Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 08:57 PM EST

PDB ID	:	7MQ8
EMDB ID	:	EMD-23936
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	:	3.60 Å(reported)
Based on initial models	:	5FAI, 5WLC, 2OZB, 6ZOJ, 6G4S, 6ZQD, 2IPX, 6G18, 4JXM

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

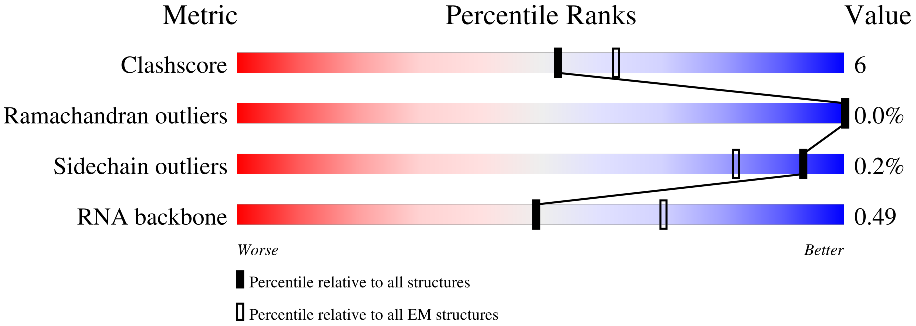
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

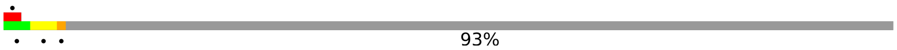
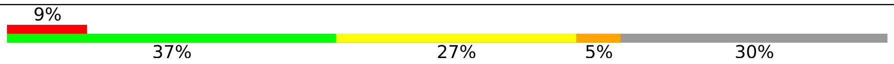
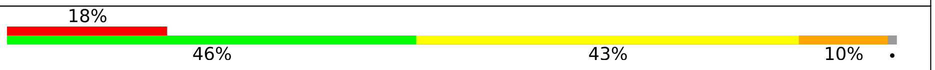
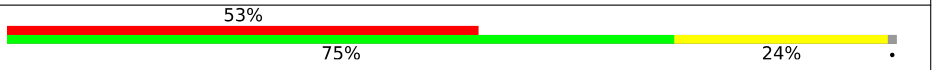
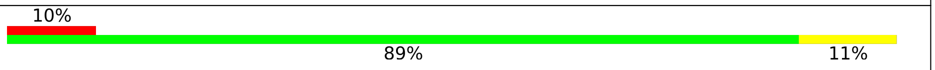
The reported resolution of this entry is 3.60 Å.

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	
2	L1	1869	
3	L2	217	
4	L3	116	
5	L4	263	
6	L5	204	
7	L6	249	

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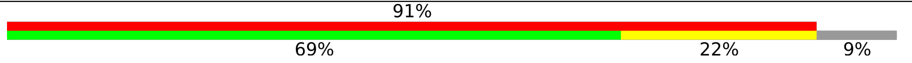
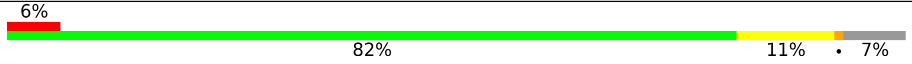
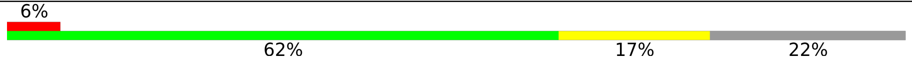
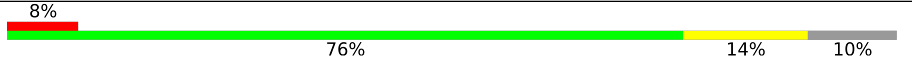
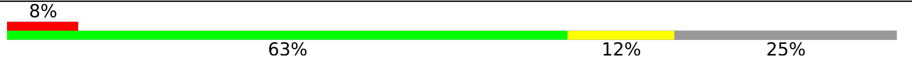
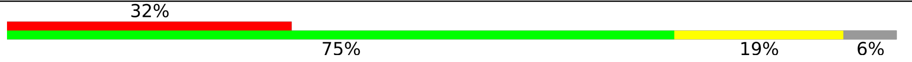
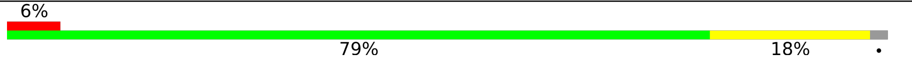
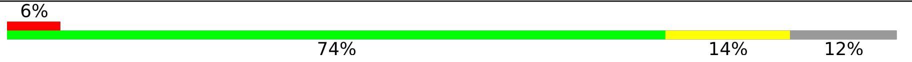
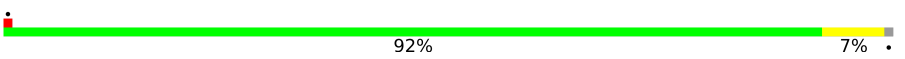
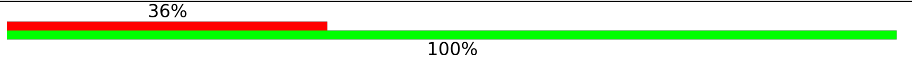
Mol	Chain	Length	Quality of chain
8	L7	194	
9	L8	208	
10	L9	194	
11	LA	132	
12	LC	146	
13	LD	158	
14	LF	133	
15	LG	69	
16	LH	830	
17	LI	678	
18	LJ	518	
19	LK	677	
19	LL	677	
20	LM	2144	
21	LN	686	
22	LO	919	
23	LP	597	
24	LQ	943	
25	LR	808	
26	LS	556	
27	LT	951	
28	LU	445	
29	LW	610	
30	LZ	184	
31	N0	22	

