Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:24 PM EST

PDB ID	:	7MQ9
EMDB ID	:	EMD-23937
Title	:	Cryo-EM structure of the human SSU processome, state pre-A1*
Authors	:	Vanden Broeck, A.; Singh, S.; Klinge, S.
Deposited on	:	2021-05-05
Resolution	:	3.87 Å(reported)
Based on initial models	:	6ZQD, 2OZB, 5FAI, 6G18, 5WLC, 6G4S, 4JXM, 6ZOJ, 2IPX

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

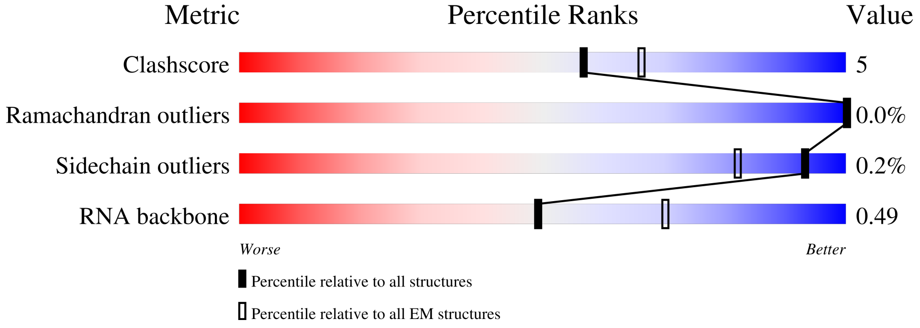
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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

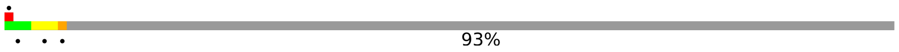
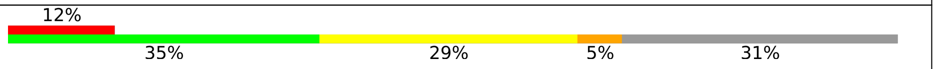
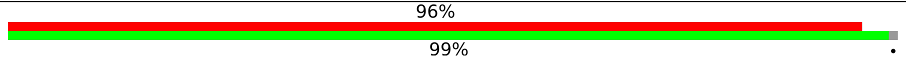
The reported resolution of this entry is 3.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	L0	3617	 • • • • 93%
2	L1	1872	 12% 35% 29% 5% 31%
3	L2	217	 • 43% 47% 9% •
4	L3	116	 96% 99% •
5	L4	263	 78% 13% 9%
6	L5	204	 • 80% 13% 7%
7	L6	249	 • 70% 19% 10%

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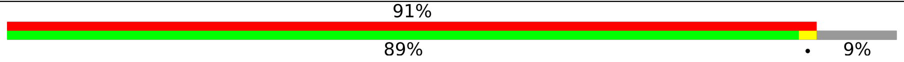
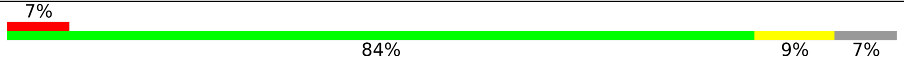
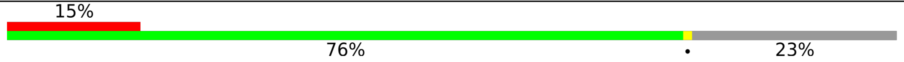
Mol	Chain	Length	Quality of chain
8	L7	194	
9	L8	208	
10	L9	194	
11	LA	132	
12	LC	146	
13	LD	158	
14	LF	133	
15	LG	69	
16	LH	830	
17	LI	699	
18	LJ	518	
19	LK	677	
19	LL	677	
20	LN	686	
21	LO	919	
22	LP	597	
23	LQ	943	
24	LS	556	
25	LT	951	
26	LU	445	
27	LW	610	
28	LZ	184	
29	NA	681	
30	NB	479	
31	ND	257	

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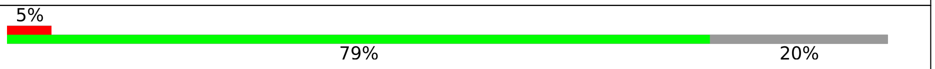
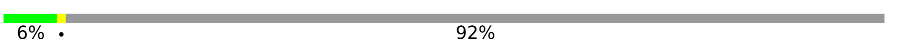
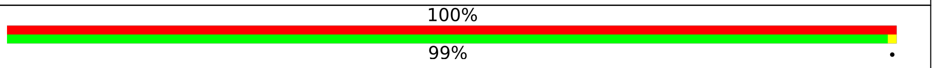
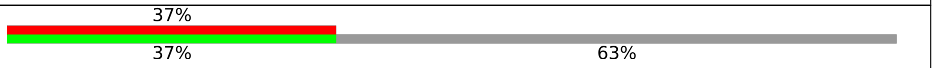
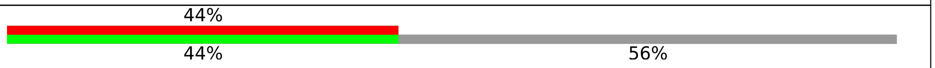
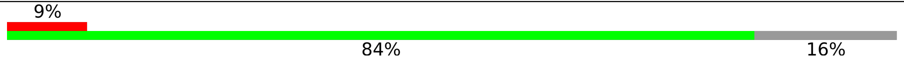
Mol	Chain	Length	Quality of chain
32	NE	293	
33	NF	151	
34	NG	151	
35	NJ	1025	
35	NK	1025	
36	NM	264	
37	NN	560	
38	NO	130	
39	NQ	84	
40	NR	861	
41	NT	156	
42	NU	135	
43	NW	688	
44	SA	594	
45	SB	529	
46	SC	321	
46	SD	321	
47	SE	128	
47	SF	128	
48	SH	373	
49	SI	1282	
50	SJ	244	
50	SK	244	
51	SL	198	
52	SM	291	

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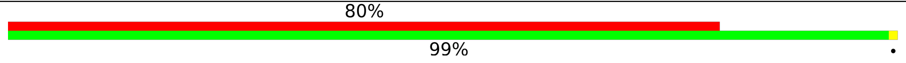
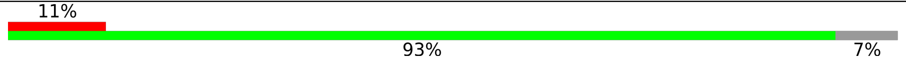
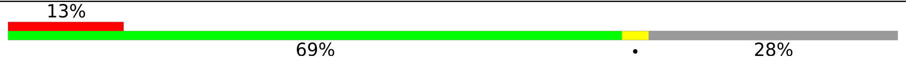
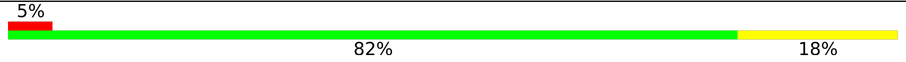
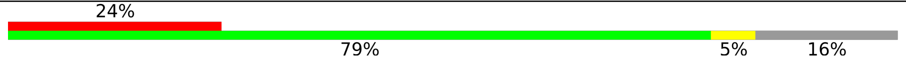
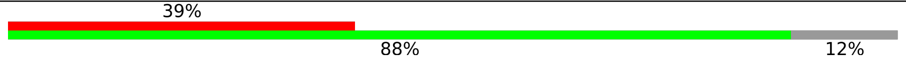
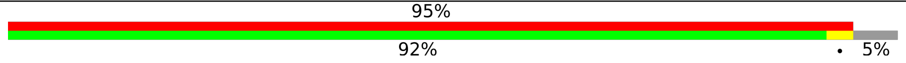
Mol	Chain	Length	Quality of chain
53	SQ	756	
54	SR	143	
55	SS	771	
56	SX	177	
57	SY	253	
58	NH	1146	
59	SP	2785	
60	LR	808	
61	LM	2144	
62	N0	22	
63	SG	475	
64	NI	280	
65	SW	252	
66	ST	632	
67	SU	472	
68	NY	381	
69	SZ	304	

2 Entry composition ⓘ

There are 74 unique types of molecules in this entry. The entry contains 223184 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 5'ETS rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L0	242	5152	2289	908	1713	242	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	1301	27777	12396	5002	9078	1301	0	0

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L2	215	4589	2047	809	1518	215	0	0

- Molecule 4 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	L3	115	571	341	115	115	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4 X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L4	239	1902	1220	350	324	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L5	190	1501	939	285	270	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L6	223	1811	1133	361	311	6	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L7	168	1346	862	239	244	1	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L8	180	1474	925	294	250	5	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L9	171	1425	908	284	232	1	0	0

- Molecule 11 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	LA	120	593	353	120	120	0	0

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LC	139	1098	699	207	189	3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LD	147	1204	767	225	206	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LF	104	851	543	158	145	5	0	0

- Molecule 15 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LG	62	488	297	97	92	2	0	0

- Molecule 16 is a protein called WD repeat-containing protein 75.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LH	746	5987	3846	1005	1101	35	0	0

- Molecule 17 is a protein called Nucleolar protein 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	LI	537	2675	1601	537	537	0	0

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LJ	469	3711	2372	637	688	14	0	0

- Molecule 19 is a protein called WD repeat-containing protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LK	118	943	612	163	163	5	0	0
			Total	C	N	O	S		
19	LL	510	3982	2538	686	731	27	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LN	671	5299	3394	925	956	24	0	0

- Molecule 21 is a protein called Periodic tryptophan protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LO	848	6676	4258	1151	1234	33	0	0

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 6 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LP	567	4705	3022	808	847	28	0	0

- Molecule 23 is a protein called WD repeat-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LQ	828	6438	4103	1108	1194	33	0	0

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 18 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LS	453	3560	2235	631	671	23	0	0

- Molecule 25 is a protein called WD repeat-containing protein 36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LT	869	6756	4321	1158	1244	33	0	0

- Molecule 26 is a protein called DDB1- and CUL4-associated factor 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LU	445	3611	2282	653	651	25	0	0

- Molecule 27 is a protein called WD repeat-containing protein 46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LW	453	3519	2221	637	646	15	0	0

- Molecule 28 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LZ	183	1532	966	292	270	4	0	0

- Molecule 29 is a protein called U3 small nucleolar ribonucleoprotein protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	NA	249	2055	1299	359	391	6	0	0

- Molecule 30 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	NB	73	617	379	140	98	0	0

- Molecule 31 is a protein called Nucleolar protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	ND	84	696	438	143	114	1	0	0

- Molecule 32 is a protein called Uncharacterized protein C1orf131.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	NE	100	799	509	143	146	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	NF	149	1202	770	228	203	1	0	0

- Molecule 34 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	NG	116	861	531	159	165	6	0	0

- Molecule 35 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NJ	827	Total 6526	C 4187	N 1126	O 1178	S 35	0	0
35	NK	815	Total 4030	C 2400	N 815	O 815		0	0

- Molecule 36 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NM	233	Total 1873	C 1186	N 339	O 334	S 14	0	0

- Molecule 37 is a protein called Protein AATF.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NN	42	Total 340	C 215	N 63	O 60	S 2	0	0

- Molecule 38 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NO	129	Total 1034	C 659	N 193	O 176	S 6	0	0

- Molecule 39 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NQ	82	Total 640	C 402	N 118	O 113	S 7	0	0

- Molecule 40 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	NR	861	Total 4305	C 2583	N 861	O 861	0	0

- Molecule 41 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	NT	58	Total 286	C 170	N 58	O 58	0	0

- Molecule 42 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms	AltConf	Trace
42	NU	60	Total C N O 297 177 60 60	0	0

- Molecule 43 is a protein called Nucleolar protein 10.

Mol	Chain	Residues	Atoms	AltConf	Trace
43	NW	311	Total C N O S 2498 1599 413 472 14	0	0

- Molecule 44 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms	AltConf	Trace
44	SA	396	Total C N O S 3077 1948 542 575 12	0	0

- Molecule 45 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms	AltConf	Trace
45	SB	440	Total C N O S 3439 2179 596 642 22	0	0

- Molecule 46 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms	AltConf	Trace
46	SC	229	Total C N O S 1781 1129 322 323 7	0	0
46	SD	237	Total C N O S 1841 1163 337 334 7	0	0

- Molecule 47 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
47	SE	125	Total C N O S 968 611 172 180 5	0	0
47	SF	123	Total C N O S 955 604 170 176 5	0	0

- Molecule 48 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
48	SH	368	Total C N O S 2832 1803 495 518 16	0	0

- Molecule 49 is a protein called Ribosome biogenesis protein BMS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SI	844	Total	C	N	O	S	0	0
			6801	4349	1230	1188	34		

- Molecule 50 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SK	204	Total	C	N	O	S	0	0
			1579	1012	272	286	9		
50	SJ	204	Total	C	N	O		0	0
			1008	600	204	204			

- Molecule 51 is a protein called rRNA-processing protein FCF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SL	192	Total	C	N	O	S	0	0
			1586	1006	290	275	15		

- Molecule 52 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SM	290	Total	C	N	O	S	0	0
			2369	1485	451	424	9		

- Molecule 53 is a protein called Deoxynucleotidyltransferase terminal-interacting protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SQ	187	Total	C	N	O	S	0	0
			1533	972	278	277	6		

- Molecule 54 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SR	108	Total	C	N	O	S	0	0
			816	521	153	140	2		

- Molecule 55 is a protein called U3 small nucleolar RNA-associated protein 14 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SS	197	Total	C	N	O	S	0	0
			1626	1039	301	285	1		

- Molecule 56 is a protein called Unassigned peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	SX	177	Total 885	C 531	N 177	O 177	0	0

- Molecule 57 is a protein called Probable U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SY	238	Total 2024	C 1280	N 385	O 353	S 6	0	0

- Molecule 58 is a protein called Nucleolar protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	NH	1066	Total 5265	C 3133	N 1066	O 1066	0	0

- Molecule 59 is a protein called Small subunit processome component 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SP	1993	Total 11768	C 7248	N 2243	O 2262	S 15	0	0

- Molecule 60 is a protein called Transducin beta-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LR	773	Total 4321	C 2606	N 860	O 850	S 5	0	0

- Molecule 61 is a protein called HEAT repeat-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LM	2005	Total 13156	C 8305	N 2316	O 2493	S 42	0	0

- Molecule 62 is a RNA chain called 5' ETS rRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	N0	22	Total 264	C 110	O 132	P 22	0	0

- Molecule 63 is a protein called U3 small nucleolar RNA-interacting protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SG	389	Total 2878	C 1806	N 531	O 528	S 13	1	0

- Molecule 64 is a protein called Ribosomal RNA-processing protein 7 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	NI	234	Total 1459	C 885	N 287	O 285	S 2	0	0

- Molecule 65 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	SW	180	Total 890	C 530	N 180	O 180	0	0

- Molecule 66 is a protein called Nucleolar protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ST	568	Total 3064	C 1844	N 620	O 598	S 2	0	0

- Molecule 67 is a protein called Nucleolar complex protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	SU	413	Total 2057	C 1231	N 413	O 413	0	0

- Molecule 68 is a protein called KRR1 small subunit processome component homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	NY	274	Total 2094	C 1337	N 366	O 383	S 8	0	0

- Molecule 69 is a protein called Bystin.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	SZ	290	Total 1442	C 862	N 290	O 290	0	0

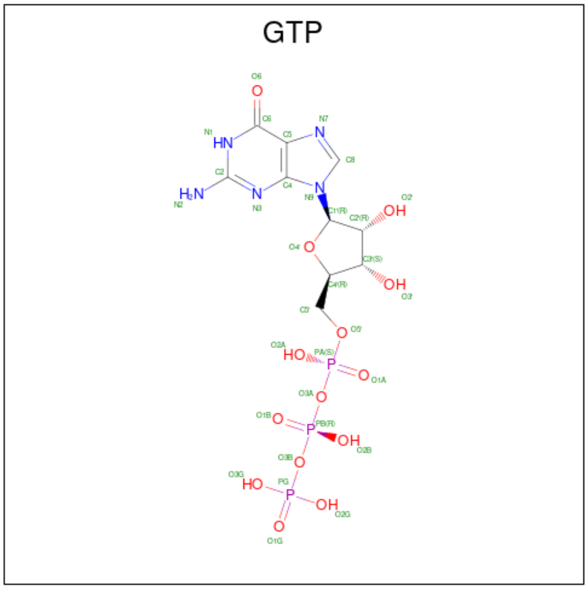
- Molecule 70 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
70	L1	19	Total Mg 19 19	0
70	SI	1	Total Mg 1 1	0
70	SL	1	Total Mg 1 1	0
70	NH	1	Total Mg 1 1	0

- Molecule 71 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
71	NQ	1	Total Zn 1 1	0
71	NT	1	Total Zn 1 1	0
71	SL	1	Total Zn 1 1	0

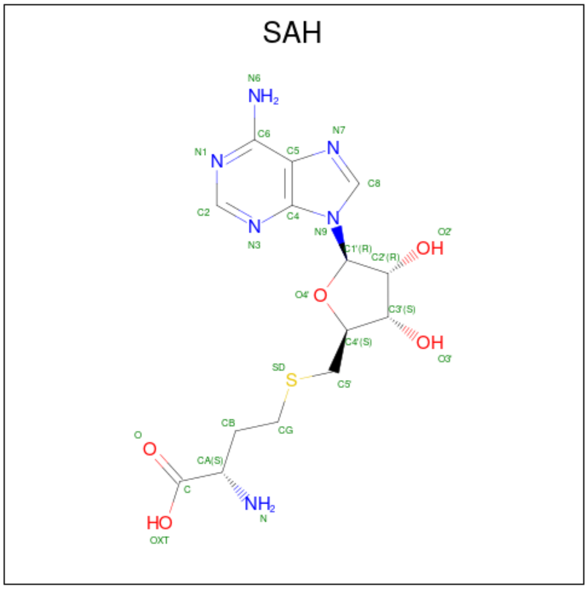
- Molecule 72 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	AltConf
72	SI	1	Total C N O P 32 10 5 14 3	0

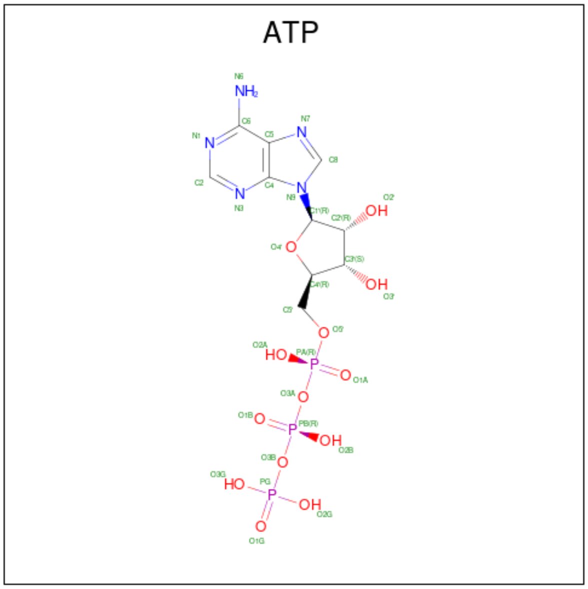
- Molecule 73 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:

$C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms	AltConf
73	SK	1	Total C N O S 26 14 6 5 1	0
73	SJ	1	Total C N O S 26 14 6 5 1	0

- Molecule 74 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

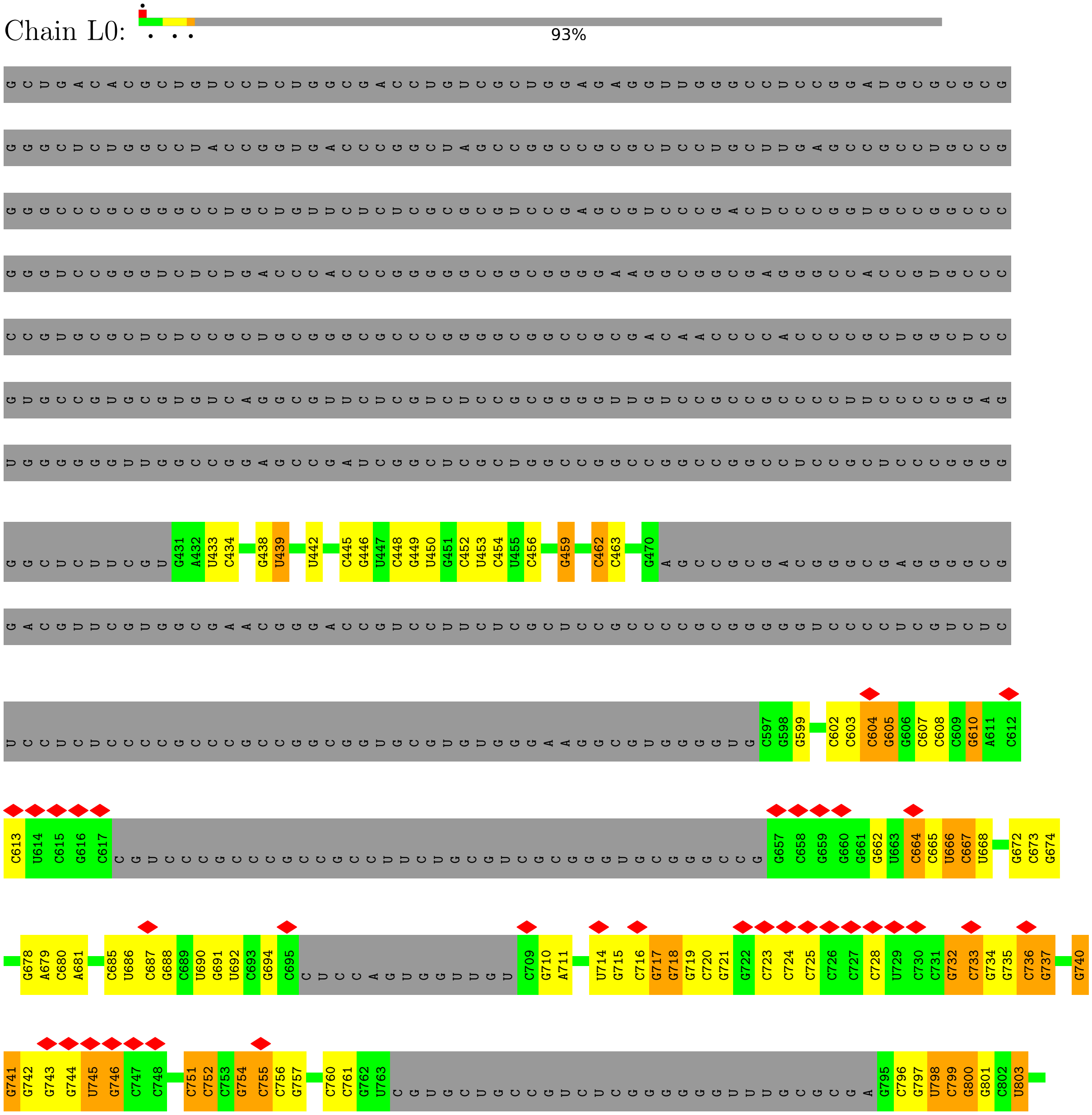


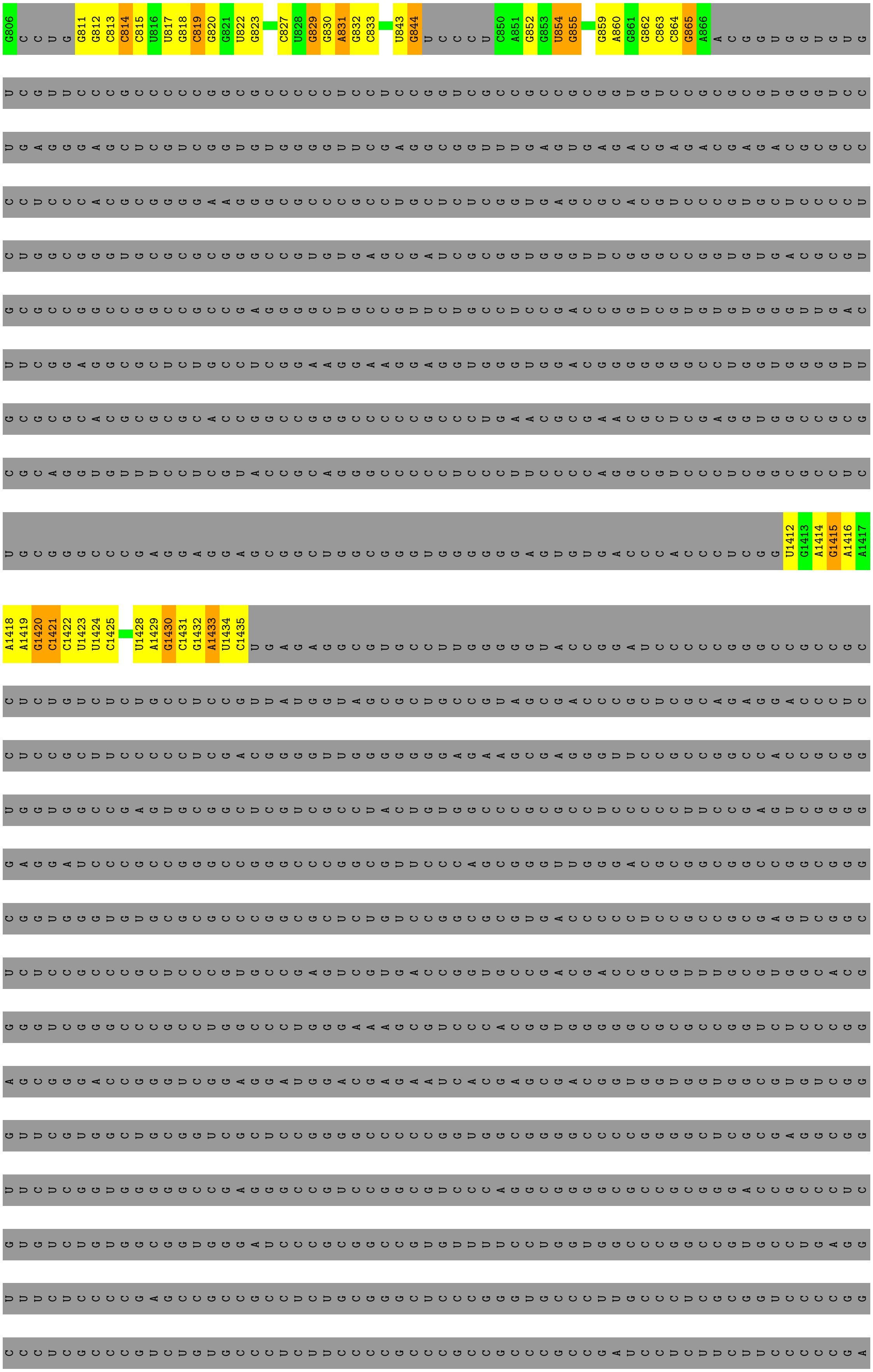
Mol	**Chain**	**Residues**	**Atoms**					**AltConf**
74	NH	1	Total	C	N	O	P	0
			31	10	5	13	3	
74	NK	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots ⓘ

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

- Molecule 1: 5'ETS rRNA




G806
G811
G812
C813
C814
C815
U816
U817
G818
C819
G820
G821
U822
G823
C827
U828
G829
G830
A831
G832
C833
U843
G844
C850
A851
G852
G853
U854
G855
G859
A860
G861
G862
C863
C864
G865
A866
U1412
G1413
A1414
G1415
A1416
A1417
A1418
A1419
G1420
C1421
C1422
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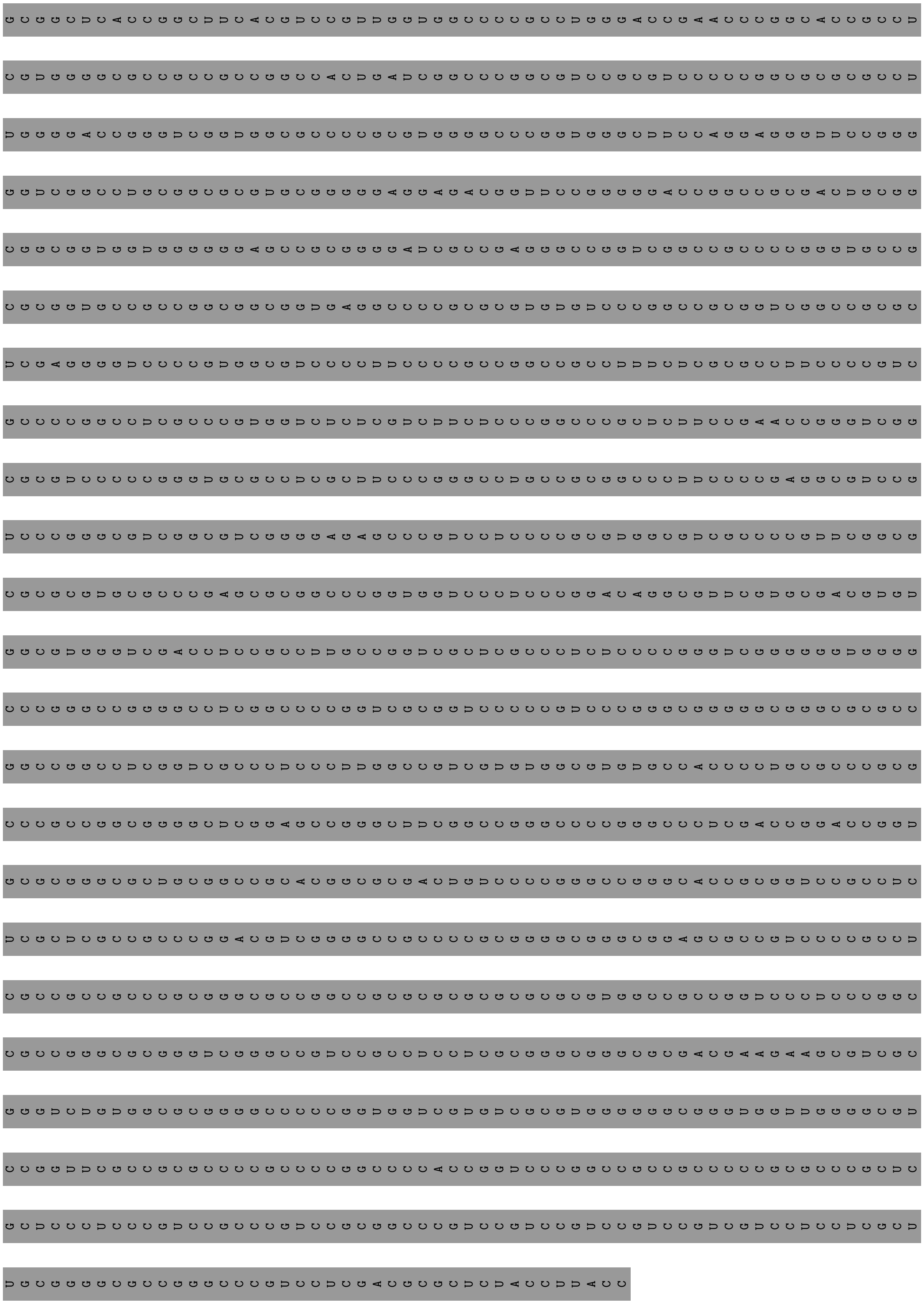
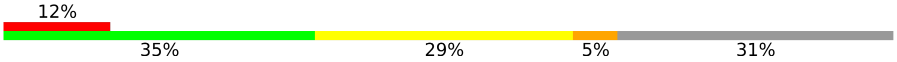
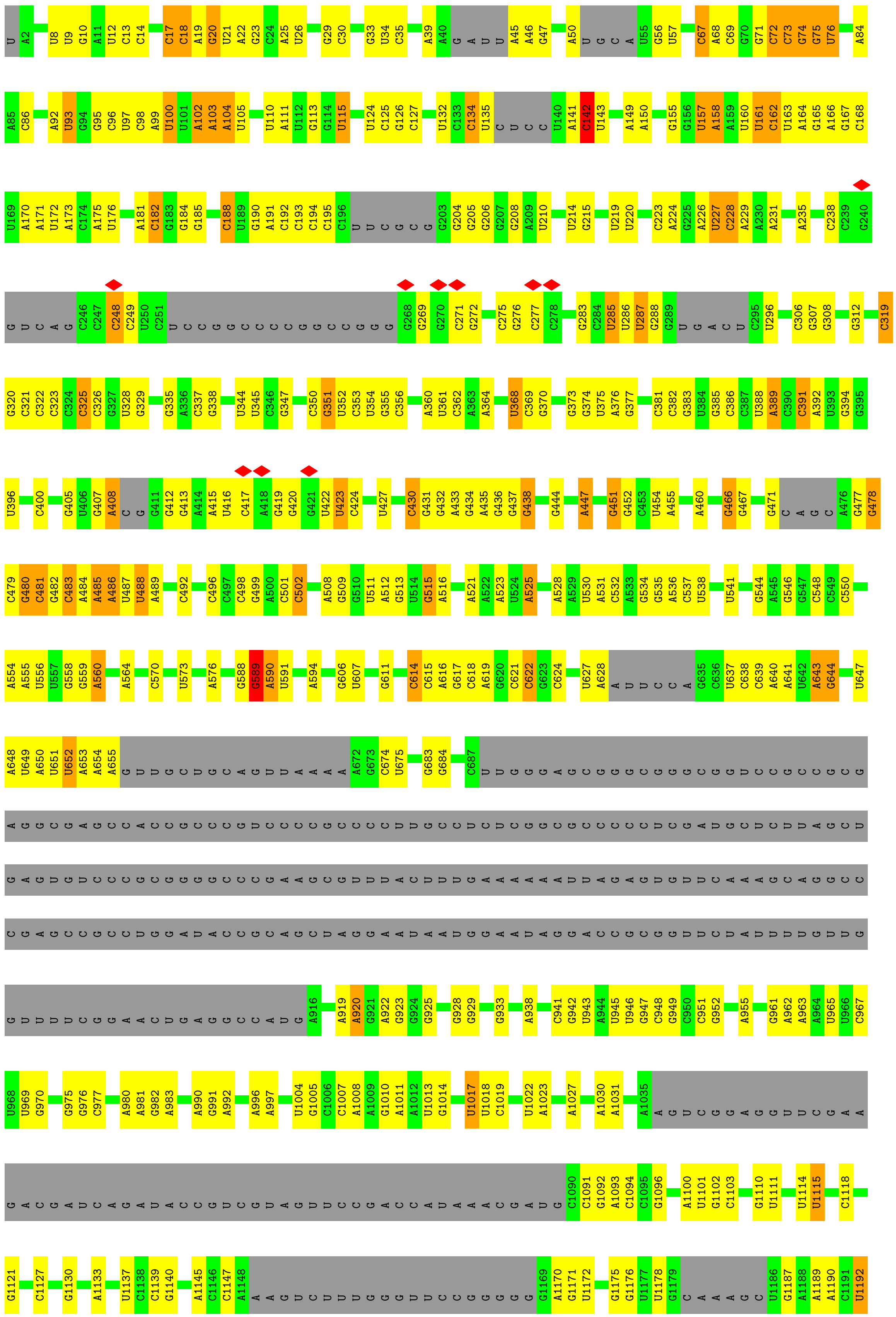
C1425
U1428
A1429
G1430
C1431
G1432
A1433
U1434
C1435

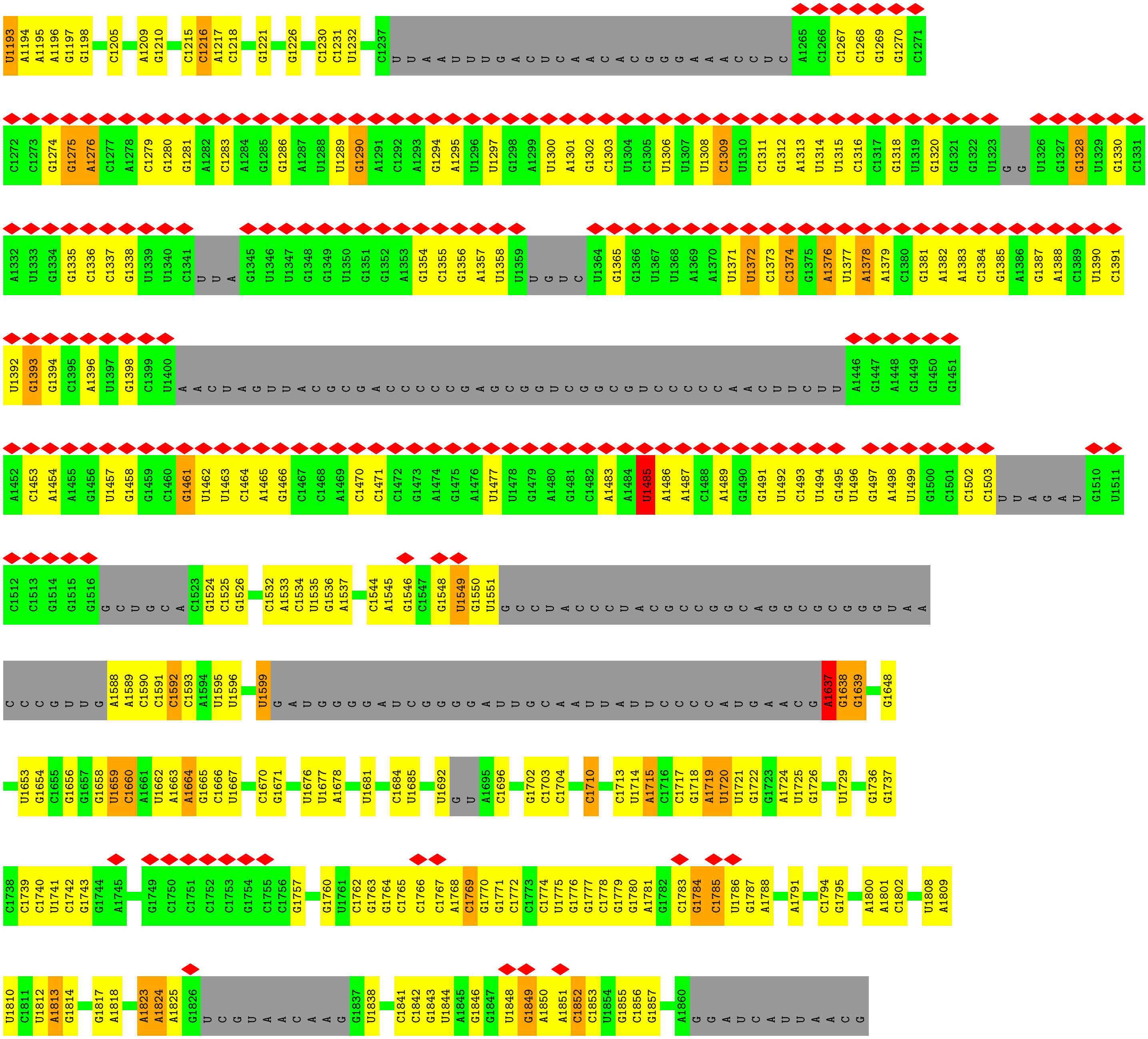


- Molecule 2: 18S rRNA

Chain L1:

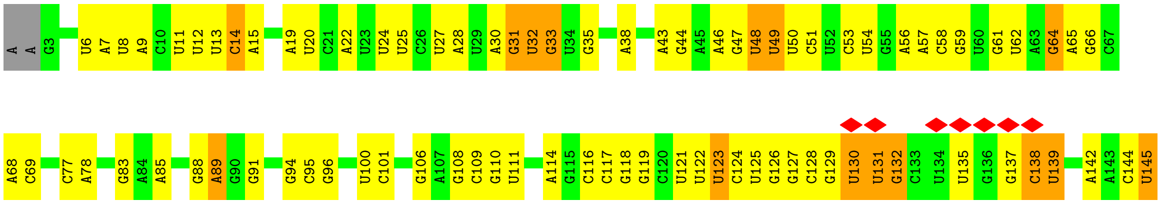


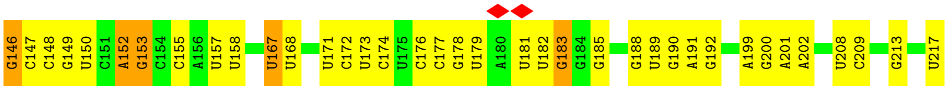

U A2 U8 U9 G10 A11 U12 C13 C14 C17 C18 A19 G20 U21 A22 G23 C24 A25 U26 G29 C30 G33 U34 C35 A39 A40 G A U U A45 A46 G47 A50 U G C A U55 G56 U57 C67 A68 C69 G70 G71 C72 C73 G74 G75 U76 A84
A85 C86 A92 U93 G94 G95 C96 U97 C98 A99 U100 U101 A102 A103 A104 U105 U110 A111 U112 G113 G114 U115 U124 C125 G126 C127 U132 C133 C134 U135 C U C C U140 A141 C142 U143 A149 A150 G155 G156 U157 A158 A159 U160 U161 C162 U163 A164 G165 A166 G167 C168
U169 A170 A171 U172 A173 C174 A175 U176 A181 C182 G183 G184 G185 C188 U189 G190 A191 C192 C193 C194 C195 C196 U U C G C G G203 G204 G205 G206 G207 G208 A209 U210 U214 G215 U219 U220 C223 A224 G225 A226 U227 C228 A229 A230 A231 A235 C238 C239 G240
G U C A G C246 C247 C248 C249 U250 C251 U C C G G C C C C G G C C G G G G268 G269 G270 C271 G272 C275 G276 C277 C278 G283 C284 U285 U286 U287 G288 G289 U G A C U C295 U296 C306 G307 G308 G312 C319
G320 C321 C322 C323 C324 C325 C326 G327 U328 G329 G335 A336 C337 G338 U344 U345 C346 G347 C350 G351 U352 C353 U354 G355 C356 A360 U361 C362 A363 A364 U368 C369 G370 G373 G374 U375 A376 G377 C381 C382 G383 U384 G385 C386 C387 U388 A389 C390 C391 A392 U393 G394 G395
U396 C400 G405 U406 G407 A408 C G G411 G412 G413 A414 A415 U416 C417 A418 G419 G420 G421 U422 U423 C424 U427 C430 G431 G432 A433 G434 A435 G436 G437 G438 G444 A447 G451 G452 G453 U454 A455 A460 G466 G467 G471 C A G C A476 G477 G478
C479 G480 C481 G482 C483 A484 A485 A486 U487 U488 A489 C492 C496 C497 C498 G499 A500 C501 C502 A508 G509 G510 U511 A512 G513 U514 G515 A516 A521 A522 A523 U524 A525 A528 A529 U530 A531 C532 A533 G534 G535 A536 C537 U538 U541 G544 A545 G546 G547 C548 C549 C550
A554 A555 U556 U557 G558 G559 A560 A564 C570 U573 A576 G588 G589 A590 U591 A594 G606 U607 G611 C614 C615 A616 G617 C618 A619 G620 C621 C622 G623 C624 U627 A628 A U U C C A G635 C636 U637 C638 C639 A640 A641 U642 A643 G644 U647
A648 U649 A650 U651 U652 A653 A654 A655 G U U G C U G C A G U U A A A A A672 G673 C674 U675 G683 G684 C687 U U G G G A G C G G G C G G G C G G U C C G C C C G
A G G C G A G C C A C C G C C C G U C C C G C C C C U U G C C U C U C G G C G C C C C C U C G A U G C U C U U A G C U
G A G U G U C C C G C G G G C C C G A A G C G U U U A C U U U G A A A A A U U A G A G U G U U U C A A A G C A G G C C
C G A G C C C C C U G G A U A C C G C A G C U A G G A A U A A U G G A A U A G G A C C C G C G G U U C U A U U U U G U U G
G U U U U C G G A A C U G A G G C C A U G A916 A919 A920 G921 A922 G923 G924 G925 G928 G929 G933 A938 C941 G942 U943 A944 U945 U946 G947 C948 G949 C950 C951 G952 A955 G961 A962 A963 A964 U965 U966 C967
U968 U969 G970 G975 G976 C977 A980 A981 G982 A983 A990 G991 A992 A996 A997 U1004 G1005 C1006 C1007 A1008 A1009 G1010 A1011 A1012 U1013 G1014 U1017 U1018 C1019 U1022 A1023 A1027 A1030 A1031 A1035 A G U C G G A G G U U C G A A
G A C G A U C A G A U A C C G U C G U A G U U C C G A C C A U A A A C G A U G C1090 C1091 G1092 A1093 C1094 C1095 G1096 A1100 U1101 G1102 C1103 G1110 U1111 U1114 U1115 C1118
G1121 C1127 G1130 A1133 U1137 C1138 C1139 G1140 A1145 C1146 C1147 A1148 A A G U C U U U G G G U U C C G G G G G1169 A1170 G1171 U1172 G1175 G1176 U1177 U1178 G1179 C A A A G C U1186 G1187 A1188 A1189 A1190 C1191 U1192



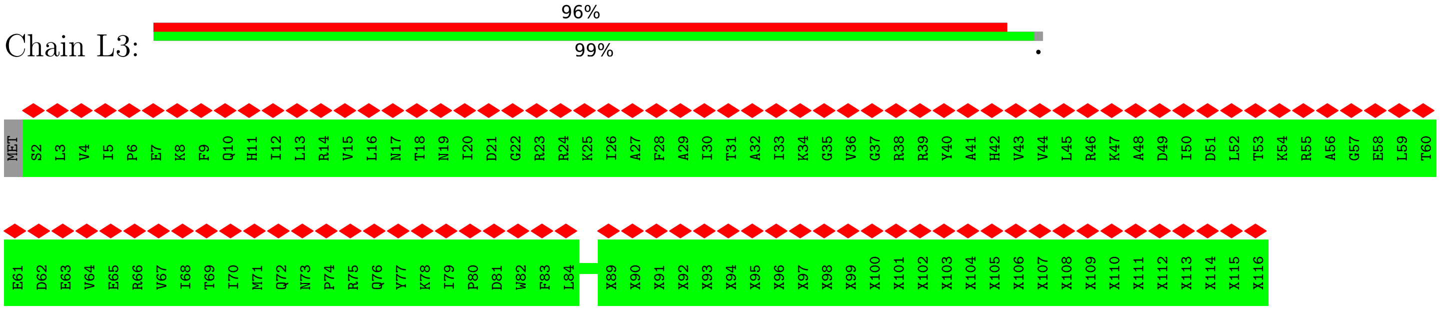
- Molecule 3: U3 snoRNA

Chain L2:

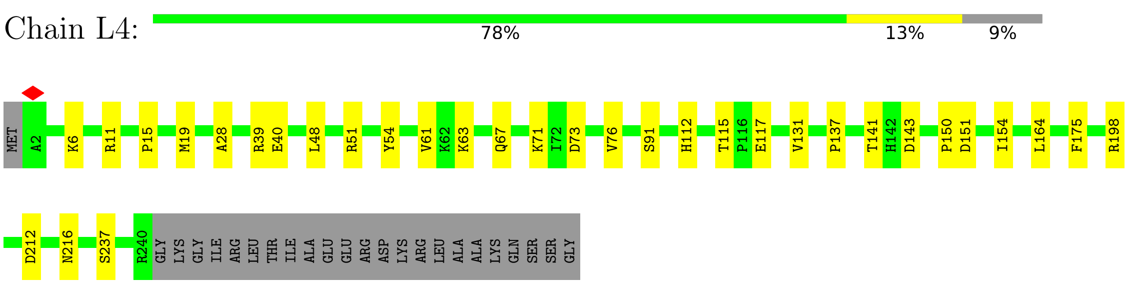




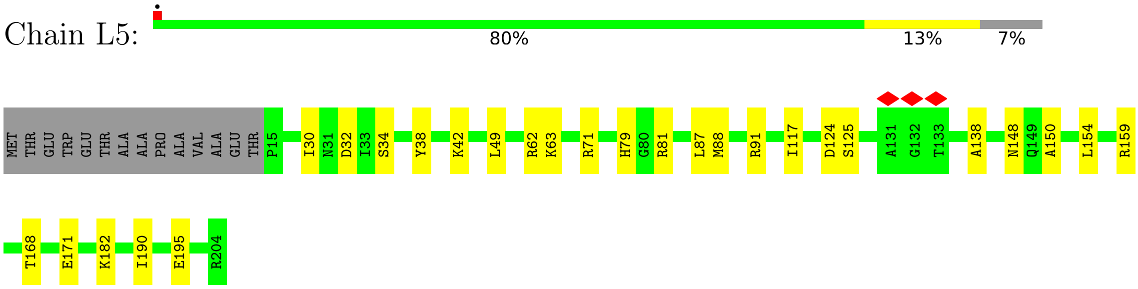
- Molecule 4: 40S ribosomal protein S18



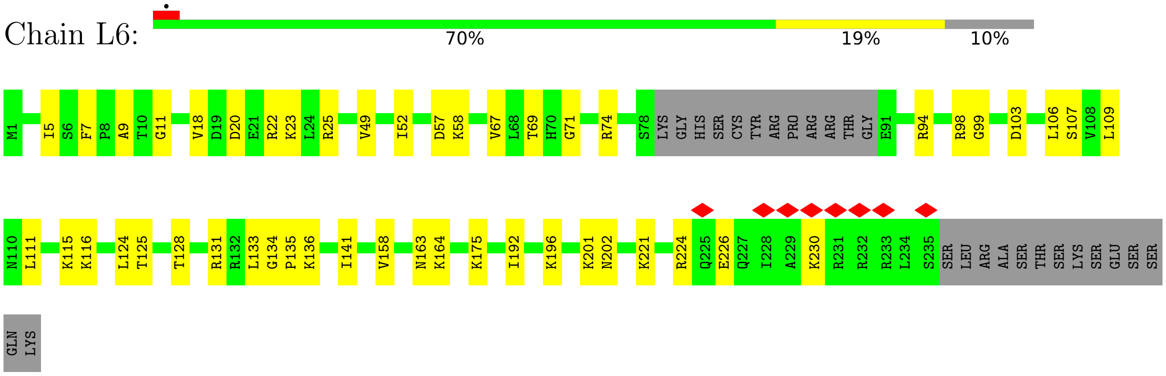
- Molecule 5: 40S ribosomal protein S4 X isoform



- Molecule 6: 40S ribosomal protein S5

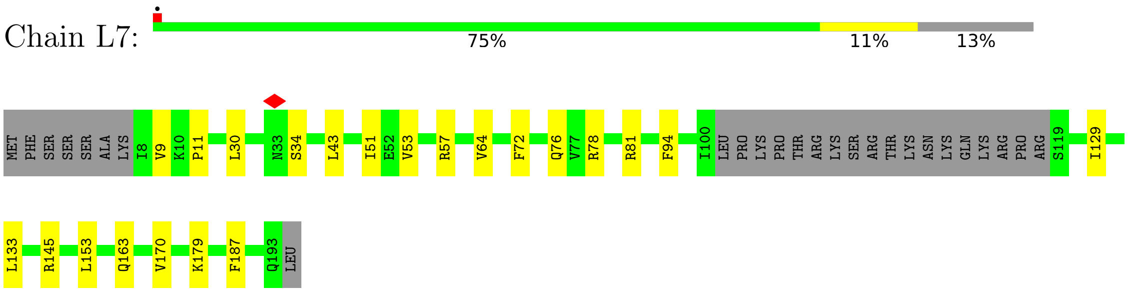


- Molecule 7: 40S ribosomal protein S6



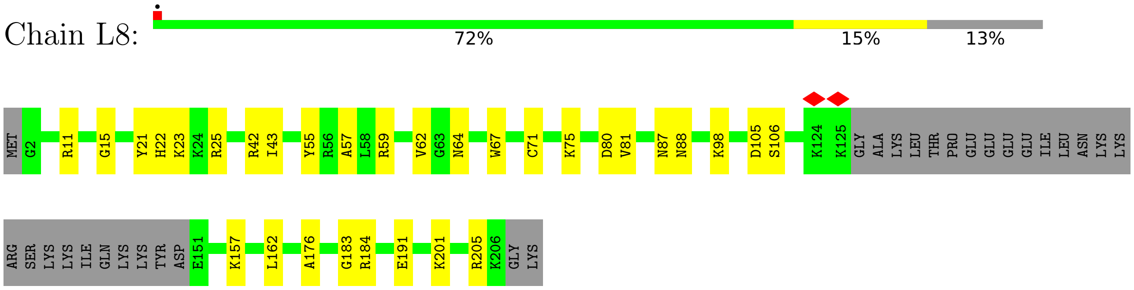
- Molecule 8: 40S ribosomal protein S7

Chain L7:



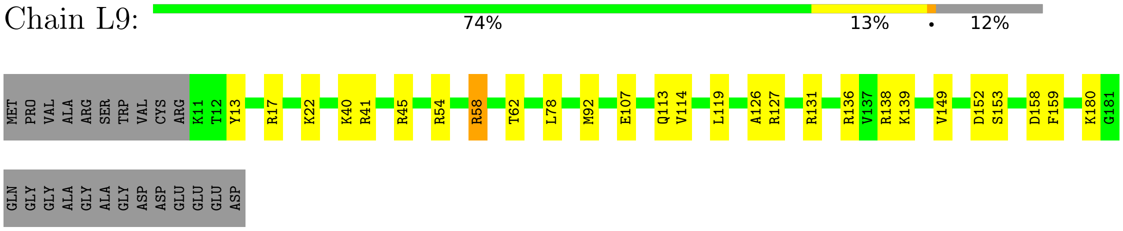
- Molecule 9: 40S ribosomal protein S8

Chain L8:



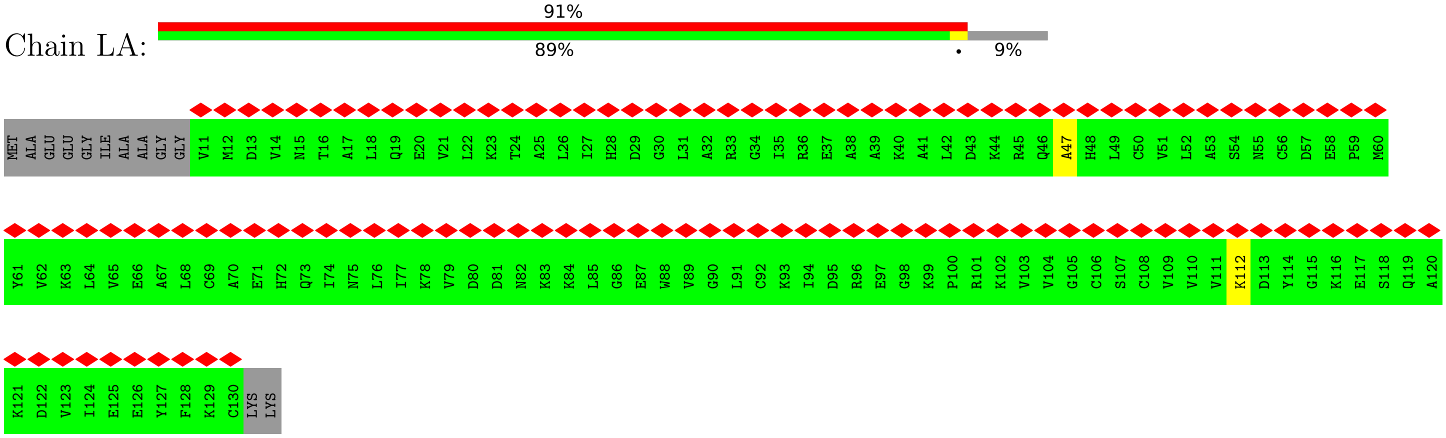
- Molecule 10: 40S ribosomal protein S9

Chain L9:



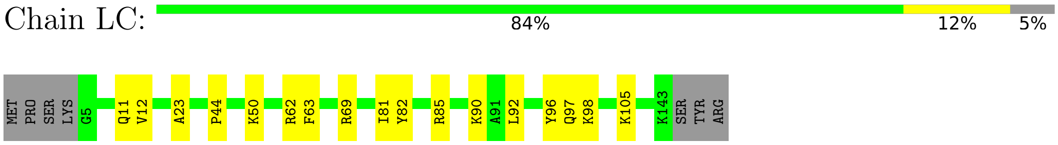
- Molecule 11: 40S ribosomal protein S12

Chain LA:



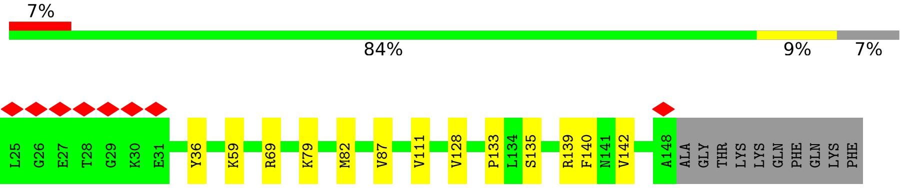
- Molecule 12: 40S ribosomal protein S16

Chain LC:



