54
17:BB:538:ARG:NH1	17:BB:539:VAL:O	2.40	0.54
23:E1:111:GLN:NE2	23:E1:113:TYR:OH	2.41	0.54
25:E4:160:UNK:O	25:E4:168:UNK:N	2.41	0.54
25:E4:272:UNK:O	25:E4:283:UNK:HA	2.08	0.54
33:S1:221:UNK:N	33:S1:225:UNK:O	2.40	0.54
54:U1:150:UNK:HA	54:U1:160:UNK:HA	1.89	0.54
2:3C:252:ILE:O	2:3C:256:ASN:ND2	2.40	0.53
14:AG:97:UNK:HA	14:AG:113:UNK:HA	1.90	0.53
17:BB:530:LEU:HB3	17:BB:551:LEU:HB3	1.90	0.53
20:BE:62:ASP:OD2	20:BE:65:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:1163:A:H4'	37:SG:166:ARG:NH1	2.23	0.53
42:SM:3:THR:OG1	42:SM:4:GLU:N	2.41	0.53
1:3A:83:A:H61	1:3A:327:G:H1'	1.73	0.53
8:AA:394:UNK:O	8:AA:401:UNK:HA	2.08	0.53
17:BB:536:CYS:H	17:BB:549:SER:HB2	1.73	0.53
20:BE:60:ILE:HB	20:BE:70:PHE:HB2	1.89	0.53
22:CB:162:PHE:HB2	22:CB:597:ARG:HD2	1.89	0.53
24:E3:301:TYR:OH	34:SA:1217:A:C2	2.55	0.53
27:MA:70:PHE:O	27:MA:74:HIS:ND1	2.40	0.53
28:MB:167:LEU:HA	28:MB:256:MET:HG2	1.90	0.53
34:SA:485:A:H1'	34:SA:503:G:H22	1.73	0.53
34:SA:1175:U:O4	34:SA:1464:G:O6	2.25	0.53
40:SJ:101:ILE:HD12	40:SJ:184:LEU:HD21	1.89	0.53
44:SO:119:GLU:O	44:SO:123:HIS:ND1	2.38	0.53
4:3E:68:VAL:HG13	4:3E:72:LEU:HD22	1.90	0.53
5:3F:190:VAL:HA	5:3F:195:GLN:O	2.08	0.53
6:3G:53:ILE:HB	6:3G:100:ALA:HB3	1.89	0.53
9:AB:259:UNK:O	9:AB:277:UNK:N	2.41	0.53
12:AE:630:TYR:OH	12:AE:637:ILE:CD1	2.35	0.53
19:BD:530:LEU:HB3	19:BD:544:VAL:HB	1.90	0.53
21:CA:103:LEU:O	22:CB:869:ASN:ND2	2.38	0.53
23:E2:104:ILE:N	23:E2:246:GLU:OE2	2.41	0.53
49:SZ:29:HIS:ND1	49:SZ:32:ARG:O	2.37	0.53
54:U1:197:UNK:O	54:U1:215:UNK:N	2.41	0.53
2:3B:171:LEU:HB3	2:3B:240:VAL:HG23	1.91	0.53
7:5A:403:C:OP2	7:5A:404:G:O2'	2.17	0.53
15:B1:822:PHE:HA	15:B1:888:PRO:HA	1.91	0.53
18:BC:510:SER:OG	18:BC:512:ASP:OD1	2.25	0.53
33:S1:208:UNK:N	33:S1:220:UNK:O	2.42	0.53
33:S1:290:UNK:N	33:S1:302:UNK:O	2.41	0.53
44:SO:111:ALA:HA	44:SO:114:ARG:HB2	1.90	0.53
46:SR:50:GLU:OE1	46:SR:82:ARG:NH2	2.41	0.53
1:3A:7:G:O6	34:SA:1117:U:O4	2.27	0.53
3:3D:223:ILE:HG22	3:3D:225:ASP:H	1.74	0.53
16:BA:328:LEU:HG	16:BA:343:GLY:HA2	1.90	0.53
18:BC:533:LYS:HB2	18:BC:554:ASP:HB3	1.90	0.53
18:BC:576:ASN:HD22	18:BC:596:ASP:HA	1.74	0.53
20:BE:418:ALA:HB3	20:BE:431:ILE:HB	1.89	0.53
22:CB:751:LYS:N	22:CB:785:GLU:O	2.41	0.53
12:AE:478:THR:HA	12:AE:490:ARG:HD2	1.90	0.53
12:AE:566:CYS:O	12:AE:570:ALA:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B1:943:LYS:HD2	34:SA:573:C:OP2	2.09	0.53
16:BA:131:ARG:HG3	20:BE:27:PHE:HA	1.91	0.53
22:CB:797:THR:HG23	22:CB:836:GLU:HG3	1.90	0.53
23:E1:103:PRO:HG3	23:E2:232:LEU:HD21	1.90	0.53
24:E3:378:LYS:O	34:SA:1220:C:O2'	2.25	0.53
34:SA:38:C:O2'	34:SA:470:A:N6	2.42	0.53
35:SC:144:ARG:NH2	35:SC:207:LEU:O	2.39	0.53
40:SJ:79:ALA:HB3	40:SJ:164:ARG:HH11	1.73	0.53
12:AE:78:SER:HB2	12:AE:125:PHE:HZ	1.73	0.53
12:AE:354:SER:O	12:AE:357:ARG:NH2	2.42	0.53
17:BB:38:PRO:HD2	17:BB:41:LEU:HB2	1.91	0.53
20:BE:526:VAL:O	20:BE:539:LYS:HA	2.09	0.53
33:S1:220:UNK:HA	33:S1:226:UNK:HA	1.90	0.53
35:SC:223:PHE:HD2	35:SC:225:VAL:HG23	1.74	0.53
36:SF:54:TYR:HB3	49:SZ:17:LEU:HD11	1.91	0.53
1:3A:18:G:H2'	1:3A:19:A:C8	2.44	0.53
5:3F:287:ALA:HB3	5:3F:296:TYR:HB2	1.91	0.53
7:5A:174:U:O4	7:5A:222:G:O6	2.26	0.53
7:5A:534:A:H8	7:5A:534:A:OP2	1.92	0.53
17:BB:165:SER:HB2	17:BB:182:LYS:HD2	1.91	0.53
17:BB:478:SER:O	17:BB:491:GLY:N	2.41	0.53
17:BB:553:ASN:HB3	17:BB:572:HIS:HB2	1.91	0.53
17:BB:559:PHE:HE1	17:BB:564:LYS:HB2	1.74	0.53
18:BC:16:TYR:HB3	18:BC:641:PHE:H	1.74	0.53
20:BE:459:ASP:O	20:BE:481:ASN:ND2	2.42	0.53
22:CB:578:ILE:HA	22:CB:620:ASN:H	1.74	0.53
31:R1:202:PRO:HG3	31:R1:229:VAL:HG11	1.91	0.53
33:S1:342:UNK:O	33:S1:350:UNK:N	2.42	0.53
34:SA:298:C:H5"	36:SF:38:LEU:HB2	1.90	0.53
34:SA:478:A:O2'	41:SK:124:HIS:ND1	2.42	0.53
34:SA:1663:G:O6	34:SA:1738:U:O4	2.27	0.53
40:SJ:8:ARG:NE	40:SJ:19:ALA:O	2.40	0.53
47:SX:18:GLU:HG3	47:SX:69:LEU:HD12	1.91	0.53
54:U1:61:UNK:N	54:U1:66:UNK:O	2.41	0.53
18:BC:174:VAL:HB	18:BC:184:HIS:HB2	1.90	0.53
34:SA:299:A:OP2	36:SF:38:LEU:HG	2.09	0.53
34:SA:1042:G:H22	34:SA:1076:A:H2	1.57	0.53
34:SA:1647:U:H2'	34:SA:1648:A:H8	1.74	0.53
1:3A:66:U:H2'	1:3A:67:G:H8	1.73	0.53
5:3F:297:ALA:HB3	5:3F:305:ARG:O	2.09	0.53
7:5A:545:G:OP1	7:5A:547:C:N4	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BA:36:ARG:HG2	16:BA:52:TYR:HB2	1.91	0.53
17:BB:898:LEU:HD11	18:BC:789:THR:HB	1.91	0.53
20:BE:275:PHE:O	20:BE:284:ILE:N	2.42	0.53
21:CA:46:ASN:HB3	21:CA:49:GLU:HB2	1.91	0.53
22:CB:174:TYR:HB3	22:CB:223:ARG:NH1	2.24	0.53
25:E4:190:UNK:O	25:E4:201:UNK:HA	2.09	0.53
34:SA:1216:C:H4'	34:SA:1217:A:OP1	2.09	0.53
36:SF:112:HIS:NE2	36:SF:237:SER:OG	2.38	0.53
34:SA:865:A:OP1	47:SX:28:ARG:NH1	2.43	0.52
34:SA:1611:A:O2'	37:SG:95:ASN:O	2.26	0.52
49:SZ:92:VAL:HG13	49:SZ:99:LYS:HD2	1.90	0.52
24:E3:418:HIS:O	24:E3:422:LEU:CB	2.57	0.52
34:SA:1217:A:H2'	34:SA:1217:A:N3	2.24	0.52
54:U1:19:UNK:HA	54:U1:26:UNK:HA	1.90	0.52
2:3B:271:ILE:HB	2:3B:314:CYS:O	2.08	0.52
12:AE:105:ALA:O	12:AE:109:TRP:NE1	2.42	0.52
17:BB:185:MET:HA	17:BB:201:ILE:HG22	1.90	0.52
17:BB:426:ARG:HD2	17:BB:457:PHE:HB3	1.91	0.52
18:BC:257:ILE:HG12	18:BC:299:ASN:HD22	1.74	0.52
24:E3:208:GLU:O	24:E3:209:LYS:HE2	2.09	0.52
33:S1:180:UNK:N	33:S1:184:UNK:O	2.43	0.52
34:SA:354:C:H5'	40:SJ:14:THR:HG21	1.92	0.52
41:SK:53:ARG:NH2	41:SK:97:LEU:O	2.41	0.52
2:3B:88:ILE:HD13	2:3B:107:VAL:HG21	1.90	0.52
23:E1:112:VAL:O	23:E1:124:VAL:HB	2.08	0.52
1:3A:66:U:H3	7:5A:287:G:H1	1.57	0.52
8:AA:382:UNK:N	8:AA:395:UNK:O	2.42	0.52
9:AB:4:UNK:HA	9:AB:283:UNK:O	2.09	0.52
18:BC:346:VAL:HB	18:BC:352:LYS:HB3	1.92	0.52
23:E2:178:VAL:HG12	23:E2:223:GLU:HB3	1.91	0.52
28:MB:143:HIS:HB2	34:SA:1604:U:H5"	1.91	0.52
31:R1:176:GLN:HG3	31:R1:305:LYS:HB3	1.92	0.52
34:SA:404:G:O2'	38:SH:88:ARG:NH1	2.42	0.52
38:SH:2:LYS:HB3	38:SH:108:VAL:HG22	1.92	0.52
39:SI:62:VAL:HG12	39:SI:64:VAL:H	1.74	0.52
42:SM:97:TYR:HB3	42:SM:99:ARG:HH11	1.74	0.52
48:SY:107:PHE:HE1	48:SY:123:LYS:HB3	1.74	0.52
7:5A:242:C:H2'	7:5A:243:A:H8	1.74	0.52
12:AE:316:PRO:HA	12:AE:319:ILE:HG22	1.91	0.52
16:BA:60:ALA:HB3	16:BA:73:ILE:HB	1.91	0.52
16:BA:206:ILE:O	16:BA:217:VAL:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BC:691:PRO:HG3	18:BC:742:ARG:HE	1.74	0.52
34:SA:25:C:N4	34:SA:470:A:OP1	2.43	0.52
42:SM:33:ARG:HH11	42:SM:61:THR:HG21	1.75	0.52
2:3B:122:ARG:HG2	2:3B:142:ARG:HG2	1.91	0.52
7:5A:178:G:O6	7:5A:219:U:O2	2.26	0.52
16:BA:92:HIS:HD2	16:BA:135:PRO:HD2	1.74	0.52
19:BD:575:GLY:O	19:BD:591:LEU:N	2.43	0.52
23:E2:211:ARG:HH12	34:SA:1190:C:H3'	1.75	0.52
34:SA:283:U:C4	38:SH:188:ARG:CB	2.73	0.52
34:SA:361:C:H3'	34:SA:378:A:OP2	2.09	0.52
39:SI:161:GLN:HG2	39:SI:162:ILE:HG13	1.92	0.52
57:U4:66:LEU:N	57:U4:152:ILE:O	2.42	0.52
22:CB:904:HIS:O	22:CB:907:GLN:NE2	2.42	0.52
37:SG:80:LYS:HB2	37:SG:83:ARG:NH1	2.24	0.52
4:3E:125:PRO:HB3	4:3E:132:SER:HA	1.91	0.52
4:3E:249:GLN:HA	4:3E:252:LEU:HD12	1.92	0.52
17:BB:456:LEU:HB3	17:BB:466:ASP:O	2.10	0.52
20:BE:471:CYS:SG	20:BE:473:ASN:ND2	2.83	0.52
20:BE:641:LEU:HB3	20:BE:654:TRP:HB2	1.91	0.52
23:E1:188:ARG:HD3	23:E1:191:ASP:OD2	2.10	0.52
26:K1:61:THR:HA	26:K1:64:LEU:HB3	1.92	0.52
32:R2:1509:GLU:HB3	32:R2:1512:GLU:HB3	1.91	0.52
34:SA:297:U:OP1	36:SF:37:LYS:NZ	2.42	0.52
38:SH:4:ASN:HA	38:SH:15:THR:HG22	1.92	0.52
12:AE:478:THR:HG22	12:AE:490:ARG:HB3	1.91	0.52
18:BC:211:LEU:O	18:BC:223:TRP:HB2	2.10	0.52
19:BD:302:THR:HG21	19:BD:364:GLN:HB3	1.92	0.52
21:CA:169:VAL:HG23	21:CA:173:LYS:NZ	2.25	0.52
22:CB:748:LEU:HD21	22:CB:791:LYS:HD2	1.92	0.52
26:K1:61:THR:O	26:K1:65:ASP:HB3	2.10	0.52
26:K1:159:LEU:HD13	26:K1:203:LEU:HB2	1.92	0.52
35:SC:141:ALA:HA	35:SC:210:ILE:HG12	1.91	0.52
37:SG:76:ARG:HH11	46:SR:120:ASP:CG	2.13	0.52
43:SN:42:ALA:HB3	43:SN:122:VAL:HB	1.92	0.52
6:3G:24:VAL:HG22	6:3G:102:ILE:HD11	1.93	0.51
6:3H:106:ASP:O	6:3H:111:LYS:NZ	2.33	0.51
18:BC:122:THR:HG23	18:BC:124:GLY:H	1.75	0.51
19:BD:406:ASP:OD1	20:BE:371:LYS:NZ	2.43	0.51
33:S1:118:UNK:O	33:S1:127:UNK:N	2.43	0.51
35:SC:107:THR:HB	35:SC:111:ARG:NH1	2.24	0.51
42:SM:127:GLN:NE2	42:SM:128:CYS:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:188:VAL:HG22	2:3B:192:GLY:HA3	1.91	0.51
5:3F:254:GLY:HA3	5:3F:260:LEU:HD23	1.93	0.51
9:AB:59:UNK:N	9:AB:68:UNK:O	2.43	0.51
17:BB:624:LEU:HB2	17:BB:629:ASN:H	1.75	0.51
20:BE:412:PRO:HD2	20:BE:441:ARG:HH12	1.75	0.51
22:CB:127:PHE:HD1	22:CB:283:TYR:HB3	1.75	0.51
22:CB:165:PRO:HD2	22:CB:222:PHE:HE2	1.75	0.51
36:SF:59:ARG:HG3	36:SF:62:LYS:HZ3	1.74	0.51
39:SI:67:LEU:HG	39:SI:71:HIS:HE1	1.75	0.51
14:AG:36:UNK:O	14:AG:48:UNK:HA	2.10	0.51
16:BA:161:ILE:HB	16:BA:173:TRP:O	2.10	0.51
21:CA:134:ILE:O	21:CA:138:TRP:CB	2.57	0.51
26:K1:130:ASN:ND2	34:SA:930:A:OP1	2.42	0.51
28:MB:233:VAL:HB	28:MB:254:PHE:HB2	1.93	0.51
34:SA:1157:A:N6	34:SA:1618:C:O2	2.42	0.51
37:SG:38:THR:HG21	46:SR:57:LEU:HB3	1.91	0.51
40:SJ:11:ARG:HH12	40:SJ:17:LYS:HB2	1.75	0.51
44:SO:18:TYR:O	47:SX:56:HIS:NE2	2.43	0.51
5:3F:365:PRO:O	5:3F:368:LEU:HB2	2.10	0.51
7:5A:21:A:H2'	7:5A:22:A:H8	1.74	0.51
13:AF:4:UNK:HA	13:AF:284:UNK:HA	1.93	0.51
20:BE:611:THR:HB	20:BE:621:ASP:HB3	1.93	0.51
22:CB:99:LYS:O	22:CB:103:PHE:CB	2.57	0.51
34:SA:485:A:H3'	34:SA:486:G:H21	1.76	0.51
34:SA:1175:U:O2	34:SA:1464:G:N2	2.42	0.51
39:SI:46:ILE:HD11	39:SI:58:LEU:HB3	1.91	0.51
5:3F:358:THR:O	5:3F:430:LYS:NZ	2.34	0.51
16:BA:142:HIS:NE2	16:BA:174:SER:O	2.40	0.51
17:BB:188:LEU:HD12	17:BB:198:GLU:HB3	1.93	0.51
31:R1:199:ARG:NH2	31:R1:236:GLY:O	2.38	0.51
33:S1:320:UNK:N	33:S1:334:UNK:O	2.44	0.51
34:SA:265:A:OP2	38:SH:194:LYS:NZ	2.29	0.51
34:SA:931:C:H5"	35:SC:116:LYS:HG2	1.93	0.51
35:SC:87:ARG:HH11	35:SC:99:ASN:ND2	2.08	0.51
3:3D:62:ALA:O	3:3D:66:ALA:HB2	2.10	0.51
18:BC:599:ILE:O	18:BC:613:LEU:HB2	2.10	0.51
19:BD:581:ASN:OD1	19:BD:585:LYS:N	2.43	0.51
20:BE:33:VAL:N	20:BE:317:ASN:OD1	2.41	0.51
22:CB:1222:GLU:O	22:CB:1226:PHE:HB2	2.11	0.51
33:S1:178:UNK:O	33:S1:186:UNK:N	2.43	0.51
7:5A:357:G:O6	7:5A:368:U:O2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AG:528:UNK:O	14:AG:536:UNK:N	2.44	0.51
16:BA:163:THR:O	16:BA:170:ALA:HA	2.11	0.51
16:BA:165:SER:OG	16:BA:166:LYS:N	2.43	0.51
17:BB:225:GLN:HG2	17:BB:243:THR:HA	1.93	0.51
22:CB:186:ILE:HG22	22:CB:346:LEU:HD22	1.93	0.51
22:CB:842:ILE:O	22:CB:849:GLY:HA2	2.10	0.51
23:E2:174:LYS:HE2	23:E2:200:GLU:HB2	1.92	0.51
31:R1:96:VAL:HG22	31:R1:122:THR:HA	1.92	0.51
31:R1:201:SER:HB3	31:R1:204:LEU:HD13	1.93	0.51
34:SA:512:A:OP2	41:SK:172:VAL:HG13	2.10	0.51
34:SA:1217:A:N3	34:SA:1217:A:C2'	2.73	0.51
35:SC:134:VAL:HB	35:SC:219:LYS:HB3	1.92	0.51
45:SP:85:ALA:H	45:SP:119:THR:HG22	1.75	0.51
46:SR:39:VAL:HG22	46:SR:41:PRO:HD2	1.92	0.51
3:3D:180:LEU:HD13	4:3E:183:ARG:HG2	1.93	0.51
10:AC:603:UNK:O	10:AC:607:UNK:CB	2.59	0.51
12:AE:43:GLN:HE21	12:AE:47:PHE:HB2	1.75	0.51
12:AE:288:ALA:HB3	12:AE:326:LYS:HB3	1.93	0.51
14:AG:117:UNK:HA	14:AG:131:UNK:O	2.11	0.51
16:BA:39:VAL:HB	16:BA:48:PHE:HB2	1.92	0.51
16:BA:78:ARG:HB2	16:BA:93:PHE:HA	1.91	0.51
18:BC:47:PRO:HD2	18:BC:51:LYS:H	1.76	0.51
19:BD:383:TRP:HZ3	19:BD:397:GLY:HA3	1.75	0.51
36:SF:85:GLY:N	36:SF:88:ASP:OD2	2.40	0.51
37:SG:156:ARG:HH12	37:SG:158:GLN:HB2	1.76	0.51
41:SK:83:VAL:O	41:SK:107:ARG:NE	2.39	0.51
3:3D:107:PRO:O	3:3D:111:GLU:HB2	2.11	0.51
3:3D:323:THR:HG22	3:3D:327:LYS:HZ2	1.74	0.51
5:3F:345:THR:HA	5:3F:359:PHE:O	2.10	0.51
6:3G:33:LEU:HA	6:3G:101:SER:O	2.11	0.51
8:AA:5:UNK:N	8:AA:565:UNK:O	2.44	0.51
8:AA:161:UNK:N	8:AA:165:UNK:O	2.44	0.51
12:AE:303:PHE:HB3	12:AE:346:LYS:HB3	1.92	0.51
12:AE:695:TYR:OH	12:AE:699:ARG:NH2	2.44	0.51
16:BA:752:ASN:O	16:BA:756:GLU:HB2	2.10	0.51
22:CB:215:GLU:N	22:CB:218:ASP:OD2	2.43	0.51
22:CB:738:TYR:O	22:CB:742:PHE:CB	2.59	0.51
23:E2:112:VAL:O	23:E2:124:VAL:HB	2.10	0.51
33:S1:301:UNK:O	33:S1:309:UNK:N	2.44	0.51
47:SX:118:ARG:NH1	47:SX:119:LYS:HZ1	2.09	0.51
57:U4:64:GLN:HA	57:U4:95:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3F:200:ASP:HB3	5:3F:209:LYS:HB2	1.93	0.51
16:BA:37:VAL:HB	16:BA:51:GLU:HB2	1.92	0.51
17:BB:629:ASN:ND2	17:BB:642:TRP:O	2.44	0.51
17:BB:674:SER:H	17:BB:681:ILE:HG23	1.76	0.51
34:SA:913:G:H5"	34:SA:914:G:H5'	1.92	0.51
36:SF:212:ASP:OD1	36:SF:216:ASN:N	2.43	0.51
45:SP:17:ALA:HA	45:SP:30:VAL:HA	1.92	0.51
6:3H:34:LYS:HB2	6:3H:101:SER:HB3	1.92	0.50
12:AE:572:ARG:N	12:AE:630:TYR:CE2	2.79	0.50
13:AF:221:UNK:O	13:AF:234:UNK:N	2.44	0.50
14:AG:111:UNK:CB	14:AG:119:UNK:O	2.59	0.50
19:BD:352:GLN:HG3	19:BD:371:VAL:HG13	1.92	0.50
22:CB:649:TRP:HB2	22:CB:653:SER:HB2	1.93	0.50
34:SA:548:G:H2'	34:SA:549:G:H8	1.76	0.50
34:SA:863:A:N7	34:SA:964:U:O4	2.44	0.50
54:U1:117:UNK:N	54:U1:130:UNK:O	2.44	0.50
12:AE:750:ASN:O	12:AE:754:GLU:CB	2.59	0.50
17:BB:180:THR:HG22	17:BB:186:ILE:HG23	1.92	0.50
22:CB:235:LEU:O	22:CB:239:LEU:CB	2.60	0.50
28:MB:215:LYS:HZ2	34:SA:1625:C:H5'	1.76	0.50
35:SC:190:PRO:HG2	35:SC:192:VAL:HG23	1.93	0.50
48:SY:54:LEU:HD12	48:SY:82:LYS:HD3	1.93	0.50
8:AA:506:UNK:HA	8:AA:516:UNK:O	2.11	0.50
12:AE:333:LEU:HD11	12:AE:369:LEU:HD12	1.92	0.50
12:AE:630:TYR:CD1	12:AE:637:ILE:HD12	2.31	0.50
16:BA:28:GLN:HA	16:BA:41:ASP:HA	1.92	0.50
16:BA:87:ARG:HH11	16:BA:89:VAL:HG22	1.75	0.50
20:BE:135:ASN:HB3	20:BE:159:VAL:HB	1.93	0.50
22:CB:334:PHE:O	22:CB:338:SER:CB	2.59	0.50
36:SF:48:LEU:HD11	36:SF:61:VAL:HG22	1.94	0.50
47:SX:103:ILE:HA	47:SX:112:ASP:HA	1.93	0.50
48:SY:76:LEU:HD12	48:SY:81:LYS:HB2	1.93	0.50
8:AA:425:UNK:O	8:AA:434:UNK:N	2.44	0.50
9:AB:203:UNK:N	9:AB:207:UNK:O	2.45	0.50
15:B1:840:LYS:HG2	15:B1:874:TYR:HB3	1.94	0.50
15:B1:978:ARG:HB3	15:B1:988:ARG:HE	1.77	0.50
15:B1:988:ARG:NH1	28:MB:146:ARG:HH11	2.06	0.50
19:BD:448:LYS:HE2	20:BE:563:ASP:HB3	1.93	0.50
19:BD:522:GLN:HB2	19:BD:531:CYS:HB3	1.92	0.50
22:CB:861:ILE:O	22:CB:865:ARG:CB	2.59	0.50
24:E3:352:SER:O	24:E3:356:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:1083:G:H1	34:SA:1090:C:H42	1.58	0.50
40:SJ:43:ILE:HA	40:SJ:57:ALA:HA	1.93	0.50
2:3B:173:LEU:HB2	2:3B:242:ALA:HA	1.94	0.50
12:AE:384:ILE:HG23	12:AE:401:VAL:HG22	1.93	0.50
16:BA:168:LEU:O	16:BA:188:ASN:ND2	2.44	0.50
17:BB:125:THR:HG21	17:BB:165:SER:HB3	1.92	0.50
20:BE:438:LYS:NZ	20:BE:460:ASP:OD1	2.45	0.50
20:BE:485:THR:HG22	20:BE:497:LYS:HG3	1.92	0.50
30:P1:186:GLU:HG2	30:P1:188:LYS:H	1.76	0.50
46:SR:58:ASP:OD1	46:SR:58:ASP:N	2.41	0.50
12:AE:769:LEU:O	12:AE:773:GLN:NE2	2.45	0.50
15:B1:931:LYS:HB3	15:B1:1004:ARG:HE	1.76	0.50
21:CA:192:GLU:O	21:CA:196:ALA:CB	2.59	0.50
22:CB:93:GLU:O	22:CB:97:LEU:HB2	2.12	0.50
22:CB:309:LEU:O	22:CB:333:ASN:ND2	2.44	0.50
22:CB:333:ASN:O	22:CB:337:LEU:HB3	2.12	0.50
22:CB:367:ARG:O	22:CB:371:GLN:CB	2.58	0.50
24:E3:267:VAL:HG11	24:E3:310:SER:HB2	1.93	0.50
28:MB:86:PRO:O	28:MB:113:ASN:ND2	2.42	0.50
31:R1:11:PHE:HB2	31:R1:33:ILE:HG12	1.93	0.50
34:SA:327:U:OP1	42:SM:82:ARG:NH1	2.44	0.50
34:SA:1648:A:H2'	34:SA:1649:G:H8	1.76	0.50
38:SH:114:VAL:HG12	38:SH:115:LYS:HD3	1.93	0.50
42:SM:94:ILE:HG22	42:SM:97:TYR:H	1.76	0.50
58:U5:10:SER:OG	58:U5:217:GLN:NE2	2.41	0.50
12:AE:218:ILE:HG23	12:AE:263:VAL:HG11	1.92	0.50
16:BA:149:ILE:HD13	16:BA:165:SER:HB2	1.93	0.50
16:BA:751:ILE:O	16:BA:755:TYR:HB3	2.11	0.50
18:BC:80:SER:HB3	18:BC:84:LEU:HB2	1.94	0.50
19:BD:418:LYS:HB2	19:BD:422:ILE:HD11	1.93	0.50
26:K1:44:LEU:HD22	35:SC:115:ARG:NH1	2.25	0.50
34:SA:284:G:OP1	38:SH:196:ARG:NH1	2.19	0.50
34:SA:1661:U:H3	34:SA:1740:A:H61	1.59	0.50
35:SC:191:GLU:HB2	35:SC:194:ASN:HD22	1.77	0.50
47:SX:81:VAL:O	47:SX:122:SER:OG	2.30	0.50
54:U1:18:UNK:O	54:U1:27:UNK:N	2.44	0.50
56:U3:1931:UNK:HA	56:U3:1947:UNK:HA	1.93	0.50
9:AB:74:UNK:HA	9:AB:95:UNK:HA	1.94	0.50
19:BD:286:THR:HG21	19:BD:335:GLN:HE22	1.76	0.50
19:BD:357:ASN:O	19:BD:369:ASN:ND2	2.45	0.50
34:SA:1739:C:H2'	34:SA:1740:A:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SC:143:THR:HB	35:SC:205:PHE:HE2	1.77	0.50
7:5A:554:G:H1	7:5A:583:U:H3	1.59	0.50
12:AE:141:ASN:ND2	12:AE:206:TYR:OH	2.44	0.50
13:AF:201:UNK:CB	13:AF:210:UNK:O	2.60	0.50
15:B1:941:ILE:HG21	15:B1:995:ILE:H	1.76	0.50
17:BB:624:LEU:HB3	17:BB:628:HIS:H	1.77	0.50
18:BC:805:ILE:HD12	20:BE:932:VAL:HG23	1.94	0.50
20:BE:349:HIS:HD1	20:BE:374:SER:HG	1.46	0.50
25:E4:96:UNK:HA	25:E4:111:UNK:O	2.11	0.50
26:K1:152:THR:O	26:K1:155:ALA:HB3	2.11	0.50
31:R1:30:PRO:HB3	31:R1:77:ARG:HG2	1.94	0.50
34:SA:1216:C:O2'	34:SA:1217:A:H2'	2.12	0.50
34:SA:1615:C:N4	37:SG:78:ALA:O	2.44	0.50
41:SK:20:GLU:HB3	41:SK:23:ARG:HE	1.77	0.50
48:SY:109:ARG:NH1	48:SY:114:LYS:O	2.44	0.50
5:3F:515:SER:O	5:3F:518:LYS:NZ	2.29	0.49
8:AA:463:UNK:CB	8:AA:477:UNK:O	2.60	0.49
14:AG:405:UNK:O	14:AG:413:UNK:N	2.44	0.49
14:AG:843:UNK:O	14:AG:847:UNK:N	2.45	0.49
17:BB:622:LYS:O	17:BB:630:PHE:HA	2.12	0.49
20:BE:40:ALA:HB3	20:BE:51:VAL:HB	1.94	0.49
33:S1:239:UNK:O	33:S1:252:UNK:N	2.45	0.49
38:SH:33:GLY:HA2	38:SH:51:LYS:NZ	2.27	0.49
42:SM:77:SER:HB3	42:SM:85:VAL:HB	1.93	0.49
4:3E:358:LYS:HG2	4:3E:361:ARG:HH12	1.77	0.49
12:AE:469:LEU:O	12:AE:473:SER:CB	2.60	0.49
16:BA:171:LYS:HG2	16:BA:186:THR:HG22	1.93	0.49
16:BA:356:ASP:OD2	16:BA:830:ARG:NH2	2.45	0.49
16:BA:825:GLN:HE22	20:BE:937:THR:HG1	1.56	0.49
17:BB:229:TRP:HZ3	17:BB:236:ASP:HB2	1.77	0.49
18:BC:226:ASN:HB3	18:BC:229:LYS:HB2	1.95	0.49
18:BC:344:ARG:NH1	18:BC:345:TYR:O	2.45	0.49
22:CB:777:ASP:O	22:CB:780:GLN:NE2	2.45	0.49
27:MA:108:ARG:HA	27:MA:113:VAL:HG11	1.94	0.49
36:SF:62:LYS:HA	36:SF:65:LEU:HB2	1.94	0.49
41:SK:121:SER:HB3	41:SK:124:HIS:HB3	1.95	0.49
1:3A:63:C:H2'	1:3A:64:A:H8	1.76	0.49
2:3B:124:SER:HA	2:3B:139:VAL:O	2.11	0.49
2:3B:299:LYS:O	2:3B:318:GLY:HA2	2.12	0.49
3:3D:21:LYS:NZ	3:3D:138:LEU:O	2.45	0.49
8:AA:37:UNK:HA	8:AA:43:UNK:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B1:634:ARG:NH1	31:R1:186:PRO:O	2.46	0.49
20:BE:35:ASN:ND2	20:BE:53:CYS:SG	2.80	0.49
34:SA:190:C:N4	34:SA:196:G:O6	2.45	0.49
34:SA:886:U:H2'	34:SA:887:A:H8	1.76	0.49
47:SX:15:ASN:HD21	47:SX:72:CYS:H	1.60	0.49
12:AE:8:LEU:O	12:AE:12:ALA:HB3	2.12	0.49
19:BD:411:TYR:CZ	19:BD:423:LEU:O	2.66	0.49
22:CB:841:ASN:HA	22:CB:850:PHE:O	2.13	0.49
34:SA:283:U:C2	38:SH:188:ARG:HB2	2.47	0.49
37:SG:72:HIS:ND1	46:SR:79:TYR:OH	2.43	0.49
2:3C:204:GLY:HA2	2:3C:207:LEU:HD12	1.94	0.49
7:5A:447:G:H2'	7:5A:448:G:C8	2.47	0.49
12:AE:1689:UNK:O	12:AE:1693:UNK:CB	2.60	0.49
16:BA:603:LEU:HB2	16:BA:612:LEU:H	1.76	0.49
16:BA:817:PHE:O	16:BA:821:MET:CB	2.59	0.49
23:E1:178:VAL:HG12	23:E1:223:GLU:HB3	1.93	0.49
28:MB:187:PRO:HB3	28:MB:220:ARG:HG3	1.95	0.49
34:SA:128:U:OP1	34:SA:264:G:O2'	2.28	0.49
34:SA:445:A:H61	34:SA:462:G:H1'	1.77	0.49
2:3B:88:ILE:HG12	2:3B:99:ALA:HA	1.93	0.49
2:3B:205:ARG:NH2	3:3D:163:VAL:O	2.45	0.49
5:3F:260:LEU:HD21	5:3F:283:VAL:HG11	1.94	0.49
5:3F:342:ARG:HH22	6:3G:90:ALA:HA	1.77	0.49
5:3F:348:LEU:O	5:3F:356:ARG:HA	2.12	0.49
12:AE:980:UNK:O	12:AE:984:UNK:CB	2.61	0.49
31:R1:119:LYS:HG2	31:R1:165:GLU:HG2	1.94	0.49
33:S1:371:UNK:HA	33:S1:385:UNK:HA	1.93	0.49
36:SF:182:TYR:HB2	36:SF:228:ILE:HD11	1.95	0.49
38:SH:12:SER:OG	38:SH:127:THR:O	2.31	0.49
38:SH:187:LYS:HZ1	38:SH:191:ARG:NH1	2.08	0.49
3:3D:146:ASP:HB2	4:3E:241:VAL:HG11	1.93	0.49
7:5A:62:C:H2'	7:5A:63:G:H8	1.77	0.49
9:AB:80:UNK:N	9:AB:84:UNK:O	2.45	0.49
10:AC:599:UNK:O	10:AC:603:UNK:CB	2.61	0.49
17:BB:574:LEU:HD23	17:BB:594:ASP:HB3	1.95	0.49
22:CB:577:ARG:NH1	22:CB:624:CYS:O	2.45	0.49
22:CB:1189:LEU:HD13	32:R2:1472:PRO:HD2	1.93	0.49
28:MB:267:GLU:HG2	61:UC:9:UNK:HA	1.95	0.49
30:P1:105:ARG:HH21	30:P1:163:THR:HA	1.77	0.49
31:R1:150:ALA:HB3	31:R1:169:VAL:HB	1.95	0.49
33:S1:301:UNK:N	33:S1:310:UNK:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SC:129:THR:HA	35:SC:177:GLN:HA	1.94	0.49
42:SM:108:PRO:HB2	42:SM:135:VAL:HG22	1.93	0.49
54:U1:203:UNK:N	54:U1:207:UNK:O	2.46	0.49
3:3D:198:TRP:NE1	3:3D:268:MET:SD	2.78	0.49
3:3D:231:ASP:HA	3:3D:237:LEU:HB2	1.95	0.49
4:3E:76:LEU:HD11	4:3E:98:ILE:HG12	1.94	0.49
5:3F:200:ASP:HB2	5:3F:211:LEU:HD11	1.94	0.49
5:3F:303:LYS:HG3	5:3F:319:TYR:HE1	1.78	0.49
7:5A:184:U:H2'	7:5A:185:A:H8	1.76	0.49
10:AC:96:UNK:HA	10:AC:112:UNK:HA	1.95	0.49
12:AE:917:UNK:O	12:AE:921:UNK:CB	2.61	0.49
12:AE:1490:UNK:O	12:AE:1494:UNK:CB	2.61	0.49
16:BA:825:GLN:HE21	20:BE:933:ALA:HB1	1.77	0.49
22:CB:628:VAL:HA	22:CB:667:CYS:O	2.12	0.49
22:CB:814:LEU:HD12	22:CB:818:SER:HB2	1.94	0.49
23:E2:48:ALA:O	23:E2:117:SER:N	2.45	0.49
24:E3:258:VAL:O	24:E3:262:ALA:CB	2.60	0.49
33:S1:208:UNK:O	33:S1:220:UNK:N	2.45	0.49
37:SG:149:VAL:HG13	37:SG:156:ARG:HG3	1.95	0.49
5:3F:526:VAL:HG22	5:3F:539:ILE:HG12	1.94	0.49
12:AE:750:ASN:O	12:AE:754:GLU:HB2	2.12	0.49
14:AG:204:UNK:N	14:AG:208:UNK:O	2.45	0.49
15:B1:831:ARG:HE	15:B1:835:HIS:HB3	1.77	0.49
16:BA:8:SER:HB2	16:BA:703:ILE:HD11	1.94	0.49
22:CB:100:SER:O	22:CB:104:LYS:CB	2.61	0.49
23:E1:91:ILE:HG12	23:E2:132:ARG:NH1	2.28	0.49
34:SA:1213:G:O6	34:SA:1450:U:O4	2.30	0.49
35:SC:89:ASP:OD2	35:SC:99:ASN:HB2	2.13	0.49
4:3E:280:MET:HG2	4:3E:293:GLU:HA	1.94	0.49
15:B1:143:MET:O	48:SY:144:ARG:NH1	2.46	0.49
17:BB:49:VAL:HB	17:BB:63:LEU:HB2	1.94	0.49