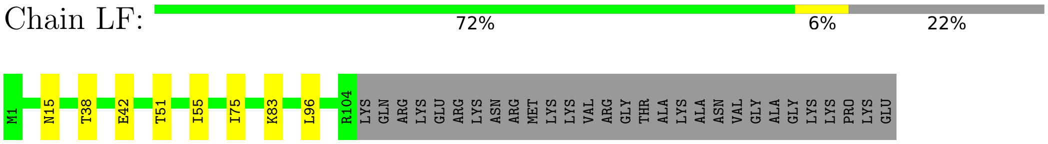
- Molecule 13: 40S ribosomal protein S11

Chain LD:



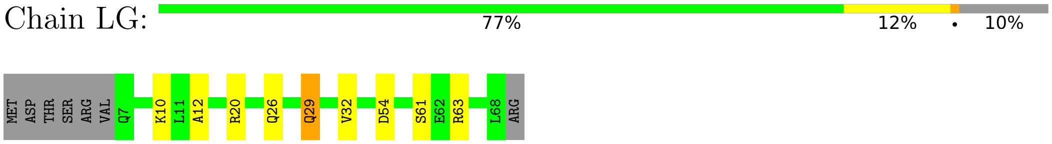
- Molecule 14: 40S ribosomal protein S24

Chain LF:



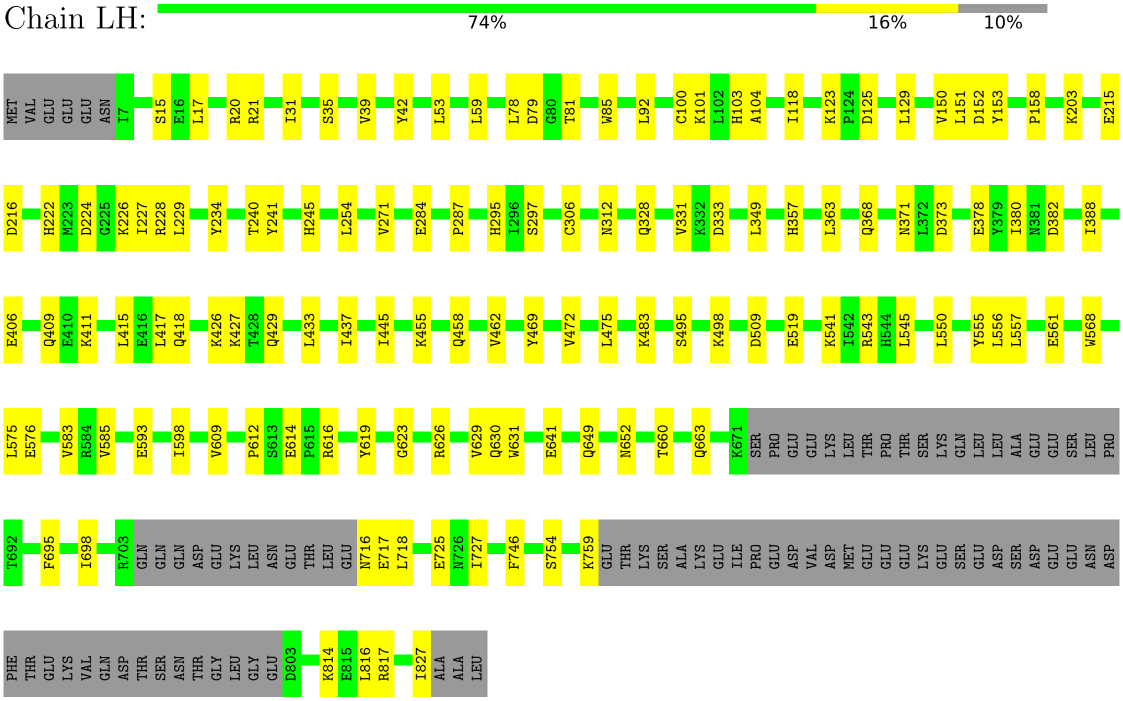
- Molecule 15: 40S ribosomal protein S28

Chain LG:



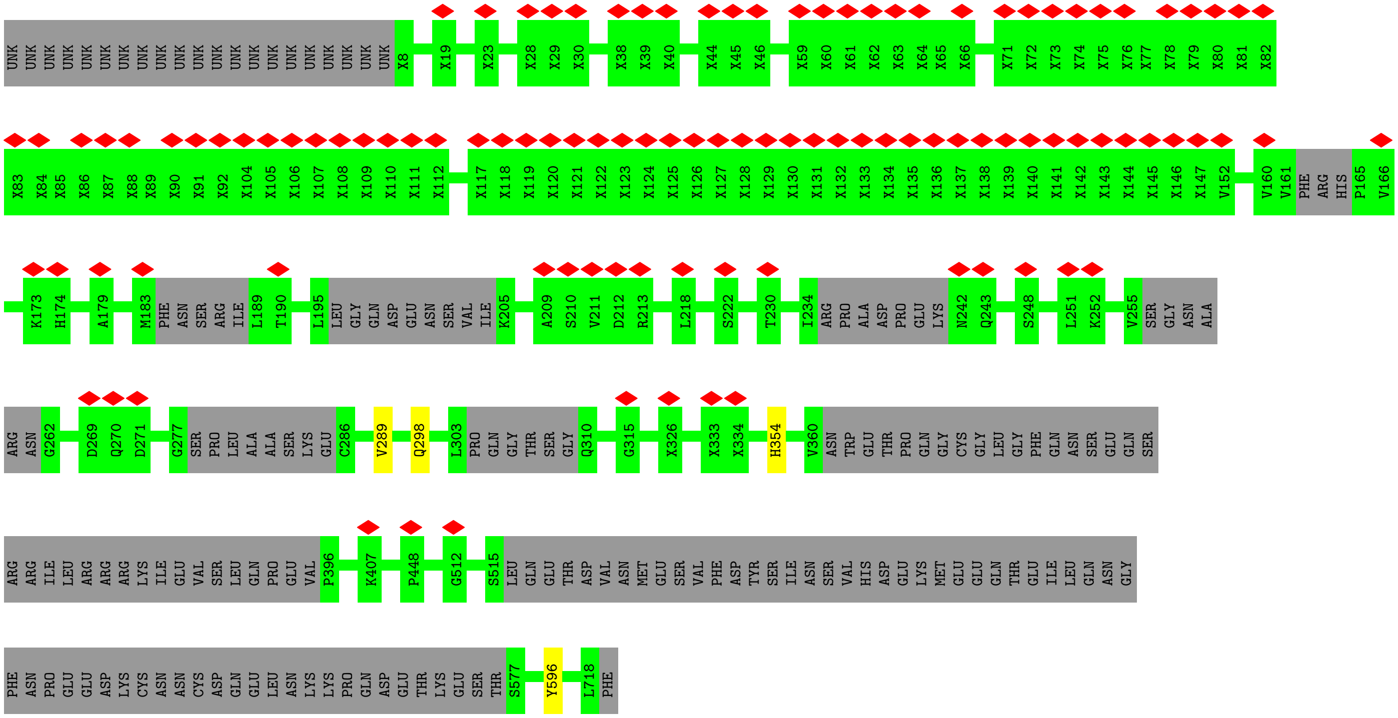
- Molecule 16: WD repeat-containing protein 75

Chain LH:



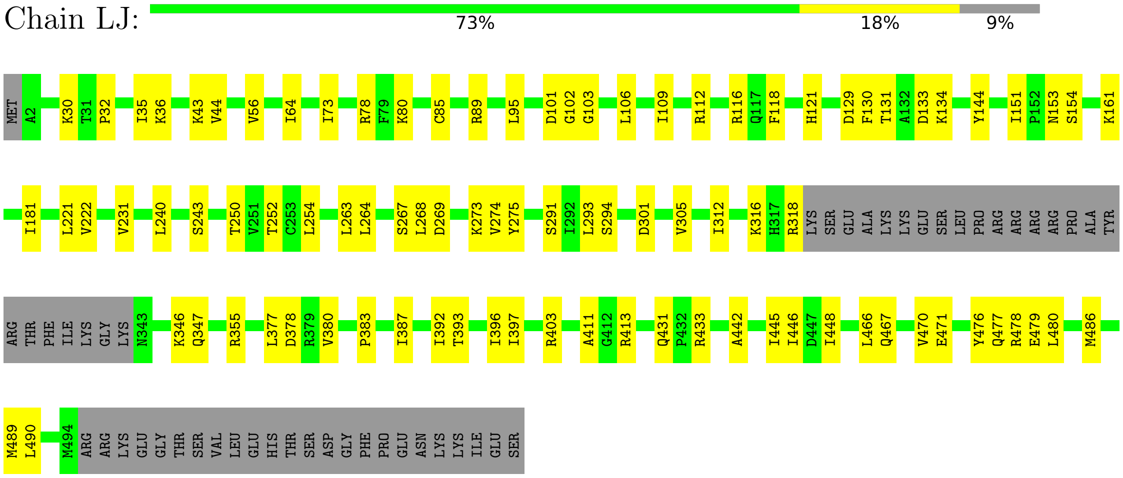
- Molecule 17: Nucleolar protein 11

Chain LI:



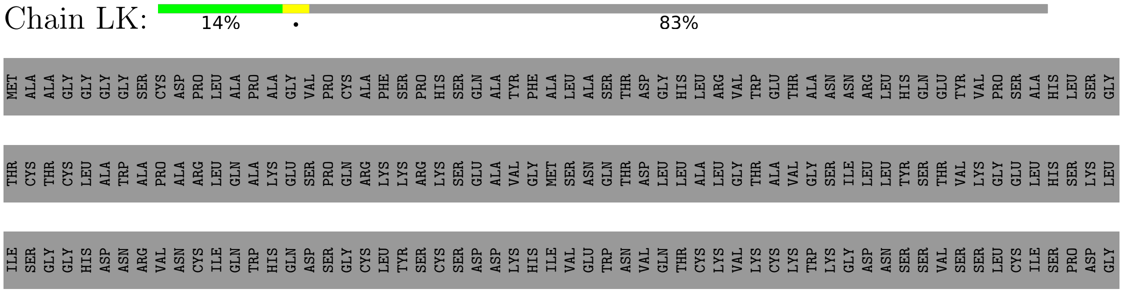
- Molecule 18: U3 small nucleolar RNA-associated protein 15 homolog

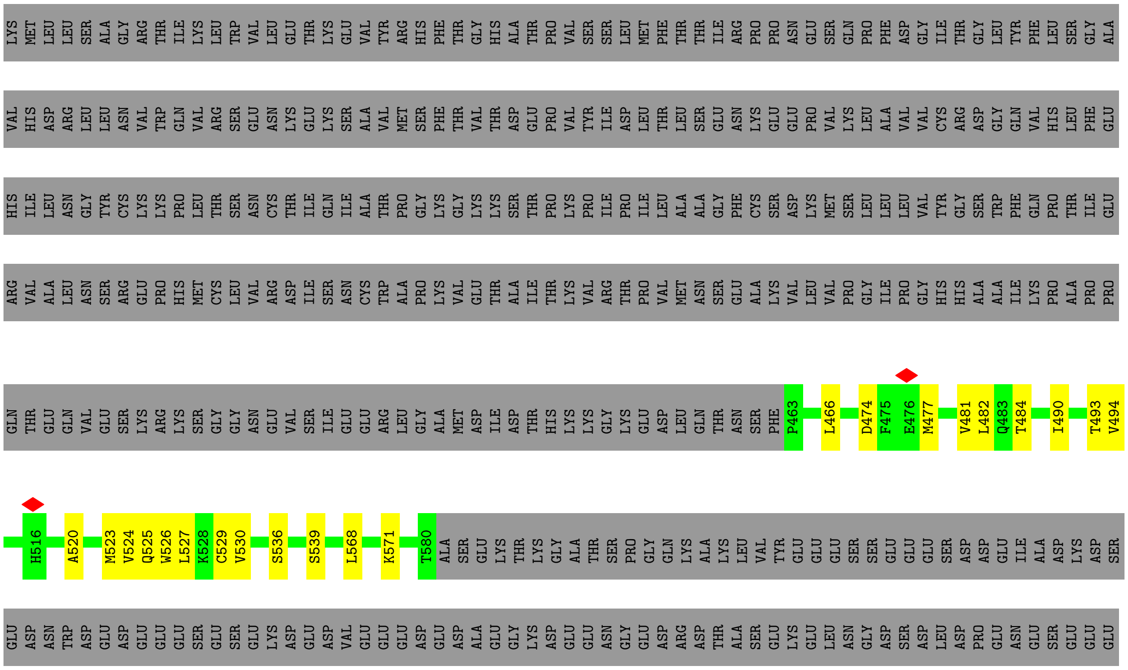
Chain LJ:



- Molecule 19: WD repeat-containing protein 43

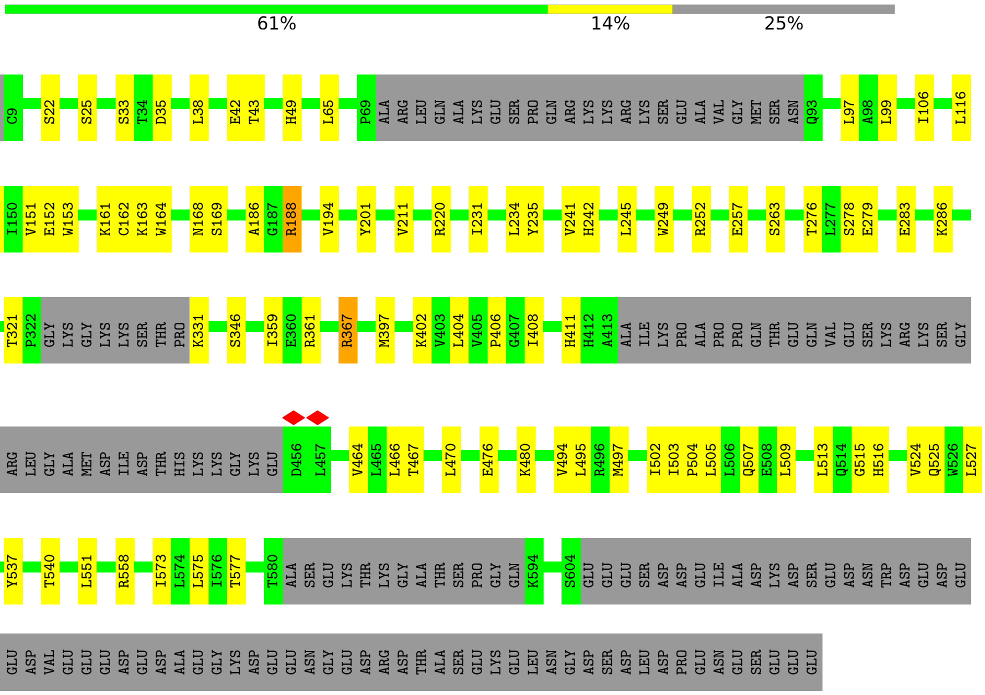
Chain LK:





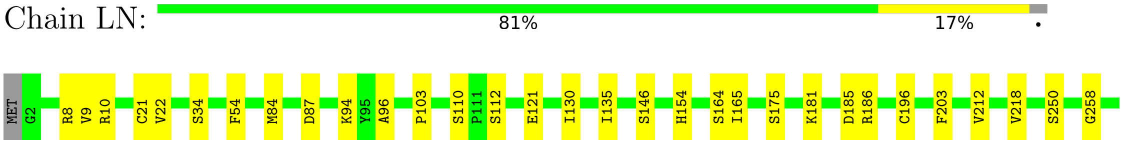
- Molecule 19: WD repeat-containing protein 43

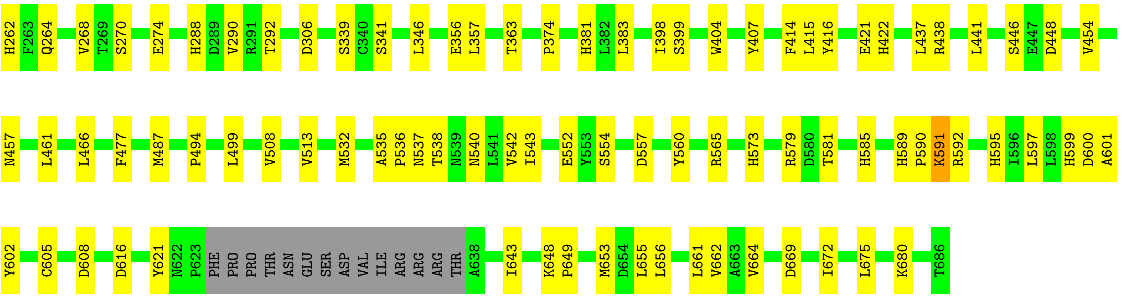
Chain LL:



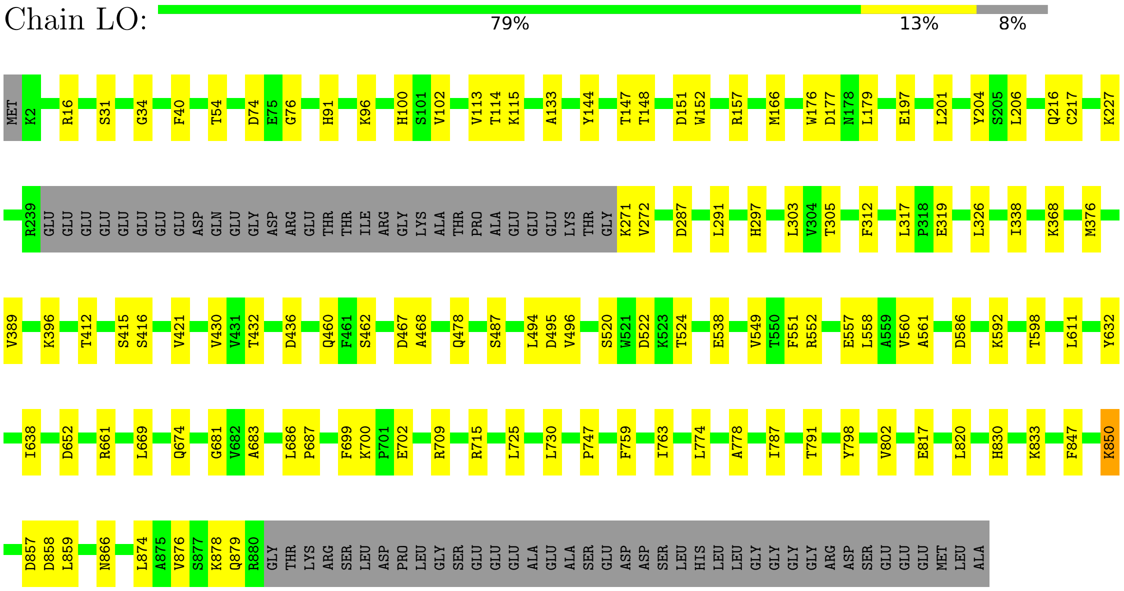
- Molecule 20: U3 small nucleolar RNA-associated protein 4 homolog

Chain LN:

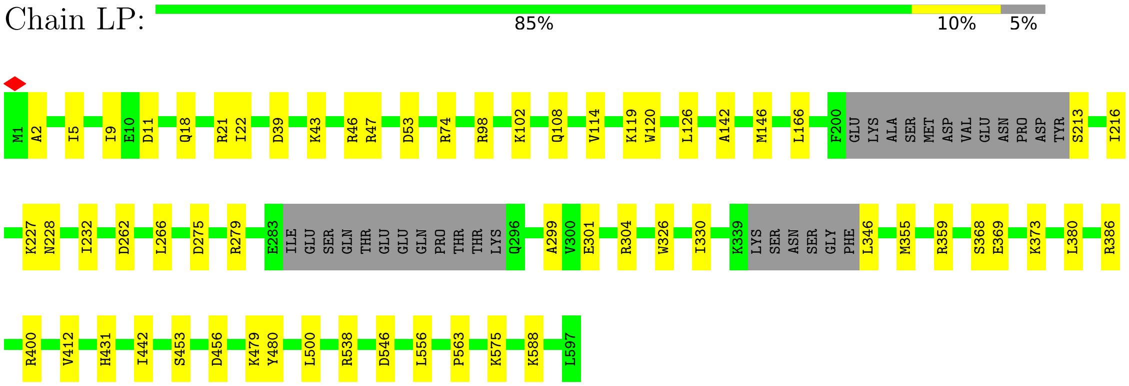




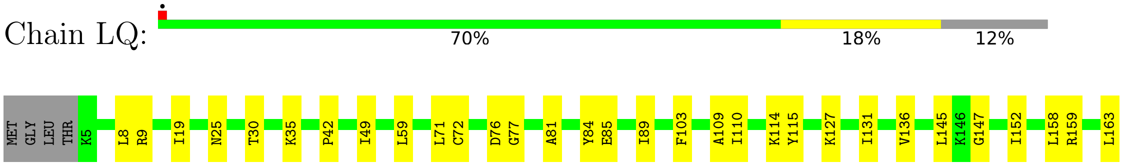
- Molecule 21: Periodic tryptophan protein 2 homolog

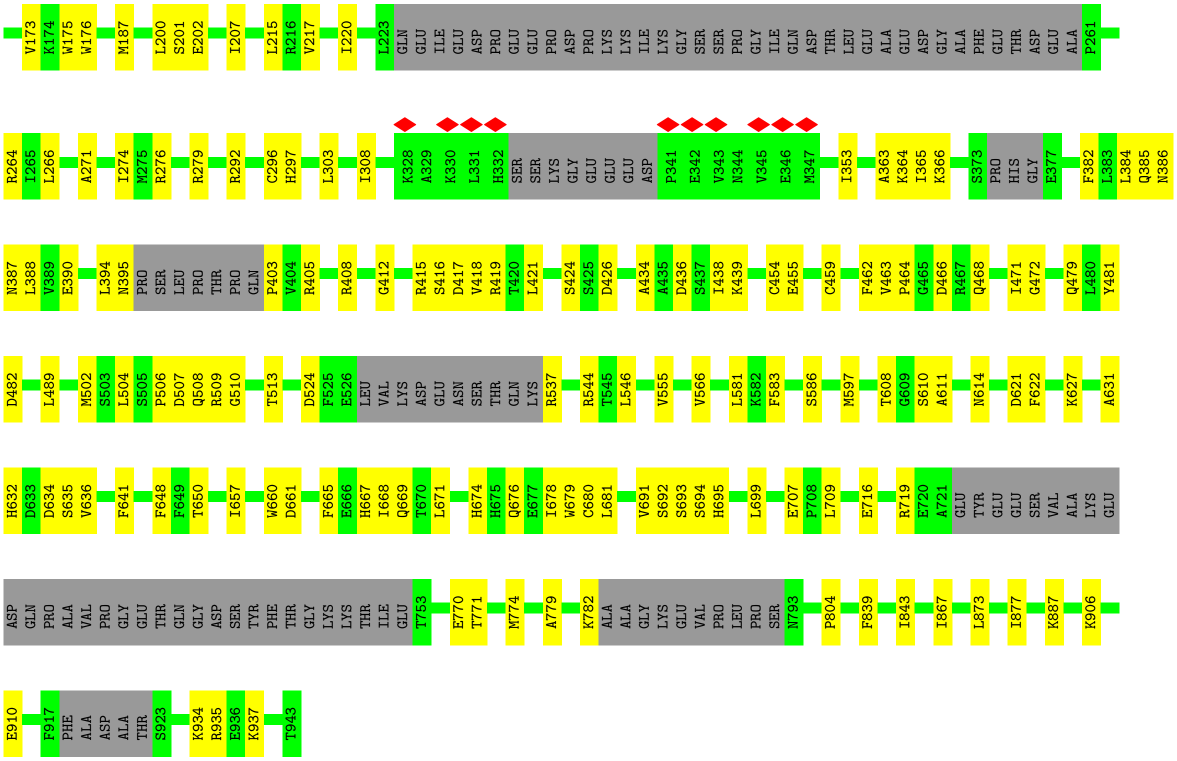


- Molecule 22: U3 small nucleolar RNA-associated protein 6 homolog



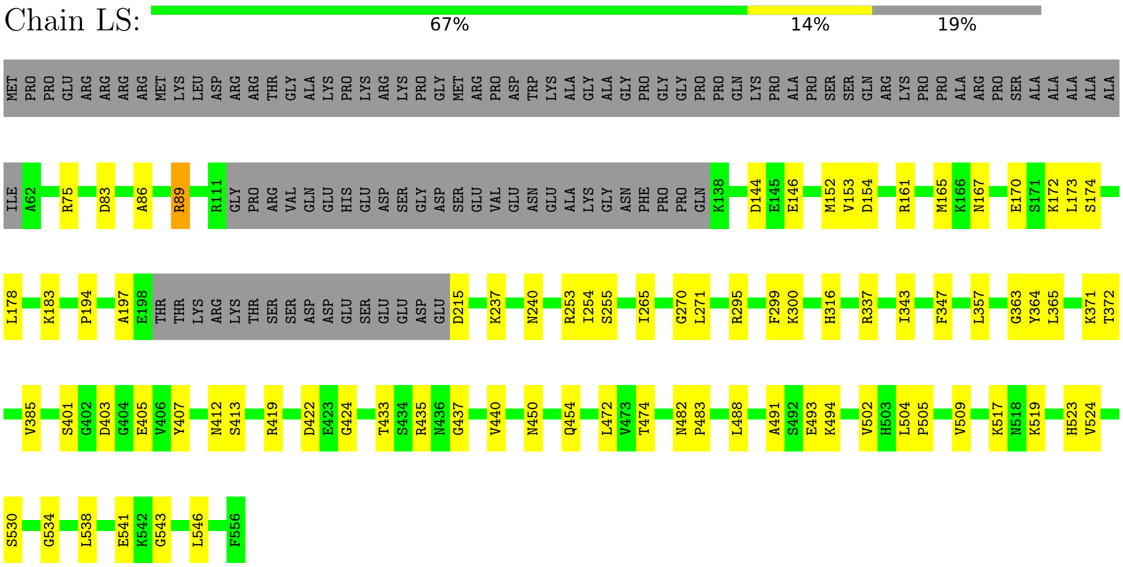
- Molecule 23: WD repeat-containing protein 3





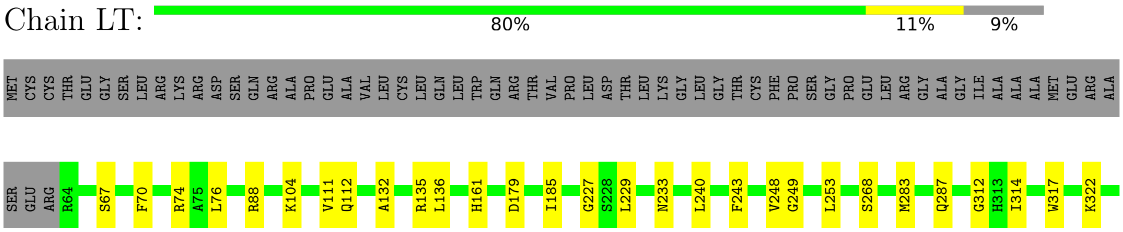
- Molecule 24: U3 small nucleolar RNA-associated protein 18 homolog

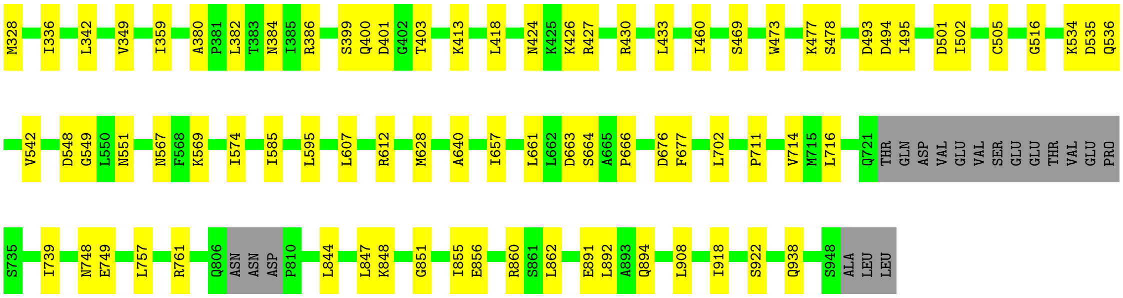
Chain LS:



- Molecule 25: WD repeat-containing protein 36

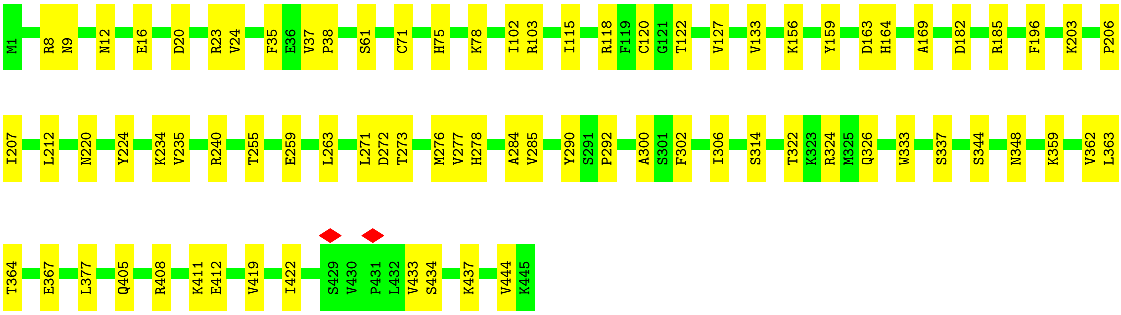
Chain LT:





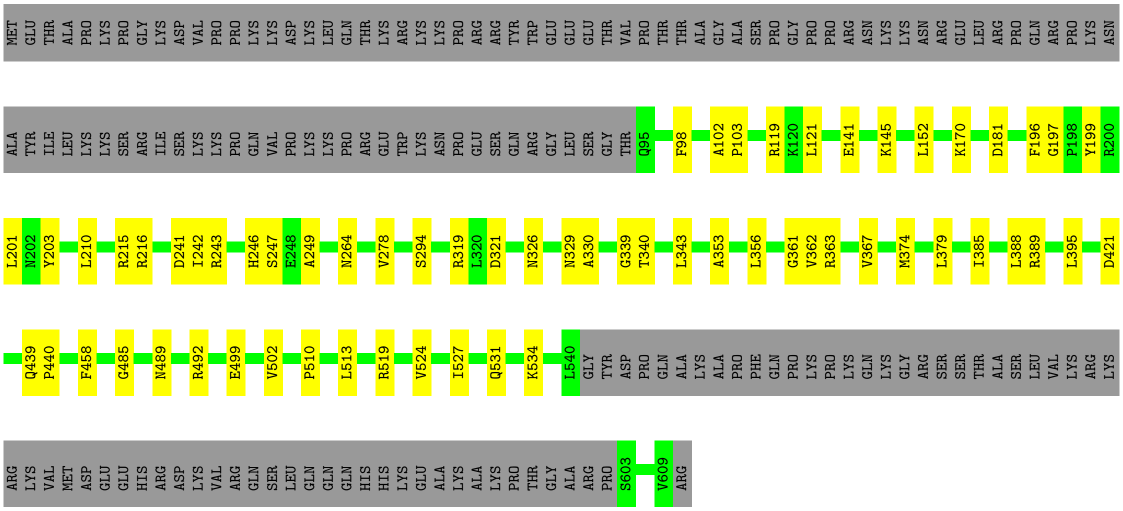
- Molecule 26: DDB1- and CUL4-associated factor 13

Chain LU:



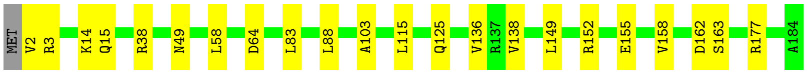
- Molecule 27: WD repeat-containing protein 46

Chain LW:



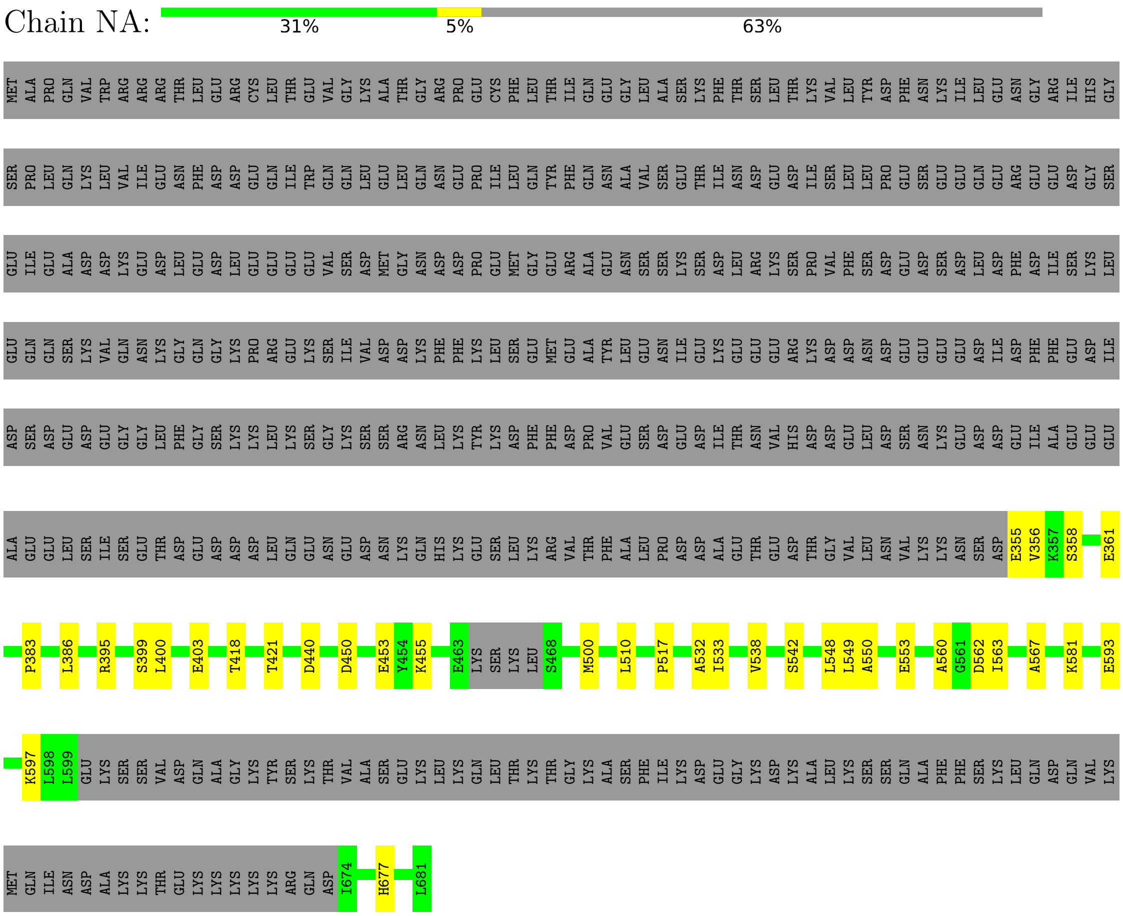
- Molecule 28: U3 small nucleolar ribonucleoprotein protein IMP3

Chain LZ:



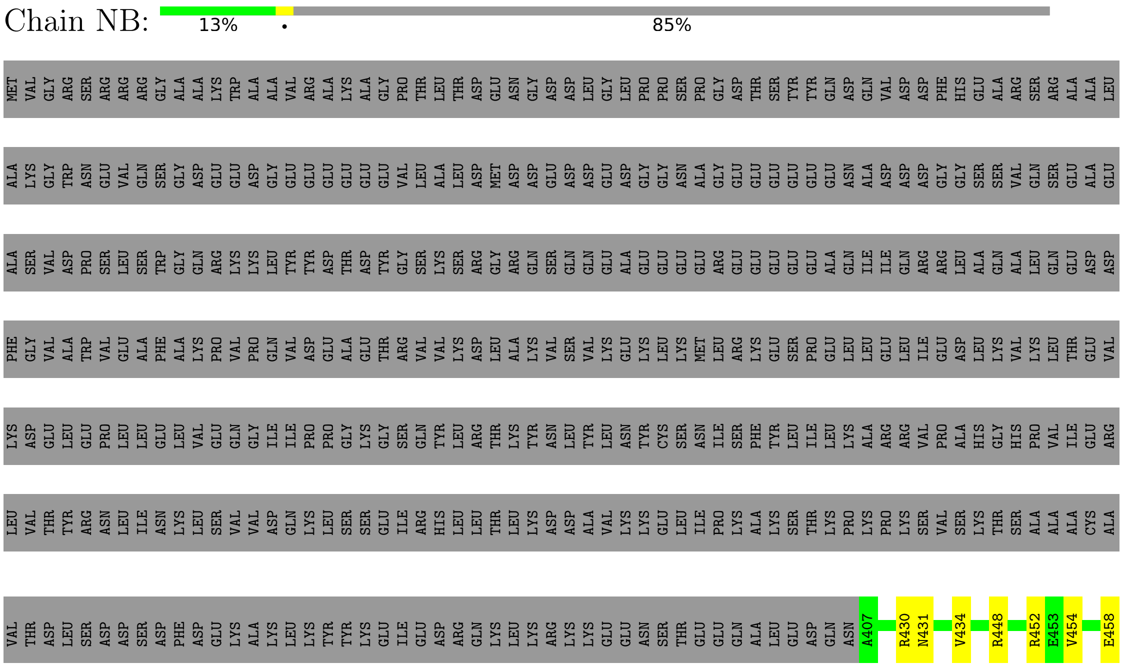
- Molecule 29: U3 small nucleolar ribonucleoprotein protein MPP10

Chain NA:

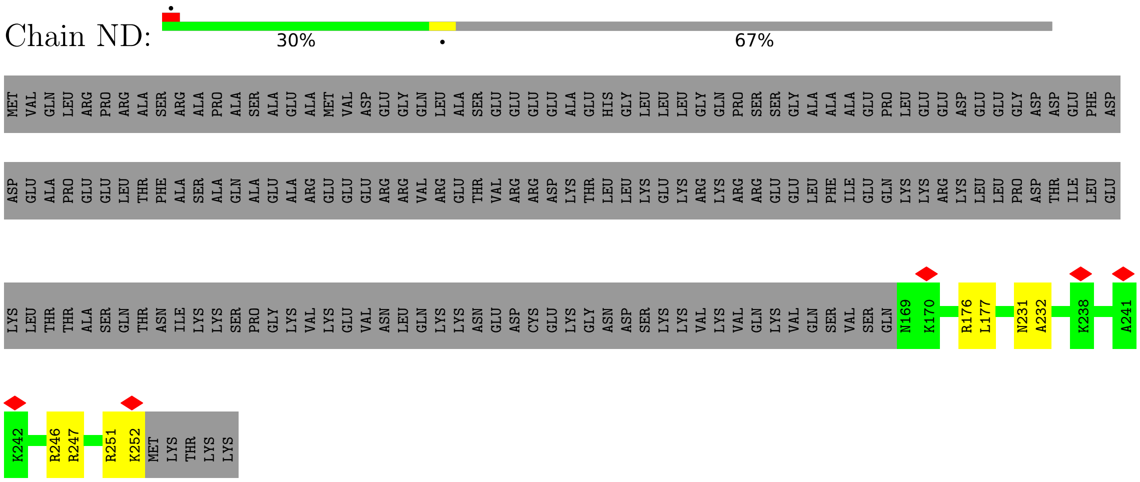


- Molecule 30: Something about silencing protein 10

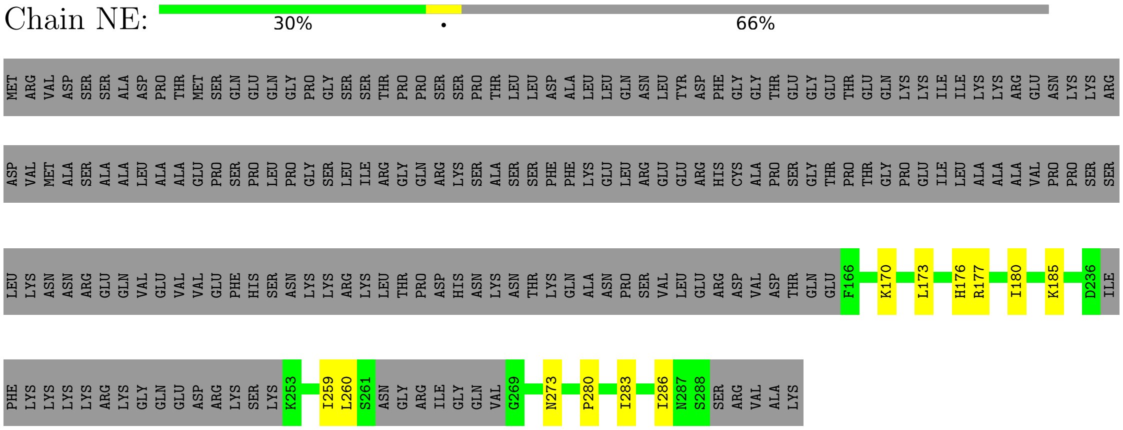
Chain NB:



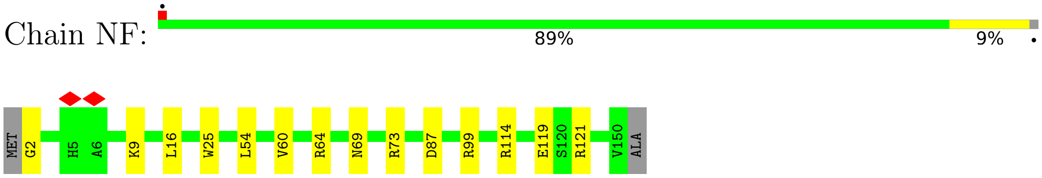
- Molecule 31: Nucleolar protein 7



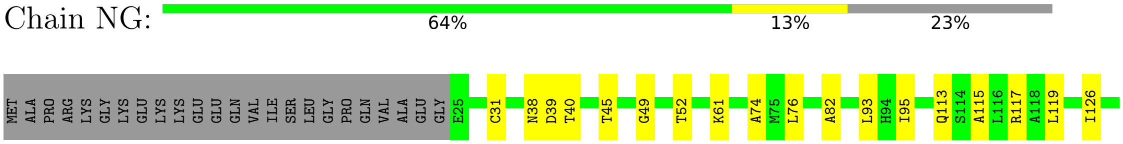
- Molecule 32: Uncharacterized protein C1orf131



- Molecule 33: 40S ribosomal protein S13

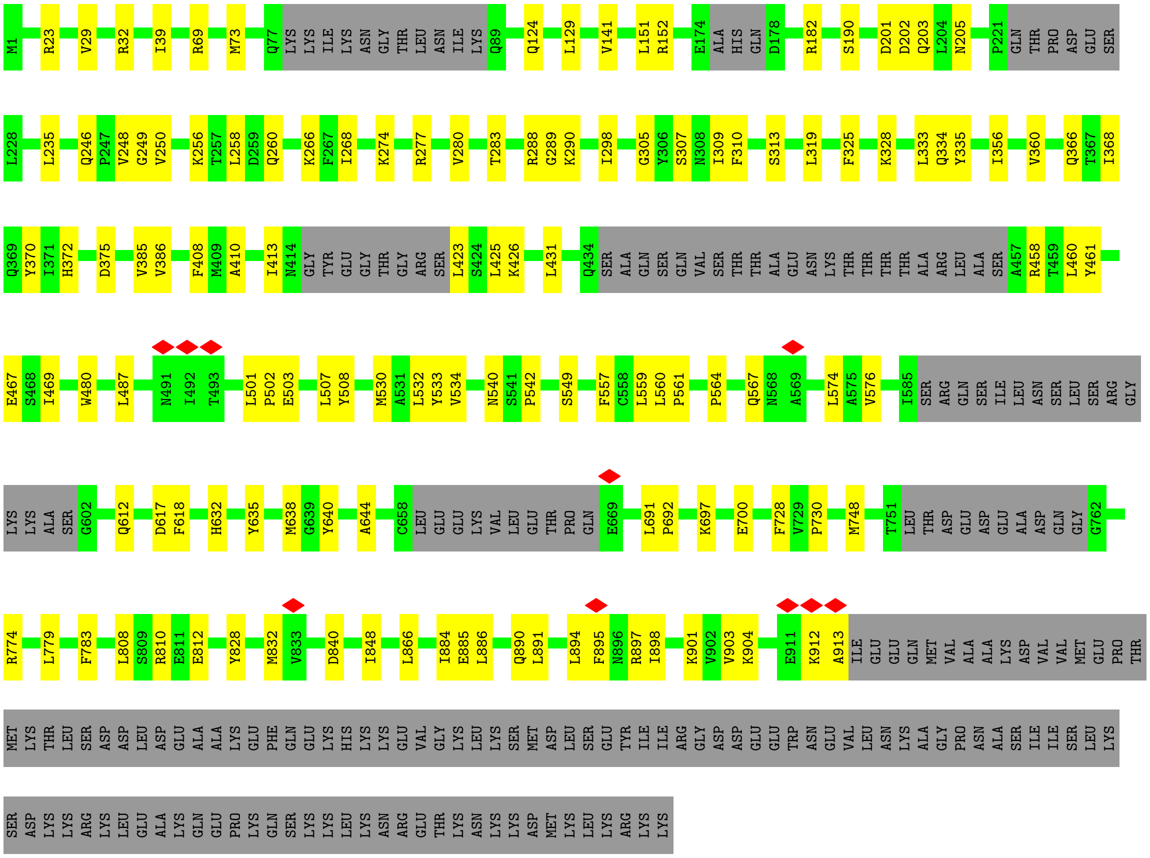


- Molecule 34: 40S ribosomal protein S14



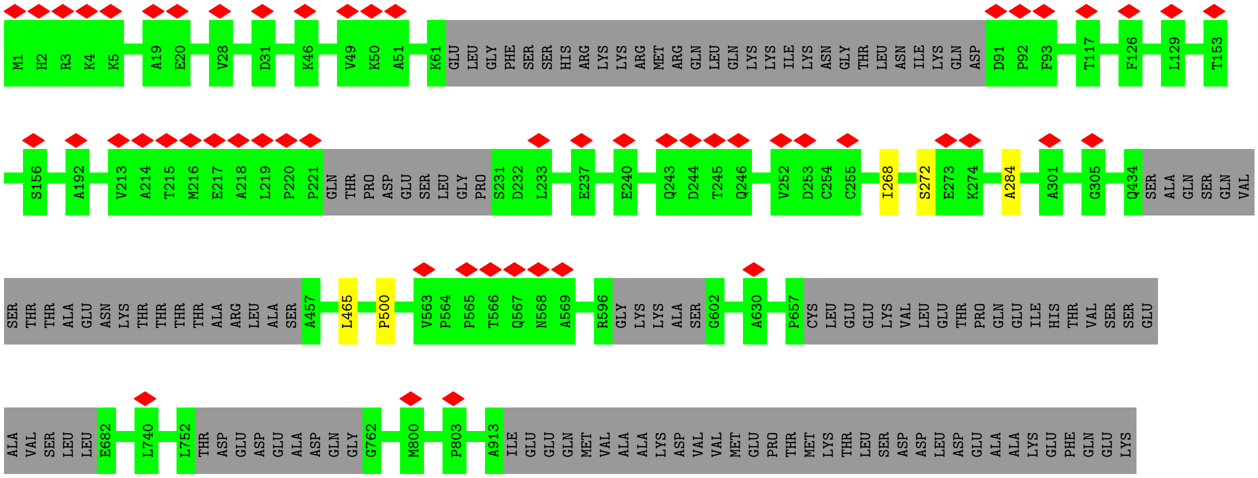
- Molecule 35: RNA cytidine acetyltransferase

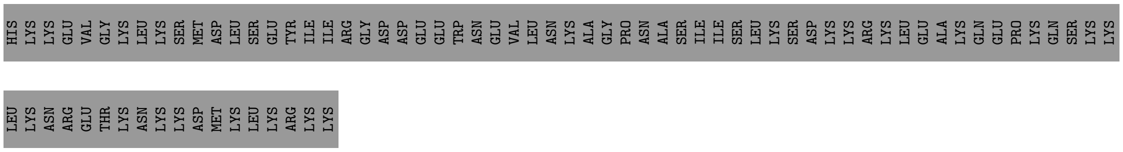
Chain NJ:



- Molecule 35: RNA cytidine acetyltransferase

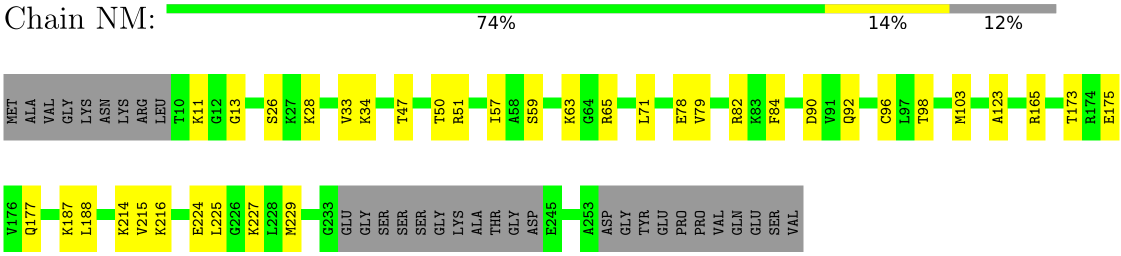
Chain NK:





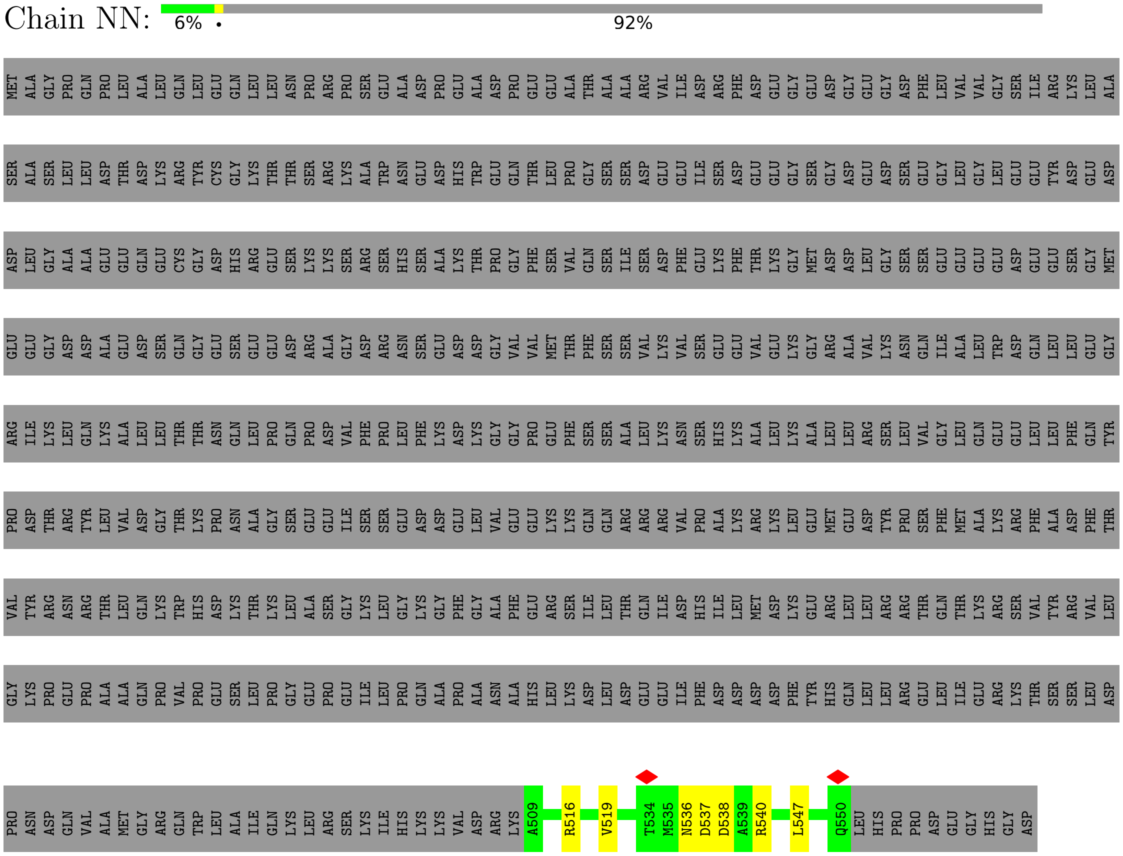
- Molecule 36: 40S ribosomal protein S3a

Chain NM:



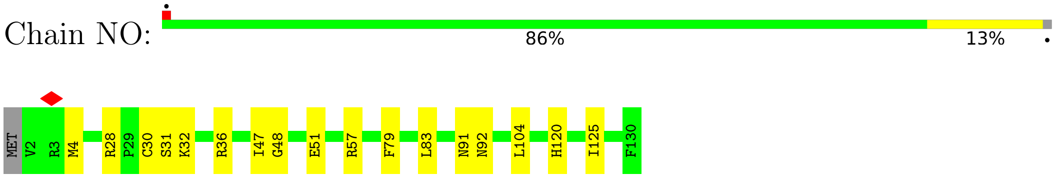
- Molecule 37: Protein AATF

Chain NN:



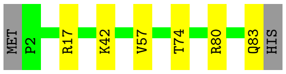
- Molecule 38: 40S ribosomal protein S15a

Chain NO:



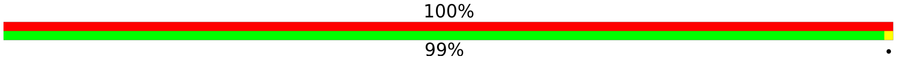
- Molecule 39: 40S ribosomal protein S27

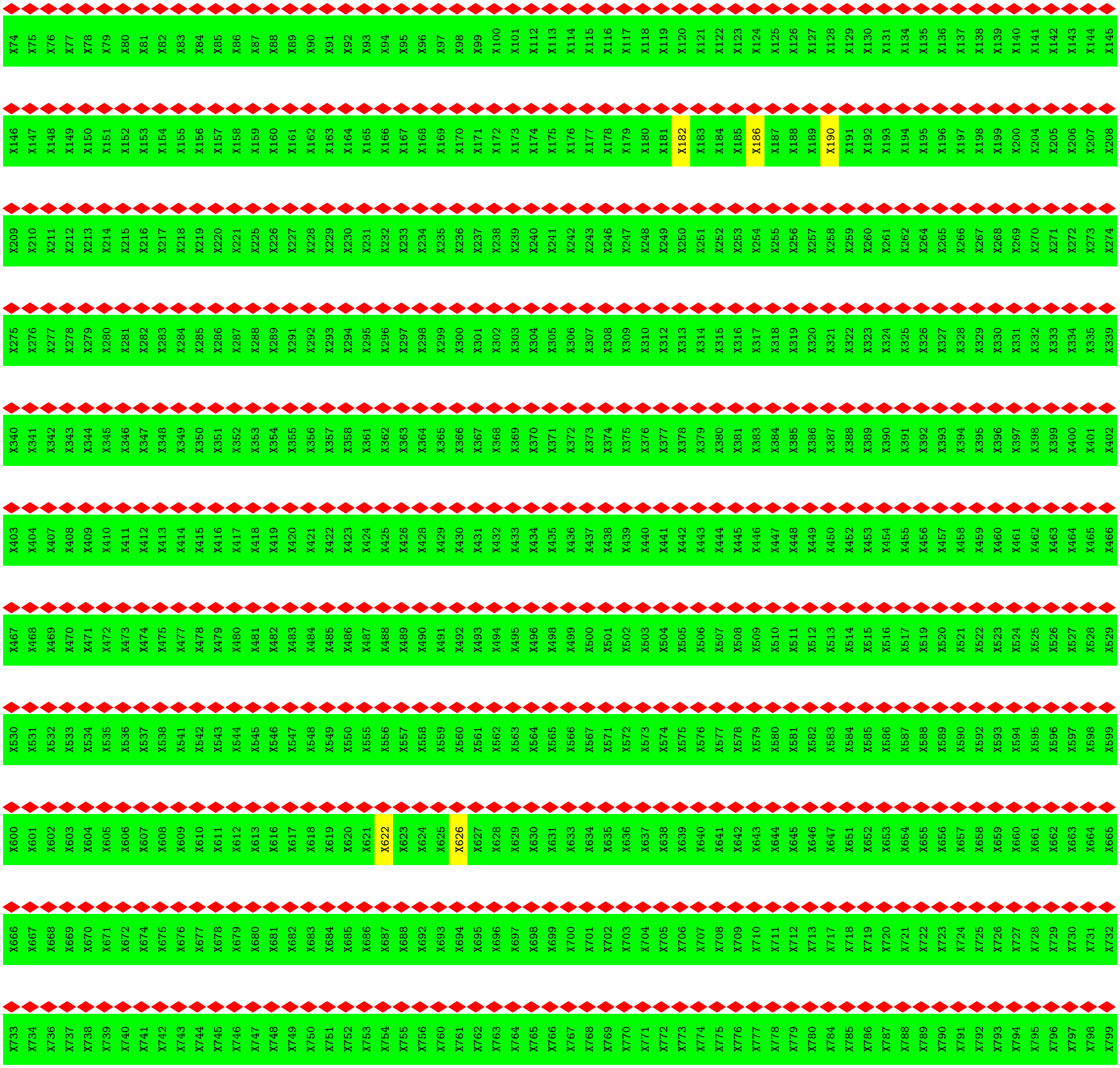
Chain NQ:

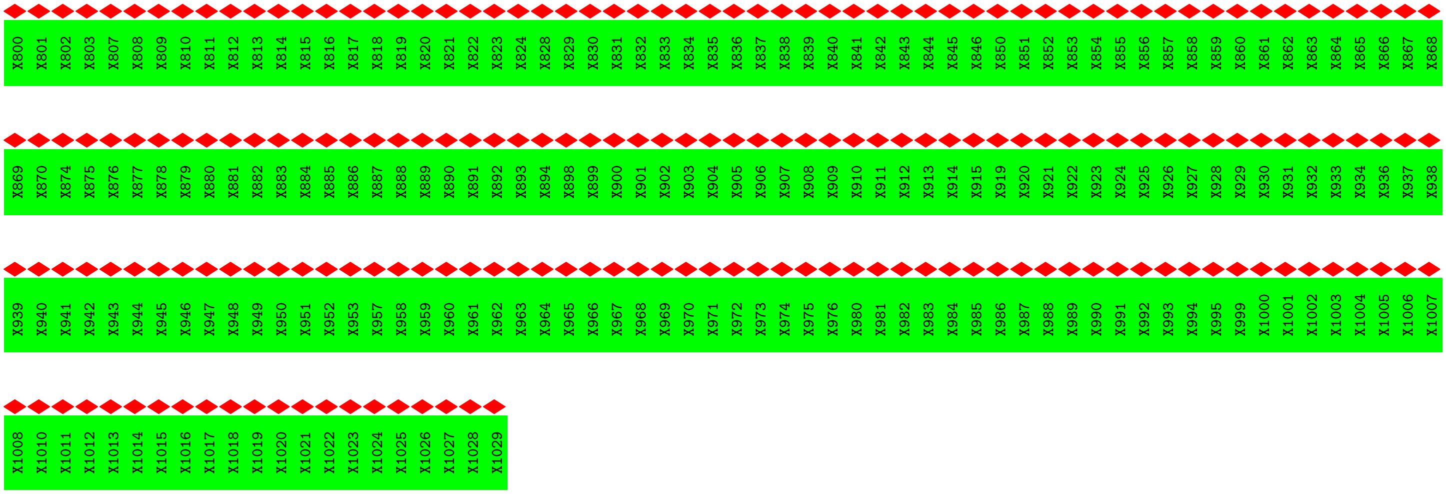


- Molecule 40: RRP12-like protein

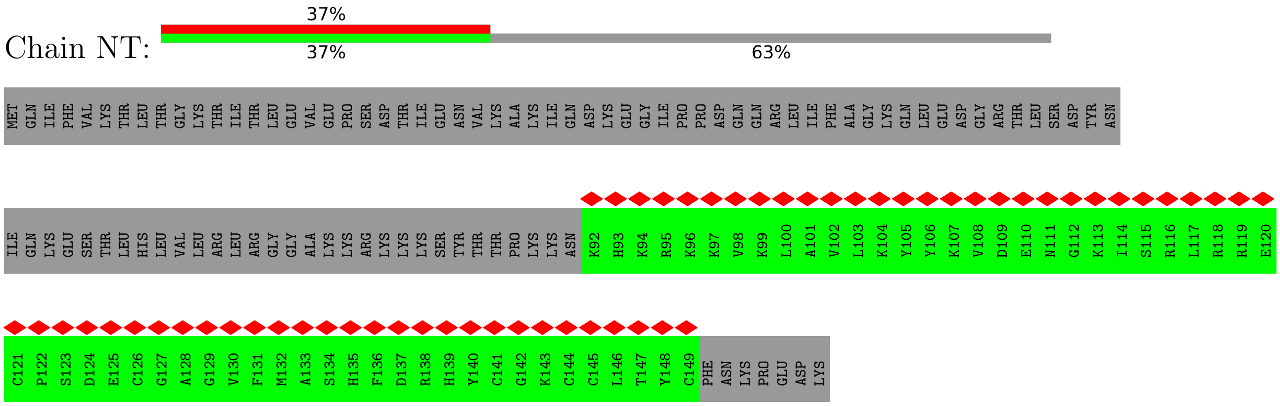
Chain NR:



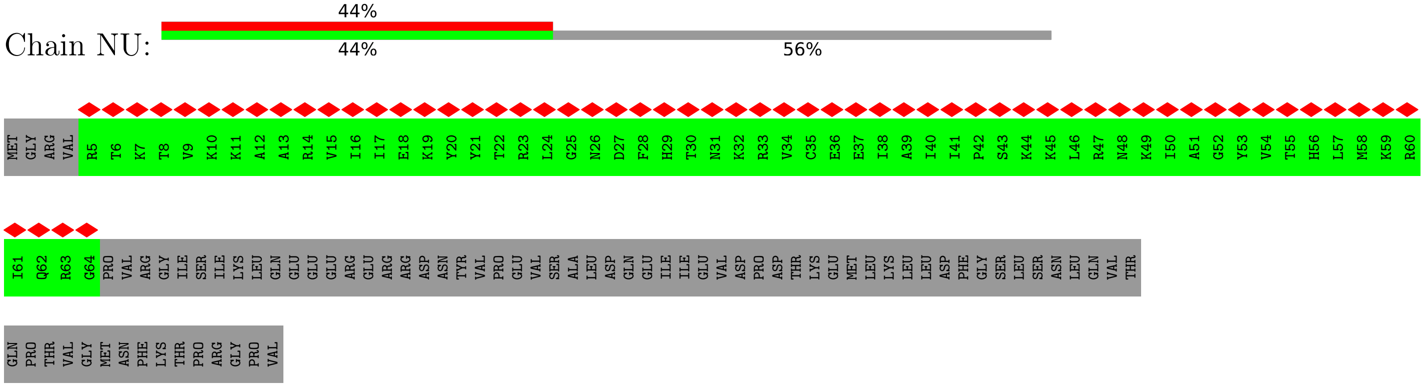




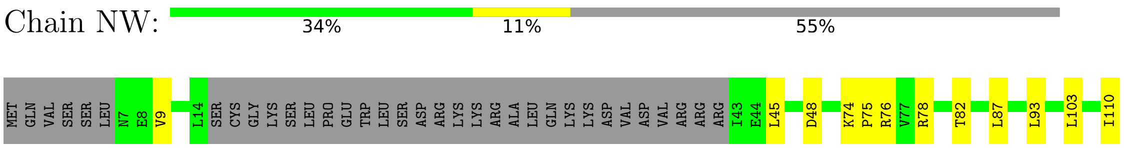
- Molecule 41: Ubiquitin-40S ribosomal protein S27a

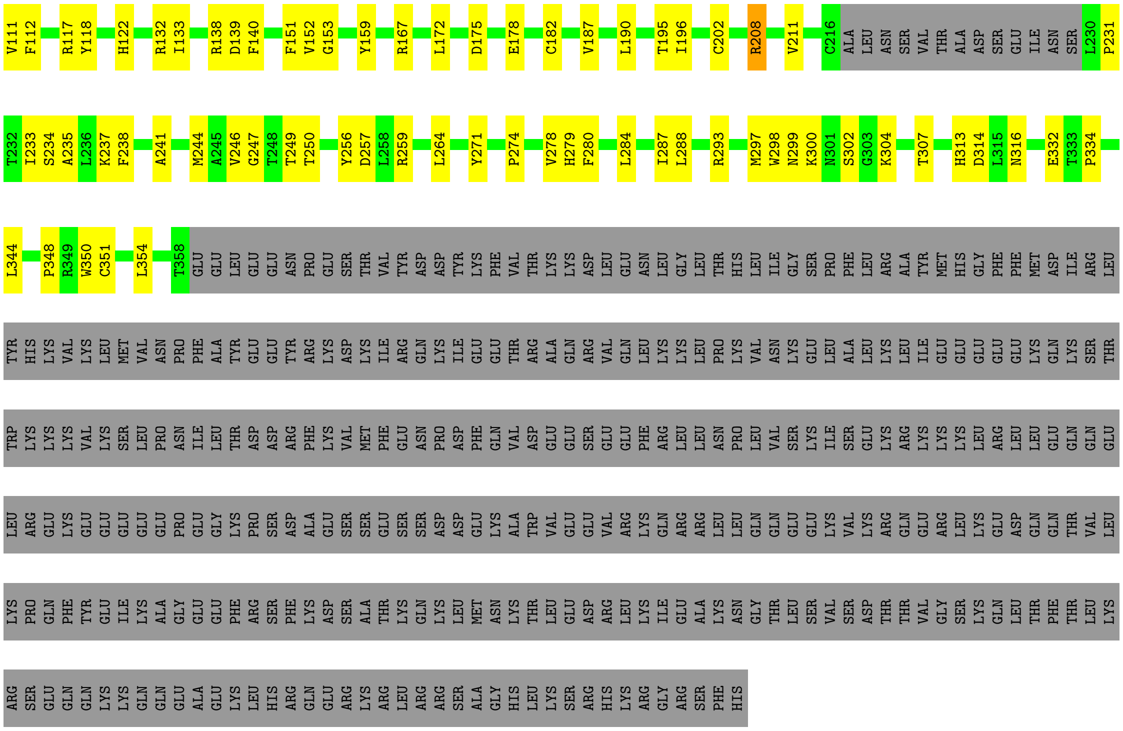


- Molecule 42: 40S ribosomal protein S17



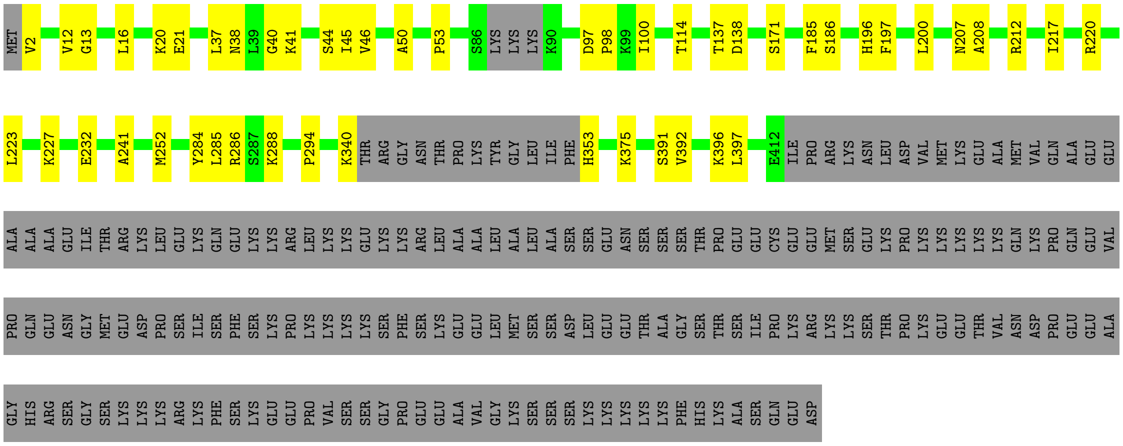
- Molecule 43: Nucleolar protein 10





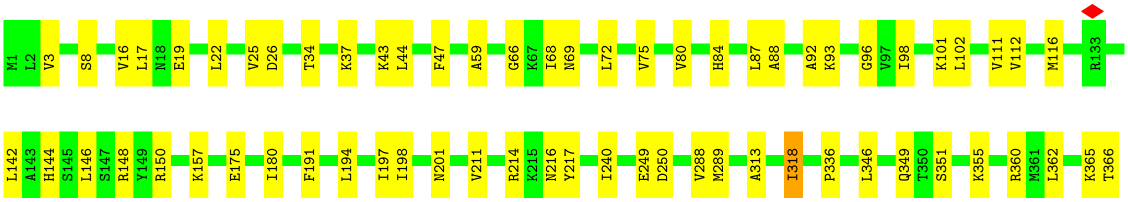
- Molecule 44: Nucleolar protein 56

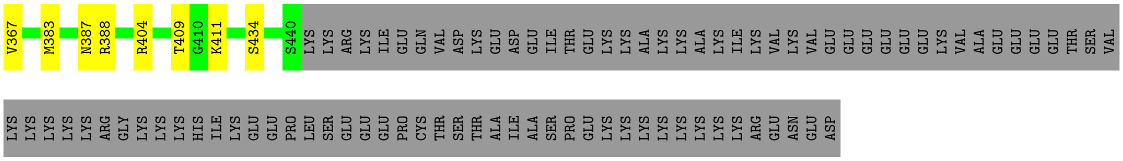
Chain SA:



- Molecule 45: Nucleolar protein 58

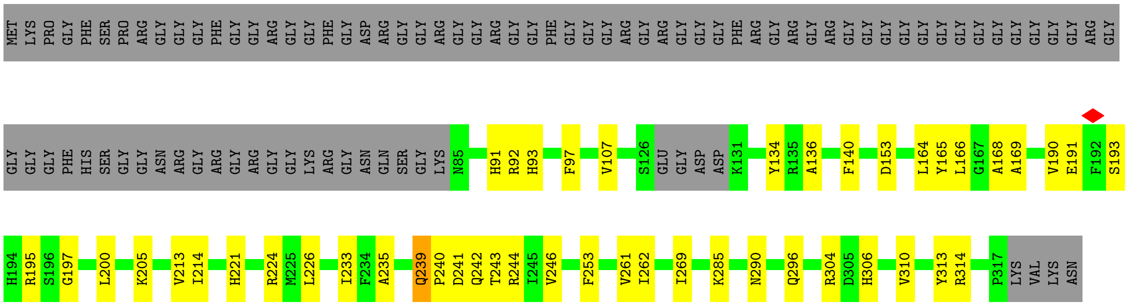
Chain SB:





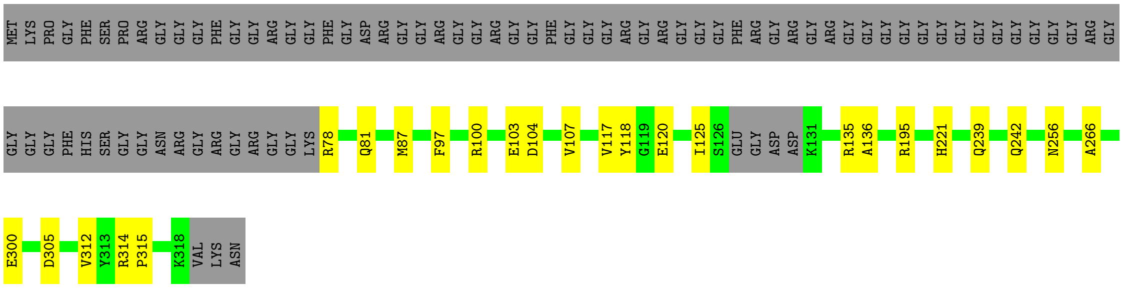
- Molecule 46: rRNA 2'-O-methyltransferase fibrillarin

Chain SC:



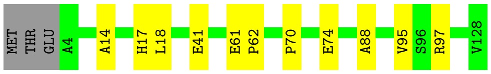
- Molecule 46: rRNA 2'-O-methyltransferase fibrillarin

Chain SD:



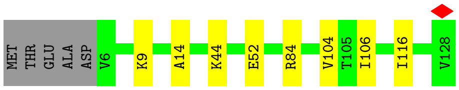
- Molecule 47: NHP2-like protein 1

Chain SE:



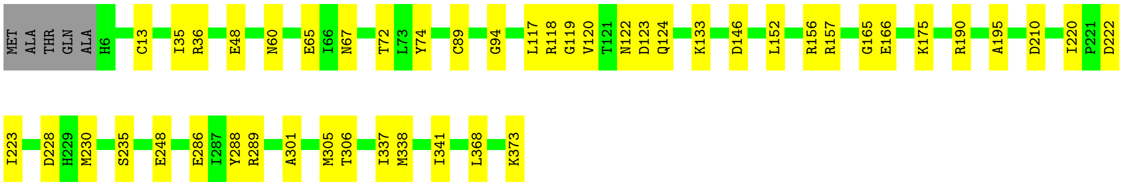
- Molecule 47: NHP2-like protein 1

Chain SF:



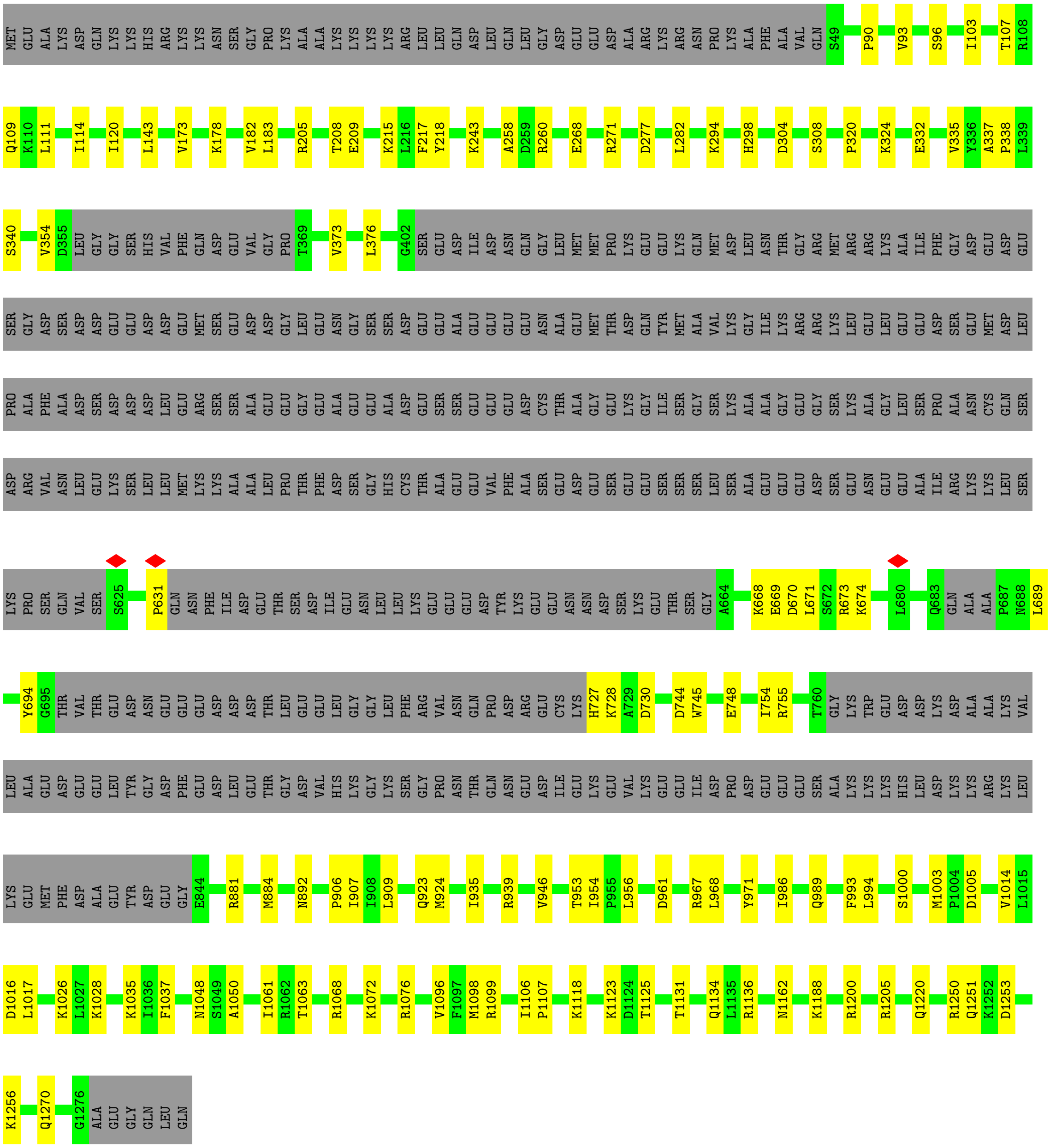
- Molecule 48: RNA 3'-terminal phosphate cyclase-like protein

Chain SH:



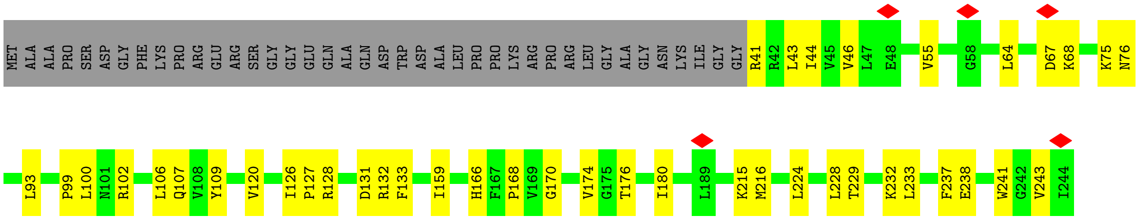
- Molecule 49: Ribosome biogenesis protein BMS1 homolog

Chain SI:

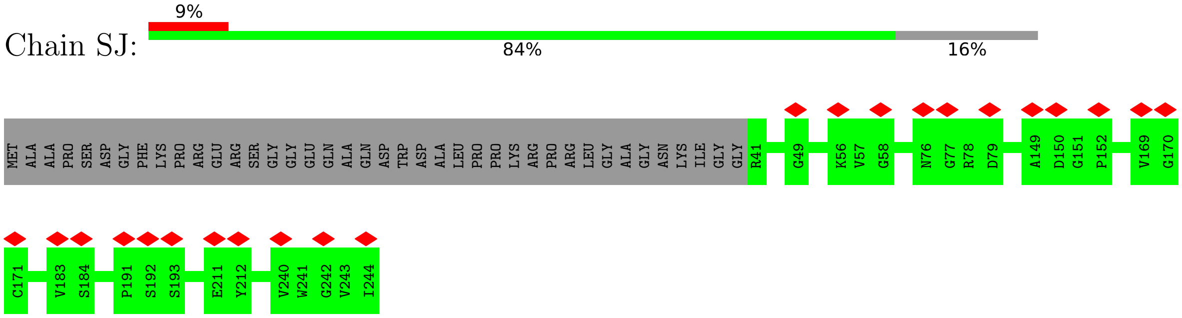


- Molecule 50: Ribosomal RNA small subunit methyltransferase NEP1

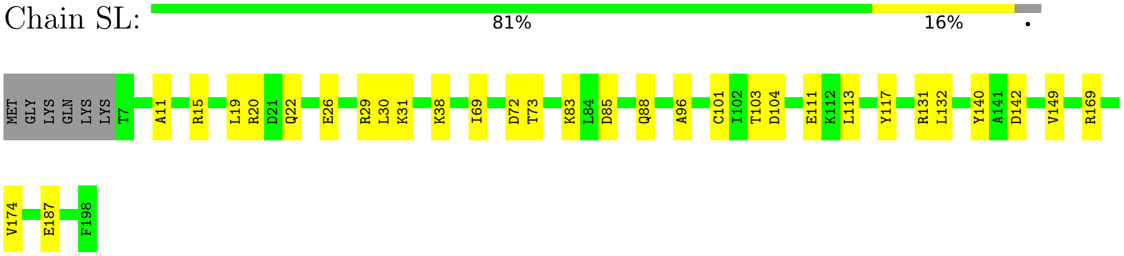
Chain SK:



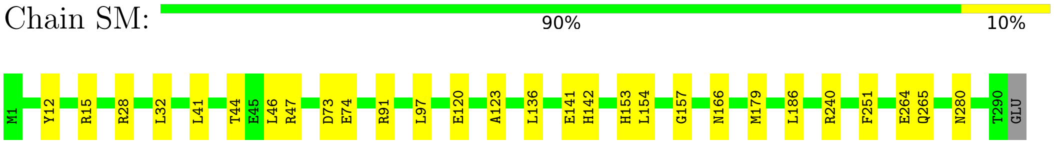
- Molecule 50: Ribosomal RNA small subunit methyltransferase NEP1



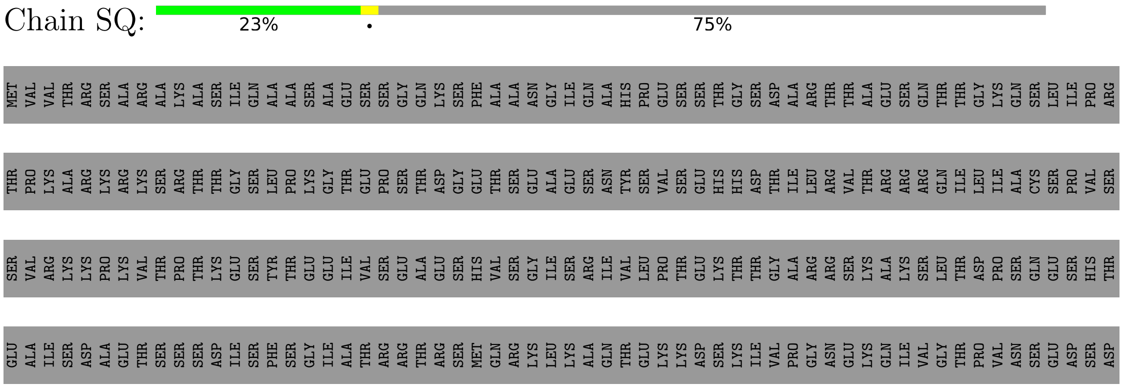
- Molecule 51: rRNA-processing protein FCF1 homolog

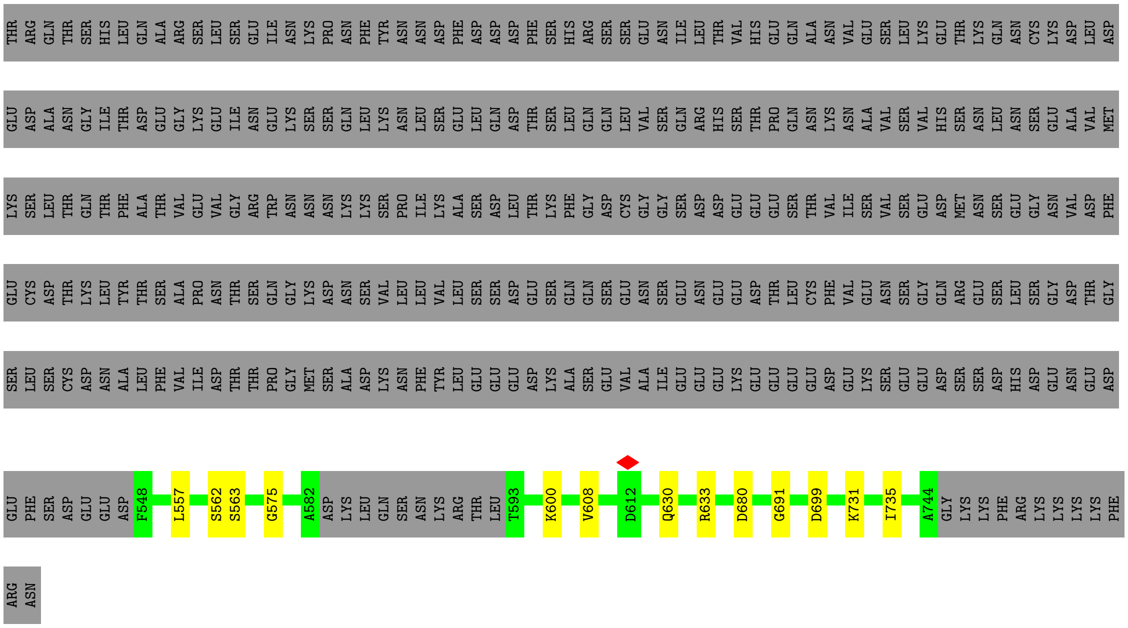


- Molecule 52: U3 small nucleolar ribonucleoprotein protein IMP4

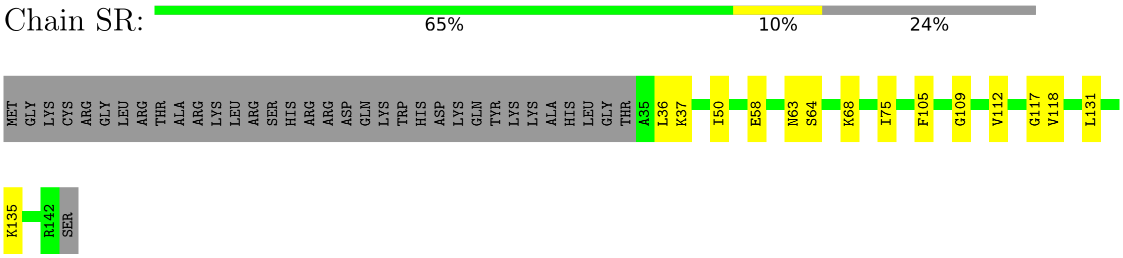


- Molecule 53: Deoxynucleotidyltransferase terminal-interacting protein 2

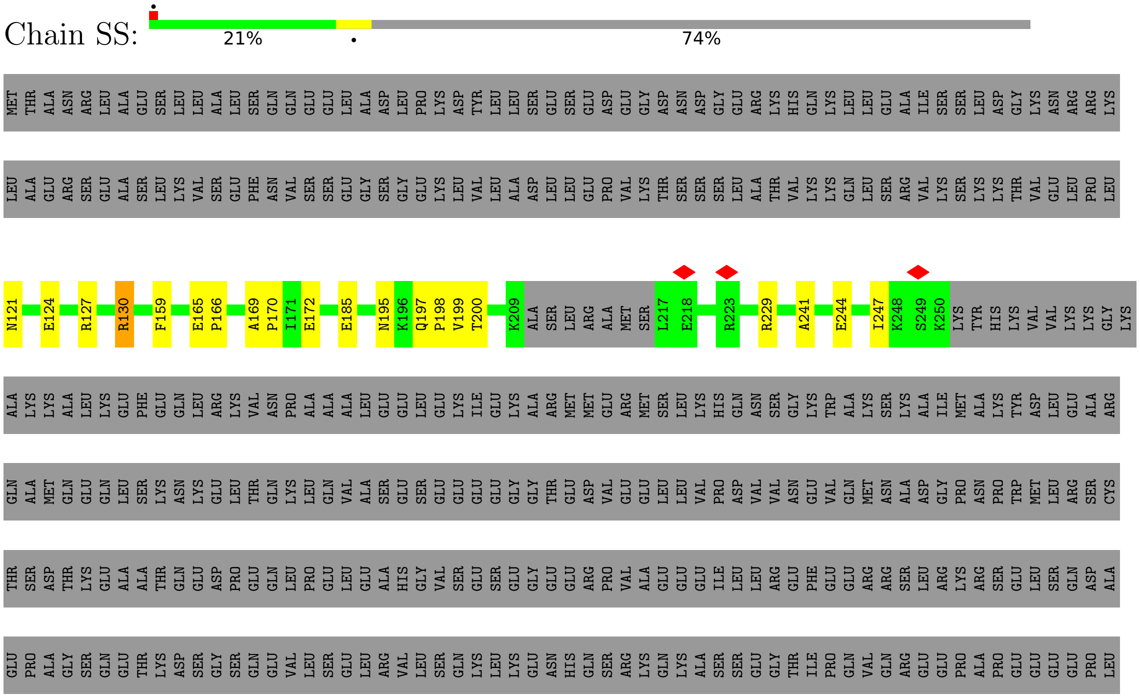


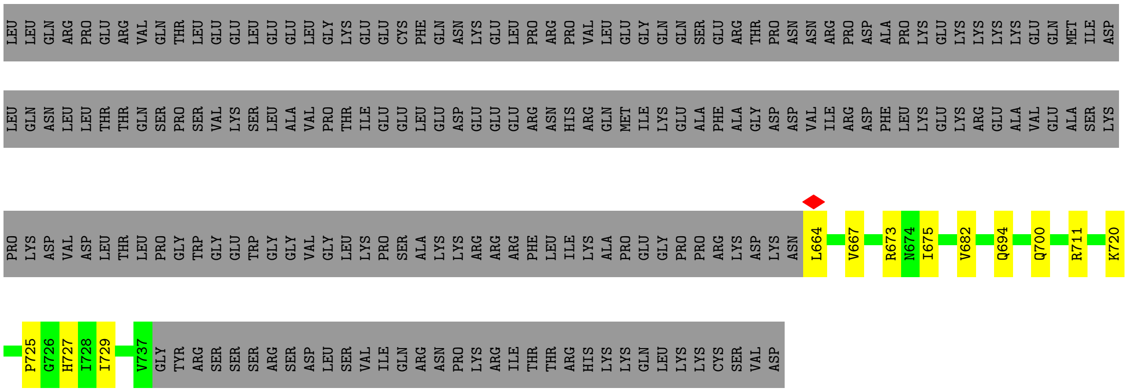


- Molecule 54: 40S ribosomal protein S23



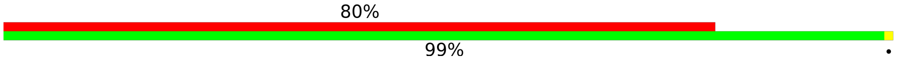
- Molecule 55: U3 small nucleolar RNA-associated protein 14 homolog A

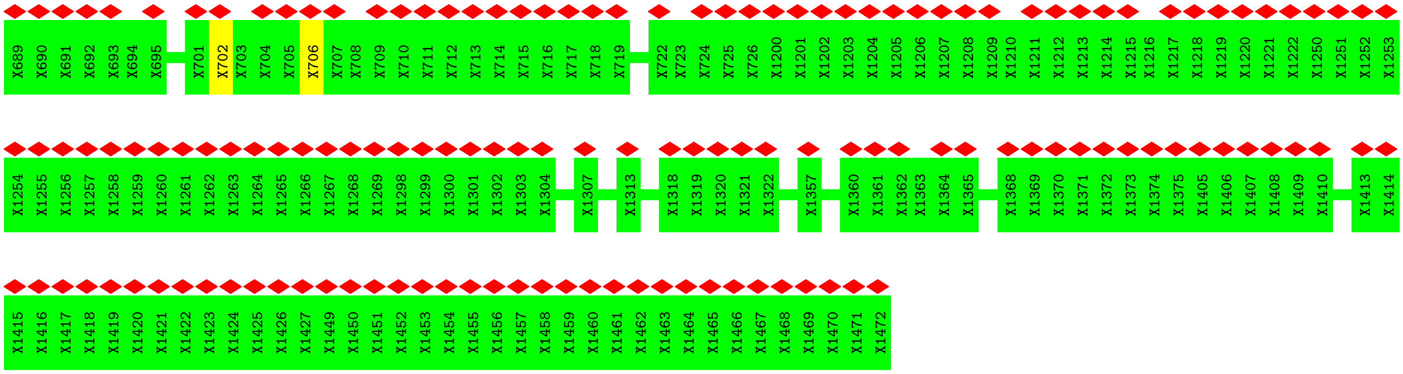




- Molecule 56: Unassigned peptides

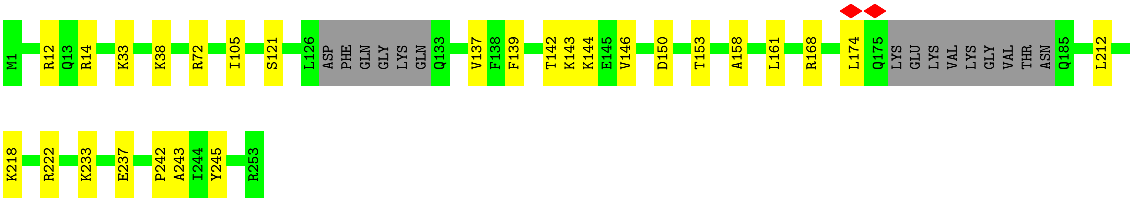
Chain SX:





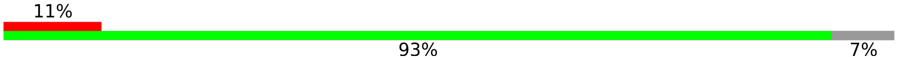
- Molecule 57: Probable U3 small nucleolar RNA-associated protein 11

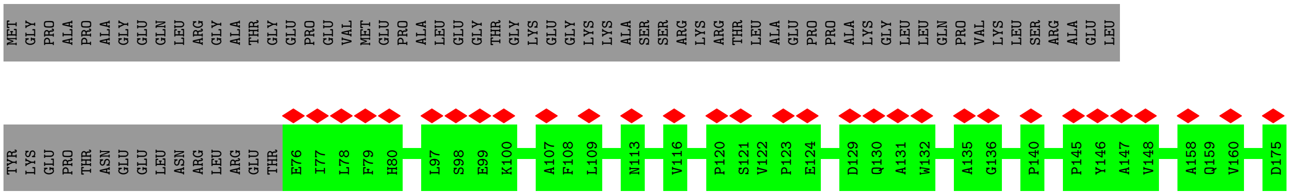
Chain SY:

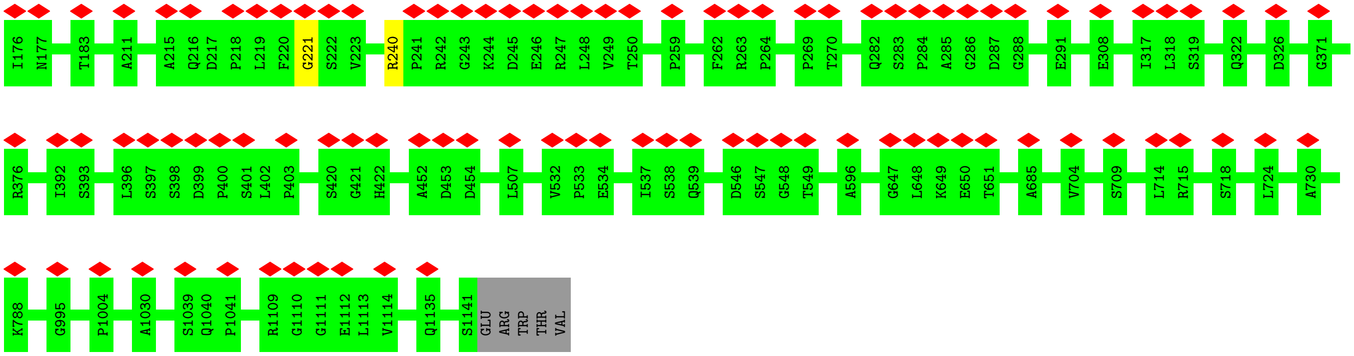


- Molecule 58: Nucleolar protein 6

Chain NH:

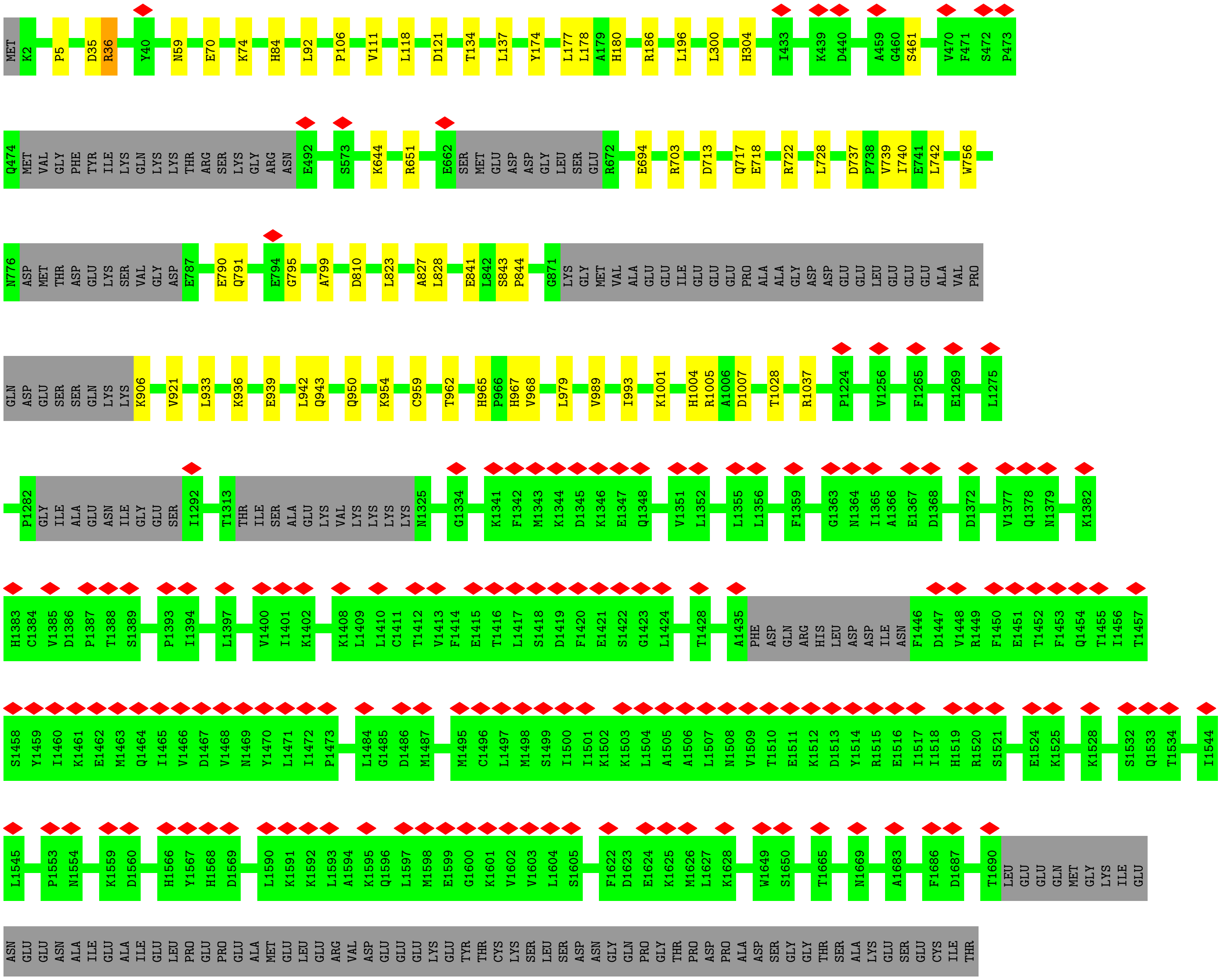


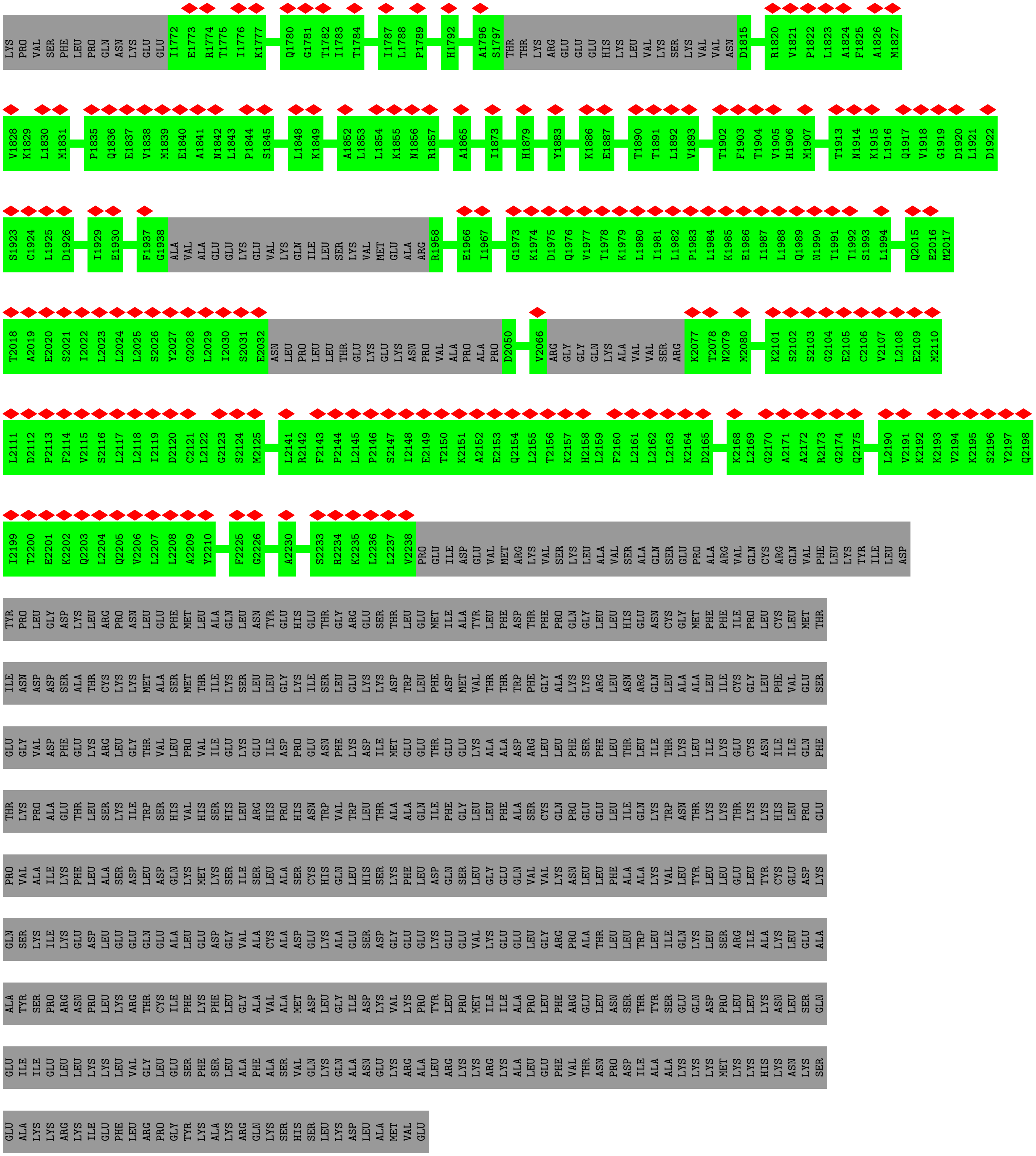




- Molecule 59: Small subunit processome component 20 homolog

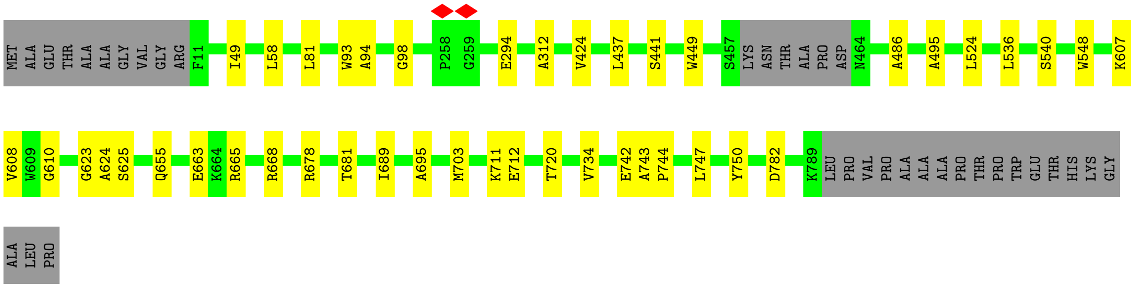
Chain SP:





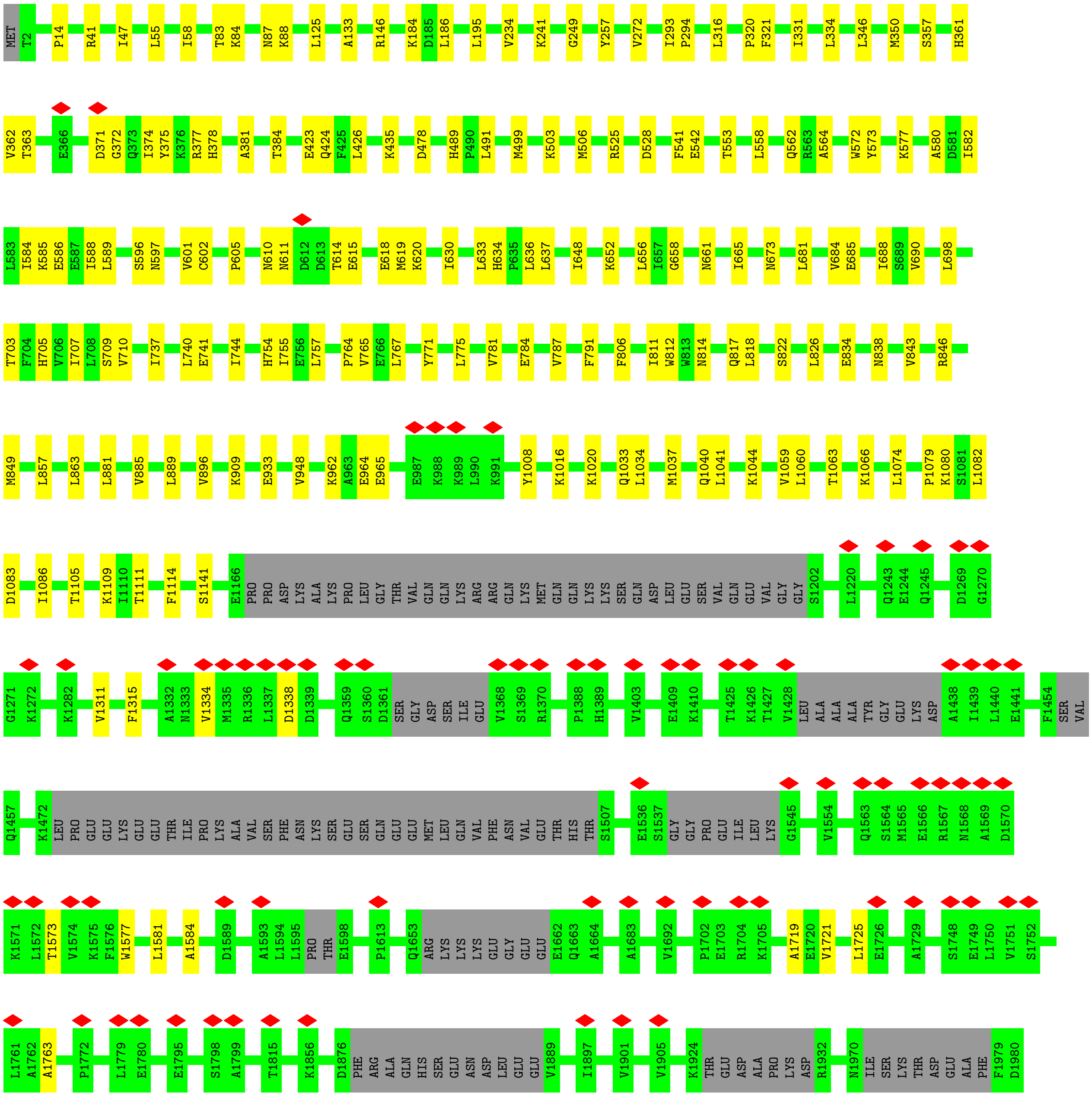
- Molecule 60: Transducin beta-like protein 3

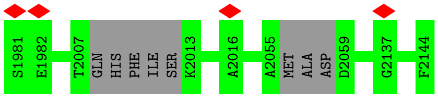
Chain LR:



- Molecule 61: HEAT repeat-containing protein 1

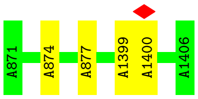
Chain LM:





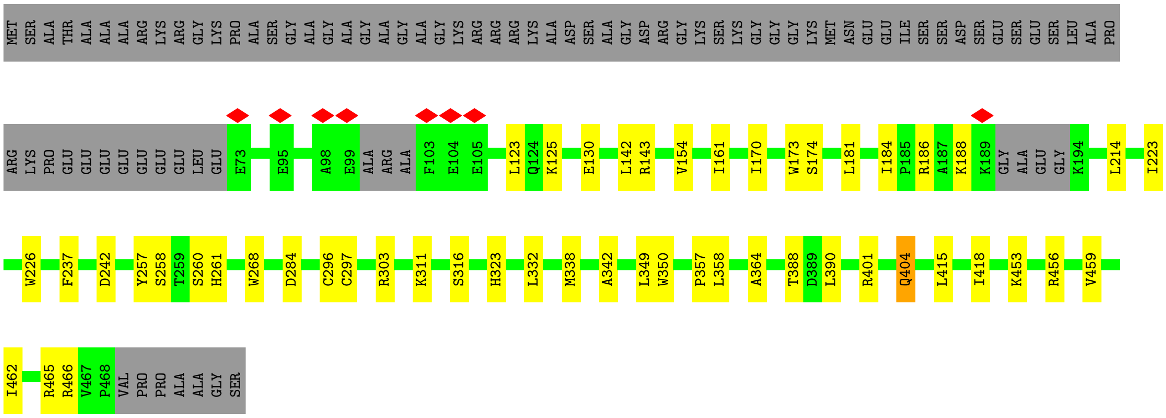
• Molecule 62: 5’ ETS rRNA

Chain N0:



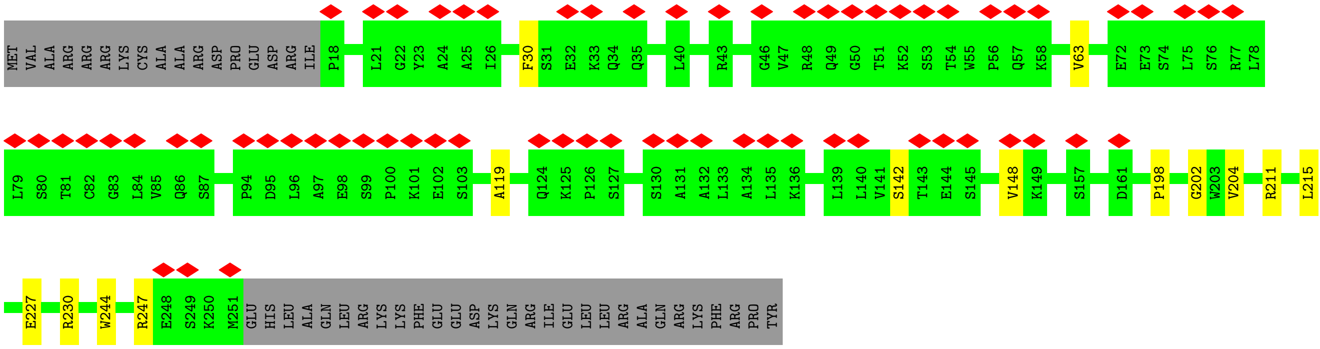
• Molecule 63: U3 small nucleolar RNA-interacting protein 2

Chain SG:



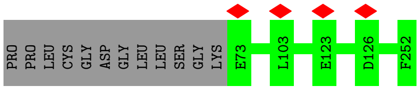
• Molecule 64: Ribosomal RNA-processing protein 7 homolog A

Chain NI:



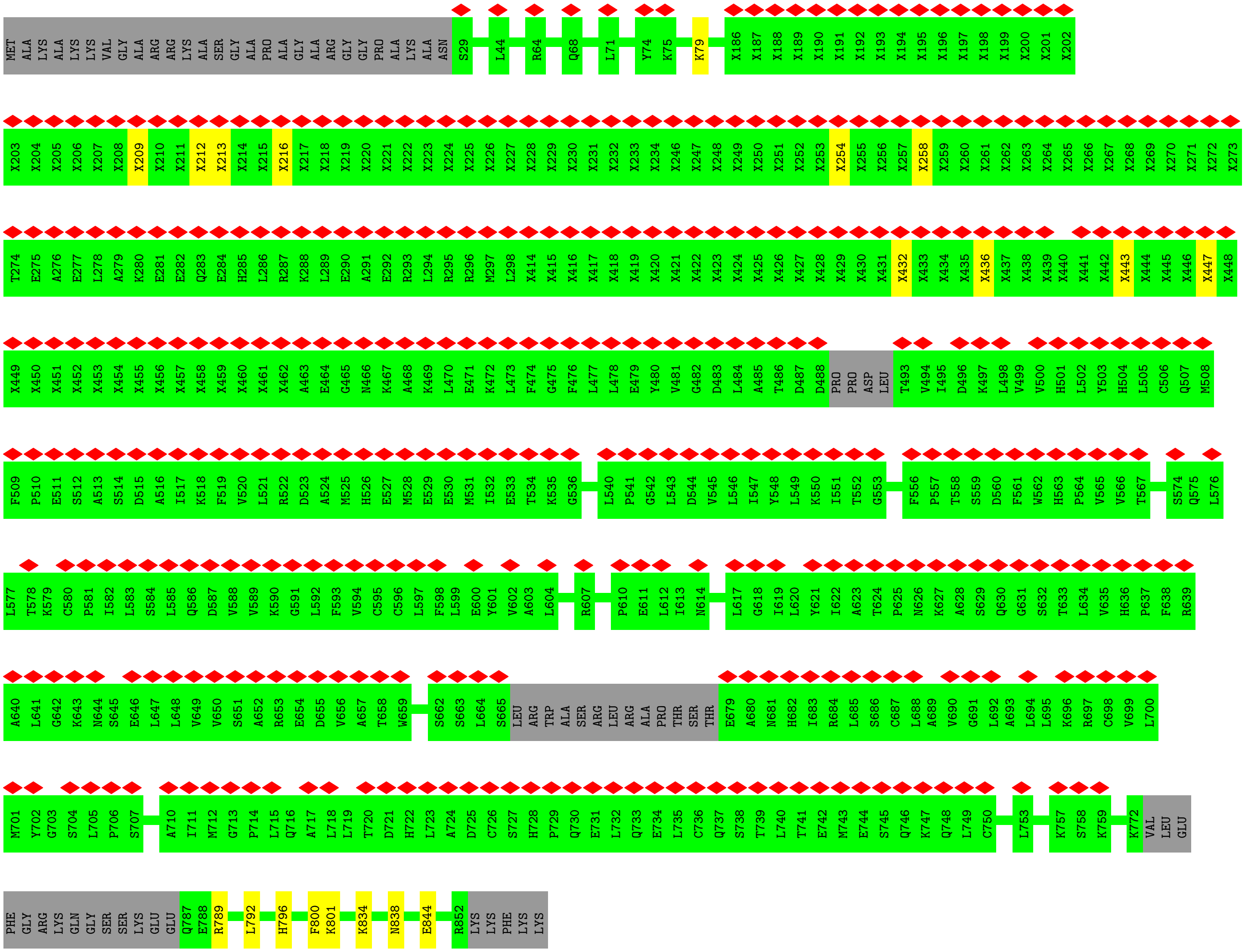
• Molecule 65: RNA-binding protein PNO1

Chain SW:



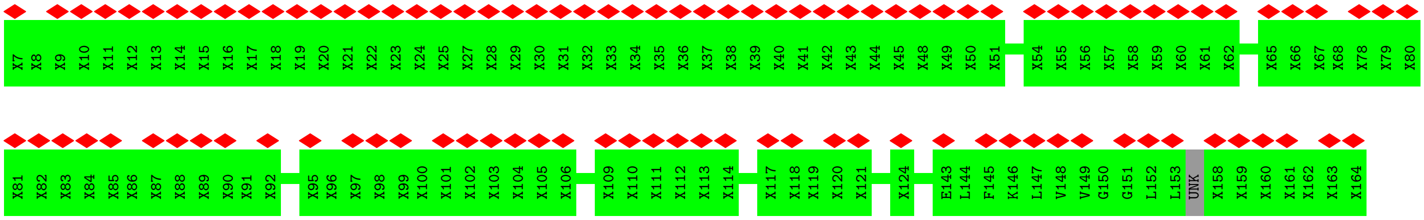
- Molecule 66: Nucleolar protein 14

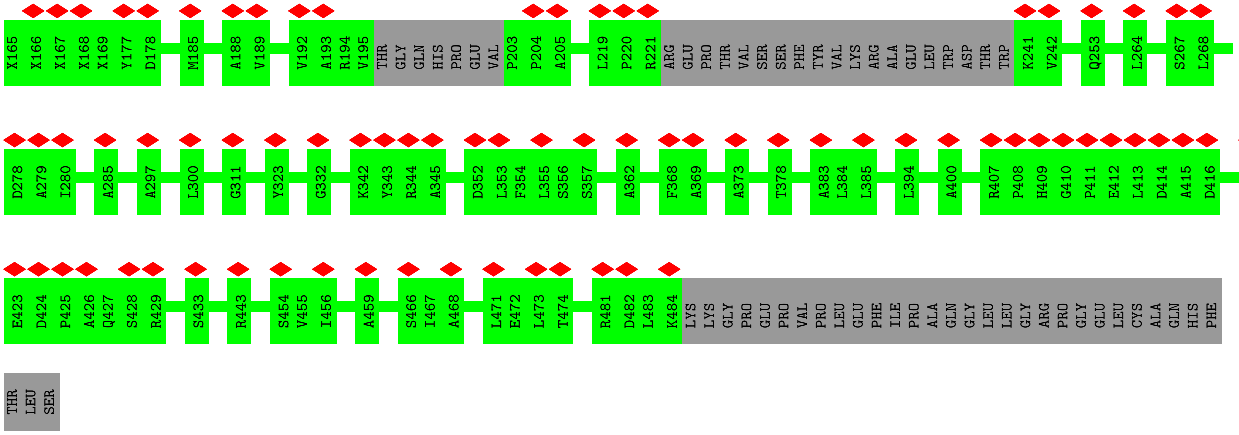
Chain ST:



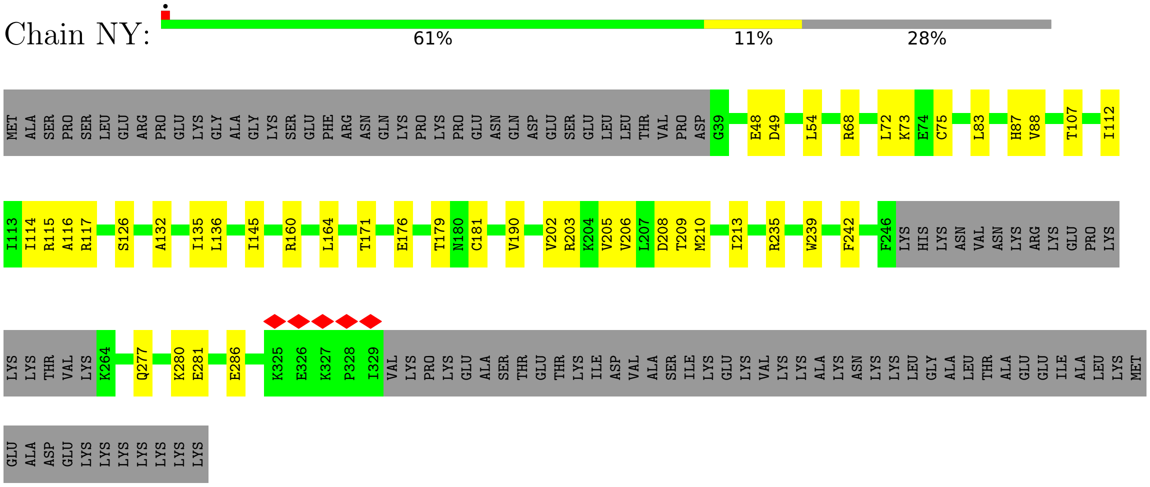
- Molecule 67: Nucleolar complex protein 4 homolog

Chain SU:

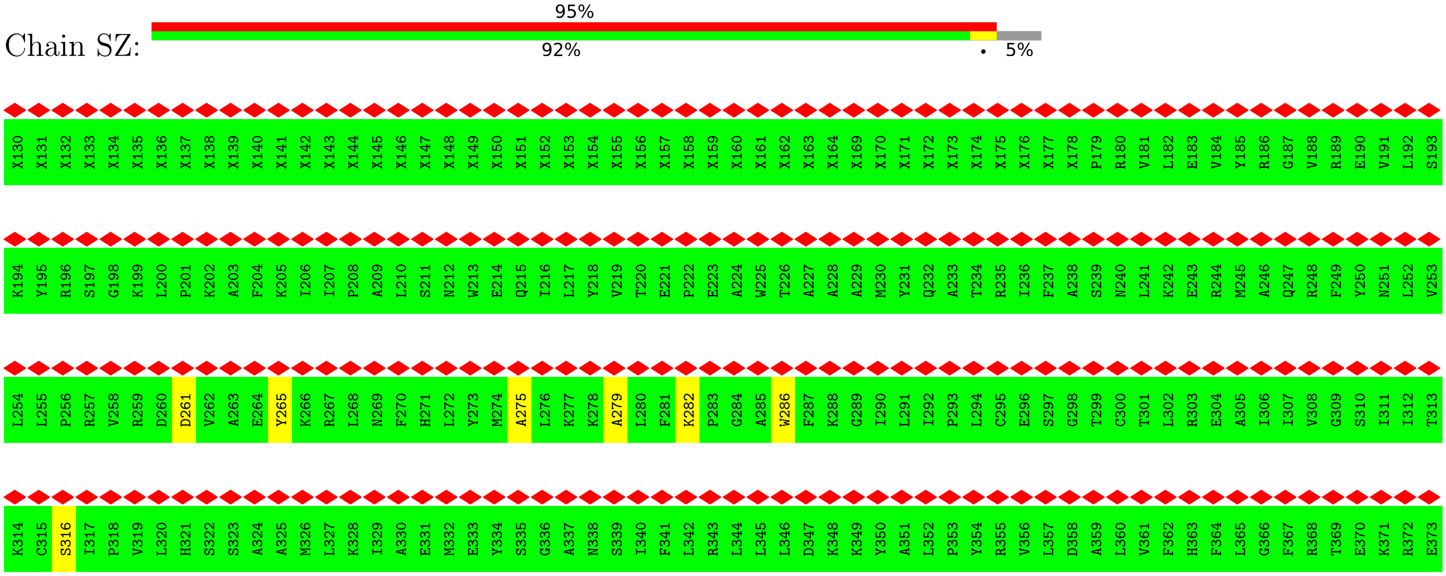


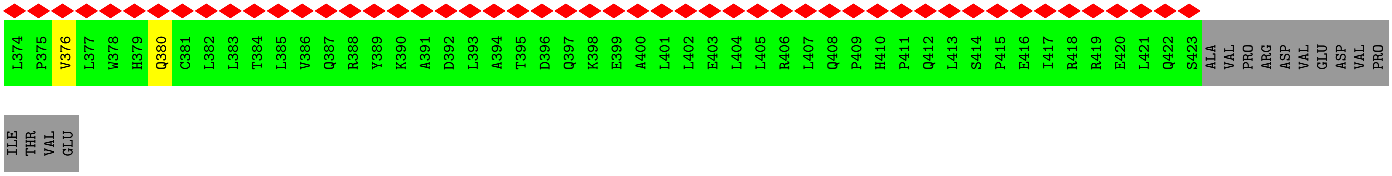


- Molecule 68: KRR1 small subunit processome component homolog



- Molecule 69: Bystin




L374
P375
V376
L377
W378
H379
Q380
C381
L382
L383
T384
L385
V386
Q387
R388
Y389
K390
A391
D392
L393
A394
T395
D396
Q397
K398
E399
A400
L401
L402
E403
L404
L405
R406
L407
Q408
P409
H410
P411
Q412
L413
S414
P415
E416
I417
R418
R419
E420
L421
Q422
S423
ALA
VAL
PRO
ARG
ASP
VAL
GLU
ASP
VAL
PRO
ILE
THR
VAL
GLU

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	58	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0088	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, SAH, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	L0	0.20	0/5739	0.82	1/8931 (0.0%)
2	L1	0.23	0/31039	0.82	54/48327 (0.1%)
3	L2	0.24	0/5130	0.79	2/7996 (0.0%)
4	L3	0.24	0/425	0.40	0/591
5	L4	0.25	0/1944	0.53	0/2621
6	L5	0.27	0/1523	0.55	0/2048
7	L6	0.26	0/1830	0.56	0/2434
8	L7	0.26	0/1365	0.51	0/1830
9	L8	0.27	0/1500	0.58	0/2002
10	L9	0.27	0/1447	0.57	0/1930
11	LA	0.23	0/592	0.39	0/823
12	LC	0.29	0/1115	0.56	0/1494
13	LD	0.25	0/1225	0.54	0/1640
14	LF	0.26	0/868	0.52	0/1159
15	LG	0.24	0/490	0.58	0/656
16	LH	0.26	0/6127	0.51	0/8292
17	LI	0.23	0/1959	0.38	0/2719
18	LJ	0.27	0/3788	0.54	0/5128
19	LK	0.24	0/959	0.48	0/1302
19	LL	0.25	0/4072	0.51	0/5539
20	LN	0.26	0/5438	0.51	0/7377
21	LO	0.28	0/6835	0.54	1/9256 (0.0%)
22	LP	0.26	0/4806	0.47	0/6455
23	LQ	0.25	0/6548	0.53	0/8839
24	LS	0.27	0/3621	0.52	0/4876
25	LT	0.26	0/6907	0.50	0/9359
26	LU	0.26	0/3695	0.52	0/4986
27	LW	0.27	0/3594	0.54	0/4867
28	LZ	0.26	0/1560	0.56	0/2104
29	NA	0.27	0/2084	0.48	0/2789
30	NB	0.26	0/622	0.62	0/816
31	ND	0.25	0/708	0.53	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	NE	0.27	0/807	0.49	0/1069
33	NF	0.24	0/1226	0.48	0/1649
34	NG	0.24	0/873	0.51	0/1177
35	NJ	0.25	0/6652	0.51	0/9006
35	NK	0.24	0/4023	0.44	0/5594
36	NM	0.24	0/1899	0.50	0/2533
37	NN	0.24	0/346	0.57	0/462
38	NO	0.26	0/1051	0.53	0/1406
39	NQ	0.24	0/653	0.50	0/876
41	NT	0.23	0/285	0.45	0/395
42	NU	0.22	0/296	0.34	0/411
43	NW	0.27	0/2556	0.54	1/3469 (0.0%)
44	SA	0.26	0/3122	0.47	0/4208
45	SB	0.25	0/3491	0.48	1/4695 (0.0%)
46	SC	0.26	0/1818	0.52	0/2463
46	SD	0.28	0/1878	0.51	0/2540
47	SE	0.26	0/980	0.50	0/1323
47	SF	0.29	0/967	0.53	0/1305
48	SH	0.26	0/2882	0.51	0/3887
49	SI	0.27	0/6949	0.50	1/9339 (0.0%)
50	SJ	0.27	0/1007	0.47	0/1401
50	SK	0.28	0/1609	0.54	1/2181 (0.0%)
51	SL	0.27	0/1619	0.53	0/2174
52	SM	0.27	0/2420	0.56	0/3264
53	SQ	0.27	0/1561	0.49	0/2083
54	SR	0.28	0/828	0.52	0/1110
55	SS	0.28	0/1663	0.53	1/2250 (0.0%)
57	SY	0.25	0/2051	0.50	0/2723
58	NH	0.26	0/5264	0.45	0/7329
59	SP	0.24	0/11868	0.43	0/16336
60	LR	0.24	0/4340	0.49	0/5985
61	LM	0.26	0/13315	0.45	0/18214
62	N0	0.13	0/284	0.87	0/432
63	SG	0.25	0/2935	0.52	0/3981
64	NI	0.25	0/1471	0.52	0/2009
65	SW	0.24	0/889	0.44	0/1237
66	ST	0.23	0/2435	0.43	0/3343
67	SU	0.24	0/1463	0.41	0/2037
68	NY	0.27	0/2133	0.48	0/2887
69	SZ	0.23	0/1216	0.42	0/1696
All	All	0.25	0/222680	0.58	63/310612 (0.0%)

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
64	NI	0	1

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	1453	C	N1-C2-O2	8.87	124.22	118.90
2	L1	1453	C	C2-N1-C1'	8.84	128.52	118.80
2	L1	1535	U	C2-N1-C1'	8.36	127.73	117.70
2	L1	1535	U	N1-C2-O2	8.18	128.52	122.80
2	L1	1742	C	C2-N1-C1'	7.78	127.36	118.80
2	L1	1535	U	N3-C2-O2	-7.50	116.95	122.20
2	L1	100	U	C2-N1-C1'	7.41	126.59	117.70
2	L1	483	C	C2-N1-C1'	7.19	126.71	118.80
2	L1	483	C	N1-C2-O2	7.14	123.19	118.90
2	L1	1453	C	N3-C2-O2	-7.10	116.93	121.90
2	L1	481	C	C2-N1-C1'	6.58	126.04	118.80
2	L1	1742	C	N1-C2-O2	6.47	122.78	118.90
55	SS	198	PRO	N-CD-CG	-6.31	93.73	103.20
2	L1	481	C	N1-C2-O2	6.19	122.61	118.90
2	L1	1637	A	OP2-P-O3'	6.15	118.73	105.20
2	L1	1218	C	N1-C2-O2	6.11	122.56	118.90
2	L1	1453	C	C6-N1-C1'	-6.07	113.52	120.80
45	SB	318	ILE	CG1-CB-CG2	-6.06	98.06	111.40
2	L1	100	U	N1-C2-O2	6.03	127.02	122.80
43	NW	175	ASP	CB-CG-OD1	5.95	123.66	118.30
2	L1	391	C	C2-N1-C1'	5.94	125.33	118.80
49	SI	631	PRO	N-CA-CB	5.93	110.41	103.30
2	L1	1453	C	C6-N1-C2	-5.89	117.94	120.30
2	L1	100	U	N3-C2-O2	-5.82	118.13	122.20
2	L1	1637	A	P-O3'-C3'	5.70	126.54	119.70
2	L1	483	C	N3-C2-O2	-5.67	117.93	121.90
2	L1	188	C	N1-C2-O2	5.61	122.27	118.90
2	L1	1802	C	N1-C2-O2	5.55	122.23	118.90
2	L1	1664	A	P-O3'-C3'	5.55	126.36	119.70
2	L1	142	C	N1-C2-O2	5.53	122.22	118.90
21	LO	166	MET	CA-CB-CG	5.53	122.70	113.30
2	L1	325	C	P-O3'-C3'	5.52	126.32	119.70
2	L1	1742	C	C6-N1-C1'	-5.47	114.23	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	1314	U	C2-N1-C1'	5.47	124.26	117.70
3	L2	14	C	P-O3'-C3'	5.41	126.20	119.70
2	L1	423	U	P-O3'-C3'	5.38	126.16	119.70
2	L1	1535	U	C6-N1-C1'	-5.36	113.70	121.20
2	L1	965	U	N1-C2-O2	5.36	126.55	122.80
2	L1	1549	U	N1-C2-O2	5.35	126.55	122.80
3	L2	130	U	C2-N1-C1'	5.35	124.12	117.70
2	L1	188	C	C2-N1-C1'	5.34	124.67	118.80
2	L1	589	G	P-O3'-C3'	5.32	126.09	119.70
2	L1	1549	U	C2-N1-C1'	5.32	124.08	117.70
2	L1	1710	C	N1-C2-O2	5.30	122.08	118.90
2	L1	391	C	N1-C2-O2	5.29	122.07	118.90
2	L1	423	U	OP1-P-O3'	5.28	116.82	105.20
2	L1	1742	C	C6-N1-C2	-5.21	118.22	120.30
2	L1	1485	U	C2-N1-C1'	5.18	123.92	117.70
2	L1	1742	C	N3-C2-O2	-5.18	118.27	121.90
1	L0	456	C	N1-C2-O2	5.17	122.00	118.90
2	L1	1218	C	N3-C2-O2	-5.16	118.29	121.90
2	L1	100	U	C6-N1-C1'	-5.15	113.99	121.20
2	L1	451	G	N3-C4-C5	-5.15	126.03	128.60
2	L1	73	C	C2-N1-C1'	5.13	124.44	118.80
2	L1	1461	G	C3'-C2'-C1'	5.13	105.60	101.50
2	L1	483	C	C6-N1-C1'	-5.12	114.66	120.80
50	SK	168	PRO	CA-N-CD	-5.11	104.34	111.50
2	L1	275	C	N1-C2-O2	5.10	121.96	118.90
2	L1	1275	G	C4-N9-C1'	5.10	133.13	126.50
2	L1	1549	U	N3-C2-O2	-5.09	118.63	122.20
2	L1	481	C	N3-C2-O2	-5.08	118.34	121.90
2	L1	1309	C	N1-C2-O2	5.07	121.94	118.90
2	L1	1218	C	C2-N1-C1'	5.02	124.32	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
64	NI	148	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L0	5152	0	2630	61	0
2	L1	27777	0	14063	275	0
3	L2	4589	0	2306	54	0
4	L3	571	0	220	0	0
5	L4	1902	0	1990	20	0
6	L5	1501	0	1557	21	0
7	L6	1811	0	1974	33	0
8	L7	1346	0	1410	13	0
9	L8	1474	0	1542	19	0
10	L9	1425	0	1541	20	0
11	LA	593	0	277	1	0
12	LC	1098	0	1168	11	0
13	LD	1204	0	1274	9	0
14	LF	851	0	894	5	0
15	LG	488	0	514	7	0
16	LH	5987	0	5953	84	0
17	LI	2675	0	993	3	0
18	LJ	3711	0	3758	66	0
19	LK	943	0	1023	15	0
19	LL	3982	0	4031	64	0
20	LN	5299	0	5269	75	0
21	LO	6676	0	6579	75	0
22	LP	4705	0	4720	44	0
23	LQ	6438	0	6400	108	0
24	LS	3560	0	3570	55	0
25	LT	6756	0	6768	68	0
26	LU	3611	0	3618	51	0
27	LW	3519	0	3518	46	0
28	LZ	1532	0	1553	16	0
29	NA	2055	0	2135	26	0
30	NB	617	0	685	9	0
31	ND	696	0	729	9	0
32	NE	799	0	854	9	0
33	NF	1202	0	1289	11	0
34	NG	861	0	871	10	0
35	NJ	6526	0	6599	77	0
35	NK	4030	0	1806	3	0
36	NM	1873	0	1968	23	0
37	NN	340	0	345	5	0
38	NO	1034	0	1080	14	0
39	NQ	640	0	661	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	NR	4305	0	945	3	0
41	NT	286	0	127	0	0
42	NU	297	0	133	0	0
43	NW	2498	0	2456	56	0
44	SA	3077	0	3139	34	0
45	SB	3439	0	3559	57	0
46	SC	1781	0	1803	32	0
46	SD	1841	0	1867	19	0
47	SE	968	0	1017	7	0
47	SF	955	0	1008	7	0
48	SH	2832	0	2937	32	0
49	SI	6801	0	6971	81	0
50	SJ	1008	0	440	0	0
50	SK	1579	0	1646	26	0
51	SL	1586	0	1641	21	0
52	SM	2369	0	2376	20	0
53	SQ	1533	0	1579	14	0
54	SR	816	0	871	8	0
55	SS	1626	0	1677	24	0
56	SX	885	0	192	1	0
57	SY	2024	0	2148	21	0
58	NH	5265	0	2357	1	0
59	SP	11768	0	7711	44	0
60	LR	4321	0	2717	30	0
61	LM	13156	0	10845	106	0
62	N0	264	0	134	0	0
63	SG	2878	0	2740	30	0
64	NI	1459	0	1045	8	0
65	SW	890	0	407	0	0
66	ST	3064	0	1559	11	0
67	SU	2057	0	804	0	0
68	NY	2094	0	2044	26	0
69	SZ	1442	0	604	5	0
70	L1	19	0	0	0	0
70	NH	1	0	0	0	0
70	SI	1	0	0	0	0
70	SL	1	0	0	0	0
71	NQ	1	0	0	0	0
71	NT	1	0	0	0	0
71	SL	1	0	0	0	0
72	SI	32	0	12	1	0
73	SJ	26	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	SK	26	0	19	2	0
74	NH	31	0	12	0	0
74	NK	31	0	12	0	0
All	All	223184	0	181708	1972	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 5.

All (1972) 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)
3:L2:12:U:HO2’	52:SM:44:THR:HG1	1.17	0.85
20:LN:461:LEU:HB2	20:LN:477:PHE:HB2	1.64	0.78
61:LM:843:VAL:HG22	61:LM:846:ARG:HH21	1.48	0.78
19:LL:276:THR:HB	19:LL:286:LYS:HB2	1.65	0.77
18:LJ:103:GLY:HA2	18:LJ:118:PHE:O	1.83	0.77
19:LL:245:LEU:HD11	19:LL:263:SER:HB2	1.66	0.77
44:SA:37:LEU:HD21	46:SD:256:ASN:HD22	1.49	0.76
6:L5:138:ALA:HB3	15:LG:63:ARG:HH12	1.51	0.76
23:LQ:668:ILE:HG22	23:LQ:669:GLN:HG3	1.68	0.76
24:LS:152:MET:HG2	24:LS:172:LYS:HG2	1.67	0.75
6:L5:81:ARG:NH1	6:L5:88:MET:SD	2.59	0.75
35:NJ:305:GLY:H	49:SI:671:LEU:HD11	1.51	0.75
48:SH:220:ILE:HG22	48:SH:222:ASP:H	1.52	0.74
22:LP:108:GLN:NE2	53:SQ:575:GLY:O	2.20	0.74
43:NW:151:PHE:HB2	43:NW:159:TYR:HB2	1.69	0.74
2:L1:1396:A:O2’	2:L1:1398:G:N7	2.21	0.74
51:SL:104:ASP:OD1	51:SL:131:ARG:NH2	2.21	0.73
3:L2:157:U:OP2	63:SG:453:LYS:NZ	2.20	0.73
49:SI:1063:THR:HG22	49:SI:1096:VAL:HG12	1.70	0.73
20:LN:186:ARG:HA	20:LN:196:CYS:HB2	1.71	0.73
2:L1:164:A:H3’	2:L1:165:G:H21	1.52	0.72
46:SC:296:GLN:HB3	57:SY:137:VAL:HB	1.71	0.72
2:L1:1192:U:H4’	2:L1:1193:U:H5’	1.71	0.72
12:LC:62:ARG:O	12:LC:96:TYR:OH	2.06	0.72
3:L2:59:G:H5”	21:LO:598:THR:HG23	1.71	0.72
20:LN:494:PRO:HG2	20:LN:536:PRO:HA	1.71	0.72
45:SB:80:VAL:HG11	45:SB:87:LEU:HD23	1.71	0.71
2:L1:1392:U:H2’	2:L1:1393:G:H8	1.55	0.71
2:L1:1824:A:OP1	29:NA:581:LYS:NZ	2.23	0.71
49:SI:1270:GLN:HE21	52:SM:41:LEU:HG	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:852:G:N2	21:LO:287:ASP:O	2.24	0.71
35:NJ:612:GLN:HB3	35:NJ:774:ARG:HH12	1.55	0.71
20:LN:250:SER:HG	20:LN:262:HIS:HE2	1.38	0.71
16:LH:21:ARG:HG2	16:LH:295:HIS:HB3	1.73	0.70
1:L0:1420:G:H1	3:L2:49:U:H3	1.38	0.70
21:LO:389:VAL:HG21	21:LO:430:VAL:HG21	1.71	0.70
1:L0:1434:U:H5'	44:SA:44:SER:HA	1.73	0.70
1:L0:668:U:H5'	31:ND:247:ARG:HD2	1.71	0.70
19:LL:503:ILE:HG22	19:LL:507:GLN:HE22	1.56	0.70
2:L1:389:A:OP1	43:NW:117:ARG:NH1	2.23	0.70
23:LQ:546:LEU:HD12	23:LQ:581:LEU:HG	1.73	0.70
45:SB:289:MET:O	45:SB:388:ARG:NH1	2.25	0.69
50:SK:224:LEU:HD12	50:SK:228:LEU:HD13	1.75	0.69
52:SM:153:HIS:HB3	52:SM:157:GLY:HA3	1.74	0.69
19:LL:466:LEU:HD21	19:LL:505:LEU:HD11	1.74	0.69
23:LQ:657:ILE:HB	23:LQ:671:LEU:HB2	1.74	0.69
2:L1:1354:G:N2	2:L1:1357:A:OP2	2.25	0.69
24:LS:371:LYS:HG3	24:LS:372:THR:HG23	1.75	0.69
30:NB:448:ARG:O	30:NB:452:ARG:NH2	2.25	0.69
43:NW:259:ARG:HD2	35:NK:500:PRO:HA	1.74	0.69
1:L0:1433:A:N6	44:SA:38:ASN:OD1	2.26	0.69
7:L6:134:GLY:HA3	7:L6:158:VAL:HG11	1.74	0.69
1:L0:604:C:H41	18:LJ:431:GLN:HB3	1.58	0.69
16:LH:409:GLN:NE2	16:LH:411:LYS:O	2.26	0.69
20:LN:21:CYS:HA	20:LN:292:THR:HG21	1.74	0.69
1:L0:811:G:N7	25:LT:469:SER:OG	2.26	0.69
45:SB:66:GLY:HA3	45:SB:93:LYS:HE2	1.74	0.68
59:SP:950:GLN:NE2	59:SP:979:LEU:O	2.26	0.68
1:L0:865:G:H1	1:L0:1412:U:H3	1.42	0.68
29:NA:550:ALA:HB3	29:NA:553:GLU:HG3	1.75	0.68
2:L1:1130:G:N2	2:L1:1130:G:OP2	2.24	0.68
61:LM:503:LYS:O	61:LM:506:MET:HB2	1.93	0.68
2:L1:1736:G:H2'	2:L1:1737:G:H8	1.57	0.68
48:SH:13:CYS:HB3	48:SH:35:ILE:HG23	1.76	0.68
16:LH:234:TYR:HE2	20:LN:270:SER:HB2	1.59	0.68
35:NJ:431:LEU:HB3	35:NJ:460:LEU:HD21	1.74	0.68
29:NA:450:ASP:N	29:NA:453:GLU:OE2	2.26	0.68
49:SI:90:PRO:HG2	49:SI:93:VAL:HB	1.75	0.68
50:SK:180:ILE:HD11	50:SK:216:MET:HB3	1.76	0.68
5:L4:15:PRO:HG3	5:L4:39:ARG:HD3	1.74	0.67
6:L5:49:LEU:HD12	12:LC:50:LYS:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:378:GLU:OE2	18:LJ:403:ARG:NH2	2.27	0.67
33:NF:69:ASN:OD1	33:NF:73:ARG:NH1	2.27	0.67
61:LM:962:LYS:HB3	61:LM:965:GLU:HB2	1.75	0.67
45:SB:383:MET:SD	45:SB:387:ASN:ND2	2.67	0.67
61:LM:384:THR:HA	61:LM:435:LYS:HE3	1.75	0.67
2:L1:683:G:H5”	38:NO:4:MET:HB3	1.75	0.67
59:SP:950:GLN:HE22	59:SP:954:LYS:HD2	1.60	0.67
1:L0:817:U:H4’	24:LS:517:LYS:HG2	1.77	0.66
2:L1:1232:U:OP2	66:ST:801:LYS:NZ	2.27	0.66
27:LW:278:VAL:HA	27:LW:294:SER:HA	1.77	0.66
1:L0:717:G:O6	1:L0:752:C:N4	2.28	0.66
25:LT:229:LEU:HB2	25:LT:243:PHE:HB2	1.76	0.66
43:NW:313:HIS:CD2	43:NW:314:ASP:H	2.13	0.66
35:NJ:386:VAL:HG22	35:NJ:408:PHE:HB2	1.78	0.66
2:L1:922:A:OP1	38:NO:28:ARG:NH2	2.28	0.66
23:LQ:89:ILE:HB	23:LQ:103:PHE:HB2	1.78	0.66
2:L1:39:A:H61	2:L1:515:G:H1’	1.60	0.66
21:LO:592:LYS:NZ	21:LO:702:GLU:OE1	2.26	0.66
57:SY:158:ALA:HB3	57:SY:161:LEU:HD13	1.77	0.66
6:L5:62:ARG:NH2	21:LO:538:GLU:OE2	2.29	0.66
49:SI:178:LYS:NZ	49:SI:243:LYS:O	2.29	0.66
18:LJ:35:ILE:O	18:LJ:312:ILE:HA	1.95	0.66
26:LU:212:LEU:HB2	26:LU:224:TYR:HB2	1.77	0.66
8:L7:53:VAL:O	8:L7:57:ARG:HB2	1.97	0.65
20:LN:185:ASP:OD2	24:LS:364:TYR:OH	2.14	0.65
63:SG:418:ILE:HD13	63:SG:462:ILE:HG21	1.78	0.65
46:SD:78:ARG:HB3	46:SD:81:GLN:HE22	1.61	0.65
63:SG:311:LYS:HE2	63:SG:316:SER:HB3	1.78	0.65
13:LD:128:VAL:HG12	13:LD:142:VAL:HA	1.79	0.65
25:LT:283:MET:HE2	25:LT:322:LYS:HG2	1.77	0.65
19:LL:515:GLY:H	19:LL:558:ARG:HH12	1.42	0.65
23:LQ:632:HIS:HD2	23:LQ:636:VAL:HG12	1.62	0.65
2:L1:444:G:N2	2:L1:447:A:OP2	2.29	0.65
16:LH:426:LYS:O	16:LH:429:GLN:NE2	2.30	0.65
21:LO:520:SER:OG	21:LO:522:ASP:OD1	2.15	0.65
1:L0:811:G:N1	25:LT:493:ASP:OD1	2.29	0.64
1:L0:817:U:OP1	25:LT:424:ASN:ND2	2.31	0.64
24:LS:363:GLY:HA2	24:LS:385:VAL:HG23	1.79	0.64
26:LU:411:LYS:NZ	26:LU:412:GLU:OE2	2.30	0.64
23:LQ:390:GLU:HG2	23:LQ:408:ARG:HG2	1.78	0.64
2:L1:1702:G:OP2	2:L1:1702:G:N2	2.21	0.64

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
18:LJ:489:MET:HG2	19:LK:571:LYS:HG2	1.78	0.64
23:LQ:109:ALA:HB3	23:LQ:127:LYS:HD2	1.80	0.64
49:SI:294:LYS:NZ	49:SI:308:SER:O	2.30	0.64
7:L6:22:ARG:HA	7:L6:25:ARG:HE	1.62	0.64
10:L9:138:ARG:NH1	10:L9:153:SER:OG	2.31	0.64
60:LR:610:GLY:O	60:LR:623:GLY:N	2.31	0.64
2:L1:1536:G:H2'	2:L1:1537:A:H8	1.63	0.64
21:LO:857:ASP:OD1	21:LO:858:ASP:N	2.29	0.64
37:NN:537:ASP:OD1	37:NN:538:ASP:N	2.31	0.64
16:LH:462:VAL:HG22	16:LH:472:VAL:HG22	1.80	0.64
2:L1:18:C:OP2	49:SI:1250:ARG:NH1	2.30	0.64
20:LN:212:VAL:HG12	20:LN:218:VAL:HG22	1.79	0.64
21:LO:879:GLN:HE22	60:LR:744:PRO:HD3	1.62	0.64
43:NW:138:ARG:H	43:NW:153:GLY:HA2	1.63	0.64
50:SK:100:LEU:HD23	50:SK:106:LEU:HD13	1.79	0.64
63:SG:142:LEU:HB2	63:SG:459:VAL:HG23	1.79	0.64
2:L1:919:A:OP2	33:NF:64:ARG:NH2	2.31	0.63
32:NE:283:ILE:HD13	38:NO:79:PHE:HE2	1.62	0.63
2:L1:1702:G:O2'	29:NA:560:ALA:O	2.15	0.63
61:LM:814:ASN:ND2	61:LM:817:GLN:OE1	2.31	0.63
35:NJ:884:ILE:HG22	35:NJ:886:LEU:HD13	1.80	0.63
50:SK:131:ASP:OD1	50:SK:132:ARG:N	2.31	0.63
28:LZ:138:VAL:HG22	28:LZ:158:VAL:HG12	1.80	0.63
49:SI:1253:ASP:HA	49:SI:1256:LYS:HD2	1.80	0.63
24:LS:255:SER:H	24:LS:270:GLY:HA2	1.63	0.63
43:NW:118:TYR:OH	43:NW:132:ARG:NH2	2.32	0.63
43:NW:138:ARG:HG2	43:NW:153:GLY:HA2	1.80	0.63
2:L1:925:G:H1	2:L1:1017:U:H3	1.46	0.63
2:L1:1743:G:H1'	2:L1:1791:A:H61	1.64	0.63
63:SG:332:LEU:HD23	63:SG:338:MET:HB3	1.79	0.63
35:NJ:309:ILE:HB	35:NJ:368:ILE:HG12	1.79	0.63
20:LN:250:SER:OG	20:LN:262:HIS:NE2	2.26	0.63
44:SA:196:HIS:O	44:SA:220:ARG:NH1	2.32	0.62
23:LQ:438:ILE:HD11	23:LQ:471:ILE:HD13	1.80	0.62
46:SC:261:VAL:HG22	46:SC:310:VAL:HG22	1.80	0.62
54:SR:117:GLY:HA2	66:ST:844:GLU:HB3	1.81	0.62
1:L0:1415:G:N7	28:LZ:125:GLN:NE2	2.47	0.62
20:LN:560:TYR:O	20:LN:565:ARG:NH1	2.32	0.62
26:LU:118:ARG:NH1	26:LU:120:CYS:SG	2.72	0.62
52:SM:15:ARG:NH1	52:SM:73:ASP:OD2	2.32	0.62
2:L1:1719:A:O2'	23:LQ:419:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LL:106:ILE:HB	19:LL:120:LEU:HB2	1.82	0.62
22:LP:546:ASP:OD1	22:LP:588:LYS:NZ	2.29	0.62
26:LU:206:PRO:HG2	26:LU:207:ILE:HD12	1.82	0.62
26:LU:434:SER:HB3	26:LU:437:LYS:HG2	1.82	0.62
48:SH:133:LYS:NZ	48:SH:152:LEU:O	2.32	0.62
63:SG:388:THR:HG23	63:SG:390:LEU:H	1.64	0.62
35:NJ:277:ARG:HD3	35:NJ:458:ARG:HH11	1.64	0.62
2:L1:1849:G:N1	68:NY:49:ASP:OD1	2.33	0.62
18:LJ:467:GLN:NE2	18:LJ:471:GLU:OE2	2.33	0.62
61:LM:652:LYS:O	61:LM:656:LEU:N	2.30	0.62
2:L1:374:G:OP1	13:LD:59:LYS:NZ	2.31	0.62
9:L8:22:HIS:ND1	9:L8:23:LYS:O	2.30	0.62
20:LN:357:LEU:HB3	20:LN:383:LEU:HB3	1.82	0.62
24:LS:433:THR:HG22	24:LS:440:VAL:HG22	1.82	0.62
26:LU:182:ASP:HB3	26:LU:185:ARG:HB3	1.82	0.62
49:SI:1106:ILE:HD12	49:SI:1107:PRO:HD2	1.80	0.62
2:L1:454:U:H2’	2:L1:455:A:H8	1.65	0.62
7:L6:69:THR:HG22	7:L6:71:GLY:H	1.65	0.61
1:L0:813:C:O2	25:LT:427:ARG:NH2	2.33	0.61
10:L9:114:VAL:HG23	10:L9:119:LEU:HD12	1.81	0.61
30:NB:460:ARG:NH1	53:SQ:699:ASP:OD1	2.32	0.61
66:ST:834:LYS:O	66:ST:838:ASN:ND2	2.33	0.61
30:NB:431:ASN:HB3	30:NB:434:VAL:HG22	1.81	0.61
13:LD:79:LYS:HB2	13:LD:87:VAL:HB	1.83	0.61
20:LN:592:ARG:HD3	20:LN:595:HIS:HB2	1.82	0.61
23:LQ:9:ARG:NH1	23:LQ:707:GLU:OE1	2.33	0.61
46:SC:107:VAL:HB	46:SC:134:TYR:HB3	1.83	0.61
2:L1:75:G:H1’	2:L1:76:U:H2’	1.83	0.61
16:LH:458:GLN:NE2	16:LH:475:LEU:O	2.30	0.61
20:LN:154:HIS:HD2	20:LN:203:PHE:HE2	1.48	0.61
21:LO:102:VAL:HG22	21:LO:113:VAL:HG22	1.81	0.61
2:L1:1592:C:O5’	6:L5:91:ARG:NH2	2.34	0.61
3:L2:43:A:OP2	53:SQ:633:ARG:NH2	2.33	0.61
18:LJ:222:VAL:HG12	18:LJ:231:VAL:HG22	1.82	0.61
25:LT:938:GLN:NE2	60:LR:782:ASP:OD2	2.34	0.61
49:SI:956:LEU:HG	49:SI:1106:ILE:HD13	1.82	0.61
61:LM:605:PRO:HA	61:LM:703:THR:HG21	1.81	0.61
68:NY:281:GLU:HB2	68:NY:286:GLU:HB3	1.82	0.61
24:LS:401:SER:OG	24:LS:403:ASP:OD1	2.18	0.61
48:SH:118:ARG:NH1	48:SH:166:GLU:OE1	2.33	0.61
61:LM:542:GLU:HG3	61:LM:582:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1849:G:N2	68:NY:48:GLU:OE1	2.33	0.61
19:LL:42:GLU:OE2	19:LL:49:HIS:ND1	2.34	0.61
36:NM:47:THR:OG1	36:NM:65:ARG:NH1	2.34	0.61
48:SH:65:GLU:HB2	48:SH:74:TYR:HB3	1.82	0.61
49:SI:961:ASP:OD1	49:SI:967:ARG:NH1	2.33	0.61
2:L1:86:C:O2'	2:L1:171:A:N1	2.30	0.61
50:SK:176:THR:O	73:SK:301:SAH:O2'	2.19	0.61
21:LO:421:VAL:HG23	21:LO:432:THR:HG22	1.81	0.61
23:LQ:8:LEU:O	23:LQ:669:GLN:NE2	2.32	0.61
23:LQ:366:LYS:HE2	23:LQ:385:GLN:HE21	1.66	0.61
2:L1:319:C:H2'	2:L1:320:G:C8	2.36	0.60
19:LL:503:ILE:O	19:LL:507:GLN:NE2	2.34	0.60
23:LQ:158:LEU:HD12	23:LQ:163:LEU:HB2	1.83	0.60
28:LZ:38:ARG:NH2	51:SL:11:ALA:O	2.34	0.60
54:SR:112:VAL:HG11	54:SR:118:VAL:HG21	1.82	0.60
9:L8:98:LYS:NZ	9:L8:176:ALA:O	2.33	0.60
18:LJ:264:LEU:HG	18:LJ:274:VAL:HG22	1.82	0.60
25:LT:88:ARG:HD3	25:LT:132:ALA:HB1	1.83	0.60
25:LT:501:ASP:OD2	25:LT:502:ILE:N	2.34	0.60
25:LT:548:ASP:OD2	25:LT:549:GLY:N	2.33	0.60
63:SG:364:ALA:O	63:SG:401:ARG:NH1	2.29	0.60
64:NI:227:GLU:OE2	64:NI:230:ARG:NH2	2.34	0.60
2:L1:368:U:OP2	37:NN:516:ARG:NH2	2.30	0.60
2:L1:1670:C:OP2	52:SM:91:ARG:NH1	2.34	0.60
18:LJ:89:ARG:NH1	18:LJ:134:LYS:O	2.34	0.60
21:LO:495:ASP:OD1	21:LO:496:VAL:N	2.33	0.60
22:LP:538:ARG:HH22	45:SB:288:VAL:HG13	1.67	0.60
2:L1:1297:U:N3	2:L1:1300:U:OP2	2.33	0.60
16:LH:368:GLN:NE2	16:LH:371:ASN:OD1	2.34	0.60
23:LQ:303:LEU:HD13	23:LQ:382:PHE:HE2	1.67	0.60
49:SI:1061:ILE:HG22	49:SI:1098:MET:HB2	1.81	0.60
26:LU:16:GLU:OE2	61:LM:41:ARG:NH1	2.35	0.60
59:SP:967:HIS:ND1	59:SP:1007:ASP:OD2	2.35	0.60
49:SI:107:THR:HG23	49:SI:109:GLN:H	1.65	0.60
2:L1:93:U:H4'	5:L4:6:LYS:HA	1.83	0.60
2:L1:925:G:OP1	33:NF:121:ARG:NH1	2.35	0.60
5:L4:48:LEU:HD23	5:L4:61:VAL:HG13	1.81	0.60
9:L8:67:TRP:O	9:L8:71:CYS:N	2.34	0.60
19:LL:321:THR:HG1	19:LL:331:LYS:N	2.00	0.60
38:NO:91:ASN:O	51:SL:83:LYS:NZ	2.26	0.60
59:SP:59:ASN:HD22	59:SP:106:PRO:HG2	1.67	0.60

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:L1:412:G:H1	2:L1:430:C:H42	1.47	0.60
2:L1:1004:U:H2'	2:L1:1005:G:H8	1.67	0.60
2:L1:1485:U:H3'	2:L1:1486:A:H8	1.67	0.60
16:LH:59:LEU:HB3	16:LH:78:LEU:HD12	1.84	0.60
16:LH:333:ASP:O	16:LH:663:GLN:NE2	2.35	0.60
26:LU:24:VAL:HG13	27:LW:485:GLY:HA3	1.83	0.60
47:SE:95:VAL:HG12	47:SE:97:ARG:H	1.66	0.60
61:LM:648:ILE:HD13	61:LM:656:LEU:HD11	1.84	0.60
16:LH:543:ARG:NH1	16:LH:583:VAL:O	2.35	0.59
48:SH:60:ASN:ND2	66:ST:79:LYS:O	2.35	0.59
1:L0:819:C:OP2	25:LT:426:LYS:NZ	2.23	0.59
1:L0:715:G:H1	1:L0:755:C:H42	1.47	0.59
2:L1:1844:U:H3	2:L1:1855:G:H1	1.51	0.59
24:LS:422:ASP:OD1	24:LS:450:ASN:ND2	2.32	0.59
2:L1:1762:C:H2'	2:L1:1763:G:C8	2.37	0.59
20:LN:110:SER:OG	20:LN:112:SER:O	2.18	0.59
23:LQ:424:SER:OG	23:LQ:426:ASP:O	2.21	0.59
26:LU:12:ASN:O	26:LU:23:ARG:NH1	2.36	0.59
35:NJ:248:VAL:HG22	35:NJ:268:ILE:HD13	1.83	0.59
35:NJ:277:ARG:HB3	35:NJ:458:ARG:HD2	1.83	0.59
19:LL:231:ILE:HD12	19:LL:234:LEU:HD12	1.83	0.59
21:LO:858:ASP:OD1	21:LO:859:LEU:N	2.36	0.59
23:LQ:479:GLN:OE1	23:LQ:481:TYR:OH	2.17	0.59
49:SI:205:ARG:NH1	49:SI:209:GLU:OE2	2.34	0.59
10:L9:113:GLN:HG3	10:L9:149:VAL:HG21	1.85	0.59
21:LO:467:ASP:OD1	21:LO:468:ALA:N	2.35	0.59
61:LM:1311:VAL:O	61:LM:1315:PHE:N	2.28	0.59
2:L1:134:C:O2'	59:SP:906:LYS:NZ	2.35	0.59
22:LP:46:ARG:HD2	26:LU:20:ASP:HA	1.84	0.59
23:LQ:555:VAL:HG12	23:LQ:566:VAL:HG12	1.83	0.59
24:LS:502:VAL:HG22	24:LS:509:VAL:HG22	1.84	0.59
43:NW:279:HIS:HB2	43:NW:288:LEU:HB2	1.83	0.59
54:SR:36:LEU:HG	54:SR:37:LYS:HG3	1.83	0.59
59:SP:134:THR:HA	59:SP:137:LEU:HD13	1.85	0.59
8:L7:43:LEU:HB3	8:L7:72:PHE:HE1	1.66	0.59
19:LK:482:LEU:HD13	19:LK:523:MET:HE3	1.83	0.59
21:LO:179:LEU:HD12	21:LO:272:VAL:HG21	1.84	0.59
21:LO:303:LEU:HB2	21:LO:317:LEU:HD11	1.83	0.59
24:LS:152:MET:HA	24:LS:174:SER:HA	1.85	0.59
43:NW:139:ASP:OD1	43:NW:140:PHE:N	2.36	0.59
43:NW:299:ASN:HD22	43:NW:304:LYS:HZ2	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:737:G:H5’	16:LH:427:LYS:HD2	1.83	0.59
2:L1:103:A:O4’	2:L1:356:C:N4	2.35	0.59
18:LJ:181:ILE:HD13	18:LJ:221:LEU:HD22	1.84	0.59
36:NM:59:SER:OG	36:NM:63:LYS:NZ	2.36	0.59
45:SB:211:VAL:HG13	45:SB:216:ASN:HB2	1.84	0.59
46:SC:164:LEU:HB3	46:SC:233:ILE:HG12	1.85	0.59
46:SD:120:GLU:OE2	46:SD:135:ARG:NH1	2.33	0.59
51:SL:103:THR:HG22	51:SL:132:LEU:HD11	1.85	0.59
3:L2:54:U:OP1	57:SY:72:ARG:NH2	2.35	0.59
7:L6:192:ILE:HG22	7:L6:196:LYS:HE3	1.85	0.59
9:L8:11:ARG:NH1	9:L8:15:GLY:O	2.34	0.59
16:LH:20:ARG:NH2	16:LH:103:HIS:O	2.35	0.59
26:LU:263:LEU:HD21	26:LU:285:VAL:HG11	1.84	0.59
43:NW:187:VAL:HG11	43:NW:241:ALA:HB2	1.85	0.59
44:SA:217:ILE:HG22	44:SA:227:LYS:HE3	1.85	0.59
2:L1:928:G:H2’	2:L1:929:G:C8	2.38	0.58
2:L1:1546:G:HO2’	2:L1:1670:C:HO2’	1.50	0.58
19:LL:278:SER:HB2	19:LL:283:GLU:HB3	1.83	0.58
23:LQ:510:GLY:HA2	23:LQ:524:ASP:HA	1.84	0.58
46:SC:92:ARG:NH1	57:SY:168:ARG:O	2.35	0.58
18:LJ:479:GLU:HB3	19:LL:524:VAL:HG11	1.85	0.58
21:LO:638:ILE:HD11	25:LT:505:CYS:HB3	1.85	0.58
16:LH:284:GLU:OE2	24:LS:337:ARG:NH1	2.35	0.58
47:SF:52:GLU:HG2	47:SF:116:ILE:HG21	1.85	0.58
5:L4:112:HIS:NE2	5:L4:237:SER:OG	2.29	0.58
20:LN:399:SER:HB3	20:LN:404:TRP:HB2	1.85	0.58
2:L1:1115:U:O2’	2:L1:1118:C:N4	2.37	0.58
10:L9:107:GLU:O	10:L9:113:GLN:NE2	2.34	0.58
32:NE:286:ILE:HG23	38:NO:92:ASN:HD22	1.68	0.58
2:L1:1216:C:H42	52:SM:179:MET:HB2	1.68	0.58
3:L2:46:A:H2’	3:L2:47:G:H8	1.68	0.58
59:SP:939:GLU:HA	59:SP:942:LEU:HB2	1.85	0.58
19:LL:537:TYR:O	19:LL:540:THR:OG1	2.19	0.58
21:LO:151:ASP:OD1	21:LO:152:TRP:N	2.36	0.58
22:LP:442:ILE:HD12	22:LP:479:LYS:HD2	1.85	0.58
35:NJ:507:LEU:HD11	35:NJ:557:PHE:HB3	1.86	0.58
45:SB:19:GLU:HA	45:SB:22:LEU:HD12	1.86	0.58
39:NQ:42:LYS:HZ1	39:NQ:57:VAL:H	1.52	0.57
61:LM:658:GLY:HA3	61:LM:765:VAL:HG13	1.85	0.57
68:NY:190:VAL:HG21	68:NY:206:VAL:HG11	1.85	0.57
1:L0:812:G:OP2	1:L0:812:G:N2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1545:A:H2	2:L1:1654:G:H21	1.53	0.57
14:LF:83:LYS:HE2	14:LF:96:LEU:HD12	1.86	0.57
20:LN:146:SER:OG	20:LN:164:SER:OG	2.21	0.57
25:LT:661:LEU:HD23	25:LT:714:VAL:HG12	1.86	0.57
26:LU:263:LEU:HB2	26:LU:278:HIS:HB2	1.87	0.57
47:SF:52:GLU:OE1	47:SF:106:ILE:HD13	2.04	0.57
2:L1:530:U:H2'	2:L1:531:A:H8	1.70	0.57
43:NW:287:ILE:HD11	43:NW:300:LYS:HG3	1.85	0.57
44:SA:45:ILE:HG13	44:SA:46:VAL:HG23	1.85	0.57
45:SB:289:MET:HE1	45:SB:365:LYS:HB3	1.87	0.57
21:LO:715:ARG:HD3	21:LO:730:LEU:HD12	1.86	0.57
36:NM:33:VAL:HA	36:NM:96:CYS:HB2	1.85	0.57
35:NJ:697:LYS:HB2	35:NJ:700:GLU:HG3	1.86	0.57
46:SC:166:LEU:HD12	46:SC:235:ALA:HB2	1.86	0.57
48:SH:368:LEU:O	49:SI:989:GLN:NE2	2.36	0.57
59:SP:713:ASP:OD1	59:SP:717:GLN:NE2	2.37	0.57
61:LM:374:ILE:HG13	61:LM:378:HIS:CE1	2.39	0.57
22:LP:369:GLU:HG2	22:LP:373:LYS:HE2	1.86	0.57
48:SH:286:GLU:OE1	48:SH:289:ARG:NH2	2.35	0.57
61:LM:334:LEU:HD21	61:LM:346:LEU:HD23	1.85	0.57
61:LM:1041:LEU:HD23	61:LM:1060:LEU:HB2	1.86	0.57
7:L6:5:ILE:HD12	7:L6:124:LEU:HD11	1.85	0.57
9:L8:67:TRP:NE1	9:L8:191:GLU:OE2	2.35	0.57
23:LQ:49:ILE:HD11	23:LQ:59:LEU:HB3	1.86	0.57
61:LM:186:LEU:HB3	61:LM:241:LYS:HE3	1.86	0.57
16:LH:129:LEU:HB3	16:LH:151:LEU:HB2	1.85	0.57
60:LR:665:ARG:HE	60:LR:668:ARG:HH21	1.51	0.57
61:LM:1111:THR:H	61:LM:1114:PHE:HB3	1.70	0.57
2:L1:621:C:O4'	57:SY:12:ARG:NH2	2.37	0.57
2:L1:1525:C:H2'	2:L1:1526:G:H8	1.68	0.57
10:L9:136:ARG:NH1	10:L9:159:PHE:O	2.38	0.57
18:LJ:479:GLU:OE1	19:LL:525:GLN:NE2	2.38	0.57
19:LK:536:SER:O	19:LK:539:SER:OG	2.20	0.57
23:LQ:416:SER:OG	23:LQ:417:ASP:N	2.37	0.57
45:SB:197:ILE:HG23	45:SB:198:ILE:HG13	1.86	0.57
12:LC:11:GLN:NE2	28:LZ:177:ARG:O	2.37	0.57
28:LZ:162:ASP:OD1	28:LZ:163:SER:N	2.38	0.57
35:NJ:235:LEU:HD13	35:NJ:258:LEU:HA	1.86	0.57
43:NW:233:ILE:HG23	43:NW:246:VAL:HG13	1.85	0.57
48:SH:119:GLY:O	48:SH:165:GLY:N	2.36	0.57
48:SH:230:MET:O	48:SH:235:SER:OG	2.22	0.57

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
55:SS:244:GLU:HA	55:SS:247:ILE:HB	1.87	0.57
69:SZ:275:ALA:O	69:SZ:279:ALA:N	2.37	0.57
2:L1:102:A:OP2	2:L1:408:A:N6	2.37	0.56
2:L1:1762:C:H2'	2:L1:1763:G:H8	1.70	0.56
21:LO:561:ALA:HB2	21:LO:611:LEU:HD11	1.86	0.56
24:LS:357:LEU:HD11	24:LS:365:LEU:HB3	1.87	0.56
2:L1:589:G:O2'	2:L1:590:A:O5'	2.20	0.56
8:L7:76:GLN:HE22	8:L7:94:PHE:HD2	1.53	0.56
64:NI:198:PRO:HB3	64:NI:204:VAL:HG22	1.87	0.56
2:L1:103:A:H4'	2:L1:104:A:C8	2.41	0.56
2:L1:433:A:H2'	2:L1:434:G:C8	2.41	0.56
2:L1:923:G:OP1	33:NF:2:GLY:N	2.38	0.56
2:L1:981:A:H2'	2:L1:982:G:C8	2.40	0.56
2:L1:1551:U:OP2	49:SI:1162:ASN:ND2	2.38	0.56
23:LQ:147:GLY:HA3	23:LQ:176:TRP:HH2	1.70	0.56
23:LQ:158:LEU:HD11	23:LQ:175:TRP:HZ3	1.70	0.56
61:LM:834:GLU:OE2	61:LM:838:ASN:ND2	2.38	0.56
1:L0:459:G:N7	31:ND:252:LYS:NZ	2.51	0.56
16:LH:498:LYS:NZ	17:LI:596:TYR:O	2.39	0.56
16:LH:557:LEU:HD11	16:LH:612:PRO:HB3	1.86	0.56
19:LL:290:VAL:HG22	19:LL:296:VAL:HG22	1.88	0.56
24:LS:75:ARG:HG2	24:LS:75:ARG:HH11	1.70	0.56
16:LH:15:SER:O	16:LH:312:ASN:ND2	2.39	0.56
19:LL:404:LEU:HD13	19:LL:408:ILE:HD11	1.88	0.56
20:LN:21:CYS:HB2	20:LN:34:SER:HB3	1.85	0.56
23:LQ:621:ASP:OD1	23:LQ:622:PHE:N	2.39	0.56
28:LZ:2:VAL:HG23	28:LZ:3:ARG:H	1.69	0.56
50:SK:46:VAL:HG22	50:SK:109:TYR:HB2	1.87	0.56
53:SQ:557:LEU:HD21	55:SS:241:ALA:HA	1.86	0.56
63:SG:223:ILE:HB	63:SG:237:PHE:HB2	1.86	0.56
1:L0:610:G:O4'	31:ND:246:ARG:NH2	2.39	0.56
3:L2:137:G:N2	3:L2:139:U:O2'	2.38	0.56
16:LH:53:LEU:HD23	16:LH:85:TRP:CE3	2.41	0.56
43:NW:152:VAL:HG21	43:NW:182:CYS:HB3	1.87	0.56
2:L1:125:C:OP1	7:L6:202:ASN:ND2	2.39	0.56
16:LH:698:ILE:HG22	24:LS:265:ILE:HD11	1.88	0.56
23:LQ:937:LYS:HG3	29:NA:549:LEU:HD21	1.88	0.56
25:LT:640:ALA:HB1	25:LT:666:PRO:HG2	1.85	0.56
35:NJ:895:PHE:HA	35:NJ:898:ILE:HD12	1.88	0.56
46:SC:221:HIS:O	46:SC:224:ARG:NH1	2.39	0.56
61:LM:423:GLU:HA	61:LM:426:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:223:C:H2'	2:L1:224:A:H8	1.71	0.56
59:SP:92:LEU:HD13	59:SP:111:VAL:HG22	1.88	0.56
2:L1:373:G:H2'	2:L1:374:G:H8	1.70	0.56
2:L1:1010:G:H2'	2:L1:1011:A:H8	1.71	0.56
2:L1:1532:C:O2	2:L1:1638:G:N2	2.35	0.56
35:NJ:423:LEU:HD23	35:NJ:425:LEU:H	1.71	0.56
27:LW:485:GLY:O	27:LW:489:ASN:ND2	2.39	0.56
63:SG:349:LEU:O	63:SG:358:LEU:N	2.39	0.56
68:NY:87:HIS:O	68:NY:107:THR:OG1	2.24	0.56
21:LO:144:TYR:HD1	27:LW:363:ARG:HH11	1.53	0.55
2:L1:286:U:H2'	2:L1:287:U:H4'	1.88	0.55
2:L1:525:A:H5'	30:NB:431:ASN:HD22	1.71	0.55
8:L7:76:GLN:NE2	8:L7:94:PHE:HD2	2.04	0.55
20:LN:22:VAL:HG22	20:LN:292:THR:HB	1.89	0.55
23:LQ:418:VAL:HG21	23:LQ:699:LEU:HD21	1.88	0.55
43:NW:302:SER:HB2	43:NW:304:LYS:HZ1	1.71	0.55
50:SK:107:GLN:NE2	50:SK:120:VAL:O	2.34	0.55
61:LM:133:ALA:HB1	61:LM:195:LEU:HD13	1.88	0.55
3:L2:48:U:O2'	51:SL:15:ARG:NH1	2.39	0.55
43:NW:103:LEU:HD11	43:NW:111:VAL:HG23	1.86	0.55
59:SP:1028:THR:HB	59:SP:1037:ARG:HG2	1.88	0.55
2:L1:1194:A:N6	23:LQ:614:ASN:OD1	2.39	0.55
19:LL:346:SER:OG	19:LL:361:ARG:NH2	2.39	0.55
37:NN:519:VAL:HG22	43:NW:167:ARG:HD2	1.88	0.55
57:SY:237:GLU:HB2	57:SY:243:ALA:HB2	1.89	0.55
59:SP:993:ILE:O	59:SP:1005:ARG:NH2	2.36	0.55
16:LH:203:LYS:H	16:LH:224:ASP:HB3	1.72	0.55
25:LT:135:ARG:HB2	25:LT:136:LEU:HD12	1.89	0.55
60:LR:81:LEU:O	60:LR:93:TRP:N	2.38	0.55
2:L1:1599:U:OP2	18:LJ:78:ARG:NH2	2.40	0.55
3:L2:56:A:H2'	3:L2:57:A:C8	2.42	0.55
35:NJ:559:LEU:HD23	35:NJ:644:ALA:HB2	1.88	0.55
37:NN:547:LEU:HD12	43:NW:211:VAL:HG21	1.88	0.55
2:L1:45:A:N1	2:L1:480:G:O2'	2.37	0.55
16:LH:123:LYS:NZ	16:LH:125:ASP:OD2	2.40	0.55
16:LH:380:ILE:HG22	16:LH:382:ASP:H	1.72	0.55
31:ND:177:LEU:HG	57:SY:139:PHE:HB3	1.87	0.55
45:SB:25:VAL:HB	45:SB:111:VAL:HG12	1.89	0.55
46:SC:241:ASP:OD2	46:SC:244:ARG:NH2	2.33	0.55
1:L0:603:C:H4'	19:LL:516:HIS:CG	2.41	0.55
20:LN:415:LEU:HD21	20:LN:466:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LQ:297:HIS:CE1	23:LQ:365:ILE:HB	2.41	0.55
25:LT:460:ILE:HB	25:LT:473:TRP:HB2	1.88	0.55
48:SH:175:LYS:NZ	49:SI:989:GLN:OE1	2.40	0.55
49:SI:946:VAL:HG22	49:SI:993:PHE:HB2	1.88	0.55
50:SK:93:LEU:HD11	50:SK:128:ARG:HG3	1.89	0.55
73:SJ:301:SAH:H8	73:SJ:301:SAH:SD	2.47	0.55
2:L1:1546:G:O2’	2:L1:1670:C:O2’	2.24	0.55
7:L6:74:ARG:O	7:L6:94:ARG:NH1	2.39	0.55
23:LQ:200:LEU:HD12	23:LQ:201:SER:H	1.70	0.55
33:NF:99:ARG:NH2	33:NF:119:GLU:OE2	2.40	0.55
44:SA:252:MET:SD	46:SC:205:LYS:HA	2.47	0.55
46:SD:100:ARG:NH2	53:SQ:680:ASP:OD2	2.40	0.55
61:LM:601:VAL:HG11	61:LM:690:VAL:HG21	1.89	0.55
1:L0:454:C:OP1	20:LN:680:LYS:NZ	2.37	0.55
21:LO:216:GLN:NE2	21:LO:217:CYS:O	2.40	0.55
21:LO:879:GLN:HE22	60:LR:743:ALA:HA	1.72	0.55
26:LU:326:GLN:O	26:LU:344:SER:OG	2.25	0.55
68:NY:160:ARG:NH1	68:NY:210:MET:O	2.40	0.55
2:L1:1392:U:H2’	2:L1:1393:G:C8	2.39	0.54
2:L1:1813:A:H2’	2:L1:1814:G:C8	2.42	0.54
3:L2:95:C:H2’	3:L2:96:G:H8	1.72	0.54
8:L7:51:ILE:HG21	8:L7:179:LYS:HG2	1.89	0.54
16:LH:433:LEU:HB2	19:LL:397:MET:HG2	1.89	0.54
20:LN:499:LEU:HD23	20:LN:513:VAL:HG22	1.89	0.54
21:LO:368:LYS:HB3	29:NA:538:VAL:HG11	1.88	0.54
26:LU:364:THR:HG23	26:LU:367:GLU:H	1.72	0.54
29:NA:533:ILE:HD12	29:NA:542:SER:HB2	1.89	0.54
44:SA:21:GLU:HB2	55:SS:725:PRO:HG2	1.88	0.54
52:SM:264:GLU:HG3	52:SM:265:GLN:HG3	1.89	0.54
59:SP:739:VAL:HA	59:SP:742:LEU:HD12	1.88	0.54
61:LM:1334:VAL:O	61:LM:1338:ASP:N	2.36	0.54
19:LL:528:LYS:O	19:LL:532:THR:OG1	2.22	0.54
20:LN:605:CYS:HB2	20:LN:643:ILE:HG22	1.90	0.54
35:NJ:23:ARG:NH1	35:NJ:141:VAL:O	2.40	0.54
49:SI:1200:ARG:O	49:SI:1205:ARG:NH1	2.40	0.54
54:SR:131:LEU:HD11	54:SR:135:LYS:HE3	1.89	0.54
59:SP:933:LEU:HD21	59:SP:936:LYS:HD2	1.88	0.54
61:LM:541:PHE:HZ	61:LM:553:THR:HG22	1.72	0.54
12:LC:82:TYR:HA	12:LC:85:ARG:HD3	1.89	0.54
18:LJ:106:LEU:HD12	18:LJ:116:ARG:HB2	1.89	0.54
19:LL:464:VAL:HA	19:LL:467:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SY:142:THR:HG22	57:SY:144:LYS:H	1.72	0.54
23:LQ:506:PRO:O	23:LQ:508:GLN:NE2	2.41	0.54
25:LT:67:SER:OG	25:LT:70:PHE:O	2.26	0.54
45:SB:68:ILE:HG13	45:SB:72:LEU:HD23	1.89	0.54
2:L1:674:C:H2'	2:L1:675:U:C6	2.42	0.54
8:L7:78:ARG:HH21	8:L7:81:ARG:HE	1.54	0.54
13:LD:135:SER:O	13:LD:139:ARG:NH1	2.37	0.54
24:LS:161:ARG:NH2	45:SB:434:SER:O	2.41	0.54
3:L2:43:A:OP2	53:SQ:630:GLN:NE2	2.40	0.54
14:LF:55:ILE:HG13	14:LF:75:ILE:HG12	1.90	0.54
16:LH:746:PHE:CE2	22:LP:563:PRO:HG2	2.43	0.54
49:SI:143:LEU:HD21	49:SI:906:PRO:HG2	1.88	0.54
35:NK:284:ALA:HB2	35:NK:465:LEU:H	1.73	0.54
20:LN:537:ASN:OD1	20:LN:538:THR:N	2.41	0.54
20:LN:621:TYR:HB2	20:LN:643:ILE:HD11	1.90	0.54
27:LW:197:GLY:HA3	27:LW:215:ARG:HB3	1.89	0.54
35:NJ:290:LYS:HD3	35:NJ:410:ALA:HB1	1.90	0.54
43:NW:178:GLU:HB3	43:NW:196:ILE:HB	1.88	0.54
63:SG:418:ILE:HG21	63:SG:462:ILE:HD13	1.89	0.54
69:SZ:282:LYS:O	69:SZ:286:TRP:N	2.36	0.54
9:L8:21:TYR:CZ	9:L8:22:HIS:HD2	2.26	0.54
16:LH:576:GLU:O	17:LI:354:HIS:N	2.40	0.54
18:LJ:78:ARG:HD2	18:LJ:112:ARG:HH12	1.73	0.54
23:LQ:843:ILE:O	23:LQ:887:LYS:NZ	2.38	0.54
35:NJ:779:LEU:HA	35:NJ:783:PHE:HB2	1.88	0.54
45:SB:146:LEU:HD23	46:SC:226:LEU:HD11	1.90	0.54
2:L1:948:C:H2'	2:L1:949:G:H8	1.73	0.54
21:LO:376:MET:HE1	21:LO:725:LEU:HB2	1.90	0.54
43:NW:195:THR:H	43:NW:233:ILE:HD12	1.71	0.54
46:SC:92:ARG:NH2	46:SC:153:ASP:OD1	2.40	0.54
46:SC:169:ALA:H	46:SC:191:GLU:HG3	1.73	0.54
49:SI:881:ARG:HG2	49:SI:884:MET:SD	2.47	0.54
2:L1:432:G:H2'	2:L1:433:A:C8	2.43	0.53
22:LP:22:ILE:HD13	27:LW:98:PHE:HZ	1.70	0.53
29:NA:358:SER:HB3	29:NA:361:GLU:HG3	1.90	0.53
49:SI:103:ILE:HG21	49:SI:111:LEU:HD12	1.88	0.53
1:L0:710:G:H2'	1:L0:711:A:H8	1.73	0.53
2:L1:559:G:O2'	2:L1:560:A:O5'	2.23	0.53
3:L2:85:A:OP2	45:SB:360:ARG:NH2	2.39	0.53
16:LH:609:VAL:HB	16:LH:619:TYR:HB3	1.91	0.53
19:LL:404:LEU:HA	19:LL:408:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LP:213:SER:OG	55:SS:195:ASN:ND2	2.41	0.53
49:SI:1118:LYS:O	49:SI:1123:LYS:NZ	2.41	0.53
60:LR:712:GLU:HG2	60:LR:750:TYR:HD1	1.73	0.53
20:LN:54:PHE:H	20:LN:487:MET:HE3	1.73	0.53
25:LT:399:SER:OG	25:LT:400:GLN:N	2.42	0.53
36:NM:123:ALA:HB2	36:NM:165:ARG:HG3	1.90	0.53
43:NW:172:LEU:HD11	43:NW:208:ARG:HB3	1.91	0.53
44:SA:232:GLU:HG3	44:SA:241:ALA:HB3	1.90	0.53
44:SA:288:LYS:NZ	45:SB:249:GLU:OE2	2.41	0.53
45:SB:313:ALA:HA	45:SB:367:VAL:HG11	1.90	0.53
54:SR:64:SER:O	54:SR:68:LYS:NZ	2.41	0.53
24:LS:253:ARG:HG2	24:LS:541:GLU:HA	1.91	0.53
26:LU:127:VAL:HG22	26:LU:133:VAL:HG22	1.90	0.53
35:NJ:310:PHE:HB2	35:NJ:385:VAL:HG22	1.91	0.53
61:LM:611:ASN:ND2	61:LM:618:GLU:OE2	2.35	0.53
2:L1:627:U:OP1	49:SI:1136:ARG:NH2	2.37	0.53
2:L1:951:C:H2’	2:L1:952:G:H8	1.73	0.53
26:LU:255:THR:OG1	26:LU:290:TYR:OH	2.17	0.53
29:NA:563:ILE:HG22	60:LR:720:THR:HG21	1.91	0.53
68:NY:83:LEU:HD12	68:NY:88:VAL:HB	1.91	0.53
2:L1:1110:G:N7	64:NI:211:ARG:NH2	2.56	0.53
3:L2:77:C:H2’	3:L2:78:A:H8	1.73	0.53
6:L5:138:ALA:O	15:LG:63:ARG:NH2	2.41	0.53
16:LH:229:LEU:O	16:LH:241:TYR:HA	2.08	0.53
20:LN:532:MET:HG2	20:LN:543:ILE:HG12	1.91	0.53
23:LQ:200:LEU:HD11	23:LQ:308:ILE:HD13	1.91	0.53
27:LW:499:GLU:OE2	28:LZ:3:ARG:NH1	2.42	0.53
51:SL:149:VAL:HG13	51:SL:174:VAL:HG21	1.91	0.53
2:L1:175:A:H2’	2:L1:176:U:C6	2.44	0.53
2:L1:1659:U:H5’	2:L1:1660:C:H5’	1.89	0.53
16:LH:816:LEU:HB3	61:LM:933:GLU:HG2	1.90	0.53
18:LJ:44:VAL:HG22	18:LJ:56:VAL:HG22	1.90	0.53
19:LL:186:ALA:HB1	19:LL:211:VAL:HB	1.89	0.53
27:LW:181:ASP:HA	61:LM:83:THR:HA	1.90	0.53
29:NA:567:ALA:HB1	60:LR:678:ARG:HH21	1.72	0.53
35:NJ:534:VAL:O	35:NJ:540:ASN:ND2	2.38	0.53
16:LH:15:SER:OG	16:LH:35:SER:OG	2.24	0.53
26:LU:234:LYS:HD2	26:LU:444:VAL:HG21	1.91	0.53
26:LU:276:MET:HE1	26:LU:314:SER:HB3	1.91	0.53
35:NJ:283:THR:HG22	35:NJ:413:ILE:HD11	1.91	0.53
46:SC:193:SER:OG	46:SC:195:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:LM:361:HIS:CG	61:LM:372:GLY:HA3	2.44	0.53
2:L1:647:U:H2’	2:L1:648:A:H8	1.73	0.53
19:LL:33:SER:OG	19:LL:35:ASP:OD1	2.21	0.53
9:L8:62:VAL:HG11	59:SP:989:VAL:HG11	1.91	0.53
19:LL:298:LEU:HB2	19:LL:315:CYS:HB2	1.89	0.53
20:LN:535:ALA:HB3	20:LN:540:ASN:H	1.74	0.53
22:LP:556:LEU:HD23	22:LP:563:PRO:HB3	1.90	0.53
23:LQ:220:ILE:HD11	23:LQ:266:LEU:HD22	1.90	0.53
2:L1:546:G:H5’	30:NB:472:VAL:HG11	1.91	0.52
7:L6:94:ARG:NH2	43:NW:87:LEU:O	2.42	0.52
16:LH:555:TYR:HE1	16:LH:576:GLU:HG3	1.74	0.52
35:NJ:124:GLN:HG2	35:NJ:152:ARG:HH21	1.74	0.52
43:NW:297:MET:HB2	43:NW:307:THR:H	1.73	0.52
52:SM:12:TYR:OH	52:SM:74:GLU:OE2	2.25	0.52
2:L1:649:U:H2’	2:L1:650:A:C8	2.44	0.52
19:LL:140:CYS:SG	19:LL:161:LYS:NZ	2.68	0.52
25:LT:516:GLY:HA2	25:LT:542:VAL:HG23	1.91	0.52
27:LW:527:ILE:HD11	55:SS:673:ARG:NH1	2.25	0.52
39:NQ:74:THR:HA	64:NI:215:LEU:HB3	1.92	0.52
2:L1:1589:A:H1’	2:L1:1654:G:H4’	1.91	0.52
2:L1:1823:A:H4’	2:L1:1824:A:O5’	2.10	0.52
9:L8:64:ASN:HA	9:L8:75:LYS:HA	1.91	0.52
24:LS:412:ASN:OD1	24:LS:413:SER:N	2.42	0.52
35:NJ:256:LYS:HD3	35:NJ:469:ILE:HG23	1.91	0.52
35:NJ:691:LEU:HD12	35:NJ:692:PRO:HD2	1.89	0.52
40:NR:186:UNK:O	40:NR:190:UNK:N	2.43	0.52
48:SH:36:ARG:NH1	48:SH:48:GLU:OE1	2.39	0.52
2:L1:276:G:H2’	2:L1:277:C:C6	2.44	0.52
20:LN:181:LYS:HD2	47:SE:17:HIS:CD2	2.45	0.52
20:LN:441:LEU:HG	20:LN:457:ASN:HA	1.92	0.52
27:LW:502:VAL:HG21	28:LZ:3:ARG:HD3	1.90	0.52
35:NJ:808:LEU:HD22	35:NJ:812:GLU:OE1	2.09	0.52
38:NO:104:LEU:HD23	38:NO:125:ILE:HA	1.92	0.52
59:SP:718:GLU:OE2	59:SP:722:ARG:NE	2.41	0.52
61:LM:1719:ALA:HB2	61:LM:1763:ALA:HA	1.90	0.52
16:LH:215:GLU:HG3	20:LN:268:VAL:HG13	1.89	0.52
35:NJ:298:ILE:HD11	35:NJ:386:VAL:HG21	1.91	0.52
61:LM:362:VAL:HG12	61:LM:363:THR:HG23	1.92	0.52
68:NY:114:ILE:HG23	68:NY:117:ARG:HH12	1.74	0.52
2:L1:1013:U:H2’	2:L1:1014:G:H8	1.75	0.52
18:LJ:116:ARG:NH1	18:LJ:154:SER:OG	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LP:21:ARG:HH11	27:LW:102:ALA:HA	1.75	0.52
23:LQ:274:ILE:HG21	23:LQ:353:ILE:HD11	1.91	0.52
25:LT:847:LEU:HD12	25:LT:855:ILE:HD12	1.92	0.52
26:LU:35:PHE:HZ	27:LW:330:ALA:HB2	1.74	0.52
29:NA:386:LEU:HD13	49:SI:939:ARG:HH12	1.75	0.52
35:NJ:423:LEU:HB3	35:NJ:426:LYS:HD3	1.92	0.52
46:SD:125:ILE:HD13	53:SQ:691:GLY:HA3	1.91	0.52
1:L0:1433:A:N7	44:SA:40:GLY:HA3	2.25	0.52
2:L1:1720:U:O2’	29:NA:677:HIS:NE2	2.37	0.52
23:LQ:217:VAL:HG13	23:LQ:271:ALA:HB3	1.91	0.52
25:LT:104:LYS:HE2	25:LT:716:LEU:HB3	1.91	0.52
73:SK:301:SAH:SD	73:SK:301:SAH:H8	2.49	0.52
59:SP:965:HIS:HB3	59:SP:968:VAL:HG12	1.92	0.52
48:SH:338:MET:HG3	49:SI:694:TYR:CZ	2.45	0.52
1:L0:830:G:H3’	1:L0:831:A:H5”	1.92	0.52
6:L5:30:ILE:HG23	6:L5:117:ILE:HD11	1.92	0.52
12:LC:44:PRO:HD2	12:LC:81:ILE:HD11	1.92	0.52
18:LJ:477:GLN:HA	18:LJ:480:LEU:HD12	1.92	0.52
25:LT:663:ASP:OD1	25:LT:664:SER:N	2.43	0.52
35:NJ:280:VAL:HG22	35:NJ:461:TYR:HD2	1.74	0.52
35:NJ:532:LEU:HD22	35:NJ:576:VAL:HG22	1.91	0.52
44:SA:208:ALA:HB1	44:SA:212:ARG:HH12	1.74	0.52
50:SK:67:ASP:HB3	50:SK:68:LYS:NZ	2.25	0.52
61:LM:707:ILE:HA	61:LM:710:VAL:HG22	1.92	0.52
64:NI:244:TRP:HA	64:NI:247:ARG:HG2	1.92	0.52
16:LH:641:GLU:HB2	16:LH:652:ASN:HA	1.92	0.52
27:LW:343:LEU:HD12	27:LW:353:ALA:HB3	1.92	0.52
35:NJ:866:LEU:HD21	35:NJ:891:LEU:HD22	1.92	0.52
50:SK:75:LYS:HD3	50:SK:76:ASN:H	1.74	0.52
60:LR:703:MET:HE1	60:LR:734:VAL:HG13	1.92	0.52
2:L1:1787:G:H2’	2:L1:1788:A:C8	2.45	0.51
25:LT:287:GLN:HG2	25:LT:317:TRP:HZ2	1.75	0.51
35:NJ:250:VAL:HG21	35:NJ:333:LEU:HD21	1.90	0.51
35:NJ:810:ARG:HH21	35:NJ:912:LYS:HB3	1.75	0.51
51:SL:169:ARG:NH1	51:SL:187:GLU:OE2	2.43	0.51
22:LP:2:ALA:HA	22:LP:5:ILE:HD12	1.91	0.51
23:LQ:463:VAL:HG11	23:LQ:468:GLN:HB2	1.93	0.51
46:SC:239:GLN:O	46:SC:242:GLN:HG3	2.09	0.51
24:LS:194:PRO:HG2	24:LS:197:ALA:HB2	1.91	0.51
24:LS:424:GLY:HA2	47:SE:88:ALA:HA	1.91	0.51
24:LS:437:GLY:O	24:LS:454:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SA:16:LEU:HB3	44:SA:50:ALA:HB3	1.92	0.51
59:SP:959:CYS:O	59:SP:962:THR:OG1	2.24	0.51
3:L2:46:A:H4'	51:SL:22:GLN:HE22	1.76	0.51
3:L2:131:U:O4	3:L2:138:C:N4	2.43	0.51
16:LH:328:GLN:NE2	16:LH:331:VAL:HG22	2.25	0.51
18:LJ:355:ARG:HH21	24:LS:295:ARG:HG3	1.74	0.51
20:LN:595:HIS:CE1	20:LN:608:ASP:OD1	2.63	0.51
23:LQ:264:ARG:NE	60:LR:663:GLU:OE2	2.43	0.51
26:LU:102:ILE:HG22	26:LU:103:ARG:HG3	1.91	0.51
45:SB:72:LEU:HA	45:SB:75:VAL:HG12	1.92	0.51
45:SB:150:ARG:HH12	46:SC:214:ILE:H	1.58	0.51
2:L1:1588:A:H2'	2:L1:1589:A:C8	2.45	0.51
19:LL:220:ARG:NH2	19:LL:279:GLU:O	2.38	0.51
25:LT:384:ASN:HD21	25:LT:386:ARG:HH21	1.59	0.51
46:SC:224:ARG:HA	46:SC:253:PHE:HZ	1.76	0.51
61:LM:293:ILE:HD12	61:LM:294:PRO:HD2	1.92	0.51
1:L0:844:G:N7	21:LO:271:LYS:NZ	2.54	0.51
3:L2:46:A:H2'	3:L2:47:G:C8	2.46	0.51
3:L2:135:U:H3	3:L2:138:C:P	2.34	0.51
16:LH:614:GLU:OE1	16:LH:616:ARG:HG2	2.11	0.51
19:LK:477:MET:O	19:LK:481:VAL:HG23	2.11	0.51
20:LN:589:HIS:CD2	20:LN:591:LYS:HG3	2.46	0.51
22:LP:43:LYS:HB3	22:LP:53:ASP:OD1	2.10	0.51
23:LQ:464:PRO:HD3	23:LQ:504:LEU:HD11	1.92	0.51
23:LQ:674:HIS:HE2	23:LQ:692:SER:HG	1.58	0.51
35:NJ:190:SER:O	35:NJ:480:TRP:NE1	2.43	0.51
44:SA:294:PRO:HB2	44:SA:391:SER:HB3	1.92	0.51
61:LM:665:ILE:HA	61:LM:710:VAL:HG12	1.91	0.51
61:LM:1040:GLN:HB3	61:LM:1044:LYS:NZ	2.25	0.51
2:L1:942:G:H2'	2:L1:943:U:C6	2.46	0.51
16:LH:695:PHE:HA	16:LH:698:ILE:HD12	1.93	0.51
20:LN:87:ASP:HB2	20:LN:94:LYS:HG3	1.93	0.51
61:LM:1721:VAL:O	61:LM:1725:LEU:N	2.41	0.51
63:SG:404:GLN:HB3	63:SG:415:LEU:HD11	1.92	0.51
1:L0:814:C:N4	24:LS:240:ASN:HD22	2.09	0.51
19:LL:169:SER:OG	19:LL:188:ARG:NH1	2.44	0.51
22:LP:142:ALA:O	22:LP:146:MET:HG3	2.10	0.51
22:LP:453:SER:OG	22:LP:456:ASP:OD2	2.29	0.51
25:LT:426:LYS:HB3	25:LT:430:ARG:HH22	1.76	0.51
26:LU:75:HIS:CD2	26:LU:78:LYS:H	2.29	0.51
43:NW:237:LYS:HD2	43:NW:278:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SH:373:LYS:NZ	54:SR:58:GLU:OE1	2.44	0.51
49:SI:1050:ALA:HB3	66:ST:800:PHE:HZ	1.75	0.51
68:NY:179:THR:HG21	68:NY:202:VAL:HG23	1.91	0.51
19:LL:38:LEU:HD22	19:LL:99:LEU:HD21	1.93	0.51
19:LL:241:VAL:HG12	19:LL:242:HIS:ND1	2.26	0.51
23:LQ:597:MET:HG2	23:LQ:608:THR:HG22	1.92	0.51
26:LU:292:PRO:HG2	26:LU:337:SER:HB3	1.91	0.51
43:NW:237:LYS:HD3	43:NW:280:PHE:HD1	1.76	0.51
2:L1:13:C:H2’	2:L1:14:C:C6	2.46	0.51
3:L2:152:A:O2’	3:L2:153:G:OP1	2.24	0.51
8:L7:64:VAL:HB	8:L7:72:PHE:HE2	1.76	0.51
23:LQ:363:ALA:HB3	23:LQ:384:LEU:HD13	1.93	0.51
24:LS:255:SER:OG	24:LS:299:PHE:O	2.29	0.51
25:LT:314:ILE:HB	25:LT:328:MET:HB2	1.93	0.51
44:SA:97:ASP:OD1	46:SD:221:HIS:ND1	2.44	0.51
49:SI:96:SER:OG	72:SI:2001:GTP:O1A	2.29	0.51
2:L1:1717:C:H2’	2:L1:1718:G:C8	2.46	0.50
16:LH:545:LEU:HD11	16:LH:556:LEU:HD21	1.92	0.50
35:NJ:728:PHE:HB3	35:NJ:748:MET:HB3	1.93	0.50
38:NO:30:CYS:SG	38:NO:31:SER:N	2.84	0.50
45:SB:84:HIS:HB3	61:LM:1141:SER:HA	1.93	0.50
46:SC:165:TYR:CE2	46:SC:168:ALA:HA	2.46	0.50
2:L1:521:A:OP1	10:L9:45:ARG:NH1	2.36	0.50
2:L1:961:G:N2	68:NY:235:ARG:O	2.44	0.50
16:LH:104:ALA:HB2	16:LH:158:PRO:HG3	1.93	0.50
46:SD:107:VAL:HG12	46:SD:136:ALA:HA	1.93	0.50
48:SH:94:GLY:HA2	48:SH:120:VAL:HG13	1.92	0.50
55:SS:127:ARG:HA	55:SS:130:ARG:HE	1.76	0.50
2:L1:227:U:H4’	2:L1:228:C:O5’	2.11	0.50
3:L2:31:G:N2	26:LU:61:SER:OG	2.45	0.50
16:LH:349:LEU:HD22	16:LH:363:LEU:HD21	1.94	0.50
21:LO:16:ARG:HB3	21:LO:34:GLY:H	1.76	0.50
23:LQ:418:VAL:HG23	23:LQ:693:SER:HB2	1.93	0.50
34:NG:31:CYS:HB2	34:NG:93:LEU:HD13	1.92	0.50
39:NQ:80:ARG:HG2	64:NI:202:GLY:O	2.12	0.50
59:SP:1001:LYS:HD2	59:SP:1004:HIS:CE1	2.46	0.50
2:L1:1856:C:H2’	2:L1:1857:G:C8	2.47	0.50
12:LC:97:GLN:HB2	12:LC:105:LYS:HG3	1.94	0.50
23:LQ:394:LEU:HD22	23:LQ:403:PRO:HB3	1.93	0.50
27:LW:524:VAL:HG13	55:SS:682:VAL:HG13	1.92	0.50
35:NJ:182:ARG:NH1	35:NJ:549:SER:O	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LL:402:LYS:HE3	19:LL:404:LEU:HD21	1.94	0.50
45:SB:214:ARG:HA	45:SB:217:TYR:HD1	1.77	0.50
49:SI:748:GLU:OE2	49:SI:755:ARG:NH1	2.45	0.50
50:SK:238:GLU:HB3	50:SK:243:VAL:O	2.12	0.50
55:SS:121:ASN:N	55:SS:124:GLU:OE2	2.45	0.50
2:L1:460:A:H5"	49:SI:324:LYS:HD3	1.94	0.50
6:L5:124:ASP:OD1	6:L5:125:SER:N	2.36	0.50
16:LH:104:ALA:HB3	16:LH:118:ILE:HD12	1.92	0.50
18:LJ:252:THR:HG21	18:LJ:293:LEU:HA	1.93	0.50
22:LP:380:LEU:HD21	22:LP:412:VAL:HG22	1.93	0.50
25:LT:551:ASN:O	25:LT:569:LYS:NZ	2.37	0.50
26:LU:272:ASP:OD1	26:LU:273:THR:N	2.45	0.50
35:NJ:307:SER:HA	35:NJ:366:GLN:HG2	1.93	0.50
5:L4:137:PRO:HG2	5:L4:150:PRO:HD2	1.93	0.50
22:LP:114:VAL:HG13	22:LP:126:LEU:HD11	1.94	0.50
27:LW:367:VAL:HG12	27:LW:374:MET:HG3	1.94	0.50
44:SA:12:VAL:HG21	44:SA:137:THR:HG21	1.92	0.50
45:SB:44:LEU:HD21	45:SB:47:PHE:HB2	1.94	0.50
60:LR:486:ALA:HB3	60:LR:495:ALA:HB3	1.93	0.50
1:L0:686:U:OP1	20:LN:186:ARG:NH2	2.30	0.50
2:L1:1696:C:OP2	29:NA:455:LYS:NZ	2.36	0.50
3:L2:32:U:O2'	3:L2:33:G:O5'	2.25	0.50
3:L2:49:U:H2'	3:L2:50:U:C6	2.46	0.50
16:LH:271:VAL:HG13	16:LH:287:PRO:HA	1.94	0.50
24:LS:154:ASP:HA	24:LS:172:LYS:HG3	1.94	0.50
2:L1:17:C:O2'	49:SI:1251:GLN:OE1	2.26	0.50
2:L1:1384:C:H2'	2:L1:1385:G:H8	1.77	0.50
20:LN:363:THR:OG1	20:LN:374:PRO:O	2.30	0.50
24:LS:253:ARG:HH21	24:LS:271:LEU:HD21	1.77	0.50
24:LS:488:LEU:HB2	24:LS:504:LEU:HD21	1.93	0.50
35:NJ:334:GLN:HG2	35:NJ:335:TYR:H	1.77	0.50
36:NM:71:LEU:HD12	36:NM:84:PHE:HE1	1.76	0.50
43:NW:75:PRO:HB2	43:NW:93:LEU:HB2	1.94	0.50
23:LQ:159:ARG:NH2	23:LQ:202:GLU:OE2	2.41	0.49
45:SB:346:LEU:HD12	45:SB:362:LEU:HD13	1.93	0.49
48:SH:122:ASN:OD1	48:SH:157:ARG:NH1	2.45	0.49
2:L1:1007:C:H2'	2:L1:1008:A:C8	2.47	0.49
18:LJ:267:SER:OG	18:LJ:269:ASP:OD1	2.30	0.49
21:LO:416:SER:N	21:LO:436:ASP:OD1	2.39	0.49
23:LQ:387:ASN:OD1	23:LQ:415:ARG:NH2	2.40	0.49
23:LQ:660:TRP:CZ3	23:LQ:667:HIS:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LU:359:LYS:NZ	26:LU:367:GLU:OE2	2.45	0.49
26:LU:405:GLN:OE1	26:LU:408:ARG:NH1	2.41	0.49
32:NE:283:ILE:HD13	38:NO:79:PHE:CE2	2.45	0.49
35:NJ:360:VAL:HG13	35:NJ:366:GLN:HB2	1.94	0.49
43:NW:110:ILE:HG13	43:NW:122:HIS:HB2	1.94	0.49
48:SH:195:ALA:O	48:SH:228:ASP:N	2.44	0.49
61:LM:83:THR:O	61:LM:87:ASN:ND2	2.45	0.49
61:LM:634:HIS:HD2	61:LM:636:LEU:HB2	1.77	0.49
6:L5:32:ASP:OD1	6:L5:34:SER:OG	2.27	0.49
16:LH:727:ILE:HD13	16:LH:754:SER:HB3	1.95	0.49
23:LQ:19:ILE:HB	23:LQ:387:ASN:HB2	1.94	0.49
63:SG:258:SER:OG	63:SG:268:TRP:NE1	2.33	0.49
9:L8:57:ALA:HB2	9:L8:183:GLY:HA2	1.94	0.49
20:LN:154:HIS:CD2	20:LN:203:PHE:HE2	2.29	0.49
21:LO:312:PHE:CE1	21:LO:326:LEU:HB2	2.47	0.49
23:LQ:676:GLN:HB3	23:LQ:695:HIS:HB3	1.93	0.49
25:LT:595:LEU:HD23	25:LT:607:LEU:HD11	1.94	0.49
44:SA:375:LYS:HD3	44:SA:397:LEU:HD22	1.94	0.49
51:SL:85:ASP:HB3	51:SL:88:GLN:HB2	1.94	0.49
60:LR:94:ALA:O	60:LR:98:GLY:N	2.33	0.49
61:LM:705:HIS:CE1	61:LM:771:TYR:CZ	3.01	0.49
35:NK:268:ILE:O	35:NK:272:SER:N	2.41	0.49
2:L1:486:A:OP2	2:L1:487:U:O2’	2.28	0.49
7:L6:20:ASP:HB3	7:L6:23:LYS:HE2	1.95	0.49
10:L9:13:TYR:OH	10:L9:41:ARG:NH1	2.45	0.49
15:LG:12:ALA:HB1	15:LG:32:VAL:HB	1.94	0.49
16:LH:17:LEU:N	16:LH:312:ASN:OD1	2.37	0.49
22:LP:18:GLN:O	22:LP:22:ILE:HG12	2.12	0.49
34:NG:39:ASP:OD1	34:NG:40:THR:N	2.45	0.49
35:NJ:246:GLN:HA	35:NJ:249:GLY:H	1.78	0.49
36:NM:26:SER:O	36:NM:51:ARG:NH1	2.45	0.49
49:SI:1003:MET:HG2	49:SI:1005:ASP:H	1.76	0.49
59:SP:644:LYS:NZ	59:SP:810:ASP:O	2.32	0.49
1:L0:740:G:H3’	1:L0:741:G:H5”	1.94	0.49
1:L0:1423:U:H2’	1:L0:1424:U:C6	2.48	0.49
2:L1:396:U:OP2	13:LD:79:LYS:NZ	2.36	0.49
2:L1:1378:A:OP2	2:L1:1379:A:O2’	2.27	0.49
20:LN:414:PHE:HB3	20:LN:416:TYR:CE1	2.47	0.49
20:LN:581:THR:HG21	20:LN:601:ALA:HB3	1.94	0.49
24:LS:153:VAL:HB	24:LS:178:LEU:HD11	1.95	0.49
26:LU:240:ARG:NH2	26:LU:259:GLU:OE2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SB:16:VAL:HG11	45:SB:22:LEU:HD11	1.94	0.49
46:SC:97:PHE:HB2	46:SC:107:VAL:HG23	1.94	0.49
49:SI:1220:GLN:HG2	53:SQ:735:ILE:HD12	1.94	0.49
1:L0:718:G:N2	1:L0:752:C:N3	2.60	0.49
1:L0:732:G:O2'	1:L0:733:C:OP1	2.29	0.49
21:LO:652:ASP:OD1	21:LO:700:LYS:HE2	2.13	0.49
23:LQ:30:THR:HG22	23:LQ:35:LYS:HG3	1.94	0.49
23:LQ:276:ARG:NE	23:LQ:296:CYS:SG	2.76	0.49
36:NM:82:ARG:HD2	36:NM:103:MET:SD	2.51	0.49
48:SH:123:ASP:OD1	48:SH:124:GLN:N	2.46	0.49
2:L1:1659:U:OP2	2:L1:1663:A:N6	2.44	0.49
9:L8:42:ARG:HH22	43:NW:334:PRO:HD3	1.78	0.49
18:LJ:378:ASP:OD1	18:LJ:413:ARG:NH1	2.41	0.49
20:LN:437:LEU:HD22	20:LN:454:VAL:HG11	1.94	0.49
21:LO:396:LYS:HE3	21:LO:412:THR:HG22	1.94	0.49
21:LO:586:ASP:OD2	21:LO:632:TYR:OH	2.23	0.49
21:LO:830:HIS:HA	21:LO:833:LYS:HE2	1.95	0.49
26:LU:75:HIS:HD2	26:LU:78:LYS:H	1.60	0.49
44:SA:197:PHE:CD2	44:SA:200:LEU:HB2	2.48	0.49
55:SS:165:GLU:HG2	55:SS:166:PRO:HD2	1.95	0.49
60:LR:424:VAL:HA	60:LR:441:SER:HA	1.95	0.49
2:L1:1787:G:H2'	2:L1:1788:A:H8	1.76	0.49
16:LH:227:ILE:HD13	16:LH:254:LEU:HD11	1.95	0.49
18:LJ:393:THR:O	18:LJ:397:ILE:HG13	2.12	0.49
21:LO:197:GLU:OE2	21:LO:204:TYR:OH	2.19	0.49
29:NA:395:ARG:NH1	29:NA:399:SER:OG	2.45	0.49
49:SI:670:ASP:HB2	49:SI:674:LYS:HE3	1.95	0.49
51:SL:19:LEU:HB3	51:SL:30:LEU:HB2	1.95	0.49
61:LM:374:ILE:HD13	61:LM:377:ARG:HH21	1.76	0.49
61:LM:499:MET:O	61:LM:503:LYS:N	2.39	0.49
1:L0:757:G:H1	1:L0:803:U:H3	1.59	0.49
1:L0:798:U:C5	12:LC:69:ARG:HD3	2.48	0.49
2:L1:69:C:OP2	7:L6:164:LYS:NZ	2.42	0.49
2:L1:124:U:OP1	7:L6:201:LYS:NZ	2.33	0.49
19:LL:476:GLU:HG3	19:LL:480:LYS:HE2	1.95	0.49
36:NM:78:GLU:HG3	36:NM:79:VAL:H	1.78	0.49
48:SH:220:ILE:HB	48:SH:223:ILE:HD11	1.95	0.49
49:SI:298:HIS:ND1	49:SI:304:ASP:OD1	2.42	0.49
2:L1:84:A:N3	2:L1:150:A:O2'	2.44	0.48
2:L1:1127:C:H4'	39:NQ:17:ARG:HH11	1.78	0.48
6:L5:168:THR:OG1	6:L5:171:GLU:OE1	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LU:300:ALA:HA	26:LU:306:ILE:HG22	1.95	0.48
63:SG:186:ARG:NH1	63:SG:188:LYS:HA	2.27	0.48
2:L1:1768:A:H2'	2:L1:1769:C:H4'	1.95	0.48
5:L4:54:TYR:O	14:LF:15:ASN:ND2	2.46	0.48
23:LQ:657:ILE:HD11	23:LQ:678:ILE:HD13	1.96	0.48
36:NM:103:MET:HG3	36:NM:188:LEU:HD21	1.95	0.48
45:SB:26:ASP:OD1	45:SB:26:ASP:N	2.46	0.48
46:SD:195:ARG:NH2	47:SF:9:LYS:O	2.47	0.48
48:SH:190:ARG:NH2	48:SH:248:GLU:OE1	2.44	0.48
59:SP:828:LEU:HD22	59:SP:921:VAL:HB	1.95	0.48
61:LM:1105:THR:O	61:LM:1109:LYS:HG2	2.14	0.48
27:LW:519:ARG:NH1	55:SS:700:GLN:OE1	2.47	0.48
31:ND:231:ASN:OD1	31:ND:232:ALA:N	2.46	0.48
61:LM:775:LEU:HD23	61:LM:781:VAL:HG21	1.95	0.48
2:L1:607:U:OP1	49:SI:1099:ARG:NH1	2.46	0.48
19:LK:520:ALA:O	19:LK:523:MET:HB2	2.13	0.48
19:LL:65:LEU:HD22	19:LL:97:LEU:HD21	1.95	0.48
21:LO:747:PRO:HG3	25:LT:739:ILE:HD11	1.95	0.48
21:LO:879:GLN:NE2	60:LR:743:ALA:HA	2.28	0.48
22:LP:119:LYS:HG2	22:LP:120:TRP:CD1	2.48	0.48
23:LQ:114:LYS:HE2	23:LQ:114:LYS:HB2	1.64	0.48
23:LQ:583:PHE:HZ	23:LQ:586:SER:HB2	1.77	0.48
52:SM:97:LEU:HD22	52:SM:141:GLU:HG2	1.95	0.48
1:L0:673:C:N4	1:L0:674:G:O6	2.47	0.48
2:L1:1794:C:H2'	2:L1:1795:G:H8	1.79	0.48
5:L4:19:MET:HB2	5:L4:51:ARG:HH22	1.79	0.48
7:L6:58:LYS:HA	7:L6:107:SER:HB3	1.95	0.48
16:LH:152:ASP:OD1	16:LH:153:TYR:N	2.45	0.48
18:LJ:392:ILE:O	18:LJ:396:ILE:HG13	2.13	0.48
18:LJ:411:ALA:HB2	18:LJ:448:ILE:HD13	1.94	0.48
26:LU:127:VAL:HG11	26:LU:159:TYR:HB2	1.96	0.48
44:SA:286:ARG:NH1	44:SA:286:ARG:HB2	2.28	0.48
51:SL:20:ARG:HH12	51:SL:31:LYS:HB3	1.78	0.48
22:LP:575:LYS:HD3	45:SB:349:GLN:HB3	1.96	0.48
26:LU:419:VAL:HA	26:LU:422:ILE:HG22	1.95	0.48
48:SH:306:THR:HG22	48:SH:337:ILE:HD13	1.94	0.48
49:SI:282:LEU:HD12	49:SI:909:LEU:HD21	1.96	0.48
52:SM:136:LEU:HB2	52:SM:154:LEU:HD21	1.95	0.48
61:LM:564:ALA:HA	61:LM:572:TRP:CZ3	2.48	0.48
2:L1:375:U:H2'	2:L1:376:A:C8	2.49	0.48
2:L1:1739:C:H2'	2:L1:1740:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L2:43:A:P	53:SQ:633:ARG:HH21	2.37	0.48
18:LJ:80:LYS:NZ	18:LJ:101:ASP:HB2	2.28	0.48
20:LN:341:SER:HB3	20:LN:346:LEU:HB2	1.96	0.48
21:LO:462:SER:HB3	21:LO:478:GLN:OE1	2.14	0.48
23:LQ:131:ILE:HD11	23:LQ:152:ILE:HG21	1.95	0.48
25:LT:418:LEU:HD22	25:LT:478:SER:HA	1.95	0.48
35:NJ:564:PRO:O	35:NJ:567:GLN:NE2	2.45	0.48
61:LM:585:LYS:HB2	61:LM:588:ILE:HD12	1.95	0.48
61:LM:586:GLU:HA	61:LM:633:LEU:HD11	1.94	0.48
61:LM:909:LYS:HB3	61:LM:948:VAL:HG21	1.95	0.48
2:L1:622:C:O2	49:SI:967:ARG:NH2	2.47	0.48
16:LH:469:TYR:HD1	16:LH:495:SER:HB3	1.78	0.48
18:LJ:254:LEU:HD21	18:LJ:263:LEU:HD11	1.96	0.48
20:LN:653:MET:HA	20:LN:662:VAL:O	2.14	0.48
23:LQ:85:GLU:HG3	23:LQ:109:ALA:HB2	1.95	0.48
25:LT:111:VAL:HG11	25:LT:342:LEU:HD11	1.96	0.48
51:SL:140:TYR:CZ	51:SL:142:ASP:HB2	2.48	0.48
2:L1:375:U:H2’	2:L1:376:A:H8	1.78	0.48
2:L1:1658:G:H2’	49:SI:1037:PHE:HB3	1.96	0.48
19:LK:524:VAL:O	19:LK:527:LEU:HB3	2.14	0.48
22:LP:22:ILE:HD13	27:LW:98:PHE:CZ	2.48	0.48
44:SA:98:PRO:HA	44:SA:114:THR:HG21	1.95	0.48
24:LS:435:ARG:HD3	24:LS:483:PRO:HA	1.96	0.47
29:NA:400:LEU:HA	29:NA:403:GLU:HG2	1.96	0.47
35:NJ:260:GLN:HE21	35:NJ:289:GLY:HA3	1.79	0.47
49:SI:669:GLU:O	49:SI:673:ARG:NH2	2.47	0.47
61:LM:764:PRO:HG2	61:LM:767:LEU:HB2	1.95	0.47
1:L0:1421:C:H2’	1:L0:1422:C:C6	2.49	0.47
16:LH:226:LYS:HG2	16:LH:245:HIS:CG	2.49	0.47
19:LL:476:GLU:O	19:LL:480:LYS:HG3	2.13	0.47
34:NG:61:LYS:NZ	34:NG:76:LEU:HB3	2.29	0.47
59:SP:756:TRP:NE1	59:SP:841:GLU:OE1	2.47	0.47
61:LM:589:LEU:O	61:LM:596:SER:OG	2.31	0.47
61:LM:615:GLU:O	61:LM:620:LYS:NZ	2.47	0.47
68:NY:132:ALA:O	68:NY:135:ILE:HG12	2.14	0.47
2:L1:683:G:N2	2:L1:1022:U:OP2	2.28	0.47
23:LQ:632:HIS:CD2	23:LQ:636:VAL:HG12	2.48	0.47
24:LS:300:LYS:NZ	24:LS:347:PHE:O	2.40	0.47
3:L2:111:U:OP2	47:SF:44:LYS:NZ	2.44	0.47
10:L9:152:ASP:OD1	10:L9:153:SER:N	2.47	0.47
16:LH:746:PHE:CZ	22:LP:563:PRO:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LK:523:MET:O	19:LK:526:TRP:HB2	2.15	0.47
21:LO:319:GLU:N	21:LO:319:GLU:OE2	2.47	0.47
23:LQ:459:CYS:O	23:LQ:472:GLY:N	2.40	0.47
23:LQ:669:GLN:HE21	23:LQ:709:LEU:HD13	1.79	0.47
28:LZ:149:LEU:HD12	29:NA:510:LEU:HB3	1.96	0.47
29:NA:395:ARG:NH2	49:SI:1048:ASN:OD1	2.47	0.47
49:SI:260:ARG:HD3	49:SI:338:PRO:HB2	1.96	0.47
50:SK:99:PRO:HA	50:SK:102:ARG:HB2	1.96	0.47
68:NY:164:LEU:O	68:NY:171:THR:OG1	2.32	0.47
2:L1:573:U:N3	2:L1:576:A:OP2	2.32	0.47
2:L1:1786:U:H2’	2:L1:1787:G:H8	1.80	0.47
3:L2:50:U:H2’	3:L2:51:C:C6	2.49	0.47
3:L2:89:A:H5’	45:SB:336:PRO:HB3	1.96	0.47
5:L4:115:THR:HG22	5:L4:117:GLU:H	1.79	0.47
19:LL:513:LEU:HD12	19:LL:551:LEU:HD11	1.95	0.47
21:LO:866:ASN:ND2	25:LT:894:GLN:OE1	2.47	0.47
34:NG:113:GLN:HE21	34:NG:117:ARG:HE	1.61	0.47
35:NJ:29:VAL:HG22	35:NJ:151:LEU:HD12	1.97	0.47
45:SB:191:PHE:HD2	45:SB:194:LEU:HB2	1.79	0.47
1:L0:760:C:OP1	57:SY:245:TYR:OH	2.28	0.47
2:L1:1713:C:H2’	2:L1:1714:U:C6	2.49	0.47
20:LN:589:HIS:HD2	20:LN:591:LYS:HG3	1.79	0.47
27:LW:531:GLN:HA	27:LW:534:LYS:HE2	1.96	0.47
50:SK:229:THR:HA	50:SK:232:LYS:HE2	1.97	0.47
52:SM:28:ARG:HB2	52:SM:46:LEU:HD21	1.97	0.47
61:LM:885:VAL:HG13	61:LM:889:LEU:HD23	1.96	0.47
61:LM:1008:TYR:OH	61:LM:1033:GLN:O	2.31	0.47
2:L1:1336:C:H2’	2:L1:1337:C:C6	2.50	0.47
2:L1:1667:U:H5”	52:SM:142:HIS:HA	1.96	0.47
12:LC:12:VAL:HG11	12:LC:90:LYS:HB3	1.97	0.47
16:LH:519:GLU:HA	16:LH:541:LYS:HA	1.97	0.47
20:LN:274:GLU:OE2	20:LN:274:GLU:N	2.47	0.47
22:LP:538:ARG:NH2	45:SB:288:VAL:HG13	2.29	0.47
23:LQ:482:ASP:OD1	23:LQ:489:LEU:HD21	2.15	0.47
29:NA:383:PRO:HD2	29:NA:386:LEU:HD12	1.97	0.47
35:NJ:903:VAL:HG23	35:NJ:904:LYS:HD3	1.97	0.47
38:NO:83:LEU:HD22	38:NO:120:HIS:HA	1.96	0.47
44:SA:97:ASP:HB3	44:SA:100:ILE:HG22	1.97	0.47
46:SD:239:GLN:O	46:SD:242:GLN:HG3	2.15	0.47
49:SI:205:ARG:NH1	49:SI:208:THR:OG1	2.48	0.47
55:SS:673:ARG:HH21	55:SS:675:ILE:HG22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:LM:362:VAL:HG22	61:LM:424:GLN:HG3	1.96	0.47
61:LM:580:ALA:O	61:LM:584:ILE:HG22	2.15	0.47
63:SG:214:LEU:HB3	63:SG:226:TRP:HB2	1.97	0.47
63:SG:338:MET:HG2	63:SG:350:TRP:HB2	1.96	0.47
68:NY:277:GLN:HA	68:NY:280:LYS:NZ	2.29	0.47
1:L0:1416:A:H61	3:L2:53:C:H42	1.63	0.47
16:LH:814:LYS:HG2	16:LH:817:ARG:NH2	2.30	0.47
19:LL:527:LEU:HA	19:LL:530:VAL:HG12	1.97	0.47
20:LN:589:HIS:HB2	20:LN:655:LEU:HD13	1.97	0.47
23:LQ:502:MET:HG3	23:LQ:513:THR:HG22	1.96	0.47
23:LQ:679:TRP:HE1	23:LQ:695:HIS:HA	1.80	0.47
30:NB:465:LEU:HD23	46:SD:103:GLU:HG2	1.96	0.47
43:NW:257:ASP:HB2	43:NW:264:LEU:HD11	1.97	0.47
66:ST:792:LEU:HG	66:ST:796:HIS:CE1	2.48	0.47
2:L1:508:A:H3’	2:L1:509:G:H8	1.80	0.47
2:L1:1457:U:H2’	2:L1:1458:G:H8	1.79	0.47
2:L1:1591:C:H2’	2:L1:1592:C:H5’	1.97	0.47
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.23	0.47
16:LH:406:GLU:OE2	16:LH:418:GLN:NE2	2.47	0.47
19:LK:466:LEU:HD13	19:LK:481:VAL:HG11	1.97	0.47
20:LN:9:VAL:HB	20:LN:664:VAL:HA	1.96	0.47
23:LQ:418:VAL:HG12	23:LQ:434:ALA:HB2	1.97	0.47
35:NJ:201:ASP:OD2	49:SI:373:VAL:HG11	2.14	0.47
2:L1:353:C:H2’	2:L1:354:U:C6	2.50	0.47
20:LN:446:SER:OG	20:LN:448:ASP:O	2.33	0.47
25:LT:74:ARG:HH21	25:LT:76:LEU:HD21	1.80	0.47
25:LT:757:LEU:HG	25:LT:761:ARG:HD3	1.97	0.47
47:SF:14:ALA:O	47:SF:84:ARG:NH1	2.31	0.47
53:SQ:731:LYS:O	53:SQ:735:ILE:HG12	2.15	0.47
60:LR:608:VAL:HA	60:LR:624:ALA:HA	1.96	0.47
61:LM:1034:LEU:HD23	61:LM:1066:LYS:HG3	1.97	0.47
2:L1:477:G:HO2’	2:L1:478:G:H8	1.63	0.46
16:LH:100:CYS:SG	16:LH:101:LYS:N	2.88	0.46
28:LZ:152:ARG:O	28:LZ:155:GLU:HG2	2.14	0.46
49:SI:120:ILE:HG22	49:SI:335:VAL:HG22	1.97	0.46
60:LR:655:GLN:O	60:LR:655:GLN:NE2	2.48	0.46
2:L1:141:A:H4’	2:L1:142:C:H5’	1.96	0.46
2:L1:170:A:H2’	2:L1:171:A:C8	2.50	0.46
2:L1:377:G:H5”	9:L8:98:LYS:HB3	1.96	0.46
2:L1:1230:C:H2’	2:L1:1231:C:C6	2.50	0.46
14:LF:38:THR:O	14:LF:42:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:490:LEU:HG	19:LL:531:LEU:HD11	1.97	0.46
26:LU:348:ASN:ND2	51:SL:111:GLU:OE1	2.35	0.46
61:LM:558:LEU:HD11	61:LM:602:CYS:HB2	1.97	0.46
2:L1:29:G:H2'	2:L1:30:C:C6	2.50	0.46
2:L1:498:C:H2'	2:L1:499:G:H8	1.80	0.46
3:L2:64:G:H2'	3:L2:65:A:C8	2.49	0.46
21:LO:177:ASP:HB2	21:LO:227:LYS:HA	1.97	0.46
23:LQ:412:GLY:H	23:LQ:439:LYS:NZ	2.13	0.46
36:NM:28:LYS:HG2	36:NM:50:THR:HG22	1.96	0.46
3:L2:152:A:HO2'	3:L2:153:G:P	2.38	0.46
3:L2:178:G:H1'	3:L2:183:G:C2	2.51	0.46
7:L6:221:LYS:HD3	7:L6:224:ARG:HH11	1.80	0.46
16:LH:543:ARG:NE	16:LH:561:GLU:OE1	2.44	0.46
23:LQ:421:LEU:HD21	23:LQ:691:VAL:HG12	1.97	0.46
24:LS:144:ASP:OD2	24:LS:146:GLU:HG2	2.15	0.46
43:NW:231:PRO:HB3	43:NW:250:THR:HG23	1.98	0.46
43:NW:246:VAL:HB	43:NW:256:TYR:HE2	1.80	0.46
48:SH:288:TYR:HD1	49:SI:754:ILE:HD11	1.81	0.46
61:LM:665:ILE:HD12	61:LM:709:SER:HB2	1.97	0.46
68:NY:115:ARG:NH1	68:NY:135:ILE:O	2.48	0.46
2:L1:1091:C:H2'	2:L1:1092:G:C8	2.50	0.46
21:LO:522:ASP:OD1	21:LO:524:THR:OG1	2.32	0.46
23:LQ:661:ASP:HB2	23:LQ:668:ILE:HD11	1.96	0.46
23:LQ:680:CYS:SG	23:LQ:681:LEU:N	2.89	0.46
47:SE:70:PRO:O	47:SE:74:GLU:HG2	2.16	0.46
50:SK:159:ILE:HD12	50:SK:166:HIS:CE1	2.51	0.46
61:LM:737:ILE:O	61:LM:741:GLU:HG3	2.16	0.46
3:L2:217:U:OP2	45:SB:404:ARG:NH1	2.35	0.46
6:L5:38:TYR:OH	15:LG:54:ASP:OD2	2.28	0.46
12:LC:11:GLN:HA	12:LC:23:ALA:O	2.15	0.46
23:LQ:131:ILE:HD11	23:LQ:152:ILE:HG13	1.97	0.46
23:LQ:906:LYS:NZ	23:LQ:910:GLU:OE2	2.48	0.46
27:LW:385:ILE:O	27:LW:395:LEU:N	2.44	0.46
35:NJ:487:LEU:HD21	35:NJ:542:PRO:HB3	1.97	0.46
46:SD:87:MET:O	46:SD:100:ARG:N	2.48	0.46
49:SI:258:ALA:HB3	49:SI:907:ILE:HG13	1.98	0.46
60:LR:294:GLU:O	60:LR:312:ALA:N	2.43	0.46
64:NI:30:PHE:O	64:NI:142:SER:N	2.41	0.46
1:L0:799:C:O2'	1:L0:800:G:OP2	2.30	0.46
2:L1:946:U:H2'	2:L1:947:G:C8	2.51	0.46
3:L2:176:C:H2'	3:L2:177:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L4:175:PHE:HE2	5:L4:198:ARG:HD2	1.79	0.46
10:L9:78:LEU:HD22	10:L9:92:MET:HA	1.97	0.46
16:LH:17:LEU:HG	16:LH:312:ASN:HD21	1.81	0.46
16:LH:85:TRP:CD1	16:LH:92:LEU:HA	2.50	0.46
18:LJ:131:THR:OG1	18:LJ:133:ASP:O	2.34	0.46
20:LN:414:PHE:HB3	20:LN:416:TYR:HE1	1.81	0.46
21:LO:879:GLN:NE2	60:LR:744:PRO:HD3	2.27	0.46
23:LQ:674:HIS:NE2	23:LQ:692:SER:OG	2.46	0.46
25:LT:908:LEU:HD21	25:LT:918:ILE:HD11	1.97	0.46
36:NM:224:GLU:OE1	36:NM:227:LYS:N	2.45	0.46
46:SC:190:VAL:HA	46:SC:213:VAL:O	2.16	0.46
49:SI:1188:LYS:HB3	49:SI:1188:LYS:HE3	1.84	0.46
51:SL:26:GLU:HG3	51:SL:29:ARG:NH2	2.31	0.46
2:L1:1852:C:H2'	2:L1:1853:C:C6	2.51	0.46
23:LQ:200:LEU:HD12	23:LQ:201:SER:N	2.30	0.46
27:LW:339:GLY:HA2	27:LW:362:VAL:HG23	1.98	0.46
36:NM:214:LYS:HE2	36:NM:216:LYS:HE3	1.98	0.46
43:NW:287:ILE:HD12	43:NW:298:TRP:CZ3	2.51	0.46
45:SB:68:ILE:HB	45:SB:101:LYS:HE3	1.96	0.46
63:SG:130:GLU:HB3	63:SG:466:ARG:HB3	1.97	0.46
2:L1:941:C:H2'	2:L1:942:G:H8	1.81	0.46
2:L1:1591:C:C2'	2:L1:1592:C:H5'	2.46	0.46
18:LJ:78:ARG:NH1	18:LJ:112:ARG:HH22	2.14	0.46
19:LL:116:LEU:HD21	19:LL:119:LYS:HG3	1.98	0.46
20:LN:130:ILE:HG12	20:LN:135:ILE:HG22	1.97	0.46
20:LN:542:VAL:HG12	20:LN:552:GLU:HG3	1.97	0.46
45:SB:98:ILE:HD11	45:SB:102:LEU:HD12	1.98	0.46
46:SC:165:TYR:HE2	46:SC:168:ALA:HA	1.80	0.46
49:SI:1026:LYS:HE2	49:SI:1028:LYS:HD3	1.96	0.46
60:LR:524:LEU:HA	60:LR:540:SER:HA	1.96	0.46
60:LR:711:LYS:NZ	60:LR:742:GLU:OE1	2.38	0.46
1:L0:604:C:H42	18:LJ:433:ARG:HE	1.64	0.46
1:L0:666:U:H4'	1:L0:667:C:OP2	2.16	0.46
1:L0:736:C:O2'	16:LH:426:LYS:HD2	2.16	0.46
16:LH:39:VAL:HB	16:LH:53:LEU:HB2	1.98	0.46
23:LQ:9:ARG:HA	23:LQ:669:GLN:NE2	2.31	0.46
27:LW:326:ASN:HB3	27:LW:329:ASN:HB3	1.97	0.46
35:NJ:884:ILE:O	35:NJ:885:GLU:HG2	2.16	0.46
43:NW:190:LEU:HD11	43:NW:202:CYS:HB3	1.98	0.46
49:SI:320:PRO:HB3	49:SI:332:GLU:OE1	2.15	0.46
49:SI:1270:GLN:NE2	52:SM:41:LEU:HG	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SK:55:VAL:HG11	50:SK:64:LEU:HD13	1.97	0.46
59:SP:939:GLU:O	59:SP:943:GLN:N	2.40	0.46
64:NI:63:VAL:O	64:NI:119:ALA:N	2.43	0.46
1:L0:815:C:H41	24:LS:237:LYS:HE2	1.81	0.45
1:L0:827:C:H2’	21:LO:661:ARG:HH21	1.81	0.45
1:L0:827:C:C4	25:LT:413:LYS:HA	2.51	0.45
2:L1:1279:C:H2’	2:L1:1280:G:H8	1.81	0.45
2:L1:1856:C:H2’	2:L1:1857:G:H8	1.79	0.45
19:LL:470:LEU:HD22	19:LL:504:PRO:HB2	1.98	0.45
21:LO:759:PHE:O	21:LO:763:ILE:HG12	2.16	0.45
21:LO:763:ILE:HD13	21:LO:778:ALA:HB1	1.98	0.45
22:LP:355:MET:HB3	22:LP:359:ARG:NH1	2.30	0.45
24:LS:407:TYR:CD1	24:LS:419:ARG:HG2	2.51	0.45
27:LW:340:THR:HG22	27:LW:356:LEU:HD13	1.97	0.45
27:LW:439:GLN:HG3	27:LW:440:PRO:HD2	1.98	0.45
44:SA:20:LYS:HB3	44:SA:20:LYS:HE2	1.77	0.45
45:SB:289:MET:HE2	45:SB:362:LEU:HD12	1.97	0.45
59:SP:118:LEU:HB3	59:SP:121:ASP:HB2	1.98	0.45
61:LM:685:GLU:HA	61:LM:688:ILE:HG22	1.96	0.45
2:L1:115:U:O2’	2:L1:381:C:O2	2.23	0.45
2:L1:525:A:OP2	30:NB:430:ARG:NH2	2.37	0.45
2:L1:640:A:H2’	2:L1:641:A:C8	2.51	0.45
2:L1:1269:G:H2’	2:L1:1270:G:H8	1.80	0.45
3:L2:144:C:H3’	3:L2:145:U:C5’	2.47	0.45
7:L6:5:ILE:HG22	7:L6:111:LEU:HB2	1.98	0.45
21:LO:551:PHE:CE1	21:LO:558:LEU:HD12	2.52	0.45
23:LQ:173:VAL:HB	23:LQ:187:MET:HB2	1.98	0.45
28:LZ:14:LYS:O	28:LZ:15:GLN:HG2	2.15	0.45
45:SB:144:HIS:CE1	45:SB:148:ARG:HG3	2.50	0.45
49:SI:744:ASP:OD1	49:SI:745:TRP:N	2.48	0.45
59:SP:70:GLU:O	59:SP:74:LYS:NZ	2.47	0.45
61:LM:661:ASN:O	61:LM:665:ILE:HG12	2.16	0.45
20:LN:508:VAL:HG21	20:LN:543:ILE:HD13	1.98	0.45
36:NM:28:LYS:HA	36:NM:50:THR:HA	1.98	0.45
49:SI:182:VAL:HG22	49:SI:217:PHE:HB3	1.98	0.45
2:L1:454:U:H2’	2:L1:455:A:C8	2.48	0.45
2:L1:641:A:OP1	10:L9:40:LYS:NZ	2.43	0.45
2:L1:975:G:O2’	34:NG:49:GLY:O	2.29	0.45
2:L1:1004:U:H2’	2:L1:1005:G:C8	2.49	0.45
2:L1:1373:C:H2’	2:L1:1374:C:C6	2.51	0.45
3:L2:19:A:H2’	3:L2:20:U:C6	2.51	0.45