18:BC:331:SER:HB2	18:BC:381:VAL:HG23	1.95	0.49
20:BE:613:ASP:HB2	20:BE:620:ILE:HD13	1.95	0.49
21:CA:91:ASP:OD1	21:CA:95:LEU:N	2.45	0.49
33:S1:372:UNK:N	33:S1:384:UNK:O	2.45	0.49
36:SF:100:ARG:NH2	36:SF:121:TYR:O	2.45	0.49
40:SJ:36:THR:HG23	40:SJ:96:LEU:HB2	1.95	0.49
6:3G:33:LEU:HD11	6:3G:100:ALA:HB1	1.94	0.48
12:AE:487:THR:HG21	12:AE:490:ARG:HE	1.78	0.48
19:BD:486:SER:OG	19:BD:487:GLU:N	2.45	0.48
23:E2:144:LEU:HD22	23:E2:160:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:E3:229:LEU:HD21	24:E3:258:VAL:HG22	1.94	0.48
34:SA:340:U:H2'	34:SA:341:A:C8	2.48	0.48
9:AB:429:UNK:O	9:AB:433:UNK:CB	2.61	0.48
12:AE:1511:UNK:O	12:AE:1515:UNK:CB	2.61	0.48
15:B1:236:LEU:O	15:B1:239:THR:OG1	2.32	0.48
15:B1:252:GLY:O	15:B1:788:TYR:HA	2.13	0.48
20:BE:116:ALA:HB1	20:BE:133:ASP:OD1	2.13	0.48
23:E2:178:VAL:HG23	23:E2:204:VAL:HG23	1.95	0.48
34:SA:126:A:H62	34:SA:291:G:H21	0.74	0.48
47:SX:23:ARG:NH1	47:SX:66:ASN:HA	2.17	0.48
2:3C:107:VAL:HG12	2:3C:143:VAL:HA	1.94	0.48
2:3C:238:ASP:OD1	2:3C:262:LYS:NZ	2.40	0.48
4:3E:76:LEU:HD13	4:3E:101:LEU:HD22	1.95	0.48
6:3H:56:ALA:N	6:3H:81:VAL:O	2.39	0.48
15:B1:266:ARG:HB3	15:B1:815:LEU:HD12	1.95	0.48
16:BA:548:LYS:HB2	46:SR:110:THR:HG21	1.93	0.48
16:BA:584:HIS:CG	16:BA:685:GLN:HA	2.48	0.48
18:BC:231:CYS:SG	18:BC:232:LYS:N	2.87	0.48
18:BC:559:ILE:HG22	18:BC:568:MET:HB3	1.95	0.48
20:BE:588:ILE:HG12	20:BE:604:SER:HB2	1.95	0.48
20:BE:632:VAL:HG12	20:BE:643:THR:HG22	1.95	0.48
37:SG:97:LEU:O	37:SG:180:ARG:NH2	2.47	0.48
42:SM:123:VAL:HG23	42:SM:142:VAL:HA	1.95	0.48
47:SX:11:LEU:HD23	47:SX:14:ILE:HD12	1.95	0.48
58:U5:73:LEU:HD13	58:U5:101:ILE:HD12	1.95	0.48
2:3C:220:ILE:HG21	2:3C:233:LEU:HD13	1.94	0.48
7:5A:12:G:N2	7:5A:70:A:OP2	2.42	0.48
12:AE:37:SER:O	12:AE:41:ALA:CB	2.61	0.48
12:AE:748:LEU:O	12:AE:752:ALA:HB2	2.13	0.48
12:AE:1688:UNK:O	12:AE:1692:UNK:CB	2.61	0.48
16:BA:751:ILE:O	16:BA:755:TYR:CB	2.61	0.48
17:BB:851:PRO:O	17:BB:855:LYS:CB	2.61	0.48
18:BC:298:SER:OG	18:BC:299:ASN:N	2.45	0.48
31:R1:107:ALA:HB1	31:R1:170:VAL:HG11	1.94	0.48
34:SA:883:C:H2'	34:SA:884:A:C8	2.49	0.48
49:SZ:10:ARG:O	49:SZ:24:VAL:N	2.44	0.48
54:U1:110:UNK:N	54:U1:118:UNK:O	2.46	0.48
3:3D:92:LYS:HA	3:3D:115:TYR:HB3	1.95	0.48
15:B1:66:ARG:HA	15:B1:69:VAL:HG22	1.96	0.48
15:B1:948:ILE:HG21	15:B1:951:MET:HB2	1.95	0.48
16:BA:538:GLN:HE21	16:BA:551:GLY:HA3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BB:218:ILE:HG22	17:BB:228:ILE:HG22	1.94	0.48
18:BC:127:ILE:HG23	18:BC:140:PHE:HB2	1.94	0.48
19:BD:310:GLN:HA	19:BD:326:LEU:HB2	1.95	0.48
34:SA:283:U:OP2	38:SH:188:ARG:NH1	2.42	0.48
35:SC:214:LYS:NZ	35:SC:216:LYS:HB3	2.29	0.48
40:SJ:26:LYS:NZ	40:SJ:29:LEU:HD13	2.28	0.48
41:SK:78:ARG:HH12	41:SK:91:LYS:HD3	1.78	0.48
43:SN:29:LYS:HE2	43:SN:100:TRP:HE1	1.78	0.48
56:U3:649:UNK:HA	56:U3:666:UNK:HA	1.96	0.48
5:3F:366:GLN:O	5:3F:369:LEU:HB2	2.13	0.48
7:5A:334:G:O6	7:5A:390:C:N4	2.43	0.48
8:AA:239:UNK:CB	8:AA:252:UNK:O	2.61	0.48
15:B1:610:LYS:O	31:R1:321:ARG:NH2	2.40	0.48
16:BA:499:ILE:HG22	16:BA:510:GLU:HA	1.95	0.48
22:CB:855:LEU:HD22	22:CB:889:TYR:HB3	1.95	0.48
22:CB:1099:VAL:HB	22:CB:1235:GLU:HB2	1.96	0.48
32:R2:1475:SER:N	32:R2:1512:GLU:OE2	2.45	0.48
34:SA:1512:G:H2'	34:SA:1513:G:C8	2.49	0.48
4:3E:76:LEU:HA	4:3E:84:LYS:NZ	2.29	0.48
16:BA:784:ASP:OD1	16:BA:826:ARG:NH2	2.46	0.48
22:CB:807:LEU:HD23	22:CB:810:ILE:HD12	1.95	0.48
26:K1:140:LYS:O	26:K1:144:ARG:CB	2.61	0.48
27:MA:47:TYR:HD1	27:MA:50:ILE:HD12	1.79	0.48
31:R1:23:LEU:HB3	31:R1:332:ILE:HG13	1.95	0.48
36:SF:122:LYS:HG2	36:SF:164:LEU:HD21	1.96	0.48
57:U4:117:LEU:HG	57:U4:121:ARG:HE	1.79	0.48
61:UC:923:UNK:O	61:UC:927:UNK:N	2.46	0.48
1:3A:1:G:N1	34:SA:1124:A:C2	2.82	0.48
8:AA:385:UNK:HA	8:AA:392:UNK:HA	1.96	0.48
8:AA:466:UNK:O	8:AA:475:UNK:N	2.47	0.48
12:AE:81:LEU:HD11	12:AE:85:VAL:HG22	1.95	0.48
12:AE:1065:UNK:O	12:AE:1069:UNK:CB	2.62	0.48
14:AG:447:UNK:HA	14:AG:453:UNK:HA	1.95	0.48
18:BC:680:ASN:O	18:BC:684:LEU:CB	2.61	0.48
19:BD:539:ASP:HA	19:BD:562:LEU:HB2	1.95	0.48
34:SA:359:A:OP2	34:SA:360:A:N6	2.47	0.48
37:SG:54:LYS:NZ	37:SG:131:GLN:HE22	2.12	0.48
38:SH:77:LEU:HD13	38:SH:84:TYR:HB2	1.95	0.48
46:SR:5:PRO:HG2	46:SR:24:ALA:HB2	1.96	0.48
2:3C:208:ILE:HD12	4:3E:156:ALA:HA	1.95	0.48
4:3E:397:ARG:HE	4:3E:401:LEU:HG	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3F:402:ILE:HA	5:3F:417:SER:HA	1.96	0.48
16:BA:81:LEU:HB2	16:BA:90:LEU:HB2	1.96	0.48
16:BA:825:GLN:NE2	20:BE:937:THR:OG1	2.37	0.48
20:BE:97:LYS:HD3	20:BE:109:LEU:HD21	1.96	0.48
20:BE:132:THR:OG1	20:BE:136:SER:O	2.32	0.48
20:BE:567:ILE:HB	20:BE:581:LEU:HB2	1.95	0.48
22:CB:551:GLU:O	22:CB:555:PHE:HB2	2.13	0.48
4:3E:363:LEU:O	4:3E:367:ALA:HB2	2.13	0.48
12:AE:817:UNK:O	12:AE:821:UNK:CB	2.62	0.48
15:B1:145:ARG:NE	15:B1:210:LYS:O	2.39	0.48
16:BA:446:CYS:HA	16:BA:456:HIS:O	2.14	0.48
17:BB:603:ASP:HA	31:R1:200:VAL:HG12	1.96	0.48
18:BC:38:ASP:OD2	18:BC:309:GLN:NE2	2.47	0.48
21:CA:183:ASP:O	21:CA:187:HIS:CB	2.62	0.48
22:CB:656:ARG:HH11	22:CB:658:PHE:HD1	1.62	0.48
22:CB:761:ARG:HB3	22:CB:896:THR:HG23	1.95	0.48
22:CB:1100:VAL:O	22:CB:1181:VAL:HA	2.13	0.48
46:SR:110:THR:HA	46:SR:113:ASP:HB2	1.95	0.48
5:3F:134:ARG:HB2	5:3F:484:SER:HA	1.94	0.47
5:3F:152:VAL:HG22	5:3F:562:GLY:HA2	1.96	0.47
5:3F:541:ALA:O	5:3F:563:ILE:HA	2.14	0.47
7:5A:98:G:O6	7:5A:146:G:O6	2.31	0.47
12:AE:608:ASN:HD21	12:AE:662:PRO:HG3	1.79	0.47
15:B1:548:ASN:HD22	15:B1:551:LYS:HE3	1.78	0.47
16:BA:355:PRO:O	16:BA:822:ARG:NH1	2.47	0.47
19:BD:296:GLN:HG3	19:BD:353:ARG:HH12	1.78	0.47
21:CA:94:GLY:HA3	21:CA:121:ARG:HH12	1.79	0.47
34:SA:539:G:OP2	34:SA:539:G:H8	1.97	0.47
35:SC:139:ALA:HA	35:SC:212:VAL:HA	1.97	0.47
1:3A:260:U:O4	3:3D:377:ARG:NH2	2.46	0.47
7:5A:184:U:H2'	7:5A:185:A:C8	2.49	0.47
12:AE:347:PHE:O	12:AE:351:TYR:CB	2.62	0.47
12:AE:600:LEU:HD22	12:AE:611:ILE:HG22	1.96	0.47
14:AG:244:UNK:HA	14:AG:250:UNK:HA	1.96	0.47
15:B1:977:LYS:H	15:B1:989:ALA:HA	1.80	0.47
16:BA:57:ASN:OD1	16:BA:619:ARG:NH2	2.47	0.47
20:BE:583:GLY:C	20:BE:610:ARG:HH12	2.16	0.47
22:CB:545:ALA:HB2	22:CB:565:LYS:HE2	1.96	0.47
22:CB:589:LYS:O	22:CB:609:ASN:ND2	2.47	0.47
23:E2:115:GLN:HE21	23:E2:119:GLY:HA2	1.79	0.47
33:S1:167:UNK:N	33:S1:179:UNK:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:283:U:C6	34:SA:283:U:O4'	2.67	0.47
34:SA:871:G:H2'	34:SA:872:G:C8	2.49	0.47
34:SA:1217:A:H2	34:SA:1448:G:N2	2.10	0.47
34:SA:1474:G:H2'	34:SA:1475:A:H8	1.78	0.47
35:SC:146:GLN:HB2	35:SC:149:GLN:HE21	1.78	0.47
37:SG:76:ARG:O	37:SG:83:ARG:NE	2.40	0.47
39:SI:14:THR:OG1	39:SI:15:GLU:N	2.46	0.47
44:SO:67:THR:HG23	44:SO:69:ASN:H	1.79	0.47
1:3A:80:U:OP2	6:3H:95:ARG:HD2	2.14	0.47
2:3B:233:LEU:O	3:3D:151:GLN:NE2	2.47	0.47
12:AE:261:LEU:O	12:AE:265:ALA:CB	2.62	0.47
12:AE:288:ALA:HB1	12:AE:292:LYS:HG2	1.96	0.47
12:AE:728:GLU:HG3	12:AE:730:GLN:H	1.79	0.47
13:AF:39:UNK:N	13:AF:43:UNK:O	2.47	0.47
17:BB:20:ASN:HD21	17:BB:23:CYS:H	1.61	0.47
18:BC:487:ARG:HH11	18:BC:523:GLY:HA2	1.79	0.47
24:E3:411:ARG:O	24:E3:447:ARG:NH2	2.48	0.47
36:SF:19:LEU:HD21	36:SF:108:ARG:HH21	1.79	0.47
38:SH:63:MET:SD	38:SH:98:ARG:NH2	2.87	0.47
40:SJ:64:ASN:HA	40:SJ:75:LYS:HA	1.96	0.47
5:3F:189:THR:HG21	5:3F:563:ILE:HD11	1.97	0.47
6:3G:77:PRO:HG2	6:3G:118:LYS:HE3	1.96	0.47
12:AE:134:MET:HA	12:AE:137:LEU:HD12	1.97	0.47
12:AE:196:LEU:HD11	12:AE:213:THR:HG21	1.95	0.47
17:BB:261:PHE:O	17:BB:272:PHE:HA	2.15	0.47
20:BE:865:ILE:HA	20:BE:868:LEU:HD12	1.95	0.47
22:CB:173:ASN:ND2	34:SA:1686:C:OP1	2.46	0.47
22:CB:508:SER:HA	22:CB:512:LEU:HB2	1.96	0.47
24:E3:301:TYR:O	24:E3:304:TYR:HB3	2.13	0.47
32:R2:1629:PHE:HB2	32:R2:1661:GLN:HE21	1.79	0.47
34:SA:549:G:H2'	34:SA:550:A:H8	1.78	0.47
34:SA:629:U:H2'	34:SA:630:A:H8	1.80	0.47
34:SA:899:G:H2'	34:SA:900:A:H8	1.79	0.47
40:SJ:44:HIS:O	40:SJ:56:ARG:N	2.47	0.47
41:SK:17:ARG:O	41:SK:23:ARG:NH2	2.47	0.47
48:SY:127:VAL:HG13	48:SY:132:LEU:HD21	1.96	0.47
58:U5:87:LEU:HA	58:U5:88:THR:HA	1.66	0.47
1:3A:246:A:OP2	5:3F:207:ARG:NH2	2.48	0.47
3:3D:176:GLN:O	3:3D:180:LEU:CB	2.62	0.47
3:3D:221:LEU:HD13	3:3D:275:ALA:HB3	1.95	0.47
8:AA:152:UNK:CB	8:AA:156:UNK:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AA:273:UNK:CB	8:AA:281:UNK:O	2.62	0.47
8:AA:302:UNK:O	8:AA:311:UNK:N	2.47	0.47
8:AA:384:UNK:O	8:AA:393:UNK:N	2.47	0.47
12:AE:261:LEU:O	12:AE:265:ALA:HB2	2.14	0.47
12:AE:1148:UNK:O	12:AE:1152:UNK:CB	2.62	0.47
18:BC:304:LEU:HD22	18:BC:311:LEU:HD11	1.97	0.47
18:BC:465:LYS:HE3	18:BC:520:LEU:HD11	1.95	0.47
22:CB:235:LEU:O	22:CB:239:LEU:HB3	2.15	0.47
22:CB:1159:ASN:HD22	22:CB:1201:ASP:HB3	1.79	0.47
25:E4:141:UNK:O	25:E4:150:UNK:N	2.46	0.47
34:SA:418:G:O2'	38:SH:72:ARG:NH1	2.48	0.47
41:SK:57:ARG:NH1	57:U4:88:ASP:O	2.47	0.47
2:3C:240:VAL:HG23	2:3C:261:LEU:HD13	1.95	0.47
5:3F:553:ILE:HD13	5:3F:556:VAL:HG12	1.95	0.47
7:5A:145:A:H2'	7:5A:146:G:C8	2.50	0.47
14:AG:823:UNK:O	14:AG:827:UNK:CB	2.63	0.47
18:BC:15:ILE:N	18:BC:641:PHE:O	2.47	0.47
18:BC:585:ASN:O	18:BC:587:GLN:NE2	2.47	0.47
22:CB:715:SER:O	22:CB:719:THR:OG1	2.30	0.47
23:E1:48:ALA:HB3	23:E1:116:THR:HA	1.97	0.47
24:E3:268:SER:HB2	34:SA:1233:G:H5'	1.97	0.47
30:P1:158:PHE:HE1	30:P1:174:LEU:HB2	1.80	0.47
37:SG:113:ILE:HG23	37:SG:191:ALA:HB2	1.97	0.47
42:SM:33:ARG:NH1	42:SM:61:THR:HG21	2.29	0.47
46:SR:21:HIS:CE1	46:SR:68:ARG:HH12	2.32	0.47
1:3A:1:G:C6	34:SA:1124:A:C2	3.02	0.47
1:3A:47:G:H2'	1:3A:48:A:H8	1.79	0.47
4:3E:76:LEU:HD23	4:3E:84:LYS:HZ1	1.80	0.47
5:3F:316:GLU:OE2	5:3F:351:ILE:HG23	2.15	0.47
6:3G:56:ALA:HB3	6:3G:82:PRO:HA	1.96	0.47
8:AA:507:UNK:O	8:AA:516:UNK:CB	2.62	0.47
9:AB:59:UNK:O	9:AB:68:UNK:N	2.48	0.47
11:AD:461:UNK:O	11:AD:465:UNK:CB	2.62	0.47
12:AE:506:TYR:O	12:AE:510:SER:HB2	2.14	0.47
18:BC:362:LEU:HB2	18:BC:384:TYR:HB2	1.97	0.47
19:BD:454:GLY:N	19:BD:487:GLU:OE1	2.40	0.47
21:CA:13:PHE:HA	21:CA:39:ALA:O	2.15	0.47
22:CB:207:LEU:HD11	22:CB:294:LEU:HD22	1.97	0.47
22:CB:826:SER:O	22:CB:838:VAL:HA	2.14	0.47
22:CB:924:LEU:HD21	22:CB:1181:VAL:HG13	1.95	0.47
25:E4:157:UNK:HA	25:E4:171:UNK:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R2:1502:LEU:HA	32:R2:1513:LYS:HE3	1.96	0.47
32:R2:1505:ILE:HB	32:R2:1513:LYS:HD3	1.96	0.47
34:SA:179:A:H4'	34:SA:180:A:C4	2.49	0.47
34:SA:417:A:OP1	38:SH:59:GLN:NE2	2.48	0.47
34:SA:1226:A:H3'	43:SN:116:VAL:HG11	1.96	0.47
34:SA:1584:G:N2	34:SA:1585:U:O4	2.37	0.47
34:SA:1718:G:H5'	34:SA:1719:A:OP2	2.15	0.47
36:SF:139:VAL:HG13	36:SF:150:PRO:HG3	1.97	0.47
39:SI:137:GLY:HA3	39:SI:153:LEU:HD12	1.96	0.47
39:SI:139:ARG:HB3	47:SX:51:GLU:OE2	2.14	0.47
41:SK:171:ARG:HH21	41:SK:175:ARG:HH22	1.63	0.47
49:SZ:83:LYS:HD2	49:SZ:84:LYS:NZ	2.29	0.47
2:3C:96:VAL:HG11	2:3C:155:ILE:HG21	1.97	0.47
2:3C:231:ARG:NH1	4:3E:7:GLU:O	2.41	0.47
3:3D:199:TYR:HE2	3:3D:206:LEU:HB3	1.80	0.47
4:3E:191:HIS:O	4:3E:215:ARG:NH2	2.48	0.47
5:3F:195:GLN:HE21	5:3F:213:TYR:HB2	1.79	0.47
8:AA:319:UNK:CB	8:AA:332:UNK:O	2.63	0.47
16:BA:155:SER:HB2	16:BA:160:PHE:HB3	1.97	0.47
18:BC:345:TYR:HD2	18:BC:350:LEU:HD12	1.80	0.47
20:BE:275:PHE:HE2	20:BE:287:LEU:HG	1.80	0.47
20:BE:551:TYR:OH	20:BE:556:ASP:OD1	2.30	0.47
22:CB:207:LEU:HB2	22:CB:295:LEU:O	2.14	0.47
34:SA:870:C:H2'	34:SA:871:G:H8	1.79	0.47
1:3A:329:C:H2'	1:3A:330:A:C8	2.50	0.47
2:3B:169:LYS:O	2:3B:238:ASP:N	2.47	0.47
7:5A:226:U:O2'	7:5A:228:A:N7	2.48	0.47
12:AE:8:LEU:O	12:AE:12:ALA:CB	2.63	0.47
16:BA:50:PHE:H	16:BA:86:ALA:HB2	1.80	0.47
16:BA:605:ASP:HB3	16:BA:611:LEU:HD21	1.96	0.47
17:BB:621:VAL:HA	17:BB:631:PHE:O	2.14	0.47
33:S1:118:UNK:N	33:S1:127:UNK:O	2.48	0.47
61:UC:702:UNK:O	61:UC:706:UNK:N	2.48	0.47
12:AE:1439:UNK:O	12:AE:1443:UNK:CB	2.63	0.47
17:BB:125:THR:H	17:BB:140:SER:HA	1.80	0.47
17:BB:545:TYR:HA	17:BB:559:PHE:HA	1.97	0.47
18:BC:455:LEU:HD13	18:BC:465:LYS:HD3	1.96	0.47
20:BE:511:ASP:OD2	20:BE:515:ARG:HB2	2.15	0.47
21:CA:169:VAL:HB	22:CB:1140:SER:HB2	1.95	0.47
24:E3:332:VAL:H	34:SA:1435:G:H5'	1.80	0.47
34:SA:1463:C:H2'	34:SA:1464:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:SG:103:ASN:HA	37:SG:106:LYS:HD2	1.97	0.47
38:SH:188:ARG:HD3	38:SH:188:ARG:HA	1.40	0.47
41:SK:53:ARG:HH12	57:U4:92:ALA:HB2	1.80	0.47
47:SX:72:CYS:HB3	47:SX:129:VAL:HG23	1.96	0.47
54:U1:272:UNK:N	54:U1:284:UNK:O	2.48	0.47
2:3B:110:ASN:HB3	2:3B:140:GLU:HB2	1.98	0.46
6:3H:111:LYS:HA	6:3H:114:ILE:HD12	1.96	0.46
7:5A:340:U:H2'	7:5A:341:G:H8	1.81	0.46
7:5A:578:G:H2'	7:5A:579:G:H8	1.80	0.46
8:AA:405:UNK:N	8:AA:409:UNK:O	2.47	0.46
12:AE:109:TRP:HH2	12:AE:118:THR:HG21	1.80	0.46
12:AE:738:LEU:HD22	12:AE:774:ASN:HB3	1.96	0.46
12:AE:1742:UNK:O	12:AE:1746:UNK:CB	2.63	0.46
16:BA:193:TYR:HB3	16:BA:211:LYS:HD3	1.97	0.46
20:BE:53:CYS:HB2	20:BE:83:LEU:HD11	1.96	0.46
20:BE:633:LYS:HB2	20:BE:642:ALA:HB3	1.95	0.46
21:CA:181:LYS:HZ3	22:CB:808:LEU:HB3	1.80	0.46
24:E3:335:ALA:O	24:E3:339:GLY:HA3	2.15	0.46
34:SA:884:A:H2'	34:SA:885:G:C8	2.50	0.46
34:SA:1588:G:N2	34:SA:1608:U:O2	2.31	0.46
35:SC:34:ALA:HB3	35:SC:41:ARG:HA	1.96	0.46
39:SI:76:LYS:HA	39:SI:79:ARG:NH1	2.30	0.46
40:SJ:48:THR:OG1	40:SJ:52:ASN:O	2.28	0.46
43:SN:131:ASP:HA	43:SN:134:SER:HB2	1.98	0.46
48:SY:75:GLN:HA	48:SY:82:LYS:HA	1.97	0.46
10:AC:411:UNK:O	10:AC:415:UNK:CB	2.63	0.46
10:AC:613:UNK:O	10:AC:617:UNK:CB	2.63	0.46
12:AE:120:TRP:O	12:AE:124:ARG:CB	2.63	0.46
20:BE:257:ARG:HD3	20:BE:263:HIS:HD2	1.79	0.46
23:E2:164:LYS:NZ	34:SA:1575:G:OP1	2.48	0.46
34:SA:356:G:H2'	34:SA:357:G:H8	1.80	0.46
35:SC:70:LEU:HA	35:SC:73:LEU:HB2	1.96	0.46
36:SF:79:ASP:HB3	36:SF:82:TYR:HB2	1.97	0.46
58:U5:242:ILE:HB	58:U5:254:ILE:HB	1.97	0.46
3:3D:373:GLY:O	3:3D:377:ARG:HB2	2.15	0.46
12:AE:1382:UNK:O	12:AE:1386:UNK:CB	2.64	0.46
17:BB:149:ASP:HB3	17:BB:153:GLU:H	1.80	0.46
17:BB:437:LYS:HG2	17:BB:481:LEU:HD13	1.97	0.46
19:BD:275:TYR:HE2	19:BD:282:ASN:HD22	1.62	0.46
22:CB:419:TYR:O	22:CB:423:LYS:HB2	2.14	0.46
24:E3:206:LEU:N	24:E3:207:PRO:HD2	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:MC:54:UNK:O	29:MC:58:UNK:N	2.49	0.46
30:P1:103:PRO:HB3	30:P1:135:LYS:HE2	1.96	0.46
33:S1:210:UNK:N	33:S1:218:UNK:O	2.48	0.46
39:SI:48:GLU:OE2	39:SI:88:ARG:NE	2.48	0.46
45:SP:29:HIS:HB3	45:SP:41:ARG:HG3	1.96	0.46
54:U1:158:UNK:N	54:U1:171:UNK:O	2.49	0.46
3:3D:291:TYR:OH	4:3E:251:ASP:OD1	2.12	0.46
7:5A:349:G:OP2	7:5A:349:G:H8	1.98	0.46
8:AA:219:UNK:N	8:AA:233:UNK:O	2.48	0.46
12:AE:227:ASN:HD22	12:AE:230:LYS:HD2	1.81	0.46
16:BA:307:THR:O	16:BA:320:GLY:N	2.47	0.46
17:BB:351:LEU:HA	17:BB:372:ARG:HG2	1.97	0.46
23:E1:91:ILE:HG12	23:E2:132:ARG:HH12	1.81	0.46
23:E1:103:PRO:O	23:E1:107:ALA:N	2.44	0.46
12:AE:736:PHE:O	12:AE:740:ALA:HB2	2.16	0.46
12:AE:1743:UNK:O	12:AE:1747:UNK:CB	2.63	0.46
15:B1:895:PRO:HA	15:B1:918:ILE:HG13	1.98	0.46
17:BB:88:HIS:CD2	17:BB:90:ASP:H	2.33	0.46
23:E1:149:SER:HB2	23:E1:158:LYS:HG2	1.98	0.46
26:K1:100:LEU:O	26:K1:103:LEU:HB2	2.16	0.46
34:SA:384:G:H5”	40:SJ:22:ARG:HB3	1.97	0.46
35:SC:39:GLU:N	35:SC:74:GLN:OE1	2.48	0.46
37:SG:200:ASN:HB2	37:SG:208:SER:HB3	1.97	0.46
43:SN:40:GLY:O	43:SN:124:LYS:N	2.40	0.46
1:3A:254:A:H5’	1:3A:255:U:H3’	1.97	0.46
2:3B:291:GLN:OE1	2:3B:294:ARG:NH2	2.45	0.46
7:5A:447:G:H2’	7:5A:448:G:H8	1.79	0.46
12:AE:502:ILE:HA	12:AE:508:ALA:HB2	1.96	0.46
15:B1:824:ILE:HA	15:B1:886:TYR:HA	1.96	0.46
17:BB:20:ASN:ND2	17:BB:23:CYS:H	2.14	0.46
17:BB:368:PRO:HA	17:BB:374:PRO:HA	1.97	0.46
19:BD:305:SER:OG	19:BD:306:ASN:N	2.49	0.46
22:CB:1059:PRO:O	22:CB:1063:ARG:CB	2.63	0.46
23:E2:31:LEU:HB3	23:E2:111:GLN:HE21	1.79	0.46
24:E3:269:ASN:ND2	34:SA:1233:G:O2’	2.33	0.46
34:SA:294:C:H2’	34:SA:295:A:C8	2.50	0.46
34:SA:1483:A:H2’	34:SA:1484:G:C8	2.50	0.46
38:SH:88:ARG:HB3	38:SH:91:GLU:HB2	1.98	0.46
41:SK:70:LEU:O	41:SK:74:ASN:ND2	2.49	0.46
48:SY:103:LEU:N	48:SY:126:LYS:O	2.47	0.46
58:U5:75:ILE:HG12	58:U5:101:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3D:19:LYS:HE3	3:3D:142:LEU:HD13	1.97	0.46
5:3F:405:VAL:HG23	5:3F:415:THR:HG22	1.98	0.46
9:AB:442:UNK:O	9:AB:446:UNK:CB	2.64	0.46
16:BA:8:SER:H	16:BA:703:ILE:HD11	1.79	0.46
16:BA:597:ASN:ND2	16:BA:681:VAL:O	2.48	0.46
17:BB:103:ILE:HB	17:BB:117:PHE:HB2	1.97	0.46
20:BE:82:ALA:H	20:BE:93:ALA:HB3	1.81	0.46
20:BE:578:VAL:HB	20:BE:579:ARG:HH11	1.81	0.46
22:CB:805:ALA:HA	22:CB:808:LEU:HD12	1.97	0.46
34:SA:153:G:H1	34:SA:161:U:H3	1.63	0.46
40:SJ:11:ARG:NH1	40:SJ:17:LYS:HB2	2.31	0.46
40:SJ:105:ASP:OD2	40:SJ:108:PRO:HD3	2.15	0.46
46:SR:29:ILE:HA	46:SR:65:ILE:HB	1.98	0.46
49:SZ:8:ARG:HB2	49:SZ:26:ASP:HB3	1.96	0.46
2:3B:268:VAL:HG22	2:3B:317:VAL:HG22	1.98	0.46
5:3F:192:LYS:NZ	5:3F:550:GLY:HA2	2.31	0.46
9:AB:276:UNK:CB	9:AB:280:UNK:O	2.64	0.46
12:AE:1069:UNK:O	12:AE:1073:UNK:CB	2.64	0.46
16:BA:495:LYS:N	16:BA:517:ASP:OD1	2.48	0.46
19:BD:436:ASP:HB2	19:BD:444:ILE:HD11	1.98	0.46
19:BD:521:LEU:HA	19:BD:531:CYS:O	2.15	0.46
33:S1:241:UNK:O	33:S1:250:UNK:N	2.49	0.46
34:SA:1648:A:H2'	34:SA:1649:G:C8	2.51	0.46
41:SK:67:PRO:HA	41:SK:70:LEU:HB2	1.98	0.46
41:SK:84:GLY:HA2	41:SK:150:LEU:HD22	1.98	0.46
7:5A:250:G:O6	7:5A:262:U:O4	2.34	0.46
7:5A:291:G:H2'	7:5A:292:A:C8	2.51	0.46
7:5A:334:G:H1	7:5A:389:U:H3	1.62	0.46
12:AE:347:PHE:O	12:AE:351:TYR:HB2	2.16	0.46
14:AG:302:UNK:O	14:AG:315:UNK:CB	2.64	0.46
16:BA:75:GLU:HA	16:BA:98:LYS:HB3	1.98	0.46
18:BC:269:LEU:O	18:BC:278:LEU:N	2.41	0.46
20:BE:143:SER:OG	20:BE:147:ASP:OD2	2.30	0.46
22:CB:96:GLU:O	22:CB:100:SER:HB2	2.16	0.46
26:K1:126:ILE:HB	26:K1:171:VAL:HB	1.98	0.46
33:S1:249:UNK:N	33:S1:261:UNK:O	2.49	0.46
34:SA:478:A:H62	34:SA:539:G:H22	1.64	0.46
34:SA:1268:G:H2'	34:SA:1270:G:H8	1.80	0.46
34:SA:1474:G:H2'	34:SA:1475:A:C8	2.51	0.46
40:SJ:36:THR:OG1	40:SJ:59:ARG:N	2.44	0.46
1:3A:46:U:H2'	1:3A:47:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:113:G:H1'	1:3A:257:A:H61	1.80	0.46
5:3F:160:ILE:HB	5:3F:542:SER:HB3	1.98	0.46
7:5A:271:G:H2'	7:5A:272:A:H8	1.81	0.46
7:5A:511:G:O6	7:5A:525:U:O4	2.33	0.46
8:AA:355:UNK:CB	8:AA:359:UNK:O	2.64	0.46
16:BA:300:MET:N	16:BA:300:MET:SD	2.89	0.46
19:BD:372:HIS:HA	19:BD:407:PHE:H	1.81	0.46
21:CA:146:ASN:HB3	21:CA:150:LYS:HZ2	1.81	0.46
21:CA:175:LEU:HD21	22:CB:827:ARG:HG2	1.97	0.46
22:CB:179:LYS:HB2	22:CB:210:PRO:HG2	1.97	0.46
34:SA:870:C:H2'	34:SA:871:G:C8	2.51	0.46
10:AC:646:UNK:O	10:AC:650:UNK:CB	2.65	0.45
13:AF:71:UNK:CB	13:AF:75:UNK:O	2.64	0.45
16:BA:150:THR:H	16:BA:165:SER:HA	1.80	0.45
16:BA:368:LYS:HG2	16:BA:384:GLU:HG2	1.97	0.45
22:CB:142:GLU:HB2	22:CB:144:LYS:HE2	1.97	0.45
22:CB:218:ASP:OD2	22:CB:227:LYS:NZ	2.50	0.45
22:CB:671:THR:OG1	22:CB:718:LYS:O	2.34	0.45
22:CB:738:TYR:O	22:CB:742:PHE:HB2	2.17	0.45
33:S1:137:UNK:N	33:S1:146:UNK:O	2.48	0.45
34:SA:429:G:H2'	34:SA:430:G:H8	1.81	0.45
34:SA:1588:G:O6	34:SA:1608:U:O4	2.34	0.45
47:SX:12:ASN:O	47:SX:16:ASN:ND2	2.49	0.45
49:SZ:7:ILE:HG21	49:SZ:44:LEU:HD21	1.98	0.45
5:3F:188:TYR:HB3	5:3F:196:LEU:HD11	1.97	0.45
15:B1:623:LYS:HA	15:B1:626:LYS:HE2	1.97	0.45
17:BB:749:GLY:HA2	17:BB:752:LEU:HD12	1.98	0.45
22:CB:975:LEU:HD23	22:CB:1041:VAL:HG22	1.97	0.45
36:SF:75:LYS:HZ1	36:SF:77:ARG:HH12	1.57	0.45
1:3A:46:U:H2'	1:3A:47:G:C8	2.51	0.45
12:AE:163:CYS:HA	12:AE:164:LEU:HA	1.70	0.45
12:AE:1057:UNK:HA	12:AE:1065:UNK:HA	1.99	0.45
13:AF:474:UNK:O	13:AF:478:UNK:CB	2.65	0.45
15:B1:965:GLN:HA	15:B1:975:GLU:HG2	1.98	0.45
18:BC:220:ILE:HB	18:BC:237:LEU:HB3	1.99	0.45
20:BE:430:ILE:O	20:BE:442:THR:HA	2.16	0.45
22:CB:897:ARG:HE	35:SC:179:SER:HB2	1.81	0.45
31:R1:155:LYS:HG2	31:R1:234:ASN:HA	1.97	0.45
34:SA:215:A:H3'	34:SA:215:A:OP2	2.17	0.45
34:SA:1082:C:OP2	34:SA:1083:G:OP2	2.35	0.45
39:SI:143:LEU:HD22	39:SI:147:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SO:101:HIS:HA	44:SO:104:ARG:HE	1.82	0.45
54:U1:151:UNK:N	54:U1:159:UNK:O	2.50	0.45
2:3B:107:VAL:HG12	2:3B:143:VAL:HA	1.99	0.45
2:3B:299:LYS:HB2	2:3B:319:ARG:HB2	1.97	0.45
4:3E:373:TYR:HB3	4:3E:379:ASP:OD2	2.16	0.45
16:BA:514:VAL:HA	46:SR:118:ILE:HD13	1.98	0.45
17:BB:59:LEU:H	17:BB:383:HIS:HB3	1.79	0.45
20:BE:383:ASP:OD1	20:BE:384:ALA:N	2.49	0.45
20:BE:474:PHE:HA	20:BE:487:TYR:O	2.17	0.45
23:E2:28:PRO:HA	23:E2:29:PRO:HD3	1.88	0.45
24:E3:449:HIS:CD2	24:E3:451:ASP:H	2.34	0.45
25:E4:112:UNK:CB	25:E4:116:UNK:O	2.65	0.45
34:SA:93:A:H61	34:SA:396:G:H1'	1.80	0.45
34:SA:332:U:H5'	40:SJ:30:GLY:HA2	1.98	0.45
34:SA:1118:G:H2'	34:SA:1119:G:C8	2.51	0.45
34:SA:1647:U:H2'	34:SA:1648:A:C8	2.52	0.45
38:SH:57:ASP:HB3	38:SH:106:LEU:HD23	1.98	0.45
40:SJ:81:VAL:HA	40:SJ:102:VAL:HG12	1.97	0.45
4:3E:296:GLY:HA2	4:3E:299:LEU:HD12	1.99	0.45
7:5A:529:A:H2'	7:5A:530:A:C8	2.52	0.45
8:AA:283:UNK:HA	8:AA:289:UNK:HA	1.98	0.45
12:AE:29:HIS:CD2	12:AE:123:ARG:HH21	2.35	0.45
14:AG:394:UNK:O	14:AG:406:UNK:CB	2.64	0.45
16:BA:263:VAL:HG22	16:BA:279:PHE:HE1	1.82	0.45
17:BB:226:VAL:O	17:BB:241:LYS:HA	2.17	0.45
17:BB:386:GLU:HB3	17:BB:390:GLN:HE22	1.80	0.45
17:BB:617:SER:O	17:BB:634:SER:OG	2.29	0.45
18:BC:377:LEU:HD12	18:BC:381:VAL:HG12	1.99	0.45
22:CB:345:TYR:HH	22:CB:472:THR:HG1	1.60	0.45
22:CB:949:PHE:O	22:CB:960:LYS:NZ	2.49	0.45