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
7:L6:7:PHE:O	7:L6:11:GLY:N	2.47	0.45
7:L6:136:LYS:NZ	7:L6:175:LYS:O	2.38	0.45
18:LJ:478:ARG:NH1	18:LJ:479:GLU:OE2	2.49	0.45
19:LL:194:VAL:HG23	19:LL:201:TYR:HB2	1.98	0.45
27:LW:119:ARG:HE	27:LW:121:LEU:HB3	1.82	0.45
43:NW:117:ARG:NE	43:NW:133:ILE:O	2.45	0.45
45:SB:240:ILE:O	45:SB:240:ILE:HG13	2.17	0.45
51:SL:113:LEU:HB3	51:SL:117:TYR:CD1	2.51	0.45
2:L1:614:C:O3'	57:SY:38:LYS:NZ	2.37	0.45
2:L1:1842:C:H2'	2:L1:1843:G:H8	1.82	0.45
5:L4:71:LYS:HG2	5:L4:76:VAL:HG12	1.97	0.45
6:L5:63:LYS:HD2	6:L5:71:ARG:HH12	1.81	0.45
16:LH:630:GLN:HG3	16:LH:631:TRP:CD1	2.52	0.45
18:LJ:116:ARG:NH1	18:LJ:151:ILE:O	2.50	0.45
18:LJ:377:LEU:HA	18:LJ:380:VAL:HG22	1.99	0.45
22:LP:166:LEU:HD22	55:SS:185:GLU:HG2	1.98	0.45
23:LQ:631:ALA:HA	23:LQ:660:TRP:CZ2	2.52	0.45
28:LZ:58:LEU:HD21	29:NA:500:MET:HG2	1.98	0.45
35:NJ:266:LYS:HE2	35:NJ:461:TYR:HB3	1.99	0.45
38:NO:47:ILE:HG13	38:NO:48:GLY:H	1.82	0.45
45:SB:157:LYS:HA	45:SB:157:LYS:HD2	1.83	0.45
45:SB:191:PHE:CD2	45:SB:194:LEU:HB2	2.51	0.45
48:SH:67:ASN:HB2	48:SH:72:THR:HG22	1.98	0.45
61:LM:1581:LEU:HA	61:LM:1584:ALA:HB3	1.99	0.45
1:L0:829:G:O2'	21:LO:76:GLY:O	2.29	0.45
2:L1:996:A:H2'	2:L1:997:A:C8	2.51	0.45
2:L1:1269:G:H2'	2:L1:1270:G:C8	2.51	0.45
18:LJ:36:LYS:HD3	18:LJ:312:ILE:HG22	1.98	0.45
18:LJ:387:ILE:HD12	31:ND:251:ARG:HD3	1.98	0.45
23:LQ:84:TYR:H	23:LQ:110:ILE:HD12	1.81	0.45
25:LT:918:ILE:O	25:LT:922:SER:N	2.37	0.45
27:LW:485:GLY:HA2	27:LW:489:ASN:OD1	2.16	0.45
36:NM:173:THR:O	36:NM:177:GLN:HG2	2.16	0.45
43:NW:249:THR:HA	43:NW:274:PRO:HB3	1.99	0.45
45:SB:92:ALA:O	45:SB:96:GLY:N	2.49	0.45
45:SB:362:LEU:O	45:SB:366:THR:OG1	2.22	0.45
48:SH:220:ILE:HG22	48:SH:222:ASP:N	2.26	0.45
53:SQ:608:VAL:CG2	61:LM:146:ARG:HH12	2.30	0.45
55:SS:199:VAL:HG12	55:SS:200:THR:HG23	1.98	0.45
63:SG:143:ARG:HH12	63:SG:456[A]:ARG:HD2	1.81	0.45
2:L1:394:G:O2'	13:LD:82:MET:SD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:498:C:H2'	2:L1:499:G:C8	2.52	0.45
2:L1:1336:C:H2'	2:L1:1337:C:H6	1.82	0.45
6:L5:71:ARG:NH2	6:L5:148:ASN:OD1	2.49	0.45
7:L6:116:LYS:HB3	59:SP:703:ARG:HH22	1.80	0.45
18:LJ:78:ARG:HD2	18:LJ:112:ARG:NH1	2.31	0.45
20:LN:669:ASP:HA	20:LN:672:ILE:HD12	1.99	0.45
21:LO:674:GLN:HA	21:LO:699:PHE:CZ	2.51	0.45
24:LS:170:GLU:HB3	24:LS:173:LEU:HD11	1.99	0.45
25:LT:349:VAL:HG22	25:LT:359:ILE:HD12	1.99	0.45
27:LW:121:LEU:HD13	55:SS:694:GLN:HG2	1.99	0.45
33:NF:114:ARG:HA	33:NF:114:ARG:HD3	1.81	0.45
35:NJ:730:PRO:HA	35:NJ:748:MET:HG2	1.99	0.45
48:SH:210:ASP:N	48:SH:210:ASP:OD1	2.48	0.45
53:SQ:562:SER:OG	53:SQ:563:SER:N	2.49	0.45
61:LM:55:LEU:HD23	61:LM:58:ILE:HD12	1.99	0.45
68:NY:277:GLN:HA	68:NY:280:LYS:HZ3	1.82	0.45
1:L0:751:C:H2'	1:L0:752:C:C6	2.51	0.45
2:L1:1091:C:H2'	2:L1:1092:G:H8	1.81	0.45
16:LH:417:LEU:HD21	16:LH:445:ILE:HD11	1.99	0.45
25:LT:248:VAL:HG11	25:LT:268:SER:H	1.82	0.45
25:LT:856:GLU:OE2	25:LT:860:ARG:NE	2.29	0.45
25:LT:908:LEU:HD11	25:LT:918:ILE:HD11	1.98	0.45
27:LW:203:TYR:CE1	27:LW:210:LEU:HD12	2.52	0.45
35:NJ:574:LEU:HD13	35:NJ:640:TYR:CZ	2.52	0.45
45:SB:8:SER:HB3	45:SB:142:LEU:HD12	1.97	0.45
46:SC:107:VAL:HG12	46:SC:136:ALA:HA	1.99	0.45
46:SC:168:ALA:H	46:SC:191:GLU:HB2	1.82	0.45
46:SD:97:PHE:HB2	46:SD:107:VAL:HG23	1.99	0.45
59:SP:180:HIS:O	59:SP:186:ARG:HD2	2.17	0.45
61:LM:371:ASP:O	61:LM:374:ILE:HG22	2.16	0.45
61:LM:740:LEU:O	61:LM:744:ILE:HG12	2.17	0.45
2:L1:437:G:H2'	2:L1:438:G:C8	2.52	0.45
2:L1:1457:U:H2'	2:L1:1458:G:C8	2.52	0.45
10:L9:131:ARG:HA	10:L9:131:ARG:HD2	1.79	0.45
11:LA:47:ALA:HA	11:LA:112:LYS:HA	1.98	0.45
18:LJ:30:LYS:NZ	18:LJ:318:ARG:O	2.37	0.45
19:LL:573:ILE:O	19:LL:577:THR:HG23	2.16	0.45
23:LQ:115:TYR:HE1	23:LQ:136:VAL:HG21	1.81	0.45
25:LT:233:ASN:HB2	25:LT:240:LEU:HD11	1.99	0.45
37:NN:536:ASN:O	37:NN:540:ARG:HG3	2.17	0.45
45:SB:180:ILE:HD13	45:SB:201:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SD:100:ARG:NH1	46:SD:104:ASP:OD2	2.50	0.45
52:SM:166:ASN:O	52:SM:251:PHE:HA	2.17	0.45
55:SS:124:GLU:HA	55:SS:127:ARG:HG2	1.99	0.45
60:LR:437:LEU:N	60:LR:449:TRP:O	2.49	0.45
63:SG:123:LEU:HD23	63:SG:125:LYS:HE2	1.99	0.45
2:L1:1714:U:H2’	2:L1:1715:A:C8	2.52	0.45
16:LH:814:LYS:HG2	16:LH:817:ARG:HH21	1.82	0.45
19:LK:474:ASP:HB2	19:LK:477:MET:HB3	1.99	0.45
19:LL:494:VAL:HG21	19:LL:530:VAL:HG23	1.98	0.45
21:LO:787:ILE:O	21:LO:791:THR:HG23	2.16	0.45
22:LP:480:TYR:HD2	22:LP:500:LEU:HD11	1.80	0.45
23:LQ:405:ARG:HH11	23:LQ:408:ARG:HD3	1.81	0.45
24:LS:491:ALA:HB1	24:LS:524:VAL:HG21	1.98	0.45
26:LU:433:VAL:HG23	26:LU:437:LYS:HZ2	1.82	0.45
28:LZ:83:LEU:HD22	28:LZ:88:LEU:HD12	1.99	0.45
32:NE:259:ILE:HG23	32:NE:260:LEU:HG	1.99	0.45
35:NJ:617:ASP:OD2	35:NJ:618:PHE:N	2.50	0.45
43:NW:75:PRO:O	43:NW:93:LEU:N	2.50	0.45
49:SI:373:VAL:HA	49:SI:376:LEU:HD12	1.99	0.45
49:SI:956:LEU:HD22	49:SI:968:LEU:HD11	1.99	0.45
61:LM:489:HIS:CE1	61:LM:491:LEU:HB3	2.52	0.45
2:L1:618:C:H2’	2:L1:619:A:O4’	2.17	0.44
9:L8:59:ARG:NH2	43:NW:332:GLU:OE1	2.50	0.44
18:LJ:44:VAL:HG11	18:LJ:305:VAL:HG11	1.99	0.44
18:LJ:102:GLY:O	18:LJ:121:HIS:HB2	2.17	0.44
24:LS:316:HIS:CD2	24:LS:343:ILE:HD13	2.52	0.44
44:SA:138:ASP:OD2	44:SA:138:ASP:N	2.50	0.44
45:SB:3:VAL:HG23	45:SB:88:ALA:HB3	1.99	0.44
45:SB:34:THR:HG23	45:SB:37:LYS:H	1.81	0.44
59:SP:740:ILE:HD11	59:SP:827:ALA:HA	1.99	0.44
60:LR:607:LYS:O	60:LR:625:SER:N	2.45	0.44
1:L0:453:U:H2’	1:L0:454:C:C6	2.53	0.44
2:L1:1470:C:H2’	2:L1:1471:C:H6	1.81	0.44
2:L1:1842:C:H2’	2:L1:1843:G:C8	2.52	0.44
7:L6:49:VAL:HB	7:L6:115:LYS:HB2	1.99	0.44
9:L8:105:ASP:OD1	9:L8:106:SER:N	2.50	0.44
16:LH:150:VAL:HG12	16:LH:151:LEU:HD23	1.98	0.44
16:LH:437:ILE:HG12	19:LL:404:LEU:HB2	1.98	0.44
20:LN:421:GLU:HG3	20:LN:422:HIS:ND1	2.32	0.44
20:LN:602:TYR:HA	20:LN:648:LYS:O	2.18	0.44
20:LN:672:ILE:HA	20:LN:675:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LO:206:LEU:HD23	21:LO:291:LEU:HD11	2.00	0.44
25:LT:661:LEU:HB2	25:LT:711:PRO:HG2	1.99	0.44
27:LW:319:ARG:NH2	27:LW:321:ASP:OD2	2.50	0.44
35:NJ:810:ARG:HD2	35:NJ:913:ALA:HB2	1.97	0.44
44:SA:197:PHE:HD2	44:SA:200:LEU:HB2	1.81	0.44
57:SY:150:ASP:HB3	57:SY:153:THR:HB	1.98	0.44
60:LR:747:LEU:HA	60:LR:750:TYR:CD2	2.53	0.44
63:SG:323:HIS:CD2	63:SG:342:ALA:HB2	2.53	0.44
3:L2:64:G:H4’	25:LT:477:LYS:O	2.17	0.44
6:L5:79:HIS:HB3	6:L5:159:ARG:HD3	1.99	0.44
19:LL:494:VAL:HG22	19:LL:534:HIS:CD2	2.53	0.44
20:LN:648:LYS:HB2	20:LN:649:PRO:HD3	1.99	0.44
22:LP:262:ASP:HB3	22:LP:266:LEU:HD13	1.98	0.44
25:LT:227:GLY:HA2	25:LT:249:GLY:HA2	1.99	0.44
31:ND:176:ARG:NH1	57:SY:143:LYS:HG2	2.32	0.44
35:NJ:730:PRO:HG3	35:NJ:748:MET:HE2	2.00	0.44
44:SA:217:ILE:HG21	44:SA:223:LEU:HD12	1.99	0.44
44:SA:284:TYR:OH	45:SB:250:ASP:OD1	2.26	0.44
45:SB:194:LEU:HD12	45:SB:194:LEU:HA	1.88	0.44
49:SI:954:ILE:HG22	49:SI:1106:ILE:HD11	1.98	0.44
51:SL:22:GLN:HA	51:SL:29:ARG:HH11	1.82	0.44
59:SP:174:TYR:CZ	59:SP:178:LEU:HD21	2.52	0.44
59:SP:461:SER:H	59:SP:651:ARG:NH2	2.14	0.44
61:LM:374:ILE:HD12	61:LM:377:ARG:HE	1.81	0.44
63:SG:296:CYS:SG	63:SG:297:CYS:N	2.91	0.44
6:L5:195:GLU:HG3	50:SK:170:GLY:HA2	2.00	0.44
16:LH:568:TRP:HA	16:LH:575:LEU:HA	1.99	0.44
20:LN:579:ARG:HH22	20:LN:600:ASP:HB2	1.82	0.44
21:LO:669:LEU:HD13	27:LW:216:ARG:HG2	1.99	0.44
21:LO:876:VAL:O	21:LO:879:GLN:HG2	2.18	0.44
24:LS:86:ALA:HA	24:LS:89:ARG:HE	1.82	0.44
25:LT:535:ASP:OD1	25:LT:536:GLN:N	2.51	0.44
26:LU:120:CYS:SG	26:LU:122:THR:HG22	2.57	0.44
35:NJ:274:LYS:HG3	49:SI:668:LYS:HG3	2.00	0.44
35:NJ:561:PRO:HG3	35:NJ:574:LEU:HD11	1.98	0.44
43:NW:110:ILE:HD12	43:NW:112:PHE:CZ	2.52	0.44
46:SD:117:VAL:HG23	46:SD:118:TYR:HD1	1.82	0.44
59:SP:461:SER:H	59:SP:651:ARG:HH21	1.65	0.44
59:SP:728:LEU:HD22	59:SP:823:LEU:HD13	1.98	0.44
2:L1:296:U:O2’	5:L4:131:VAL:O	2.35	0.44
22:LP:11:ASP:OD2	55:SS:711:ARG:NH2	2.51	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
23:LQ:770:GLU:OE1	23:LQ:804:PRO:HG3	2.18	0.44
24:LS:530:SER:OG	24:LS:534:GLY:N	2.50	0.44
35:NJ:897:ARG:HB3	35:NJ:901:LYS:NZ	2.33	0.44
45:SB:17:LEU:HD11	45:SB:43:LYS:HD3	1.98	0.44
48:SH:67:ASN:HD22	48:SH:72:THR:HG22	1.83	0.44
54:SR:50:ILE:HG13	54:SR:75:ILE:HD11	1.98	0.44
57:SY:161:LEU:HD21	57:SY:174:LEU:HD11	1.98	0.44
1:L0:604:C:N4	18:LJ:431:GLN:HB3	2.28	0.44
2:L1:67:C:H41	7:L6:163:ASN:HA	1.83	0.44
2:L1:248:C:H2'	2:L1:249:C:C6	2.52	0.44
2:L1:344:U:H2'	2:L1:345:U:C6	2.52	0.44
2:L1:434:G:H2'	2:L1:435:A:C8	2.53	0.44
2:L1:639:C:H2'	2:L1:640:A:H8	1.83	0.44
2:L1:649:U:H2'	2:L1:650:A:H8	1.82	0.44
3:L2:100:U:H2'	3:L2:101:C:H6	1.82	0.44
19:LL:470:LEU:HD11	19:LL:505:LEU:HD22	1.99	0.44
23:LQ:509:ARG:HH11	23:LQ:524:ASP:HB3	1.82	0.44
27:LW:389:ARG:HD3	27:LW:389:ARG:HA	1.70	0.44
38:NO:36:ARG:HH11	38:NO:36:ARG:HG2	1.83	0.44
63:SG:260:SER:OG	63:SG:261:HIS:N	2.50	0.44
3:L2:155:C:P	63:SG:456[A]:ARG:HH12	2.39	0.44
7:L6:115:LYS:HD3	7:L6:115:LYS:HA	1.82	0.44
17:LI:289:VAL:O	17:LI:298:GLN:N	2.51	0.44
18:LJ:383:PRO:HG2	31:ND:251:ARG:NH2	2.33	0.44
22:LP:227:LYS:HE3	22:LP:227:LYS:HB3	1.77	0.44
23:LQ:455:GLU:HG3	23:LQ:479:GLN:HE22	1.82	0.44
27:LW:421:ASP:OD1	27:LW:421:ASP:N	2.47	0.44
49:SI:924:MET:HG2	49:SI:1014:VAL:HG22	1.99	0.44
59:SP:967:HIS:HA	59:SP:1004:HIS:HD2	1.83	0.44
68:NY:54:LEU:HD12	68:NY:107:THR:HB	2.00	0.44
68:NY:145:ILE:HG12	68:NY:203:ARG:NH1	2.33	0.44
69:SZ:376:VAL:O	69:SZ:380:GLN:N	2.41	0.44
2:L1:181:A:H2'	2:L1:182:C:C6	2.52	0.44
2:L1:1824:A:H2'	2:L1:1825:A:C8	2.53	0.44
3:L2:121:U:H1'	3:L2:153:G:N2	2.32	0.44
8:L7:153:LEU:HD11	26:LU:196:PHE:HB3	2.00	0.44
16:LH:222:HIS:CE1	16:LH:228:ARG:HD2	2.53	0.44
18:LJ:43:LYS:HD3	18:LJ:85:CYS:HA	2.00	0.44
21:LO:157:ARG:HD2	21:LO:176:TRP:CZ2	2.53	0.44
22:LP:9:ILE:HG21	27:LW:152:LEU:HD11	2.00	0.44
23:LQ:489:LEU:HD12	23:LQ:537:ARG:HH11	1.83	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
49:SI:277:ASP:HB3	49:SI:892:ASN:HA	2.00	0.44
49:SI:1035:LYS:HE3	49:SI:1037:PHE:CE1	2.53	0.44
50:SK:93:LEU:HA	50:SK:126:ILE:HD11	2.00	0.44
51:SL:38:LYS:HB3	51:SL:38:LYS:HE2	1.79	0.44
61:LM:249:GLY:HA2	61:LM:257:TYR:CE2	2.53	0.44
61:LM:525:ARG:NH1	61:LM:528:ASP:OD2	2.51	0.44
63:SG:242:ASP:HB3	63:SG:261:HIS:HB2	2.00	0.44
68:NY:176:GLU:HG3	68:NY:181:CYS:O	2.17	0.44
1:L0:664:C:H2’	1:L0:665:C:O4’	2.18	0.44
1:L0:854:U:H4’	1:L0:855:G:O5’	2.17	0.44
2:L1:67:C:H41	7:L6:164:LYS:H	1.64	0.44
2:L1:1855:G:H2’	2:L1:1856:C:C6	2.52	0.44
21:LO:874:LEU:O	21:LO:878:LYS:HG2	2.18	0.44
22:LP:21:ARG:HD3	27:LW:103:PRO:HD2	1.99	0.44
22:LP:74:ARG:NH1	24:LS:83:ASP:O	2.39	0.44
35:NJ:840:ASP:N	35:NJ:840:ASP:OD1	2.50	0.44
49:SI:1131:THR:HG22	49:SI:1134:GLN:HG3	2.00	0.44
57:SY:218:LYS:O	57:SY:222:ARG:HG3	2.18	0.44
60:LR:49:ILE:O	60:LR:58:LEU:N	2.44	0.44
1:L0:754:G:H2’	1:L0:755:C:C5	2.52	0.43
1:L0:1422:C:H2’	1:L0:1423:U:C6	2.52	0.43
2:L1:511:U:H2’	2:L1:512:A:C8	2.53	0.43
2:L1:1592:C:H2’	2:L1:1593:C:C6	2.53	0.43
2:L1:1778:C:H2’	2:L1:1779:G:C8	2.53	0.43
2:L1:1844:U:O2	2:L1:1855:G:N2	2.46	0.43
10:L9:136:ARG:NH1	10:L9:158:ASP:OD2	2.51	0.43
20:LN:597:LEU:HD21	20:LN:653:MET:HE3	1.99	0.43
21:LO:91:HIS:ND1	21:LO:133:ALA:HB2	2.33	0.43
25:LT:657:ILE:HG21	25:LT:702:LEU:HD22	2.00	0.43
25:LT:676:ASP:OD1	25:LT:677:PHE:N	2.51	0.43
25:LT:891:GLU:HG2	25:LT:892:LEU:HD12	2.00	0.43
44:SA:340:LYS:HD2	44:SA:353:HIS:HB2	2.00	0.43
46:SC:246:VAL:HG21	46:SC:262:ILE:HD13	2.00	0.43
52:SM:32:LEU:HB2	52:SM:46:LEU:HD13	2.00	0.43
54:SR:105:PHE:HE2	54:SR:109:GLY:HA2	1.82	0.43
1:L0:745:U:O2’	1:L0:746:G:H5”	2.18	0.43
2:L1:12:U:H2’	2:L1:13:C:H6	1.83	0.43
2:L1:25:A:H2’	2:L1:26:U:C6	2.53	0.43
6:L5:150:ALA:O	6:L5:154:LEU:HG	2.18	0.43
8:L7:145:ARG:NE	38:NO:51:GLU:OE2	2.31	0.43
19:LL:22:SER:OG	19:LL:25:SER:O	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LO:460:GLN:HG2	29:NA:517:PRO:HG3	1.99	0.43
25:LT:851:GLY:O	25:LT:855:ILE:HG12	2.18	0.43
28:LZ:64:ASP:HB3	32:NE:185:LYS:HG2	2.00	0.43
32:NE:280:PRO:HA	32:NE:283:ILE:HD12	1.99	0.43
43:NW:302:SER:HB2	43:NW:304:LYS:NZ	2.33	0.43
49:SI:1068:ARG:NH1	52:SM:280:ASN:OD1	2.51	0.43
61:LM:1080:LYS:HG2	61:LM:1083:ASP:HB2	1.99	0.43
2:L1:166:A:H2'	2:L1:167:G:H8	1.83	0.43
2:L1:1595:U:H2'	2:L1:1596:U:H6	1.83	0.43
19:LL:252:ARG:NH2	19:LL:257:GLU:OE2	2.51	0.43
21:LO:847:PHE:O	21:LO:850:LYS:HG3	2.18	0.43
26:LU:164:HIS:CE1	26:LU:169:ALA:HA	2.54	0.43
34:NG:95:ILE:HD12	34:NG:129:ILE:HG22	1.99	0.43
35:NJ:501:LEU:HG	35:NJ:638:MET:HB3	1.99	0.43
61:LM:14:PRO:HB3	61:LM:125:LEU:HB3	2.01	0.43
1:L0:1431:C:O2'	22:LP:47:ARG:O	2.29	0.43
2:L1:1289:U:H2'	2:L1:1290:G:C8	2.53	0.43
2:L1:1780:G:H2'	2:L1:1781:A:N3	2.33	0.43
3:L2:57:A:H2'	3:L2:58:C:C6	2.54	0.43
20:LN:288:HIS:HB2	20:LN:306:ASP:HB3	2.00	0.43
20:LN:339:SER:HB2	20:LN:398:ILE:HG22	1.99	0.43
23:LQ:72:CYS:O	23:LQ:81:ALA:N	2.43	0.43
23:LQ:627:LYS:HG2	23:LQ:665:PHE:HB3	2.01	0.43
24:LS:493:GLU:O	24:LS:523:HIS:ND1	2.48	0.43
26:LU:8:ARG:NH2	27:LW:458:PHE:O	2.50	0.43
44:SA:186:SER:HB2	44:SA:207:ASN:HB3	2.01	0.43
46:SC:243:THR:HG21	46:SC:285:LYS:HD3	2.00	0.43
49:SI:337:ALA:HB1	49:SI:340:SER:HB3	2.00	0.43
56:SX:702:UNK:O	56:SX:706:UNK:N	2.52	0.43
57:SY:33:LYS:HA	57:SY:33:LYS:HD3	1.88	0.43
59:SP:795:GLY:O	59:SP:799:ALA:N	2.41	0.43
68:NY:136:LEU:HD23	68:NY:136:LEU:HA	1.86	0.43
1:L0:1429:A:H2'	1:L0:1430:G:C8	2.52	0.43
2:L1:13:C:H2'	2:L1:14:C:H6	1.83	0.43
2:L1:537:C:H2'	2:L1:538:U:C6	2.54	0.43
2:L1:615:C:H2'	2:L1:616:A:C8	2.54	0.43
2:L1:1662:U:OP2	49:SI:1072:LYS:HE3	2.17	0.43
3:L2:66:G:H5'	25:LT:433:LEU:HD11	2.00	0.43
8:L7:170:VAL:HG13	8:L7:187:PHE:HB2	2.00	0.43
10:L9:54:ARG:NH2	51:SL:96:ALA:HB2	2.32	0.43
13:LD:133:PRO:HA	13:LD:139:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:297:SER:HB2	16:LH:306:CYS:SG	2.59	0.43
16:LH:550:LEU:HB2	16:LH:593:GLU:HG3	2.01	0.43
18:LJ:442:ALA:HA	18:LJ:445:ILE:HG22	2.00	0.43
20:LN:589:HIS:ND1	20:LN:590:PRO:HD2	2.34	0.43
23:LQ:462:PHE:CZ	23:LQ:466:ASP:HA	2.53	0.43
23:LQ:507:ASP:N	23:LQ:507:ASP:OD1	2.50	0.43
25:LT:494:ASP:OD1	25:LT:495:ILE:N	2.51	0.43
43:NW:74:LYS:O	43:NW:76:ARG:HG3	2.18	0.43
43:NW:316:ASN:ND2	43:NW:332:GLU:OE2	2.51	0.43
46:SD:312:VAL:HG13	46:SD:315:PRO:HG3	2.00	0.43
61:LM:1008:TYR:CD1	61:LM:1037:MET:HE3	2.54	0.43
61:LM:1016:LYS:HG2	61:LM:1020:LYS:HE2	2.01	0.43
68:NY:208:ASP:OD2	68:NY:213:ILE:HB	2.18	0.43
1:L0:1432:G:H21	3:L2:38:A:H62	1.67	0.43
2:L1:163:U:H2'	2:L1:164:A:H8	1.82	0.43
2:L1:219:U:H1'	9:L8:184:ARG:HD2	2.01	0.43
2:L1:637:U:H2'	2:L1:638:C:C6	2.53	0.43
18:LJ:78:ARG:HH11	18:LJ:112:ARG:HH12	1.64	0.43
19:LL:367:ARG:HD3	19:LL:367:ARG:H	1.82	0.43
21:LO:487:SER:HB2	21:LO:494:LEU:HD21	2.01	0.43
33:NF:54:LEU:HB3	33:NF:60:VAL:HB	1.99	0.43
45:SB:150:ARG:HH22	46:SC:214:ILE:H	1.66	0.43
46:SC:140:PHE:CE2	57:SY:121:SER:HA	2.54	0.43
49:SI:953:THR:OG1	49:SI:954:ILE:N	2.52	0.43
50:SK:43:LEU:HD13	50:SK:237:PHE:CE2	2.53	0.43
57:SY:105:ILE:HG23	57:SY:212:LEU:HD22	2.01	0.43
61:LM:814:ASN:O	61:LM:818:LEU:HG	2.18	0.43
66:ST:432:UNK:O	66:ST:436:UNK:N	2.52	0.43
2:L1:354:U:H2'	2:L1:355:G:C8	2.54	0.43
2:L1:617:G:H2'	2:L1:618:C:C6	2.54	0.43
8:L7:9:VAL:HG12	8:L7:11:PRO:HD3	2.01	0.43
16:LH:469:TYR:CD1	16:LH:495:SER:HB3	2.54	0.43
19:LK:525:GLN:NE2	19:LK:529:CYS:SG	2.92	0.43
23:LQ:25:ASN:OD1	23:LQ:71:LEU:N	2.43	0.43
23:LQ:42:PRO:HB3	23:LQ:71:LEU:HD11	2.01	0.43
24:LS:165:MET:O	27:LW:170:LYS:HE2	2.19	0.43
29:NA:562:ASP:OD1	29:NA:563:ILE:N	2.52	0.43
35:NJ:313:SER:HB3	35:NJ:319:LEU:HD11	2.00	0.43
43:NW:348:PRO:HG2	43:NW:351:CYS:HB2	2.01	0.43
48:SH:89:CYS:SG	48:SH:117:LEU:HD22	2.59	0.43
57:SY:12:ARG:HH11	57:SY:14:ARG:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SG:161:ILE:HB	63:SG:173:TRP:HB2	2.00	0.43
63:SG:174:SER:HB2	63:SG:181:LEU:HD11	2.00	0.43
2:L1:1018:U:H2'	2:L1:1019:C:H6	1.83	0.43
3:L2:49:U:H2'	3:L2:50:U:H6	1.83	0.43
16:LH:629:VAL:HG22	16:LH:660:THR:HG22	2.00	0.43
18:LJ:466:LEU:O	18:LJ:470:VAL:HG23	2.19	0.43
26:LU:220:ASN:HD22	26:LU:234:LYS:HD3	1.82	0.43
29:NA:355:GLU:HG2	29:NA:356:VAL:H	1.84	0.43
43:NW:235:ALA:O	43:NW:247:GLY:N	2.41	0.43
43:NW:299:ASN:HD22	43:NW:304:LYS:NZ	2.13	0.43
46:SC:304:ARG:O	46:SC:306:HIS:ND1	2.45	0.43
47:SE:61:GLU:CD	47:SE:62:PRO:HD3	2.39	0.43
49:SI:173:VAL:HG21	49:SI:994:LEU:HD12	2.00	0.43
60:LR:712:GLU:HG2	60:LR:750:TYR:CD1	2.52	0.43
61:LM:573:TYR:CZ	61:LM:577:LYS:HD2	2.54	0.43
61:LM:811:ILE:HG23	61:LM:812:TRP:CD1	2.54	0.43
2:L1:22:A:H61	2:L1:652:U:H3	1.66	0.43
2:L1:976:G:H2'	2:L1:977:C:C6	2.54	0.43
3:L2:8:U:H2'	3:L2:9:A:C8	2.53	0.43
18:LJ:32:PRO:HG3	18:LJ:316:LYS:NZ	2.34	0.43
21:LO:297:HIS:HB2	21:LO:338:ILE:HD13	2.00	0.43
23:LQ:394:LEU:HD12	23:LQ:395:ASN:H	1.84	0.43
23:LQ:694:SER:OG	23:LQ:695:HIS:N	2.52	0.43
24:LS:405:GLU:HG2	24:LS:407:TYR:HE1	1.84	0.43
26:LU:276:MET:HE3	26:LU:277:VAL:H	1.84	0.43
36:NM:34:LYS:O	36:NM:98:THR:OG1	2.32	0.43
43:NW:284:LEU:HD12	43:NW:344:LEU:HD12	2.01	0.43
43:NW:313:HIS:CE1	43:NW:332:GLU:HB2	2.54	0.43
46:SD:117:VAL:HG23	46:SD:118:TYR:CD1	2.53	0.43
50:SK:174:VAL:HG13	50:SK:215:LYS:HG3	2.00	0.43
51:SL:140:TYR:CE2	51:SL:142:ASP:HB2	2.54	0.43
2:L1:1101:U:H2'	2:L1:1102:G:C8	2.54	0.43
2:L1:1372:U:H2'	2:L1:1373:C:C6	2.53	0.43
2:L1:1588:A:H2	2:L1:1654:G:H1'	1.84	0.43
2:L1:1740:C:H2'	2:L1:1741:U:H6	1.84	0.43
2:L1:1784:G:H3'	2:L1:1785:C:H5"	2.00	0.43
5:L4:63:LYS:O	5:L4:67:GLN:HG3	2.19	0.43
5:L4:151:ASP:O	5:L4:154:ILE:HG22	2.19	0.43
15:LG:10:LYS:HG3	15:LG:61:SER:HB3	2.01	0.43
16:LH:215:GLU:HG2	16:LH:216:ASP:N	2.34	0.43
18:LJ:301:ASP:HB2	18:LJ:318:ARG:HH22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LO:686:LEU:HD12	21:LO:687:PRO:HD2	2.01	0.43
22:LP:216:ILE:HD12	55:SS:197:GLN:OE1	2.19	0.43
24:LS:183:LYS:HB2	24:LS:183:LYS:HE2	1.82	0.43
40:NR:622:UNK:O	40:NR:626:UNK:N	2.52	0.43
49:SI:183:LEU:HD21	49:SI:218:TYR:CD1	2.54	0.43
50:SK:127:PRO:HB3	50:SK:132:ARG:HG3	1.99	0.43
2:L1:193:C:H2'	2:L1:194:C:C6	2.54	0.42
2:L1:1226:G:N1	2:L1:1639:G:OP2	2.52	0.42
3:L2:106:G:N2	3:L2:167:U:OP2	2.38	0.42
18:LJ:273:LYS:HB3	18:LJ:275:TYR:CE1	2.53	0.42
20:LN:554:SER:HB3	20:LN:557:ASP:HB2	2.01	0.42
21:LO:96:LYS:HB2	21:LO:115:LYS:HZ1	1.85	0.42
22:LP:275:ASP:O	22:LP:279:ARG:HG2	2.19	0.42
23:LQ:76:ASP:OD1	23:LQ:77:GLY:N	2.52	0.42
23:LQ:89:ILE:N	23:LQ:103:PHE:O	2.35	0.42
23:LQ:779:ALA:HA	23:LQ:782:LYS:NZ	2.33	0.42
24:LS:254:ILE:HG12	24:LS:543:GLY:HA2	2.01	0.42
24:LS:538:LEU:O	24:LS:546:LEU:N	2.52	0.42
31:ND:176:ARG:HB2	57:SY:146:VAL:HG21	2.01	0.42
35:NJ:246:GLN:HA	35:NJ:248:VAL:N	2.33	0.42
45:SB:318:ILE:HG22	45:SB:318:ILE:O	2.18	0.42
45:SB:404:ARG:HH21	45:SB:409:THR:HA	1.84	0.42
61:LM:1074:LEU:HD12	61:LM:1079:PRO:HG3	2.01	0.42
2:L1:615:C:H2'	2:L1:616:A:H8	1.84	0.42
6:L5:182:LYS:NZ	18:LJ:153:ASN:HA	2.33	0.42
20:LN:258:GLY:HA2	20:LN:290:VAL:HG23	2.01	0.42
25:LT:567:ASN:OD1	25:LT:574:ILE:HD11	2.19	0.42
26:LU:163:ASP:OD2	26:LU:203:LYS:HD3	2.18	0.42
33:NF:87:ASP:N	33:NF:87:ASP:OD1	2.52	0.42
40:NR:182:UNK:O	40:NR:186:UNK:N	2.51	0.42
43:NW:238:PHE:HE1	43:NW:244:MET:HG3	1.84	0.42
43:NW:244:MET:SD	43:NW:246:VAL:HG23	2.60	0.42
49:SI:114:ILE:HA	49:SI:340:SER:OG	2.18	0.42
61:LM:321:PHE:HE1	61:LM:350:MET:HG3	1.84	0.42
61:LM:826:LEU:HD23	61:LM:881:LEU:HD11	2.01	0.42
63:SG:284:ASP:OD2	63:SG:303:ARG:HB3	2.18	0.42
2:L1:191:A:N6	2:L1:208:G:O2'	2.52	0.42
9:L8:201:LYS:O	9:L8:205:ARG:HG2	2.19	0.42
10:L9:114:VAL:HG13	10:L9:126:ALA:HB1	2.00	0.42
19:LK:568:LEU:HD23	19:LK:568:LEU:HA	1.88	0.42
19:LL:502:ILE:O	19:LL:505:LEU:HB2	2.19	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
21:LO:396:LYS:HB3	21:LO:396:LYS:HE2	1.75	0.42
27:LW:510:PRO:HD2	27:LW:513:LEU:HD12	2.01	0.42
32:NE:173:LEU:O	32:NE:177:ARG:HG2	2.20	0.42
34:NG:95:ILE:HD11	34:NG:126:ILE:HD12	2.01	0.42
35:NJ:39:ILE:HD13	49:SI:354:VAL:HG21	2.01	0.42
45:SB:194:LEU:HA	45:SB:197:ILE:HG22	2.00	0.42
49:SI:668:LYS:H	49:SI:668:LYS:HG2	1.70	0.42
55:SS:711:ARG:HD3	55:SS:711:ARG:HA	1.85	0.42
68:NY:72:LEU:HA	68:NY:75:CYS:SG	2.59	0.42
73:SJ:301:SAH:HG2	73:SJ:301:SAH:H3’	2.01	0.42
2:L1:71:G:H2’	2:L1:72:C:O4’	2.19	0.42
2:L1:1726:G:N2	2:L1:1808:U:O2	2.41	0.42
5:L4:11:ARG:HA	5:L4:28:ALA:HB2	2.00	0.42
10:L9:58:ARG:O	10:L9:62:THR:HG23	2.19	0.42
15:LG:29:GLN:HE21	15:LG:29:GLN:HB2	1.68	0.42
16:LH:53:LEU:HD23	16:LH:85:TRP:HE3	1.82	0.42
20:LN:165:ILE:H	20:LN:165:ILE:HD12	1.85	0.42
22:LP:98:ARG:O	22:LP:102:LYS:HG2	2.19	0.42
23:LQ:839:PHE:O	23:LQ:843:ILE:HG12	2.19	0.42
25:LT:844:LEU:HD23	25:LT:848:LYS:HD2	2.01	0.42
29:NA:593:GLU:OE2	29:NA:597:LYS:HE3	2.20	0.42
34:NG:45:THR:HG22	34:NG:52:THR:HA	2.01	0.42
36:NM:82:ARG:HD3	36:NM:82:ARG:HA	1.88	0.42
43:NW:271:TYR:CE1	43:NW:293:ARG:HG2	2.54	0.42
50:SK:67:ASP:HB3	50:SK:68:LYS:HZ2	1.83	0.42
59:SP:300:LEU:O	59:SP:304:HIS:N	2.46	0.42
2:L1:57:U:OP2	59:SP:5:PRO:HG3	2.19	0.42
2:L1:134:C:H2’	2:L1:135:U:C6	2.54	0.42
2:L1:1654:G:C2	2:L1:1671:G:C2	3.08	0.42
7:L6:128:THR:HG21	59:SP:694:GLU:HG3	2.02	0.42
12:LC:98:LYS:HE2	12:LC:98:LYS:HB2	1.84	0.42
16:LH:240:THR:HG21	20:LN:264:GLN:HE22	1.84	0.42
16:LH:409:GLN:OE1	16:LH:415:LEU:HD13	2.20	0.42
19:LK:490:ILE:O	19:LK:494:VAL:HG23	2.20	0.42
20:LN:103:PRO:HG2	20:LN:121:GLU:HB2	2.00	0.42
27:LW:361:GLY:H	27:LW:379:LEU:HD12	1.83	0.42
35:NJ:203:GLN:O	35:NJ:205:ASN:N	2.51	0.42
44:SA:13:GLY:HA3	44:SA:53:PRO:HA	2.01	0.42
61:LM:857:LEU:HD13	61:LM:863:LEU:HA	2.01	0.42
10:L9:22:LYS:HB3	10:L9:22:LYS:HE3	1.76	0.42
16:LH:585:VAL:HB	16:LH:598:ILE:HB	2.01	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
18:LJ:252:THR:H	18:LJ:267:SER:HA	1.84	0.42
18:LJ:268:LEU:O	18:LJ:291:SER:OG	2.33	0.42
22:LP:39:ASP:O	22:LP:43:LYS:HG2	2.18	0.42
22:LP:480:TYR:CD2	22:LP:500:LEU:HD11	2.55	0.42
26:LU:71:CYS:HB3	26:LU:115:ILE:HG12	2.02	0.42
26:LU:333:TRP:HE1	26:LU:337:SER:HA	1.83	0.42
28:LZ:49:ASN:HA	28:LZ:103:ALA:HB2	2.00	0.42
35:NJ:632:HIS:HB3	35:NJ:635:TYR:HD1	1.84	0.42
36:NM:90:ASP:OD2	36:NM:92:GLN:NE2	2.52	0.42
38:NO:32:LYS:O	38:NO:36:ARG:HG3	2.20	0.42
50:SK:127:PRO:HG2	50:SK:133:PHE:HA	2.02	0.42
50:SK:229:THR:O	50:SK:233:LEU:HD23	2.20	0.42
59:SP:74:LYS:HD2	59:SP:84:HIS:HB3	2.02	0.42
59:SP:137:LEU:HD22	59:SP:177:LEU:HD11	2.00	0.42
59:SP:790:GLU:O	59:SP:791:GLN:NE2	2.52	0.42
63:SG:154:VAL:HG12	63:SG:161:ILE:HG12	2.02	0.42
2:L1:168:C:OP1	7:L6:131:ARG:NH2	2.53	0.42
2:L1:501:C:H2’	2:L1:502:C:H5”	2.02	0.42
2:L1:1592:C:H5”	6:L5:91:ARG:HH12	1.84	0.42
18:LJ:95:LEU:HD23	18:LJ:109:ILE:HG22	2.01	0.42
18:LJ:240:LEU:HD21	18:LJ:243:SER:HB2	2.01	0.42
20:LN:84:MET:HG2	20:LN:96:ALA:HB2	2.01	0.42
21:LO:100:HIS:ND1	21:LO:148:THR:O	2.53	0.42
23:LQ:634:ASP:OD1	23:LQ:635:SER:N	2.45	0.42
23:LQ:771:THR:HA	23:LQ:774:MET:HG3	2.02	0.42
24:LS:144:ASP:OD1	25:LT:233:ASN:ND2	2.52	0.42
24:LS:530:SER:HG	24:LS:534:GLY:H	1.68	0.42
32:NE:176:HIS:O	32:NE:180:ILE:HG12	2.20	0.42
36:NM:57:ILE:HG22	36:NM:59:SER:H	1.85	0.42
43:NW:48:ASP:O	43:NW:78:ARG:NH2	2.53	0.42
46:SC:240:PRO:HA	46:SC:269:ILE:HD13	2.02	0.42
49:SI:935:ILE:HD12	49:SI:971:TYR:HB3	2.01	0.42
60:LR:747:LEU:HA	60:LR:750:TYR:HD2	1.84	0.42
61:LM:88:LYS:HE3	61:LM:88:LYS:HB3	1.90	0.42
66:ST:254:UNK:O	66:ST:258:UNK:N	2.52	0.42
2:L1:103:A:H4’	2:L1:104:A:H8	1.85	0.42
2:L1:558:G:H2’	2:L1:559:G:C8	2.54	0.42
2:L1:962:A:H2’	2:L1:963:A:O4’	2.20	0.42
2:L1:1376:A:O2’	2:L1:1378:A:H3’	2.20	0.42
2:L1:1536:G:H2’	2:L1:1537:A:C8	2.49	0.42
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:31:ILE:HG22	16:LH:42:TYR:HB2	2.01	0.42
19:LK:527:LEU:O	19:LK:530:VAL:HG12	2.19	0.42
27:LW:243:ARG:HD3	27:LW:243:ARG:HA	1.81	0.42
35:NJ:32:ARG:NH2	35:NJ:202:ASP:OD2	2.53	0.42
35:NJ:890:GLN:O	35:NJ:894:LEU:N	2.45	0.42
36:NM:11:LYS:HE3	36:NM:13:GLY:H	1.84	0.42
50:SK:99:PRO:HB2	50:SK:238:GLU:HG2	2.02	0.42
63:SG:170:ILE:HB	63:SG:184:ILE:HB	2.01	0.42
66:ST:209:UNK:O	66:ST:213:UNK:N	2.53	0.42
2:L1:980:A:H2’	2:L1:981:A:C8	2.55	0.42
2:L1:1010:G:H2’	2:L1:1011:A:C8	2.53	0.42
2:L1:1231:C:O3’	49:SI:1076:ARG:NH1	2.53	0.42
18:LJ:32:PRO:HG3	18:LJ:316:LYS:HZ3	1.85	0.42
23:LQ:544:ARG:HD2	23:LQ:544:ARG:HA	1.77	0.42
23:LQ:934:LYS:HD2	23:LQ:934:LYS:HA	1.83	0.42
27:LW:374:MET:HE3	27:LW:388:LEU:HD21	2.02	0.42
29:NA:418:THR:HG22	29:NA:421:THR:HG23	2.02	0.42
45:SB:351:SER:O	45:SB:355:LYS:HG3	2.20	0.42
53:SQ:608:VAL:HG21	61:LM:146:ARG:HH12	1.84	0.42
59:SP:843:SER:OG	59:SP:844:PRO:HD3	2.20	0.42
61:LM:234:VAL:HB	61:LM:272:VAL:HG11	2.02	0.42
61:LM:1074:LEU:O	61:LM:1079:PRO:HD3	2.20	0.42
61:LM:1573:THR:O	61:LM:1577:TRP:N	2.42	0.42
63:SG:257:TYR:CD2	63:SG:297:CYS:HB3	2.55	0.42
2:L1:388:U:H2’	2:L1:389:A:H8	1.84	0.42
2:L1:488:U:H2’	2:L1:489:A:H8	1.84	0.42
2:L1:523:A:OP1	10:L9:127:ARG:NE	2.51	0.42
2:L1:651:U:O2’	2:L1:652:U:H5’	2.19	0.42
2:L1:1102:G:H2’	2:L1:1103:C:C6	2.55	0.42
2:L1:1276:A:O2’	69:SZ:316:SER:N	2.53	0.42
7:L6:226:GLU:HG2	7:L6:230:LYS:HE2	2.02	0.42
9:L8:162:LEU:HD21	9:L8:191:GLU:HG2	2.01	0.42
16:LH:725:GLU:OE1	16:LH:725:GLU:N	2.45	0.42
19:LL:406:PRO:HA	19:LL:411:HIS:CG	2.55	0.42
23:LQ:292:ARG:HB2	23:LQ:308:ILE:HG12	2.02	0.42
23:LQ:641:PHE:HA	23:LQ:648:PHE:HA	2.01	0.42
24:LS:170:GLU:HA	24:LS:173:LEU:HD21	2.02	0.42
25:LT:312:GLY:HA2	25:LT:336:ILE:HG12	2.02	0.42
35:NJ:325:PHE:HA	35:NJ:328:LYS:HB2	2.02	0.42
35:NJ:333:LEU:HD23	35:NJ:333:LEU:HA	1.88	0.42
45:SB:411:LYS:HA	61:LM:184:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SI:986:ILE:HG23	49:SI:1017:LEU:HD13	2.02	0.42
52:SM:44:THR:HA	52:SM:47:ARG:HB2	2.02	0.42
59:SP:196:LEU:HD12	59:SP:196:LEU:HA	1.94	0.42
6:L5:87:LEU:O	6:L5:91:ARG:HG3	2.19	0.41
7:L6:67:VAL:HG13	7:L6:99:GLY:HA2	2.02	0.41
7:L6:98:ARG:HH22	7:L6:103:ASP:HB2	1.84	0.41
13:LD:13:GLN:NE2	13:LD:36:TYR:HB3	2.35	0.41
18:LJ:144:TYR:HB2	18:LJ:161:LYS:HE2	2.01	0.41
20:LN:565:ARG:HG2	61:LM:964:GLU:HG2	2.01	0.41
21:LO:31:SER:HB3	21:LO:40:PHE:HE1	1.84	0.41
21:LO:305:THR:O	21:LO:312:PHE:HA	2.20	0.41
21:LO:709:ARG:HD3	21:LO:709:ARG:HA	1.89	0.41
23:LQ:867:ILE:HD11	23:LQ:877:ILE:HD11	2.01	0.41
27:LW:246:HIS:CG	27:LW:247:SER:H	2.37	0.41
32:NE:170:LYS:HE3	32:NE:170:LYS:HB3	1.80	0.41
33:NF:9:LYS:HG3	33:NF:9:LYS:O	2.20	0.41
33:NF:25:TRP:HZ3	39:NQ:83:GLN:HB2	1.84	0.41
35:NJ:69:ARG:O	35:NJ:73:MET:HG2	2.20	0.41
44:SA:392:VAL:HG12	44:SA:396:LYS:HE3	2.02	0.41
45:SB:59:ALA:HA	45:SB:69:ASN:OD1	2.19	0.41
51:SL:69:ILE:O	51:SL:101:CYS:N	2.46	0.41
53:SQ:600:LYS:HG3	61:LM:47:ILE:HG12	2.02	0.41
60:LR:678:ARG:HB3	60:LR:681:THR:HB	2.02	0.41
61:LM:478:ASP:OD2	61:LM:478:ASP:N	2.50	0.41
1:L0:462:C:H2’	1:L0:463:C:C6	2.55	0.41
2:L1:1637:A:H4’	2:L1:1638:G:H5’	2.02	0.41
9:L8:80:ASP:OD2	9:L8:81:VAL:N	2.52	0.41
18:LJ:43:LYS:HA	18:LJ:294:SER:HB3	2.02	0.41
19:LL:466:LEU:HD23	19:LL:497:MET:SD	2.59	0.41
19:LL:509:LEU:O	19:LL:513:LEU:HG	2.20	0.41
23:LQ:207:ILE:HG23	23:LQ:215:LEU:HD21	2.02	0.41
25:LT:534:LYS:HE3	25:LT:534:LYS:HB3	1.91	0.41
27:LW:241:ASP:OD1	27:LW:242:ILE:N	2.53	0.41
45:SB:88:ALA:HB1	45:SB:112:VAL:HG13	2.02	0.41
51:SL:72:ASP:OD1	51:SL:73:THR:N	2.52	0.41
52:SM:120:GLU:HG3	52:SM:123:ALA:H	1.84	0.41
68:NY:68:ARG:CZ	68:NY:126:SER:HA	2.49	0.41
3:L2:132:G:H1	3:L2:142:A:H1’	1.84	0.41
5:L4:19:MET:HB2	5:L4:51:ARG:NH2	2.36	0.41
5:L4:71:LYS:HB2	5:L4:91:SER:OG	2.20	0.41
16:LH:716:ASN:HB3	16:LH:717:GLU:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LN:573:HIS:CD2	20:LN:616:ASP:HA	2.55	0.41
26:LU:37:VAL:HB	26:LU:38:PRO:HD3	2.02	0.41
26:LU:359:LYS:HD2	26:LU:363:LEU:HD21	2.02	0.41
26:LU:362:VAL:HG11	44:SA:41:LYS:HB3	2.02	0.41
29:NA:440:ASP:OD1	52:SM:186:LEU:N	2.43	0.41
30:NB:454:VAL:HG22	46:SD:300:GLU:O	2.20	0.41
2:L1:382:C:H2’	2:L1:383:G:H8	1.84	0.41
2:L1:643:A:H4’	2:L1:644:G:H5’	2.01	0.41
2:L1:1311:C:H2’	2:L1:1312:G:C8	2.56	0.41
7:L6:52:ILE:HG23	7:L6:109:LEU:HD11	2.02	0.41
7:L6:135:PRO:HG2	7:L6:141:ILE:HG12	2.03	0.41
9:L8:43:ILE:HD11	9:L8:55:TYR:HB3	2.02	0.41
10:L9:139:LYS:HA	10:L9:139:LYS:HD2	1.86	0.41
19:LL:43:THR:HG23	19:LL:359:ILE:HG21	2.01	0.41
19:LL:148:LYS:HD3	19:LL:168:ASN:O	2.21	0.41
20:LN:185:ASP:OD1	20:LN:185:ASP:N	2.52	0.41
21:LO:201:LEU:HB2	21:LO:217:CYS:SG	2.60	0.41
24:LS:482:ASN:ND2	24:LS:483:PRO:HD2	2.34	0.41
26:LU:156:LYS:H	26:LU:156:LYS:HG2	1.70	0.41
43:NW:9:VAL:HG21	43:NW:307:THR:HB	2.02	0.41
43:NW:45:LEU:HD11	43:NW:354:LEU:HD21	2.02	0.41
45:SB:191:PHE:HE2	45:SB:194:LEU:HD13	1.84	0.41
47:SE:14:ALA:HB1	47:SE:18:LEU:HB3	2.02	0.41
49:SI:727:HIS:HB3	49:SI:728:LYS:H	1.67	0.41
49:SI:923:GLN:HB2	49:SI:1016:ASP:HB2	2.02	0.41
58:NH:221:GLY:N	58:NH:240:ARG:O	2.54	0.41
60:LR:536:LEU:N	60:LR:548:TRP:O	2.45	0.41
61:LM:316:LEU:HD11	61:LM:320:PRO:HG2	2.02	0.41
61:LM:1082:LEU:O	61:LM:1086:ILE:HG12	2.21	0.41
2:L1:110:U:H2’	2:L1:111:A:C8	2.56	0.41
2:L1:161:U:H5”	2:L1:162:C:OP2	2.20	0.41
2:L1:674:C:H2’	2:L1:675:U:H6	1.85	0.41
2:L1:1030:A:H2’	2:L1:1031:A:H8	1.85	0.41
2:L1:1383:A:H2’	2:L1:1384:C:C6	2.55	0.41
3:L2:145:U:O2’	3:L2:146:G:OP2	2.31	0.41
7:L6:57:ASP:HA	7:L6:106:LEU:HA	2.02	0.41
18:LJ:64:ILE:O	18:LJ:73:ILE:HG22	2.21	0.41
21:LO:114:THR:HB	21:LO:147:THR:OG1	2.20	0.41
27:LW:489:ASN:HB2	27:LW:492:ARG:HB3	2.01	0.41
35:NJ:260:GLN:NE2	35:NJ:289:GLY:HA3	2.36	0.41
43:NW:82:THR:HB	43:NW:350:TRP:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SD:256:ASN:OD1	46:SD:314:ARG:HD2	2.20	0.41
46:SD:266:ALA:HB3	46:SD:305:ASP:HB3	2.02	0.41
47:SF:84:ARG:HH11	47:SF:84:ARG:HG3	1.85	0.41
61:LM:374:ILE:HD12	61:LM:374:ILE:HA	1.95	0.41
61:LM:597:ASN:O	61:LM:601:VAL:HG23	2.20	0.41
66:ST:443:UNK:O	66:ST:447:UNK:N	2.54	0.41
2:L1:285:U:H2’	2:L1:286:U:C6	2.55	0.41
2:L1:1139:C:H2’	2:L1:1140:G:H8	1.84	0.41
2:L1:1677:U:C2	2:L1:1678:A:C8	3.08	0.41
18:LJ:80:LYS:HZ1	18:LJ:101:ASP:N	2.17	0.41
19:LL:151:VAL:HG22	19:LL:163:LYS:HG3	2.02	0.41
19:LL:152:GLU:HG2	19:LL:162:CYS:HB3	2.02	0.41
21:LO:681:GLY:O	21:LO:683:ALA:N	2.49	0.41
21:LO:798:TYR:O	21:LO:802:VAL:HG23	2.21	0.41
22:LP:368:SER:OG	22:LP:369:GLU:N	2.53	0.41
25:LT:384:ASN:ND2	25:LT:386:ARG:HH21	2.19	0.41
55:SS:169:ALA:HA	55:SS:170:PRO:HD3	1.86	0.41
59:SP:737:ASP:O	59:SP:740:ILE:HG22	2.21	0.41
68:NY:205:VAL:O	68:NY:209:THR:HG23	2.20	0.41
3:L2:94:G:H2’	3:L2:95:C:C6	2.56	0.41
5:L4:40:GLU:HG2	5:L4:40:GLU:O	2.20	0.41
6:L5:42:LYS:HD3	6:L5:42:LYS:HA	1.84	0.41
7:L6:133:LEU:HD23	7:L6:133:LEU:HA	1.79	0.41
18:LJ:346:LYS:HG2	18:LJ:347:GLN:O	2.20	0.41
19:LL:149:HIS:HA	19:LL:164:TRP:O	2.21	0.41
20:LN:8:ARG:HH21	20:LN:10:ARG:HH21	1.69	0.41
20:LN:656:LEU:HD23	20:LN:656:LEU:HA	1.92	0.41
21:LO:552:ARG:HD3	21:LO:557:GLU:HB3	2.02	0.41
21:LO:774:LEU:HD12	21:LO:774:LEU:HA	1.94	0.41
25:LT:748:ASN:OD1	25:LT:749:GLU:N	2.54	0.41
27:LW:196:PHE:HB2	27:LW:199:TYR:OH	2.21	0.41
27:LW:249:ALA:O	27:LW:264:ASN:N	2.54	0.41
35:NJ:129:LEU:HD23	35:NJ:129:LEU:HA	1.92	0.41
43:NW:234:SER:N	43:NW:247:GLY:O	2.51	0.41
61:LM:331:ILE:HG21	61:LM:381:ALA:HB1	2.02	0.41
61:LM:610:ASN:HD21	61:LM:698:LEU:HG	1.86	0.41
68:NY:73:LYS:HB2	68:NY:73:LYS:HE2	1.83	0.41
10:L9:180:LYS:HB2	10:L9:180:LYS:HE3	1.80	0.41
15:LG:20:ARG:HD3	15:LG:26:GLN:HE21	1.86	0.41
19:LL:120:LEU:HD13	19:LL:153:TRP:CD2	2.56	0.41
22:LP:400:ARG:HH11	22:LP:431:HIS:CD2	2.38	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
23:LQ:632:HIS:NE2	23:LQ:650:THR:HG23	2.35	0.41
24:LS:215:ASP:N	24:LS:215:ASP:OD1	2.54	0.41
25:LT:585:ILE:HD11	25:LT:628:MET:HG3	2.03	0.41
28:LZ:115:LEU:HD21	28:LZ:136:VAL:HG11	2.02	0.41
35:NJ:808:LEU:HD11	35:NJ:848:ILE:HG21	2.02	0.41
61:LM:806:PHE:HD1	61:LM:822:SER:HB2	1.86	0.41
61:LM:1059:VAL:O	61:LM:1063:THR:HG23	2.21	0.41
2:L1:34:U:H2’	2:L1:35:C:H6	1.86	0.41
2:L1:466:G:H3’	2:L1:466:G:N3	2.36	0.41
2:L1:478:G:H2’	2:L1:479:C:H6	1.86	0.41
2:L1:485:A:N7	49:SI:215:LYS:NZ	2.49	0.41
2:L1:536:A:H3’	2:L1:537:C:H6	1.85	0.41
2:L1:941:C:H2’	2:L1:942:G:C8	2.56	0.41
2:L1:945:U:H2’	2:L1:946:U:C6	2.56	0.41
2:L1:1171:G:N2	3:L2:11:U:C2	2.89	0.41
2:L1:1387:G:C2	2:L1:1388:A:H1’	2.56	0.41
3:L2:83:G:N1	47:SE:41:GLU:OE2	2.39	0.41
3:L2:122:U:H2’	3:L2:123:U:C6	2.56	0.41
7:L6:7:PHE:CE2	7:L6:9:ALA:HB3	2.56	0.41
8:L7:30:LEU:O	8:L7:34:SER:HB3	2.21	0.41
16:LH:388:ILE:H	16:LH:388:ILE:HD12	1.86	0.41
18:LJ:446:ILE:HG23	19:LL:575:LEU:HD12	2.03	0.41
19:LK:481:VAL:O	19:LK:484:THR:HG23	2.21	0.41
20:LN:585:HIS:HB3	20:LN:599:HIS:CD2	2.55	0.41
22:LP:301:GLU:HA	22:LP:304:ARG:NH1	2.36	0.41
23:LQ:610:SER:OG	23:LQ:611:ALA:N	2.53	0.41
23:LQ:716:GLU:HA	23:LQ:719:ARG:HD2	2.03	0.41
25:LT:161:HIS:ND1	25:LT:179:ASP:OD1	2.54	0.41
27:LW:141:GLU:OE2	27:LW:145:LYS:HE2	2.21	0.41
27:LW:201:LEU:HD23	27:LW:201:LEU:H	1.86	0.41
35:NJ:508:TYR:HE2	35:NJ:560:LEU:HB2	1.84	0.41
45:SB:150:ARG:NH1	46:SC:214:ILE:O	2.54	0.41
47:SF:52:GLU:OE2	47:SF:104:VAL:HG12	2.20	0.41
48:SH:13:CYS:SG	49:SI:730:ASP:HA	2.61	0.41
49:SI:271:ARG:HH11	49:SI:271:ARG:HB2	1.86	0.41
55:SS:664:LEU:HB3	55:SS:667:VAL:HB	2.02	0.41
57:SY:233:LYS:HG2	57:SY:245:TYR:CE1	2.56	0.41
60:LR:689:ILE:HG23	60:LR:695:ALA:HB1	2.03	0.41
61:LM:614:THR:HA	61:LM:619:MET:HG3	2.01	0.41
61:LM:846:ARG:HA	61:LM:849:MET:SD	2.61	0.41
68:NY:239:TRP:HA	68:NY:242:PHE:HD2	1.86	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:L1:110:U:H2’	2:L1:111:A:H8	1.85	0.41
2:L1:337:C:H2’	2:L1:338:G:C8	2.55	0.41
2:L1:1328:G:H22	2:L1:1502:C:H1’	1.86	0.41
2:L1:1355:C:H2’	2:L1:1356:G:O4’	2.21	0.41
2:L1:1373:C:H2’	2:L1:1374:C:H6	1.86	0.41
2:L1:1390:U:H2’	2:L1:1391:C:C6	2.56	0.41
2:L1:1653:U:H3	2:L1:1671:G:H1	1.69	0.41
5:L4:73:ASP:HA	5:L4:164:LEU:HD13	2.03	0.41
16:LH:623:GLY:HA2	16:LH:626:ARG:HH22	1.86	0.41
19:LK:490:ILE:O	19:LK:493:THR:OG1	2.30	0.41
25:LT:380:ALA:HB1	25:LT:400:GLN:HB2	2.03	0.41
34:NG:74:ALA:HB1	34:NG:115:ALA:HB2	2.03	0.41
36:NM:188:LEU:HD11	36:NM:215:VAL:HG21	2.03	0.41
43:NW:110:ILE:HD12	43:NW:112:PHE:HZ	1.86	0.41
44:SA:2:VAL:HG12	55:SS:727:HIS:CE1	2.56	0.41
48:SH:341:ILE:HG21	49:SI:689:LEU:HD23	2.03	0.41
50:SK:41:ARG:HH21	50:SK:241:TRP:HB3	1.85	0.41
59:SP:35:ASP:OD1	59:SP:35:ASP:N	2.45	0.41
61:LM:357:SER:HB3	61:LM:375:TYR:CD2	2.56	0.41
2:L1:157:U:O2’	2:L1:158:A:OP1	2.32	0.40
2:L1:219:U:H2’	2:L1:220:U:C6	2.55	0.40
2:L1:352:U:H2’	2:L1:353:C:C6	2.55	0.40
2:L1:1221:G:O2’	2:L1:1676:U:O2	2.38	0.40
2:L1:1337:C:H2’	2:L1:1338:G:H8	1.86	0.40
8:L7:129:ILE:O	8:L7:133:LEU:HB2	2.21	0.40
13:LD:111:VAL:HG12	13:LD:140:PHE:HB2	2.02	0.40
16:LH:455:LYS:HE2	16:LH:509:ASP:HA	2.03	0.40
20:LN:407:TYR:CZ	20:LN:414:PHE:HD2	2.39	0.40
21:LO:817:GLU:HA	21:LO:820:LEU:HB2	2.02	0.40
22:LP:228:ASN:O	22:LP:232:ILE:HG12	2.22	0.40
22:LP:326:TRP:O	22:LP:330:ILE:HD12	2.21	0.40
23:LQ:873:LEU:HD23	23:LQ:873:LEU:HA	1.92	0.40
24:LS:474:THR:HG21	24:LS:494:LYS:HB2	2.03	0.40
26:LU:322:THR:HG22	26:LU:324:ARG:H	1.86	0.40
35:NJ:502:PRO:HG2	35:NJ:503:GLU:HG3	2.02	0.40
35:NJ:530:MET:HA	35:NJ:533:TYR:HB3	2.02	0.40
36:NM:225:LEU:O	36:NM:229:MET:HG2	2.21	0.40
46:SC:197:GLY:HA2	46:SC:200:LEU:HD12	2.03	0.40
46:SC:313:TYR:OH	46:SC:314:ARG:NH2	2.54	0.40
48:SH:146:ASP:OD1	48:SH:146:ASP:N	2.54	0.40
55:SS:720:LYS:HE3	55:SS:720:LYS:HB3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SG:350:TRP:CH2	63:SG:357:PRO:HG3	2.56	0.40
1:L0:439:U:HO2’	16:LH:245:HIS:HD1	1.69	0.40
2:L1:157:U:HO2’	2:L1:158:A:P	2.42	0.40
2:L1:531:A:H2’	2:L1:532:C:C6	2.56	0.40
2:L1:1589:A:H2’	2:L1:1590:C:O4’	2.21	0.40
3:L2:6:U:H2’	3:L2:7:A:C8	2.55	0.40
3:L2:31:G:H5”	3:L2:32:U:C2	2.56	0.40
9:L8:87:ASN:OD1	9:L8:88:ASN:N	2.54	0.40
10:L9:17:ARG:H	10:L9:17:ARG:HG2	1.69	0.40
14:LF:51:THR:HG21	59:SP:36:ARG:CZ	2.52	0.40
16:LH:79:ASP:OD1	16:LH:81:THR:HG22	2.21	0.40
16:LH:827:ILE:HD11	61:LM:896:VAL:HG13	2.04	0.40
18:LJ:129:ASP:OD1	18:LJ:130:PHE:N	2.54	0.40
21:LO:415:SER:OG	21:LO:436:ASP:OD1	2.31	0.40
23:LQ:145:LEU:HD12	23:LQ:176:TRP:CE3	2.56	0.40
30:NB:458:GLU:CD	30:NB:459:GLN:HG2	2.42	0.40
34:NG:82:ALA:HB2	34:NG:119:LEU:HD23	2.03	0.40
35:NJ:828:TYR:CE2	35:NJ:832:MET:HE1	2.56	0.40
44:SA:185:PHE:HZ	45:SB:175:GLU:HG3	1.86	0.40
46:SC:91:HIS:CD2	46:SC:93:HIS:H	2.39	0.40
49:SI:268:GLU:HA	49:SI:271:ARG:CZ	2.51	0.40
49:SI:1000:SER:HB2	49:SI:1125:THR:HA	2.02	0.40
50:SK:44:ILE:HD13	50:SK:107:GLN:HB3	2.03	0.40
55:SS:170:PRO:O	55:SS:172:GLU:N	2.46	0.40
61:LM:681:LEU:HA	61:LM:684:VAL:HG12	2.03	0.40
61:LM:757:LEU:HB3	61:LM:791:PHE:HE1	1.85	0.40
68:NY:112:ILE:O	68:NY:116:ALA:N	2.53	0.40
69:SZ:261:ASP:O	69:SZ:265:TYR:N	2.52	0.40
2:L1:74:G:H1’	2:L1:76:U:OP1	2.22	0.40
2:L1:639:C:H2’	2:L1:640:A:C8	2.56	0.40
2:L1:1209:A:H2’	2:L1:1210:G:C8	2.56	0.40
2:L1:1280:G:H2’	2:L1:1281:G:C8	2.57	0.40
2:L1:1294:G:N1	2:L1:1306:U:O4	2.54	0.40
3:L2:137:G:C2	3:L2:139:U:H1’	2.56	0.40
7:L6:18:VAL:HG13	7:L6:23:LYS:HE3	2.03	0.40
7:L6:116:LYS:HE3	7:L6:125:THR:HG21	2.02	0.40
18:LJ:250:THR:HB	18:LJ:268:LEU:HD13	2.03	0.40
19:LL:42:GLU:HG3	19:LL:49:HIS:HB2	2.04	0.40
19:LL:235:TYR:HA	19:LL:249:TRP:O	2.20	0.40
19:LL:470:LEU:HD11	19:LL:505:LEU:CD2	2.51	0.40
19:LL:495:LEU:HD23	19:LL:534:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LN:655:LEU:HD23	20:LN:661:LEU:HG	2.03	0.40
22:LP:299:ALA:HB1	22:LP:346:LEU:HD21	2.03	0.40
23:LQ:386:ASN:O	23:LQ:388:LEU:N	2.54	0.40
23:LQ:779:ALA:HA	23:LQ:782:LYS:HZ3	1.86	0.40
25:LT:161:HIS:NE2	25:LT:185:ILE:HD12	2.36	0.40
26:LU:284:ALA:O	26:LU:302:PHE:N	2.43	0.40
29:NA:532:ALA:HA	29:NA:548:LEU:HD13	2.03	0.40
35:NJ:356:ILE:HG23	35:NJ:370:TYR:HB3	2.03	0.40
36:NM:175:GLU:OE2	36:NM:187:LYS:NZ	2.54	0.40
45:SB:112:VAL:O	45:SB:116:MET:HG2	2.22	0.40
48:SH:156:ARG:HG3	48:SH:165:GLY:HA2	2.02	0.40
48:SH:301:ALA:O	48:SH:305:MET:HG3	2.22	0.40
61:LM:754:HIS:CD2	61:LM:755:ILE:HG23	2.56	0.40
1:L0:1414:A:H5’	1:L0:1415:G:H5”	2.04	0.40
2:L1:920:A:H4’	38:NO:57:ARG:HD3	2.03	0.40
6:L5:190:ILE:HD13	6:L5:190:ILE:HA	1.94	0.40
12:LC:63:PHE:CZ	12:LC:92:LEU:HD22	2.56	0.40
16:LH:718:LEU:HD13	24:LS:505:PRO:HG3	2.03	0.40
18:LJ:476:TYR:CZ	18:LJ:480:LEU:HD21	2.56	0.40
18:LJ:476:TYR:O	18:LJ:480:LEU:HG	2.20	0.40
20:LN:356:GLU:HB3	20:LN:381:HIS:HE1	1.86	0.40
24:LS:167:ASN:OD1	24:LS:170:GLU:HG3	2.22	0.40
24:LS:472:LEU:HD23	24:LS:472:LEU:HA	1.79	0.40
24:LS:519:LYS:HB3	24:LS:519:LYS:HE2	1.73	0.40
26:LU:9:ASN:HB2	26:LU:12:ASN:ND2	2.36	0.40
33:NF:16:LEU:HD23	33:NF:16:LEU:HA	1.95	0.40
35:NJ:288:ARG:HG3	35:NJ:467:GLU:O	2.21	0.40
35:NJ:372:HIS:O	35:NJ:375:ASP:HB2	2.22	0.40
43:NW:271:TYR:CD1	43:NW:293:ARG:HG2	2.56	0.40
44:SA:171:SER:HB2	44:SA:285:LEU:HD13	2.03	0.40
52:SM:240:ARG:O	52:SM:240:ARG:HG2	2.21	0.40
61:LM:630:ILE:HG23	61:LM:637:LEU:HD23	2.03	0.40
61:LM:784:GLU:HA	61:LM:787:VAL:HG22	2.02	0.40
66:ST:212:UNK:O	66:ST:216:UNK:N	2.54	0.40
1:L0:604:C:O2’	1:L0:605:G:OP2	2.32	0.40
2:L1:19:A:O2’	2:L1:20:G:O4’	2.35	0.40
2:L1:111:A:C6	2:L1:351:G:C6	3.09	0.40
2:L1:360:A:H4’	2:L1:361:U:H5”	2.04	0.40
3:L2:12:U:H2’	3:L2:13:U:C6	2.57	0.40
16:LH:357:HIS:CD2	16:LH:373:ASP:HB2	2.56	0.40
18:LJ:486:MET:CE	19:LL:528:LYS:HG3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LO:54:THR:HG21	21:LO:74:ASP:HB3	2.02	0.40
21:LO:549:VAL:HG22	21:LO:560:VAL:HG22	2.03	0.40
23:LQ:364:LYS:HD2	23:LQ:385:GLN:NE2	2.37	0.40
23:LQ:436:ASP:HA	23:LQ:454:CYS:O	2.21	0.40
25:LT:112:GLN:H	25:LT:112:GLN:HG2	1.72	0.40
25:LT:253:LEU:HD23	25:LT:253:LEU:HA	1.96	0.40
25:LT:382:LEU:HD23	25:LT:399:SER:HB2	2.03	0.40
25:LT:401:ASP:OD1	25:LT:403:THR:HG22	2.21	0.40
25:LT:862:LEU:HD12	25:LT:862:LEU:HA	1.85	0.40
26:LU:235:VAL:HG21	26:LU:271:LEU:HB3	2.03	0.40
26:LU:377:LEU:HD23	26:LU:377:LEU:HA	1.88	0.40
36:NM:63:LYS:HE3	36:NM:90:ASP:HA	2.02	0.40
55:SS:159:PHE:HB3	55:SS:729:ILE:HG12	2.03	0.40
57:SY:218:LYS:HG2	57:SY:242:PRO:HB3	2.02	0.40
61:LM:558:LEU:O	61:LM:562:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L3	85/116 (73%)	85 (100%)	0	0	100	100
5	L4	237/263 (90%)	237 (100%)	0	0	100	100
6	L5	188/204 (92%)	183 (97%)	5 (3%)	0	100	100
7	L6	219/249 (88%)	217 (99%)	2 (1%)	0	100	100
8	L7	164/194 (84%)	162 (99%)	2 (1%)	0	100	100
9	L8	176/208 (85%)	172 (98%)	4 (2%)	0	100	100
10	L9	169/194 (87%)	168 (99%)	1 (1%)	0	100	100
11	LA	118/132 (89%)	116 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	LC	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
13	LD	145/158 (92%)	139 (96%)	6 (4%)	0	100	100
14	LF	102/133 (77%)	101 (99%)	1 (1%)	0	100	100
15	LG	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
16	LH	738/830 (89%)	721 (98%)	17 (2%)	0	100	100
17	LI	374/699 (54%)	372 (100%)	2 (0%)	0	100	100
18	LJ	465/518 (90%)	449 (97%)	16 (3%)	0	100	100
19	LK	116/677 (17%)	112 (97%)	4 (3%)	0	100	100
19	LL	500/677 (74%)	485 (97%)	15 (3%)	0	100	100
20	LN	667/686 (97%)	647 (97%)	19 (3%)	1 (0%)	51	84
21	LO	844/919 (92%)	825 (98%)	19 (2%)	0	100	100
22	LP	559/597 (94%)	552 (99%)	7 (1%)	0	100	100
23	LQ	810/943 (86%)	793 (98%)	17 (2%)	0	100	100
24	LS	447/556 (80%)	436 (98%)	11 (2%)	0	100	100
25	LT	863/951 (91%)	846 (98%)	17 (2%)	0	100	100
26	LU	443/445 (100%)	434 (98%)	9 (2%)	0	100	100
27	LW	449/610 (74%)	433 (96%)	16 (4%)	0	100	100
28	LZ	181/184 (98%)	179 (99%)	2 (1%)	0	100	100
29	NA	243/681 (36%)	242 (100%)	1 (0%)	0	100	100
30	NB	71/479 (15%)	69 (97%)	2 (3%)	0	100	100
31	ND	82/257 (32%)	81 (99%)	1 (1%)	0	100	100
32	NE	94/293 (32%)	94 (100%)	0	0	100	100
33	NF	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
34	NG	114/151 (76%)	111 (97%)	3 (3%)	0	100	100
35	NJ	809/1025 (79%)	790 (98%)	19 (2%)	0	100	100
35	NK	801/1025 (78%)	775 (97%)	26 (3%)	0	100	100
36	NM	229/264 (87%)	224 (98%)	5 (2%)	0	100	100
37	NN	40/560 (7%)	39 (98%)	1 (2%)	0	100	100
38	NO	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
39	NQ	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
41	NT	56/156 (36%)	56 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	NU	58/135 (43%)	58 (100%)	0	0	100	100
43	NW	305/688 (44%)	292 (96%)	13 (4%)	0	100	100
44	SA	390/594 (66%)	388 (100%)	2 (0%)	0	100	100
45	SB	438/529 (83%)	432 (99%)	6 (1%)	0	100	100
46	SC	225/321 (70%)	219 (97%)	6 (3%)	0	100	100
46	SD	233/321 (73%)	228 (98%)	5 (2%)	0	100	100
47	SE	123/128 (96%)	122 (99%)	1 (1%)	0	100	100
47	SF	121/128 (94%)	118 (98%)	3 (2%)	0	100	100
48	SH	366/373 (98%)	362 (99%)	4 (1%)	0	100	100
49	SI	830/1282 (65%)	811 (98%)	19 (2%)	0	100	100
50	SJ	202/244 (83%)	195 (96%)	7 (4%)	0	100	100
50	SK	202/244 (83%)	200 (99%)	2 (1%)	0	100	100
51	SL	190/198 (96%)	184 (97%)	6 (3%)	0	100	100
52	SM	288/291 (99%)	279 (97%)	9 (3%)	0	100	100
53	SQ	183/756 (24%)	180 (98%)	3 (2%)	0	100	100
54	SR	106/143 (74%)	104 (98%)	2 (2%)	0	100	100
55	SS	191/771 (25%)	186 (97%)	5 (3%)	0	100	100
57	SY	232/253 (92%)	232 (100%)	0	0	100	100
58	NH	1064/1146 (93%)	1043 (98%)	21 (2%)	0	100	100
59	SP	1967/2785 (71%)	1940 (99%)	27 (1%)	0	100	100
60	LR	769/808 (95%)	749 (97%)	20 (3%)	0	100	100
61	LM	1977/2144 (92%)	1933 (98%)	44 (2%)	0	100	100
63	SG	383/475 (81%)	376 (98%)	7 (2%)	0	100	100
64	NI	232/280 (83%)	229 (99%)	3 (1%)	0	100	100
65	SW	178/252 (71%)	175 (98%)	3 (2%)	0	100	100
66	ST	432/632 (68%)	424 (98%)	8 (2%)	0	100	100
67	SU	287/472 (61%)	285 (99%)	2 (1%)	0	100	100
68	NY	270/381 (71%)	269 (100%)	1 (0%)	0	100	100
69	SZ	244/304 (80%)	237 (97%)	7 (3%)	0	100	100
All	All	24635/33692 (73%)	24132 (98%)	502 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	LN	175	SER