22:CB:1059:PRO:O	22:CB:1063:ARG:HB2	2.16	0.45
28:MB:169:ASN:ND2	28:MB:253:ARG:O	2.49	0.45
31:R1:281:GLU:OE2	31:R1:285:LYS:HE2	2.17	0.45
34:SA:391:A:H2'	34:SA:392:G:C8	2.51	0.45
34:SA:913:G:H4'	34:SA:914:G:OP2	2.15	0.45
38:SH:70:PRO:HD3	38:SH:101:ILE:HD12	1.98	0.45
1:3A:67:G:H2'	1:3A:68:A:H8	1.81	0.45
1:3A:330:A:H2'	1:3A:331:A:H8	1.81	0.45
7:5A:589:U:H2'	7:5A:590:G:H8	1.82	0.45
11:AD:509:UNK:O	11:AD:513:UNK:CB	2.64	0.45
17:BB:748:ALA:HA	17:BB:751:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BC:751:LYS:H	18:BC:753:HIS:CE1	2.35	0.45
20:BE:541:LYS:NZ	20:BE:542:LEU:O	2.48	0.45
28:MB:205:ILE:O	28:MB:209:LEU:N	2.49	0.45
33:S1:219:UNK:O	33:S1:227:UNK:N	2.50	0.45
34:SA:15:U:H2'	34:SA:16:G:C8	2.52	0.45
34:SA:406:U:H2'	34:SA:407:A:C8	2.52	0.45
34:SA:1584:G:H1'	34:SA:1585:U:H5	1.82	0.45
58:U5:52:ASN:HD21	58:U5:228:LYS:HE3	1.82	0.45
1:3A:3:C:H2'	1:3A:4:G:C8	2.51	0.45
4:3E:225:GLU:HG3	4:3E:226:ILE:HG13	1.99	0.45
8:AA:116:UNK:O	8:AA:129:UNK:CB	2.65	0.45
12:AE:121:LEU:HA	12:AE:125:PHE:HD2	1.82	0.45
15:B1:201:ASN:OD1	15:B1:204:ARG:NH2	2.49	0.45
16:BA:16:ARG:HB2	16:BA:34:GLY:H	1.82	0.45
16:BA:60:ALA:H	16:BA:73:ILE:H	1.64	0.45
19:BD:273:ARG:HA	19:BD:287:SER:HA	1.99	0.45
21:CA:53:LEU:HD12	21:CA:126:LEU:HD23	1.99	0.45
22:CB:167:PRO:HD3	22:CB:226:HIS:CE1	2.51	0.45
22:CB:419:TYR:HE1	22:CB:499:LEU:HD22	1.82	0.45
34:SA:445:A:C4	34:SA:525:A:H4'	2.52	0.45
57:U4:81:ASP:OD2	57:U4:84:ARG:NE	2.36	0.45
3:3D:74:VAL:HB	3:3D:78:LEU:HD22	1.99	0.45
6:3G:111:LYS:HA	6:3G:114:ILE:HD12	1.98	0.45
7:5A:71:U:H2'	7:5A:72:G:C8	2.52	0.45
7:5A:357:G:H2'	7:5A:358:G:H8	1.82	0.45
12:AE:25:ARG:O	12:AE:29:HIS:CB	2.64	0.45
12:AE:1520:UNK:O	12:AE:1524:UNK:CB	2.65	0.45
15:B1:190:ILE:H	15:B1:190:ILE:HG13	1.60	0.45
17:BB:212:VAL:HB	17:BB:217:LEU:HD23	1.98	0.45
17:BB:530:LEU:HD23	17:BB:551:LEU:HG	1.99	0.45
18:BC:43:ILE:HB	18:BC:56:ILE:O	2.17	0.45
18:BC:680:ASN:O	18:BC:684:LEU:HB3	2.17	0.45
22:CB:232:LEU:HD13	22:CB:296:ILE:HD11	1.98	0.45
22:CB:268:LEU:HB3	22:CB:294:LEU:HB2	1.98	0.45
24:E3:388:ASP:OD1	24:E3:436:GLN:NE2	2.48	0.45
35:SC:118:GLN:OE1	35:SC:208:GLN:NE2	2.49	0.45
37:SG:80:LYS:HB3	37:SG:83:ARG:HB2	1.98	0.45
38:SH:102:VAL:HG13	38:SH:106:LEU:HD12	1.98	0.45
47:SX:12:ASN:OD1	47:SX:16:ASN:ND2	2.49	0.45
54:U1:265:UNK:HA	54:U1:272:UNK:HA	1.99	0.45
58:U5:70:LEU:HB3	58:U5:123:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AC:4:UNK:HA	10:AC:284:UNK:HA	1.99	0.45
10:AC:530:UNK:O	10:AC:534:UNK:CB	2.65	0.45
12:AE:1095:UNK:O	12:AE:1099:UNK:CB	2.65	0.45
13:AF:3:UNK:O	13:AF:285:UNK:N	2.50	0.45
17:BB:426:ARG:NH1	17:BB:458:ASP:O	2.49	0.45
17:BB:555:VAL:HG22	17:BB:569:LEU:HB2	1.97	0.45
22:CB:879:GLU:O	22:CB:883:LEU:HB2	2.16	0.45
22:CB:1147:TYR:O	22:CB:1151:LYS:HB2	2.17	0.45
25:E4:230:UNK:HA	25:E4:244:UNK:HA	1.98	0.45
35:SC:88:VAL:HG13	35:SC:96:LEU:HD11	1.99	0.45
39:SI:21:ALA:HA	39:SI:24:PHE:HD2	1.82	0.45
46:SR:24:ALA:HA	46:SR:63:ILE:HA	1.99	0.45
46:SR:42:GLU:CG	46:SR:45:ARG:HH12	2.26	0.45
8:AA:478:UNK:CB	8:AA:482:UNK:O	2.65	0.45
12:AE:814:UNK:O	12:AE:818:UNK:CB	2.65	0.45
14:AG:122:UNK:N	14:AG:126:UNK:O	2.50	0.45
15:B1:143:MET:H	48:SY:144:ARG:HH11	1.64	0.45
15:B1:893:ASN:HD22	15:B1:919:VAL:HG12	1.81	0.45
16:BA:385:GLU:OE1	16:BA:421:ASN:ND2	2.49	0.45
20:BE:36:GLY:HA2	20:BE:299:THR:HG21	1.99	0.45
20:BE:418:ALA:HB1	20:BE:468:MET:HG3	1.98	0.45
32:R2:1613:PRO:HD2	32:R2:1616:ASN:HD22	1.82	0.45
34:SA:1473:U:C2	37:SG:102:ARG:NH1	2.85	0.45
34:SA:1638:G:H22	34:SA:1763:A:H2	1.64	0.45
44:SO:114:ARG:HG3	44:SO:117:LEU:HD12	1.99	0.45
1:3A:199:G:C2	5:3F:153:GLY:HA2	2.52	0.44
6:3H:84:ARG:HG3	6:3H:96:PRO:HB3	1.98	0.44
12:AE:10:GLN:O	12:AE:13:SER:OG	2.30	0.44
13:AF:505:UNK:O	13:AF:509:UNK:CB	2.65	0.44
15:B1:977:LYS:HB3	15:B1:988:ARG:HG3	1.99	0.44
16:BA:710:ILE:HA	20:BE:596:GLU:HB2	1.98	0.44
17:BB:478:SER:H	17:BB:491:GLY:HA3	1.81	0.44
18:BC:36:VAL:HB	18:BC:39:GLU:H	1.83	0.44
18:BC:308:ASP:OD1	18:BC:308:ASP:N	2.51	0.44
20:BE:666:ARG:HB3	20:BE:667:THR:H	1.64	0.44
20:BE:860:GLU:HA	20:BE:863:TRP:HE3	1.82	0.44
22:CB:315:ILE:HB	22:CB:553:VAL:HG13	1.99	0.44
22:CB:970:TRP:HZ3	22:CB:1034:GLY:HA3	1.83	0.44
23:E2:121:LEU:HD11	23:E2:167:ILE:HD13	1.99	0.44
25:E4:59:UNK:O	25:E4:68:UNK:N	2.51	0.44
34:SA:156:A:H2'	34:SA:157:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:568:G:N2	34:SA:569:C:N3	2.65	0.44
43:SN:67:THR:HG22	43:SN:68:GLU:HG3	1.99	0.44
61:UC:731:UNK:HA	61:UC:732:UNK:HA	1.74	0.44
6:3H:85:VAL:HG22	6:3H:96:PRO:HG3	1.99	0.44
7:5A:163:G:H2'	7:5A:164:G:C8	2.52	0.44
8:AA:36:UNK:O	8:AA:44:UNK:N	2.50	0.44
11:AD:411:UNK:O	11:AD:415:UNK:CB	2.65	0.44
12:AE:1070:UNK:O	12:AE:1074:UNK:CB	2.65	0.44
18:BC:213:SER:OG	18:BC:223:TRP:NE1	2.45	0.44
20:BE:349:HIS:ND1	20:BE:374:SER:OG	2.38	0.44
22:CB:643:ALA:O	22:CB:647:ASN:HB2	2.17	0.44
23:E1:98:THR:OG1	23:E1:235:SER:OG	2.30	0.44
23:E2:103:PRO:O	23:E2:107:ALA:N	2.42	0.44
23:E2:151:ARG:NH2	34:SA:1572:G:OP2	2.50	0.44
34:SA:1145:U:H3	34:SA:1633:A:H2'	1.82	0.44
42:SM:75:VAL:HG22	42:SM:86:ILE:HG22	1.99	0.44
54:U1:157:UNK:HA	54:U1:172:UNK:HA	1.99	0.44
57:U4:72:ILE:HG23	57:U4:82:ILE:HD11	1.99	0.44
2:3B:116:SER:HB3	2:3B:122:ARG:HH12	1.82	0.44
2:3B:117:VAL:HG11	2:3B:179:THR:HA	1.98	0.44
7:5A:281:G:H2'	7:5A:282:G:H8	1.82	0.44
10:AC:8:UNK:N	10:AC:281:UNK:O	2.50	0.44
12:AE:659:LEU:HD23	12:AE:692:ILE:HA	1.99	0.44
12:AE:769:LEU:HB3	12:AE:801:ILE:HG12	2.00	0.44
13:AF:427:UNK:O	13:AF:431:UNK:CB	2.65	0.44
16:BA:85:LYS:HE2	20:BE:659:GLN:HA	1.98	0.44
19:BD:423:LEU:HG	19:BD:432:VAL:HG13	1.99	0.44
19:BD:424:ILE:HD13	19:BD:433:TRP:HD1	1.81	0.44
20:BE:292:ARG:NH2	20:BE:350:SER:OG	2.46	0.44
20:BE:602:SER:O	20:BE:609:ILE:HA	2.17	0.44
21:CA:211:GLY:HA2	21:CA:214:LEU:HD12	1.99	0.44
22:CB:864:LEU:HD23	22:CB:867:ILE:HD12	1.98	0.44
24:E3:251:PRO:HA	24:E3:254:TRP:CE2	2.52	0.44
30:P1:161:ALA:HA	30:P1:232:HIS:HE1	1.83	0.44
34:SA:10:G:H2'	34:SA:11:A:C8	2.52	0.44
36:SF:100:ARG:HH12	36:SF:236:ILE:HG21	1.81	0.44
46:SR:23:LYS:O	46:SR:64:ASP:N	2.43	0.44
61:UC:58:UNK:O	61:UC:62:UNK:N	2.50	0.44
10:AC:59:UNK:O	10:AC:68:UNK:N	2.51	0.44
10:AC:466:UNK:O	10:AC:470:UNK:CB	2.66	0.44
15:B1:106:ALA:HA	15:B1:109:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BB:357:THR:OG1	17:BB:361:THR:O	2.34	0.44
18:BC:172:VAL:HB	18:BC:186:LEU:HB2	2.00	0.44
24:E3:276:GLN:O	24:E3:280:ASN:HB2	2.18	0.44
25:E4:199:UNK:O	25:E4:212:UNK:CB	2.66	0.44
26:K1:132:VAL:HG11	26:K1:137:ARG:HB3	1.98	0.44
26:K1:140:LYS:HB3	26:K1:144:ARG:HH22	1.82	0.44
34:SA:924:A:H2'	34:SA:925:G:C4	2.52	0.44
35:SC:83:LYS:HZ1	35:SC:106:THR:HA	1.82	0.44
35:SC:83:LYS:NZ	35:SC:106:THR:HA	2.33	0.44
39:SI:30:SER:HB2	39:SI:34:LEU:HB2	1.99	0.44
41:SK:78:ARG:HH11	41:SK:81:VAL:HG21	1.83	0.44
57:U4:71:PHE:HB2	57:U4:155:THR:HA	1.99	0.44
5:3F:440:HIS:HA	5:3F:497:LYS:HE3	2.00	0.44
7:5A:101:G:N2	7:5A:102:A:N1	2.61	0.44
14:AG:132:UNK:HA	14:AG:133:UNK:HA	1.73	0.44
16:BA:445:VAL:HG13	16:BA:458:TRP:HB2	2.00	0.44
28:MB:249:GLU:HB3	28:MB:253:ARG:HE	1.82	0.44
33:S1:137:UNK:O	33:S1:145:UNK:N	2.50	0.44
33:S1:179:UNK:HA	33:S1:185:UNK:HA	1.99	0.44
35:SC:129:THR:OG1	35:SC:131:ASP:O	2.29	0.44
46:SR:58:ASP:O	46:SR:60:PHE:N	2.51	0.44
46:SR:113:ASP:OD1	46:SR:116:LEU:N	2.46	0.44
6:3H:56:ALA:HB3	6:3H:82:PRO:HA	2.00	0.44
7:5A:290:G:H2'	7:5A:291:G:H8	1.83	0.44
8:AA:148:UNK:O	8:AA:159:UNK:HA	2.18	0.44
12:AE:1651:UNK:HA	12:AE:1659:UNK:HA	1.99	0.44
14:AG:284:UNK:CB	14:AG:293:UNK:O	2.66	0.44
34:SA:1216:C:O2'	34:SA:1217:A:OP1	2.35	0.44
34:SA:1650:U:H2'	34:SA:1651:A:H8	1.83	0.44
35:SC:97:LEU:HD22	35:SC:232:HIS:CE1	2.52	0.44
37:SG:92:ARG:HA	37:SG:95:ASN:HD22	1.82	0.44
42:SM:130:PRO:HA	42:SM:136:ARG:HG3	1.99	0.44
58:U5:147:SER:HA	58:U5:148:LYS:HA	1.67	0.44
10:AC:598:UNK:O	10:AC:602:UNK:CB	2.66	0.44
12:AE:528:ARG:HA	12:AE:531:ILE:HG22	1.99	0.44
12:AE:564:VAL:HB	12:AE:614:LEU:HD11	2.00	0.44
12:AE:912:UNK:HA	12:AE:913:UNK:HA	1.78	0.44
16:BA:423:ARG:NH2	16:BA:461:GLN:O	2.50	0.44
18:BC:35:PRO:HG3	18:BC:67:LEU:HG	1.99	0.44
19:BD:445:ARG:NH1	19:BD:499:ALA:O	2.50	0.44
21:CA:185:HIS:O	21:CA:189:ALA:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E4:3:UNK:O	25:E4:285:UNK:N	2.51	0.44
34:SA:361:C:N4	34:SA:384:G:O6	2.51	0.44
57:U4:63:TYR:O	57:U4:95:ASN:N	2.50	0.44
2:3B:264:GLN:HE22	2:3B:322:ARG:HA	1.81	0.44
5:3F:442:ILE:HD12	5:3F:470:LEU:HD12	1.99	0.44
7:5A:168:G:H1	7:5A:228:A:N6	2.16	0.44
15:B1:957:GLU:HG2	15:B1:960:ARG:HH11	1.82	0.44
16:BA:45:ASN:HB2	16:BA:377:GLY:HA3	1.99	0.44
18:BC:348:PRO:HB3	18:BC:399:ASP:HA	1.99	0.44
22:CB:1138:ASP:O	22:CB:1141:GLU:HB2	2.18	0.44
23:E2:67:LEU:HD11	23:E2:141:MET:HB2	1.98	0.44
30:P1:248:VAL:HA	30:P1:251:ILE:HD12	2.00	0.44
1:3A:18:G:H2'	1:3A:19:A:H8	1.82	0.44
5:3F:342:ARG:NH1	6:3G:89:ARG:O	2.51	0.44
8:AA:231:UNK:HA	8:AA:240:UNK:O	2.17	0.44
10:AC:548:UNK:O	10:AC:552:UNK:CB	2.66	0.44
12:AE:854:UNK:O	12:AE:858:UNK:CB	2.66	0.44
13:AF:428:UNK:O	13:AF:432:UNK:CB	2.66	0.44
19:BD:429:TYR:HD2	19:BD:431:GLU:HG2	1.81	0.44
20:BE:154:TYR:OH	20:BE:194:ARG:O	2.25	0.44
20:BE:230:VAL:HB	20:BE:244:ILE:HB	2.00	0.44
21:CA:146:ASN:HB3	21:CA:150:LYS:NZ	2.32	0.44
24:E3:260:TYR:HA	24:E3:306:ALA:HB2	1.99	0.44
24:E3:305:ARG:HA	34:SA:1217:A:C8	2.52	0.44
28:MB:236:HIS:HE1	28:MB:249:GLU:HG2	1.83	0.44
36:SF:136:VAL:HG21	36:SF:148:ARG:NH1	2.33	0.44
40:SJ:67:TRP:NE1	40:SJ:69:SER:OG	2.51	0.44
58:U5:213:LEU:HA	58:U5:216:ILE:HD12	1.98	0.44
1:3A:310:G:H2'	1:3A:311:G:H8	1.83	0.43
4:3E:277:SER:HA	4:3E:293:GLU:OE2	2.18	0.43
5:3F:367:LYS:HA	5:3F:370:ARG:HD3	2.00	0.43
15:B1:868:ARG:HH21	15:B1:928:ILE:HA	1.83	0.43
20:BE:38:PRO:HB3	20:BE:300:GLN:HE21	1.82	0.43
20:BE:291:HIS:HD2	20:BE:298:VAL:HG22	1.83	0.43
20:BE:412:PRO:O	20:BE:434:HIS:ND1	2.42	0.43
23:E2:219:GLU:HA	37:SG:157:ARG:HH22	1.83	0.43
24:E3:457:ARG:HE	24:E3:461:LEU:HD11	1.83	0.43
31:R1:301:MET:HG2	31:R1:354:ILE:HD13	2.01	0.43
34:SA:51:A:N6	34:SA:429:G:H21	2.14	0.43
34:SA:1585:U:H2'	34:SA:1586:A:H8	1.83	0.43
61:UC:69:UNK:O	61:UC:73:UNK:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AB:244:UNK:N	9:AB:248:UNK:O	2.51	0.43
14:AG:79:UNK:CB	14:AG:88:UNK:O	2.66	0.43
15:B1:828:ARG:HD3	48:SY:94:ASN:HA	2.00	0.43
16:BA:603:LEU:HB2	16:BA:612:LEU:O	2.18	0.43
17:BB:219:THR:HG22	17:BB:227:LYS:HB2	2.00	0.43
17:BB:253:LYS:NZ	17:BB:254:GLN:O	2.48	0.43
17:BB:444:LEU:HD13	17:BB:456:LEU:HD11	1.99	0.43
18:BC:270:ILE:HA	18:BC:277:VAL:HA	2.01	0.43
18:BC:311:LEU:HD12	18:BC:333:ILE:HD11	2.01	0.43
27:MA:114:ILE:HG13	27:MA:150:VAL:HB	2.00	0.43
34:SA:894:U:H2'	34:SA:895:G:C8	2.54	0.43
34:SA:1628:U:H2'	34:SA:1629:G:H8	1.82	0.43
39:SI:159:VAL:HG23	39:SI:163:ASP:OD2	2.17	0.43
61:UC:771:UNK:O	61:UC:775:UNK:N	2.51	0.43
9:AB:148:UNK:HA	9:AB:161:UNK:O	2.17	0.43
10:AC:235:UNK:CB	10:AC:239:UNK:O	2.66	0.43
10:AC:240:UNK:O	10:AC:253:UNK:CB	2.66	0.43
12:AE:121:LEU:HB3	12:AE:127:ILE:HD13	2.00	0.43
12:AE:595:THR:HG22	12:AE:619:SER:HA	2.00	0.43
13:AF:100:UNK:O	13:AF:109:UNK:N	2.51	0.43
13:AF:153:UNK:CB	13:AF:157:UNK:O	2.66	0.43
14:AG:264:UNK:HA	14:AG:274:UNK:O	2.17	0.43
14:AG:841:UNK:O	14:AG:845:UNK:CB	2.66	0.43
16:BA:99:CYS:SG	16:BA:115:SER:OG	2.76	0.43
16:BA:347:SER:HB2	16:BA:698:THR:HA	2.01	0.43
16:BA:522:SER:HB2	16:BA:583:ILE:HG23	1.99	0.43
17:BB:634:SER:OG	17:BB:635:LYS:N	2.49	0.43
17:BB:857:LEU:HD21	17:BB:884:LYS:HE2	2.01	0.43
22:CB:364:VAL:HA	22:CB:367:ARG:HG2	1.99	0.43
22:CB:412:LEU:HD22	22:CB:421:LEU:HA	2.01	0.43
22:CB:506:GLN:OE1	22:CB:509:ASN:ND2	2.48	0.43
30:P1:188:LYS:HD2	30:P1:191:LYS:NZ	2.34	0.43
33:S1:282:UNK:O	33:S1:291:UNK:N	2.51	0.43
34:SA:283:U:H5"	38:SH:188:ARG:NE	2.31	0.43
34:SA:328:A:H2'	34:SA:329:G:C8	2.53	0.43
34:SA:363:G:H2'	34:SA:364:G:H8	1.83	0.43
34:SA:975:C:N4	34:SA:976:G:O6	2.52	0.43
36:SF:100:ARG:NH1	36:SF:236:ILE:HG21	2.34	0.43
44:SO:85:PRO:HD2	44:SO:88:LEU:HD13	2.00	0.43
58:U5:86:THR:HA	58:U5:90:ASP:HB2	2.00	0.43
2:3B:271:ILE:O	2:3B:313:HIS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B1:819:GLU:O	15:B1:852:ARG:NH1	2.52	0.43
16:BA:308:VAL:HA	16:BA:319:PHE:HA	2.01	0.43
16:BA:475:PRO:HD2	16:BA:493:TRP:HB3	2.01	0.43
16:BA:498:ARG:HB3	16:BA:500:TRP:HE1	1.84	0.43
17:BB:166:ILE:HD11	17:BB:179:SER:HB2	1.99	0.43
17:BB:622:LYS:HB2	17:BB:631:PHE:CZ	2.54	0.43
18:BC:492:LYS:HD3	18:BC:511:TYR:HD2	1.83	0.43
20:BE:627:ASN:ND2	20:BE:647:THR:O	2.41	0.43
23:E2:53:HIS:N	23:E2:66:VAL:O	2.51	0.43
33:S1:289:UNK:HA	33:S1:303:UNK:HA	2.01	0.43
34:SA:491:C:H2'	34:SA:492:A:C8	2.53	0.43
34:SA:1679:G:N2	34:SA:1723:U:O4	2.51	0.43
34:SA:1802:A:N6	34:SA:1808:U:O4	2.50	0.43
35:SC:127:VAL:HG11	35:SC:176:VAL:HG11	2.01	0.43
37:SG:81:ARG:NH1	37:SG:82:PHE:HE2	2.16	0.43
38:SH:57:ASP:HA	38:SH:106:LEU:HA	2.01	0.43
5:3F:491:SER:OG	5:3F:492:TRP:N	2.51	0.43
7:5A:244:U:H3	7:5A:269:G:H1	1.66	0.43
7:5A:409:C:H2'	7:5A:410:A:C8	2.53	0.43
15:B1:236:LEU:HB3	15:B1:239:THR:HG23	1.99	0.43
17:BB:163:LYS:HD3	34:SA:1765:A:H4'	2.01	0.43
17:BB:385:ILE:HG23	17:BB:417:TRP:HH2	1.83	0.43
24:E3:301:TYR:O	24:E3:304:TYR:CA	2.66	0.43
28:MB:215:LYS:NZ	34:SA:1625:C:H5'	2.33	0.43
34:SA:886:U:H2'	34:SA:887:A:C8	2.53	0.43
34:SA:1210:C:H2'	34:SA:1211:A:H8	1.83	0.43
36:SF:149:TYR:HB3	38:SH:208:TYR:CZ	2.52	0.43
40:SJ:4:SER:OG	40:SJ:6:ASP:OD1	2.34	0.43
54:U1:200:UNK:HA	54:U1:211:UNK:HA	2.01	0.43
4:3E:45:ALA:HB1	4:3E:83:LYS:NZ	2.33	0.43
12:AE:272:LYS:HA	12:AE:275:ILE:HD12	2.00	0.43
12:AE:367:LEU:O	12:AE:371:LYS:CB	2.63	0.43
12:AE:894:UNK:O	12:AE:898:UNK:CB	2.66	0.43
18:BC:622:ALA:H	18:BC:635:ALA:HB3	1.84	0.43
19:BD:368:THR:HA	19:BD:385:ASN:O	2.18	0.43
20:BE:97:LYS:NZ	20:BE:111:GLU:HB2	2.30	0.43
20:BE:208:GLN:O	20:BE:226:VAL:N	2.49	0.43
34:SA:273:G:C6	34:SA:283:U:O2	2.72	0.43
34:SA:363:G:H2'	34:SA:364:G:C8	2.54	0.43
36:SF:92:LEU:HB2	36:SF:97:GLU:HB2	2.01	0.43
39:SI:67:LEU:HG	39:SI:71:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SP:20:TYR:HB3	45:SP:27:PHE:HB2	2.00	0.43
46:SR:79:TYR:HD1	46:SR:82:ARG:HD3	1.84	0.43
54:U1:77:UNK:HA	54:U1:88:UNK:HA	2.00	0.43
61:UC:243:UNK:O	61:UC:247:UNK:N	2.52	0.43
61:UC:437:UNK:O	61:UC:441:UNK:N	2.52	0.43
1:3A:47:G:H2'	1:3A:48:A:C8	2.53	0.43
1:3A:84:U:H2'	1:3A:85:G:H8	1.84	0.43
3:3D:150:ALA:O	3:3D:154:LEU:HB2	2.18	0.43
8:AA:65:UNK:HA	8:AA:78:UNK:O	2.18	0.43
15:B1:836:LYS:H	15:B1:912:ARG:HH12	1.67	0.43
16:BA:412:ARG:HA	16:BA:423:ARG:O	2.19	0.43
22:CB:812:GLU:O	22:CB:816:ALA:CB	2.67	0.43
30:P1:255:PRO:HA	30:P1:256:PRO:HD3	1.88	0.43
31:R1:67:ILE:HG23	31:R1:74:VAL:HG22	2.01	0.43
34:SA:389:G:H3'	34:SA:390:G:H21	1.83	0.43
34:SA:1263:G:C2	34:SA:1264:G:H1'	2.53	0.43
34:SA:1661:U:H2'	34:SA:1662:G:C8	2.54	0.43
35:SC:83:LYS:HB2	35:SC:104:ASP:HB3	2.01	0.43
36:SF:137:PRO:HG2	36:SF:149:TYR:HA	2.00	0.43
7:5A:274:C:H2'	7:5A:275:A:C8	2.54	0.43
7:5A:379:A:H2'	7:5A:380:A:C8	2.54	0.43
8:AA:386:UNK:N	8:AA:391:UNK:O	2.51	0.43
15:B1:189:VAL:HG13	15:B1:193:ARG:HA	2.01	0.43
16:BA:66:GLN:HG3	16:BA:68:THR:HG22	2.00	0.43
18:BC:353:LEU:HD12	18:BC:366:PRO:HG2	2.00	0.43
21:CA:6:ILE:HD13	22:CB:1206:PRO:HB2	2.00	0.43
22:CB:334:PHE:O	22:CB:338:SER:OG	2.26	0.43
22:CB:896:THR:O	22:CB:900:GLU:HB2	2.19	0.43
24:E3:228:LYS:NZ	34:SA:1245:G:OP2	2.51	0.43
34:SA:523:G:H22	34:SA:528:U:H5"	1.83	0.43
34:SA:1679:G:H1'	34:SA:1722:A:H61	1.84	0.43
35:SC:91:VAL:HG23	35:SC:96:LEU:HB2	2.01	0.43
36:SF:12:LEU:HD21	36:SF:22:LYS:HG2	2.01	0.43
40:SJ:8:ARG:HH11	40:SJ:19:ALA:HB3	1.84	0.43
2:3C:169:LYS:O	2:3C:238:ASP:N	2.42	0.43
15:B1:66:ARG:HH21	15:B1:78:ASN:HB3	1.83	0.43
18:BC:614:ASP:OD1	18:BC:614:ASP:N	2.50	0.43
22:CB:298:PHE:HB2	22:CB:340:SER:HA	2.00	0.43
22:CB:644:VAL:O	22:CB:648:PHE:HB2	2.19	0.43
22:CB:823:SER:HA	22:CB:841:ASN:O	2.19	0.43
23:E1:181:SER:OG	23:E1:214:ASP:OD2	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:MB:173:ARG:HD3	28:MB:252:PRO:HB3	2.00	0.43
32:R2:1690:PHE:HA	32:R2:1693:ASN:HD22	1.83	0.43
34:SA:205:U:H2'	34:SA:206:A:H8	1.84	0.43
37:SG:94:THR:HG22	37:SG:114:ILE:HG13	2.01	0.43
39:SI:26:GLU:OE2	39:SI:27:LEU:HG	2.19	0.43
40:SJ:85:PRO:HG3	42:SM:12:ALA:HB2	2.01	0.43
44:SO:101:HIS:HA	44:SO:104:ARG:HH11	1.83	0.43
2:3B:227:PRO:HA	2:3B:230:TYR:CE1	2.54	0.43
3:3D:62:ALA:O	3:3D:66:ALA:CB	2.67	0.43
3:3D:284:TYR:HE1	4:3E:257:ALA:HB1	1.84	0.43
4:3E:160:ASP:OD1	4:3E:163:ILE:HD12	2.18	0.43
7:5A:242:C:H2'	7:5A:243:A:C8	2.53	0.43
16:BA:114:ALA:HB1	16:BA:149:ILE:HB	2.01	0.43
16:BA:505:ARG:HH22	34:SA:1618:C:H41	1.66	0.43
16:BA:556:ARG:HB3	16:BA:557:LYS:H	1.70	0.43
17:BB:438:PHE:HA	17:BB:445:VAL:HG23	2.00	0.43
17:BB:576:VAL:HA	17:BB:592:SER:HA	2.01	0.43
18:BC:18:GLY:O	18:BC:336:ASN:N	2.52	0.43
18:BC:439:ALA:HB3	18:BC:457:ALA:HB3	2.01	0.43
20:BE:375:LEU:HB3	20:BE:389:MET:HB2	2.00	0.43
20:BE:391:GLN:HG2	20:BE:443:TRP:HH2	1.84	0.43
20:BE:588:ILE:HA	20:BE:604:SER:HA	2.01	0.43
22:CB:758:SER:O	22:CB:762:TYR:N	2.52	0.43
22:CB:1157:TYR:HB3	22:CB:1161:LEU:HB2	2.01	0.43
25:E4:33:UNK:HA	25:E4:54:UNK:HA	2.01	0.43
26:K1:99:ASP:O	26:K1:103:LEU:N	2.44	0.43
26:K1:125:VAL:O	45:SP:92:LYS:NZ	2.44	0.43
34:SA:1041:G:H2'	34:SA:1042:G:C8	2.54	0.43
39:SI:71:HIS:HD2	39:SI:131:PHE:CZ	2.36	0.43
1:3A:79:G:C5	6:3H:95:ARG:HD3	2.54	0.42
3:3D:18:PHE:CZ	3:3D:151:GLN:HB2	2.54	0.42
3:3D:158:TYR:O	3:3D:162:LYS:CB	2.62	0.42
4:3E:58:GLU:HA	4:3E:61:ASN:HD22	1.84	0.42
7:5A:133:U:H2'	7:5A:134:A:C8	2.54	0.42
7:5A:271:G:H2'	7:5A:272:A:C8	2.54	0.42
12:AE:576:ILE:HA	12:AE:579:ARG:HE	1.83	0.42
13:AF:143:UNK:N	13:AF:148:UNK:O	2.52	0.42
20:BE:559:ALA:HA	20:BE:569:VAL:HA	2.01	0.42
20:BE:592:ASP:OD1	20:BE:593:PHE:N	2.51	0.42
23:E1:105:ASN:HB2	23:E1:110:LEU:HD23	2.00	0.42
29:MC:429:GLU:N	29:MC:432:LYS:HZ2	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R1:177:PRO:HD2	31:R1:304:GLY:HA2	2.00	0.42
34:SA:878:G:O2'	44:SO:108:ASP:OD1	2.36	0.42
34:SA:891:A:H2'	34:SA:892:A:H8	1.83	0.42
34:SA:1606:C:H2'	34:SA:1607:G:C8	2.54	0.42
35:SC:36:SER:O	35:SC:38:PHE:N	2.51	0.42
37:SG:80:LYS:HZ3	37:SG:83:ARG:HH11	1.67	0.42
37:SG:142:PRO:HA	37:SG:218:GLU:OE2	2.18	0.42
41:SK:66:ASP:O	41:SK:70:LEU:N	2.49	0.42
61:UC:769:UNK:O	61:UC:773:UNK:N	2.52	0.42
2:3C:100:ARG:HA	2:3C:101:GLY:HA2	1.77	0.42
5:3F:323:ASP:OD2	5:3F:342:ARG:HD3	2.20	0.42
5:3F:345:THR:HG22	5:3F:360:ARG:HG3	2.01	0.42
12:AE:506:TYR:O	12:AE:510:SER:CB	2.67	0.42
12:AE:816:UNK:O	12:AE:820:UNK:CB	2.67	0.42
15:B1:245:ASP:HB3	15:B1:797:PRO:HA	2.00	0.42
15:B1:846:VAL:HB	15:B1:899:VAL:HG23	2.00	0.42
17:BB:15:GLY:H	17:BB:685:GLU:HB3	1.84	0.42
17:BB:656:HIS:CE1	17:BB:682:ARG:HD2	2.55	0.42
25:E4:258:UNK:HA	40:SJ:42:ARG:HH11	1.81	0.42
31:R1:153:THR:HA	31:R1:166:VAL:HG12	2.00	0.42
33:S1:101:UNK:N	33:S1:385:UNK:O	2.48	0.42
34:SA:497:G:H2'	34:SA:498:G:C8	2.54	0.42
36:SF:211:LYS:HB3	36:SF:217:THR:HG22	2.01	0.42
44:SO:55:ARG:HA	44:SO:60:VAL:HB	2.01	0.42
47:SX:65:LEU:HD22	47:SX:66:ASN:H	1.85	0.42
1:3A:330:A:H2'	1:3A:331:A:C8	2.54	0.42
2:3C:180:SER:HA	2:3C:183:HIS:HD2	1.83	0.42
8:AA:27:UNK:O	8:AA:34:UNK:HA	2.19	0.42
8:AA:404:UNK:HA	8:AA:410:UNK:HA	2.02	0.42
12:AE:1762:UNK:O	12:AE:1766:UNK:CB	2.67	0.42
14:AG:8:UNK:N	14:AG:567:UNK:O	2.51	0.42
18:BC:391:LEU:HD23	18:BC:407:SER:HB2	2.00	0.42
18:BC:397:THR:OG1	18:BC:398:GLU:N	2.53	0.42
20:BE:323:VAL:HG13	20:BE:343:LEU:HB2	2.00	0.42
22:CB:543:LEU:HG	22:CB:545:ALA:H	1.85	0.42
27:MA:111:LEU:HB2	27:MA:148:TYR:HB3	2.02	0.42
34:SA:283:U:O4'	38:SH:188:ARG:HG3	2.19	0.42
34:SA:1049:U:H2'	34:SA:1050:G:C8	2.54	0.42
34:SA:1179:G:O6	34:SA:1461:C:N4	2.53	0.42
35:SC:97:LEU:HD22	35:SC:232:HIS:HE1	1.84	0.42
36:SF:129:VAL:HB	36:SF:139:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:SF:137:PRO:HB2	36:SF:150:PRO:HD2	2.01	0.42
41:SK:58:ASP:O	41:SK:61:THR:OG1	2.32	0.42
58:U5:64:LEU:HB3	58:U5:68:ARG:HE	1.84	0.42
7:5A:251:C:H2'	7:5A:252:A:C8	2.54	0.42
12:AE:687:LEU:HB2	12:AE:691:PHE:HD2	1.83	0.42
15:B1:962:GLU:HA	15:B1:976:ILE:HB	2.01	0.42
16:BA:99:CYS:HG	16:BA:115:SER:HG	1.67	0.42
16:BA:536:LYS:HG3	16:BA:538:GLN:H	1.85	0.42
19:BD:362:HIS:H	19:BD:418:LYS:HD3	1.85	0.42
21:CA:138:TRP:CD1	21:CA:142:LYS:HE3	2.54	0.42
23:E1:122:ILE:HA	23:E1:161:LYS:O	2.19	0.42
24:E3:308:LYS:HB3	24:E3:345:VAL:HG21	2.01	0.42
28:MB:177:ILE:HG21	34:SA:1159:C:H5'	2.02	0.42
32:R2:1582:VAL:HG13	32:R2:1620:VAL:HG12	2.00	0.42
34:SA:139:C:H42	34:SA:175:G:H21	1.67	0.42
34:SA:162:A:OP2	34:SA:162:A:H8	2.00	0.42
34:SA:200:A:H2'	34:SA:201:G:H8	1.83	0.42
34:SA:868:G:H1	34:SA:960:U:H3	1.67	0.42
34:SA:890:C:H2'	34:SA:891:A:H8	1.84	0.42
34:SA:1482:C:O4'	46:SR:74:HIS:NE2	2.52	0.42
46:SR:52:LEU:C	46:SR:59:LYS:HZ1	2.20	0.42
48:SY:126:LYS:HG2	48:SY:131:SER:HA	2.01	0.42
7:5A:182:G:H2'	7:5A:183:A:H8	1.85	0.42
9:AB:54:UNK:O	9:AB:72:UNK:N	2.53	0.42
9:AB:121:UNK:N	9:AB:125:UNK:O	2.52	0.42
12:AE:132:THR:HG23	12:AE:155:ILE:HD11	2.01	0.42
16:BA:36:ARG:NH1	16:BA:699:GLU:OE2	2.53	0.42
16:BA:716:ASP:O	16:BA:744:ARG:NH2	2.46	0.42
17:BB:857:LEU:HD12	17:BB:860:ILE:HD11	2.02	0.42
18:BC:47:PRO:HD3	18:BC:53:LEU:HG	2.01	0.42
18:BC:343:MET:HB2	18:BC:353:LEU:HD21	2.01	0.42
18:BC:345:TYR:CD2	18:BC:350:LEU:HD12	2.54	0.42
18:BC:532:HIS:CG	18:BC:536:LEU:HD11	2.55	0.42
20:BE:914:ASP:OD1	20:BE:914:ASP:N	2.52	0.42
22:CB:712:ASN:HA	22:CB:1115:LEU:HG	2.00	0.42
22:CB:752:SER:HB3	22:CB:754:LEU:HG	2.01	0.42
26:K1:195:HIS:HA	26:K1:196:PRO:HD3	1.88	0.42
34:SA:340:U:H2'	34:SA:341:A:H8	1.84	0.42
34:SA:1253:U:O5'	43:SN:46:ARG:NH2	2.51	0.42
34:SA:1573:A:H4'	34:SA:1574:G:H5'	2.01	0.42
35:SC:77:GLU:OE2	45:SP:114:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5A:26:C:N4	7:5A:54:A:OP2	2.52	0.42
7:5A:125:G:H2'	7:5A:126:A:C8	2.54	0.42
8:AA:99:UNK:O	8:AA:108:UNK:N	2.51	0.42
12:AE:33:LEU:HD12	12:AE:115:LEU:HD11	2.01	0.42
12:AE:405:GLU:HA	12:AE:414:LEU:HD13	2.02	0.42
12:AE:1506:UNK:HA	12:AE:1507:UNK:HA	1.80	0.42
18:BC:13:ASN:N	18:BC:643:PHE:O	2.53	0.42
20:BE:140:TYR:HE1	20:BE:153:PHE:HD1	1.66	0.42
22:CB:559:GLU:OE2	22:CB:608:PHE:HB3	2.20	0.42
23:E1:28:PRO:HA	23:E1:29:PRO:HD3	1.88	0.42
34:SA:153:G:H2'	34:SA:154:G:C8	2.54	0.42
34:SA:283:U:N3	38:SH:188:ARG:CB	2.75	0.42
34:SA:891:A:H2'	34:SA:892:A:C8	2.54	0.42
34:SA:1158:C:N3	34:SA:1581:C:H3'	2.35	0.42
35:SC:207:LEU:HD22	35:SC:210:ILE:HD11	2.01	0.42
46:SR:44:LEU:HD12	46:SR:47:LYS:HG3	2.01	0.42
54:U1:13:UNK:O	54:U1:31:UNK:N	2.52	0.42
57:U4:66:LEU:HD13	57:U4:141:LEU:HD22	2.01	0.42
61:UC:445:UNK:O	61:UC:449:UNK:N	2.53	0.42
1:3A:63:C:H2'	1:3A:64:A:C8	2.54	0.42
1:3A:102:U:H2'	1:3A:103:A:C8	2.54	0.42
2:3C:251:ARG:HH12	8:AA:249:UNK:HA	1.85	0.42
5:3F:481:ILE:HA	5:3F:482:PRO:HD3	1.88	0.42
6:3H:93:VAL:HG12	6:3H:95:ARG:H	1.84	0.42
7:5A:352:U:H5"	7:5A:353:A:OP2	2.20	0.42
7:5A:556:G:H2'	7:5A:557:A:C8	2.51	0.42
8:AA:159:UNK:O	8:AA:167:UNK:N	2.53	0.42
12:AE:106:SER:HA	12:AE:109:TRP:HE1	1.84	0.42
12:AE:666:ALA:HA	12:AE:669:VAL:HG12	2.01	0.42
15:B1:134:PHE:HA	15:B1:137:ILE:HD12	2.00	0.42
16:BA:119:LEU:HD23	16:BA:142:HIS:HB2	2.01	0.42
17:BB:126:LEU:N	17:BB:139:GLY:O	2.52	0.42
17:BB:135:ARG:HA	17:BB:148:TRP:O	2.19	0.42
18:BC:33:ALA:H	18:BC:69:LEU:HD21	1.85	0.42
18:BC:667:GLN:HE22	18:BC:688:LEU:HB3	1.85	0.42
19:BD:519:SER:HB2	19:BD:534:SER:HA	2.02	0.42
22:CB:156:LYS:HD2	22:CB:237:HIS:CE1	2.55	0.42
22:CB:419:TYR:O	22:CB:423:LYS:CB	2.67	0.42
22:CB:883:LEU:HD11	22:CB:1051:LEU:HA	2.02	0.42
22:CB:1103:ARG:HD3	22:CB:1179:LYS:HE2	2.02	0.42
24:E3:449:HIS:HB3	24:E3:453:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E4:220:UNK:CB	25:E4:234:UNK:O	2.68	0.42
33:S1:126:UNK:N	33:S1:138:UNK:O	2.53	0.42
34:SA:156:A:H1'	34:SA:416:A:C5	2.54	0.42
34:SA:863:A:N6	34:SA:964:U:C2	2.88	0.42
34:SA:883:C:H2'	34:SA:884:A:H8	1.83	0.42
36:SF:206:ASP:HB2	36:SF:222:LEU:HB2	2.00	0.42
40:SJ:8:ARG:NH1	40:SJ:19:ALA:H	2.17	0.42
47:SX:76:SER:HA	47:SX:77:PRO:HA	1.92	0.42
1:3A:204:U:H2'	1:3A:205:G:C8	2.55	0.42
4:3E:210:LEU:HA	4:3E:256:ASN:HD22	1.84	0.42
5:3F:160:ILE:HG23	5:3F:525:GLN:HG2	2.01	0.42
5:3F:443:LEU:N	5:3F:471:GLN:O	2.46	0.42
12:AE:374:ARG:HE	12:AE:404:PHE:HE1	1.66	0.42
15:B1:133:GLU:OE1	15:B1:832:HIS:NE2	2.52	0.42
15:B1:634:ARG:HH12	31:R1:185:ARG:HG2	1.85	0.42
16:BA:516:SER:HA	16:BA:535:LEU:HB2	2.02	0.42
17:BB:630:PHE:O	17:BB:642:TRP:HB2	2.19	0.42
18:BC:222:LEU:HD12	18:BC:235:LYS:HB2	2.02	0.42
20:BE:342:TYR:OH	20:BE:345:SER:OG	2.36	0.42
22:CB:334:PHE:O	22:CB:338:SER:HB3	2.20	0.42
24:E3:260:TYR:HD1	24:E3:306:ALA:HB2	1.84	0.42
32:R2:1473:ASN:HA	32:R2:1505:ILE:HG23	2.00	0.42
32:R2:1476:VAL:O	32:R2:1480:ASN:ND2	2.52	0.42
32:R2:1644:LEU:HB3	32:R2:1654:LEU:HD13	2.02	0.42
34:SA:568:G:N2	34:SA:575:C:N3	2.65	0.42
34:SA:1042:G:H2'	34:SA:1043:A:C8	2.55	0.42
34:SA:1726:G:H2'	34:SA:1727:G:H8	1.84	0.42
35:SC:90:GLU:HB2	35:SC:97:LEU:HD21	2.01	0.42
37:SG:77:TYR:HA	37:SG:83:ARG:HE	1.84	0.42
38:SH:98:ARG:HH12	38:SH:103:GLY:N	2.17	0.42
40:SJ:78:ILE:HA	40:SJ:104:ILE:HG22	2.02	0.42
44:SO:71:ILE:HA	44:SO:74:ILE:HD12	2.01	0.42
1:3A:84:U:H2'	1:3A:85:G:C8	2.55	0.42
6:3G:56:ALA:N	6:3G:81:VAL:O	2.47	0.42
8:AA:29:UNK:CB	8:AA:33:UNK:O	2.68	0.42
15:B1:938:PRO:HB2	15:B1:941:ILE:HD11	2.02	0.42
16:BA:619:ARG:HD3	16:BA:619:ARG:H	1.85	0.42
20:BE:365:PHE:HA	20:BE:378:PHE:O	2.20	0.42
22:CB:781:ASP:OD1	22:CB:781:ASP:N	2.52	0.42
23:E1:196:LEU:HD11	23:E1:202:ILE:HD12	2.02	0.42
32:R2:1633:ASP:HB3	32:R2:1636:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:1177:C:H2'	34:SA:1178:G:C8	2.54	0.42
3:3D:54:ALA:HB2	3:3D:81:ILE:HD12	2.02	0.42
10:AC:137:UNK:HA	10:AC:152:UNK:O	2.20	0.42
15:B1:112:LYS:HB3	15:B1:141:HIS:ND1	2.35	0.42
15:B1:155:LEU:HD11	15:B1:190:ILE:HD11	2.02	0.42
15:B1:260:PRO:HG3	15:B1:282:LYS:HD3	2.00	0.42
17:BB:407:ALA:HB1	17:BB:414:LEU:HD11	2.02	0.42
17:BB:439:LEU:HD12	17:BB:440:PRO:HD2	2.01	0.42
18:BC:193:VAL:HG23	18:BC:215:GLY:H	1.85	0.42
23:E1:180:LEU:HD13	23:E1:237:ALA:HB1	2.01	0.42
31:R1:9:THR:HB	31:R1:31:ILE:HG22	2.02	0.42
31:R1:228:ASP:OD2	31:R1:230:TRP:NE1	2.52	0.42
34:SA:1202:A:H4'	34:SA:1205:C:H42	1.85	0.42
34:SA:1593:A:H2'	34:SA:1594:G:C8	2.55	0.42
7:5A:476:A:H2'	7:5A:477:G:C8	2.55	0.41
7:5A:578:G:H2'	7:5A:579:G:C8	2.55	0.41
15:B1:151:THR:HG22	15:B1:186:LEU:HB2	2.02	0.41
17:BB:255:ARG:HA	17:BB:346:VAL:HG11	2.01	0.41
18:BC:110:ALA:HB3	18:BC:150:LEU:HD11	2.01	0.41
19:BD:363:LEU:H	19:BD:418:LYS:NZ	2.18	0.41
19:BD:495:ASP:H	19:BD:498:ASN:HD22	1.68	0.41
21:CA:46:ASN:HD22	21:CA:47:SER:H	1.68	0.41
22:CB:345:TYR:OH	22:CB:472:THR:OG1	2.32	0.41
34:SA:256:A:H2'	34:SA:257:A:C8	2.54	0.41
34:SA:322:G:O3'	40:SJ:10:LYS:NZ	2.53	0.41
34:SA:1059:U:H4'	34:SA:1060:U:H5'	2.02	0.41
35:SC:196:GLU:HA	35:SC:199:ASN:HD22	1.85	0.41
38:SH:57:ASP:HA	38:SH:107:ALA:H	1.84	0.41
47:SX:17:ALA:HA	47:SX:22:LYS:HZ1	1.83	0.41
58:U5:82:LEU:HG	58:U5:174:ILE:HG21	2.02	0.41
1:3A:82:G:OP2	4:3E:365:ALA:HB1	2.20	0.41
2:3B:165:ALA:HB3	2:3B:168:LYS:HE2	2.02	0.41
3:3D:30:ARG:NH2	33:S1:204:UNK:O	2.53	0.41
4:3E:44:ILE:HG23	4:3E:127:LEU:HD22	2.02	0.41
5:3F:352:PRO:HB3	49:SZ:10:ARG:NH1	2.34	0.41
7:5A:250:G:N2	7:5A:262:U:O2	2.33	0.41
7:5A:384:U:H2'	7:5A:385:A:C8	2.55	0.41
12:AE:95:ASP:HA	12:AE:98:ILE:HD12	2.02	0.41
14:AG:475:UNK:HA	14:AG:489:UNK:HA	2.01	0.41
15:B1:63:THR:HG22	15:B1:193:ARG:HE	1.84	0.41
16:BA:111:PHE:HB3	16:BA:122:TRP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BA:743:PHE:CZ	16:BA:777:ARG:HB3	2.55	0.41
18:BC:206:GLU:HA	18:BC:209:LEU:HB2	2.03	0.41
18:BC:706:ARG:HH21	18:BC:715:LYS:HA	1.84	0.41
22:CB:130:LYS:HD2	22:CB:283:TYR:CZ	2.56	0.41
25:E4:120:UNK:HA	25:E4:126:UNK:HA	2.02	0.41
34:SA:482:U:H2'	34:SA:483:A:C8	2.54	0.41
34:SA:947:U:H2'	34:SA:948:G:C8	2.55	0.41
34:SA:1748:G:H2'	34:SA:1749:A:C8	2.54	0.41
39:SI:13:PRO:HA	39:SI:14:THR:HA	1.91	0.41
39:SI:122:HIS:HA	39:SI:125:ILE:HD12	2.02	0.41
44:SO:34:ILE:HA	44:SO:37:ILE:HD12	2.01	0.41
54:U1:116:UNK:HA	54:U1:131:UNK:HA	2.01	0.41
6:3H:79:VAL:HG23	6:3H:121:ILE:HG23	2.02	0.41
7:5A:529:A:H2'	7:5A:530:A:H8	1.85	0.41
9:AB:149:UNK:O	9:AB:160:UNK:HA	2.19	0.41
15:B1:969:VAL:HG22	15:B1:1000:ILE:H	1.84	0.41
16:BA:161:ILE:O	16:BA:172:ILE:HA	2.20	0.41
16:BA:600:SER:OG	16:BA:601:ILE:N	2.51	0.41
20:BE:828:LYS:HA	20:BE:870:GLN:HE22	1.85	0.41
20:BE:906:ALA:O	20:BE:910:GLN:HB2	2.21	0.41
22:CB:201:SER:O	22:CB:290:PHE:HA	2.20	0.41
28:MB:109:LEU:HD12	28:MB:111:PHE:HE1	1.85	0.41
34:SA:576:G:H8	34:SA:576:G:OP2	2.03	0.41
39:SI:14:THR:OG1	39:SI:15:GLU:OE1	2.38	0.41
41:SK:38:ASN:HB2	41:SK:41:GLU:HG3	2.02	0.41
41:SK:114:TYR:HD1	41:SK:119:ALA:HB3	1.86	0.41
47:SX:71:LYS:HB3	47:SX:130:TYR:CZ	2.55	0.41
56:U3:2147:UNK:O	56:U3:2151:UNK:N	2.53	0.41
2:3C:253:ILE:O	2:3C:257:SER:N	2.46	0.41
4:3E:166:ALA:HB1	4:3E:272:LEU:HD11	2.02	0.41
5:3F:485:ASN:O	5:3F:501:ILE:N	2.48	0.41
7:5A:133:U:H2'	7:5A:134:A:H8	1.84	0.41
13:AF:13:UNK:HA	13:AF:279:UNK:HA	2.03	0.41
14:AG:195:UNK:CB	14:AG:199:UNK:O	2.69	0.41
15:B1:187:SER:O	15:B1:193:ARG:NH2	2.51	0.41
16:BA:557:LYS:HE2	16:BA:598:ASN:HB2	2.02	0.41
17:BB:559:PHE:HE2	17:BB:561:ASP:HB2	1.85	0.41
20:BE:131:SER:HA	20:BE:137:ILE:HG12	2.02	0.41
23:E1:50:LEU:HD12	23:E1:116:THR:HG22	2.03	0.41
31:R1:52:PHE:HE1	31:R1:102:PRO:HG3	1.86	0.41
34:SA:283:U:OP2	38:SH:188:ARG:NE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SC:31:ASP:HB3	35:SC:45:LYS:NZ	2.35	0.41
38:SH:98:ARG:HH12	38:SH:103:GLY:H	1.67	0.41
44:SO:16:ILE:HA	44:SO:17:PRO:HD3	1.91	0.41
1:3A:60:A:H5"	1:3A:61:G:C8	2.55	0.41
3:3D:146:ASP:OD2	4:3E:237:THR:HB	2.21	0.41
5:3F:301:ASP:OD1	5:3F:301:ASP:N	2.53	0.41
7:5A:286:U:H2'	7:5A:287:G:C8	2.56	0.41
17:BB:50:ASN:ND2	17:BB:52:TRP:HE1	2.17	0.41
22:CB:381:HIS:NE2	22:CB:478:THR:O	2.44	0.41
22:CB:939:ILE:HG12	22:CB:943:VAL:HG13	2.02	0.41
34:SA:328:A:H2'	34:SA:329:G:H8	1.85	0.41
34:SA:1276:U:N3	34:SA:1437:U:O2	2.54	0.41
36:SF:130:GLN:HB2	36:SF:138:TYR:CZ	2.55	0.41
46:SR:59:LYS:HE2	46:SR:60:PHE:CZ	2.56	0.41
61:UC:297:UNK:O	61:UC:301:UNK:N	2.53	0.41
1:3A:85:G:H2'	1:3A:86:A:H8	1.85	0.41
7:5A:281:G:H2'	7:5A:282:G:C8	2.56	0.41
12:AE:345:ASP:HB3	12:AE:375:LEU:HB3	2.02	0.41
12:AE:748:LEU:O	12:AE:752:ALA:CB	2.69	0.41
12:AE:1128:UNK:O	12:AE:1133:UNK:N	2.54	0.41
13:AF:240:UNK:CB	13:AF:253:UNK:O	2.68	0.41
15:B1:560:PRO:HB2	31:R1:320:GLU:HG2	2.02	0.41
17:BB:142:ASP:OD1	17:BB:142:ASP:N	2.54	0.41
19:BD:435:PHE:HZ	19:BD:441:GLY:H	1.68	0.41
20:BE:544:ALA:HB3	20:BE:562:LEU:HD23	2.03	0.41
21:CA:94:GLY:CA	21:CA:121:ARG:HH12	2.34	0.41
22:CB:629:THR:HB	22:CB:667:CYS:HB2	2.01	0.41
23:E1:113:TYR:HE1	23:E1:123:GLU:HG3	1.86	0.41
23:E2:177:LYS:HB3	23:E2:221:VAL:HG12	2.02	0.41
31:R1:192:THR:N	31:R1:248:GLN:HE22	2.18	0.41
33:S1:178:UNK:N	33:S1:187:UNK:O	2.53	0.41
33:S1:282:UNK:N	33:S1:291:UNK:O	2.53	0.41
34:SA:1528:U:P	37:SG:109:LYS:HZ1	2.43	0.41
36:SF:72:VAL:HG12	36:SF:90:ILE:HG12	2.02	0.41
39:SI:9:LEU:HD22	39:SI:17:GLU:HB3	2.02	0.41
39:SI:129:LEU:HD11	39:SI:173:TYR:HB2	2.02	0.41
45:SP:84:ARG:HB2	45:SP:118:VAL:HG23	2.03	0.41
47:SX:86:ILE:HD11	47:SX:117:ARG:NH1	2.36	0.41
54:U1:34:UNK:HA	54:U1:49:UNK:HA	2.02	0.41
3:3D:176:GLN:O	3:3D:180:LEU:HB3	2.20	0.41
4:3E:163:ILE:HG23	4:3E:276:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3F:156:ASN:HA	5:3F:544:ALA:HB1	2.03	0.41
7:5A:191:U:H2'	7:5A:192:G:C8	2.56	0.41
12:AE:1167:UNK:O	12:AE:1171:UNK:CB	2.69	0.41
16:BA:329:VAL:HB	16:BA:342:GLN:HE21	1.85	0.41
16:BA:825:GLN:HA	16:BA:828:ILE:HD12	2.02	0.41
20:BE:503:ARG:NH1	20:BE:522:LEU:O	2.54	0.41
20:BE:592:ASP:HB3	20:BE:634:PHE:HD1	1.86	0.41
22:CB:855:LEU:HD13	22:CB:889:TYR:HD2	1.86	0.41
22:CB:1233:ASN:HD22	22:CB:1234:PHE:H	1.69	0.41
23:E1:36:LYS:HB3	23:E1:172:PRO:HA	2.02	0.41
31:R1:305:LYS:HA	31:R1:358:GLY:HA2	2.02	0.41
33:S1:364:UNK:O	33:S1:373:UNK:N	2.54	0.41
34:SA:1202:A:H1'	34:SA:1207:C:H42	1.85	0.41
36:SF:112:HIS:NE2	36:SF:237:SER:O	2.54	0.41
40:SJ:103:GLN:HG3	40:SJ:164:ARG:HB3	2.02	0.41
43:SN:29:LYS:HG3	43:SN:100:TRP:CD1	2.55	0.41
2:3C:296:GLU:HG3	2:3C:298:ILE:HG12	2.03	0.41
5:3F:334:GLU:HG2	5:3F:351:ILE:HB	2.03	0.41
7:5A:589:U:H2'	7:5A:590:G:C8	2.56	0.41
12:AE:775:ILE:O	12:AE:779:SER:OG	2.30	0.41
13:AF:141:UNK:O	13:AF:150:UNK:N	2.54	0.41
18:BC:281:THR:HG23	18:BC:327:ILE:HD13	2.02	0.41
18:BC:588:LYS:HG2	18:BC:589:GLN:HE21	1.85	0.41
20:BE:566:SER:HA	20:BE:581:LEU:O	2.21	0.41
21:CA:191:PHE:O	21:CA:195:GLU:HB2	2.21	0.41
24:E3:305:ARG:C	24:E3:307:VAL:N	2.74	0.41
31:R1:312:ARG:HH21	31:R1:347:ASN:HD21	1.69	0.41
34:SA:348:U:H5"	42:SM:106:ASN:HB2	2.02	0.41
34:SA:505:A:H2'	34:SA:507:U:H5'	2.02	0.41
34:SA:1173:C:O2'	34:SA:1601:G:N2	2.51	0.41
34:SA:1759:C:H2'	34:SA:1760:G:C8	2.56	0.41
38:SH:188:ARG:NH1	38:SH:191:ARG:CG	2.80	0.41
40:SJ:90:LEU:HD22	40:SJ:95:THR:HG21	2.02	0.41
46:SR:13:LYS:HG3	46:SR:14:LYS:H	1.85	0.41
48:SY:51:GLY:HA2	48:SY:77:ILE:HG13	2.03	0.41
1:3A:9:A:H2'	1:3A:10:C:C6	2.56	0.41
1:3A:113:G:H1'	1:3A:257:A:N6	2.35	0.41
3:3D:218:LYS:HZ1	3:3D:240:LEU:HD22	1.85	0.41
4:3E:174:ASP:O	4:3E:178:ASN:HB2	2.21	0.41
4:3E:314:ALA:HA	4:3E:317:ILE:HD12	2.02	0.41
5:3F:364:GLU:HG2	5:3F:366:GLN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AE:767:GLN:HA	12:AE:770:LYS:HB3	2.03	0.41
12:AE:1477:UNK:O	12:AE:1481:UNK:CB	2.69	0.41
12:AE:1663:UNK:O	12:AE:1667:UNK:CB	2.69	0.41
13:AF:407:UNK:O	13:AF:411:UNK:CB	2.69	0.41
14:AG:243:UNK:O	14:AG:251:UNK:N	2.53	0.41
14:AG:305:UNK:HA	14:AG:312:UNK:HA	2.02	0.41
15:B1:57:PRO:HD3	15:B1:101:ALA:HB3	2.02	0.41
15:B1:978:ARG:HG2	15:B1:980:LEU:H	1.85	0.41
16:BA:139:HIS:NE2	16:BA:176:ASP:OD1	2.50	0.41
16:BA:162:LEU:HD23	16:BA:199:PHE:HB2	2.02	0.41
16:BA:795:ASN:HA	16:BA:798:TRP:HD1	1.85	0.41
17:BB:37:GLY:HA3	17:BB:38:PRO:HD3	1.90	0.41
17:BB:214:ASP:HB2	17:BB:258:LYS:HD3	2.01	0.41
17:BB:833:LEU:HD13	17:BB:836:ILE:HD13	2.03	0.41
18:BC:256:ARG:NH1	18:BC:299:ASN:OD1	2.50	0.41
19:BD:273:ARG:HB2	19:BD:284:LEU:HD11	2.03	0.41
19:BD:543:LEU:HD23	19:BD:556:PRO:HG3	2.03	0.41
20:BE:462:PHE:O	20:BE:480:SER:N	2.54	0.41
21:CA:133:SER:O	21:CA:137:CYS:HB3	2.21	0.41
22:CB:168:ILE:HD12	22:CB:171:ASN:H	1.86	0.41
22:CB:384:SER:HB3	22:CB:588:GLN:HE22	1.85	0.41
22:CB:748:LEU:HA	22:CB:787:GLU:OE2	2.21	0.41
23:E2:104:ILE:HG23	23:E2:110:LEU:HD22	2.02	0.41
34:SA:107:C:H2'	34:SA:108:A:H8	1.85	0.41
34:SA:253:A:H2'	34:SA:254:A:C8	2.56	0.41
34:SA:453:U:OP2	34:SA:455:C:N4	2.54	0.41
34:SA:576:G:O3'	48:SY:63:GLN:NE2	2.54	0.41
34:SA:877:G:H2'	34:SA:878:G:H8	1.86	0.41
34:SA:1049:U:H2'	34:SA:1050:G:H8	1.86	0.41
34:SA:1152:A:H2'	34:SA:1153:G:C8	2.56	0.41
35:SC:161:ILE:HG22	35:SC:165:ARG:NH1	2.35	0.41
37:SG:26:ALA:HB2	46:SR:26:LYS:NZ	2.36	0.41
37:SG:130:ILE:H	37:SG:130:ILE:HG13	1.71	0.41
42:SM:55:ASP:OD2	42:SM:113:PRO:HD2	2.20	0.41
44:SO:124:ARG:HG2	44:SO:127:ARG:HH21	1.86	0.41
45:SP:31:THR:HG22	45:SP:38:THR:HA	2.03	0.41
49:SZ:55:VAL:HG22	49:SZ:75:VAL:HG23	2.02	0.41
57:U4:70:ASN:HA	57:U4:73:ASN:HD22	1.84	0.41
1:3A:252:C:H2'	1:3A:253:G:C4	2.56	0.41
4:3E:62:SER:HA	4:3E:67:LYS:HB3	2.03	0.41
4:3E:288:THR:O	4:3E:292:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AE:769:LEU:HB2	12:AE:773:GLN:HE22	1.85	0.41
17:BB:640:LYS:HE2	17:BB:652:LYS:HD2	2.02	0.41
18:BC:135:TYR:CD2	18:BC:137:THR:HG22	2.55	0.41
20:BE:797:ASP:OD1	20:BE:797:ASP:N	2.53	0.41
22:CB:563:ALA:O	22:CB:567:THR:OG1	2.24	0.41
28:MB:150:THR:HG21	28:MB:170:VAL:HG21	2.03	0.41
33:S1:159:UNK:O	33:S1:168:UNK:N	2.54	0.41
34:SA:1042:G:H2'	34:SA:1043:A:H8	1.86	0.41
34:SA:1045:C:H2'	34:SA:1046:G:H8	1.86	0.41
35:SC:91:VAL:HB	35:SC:96:LEU:HD13	2.03	0.41
40:SJ:39:GLY:O	40:SJ:59:ARG:HB3	2.21	0.41
46:SR:21:HIS:CE1	46:SR:68:ARG:NH1	2.89	0.41
56:U3:395:UNK:HA	56:U3:440:UNK:HA	2.03	0.41
1:3A:66:U:H2'	1:3A:67:G:C8	2.55	0.40
3:3D:44:PHE:CE2	3:3D:46:LYS:HB3	2.56	0.40
7:5A:244:U:H2'	7:5A:245:C:C6	2.56	0.40
10:AC:470:UNK:O	10:AC:474:UNK:CB	2.68	0.40
12:AE:756:LEU:O	12:AE:760:PHE:CB	2.65	0.40
15:B1:216:TRP:O	15:B1:220:HIS:ND1	2.44	0.40
18:BC:150:LEU:HD12	18:BC:159:LYS:HG2	2.02	0.40
18:BC:264:ASP:OD1	18:BC:264:ASP:N	2.47	0.40
19:BD:403:VAL:HG12	20:BE:605:LEU:HG	2.03	0.40
19:BD:424:ILE:O	19:BD:432:VAL:HA	2.21	0.40
22:CB:333:ASN:O	22:CB:337:LEU:CB	2.70	0.40
23:E1:129:ARG:HB3	34:SA:1192:C:H5"	2.02	0.40
23:E2:36:LYS:HD2	23:E2:172:PRO:HA	2.02	0.40
23:E2:143:GLN:O	23:E2:147:LYS:HB2	2.20	0.40
24:E3:300:ASN:HB3	24:E3:303:ILE:HG12	2.02	0.40
24:E3:334:GLU:O	24:E3:338:ALA:CB	2.60	0.40
28:MB:112:PRO:HD3	28:MB:184:GLU:HG2	2.03	0.40
32:R2:1638:ARG:NH2	32:R2:1662:GLU:OE1	2.52	0.40
34:SA:289:U:H2'	34:SA:290:G:H8	1.86	0.40
34:SA:1164:G:OP1	37:SG:166:ARG:NH2	2.55	0.40
34:SA:1224:A:H2'	34:SA:1225:U:H6	1.86	0.40
34:SA:1727:G:H2'	34:SA:1728:A:C8	2.55	0.40
49:SZ:54:ALA:O	49:SZ:76:TYR:N	2.43	0.40
2:3B:255:LEU:O	2:3B:259:MET:HB2	2.21	0.40
4:3E:234:ARG:O	4:3E:238:ALA:CB	2.69	0.40
4:3E:299:LEU:HD23	4:3E:341:LEU:HD12	2.03	0.40
5:3F:157:LEU:HA	5:3F:191:SER:HA	2.03	0.40
5:3F:230:ASN:HD21	5:3F:258:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3F:323:ASP:OD2	5:3F:342:ARG:HB2	2.21	0.40
9:AB:4:UNK:HA	9:AB:284:UNK:HA	2.04	0.40
12:AE:566:CYS:O	12:AE:570:ALA:CB	2.68	0.40
12:AE:628:ASN:O	12:AE:632:THR:OG1	2.26	0.40
14:AG:446:UNK:O	14:AG:454:UNK:N	2.55	0.40
16:BA:159:ARG:HA	16:BA:175:VAL:HB	2.03	0.40
17:BB:592:SER:HB3	17:BB:598:LYS:HZ1	1.87	0.40
17:BB:821:LEU:HB3	17:BB:863:PHE:HE2	1.87	0.40
18:BC:50:ARG:HB2	18:BC:375:ALA:HB2	2.03	0.40
18:BC:239:VAL:HB	22:CB:636:GLU:HG3	2.03	0.40
19:BD:411:TYR:CE1	19:BD:423:LEU:O	2.74	0.40
22:CB:738:TYR:O	22:CB:742:PHE:HB3	2.22	0.40
33:S1:157:UNK:N	33:S1:170:UNK:O	2.54	0.40
34:SA:1228:G:H21	43:SN:66:VAL:HG22	1.86	0.40
54:U1:14:UNK:HA	54:U1:30:UNK:HA	2.02	0.40
17:BB:405:LEU:HD22	17:BB:459:LEU:HD21	2.03	0.40
18:BC:474:SER:H	18:BC:478:GLN:NE2	2.20	0.40
19:BD:288:LEU:HD22	19:BD:324:TRP:CD1	2.56	0.40
19:BD:424:ILE:HD13	19:BD:433:TRP:CD1	2.56	0.40
20:BE:192:ASN:O	20:BE:196:GLY:N	2.54	0.40
20:BE:440:ALA:HB3	20:BE:455:PHE:HB2	2.03	0.40
22:CB:267:ILE:HG21	22:CB:295:LEU:HG	2.03	0.40
34:SA:116:U:H2'	34:SA:117:U:C6	2.57	0.40
34:SA:190:C:H1'	34:SA:191:C:H5'	2.03	0.40
34:SA:200:A:H2'	34:SA:201:G:C8	2.56	0.40
34:SA:976:G:H2'	34:SA:977:A:C8	2.56	0.40
39:SI:50:ASP:HA	39:SI:56:LYS:HA	2.02	0.40
41:SK:171:ARG:HH21	41:SK:175:ARG:NH2	2.19	0.40
7:5A:525:U:H2'	7:5A:526:U:C6	2.57	0.40
14:AG:239:UNK:HA	14:AG:260:UNK:HA	2.04	0.40
17:BB:496:THR:OG1	17:BB:520:LEU:O	2.31	0.40
18:BC:222:LEU:HB2	18:BC:235:LYS:H	1.86	0.40
19:BD:412:GLN:NE2	19:BD:459:GLN:OE1	2.46	0.40
20:BE:97:LYS:HZ3	20:BE:111:GLU:CD	2.23	0.40
22:CB:227:LYS:O	22:CB:231:TYR:HB2	2.20	0.40
22:CB:853:ARG:HH21	22:CB:889:TYR:HE1	1.69	0.40
24:E3:258:VAL:O	24:E3:262:ALA:HB3	2.21	0.40
24:E3:300:ASN:HD22	24:E3:301:TYR:H	1.70	0.40
24:E3:318:PHE:HE2	24:E3:351:HIS:HB3	1.86	0.40
24:E3:398:ARG:HB3	24:E3:443:THR:HA	2.03	0.40
26:K1:166:VAL:HA	26:K1:171:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SA:96:G:N1	34:SA:403:G:OP1	2.55	0.40
34:SA:356:G:H2'	34:SA:357:G:C8	2.55	0.40
34:SA:922:G:H2'	34:SA:923:A:C8	2.56	0.40
34:SA:936:G:OP1	34:SA:1074:G:N2	2.45	0.40
37:SG:21:THR:OG1	37:SG:21:THR:O	2.37	0.40
48:SY:95:PHE:O	48:SY:142:LYS:NZ	2.48	0.40
3:3D:233:SER:HA	3:3D:234:LEU:HA	1.92	0.40
6:3G:84:ARG:HG3	6:3G:96:PRO:HB3	2.03	0.40
7:5A:291:G:H2'	7:5A:292:A:H8	1.86	0.40
12:AE:180:ILE:HD12	12:AE:223:PHE:HZ	1.86	0.40
15:B1:53:VAL:HG13	15:B1:118:LEU:HD22	2.02	0.40
19:BD:321:MET:HG3	19:BD:342:PHE:HD2	1.86	0.40
19:BD:411:TYR:CG	19:BD:412:GLN:N	2.90	0.40
34:SA:921:U:H2'	34:SA:922:G:C8	2.57	0.40
36:SF:182:TYR:CZ	36:SF:190:GLY:HA2	2.57	0.40
47:SX:17:ALA:HA	47:SX:22:LYS:HZ3	1.86	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	
2	3B	237/327 (72%)	227 (96%)	10 (4%)	0	100	100
2	3C	237/327 (72%)	216 (91%)	21 (9%)	0	100	100
3	3D	366/504 (73%)	343 (94%)	23 (6%)	0	100	100
4	3E	378/511 (74%)	358 (95%)	20 (5%)	0	100	100
5	3F	353/573 (62%)	334 (95%)	19 (5%)	0	100	100
6	3G	120/126 (95%)	114 (95%)	6 (5%)	0	100	100
6	3H	120/126 (95%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AE	751/1769 (42%)	703 (94%)	48 (6%)	0	100	100
15	B1	528/1183 (45%)	481 (91%)	47 (9%)	0	100	100
16	BA	747/923 (81%)	669 (90%)	76 (10%)	2 (0%)	41	77
17	BB	770/943 (82%)	682 (89%)	86 (11%)	2 (0%)	41	77
18	BC	779/817 (95%)	678 (87%)	96 (12%)	5 (1%)	25	66
19	BD	317/594 (53%)	278 (88%)	39 (12%)	0	100	100
20	BE	741/939 (79%)	699 (94%)	42 (6%)	0	100	100
21	CA	190/297 (64%)	180 (95%)	10 (5%)	0	100	100
22	CB	1086/1237 (88%)	1059 (98%)	27 (2%)	0	100	100
23	E1	213/252 (84%)	209 (98%)	4 (2%)	0	100	100
23	E2	210/252 (83%)	204 (97%)	6 (3%)	0	100	100
24	E3	256/483 (53%)	242 (94%)	12 (5%)	2 (1%)	19	60
26	K1	173/316 (55%)	167 (96%)	6 (4%)	0	100	100
27	MA	131/183 (72%)	128 (98%)	3 (2%)	0	100	100
28	MB	182/290 (63%)	168 (92%)	14 (8%)	0	100	100
29	MC	24/593 (4%)	24 (100%)	0	0	100	100
30	P1	171/274 (62%)	161 (94%)	10 (6%)	0	100	100
31	R1	353/367 (96%)	348 (99%)	5 (1%)	0	100	100
32	R2	266/1729 (15%)	262 (98%)	4 (2%)	0	100	100
35	SC	212/255 (83%)	170 (80%)	37 (18%)	5 (2%)	6	33
36	SF	235/261 (90%)	210 (89%)	24 (10%)	1 (0%)	34	72
37	SG	204/225 (91%)	181 (89%)	21 (10%)	2 (1%)	15	55
38	SH	170/236 (72%)	159 (94%)	11 (6%)	0	100	100
39	SI	161/190 (85%)	142 (88%)	18 (11%)	1 (1%)	25	66
40	SJ	166/200 (83%)	146 (88%)	19 (11%)	1 (1%)	25	66
41	SK	173/197 (88%)	157 (91%)	15 (9%)	1 (1%)	25	66
42	SM	139/156 (89%)	124 (89%)	13 (9%)	2 (1%)	11	46
43	SN	122/143 (85%)	83 (68%)	35 (29%)	4 (3%)	4	26
44	SO	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
45	SP	107/137 (78%)	95 (89%)	12 (11%)	0	100	100
46	SR	123/143 (86%)	113 (92%)	8 (6%)	2 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	SX	127/130 (98%)	115 (91%)	12 (9%)	0	100 100
48	SY	101/145 (70%)	82 (81%)	16 (16%)	3 (3%)	4 28
49	SZ	99/135 (73%)	88 (89%)	11 (11%)	0	100 100
50	Sc	77/82 (94%)	67 (87%)	10 (13%)	0	100 100
51	Sd	61/67 (91%)	57 (93%)	4 (7%)	0	100 100
52	Sf	28/63 (44%)	28 (100%)	0	0	100 100
53	Sg	49/152 (32%)	37 (76%)	12 (24%)	0	100 100
57	U4	124/189 (66%)	115 (93%)	8 (6%)	1 (1%)	19 60
58	U5	246/274 (90%)	229 (93%)	17 (7%)	0	100 100
All	All	12555/19466 (64%)	11579 (92%)	942 (8%)	34 (0%)	44 77