5.3.2 Protein sidechains ⓘ

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	
5	L4	207/225 (92%)	207 (100%)	0	100	100
6	L5	160/170 (94%)	160 (100%)	0	100	100
7	L6	195/218 (89%)	195 (100%)	0	100	100
8	L7	149/174 (86%)	148 (99%)	1 (1%)	84	90
9	L8	155/180 (86%)	153 (99%)	2 (1%)	69	81
10	L9	152/168 (90%)	151 (99%)	1 (1%)	84	90
12	LC	114/121 (94%)	114 (100%)	0	100	100
13	LD	133/142 (94%)	132 (99%)	1 (1%)	81	89
14	LF	92/115 (80%)	92 (100%)	0	100	100
15	LG	55/62 (89%)	54 (98%)	1 (2%)	59	77
16	LH	670/748 (90%)	667 (100%)	3 (0%)	91	94
18	LJ	412/456 (90%)	412 (100%)	0	100	100
19	LK	112/594 (19%)	112 (100%)	0	100	100
19	LL	456/594 (77%)	454 (100%)	2 (0%)	91	94
20	LN	582/597 (98%)	580 (100%)	2 (0%)	92	95
21	LO	726/783 (93%)	725 (100%)	1 (0%)	93	97
22	LP	499/527 (95%)	498 (100%)	1 (0%)	93	96
23	LQ	690/828 (83%)	688 (100%)	2 (0%)	92	95
24	LS	393/476 (83%)	392 (100%)	1 (0%)	92	95
25	LT	744/823 (90%)	743 (100%)	1 (0%)	93	97
26	LU	399/399 (100%)	399 (100%)	0	100	100
27	LW	373/512 (73%)	373 (100%)	0	100	100
28	LZ	166/167 (99%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	NA	229/626 (37%)	229 (100%)	0	100	100
30	NB	63/413 (15%)	63 (100%)	0	100	100
31	ND	72/222 (32%)	72 (100%)	0	100	100
32	NE	86/253 (34%)	85 (99%)	1 (1%)	71	83
33	NF	130/131 (99%)	130 (100%)	0	100	100
34	NG	92/119 (77%)	91 (99%)	1 (1%)	73	84
35	NJ	707/899 (79%)	707 (100%)	0	100	100
36	NM	207/231 (90%)	207 (100%)	0	100	100
37	NN	37/484 (8%)	37 (100%)	0	100	100
38	NO	112/113 (99%)	112 (100%)	0	100	100
39	NQ	74/76 (97%)	74 (100%)	0	100	100
43	NW	282/635 (44%)	281 (100%)	1 (0%)	91	94
44	SA	334/511 (65%)	334 (100%)	0	100	100
45	SB	372/455 (82%)	372 (100%)	0	100	100
46	SC	192/234 (82%)	190 (99%)	2 (1%)	76	86
46	SD	198/234 (85%)	198 (100%)	0	100	100
47	SE	108/111 (97%)	108 (100%)	0	100	100
47	SF	107/111 (96%)	107 (100%)	0	100	100
48	SH	315/318 (99%)	315 (100%)	0	100	100
49	SI	738/1119 (66%)	738 (100%)	0	100	100
50	SK	181/209 (87%)	181 (100%)	0	100	100
51	SL	177/182 (97%)	177 (100%)	0	100	100
52	SM	253/254 (100%)	253 (100%)	0	100	100
53	SQ	165/676 (24%)	165 (100%)	0	100	100
54	SR	85/115 (74%)	84 (99%)	1 (1%)	71	83
55	SS	177/686 (26%)	175 (99%)	2 (1%)	73	84
57	SY	219/232 (94%)	219 (100%)	0	100	100
59	SP	504/2522 (20%)	503 (100%)	1 (0%)	93	96
60	LR	133/672 (20%)	133 (100%)	0	100	100
61	LM	977/1943 (50%)	975 (100%)	2 (0%)	93	96
63	SG	286/382 (75%)	284 (99%)	2 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	NI	76/246 (31%)	76 (100%)	0	100	100
66	ST	59/439 (13%)	58 (98%)	1 (2%)	60	78
68	NY	211/340 (62%)	211 (100%)	0	100	100
All	All	15592/25272 (62%)	15559 (100%)	33 (0%)	93	96

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	L7	163	GLN
9	L8	25	ARG
9	L8	157	LYS
10	L9	58	ARG
13	LD	69	ARG
15	LG	29	GLN
16	LH	483	LYS
16	LH	649	GLN
16	LH	759	LYS
19	LL	188	ARG
19	LL	367	ARG
20	LN	438	ARG
20	LN	591	LYS
21	LO	850	LYS
22	LP	386	ARG
23	LQ	279	ARG
23	LQ	935	ARG
24	LS	89	ARG
25	LT	612	ARG
32	NE	273	ASN
34	NG	38	ASN
43	NW	208	ARG
46	SC	239	GLN
46	SC	290	ASN
54	SR	63	ASN
55	SS	130	ARG
55	SS	229	ARG
59	SP	36	ARG
61	LM	84	LYS
61	LM	673	ASN
63	SG	404	GLN
63	SG	465	ARG
66	ST	789	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
8	L7	76	GLN
16	LH	429	GLN
16	LH	663	GLN
19	LL	301	HIS
19	LL	507	GLN
19	LL	547	GLN
20	LN	384	HIS
20	LN	549	GLN
20	LN	595	HIS
21	LO	879	GLN
23	LQ	632	HIS
26	LU	12	ASN
26	LU	75	HIS
26	LU	187	ASN
34	NG	113	GLN
35	NJ	260	GLN
43	NW	299	ASN
43	NW	313	HIS
46	SD	256	ASN
49	SI	1270	GLN
55	SS	195	ASN
57	SY	21	GLN
59	SP	819	ASN
61	LM	489	HIS
61	LM	705	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	234/3617 (6%)	101 (43%)	6 (2%)
2	L1	1275/1872 (68%)	334 (26%)	21 (1%)
3	L2	214/217 (98%)	74 (34%)	4 (1%)
62	N0	20/22 (90%)	4 (20%)	0
All	All	1743/5728 (30%)	513 (29%)	31 (1%)

All (513) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	434	C
1	L0	438	G

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Mol	Chain	Res	Type
1	L0	439	U
1	L0	442	U
1	L0	445	C
1	L0	446	G
1	L0	448	C
1	L0	449	G
1	L0	450	U
1	L0	452	C
1	L0	459	G
1	L0	462	C
1	L0	599	G
1	L0	602	C
1	L0	604	C
1	L0	605	G
1	L0	607	C
1	L0	608	C
1	L0	610	G
1	L0	613	C
1	L0	662	G
1	L0	664	C
1	L0	666	U
1	L0	667	C
1	L0	672	G
1	L0	678	G
1	L0	679	A
1	L0	680	C
1	L0	681	A
1	L0	685	C
1	L0	687	C
1	L0	688	G
1	L0	690	U
1	L0	691	G
1	L0	692	U
1	L0	694	G
1	L0	714	U
1	L0	716	C
1	L0	717	G
1	L0	718	G
1	L0	719	G
1	L0	720	C
1	L0	721	G
1	L0	723	C

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Mol	Chain	Res	Type
1	L0	724	C
1	L0	725	C
1	L0	728	C
1	L0	732	G
1	L0	733	C
1	L0	734	G
1	L0	735	G
1	L0	736	C
1	L0	737	G
1	L0	740	G
1	L0	741	G
1	L0	742	G
1	L0	743	G
1	L0	744	G
1	L0	745	U
1	L0	746	G
1	L0	751	C
1	L0	752	C
1	L0	754	G
1	L0	755	C
1	L0	756	C
1	L0	761	C
1	L0	796	C
1	L0	797	G
1	L0	798	U
1	L0	800	G
1	L0	801	G
1	L0	803	U
1	L0	814	C
1	L0	818	G
1	L0	819	C
1	L0	820	G
1	L0	822	U
1	L0	823	G
1	L0	829	G
1	L0	831	A
1	L0	832	G
1	L0	833	C
1	L0	843	U
1	L0	844	G
1	L0	855	G
1	L0	859	G

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Mol	Chain	Res	Type
1	L0	860	A
1	L0	862	G
1	L0	863	C
1	L0	864	C
1	L0	865	G
1	L0	1415	G
1	L0	1418	A
1	L0	1419	A
1	L0	1420	G
1	L0	1421	C
1	L0	1425	C
1	L0	1428	U
1	L0	1430	G
1	L0	1433	A
1	L0	1435	C
2	L1	8	U
2	L1	9	U
2	L1	10	G
2	L1	17	C
2	L1	18	C
2	L1	20	G
2	L1	21	U
2	L1	23	G
2	L1	33	G
2	L1	46	A
2	L1	47	G
2	L1	50	A
2	L1	56	G
2	L1	67	C
2	L1	68	A
2	L1	72	C
2	L1	73	C
2	L1	74	G
2	L1	75	G
2	L1	76	U
2	L1	92	A
2	L1	93	U
2	L1	95	G
2	L1	96	C
2	L1	97	U
2	L1	98	C
2	L1	99	A

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Mol	Chain	Res	Type
2	L1	100	U
2	L1	102	A
2	L1	103	A
2	L1	104	A
2	L1	105	U
2	L1	113	G
2	L1	115	U
2	L1	126	G
2	L1	127	C
2	L1	132	U
2	L1	134	C
2	L1	142	C
2	L1	143	U
2	L1	149	A
2	L1	155	G
2	L1	158	A
2	L1	160	U
2	L1	161	U
2	L1	162	C
2	L1	172	U
2	L1	173	A
2	L1	182	C
2	L1	184	G
2	L1	185	G
2	L1	188	C
2	L1	190	G
2	L1	192	C
2	L1	195	C
2	L1	204	G
2	L1	205	G
2	L1	206	G
2	L1	210	U
2	L1	214	U
2	L1	215	G
2	L1	226	A
2	L1	227	U
2	L1	228	C
2	L1	229	A
2	L1	231	A
2	L1	235	A
2	L1	238	C
2	L1	248	C

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Mol	Chain	Res	Type
2	L1	269	G
2	L1	271	C
2	L1	272	G
2	L1	283	G
2	L1	285	U
2	L1	287	U
2	L1	288	G
2	L1	306	C
2	L1	307	G
2	L1	308	G
2	L1	312	G
2	L1	319	C
2	L1	321	C
2	L1	322	C
2	L1	323	C
2	L1	325	C
2	L1	326	C
2	L1	328	U
2	L1	329	G
2	L1	335	G
2	L1	347	G
2	L1	350	C
2	L1	351	G
2	L1	362	C
2	L1	364	A
2	L1	368	U
2	L1	369	C
2	L1	370	G
2	L1	385	G
2	L1	386	C
2	L1	389	A
2	L1	391	C
2	L1	392	A
2	L1	400	C
2	L1	405	G
2	L1	407	G
2	L1	408	A
2	L1	413	G
2	L1	415	A
2	L1	416	U
2	L1	417	C
2	L1	419	G

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Mol	Chain	Res	Type
2	L1	420	G
2	L1	422	U
2	L1	423	U
2	L1	424	C
2	L1	427	U
2	L1	430	C
2	L1	431	G
2	L1	436	G
2	L1	438	G
2	L1	447	A
2	L1	451	G
2	L1	452	G
2	L1	467	G
2	L1	471	G
2	L1	478	G
2	L1	480	G
2	L1	481	C
2	L1	482	G
2	L1	483	C
2	L1	484	A
2	L1	485	A
2	L1	486	A
2	L1	488	U
2	L1	492	C
2	L1	496	C
2	L1	502	C
2	L1	513	G
2	L1	515	G
2	L1	516	A
2	L1	525	A
2	L1	528	A
2	L1	534	G
2	L1	535	G
2	L1	541	U
2	L1	544	G
2	L1	548	C
2	L1	550	C
2	L1	554	A
2	L1	555	A
2	L1	556	U
2	L1	560	A
2	L1	564	A

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Mol	Chain	Res	Type
2	L1	570	C
2	L1	588	G
2	L1	590	A
2	L1	591	U
2	L1	594	A
2	L1	606	G
2	L1	611	G
2	L1	614	C
2	L1	622	C
2	L1	624	C
2	L1	628	A
2	L1	643	A
2	L1	644	G
2	L1	652	U
2	L1	653	A
2	L1	654	A
2	L1	655	A
2	L1	684	G
2	L1	920	A
2	L1	933	G
2	L1	938	A
2	L1	955	A
2	L1	967	C
2	L1	969	U
2	L1	970	G
2	L1	983	A
2	L1	990	A
2	L1	991	G
2	L1	992	A
2	L1	1017	U
2	L1	1023	A
2	L1	1027	A
2	L1	1093	A
2	L1	1094	C
2	L1	1096	G
2	L1	1100	A
2	L1	1111	U
2	L1	1114	U
2	L1	1115	U
2	L1	1121	G
2	L1	1133	A
2	L1	1137	U

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Mol	Chain	Res	Type
2	L1	1145	A
2	L1	1147	C
2	L1	1170	A
2	L1	1172	U
2	L1	1175	G
2	L1	1176	G
2	L1	1178	U
2	L1	1187	G
2	L1	1189	A
2	L1	1190	A
2	L1	1192	U
2	L1	1193	U
2	L1	1195	A
2	L1	1196	A
2	L1	1197	G
2	L1	1198	G
2	L1	1205	C
2	L1	1215	C
2	L1	1216	C
2	L1	1217	A
2	L1	1267	C
2	L1	1268	C
2	L1	1274	G
2	L1	1275	G
2	L1	1276	A
2	L1	1283	C
2	L1	1286	G
2	L1	1290	G
2	L1	1295	A
2	L1	1301	A
2	L1	1302	G
2	L1	1303	C
2	L1	1308	U
2	L1	1309	C
2	L1	1313	A
2	L1	1315	U
2	L1	1316	C
2	L1	1318	G
2	L1	1320	G
2	L1	1328	G
2	L1	1330	G
2	L1	1335	G

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Mol	Chain	Res	Type
2	L1	1358	U
2	L1	1365	G
2	L1	1371	U
2	L1	1372	U
2	L1	1374	C
2	L1	1376	A
2	L1	1377	U
2	L1	1378	A
2	L1	1381	G
2	L1	1382	A
2	L1	1394	G
2	L1	1454	A
2	L1	1461	G
2	L1	1462	U
2	L1	1463	U
2	L1	1464	C
2	L1	1465	A
2	L1	1466	G
2	L1	1477	U
2	L1	1483	A
2	L1	1485	U
2	L1	1487	A
2	L1	1489	A
2	L1	1491	G
2	L1	1492	U
2	L1	1493	C
2	L1	1494	U
2	L1	1495	G
2	L1	1496	U
2	L1	1497	G
2	L1	1498	A
2	L1	1499	U
2	L1	1503	C
2	L1	1524	G
2	L1	1533	A
2	L1	1534	C
2	L1	1544	C
2	L1	1548	G
2	L1	1549	U
2	L1	1550	G
2	L1	1592	C
2	L1	1599	U

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Mol	Chain	Res	Type
2	L1	1638	G
2	L1	1639	G
2	L1	1648	G
2	L1	1656	G
2	L1	1659	U
2	L1	1660	C
2	L1	1664	A
2	L1	1665	G
2	L1	1666	C
2	L1	1681	U
2	L1	1685	U
2	L1	1692	U
2	L1	1704	C
2	L1	1710	C
2	L1	1715	A
2	L1	1720	U
2	L1	1721	U
2	L1	1722	G
2	L1	1724	A
2	L1	1725	U
2	L1	1729	U
2	L1	1757	G
2	L1	1760	G
2	L1	1764	G
2	L1	1765	C
2	L1	1766	C
2	L1	1767	C
2	L1	1769	C
2	L1	1770	G
2	L1	1771	G
2	L1	1772	C
2	L1	1774	C
2	L1	1775	U
2	L1	1776	G
2	L1	1777	G
2	L1	1783	C
2	L1	1784	G
2	L1	1785	C
2	L1	1800	A
2	L1	1801	A
2	L1	1809	A
2	L1	1810	U

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Mol	Chain	Res	Type
2	L1	1812	U
2	L1	1813	A
2	L1	1818	A
2	L1	1823	A
2	L1	1824	A
2	L1	1838	U
2	L1	1841	C
2	L1	1846	G
2	L1	1848	U
2	L1	1849	G
2	L1	1850	A
2	L1	1851	A
2	L1	1852	C
3	L2	14	C
3	L2	15	A
3	L2	22	A
3	L2	24	U
3	L2	25	U
3	L2	27	U
3	L2	28	A
3	L2	30	A
3	L2	31	G
3	L2	32	U
3	L2	33	G
3	L2	35	G
3	L2	44	G
3	L2	48	U
3	L2	49	U
3	L2	61	G
3	L2	62	U
3	L2	64	G
3	L2	68	A
3	L2	69	C
3	L2	88	G
3	L2	89	A
3	L2	91	G
3	L2	108	G
3	L2	109	C
3	L2	110	G
3	L2	114	A
3	L2	116	C
3	L2	117	C

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Mol	Chain	Res	Type
3	L2	118	G
3	L2	119	G
3	L2	123	U
3	L2	124	C
3	L2	125	U
3	L2	126	G
3	L2	127	G
3	L2	128	C
3	L2	129	G
3	L2	130	U
3	L2	131	U
3	L2	132	G
3	L2	138	C
3	L2	139	U
3	L2	145	U
3	L2	146	G
3	L2	147	C
3	L2	148	C
3	L2	149	G
3	L2	150	U
3	L2	153	G
3	L2	158	U
3	L2	167	U
3	L2	168	U
3	L2	171	U
3	L2	172	C
3	L2	173	U
3	L2	174	C
3	L2	179	U
3	L2	181	U
3	L2	182	U
3	L2	183	G
3	L2	185	G
3	L2	188	G
3	L2	189	U
3	L2	190	G
3	L2	191	A
3	L2	192	G
3	L2	199	A
3	L2	200	G
3	L2	201	A
3	L2	202	A

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Mol	Chain	Res	Type
3	L2	208	U
3	L2	209	C
3	L2	213	G
62	N0	874	A
62	N0	877	A
62	N0	1399	A
62	N0	1400	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L0	433	U
1	L0	604	C
1	L0	666	U
1	L0	732	G
1	L0	799	C
1	L0	854	U
2	L1	157	U
2	L1	226	A
2	L1	227	U
2	L1	325	C
2	L1	368	U
2	L1	369	C
2	L1	423	U
2	L1	466	G
2	L1	589	G
2	L1	969	U
2	L1	1197	G
2	L1	1393	G
2	L1	1461	G
2	L1	1637	A
2	L1	1664	A
2	L1	1684	C
2	L1	1703	C
2	L1	1719	A
2	L1	1765	C
2	L1	1817	G
2	L1	1823	A
3	L2	14	C
3	L2	145	U
3	L2	152	A
3	L2	188	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 25 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	ATP	NK	1101	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
73	SAH	SJ	301	-	24,28,28	1.20	3 (12%)	25,40,40	1.70	5 (20%)
73	SAH	SK	301	-	24,28,28	1.17	3 (12%)	25,40,40	1.68	5 (20%)
74	ATP	NH	3000	70	26,33,33	0.59	0	31,52,52	0.82	2 (6%)
72	GTP	SI	2001	70	26,34,34	1.14	2 (7%)	32,54,54	1.57	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	ATP	NK	1101	-	-	6/18/38/38	0/3/3/3
73	SAH	SJ	301	-	-	1/11/31/31	0/3/3/3
73	SAH	SK	301	-	-	5/11/31/31	0/3/3/3
74	ATP	NH	3000	70	-	7/18/38/38	0/3/3/3
72	GTP	SI	2001	70	-	7/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	SI	2001	GTP	C5-C6	-4.03	1.39	1.47
73	SJ	301	SAH	C2-N3	3.84	1.38	1.32
73	SK	301	SAH	C2-N3	3.82	1.38	1.32
73	SJ	301	SAH	C2-N1	2.54	1.38	1.33
72	SI	2001	GTP	C2-N3	2.18	1.38	1.33
73	SK	301	SAH	C2-N1	2.14	1.37	1.33
73	SK	301	SAH	OXT-C	-2.12	1.23	1.30
73	SJ	301	SAH	OXT-C	-2.11	1.23	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	SK	301	SAH	N3-C2-N1	-5.63	119.88	128.68
73	SJ	301	SAH	N3-C2-N1	-5.30	120.39	128.68
72	SI	2001	GTP	PB-O3B-PG	-3.74	120.00	132.83
73	SJ	301	SAH	C5'-SD-CG	-3.31	92.34	102.27
72	SI	2001	GTP	C5-C6-N1	3.23	119.66	113.95
73	SK	301	SAH	C5'-SD-CG	-3.12	92.91	102.27
72	SI	2001	GTP	C3'-C2'-C1'	3.02	105.53	100.98
72	SI	2001	GTP	C8-N7-C5	3.00	108.70	102.99
72	SI	2001	GTP	C2-N1-C6	-2.96	119.65	125.10
72	SI	2001	GTP	PA-O3A-PB	-2.75	123.40	132.83
73	SJ	301	SAH	OXT-C-O	-2.74	117.86	124.09
73	SJ	301	SAH	C3'-C2'-C1'	2.70	105.05	100.98
73	SK	301	SAH	C3'-C2'-C1'	2.66	104.98	100.98
73	SK	301	SAH	OXT-C-O	-2.62	118.14	124.09
74	NH	3000	ATP	C5-C6-N6	2.33	123.89	120.35
74	NK	1101	ATP	C5-C6-N6	2.27	123.80	120.35
73	SJ	301	SAH	OXT-C-CA	2.25	121.05	113.38
73	SK	301	SAH	OXT-C-CA	2.21	120.92	113.38
72	SI	2001	GTP	O6-C6-C5	-2.12	120.23	124.37
74	NK	1101	ATP	PB-O3B-PG	2.06	139.88	132.83
74	NH	3000	ATP	PB-O3B-PG	2.03	139.80	132.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
72	SI	2001	GTP	C5'-O5'-PA-O1A
73	SK	301	SAH	O-C-CA-N
73	SK	301	SAH	CA-CB-CG-SD
74	NH	3000	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
74	NH	3000	ATP	C5'-O5'-PA-O3A
74	NK	1101	ATP	C5'-O5'-PA-O1A
73	SK	301	SAH	OXT-C-CA-N
74	NH	3000	ATP	O4'-C4'-C5'-O5'
74	NH	3000	ATP	C4'-C5'-O5'-PA
74	NH	3000	ATP	PB-O3A-PA-O5'
73	SJ	301	SAH	CA-CB-CG-SD
72	SI	2001	GTP	C5'-O5'-PA-O3A
74	NK	1101	ATP	C5'-O5'-PA-O3A
72	SI	2001	GTP	C3'-C4'-C5'-O5'
72	SI	2001	GTP	PB-O3A-PA-O2A
74	NK	1101	ATP	PA-O3A-PB-O1B
74	NK	1101	ATP	C4'-C5'-O5'-PA
72	SI	2001	GTP	C5'-O5'-PA-O2A
74	NK	1101	ATP	C5'-O5'-PA-O2A
73	SK	301	SAH	C-CA-CB-CG
74	NH	3000	ATP	C3'-C4'-C5'-O5'
72	SI	2001	GTP	PG-O3B-PB-O2B
73	SK	301	SAH	N-CA-CB-CG
74	NK	1101	ATP	O4'-C4'-C5'-O5'
72	SI	2001	GTP	PG-O3B-PB-O1B
74	NH	3000	ATP	PG-O3B-PB-O2B

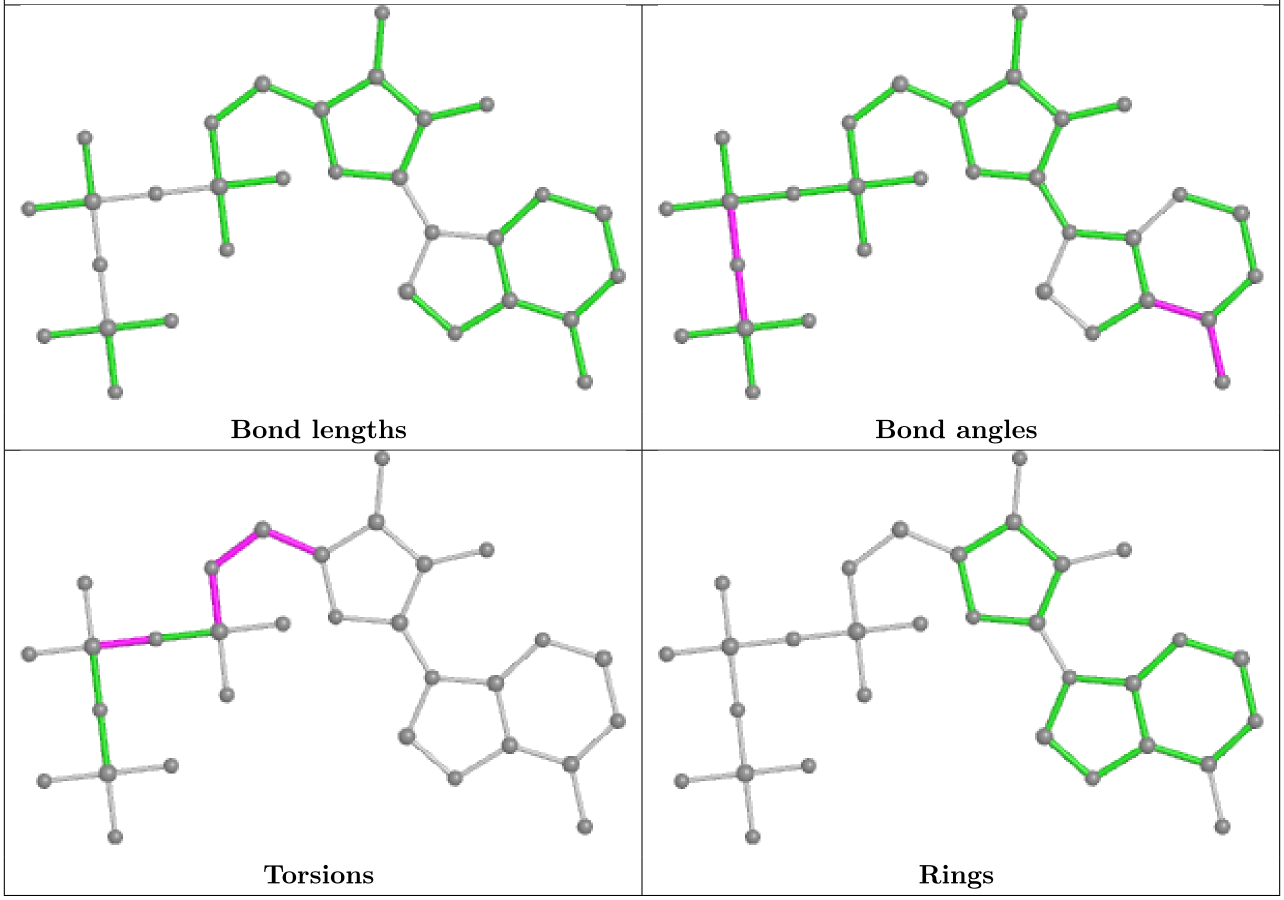
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	SJ	301	SAH	2	0
73	SK	301	SAH	2	0
72	SI	2001	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP NK 1101