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	BC	298	SER
24	E3	306	ALA
35	SC	207	LEU
35	SC	209	ASN
37	SG	50	GLU
37	SG	51	VAL
43	SN	130	THR
46	SR	59	LYS
17	BB	798	ASN
18	BC	137	THR
24	E3	206	LEU
35	SC	181	LEU
35	SC	206	PRO
36	SF	195	ILE
42	SM	4	GLU
43	SN	131	ASP
48	SY	97	ASP
16	BA	130	ASP
18	BC	297	LEU
42	SM	3	THR
43	SN	90	LYS
16	BA	556	ARG
17	BB	797	VAL
18	BC	90	LEU
18	BC	772	LEU

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Mol	Chain	Res	Type
40	SJ	23	LYS
43	SN	126	TRP
48	SY	70	LYS
35	SC	210	ILE
39	SI	131	PHE
41	SK	134	ILE
46	SR	33	GLY
48	SY	96	VAL
57	U4	175	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	3B	202/240 (84%)	200 (99%)	2 (1%)	76 86
2	3C	202/240 (84%)	202 (100%)	0	100 100
3	3D	317/435 (73%)	315 (99%)	2 (1%)	86 92
4	3E	314/433 (72%)	312 (99%)	2 (1%)	86 92
5	3F	317/503 (63%)	316 (100%)	1 (0%)	92 95
6	3G	101/104 (97%)	100 (99%)	1 (1%)	76 86
6	3H	101/104 (97%)	100 (99%)	1 (1%)	76 86
12	AE	698/744 (94%)	688 (99%)	10 (1%)	67 80
15	B1	471/1039 (45%)	466 (99%)	5 (1%)	73 84
16	BA	663/812 (82%)	653 (98%)	10 (2%)	65 80
17	BB	687/832 (83%)	676 (98%)	11 (2%)	62 79
18	BC	687/719 (96%)	683 (99%)	4 (1%)	86 92
19	BD	281/529 (53%)	277 (99%)	4 (1%)	67 80
20	BE	657/819 (80%)	654 (100%)	3 (0%)	88 93
21	CA	178/274 (65%)	177 (99%)	1 (1%)	86 92
22	CB	1000/1125 (89%)	994 (99%)	6 (1%)	86 92
23	E1	191/222 (86%)	191 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	E2	193/222 (87%)	193 (100%)	0	100	100
24	E3	232/424 (55%)	228 (98%)	4 (2%)	60	78
26	K1	158/289 (55%)	158 (100%)	0	100	100
27	MA	123/172 (72%)	121 (98%)	2 (2%)	62	79
28	MB	164/258 (64%)	164 (100%)	0	100	100
29	MC	24/148 (16%)	24 (100%)	0	100	100
30	P1	151/238 (63%)	150 (99%)	1 (1%)	84	90
31	R1	302/312 (97%)	301 (100%)	1 (0%)	92	95
32	R2	235/1544 (15%)	233 (99%)	2 (1%)	78	87
35	SC	191/224 (85%)	191 (100%)	0	100	100
36	SF	203/222 (91%)	199 (98%)	4 (2%)	55	74
37	SG	173/191 (91%)	171 (99%)	2 (1%)	71	83
38	SH	141/201 (70%)	138 (98%)	3 (2%)	53	72
39	SI	146/170 (86%)	146 (100%)	0	100	100
40	SJ	138/161 (86%)	137 (99%)	1 (1%)	84	90
41	SK	149/166 (90%)	145 (97%)	4 (3%)	44	65
42	SM	128/137 (93%)	123 (96%)	5 (4%)	32	56
43	SN	88/119 (74%)	85 (97%)	3 (3%)	37	60
44	SO	117/128 (91%)	115 (98%)	2 (2%)	60	78
45	SP	66/105 (63%)	66 (100%)	0	100	100
46	SR	105/119 (88%)	103 (98%)	2 (2%)	57	75
47	SX	110/111 (99%)	110 (100%)	0	100	100
48	SY	85/120 (71%)	84 (99%)	1 (1%)	71	83
49	SZ	85/113 (75%)	83 (98%)	2 (2%)	49	69
50	Sc	68/71 (96%)	68 (100%)	0	100	100
51	Sd	56/60 (93%)	53 (95%)	3 (5%)	22	47
52	Sf	27/54 (50%)	27 (100%)	0	100	100
53	Sg	43/135 (32%)	42 (98%)	1 (2%)	50	70
57	U4	110/169 (65%)	110 (100%)	0	100	100
58	U5	231/256 (90%)	229 (99%)	2 (1%)	78	87
All	All	11109/15813 (70%)	11001 (99%)	108 (1%)	77	86

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3B	145	ASN
2	3B	231	ARG
3	3D	285	ARG
3	3D	391	ASN
4	3E	50	PHE
4	3E	178	ASN
5	3F	555	ASN
6	3G	105	ASN
6	3H	105	ASN
12	AE	83	ARG
12	AE	134	MET
12	AE	232	ASN
12	AE	487	THR
12	AE	559	ASN
12	AE	615	ASN
12	AE	630	TYR
12	AE	648	LYS
12	AE	729	LYS
12	AE	781	ASN
15	B1	246	ARG
15	B1	812	MET
15	B1	831	ARG
15	B1	833	ARG
15	B1	853	ARG
16	BA	78	ARG
16	BA	94	ASN
16	BA	306	ASN
16	BA	418	ARG
16	BA	420	ARG
16	BA	434	ASN
16	BA	619	ARG
16	BA	777	ARG
16	BA	811	ASN
16	BA	837	ASN
17	BB	20	ASN
17	BB	22	ASN
17	BB	118	ASN
17	BB	271	PHE
17	BB	411	ASN
17	BB	587	MET
17	BB	596	ASN
17	BB	620	ASN

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Mol	Chain	Res	Type
17	BB	629	ASN
17	BB	770	ASN
17	BB	799	LYS
18	BC	58	ASN
18	BC	157	ASN
18	BC	227	MET
18	BC	487	ARG
19	BD	357	ASN
19	BD	369	ASN
19	BD	440	ASN
19	BD	446	ARG
20	BE	392	ARG
20	BE	449	ARG
20	BE	587	ARG
21	CA	46	ASN
22	CB	155	ASN
22	CB	211	LYS
22	CB	216	LYS
22	CB	261	ASN
22	CB	683	ASN
22	CB	1233	ASN
24	E3	206	LEU
24	E3	300	ASN
24	E3	304	TYR
24	E3	457	ARG
27	MA	48	ASN
27	MA	71	ARG
30	P1	142	ASN
31	R1	301	MET
32	R2	1466	ARG
32	R2	1615	ARG
36	SF	39	ARG
36	SF	59	ARG
36	SF	198	LYS
36	SF	240	LYS
37	SG	122	ASN
37	SG	157	ARG
38	SH	25	ARG
38	SH	68	LEU
38	SH	188	ARG
40	SJ	64	ASN
41	SK	99	LEU