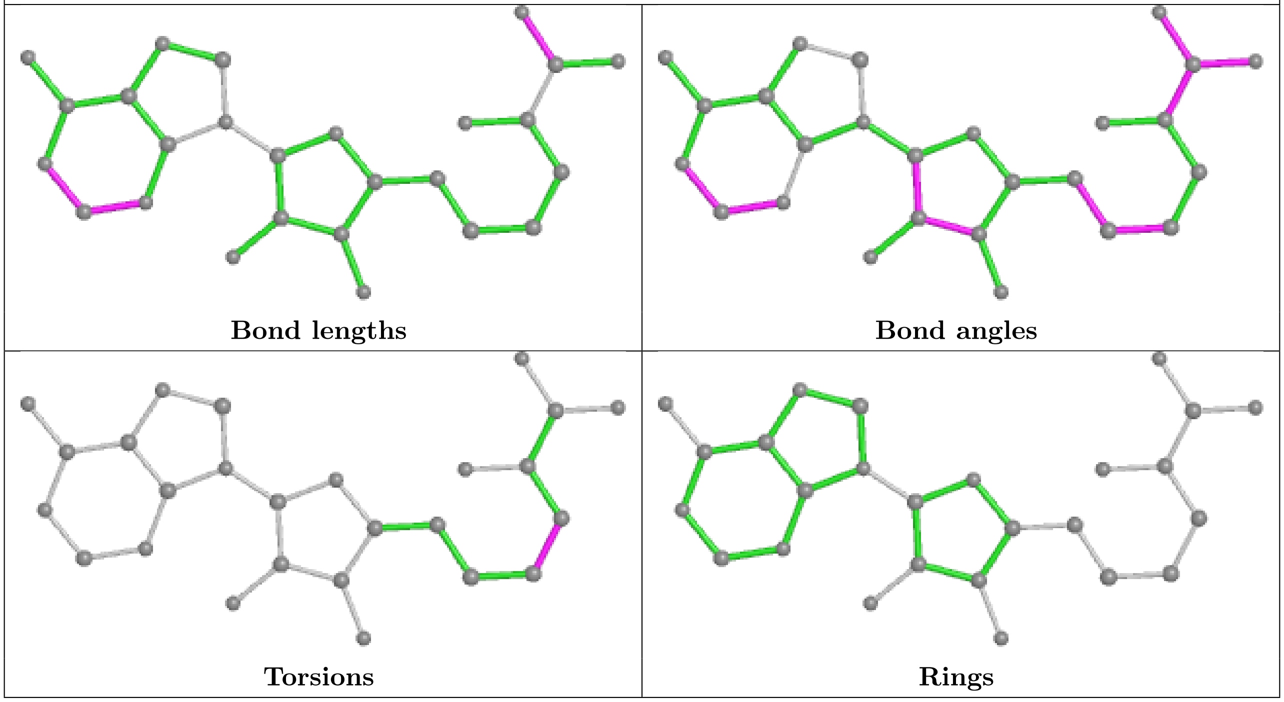
Bond lengths

Bond angles

Torsions

Rings

Ligand SAH SJ 301



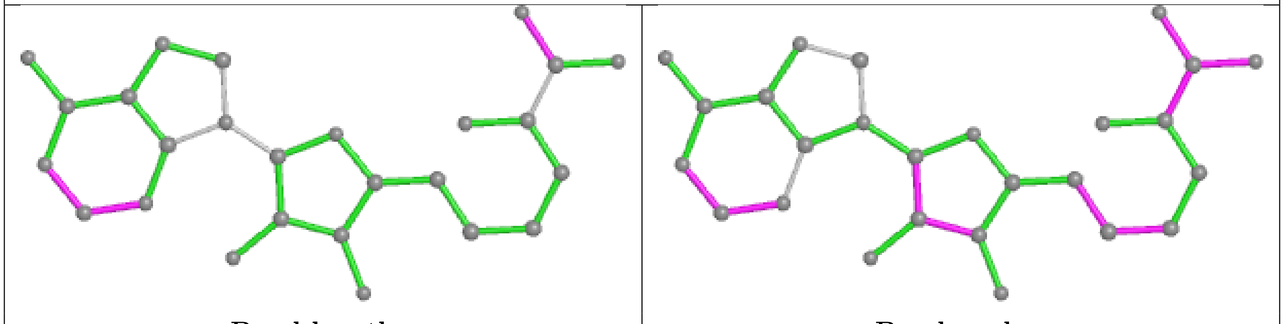
Bond lengths

Bond angles

Torsions

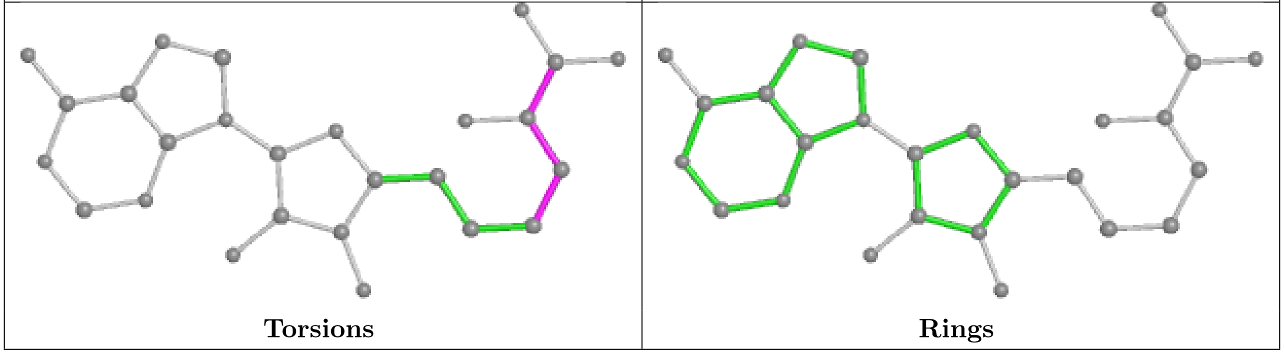
Rings

Ligand SAH SK 301



Bond lengths

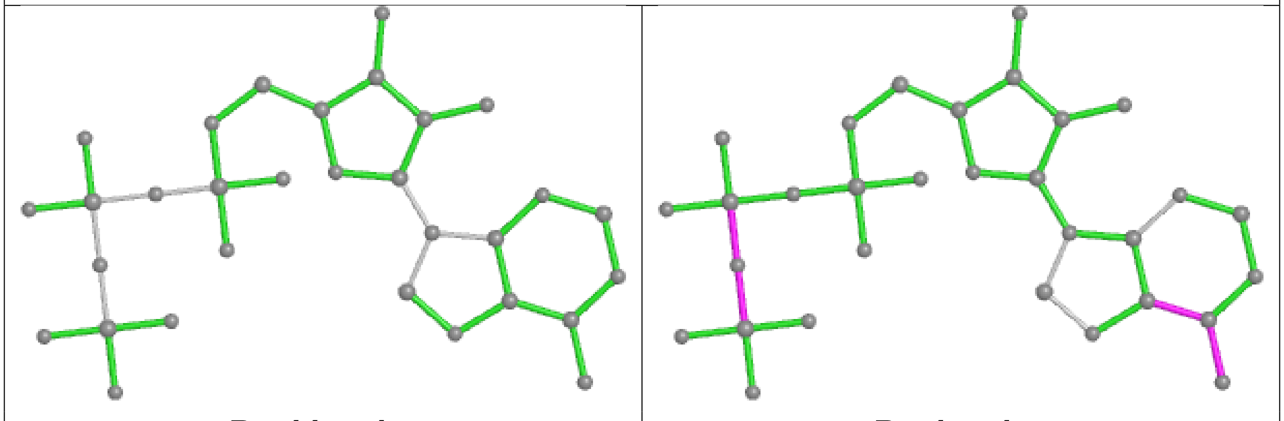
Bond angles



Torsions

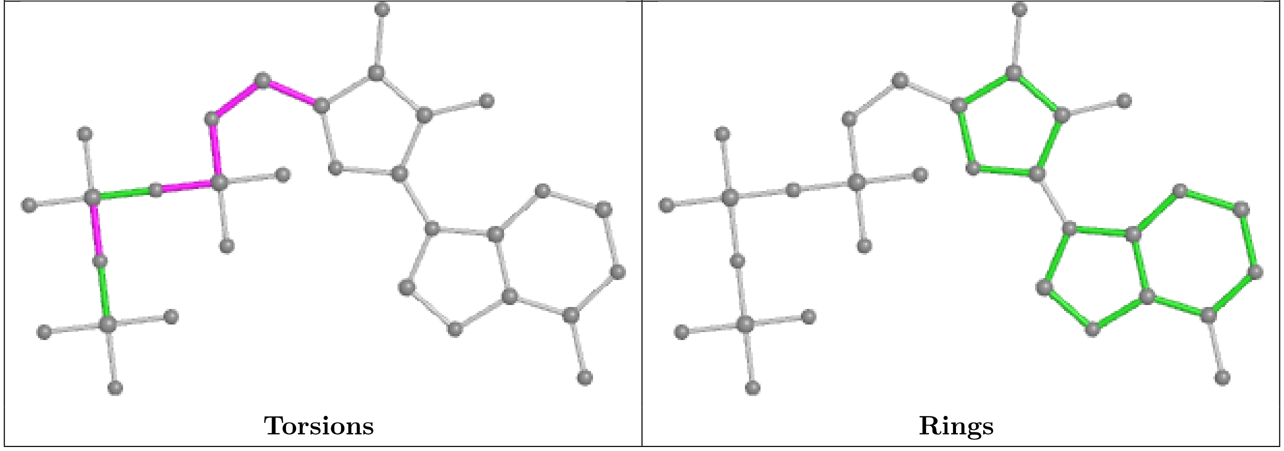
Rings

Ligand ATP NH 3000



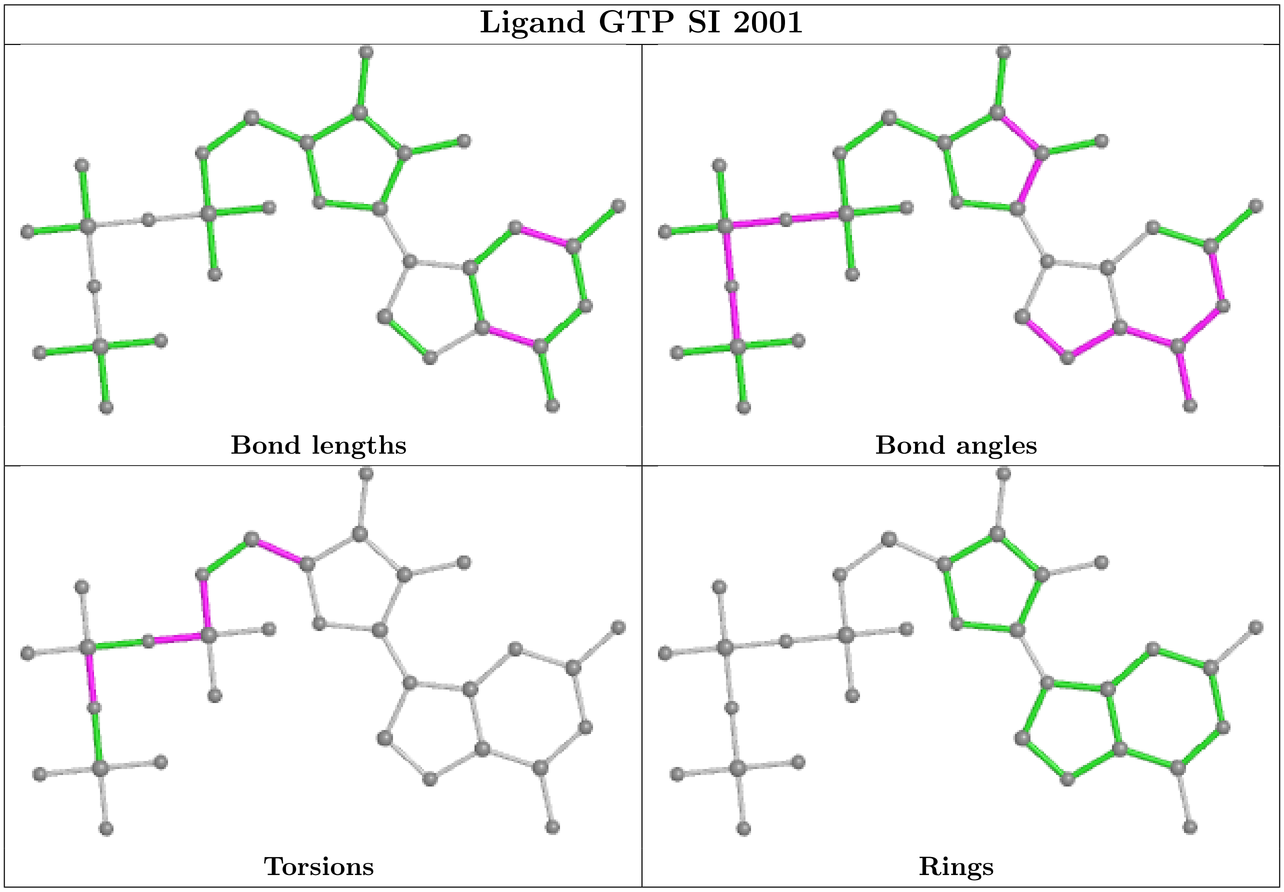
Bond lengths

Bond angles



Torsions

Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	NR	41
56	SX	6
17	LI	5
67	SU	5
66	ST	3
62	N0	1
69	SZ	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SX	726:UNK	C	1200:UNK	N	185.33
1	ST	298:LEU	C	414:UNK	N	53.15
1	SX	1269:UNK	C	1298:UNK	N	38.21
1	ST	86:LYS	C	186:UNK	N	37.03
1	SX	1427:UNK	C	1449:UNK	N	35.78
1	SX	1375:UNK	C	1405:UNK	N	33.62
1	LI	48:UNK	C	59:UNK	N	26.45
1	ST	234:UNK	C	246:UNK	N	21.92
1	LI	92:UNK	C	104:UNK	N	18.13
1	SX	1322:UNK	C	1352:UNK	N	17.58
1	NR	310:UNK	C	312:UNK	N	16.86
1	NR	567:UNK	C	571:UNK	N	16.56
1	NR	803:UNK	C	807:UNK	N	16.53
1	NR	131:UNK	C	134:UNK	N	16.06
1	SX	1222:UNK	C	1250:UNK	N	15.84
1	NR	358:UNK	C	361:UNK	N	15.73
1	N0	881:A	O3'	1396:A	P	15.63
1	LI	346:UNK	C	354:HIS	N	15.43
1	NR	976:UNK	C	980:UNK	N	14.97
1	NR	450:UNK	C	452:UNK	N	14.75
1	NR	915:UNK	C	919:UNK	N	14.25
1	SU	68:UNK	C	78:UNK	N	13.97
1	NR	496:UNK	C	498:UNK	N	13.49
1	NR	647:UNK	C	651:UNK	N	13.16
1	NR	101:UNK	C	112:UNK	N	13.09
1	NR	613:UNK	C	616:UNK	N	12.91
1	NR	953:UNK	C	957:UNK	N	12.71
1	NR	517:UNK	C	519:UNK	N	12.58
1	NR	688:UNK	C	692:UNK	N	12.22
1	NR	995:UNK	C	999:UNK	N	12.22
1	NR	475:UNK	C	477:UNK	N	12.20
1	LI	147:UNK	C	152:VAL	N	11.99
1	NR	672:UNK	C	674:UNK	N	11.97
1	NR	221:UNK	C	225:UNK	N	11.89
1	NR	426:UNK	C	428:UNK	N	11.79
1	NR	335:UNK	C	339:UNK	N	11.62
1	NR	870:UNK	C	874:UNK	N	11.34
1	NR	713:UNK	C	717:UNK	N	10.89
1	NR	934:UNK	C	936:UNK	N	10.47
1	NR	894:UNK	C	898:UNK	N	10.26
1	NR	780:UNK	C	784:UNK	N	10.25
1	SZ	164:UNK	C	169:UNK	N	10.18
1	NR	631:UNK	C	633:UNK	N	10.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	NR	846:UNK	C	850:UNK	N	9.68
1	SU	169:UNK	C	177:TYR	N	9.08
1	NR	590:UNK	C	592:UNK	N	8.89
1	NR	824:UNK	C	828:UNK	N	8.83
1	NR	538:UNK	C	541:UNK	N	8.50
1	NR	756:UNK	C	760:UNK	N	8.16
1	NR	1008:UNK	C	1010:UNK	N	8.04
1	NR	734:UNK	C	736:UNK	N	7.90
1	NR	550:UNK	C	555:UNK	N	7.83
1	SU	25:UNK	C	27:UNK	N	7.50
1	NR	262:UNK	C	264:UNK	N	7.47
1	NR	243:UNK	C	246:UNK	N	7.45
1	NR	381:UNK	C	383:UNK	N	5.92
1	NR	200:UNK	C	204:UNK	N	5.50
1	SU	124:UNK	C	141:PRO	N	5.49
1	LI	322:HIS	C	325:UNK	N	5.32
1	SU	45:UNK	C	48:UNK	N	4.87
1	NR	289:UNK	C	291:UNK	N	4.80
1	NR	404:UNK	C	407:UNK	N	4.38

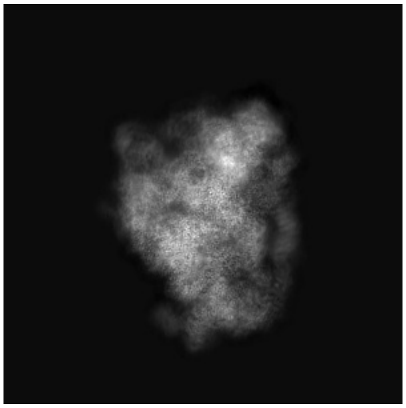
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-23937. These allow visual inspection of the internal detail of the map and identification of artifacts.

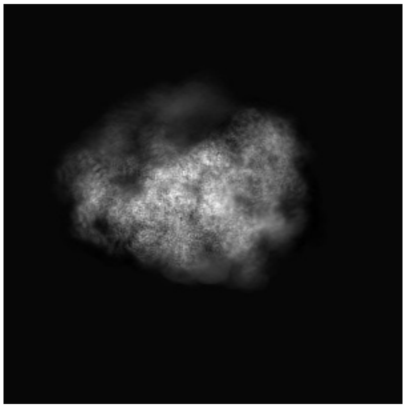
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

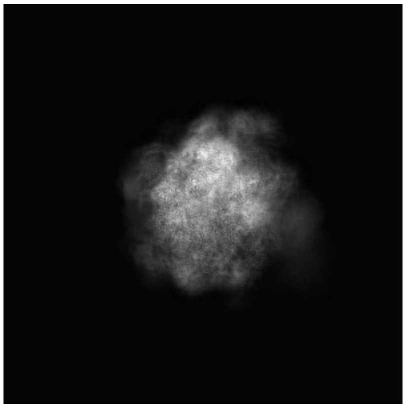
6.1.1 Primary map



X

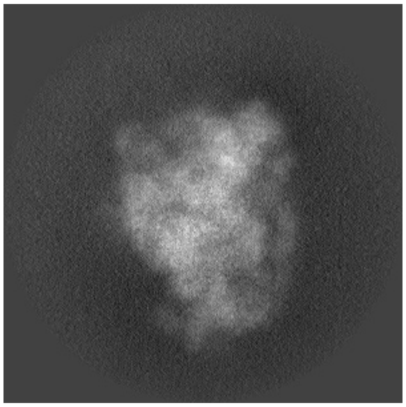


Y

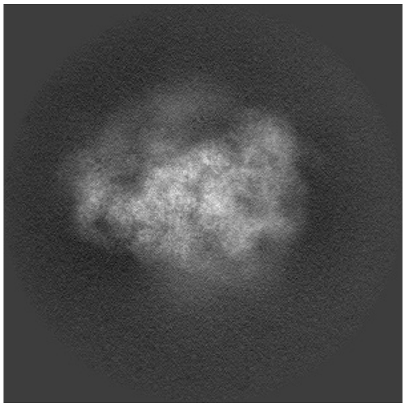


Z

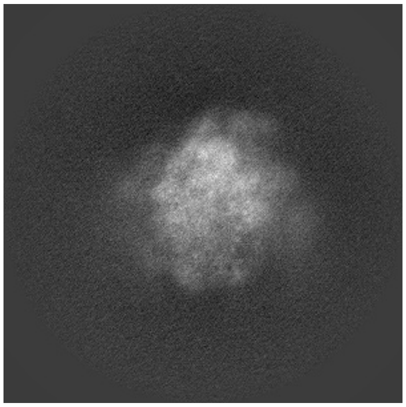
6.1.2 Raw map



X



Y

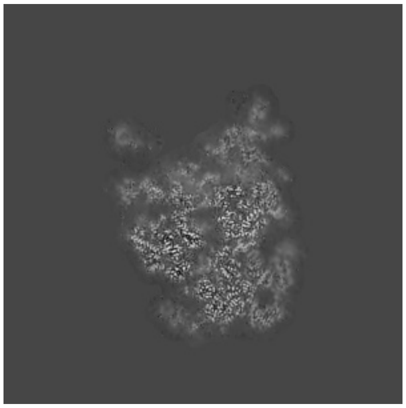


Z

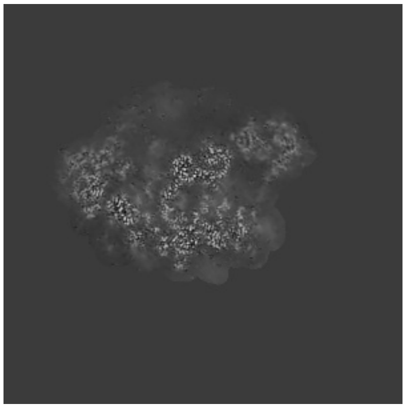
The images above show the map projected in three orthogonal directions.

6.2 Central slices

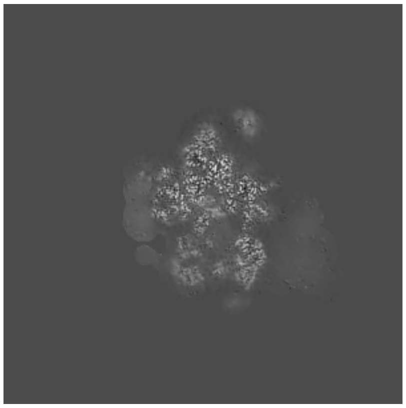
6.2.1 Primary map



X Index: 280

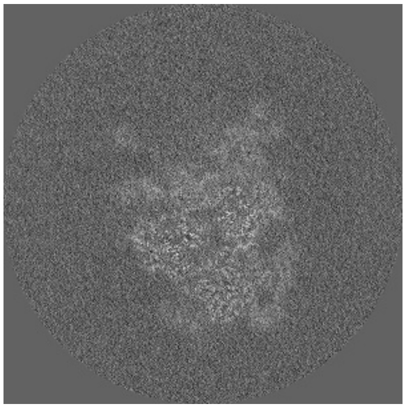


Y Index: 280

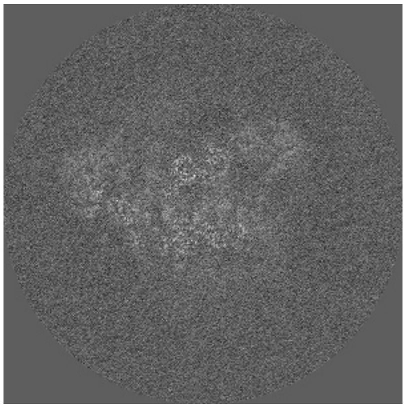


Z Index: 280

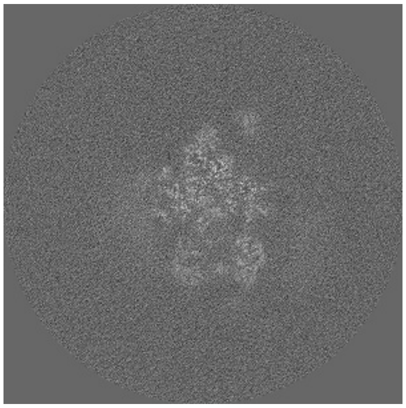
6.2.2 Raw map



X Index: 280



Y Index: 280

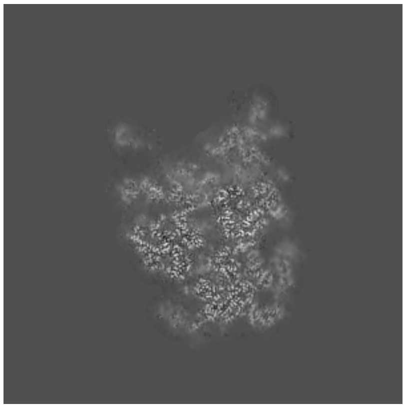


Z Index: 280

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

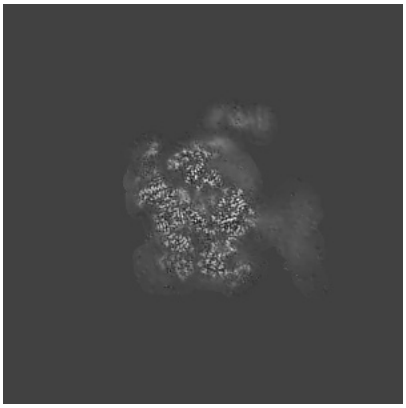
6.3 Largest variance slices

6.3.1 Primary map



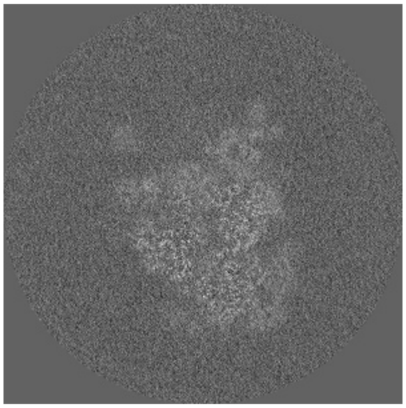
X Index: 281

Y Index: 310

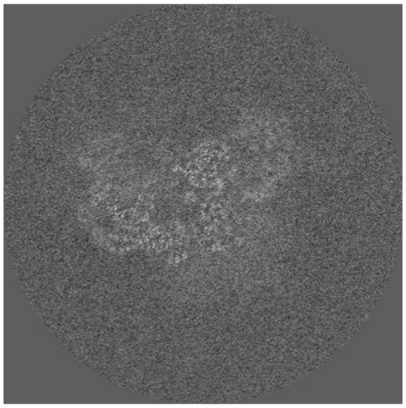


Z Index: 244

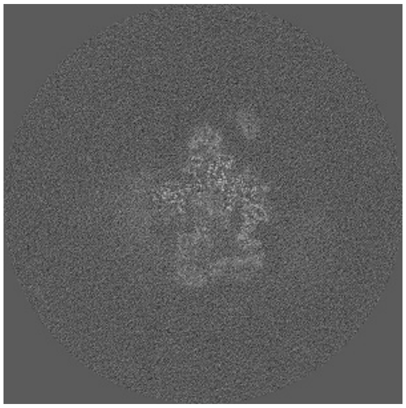
6.3.2 Raw map



X Index: 278



Y Index: 298



Z Index: 285

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

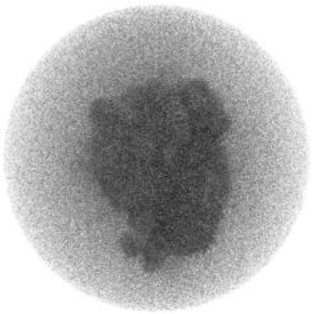
X

Y

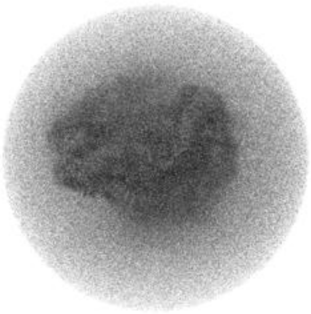
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

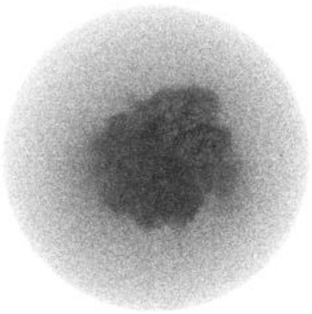
6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

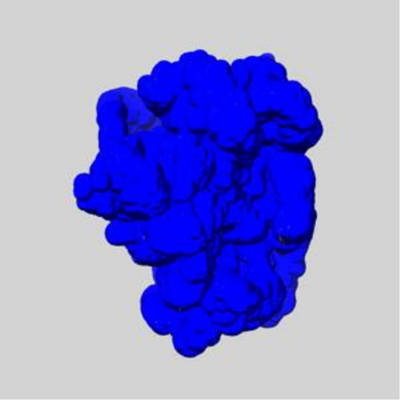
6.5 Mask visualisation ⓘ

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

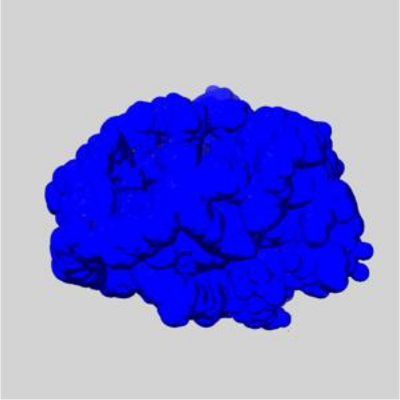
A mask typically either:

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

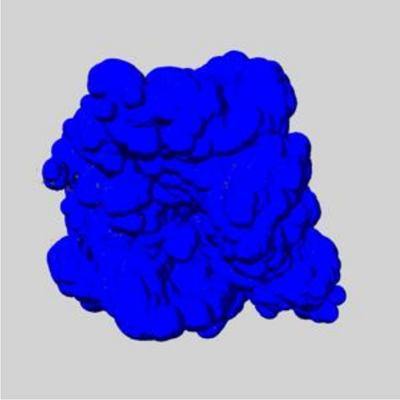
6.5.1 emd_23937_msk_1.map ⓘ



X



Y

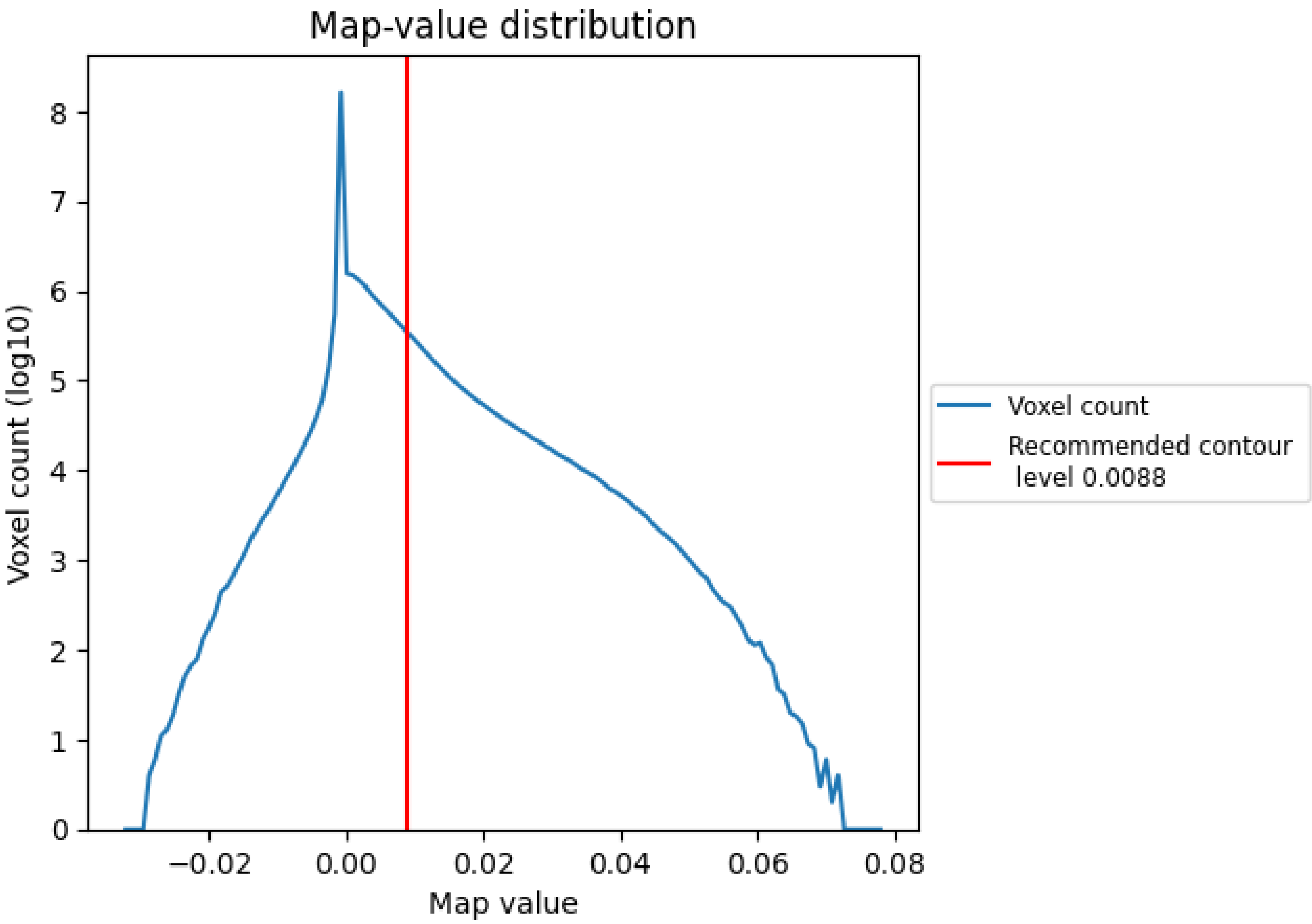


Z

7 Map analysis ⓘ

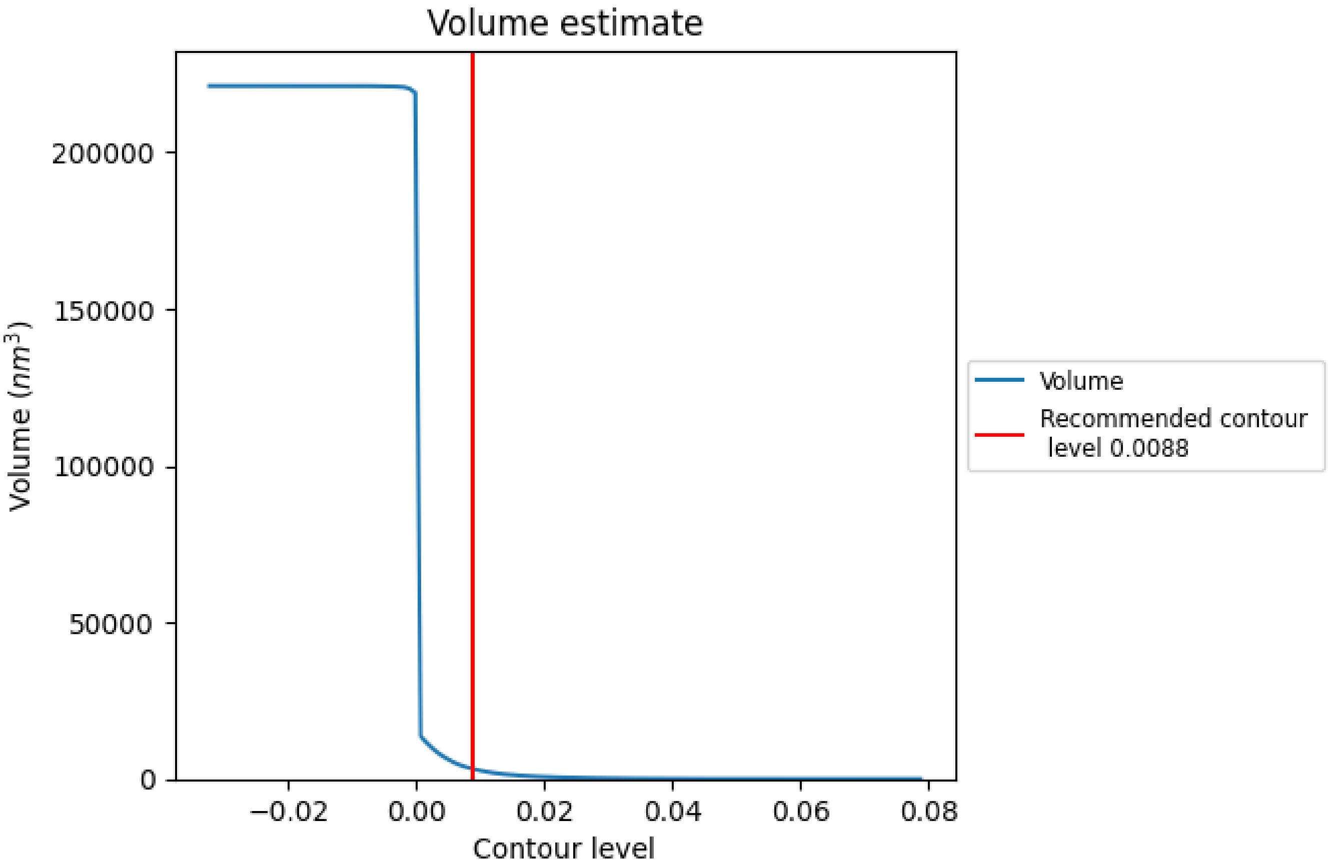
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

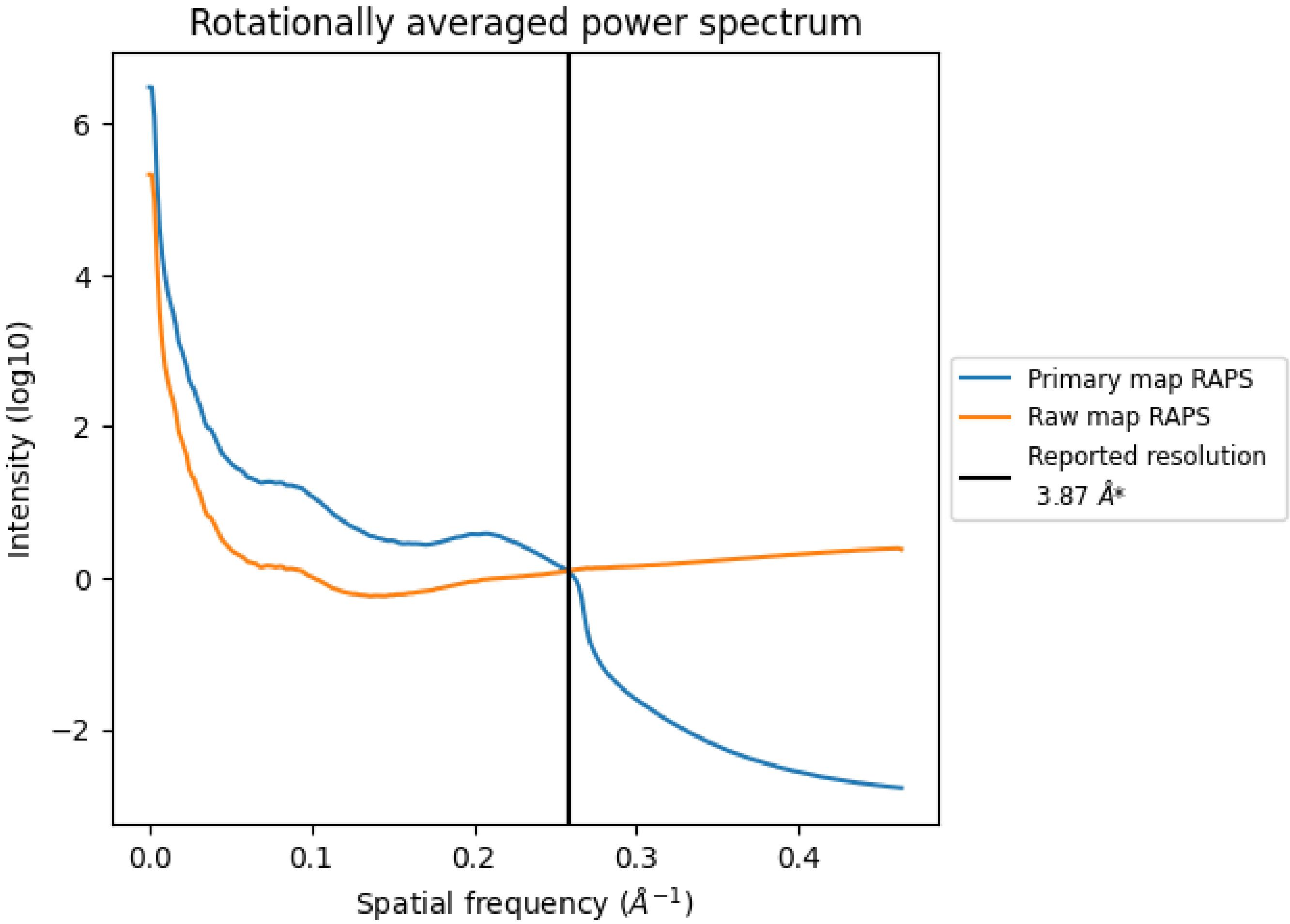
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 3275 nm^3; this corresponds to an approximate mass of 2958 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

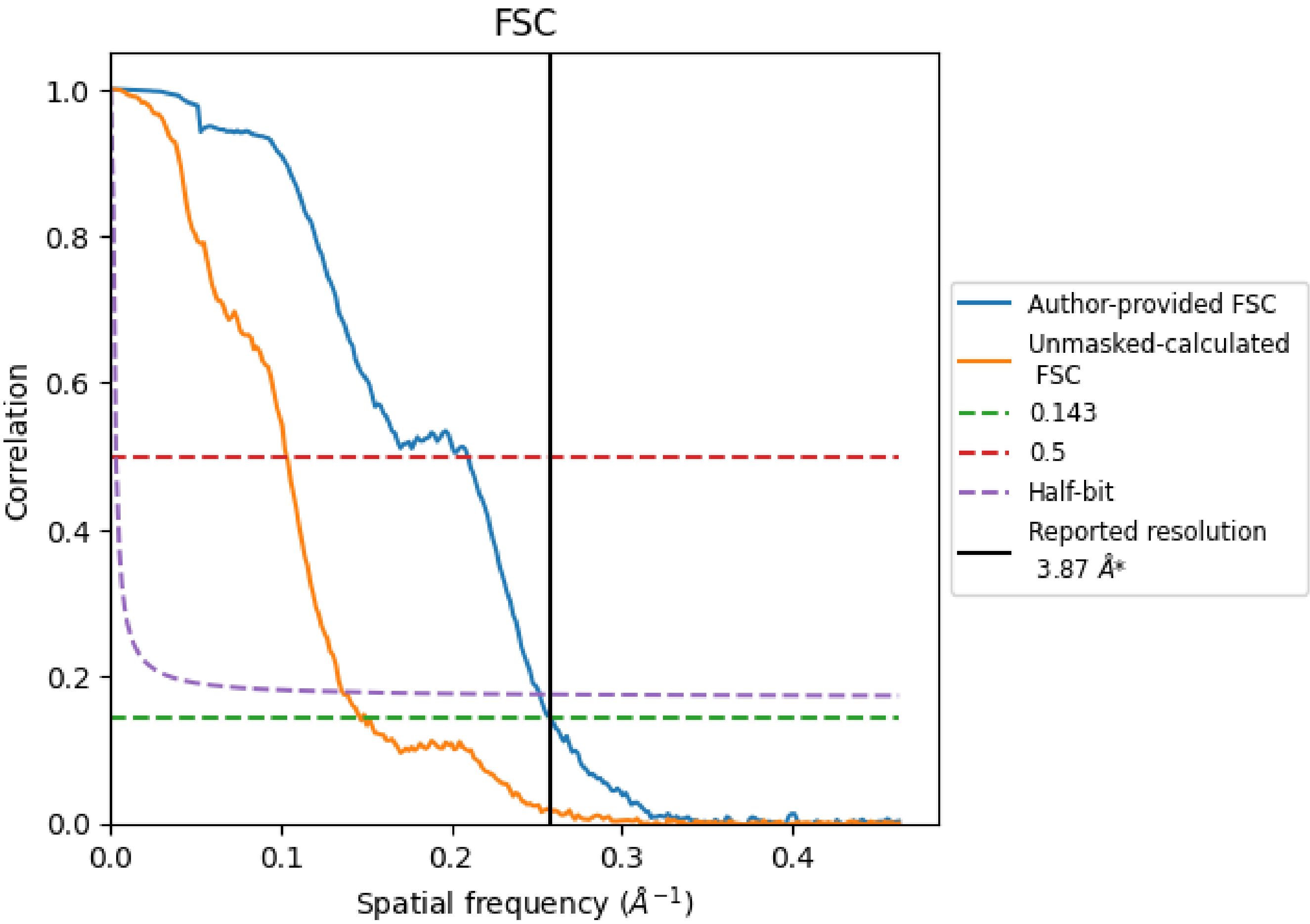


*Reported resolution corresponds to spatial frequency of 0.258 $\AA^{-1}$

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 0.258 $Å^{-1}$

8.2 Resolution estimates ⓘ

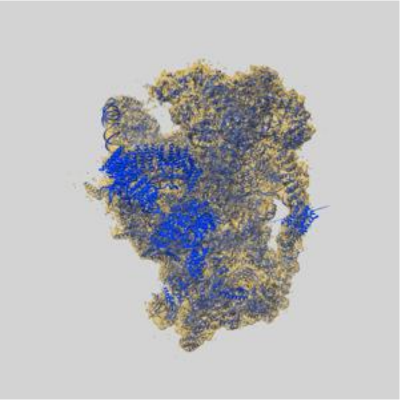
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.87	4.77	3.97
Unmasked-calculated*	6.83	9.67	7.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.83 differs from the reported value 3.87 by more than 10 %

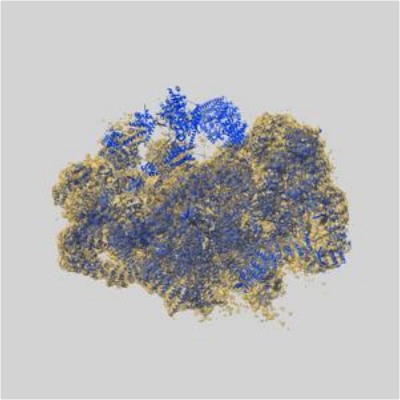
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23937 and PDB model 7MQ9. Per-residue inclusion information can be found in section 3 on page 19.

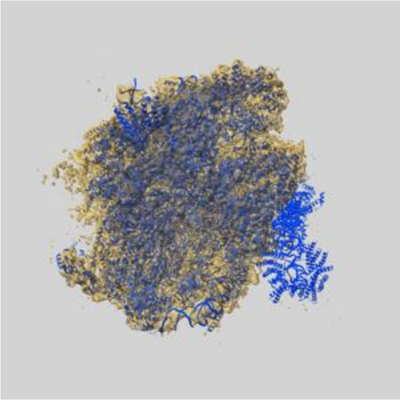
9.1 Map-model overlay ⓘ



X



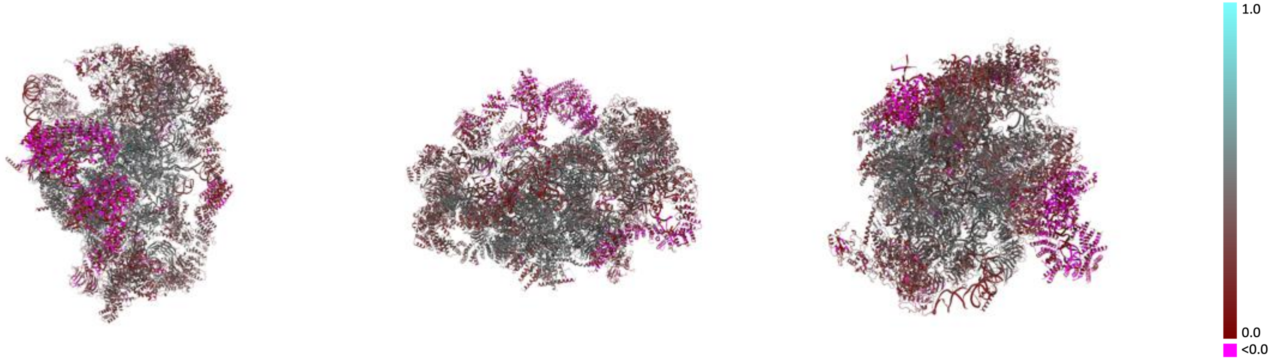
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0088 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.

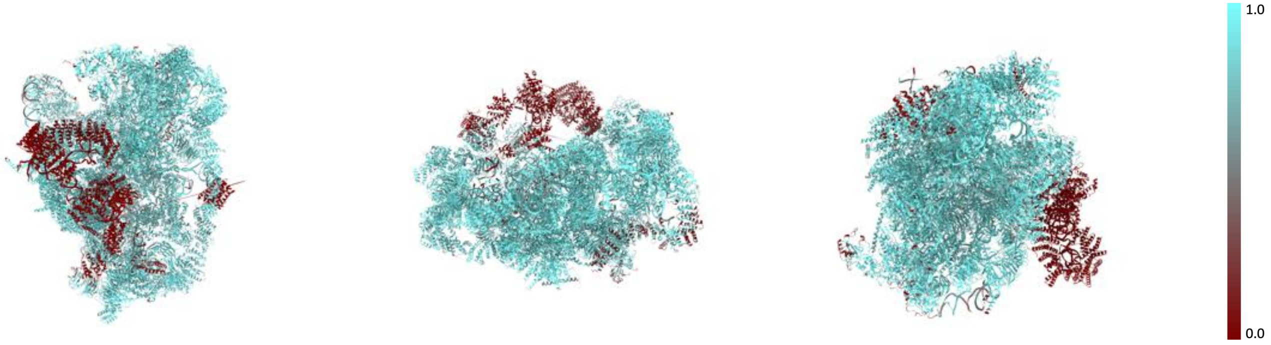
9.2 Q-score mapped to coordinate model ⓘ



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.

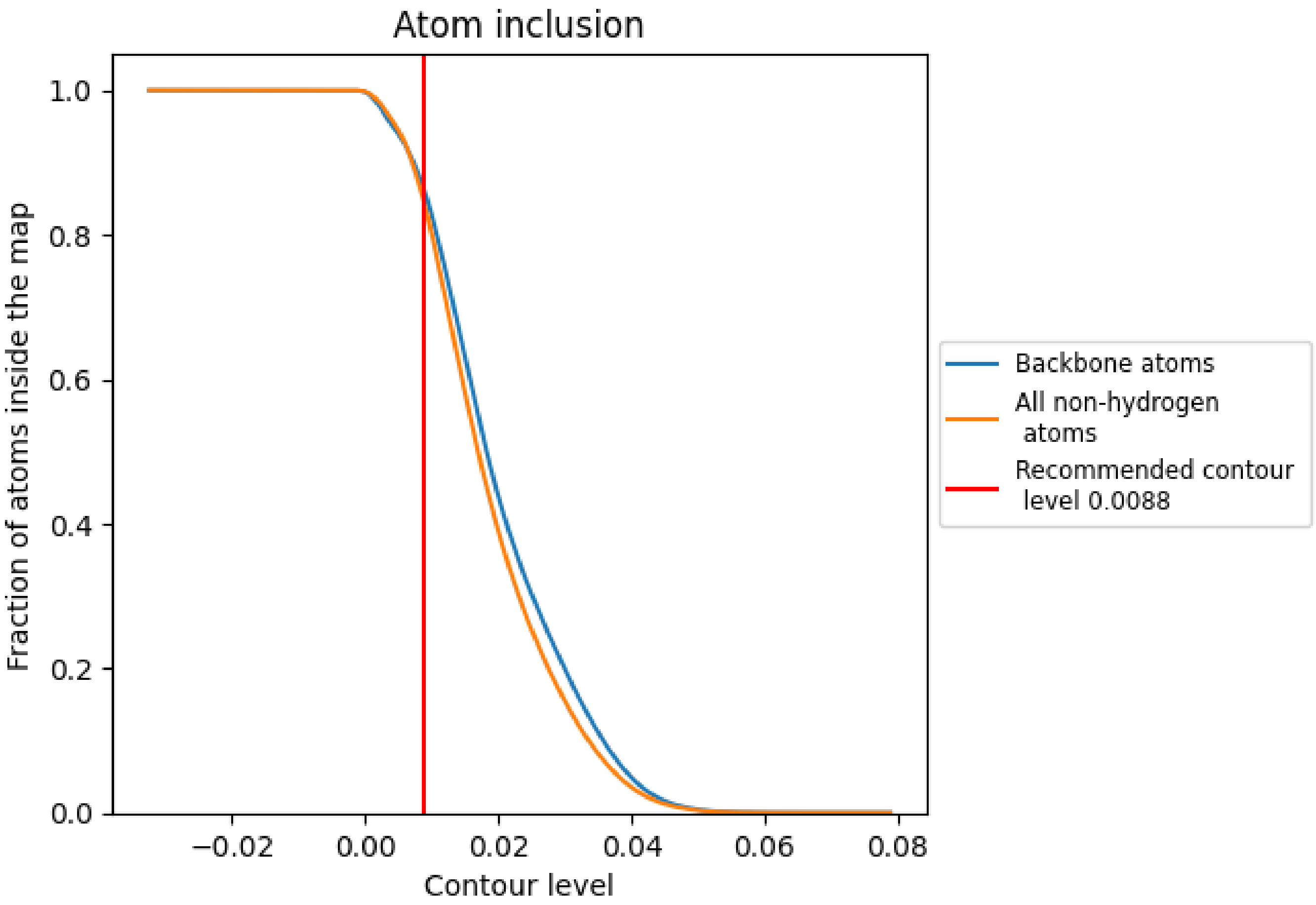
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.0088).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8484	0.3570
L0	0.7814	0.3070
L1	0.8022	0.3010
L2	0.9305	0.3620
L3	0.0543	0.0690
L4	0.9618	0.4020
L5	0.9616	0.4680
L6	0.9006	0.3800
L7	0.8445	0.3190
L8	0.9422	0.3350
L9	0.9752	0.4920
LA	0.0000	0.0350
LC	0.9671	0.4890
LD	0.8486	0.2650
LF	0.9710	0.4790
LG	0.9638	0.4600
LH	0.9374	0.4120
LI	0.7723	0.2440
LJ	0.9200	0.3950
LK	0.7908	0.2460
LL	0.9254	0.4090
LM	0.8783	0.3190
LN	0.9415	0.4040
LO	0.9584	0.4870
LP	0.9321	0.4120
LQ	0.9328	0.4070
LR	0.9678	0.3720
LS	0.9510	0.4730
LT	0.9504	0.4740
LU	0.9552	0.4700
LW	0.9430	0.4660
LZ	0.9620	0.4890
N0	0.8447	0.3530
NA	0.9347	0.4610
NB	0.9863	0.5220

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Chain	Atom inclusion	Q-score
ND	0.8497	0.3200
NE	0.9109	0.3650
NF	0.9400	0.4260
NG	0.9573	0.4040
NH	0.8267	0.2540
NI	0.6592	0.2380
NJ	0.8670	0.3300
NK	0.8966	0.2710
NM	0.8995	0.3880
NN	0.8278	0.2710
NO	0.9485	0.4490
NQ	0.9603	0.4610
NR	0.0002	0.0250
NT	0.0000	0.0080
NU	0.0000	0.0840
NW	0.9186	0.3650
NY	0.8968	0.3690
SA	0.9493	0.4350
SB	0.9130	0.4100
SC	0.8957	0.2880
SD	0.9789	0.5160
SE	0.9717	0.4910
SF	0.9649	0.4780
SG	0.9358	0.3800
SH	0.9593	0.4780
SI	0.9545	0.4650
SJ	0.7988	0.2380
SK	0.8230	0.3470
SL	0.9702	0.4910
SM	0.9655	0.4940
SP	0.7961	0.2360
SQ	0.9286	0.4500
SR	0.9676	0.4990
SS	0.8887	0.4050
ST	0.3477	0.1920
SU	0.5124	0.2310
SW	0.9169	0.3890
SX	0.2249	0.1000
SY	0.9217	0.3800
SZ	0.0062	0.0400