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Mol	Chain	Res	Type
41	SK	120	LYS
41	SK	138	LYS
41	SK	149	ARG
42	SM	5	LEU
42	SM	67	ARG
42	SM	116	ARG
42	SM	129	ARG
42	SM	141	LYS
43	SN	43	ARG
43	SN	91	VAL
43	SN	125	ASN
44	SO	55	ARG
44	SO	64	ARG
46	SR	23	LYS
46	SR	106	LYS
48	SY	144	ARG
49	SZ	32	ARG
49	SZ	34	ASN
51	Sd	14	LYS
51	Sd	49	ARG
51	Sd	64	ARG
53	Sg	123	ASN
58	U5	68	ARG
58	U5	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
2	3B	91	HIS
2	3B	145	ASN
3	3D	23	GLN
3	3D	37	GLN
3	3D	67	ASN
3	3D	125	GLN
3	3D	151	GLN
3	3D	176	GLN
3	3D	230	ASN
3	3D	318	HIS
3	3D	391	ASN
4	3E	61	ASN
4	3E	178	ASN
4	3E	256	ASN

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Mol	Chain	Res	Type
5	3F	195	GLN
5	3F	230	ASN
5	3F	555	ASN
6	3G	105	ASN
6	3H	105	ASN
12	AE	29	HIS
12	AE	43	GLN
12	AE	219	ASN
12	AE	227	ASN
12	AE	232	ASN
12	AE	258	HIS
12	AE	480	ASN
12	AE	615	ASN
12	AE	781	ASN
15	B1	136	ASN
15	B1	218	ASN
15	B1	233	HIS
15	B1	548	ASN
15	B1	893	ASN
15	B1	904	ASN
15	B1	909	ASN
16	BA	9	ASN
16	BA	17	GLN
16	BA	92	HIS
16	BA	94	ASN
16	BA	128	ASN
16	BA	306	ASN
16	BA	434	ASN
16	BA	483	GLN
16	BA	538	GLN
16	BA	552	ASN
16	BA	608	ASN
16	BA	811	ASN
16	BA	837	ASN
17	BB	20	ASN
17	BB	22	ASN
17	BB	118	ASN
17	BB	360	ASN
17	BB	390	GLN
17	BB	411	ASN
17	BB	596	ASN
17	BB	620	ASN

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Mol	Chain	Res	Type
17	BB	628	HIS
17	BB	629	ASN
17	BB	656	HIS
17	BB	770	ASN
18	BC	28	ASN
18	BC	58	ASN
18	BC	83	GLN
18	BC	184	HIS
18	BC	478	GLN
18	BC	576	ASN
18	BC	585	ASN
18	BC	587	GLN
18	BC	589	GLN
18	BC	667	GLN
19	BD	282	ASN
19	BD	335	GLN
19	BD	357	ASN
19	BD	369	ASN
19	BD	440	ASN
19	BD	498	ASN
19	BD	520	ASN
20	BE	300	GLN
20	BE	473	ASN
20	BE	900	ASN
20	BE	903	GLN
21	CA	35	HIS
21	CA	46	ASN
22	CB	120	HIS
22	CB	155	ASN
22	CB	261	ASN
22	CB	333	ASN
22	CB	409	ASN
22	CB	436	HIS
22	CB	441	GLN
22	CB	445	ASN
22	CB	560	ASN
22	CB	582	GLN
22	CB	588	GLN
22	CB	683	ASN
22	CB	904	HIS
22	CB	1029	ASN
22	CB	1078	HIS

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Mol	Chain	Res	Type
22	CB	1154	ASN
22	CB	1233	ASN
23	E1	111	GLN
23	E2	115	GLN
24	E3	250	ASN
24	E3	269	ASN
24	E3	300	ASN
24	E3	351	HIS
24	E3	449	HIS
26	K1	167	GLN
27	MA	48	ASN
28	MB	226	ASN
28	MB	236	HIS
30	P1	142	ASN
31	R1	248	GLN
32	R2	1416	GLN
32	R2	1616	ASN
32	R2	1661	GLN
32	R2	1693	ASN
35	SC	49	ASN
35	SC	118	GLN
35	SC	146	GLN
35	SC	149	GLN
35	SC	194	ASN
35	SC	199	ASN
35	SC	208	GLN
36	SF	98	ASN
37	SG	95	ASN
37	SG	100	ASN
37	SG	131	GLN
37	SG	158	GLN
38	SH	185	GLN
39	SI	147	ASN
40	SJ	64	ASN
42	SM	18	HIS
43	SN	125	ASN
44	SO	62	GLN
45	SP	80	HIS
46	SR	21	HIS
47	SX	15	ASN
47	SX	42	GLN
47	SX	80	ASN

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Mol	Chain	Res	Type
47	SX	92	ASN
48	SY	63	GLN
48	SY	79	ASN
57	U4	57	GLN
57	U4	73	ASN
58	U5	41	ASN
58	U5	105	ASN
58	U5	217	GLN
58	U5	248	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	151/333 (45%)	31 (20%)	1 (0%)
34	SA	1091/1812 (60%)	268 (24%)	22 (2%)
7	5A	452/700 (64%)	102 (22%)	4 (0%)
All	All	1694/2845 (59%)	401 (23%)	27 (1%)

All (401) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	9	A
1	3A	14	A
1	3A	15	U
1	3A	22	A
1	3A	24	U
1	3A	55	A
1	3A	58	A
1	3A	61	G
1	3A	64	A
1	3A	65	C
1	3A	79	G
1	3A	106	C
1	3A	109	G
1	3A	111	G
1	3A	114	A
1	3A	207	A
1	3A	254	A
1	3A	255	U
1	3A	256	G
1	3A	261	U

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Mol	Chain	Res	Type
1	3A	262	G
1	3A	267	A
1	3A	317	A
1	3A	318	U
1	3A	319	G
1	3A	322	A
1	3A	323	G
1	3A	324	U
1	3A	325	C
1	3A	328	A
1	3A	329	C
7	5A	12	G
7	5A	13	U
7	5A	14	U
7	5A	27	G
7	5A	58	U
7	5A	59	U
7	5A	60	G
7	5A	63	G
7	5A	67	G
7	5A	68	U
7	5A	69	U
7	5A	70	A
7	5A	76	U
7	5A	91	U
7	5A	101	G
7	5A	103	G
7	5A	106	A
7	5A	109	C
7	5A	121	G
7	5A	123	C
7	5A	124	A
7	5A	125	G
7	5A	129	U
7	5A	130	G
7	5A	142	U
7	5A	143	A
7	5A	145	A
7	5A	152	U
7	5A	153	U
7	5A	158	G
7	5A	169	A

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Mol	Chain	Res	Type
7	5A	170	U
7	5A	171	G
7	5A	176	U
7	5A	178	G
7	5A	181	A
7	5A	200	A
7	5A	211	G
7	5A	225	U
7	5A	226	U
7	5A	227	U
7	5A	234	A
7	5A	236	C
7	5A	237	A
7	5A	238	G
7	5A	239	U
7	5A	240	C
7	5A	246	G
7	5A	253	U
7	5A	261	U
7	5A	266	U
7	5A	267	U
7	5A	278	G
7	5A	280	A
7	5A	294	U
7	5A	338	A
7	5A	340	U
7	5A	349	G
7	5A	353	A
7	5A	354	G
7	5A	355	C
7	5A	361	G
7	5A	362	C
7	5A	363	A
7	5A	368	U
7	5A	370	U
7	5A	371	G
7	5A	372	A
7	5A	382	U
7	5A	383	G
7	5A	384	U
7	5A	386	A
7	5A	387	C

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Mol	Chain	Res	Type
7	5A	388	C
7	5A	391	C
7	5A	392	U
7	5A	393	C
7	5A	394	U
7	5A	395	C
7	5A	401	A
7	5A	402	G
7	5A	403	C
7	5A	404	G
7	5A	405	A
7	5A	419	A
7	5A	433	C
7	5A	434	G
7	5A	435	G
7	5A	436	G
7	5A	441	C
7	5A	442	U
7	5A	451	G
7	5A	452	A
7	5A	459	U
7	5A	464	G
7	5A	503	C
7	5A	508	C
7	5A	511	G
7	5A	514	U
7	5A	527	U
7	5A	528	G
7	5A	534	A
34	SA	8	U
34	SA	10	G
34	SA	25	C
34	SA	26	A
34	SA	27	U
34	SA	34	G
34	SA	39	A
34	SA	47	A
34	SA	50	C
34	SA	93	A
34	SA	94	U
34	SA	95	G
34	SA	103	A

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Mol	Chain	Res	Type
34	SA	114	C
34	SA	116	U
34	SA	127	G
34	SA	128	U
34	SA	129	U
34	SA	132	U
34	SA	133	U
34	SA	134	U
34	SA	135	A
34	SA	137	U
34	SA	138	A
34	SA	139	C
34	SA	140	A
34	SA	145	A
34	SA	146	U
34	SA	152	U
34	SA	153	G
34	SA	156	A
34	SA	159	U
34	SA	162	A
34	SA	179	A
34	SA	180	A
34	SA	181	A
34	SA	185	U
34	SA	186	C
34	SA	188	A
34	SA	190	C
34	SA	191	C
34	SA	192	U
34	SA	193	U
34	SA	194	U
34	SA	195	G
34	SA	196	G
34	SA	199	G
34	SA	200	A
34	SA	204	G
34	SA	215	A
34	SA	251	A
34	SA	261	U
34	SA	265	A
34	SA	266	A
34	SA	270	C

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Mol	Chain	Res	Type
34	SA	272	U
34	SA	273	G
34	SA	276	C
34	SA	277	U
34	SA	278	U
34	SA	279	G
34	SA	280	U
34	SA	281	G
34	SA	288	A
34	SA	299	A
34	SA	302	U
34	SA	316	A
34	SA	321	C
34	SA	322	G
34	SA	337	G
34	SA	338	C
34	SA	341	A
34	SA	348	U
34	SA	351	C
34	SA	352	A
34	SA	359	A
34	SA	360	A
34	SA	361	C
34	SA	369	A
34	SA	370	A
34	SA	372	G
34	SA	378	A
34	SA	379	U
34	SA	380	U
34	SA	381	C
34	SA	387	A
34	SA	399	A
34	SA	400	A
34	SA	401	A
34	SA	402	C
34	SA	403	G
34	SA	404	G
34	SA	416	A
34	SA	417	A
34	SA	418	G
34	SA	428	A
34	SA	433	C

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Mol	Chain	Res	Type
34	SA	440	U
34	SA	444	C
34	SA	452	A
34	SA	459	G
34	SA	466	U
34	SA	467	G
34	SA	468	A
34	SA	470	A
34	SA	475	A
34	SA	477	A
34	SA	484	C
34	SA	485	A
34	SA	486	G
34	SA	487	G
34	SA	488	G
34	SA	493	U
34	SA	494	U
34	SA	501	U
34	SA	503	G
34	SA	504	U
34	SA	506	A
34	SA	507	U
34	SA	508	U
34	SA	510	G
34	SA	511	A
34	SA	515	A
34	SA	522	U
34	SA	525	A
34	SA	526	A
34	SA	527	A
34	SA	528	U
34	SA	532	U
34	SA	538	A
34	SA	539	G
34	SA	540	G
34	SA	542	A
34	SA	543	C
34	SA	545	A
34	SA	546	U
34	SA	548	G
34	SA	558	U
34	SA	559	C

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Mol	Chain	Res	Type
34	SA	561	G
34	SA	570	A
34	SA	572	C
34	SA	576	G
34	SA	585	A
34	SA	592	A
34	SA	594	A
34	SA	605	A
34	SA	635	A
34	SA	862	A
34	SA	863	A
34	SA	865	A
34	SA	873	U
34	SA	876	G
34	SA	898	A
34	SA	914	G
34	SA	928	U
34	SA	929	A
34	SA	930	A
34	SA	932	U
34	SA	933	A
34	SA	935	U
34	SA	942	G
34	SA	951	A
34	SA	960	U
34	SA	966	A
34	SA	978	A
34	SA	1040	G
34	SA	1053	G
34	SA	1058	U
34	SA	1059	U
34	SA	1060	U
34	SA	1061	A
34	SA	1063	U
34	SA	1072	C
34	SA	1082	C
34	SA	1083	G
34	SA	1084	A
34	SA	1086	A
34	SA	1087	A
34	SA	1150	G
34	SA	1151	A

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Mol	Chain	Res	Type
34	SA	1155	G
34	SA	1156	C
34	SA	1157	A
34	SA	1158	C
34	SA	1159	C
34	SA	1160	A
34	SA	1164	G
34	SA	1165	G
34	SA	1167	G
34	SA	1193	A
34	SA	1207	C
34	SA	1209	C
34	SA	1212	G
34	SA	1217	A
34	SA	1218	G
34	SA	1227	A
34	SA	1228	G
34	SA	1229	G
34	SA	1238	A
34	SA	1243	G
34	SA	1244	A
34	SA	1245	G
34	SA	1246	C
34	SA	1251	U
34	SA	1256	A
34	SA	1265	G
34	SA	1269	U
34	SA	1270	G
34	SA	1272	U
34	SA	1273	G
34	SA	1275	A
34	SA	1276	U
34	SA	1278	G
34	SA	1282	U
34	SA	1427	A
34	SA	1428	G
34	SA	1431	C
34	SA	1432	U
34	SA	1433	G
34	SA	1435	G
34	SA	1436	A
34	SA	1437	U

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Mol	Chain	Res	Type
34	SA	1440	C
34	SA	1441	C
34	SA	1442	U
34	SA	1444	A
34	SA	1446	A
34	SA	1448	G
34	SA	1450	U
34	SA	1453	G
34	SA	1461	C
34	SA	1471	A
34	SA	1474	G
34	SA	1475	A
34	SA	1482	C
34	SA	1485	C
34	SA	1487	A
34	SA	1496	U
34	SA	1500	C
34	SA	1506	G
34	SA	1535	U
34	SA	1536	G
34	SA	1537	C
34	SA	1570	A
34	SA	1572	G
34	SA	1574	G
34	SA	1582	U
34	SA	1584	G
34	SA	1599	C
34	SA	1600	A
34	SA	1616	G
34	SA	1617	U
34	SA	1631	A
34	SA	1657	U
34	SA	1658	G
34	SA	1684	U
34	SA	1686	C
34	SA	1716	C
34	SA	1717	G
34	SA	1754	A
34	SA	1756	A
34	SA	1758	U
34	SA	1767	G
34	SA	1796	C

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Mol	Chain	Res	Type
34	SA	1804	A
34	SA	1806	A
34	SA	1812	U

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	78	G
7	5A	382	U
7	5A	385	A
7	5A	526	U
7	5A	527	U
34	SA	25	C
34	SA	139	C
34	SA	158	U
34	SA	192	U
34	SA	278	U
34	SA	351	C
34	SA	417	A
34	SA	467	G
34	SA	487	G
34	SA	503	G
34	SA	591	A
34	SA	913	G
34	SA	929	A
34	SA	1083	G
34	SA	1157	A
34	SA	1216	C
34	SA	1226	A
34	SA	1244	A
34	SA	1250	U
34	SA	1441	C
34	SA	1481	C
34	SA	1573	A

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

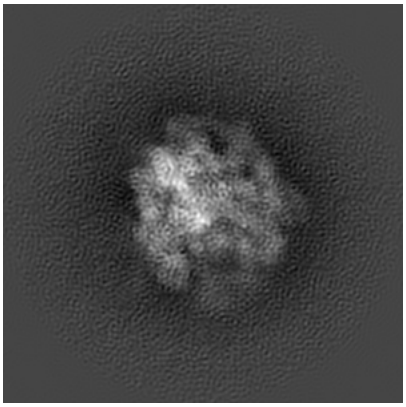
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6695. These allow visual inspection of the internal detail of the map and identification of artifacts.

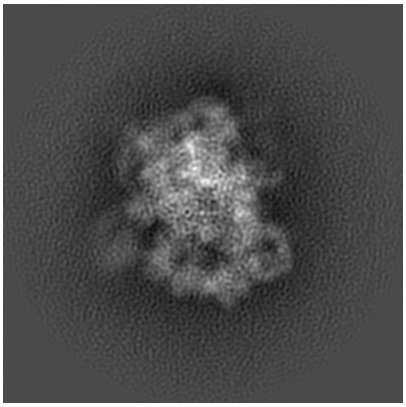
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

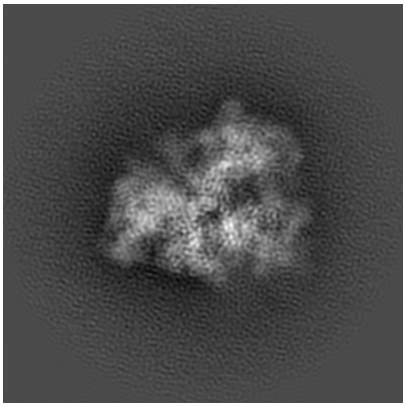
6.1.1 Primary map



X



Y

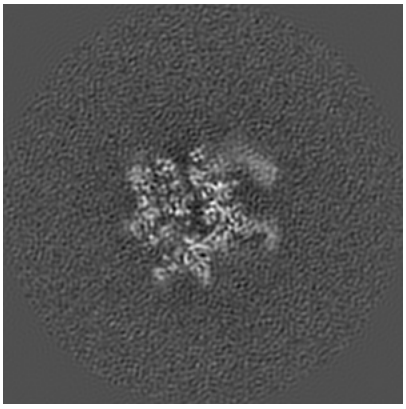


Z

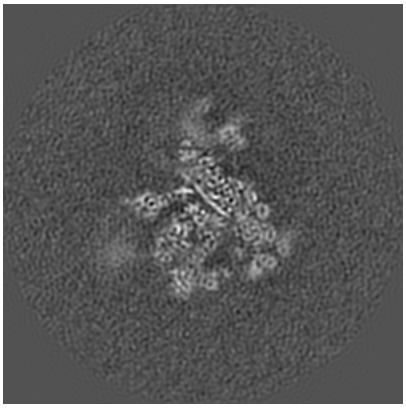
The images above show the map projected in three orthogonal directions.

6.2 Central slices

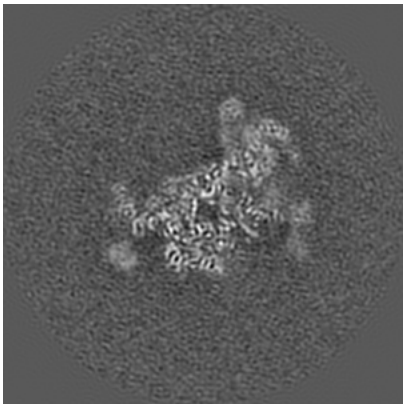
6.2.1 Primary map



X Index: 200



Y Index: 200

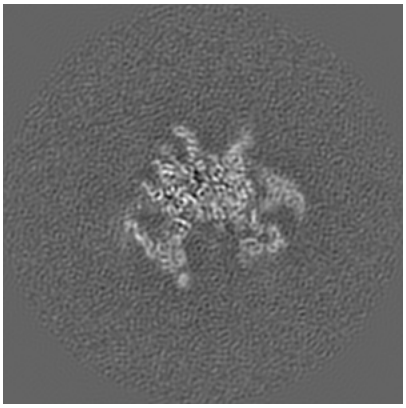


Z Index: 200

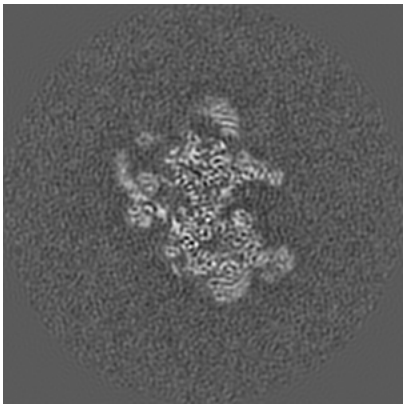
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

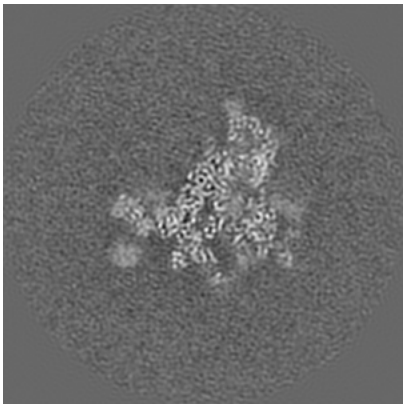
6.3.1 Primary map



X Index: 221



Y Index: 178



Z Index: 187

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

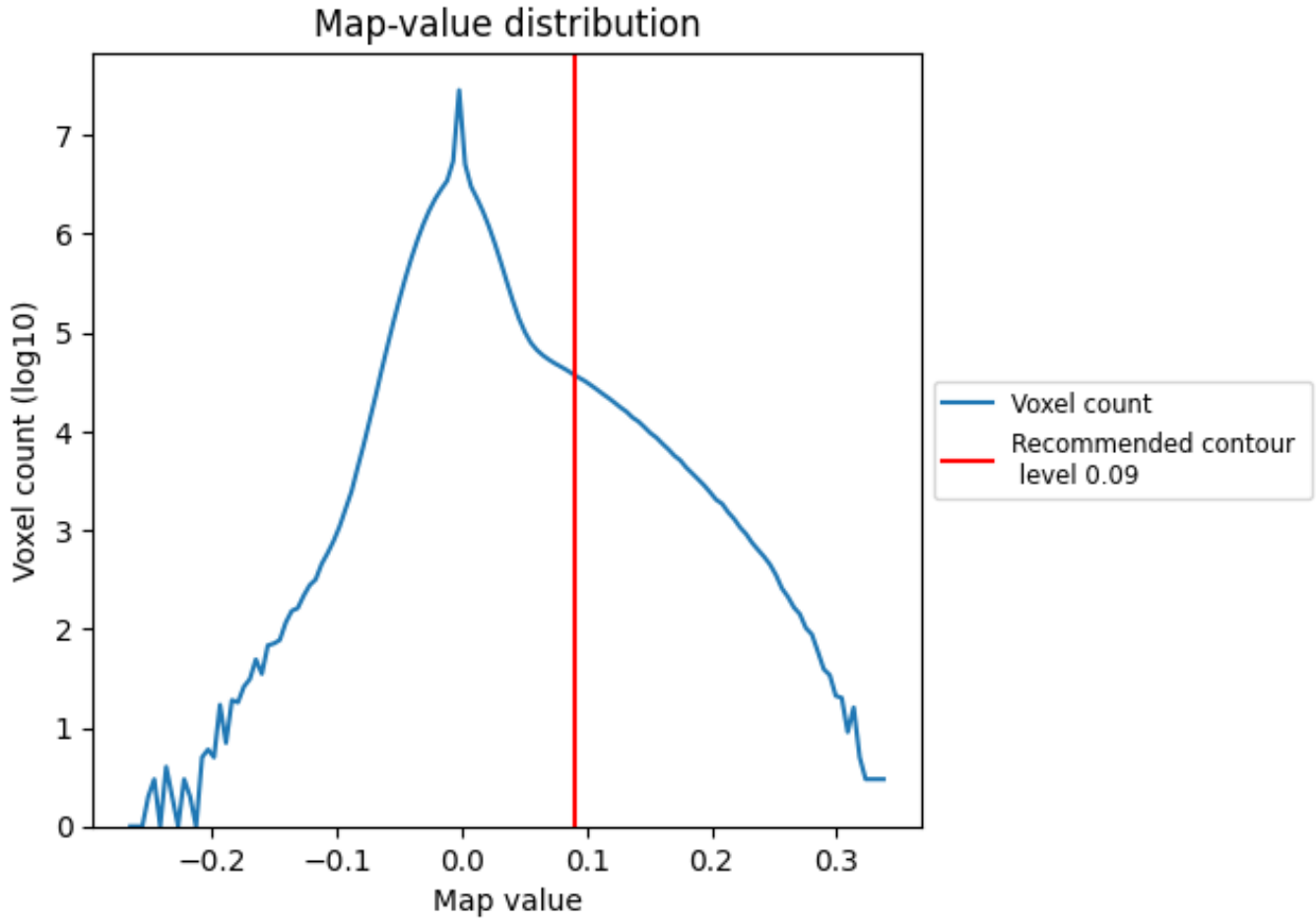
6.5 Mask visualisation (i)

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

7 Map analysis

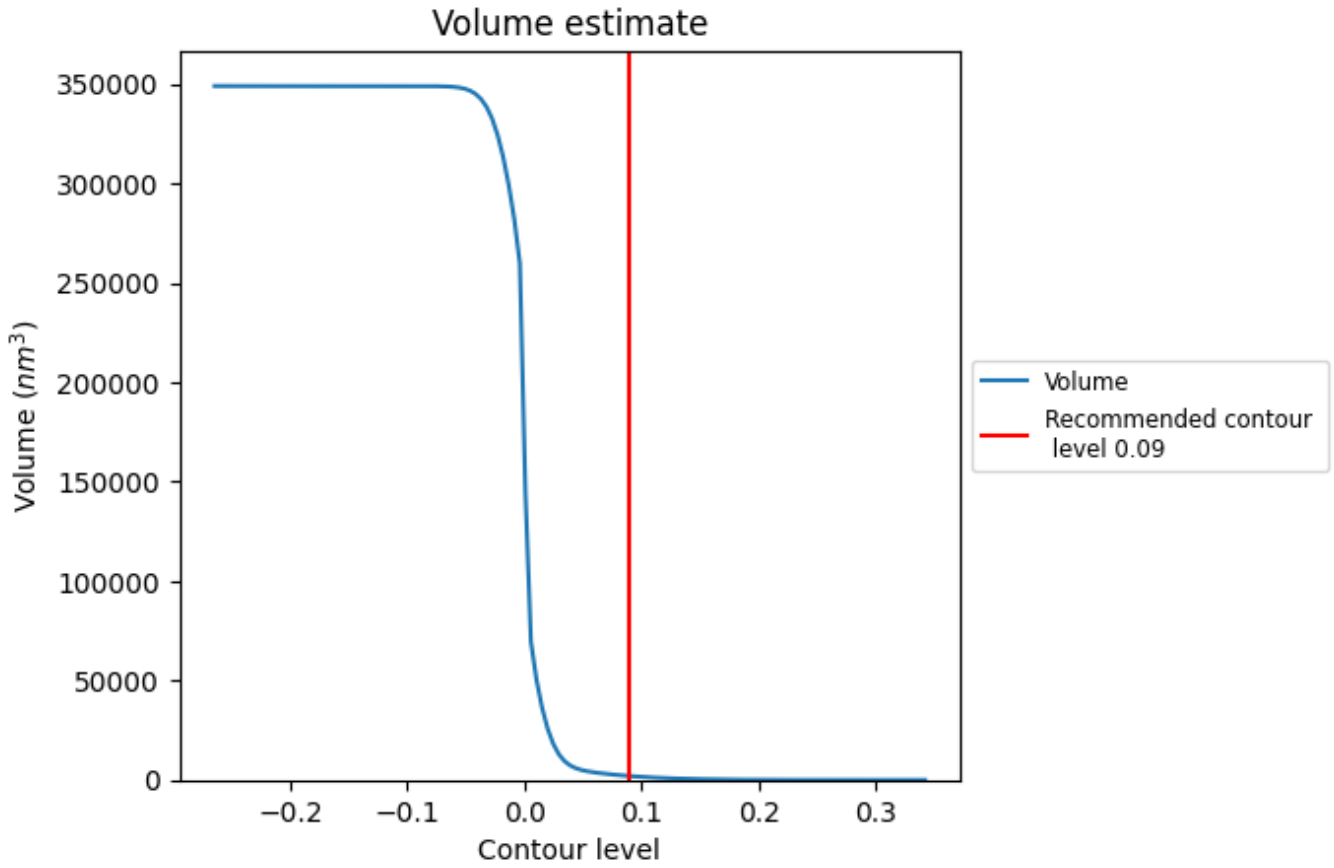
This section contains the results of statistical analysis of the map.

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.

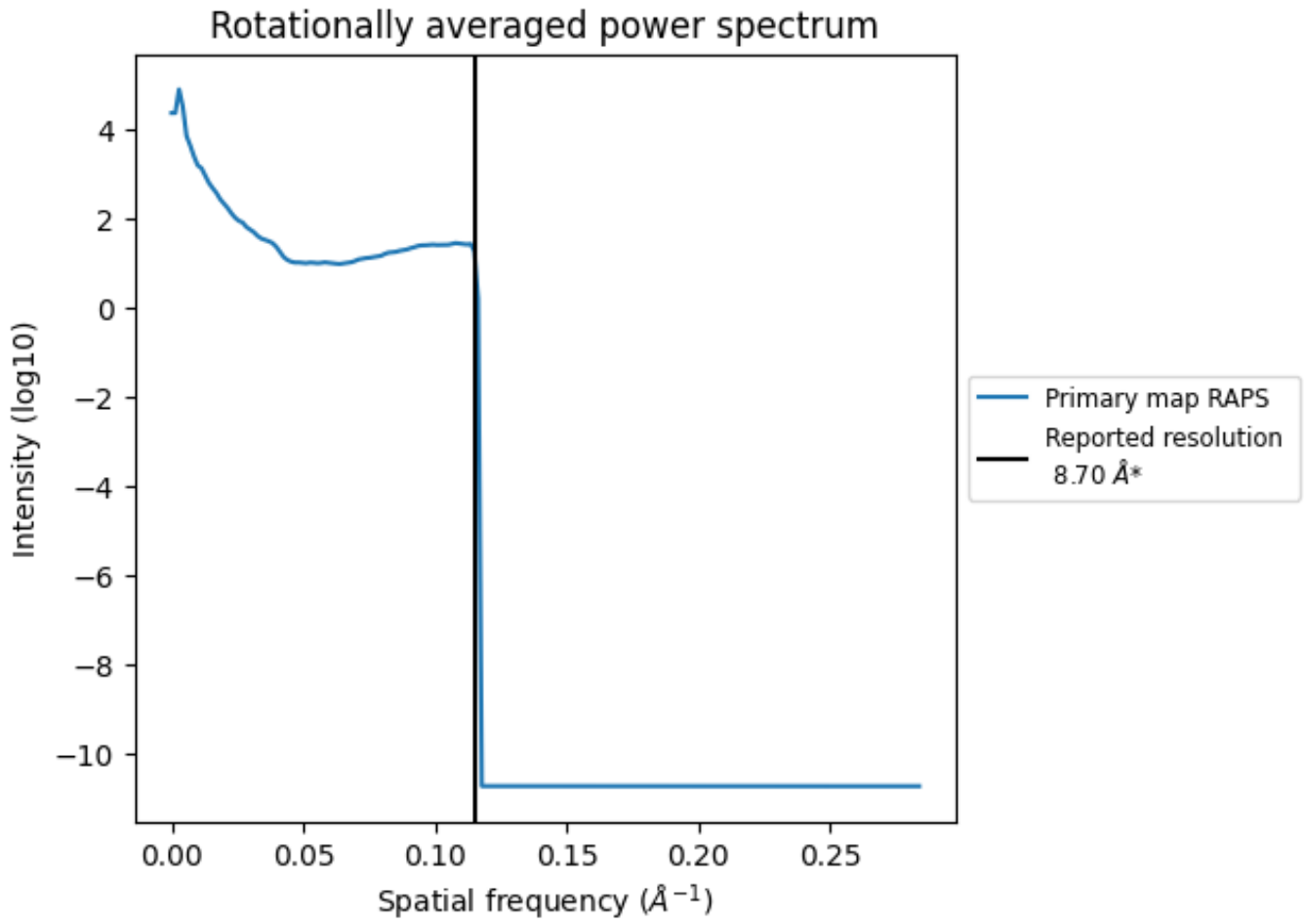
7.2 Volume estimate



The volume at the recommended contour level is 1973 nm^3; this corresponds to an approximate mass of 1782 kDa.

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

7.3 Rotationally averaged power spectrum (i)

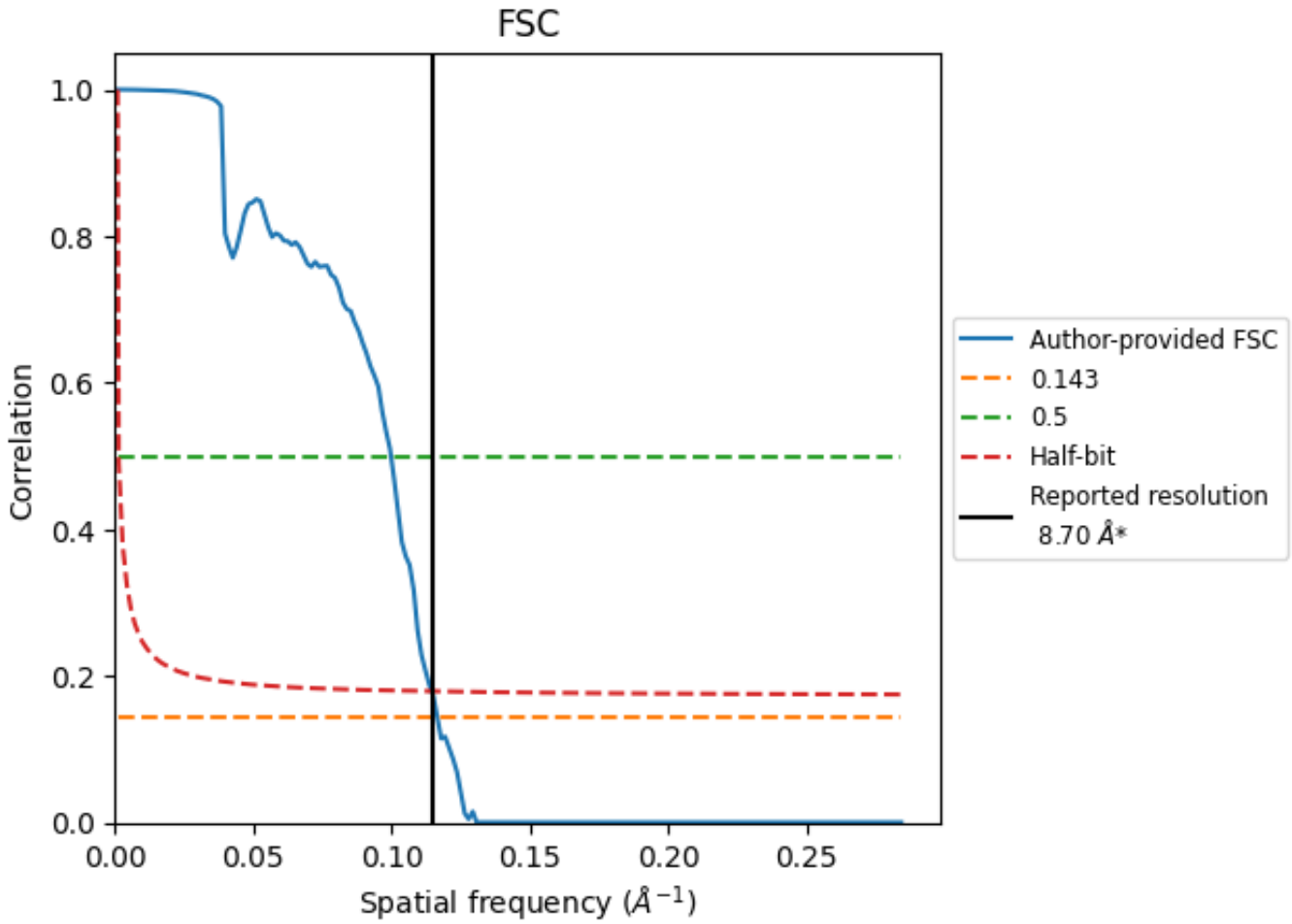


*Reported resolution corresponds to spatial frequency of 0.115 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

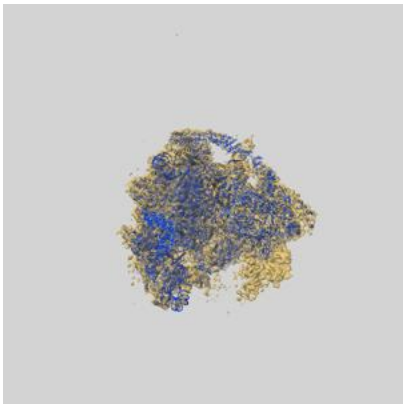
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.58	10.02	8.74
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

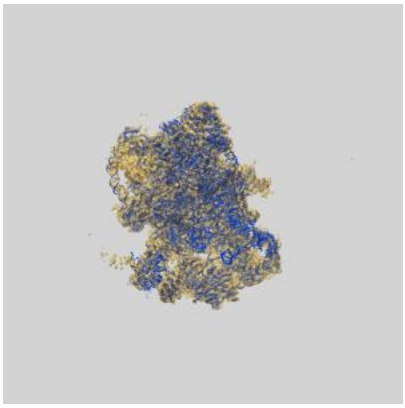
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6695 and PDB model 5WYJ. Per-residue inclusion information can be found in section 3 on page 15.

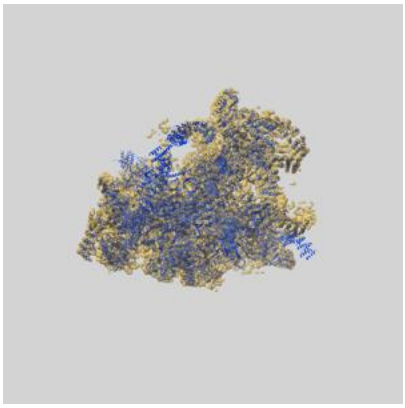
9.1 Map-model overlay



X



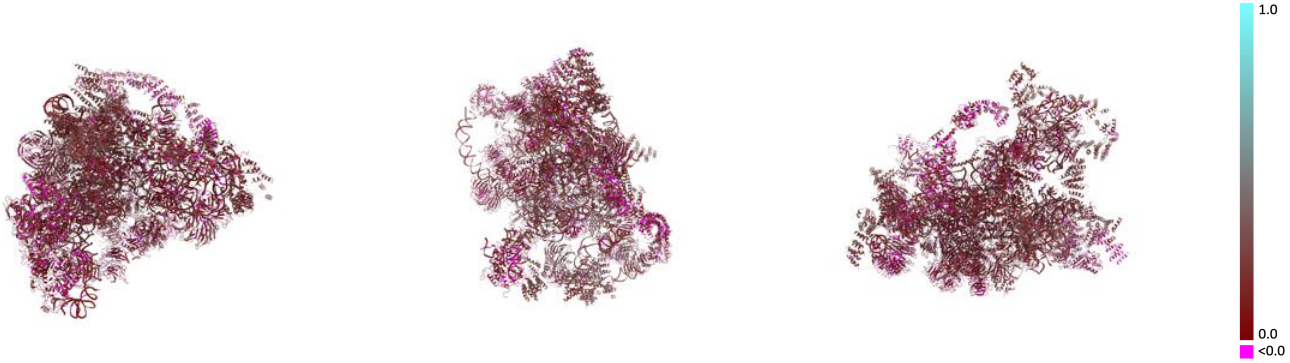
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

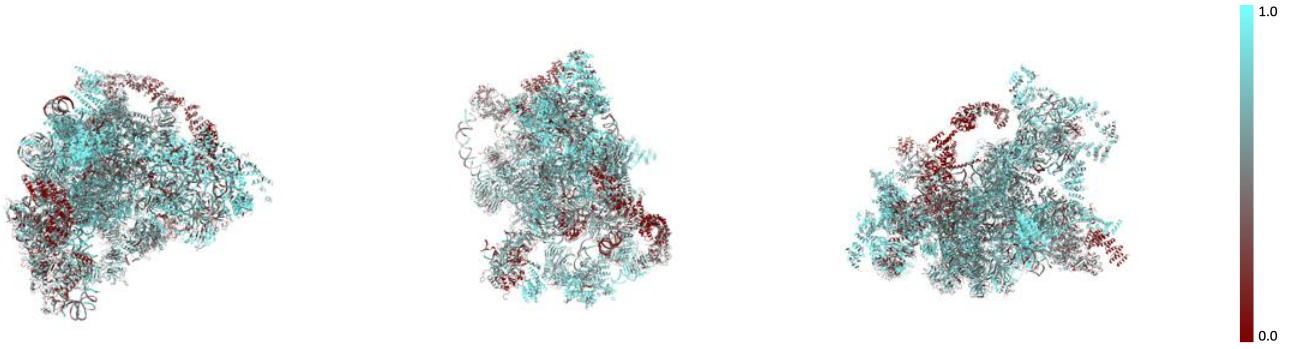
9.2 Q-score mapped to coordinate model



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.

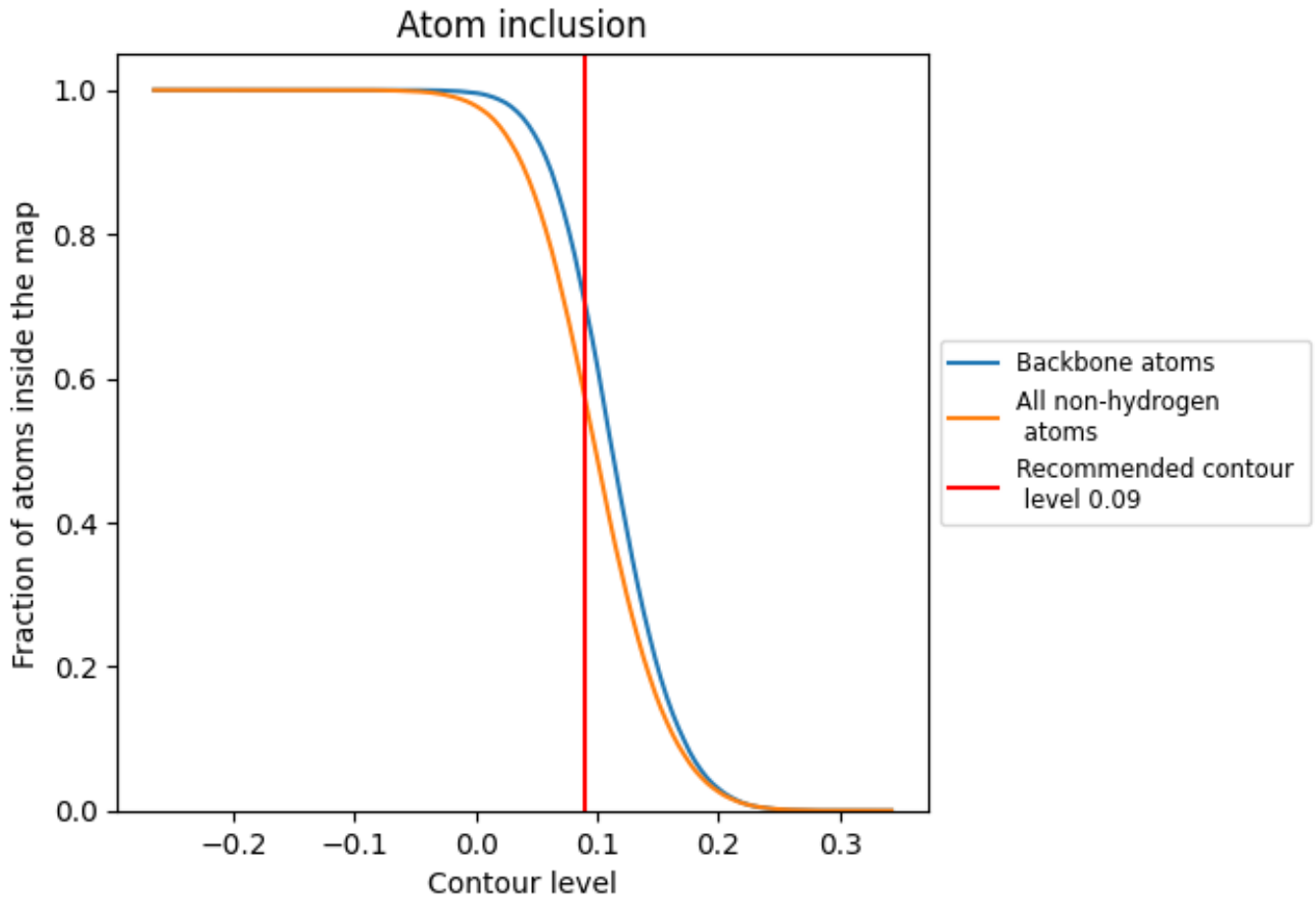
9.3 Atom inclusion mapped to coordinate model



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 57% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5717	0.1600
3A	0.7484	0.1830
3B	0.5458	0.1630
3C	0.3769	0.1290
3D	0.5854	0.1550
3E	0.5061	0.1500
3F	0.5810	0.1410
3G	0.5822	0.1580
3H	0.5548	0.1590
5A	0.4966	0.1750
AA	0.7525	0.2230
AB	0.6864	0.1990
AC	0.5123	0.1480
AD	0.7386	0.2190
AE	0.3774	0.1220
AF	0.8144	0.2410
AG	0.6980	0.2000
B1	0.5596	0.1420
BA	0.5864	0.1550
BB	0.5861	0.1320
BC	0.4752	0.1160
BD	0.5207	0.1110
BE	0.5976	0.1430
CA	0.3852	0.1130
CB	0.4158	0.1210
E1	0.4618	0.1290
E2	0.4841	0.1330
E3	0.4816	0.1220
E4	0.6484	0.2180
K1	0.4877	0.1450
MA	0.6006	0.1550
MB	0.5297	0.1350
MC	0.7115	0.2100
P1	0.5508	0.1530
R1	0.5599	0.1470

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Chain	Atom inclusion	Q-score
R2	0.0516	0.1040
S1	0.7818	0.2440
SA	0.7164	0.1710
SC	0.4735	0.1580
SF	0.5003	0.1300
SG	0.5640	0.1610
SH	0.3787	0.1150
SI	0.4751	0.1500
SJ	0.4862	0.1320
SK	0.5275	0.1470
SM	0.4038	0.1150
SN	0.0693	0.0710
SO	0.5171	0.1480
SP	0.5062	0.1440
SR	0.5839	0.1490
SX	0.5150	0.1580
SY	0.5013	0.1190
SZ	0.5134	0.1450
Sc	0.4317	0.1560
Sd	0.5178	0.1400
Sf	0.6432	0.1490
Sg	0.0181	0.0120
U1	0.8204	0.2560
U2	0.9068	0.2620
U3	0.7750	0.2360
U4	0.5397	0.1660
U5	0.1585	0.1000
UA	0.9189	0.2650
UB	0.8288	0.2540
UC	0.8200	0.2700