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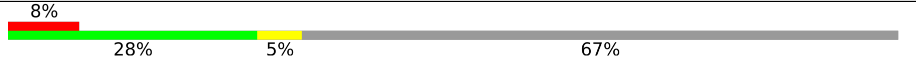
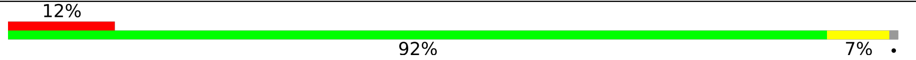
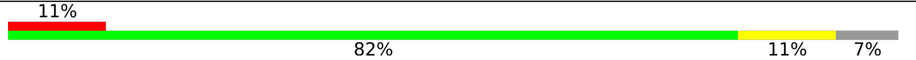
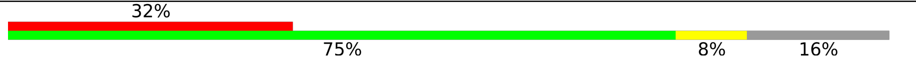
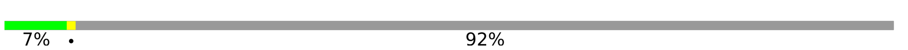
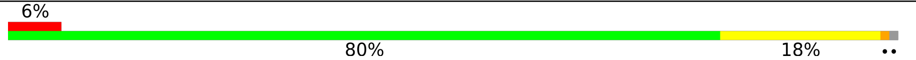
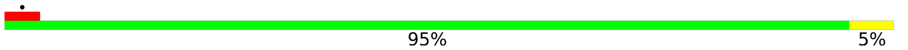
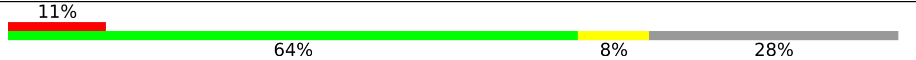
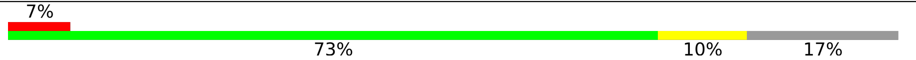
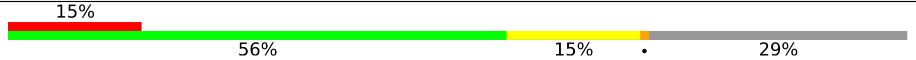
Mol	Chain	Length	Quality of chain
32	NA	681	
33	NB	479	
34	NC	315	
35	ND	257	
36	NE	293	
37	NF	151	
38	NG	151	
39	NH	1146	
40	NI	280	
41	NJ	1025	
41	NK	1025	
42	NM	264	
43	NN	560	
44	NO	130	
45	NQ	84	
46	NR	861	
47	NT	156	
48	NU	135	
49	NW	688	
50	NY	381	
51	SA	594	
52	SB	529	
53	SC	321	
53	SD	321	
54	SE	128	

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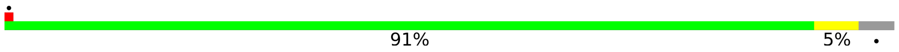
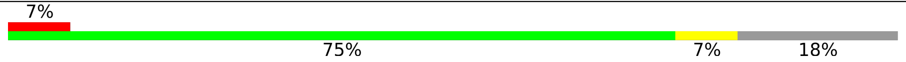
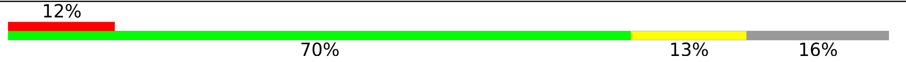
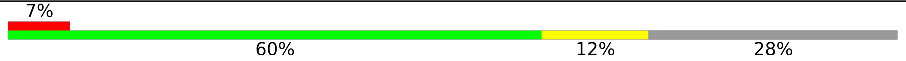
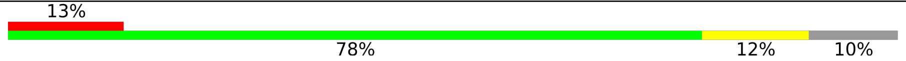
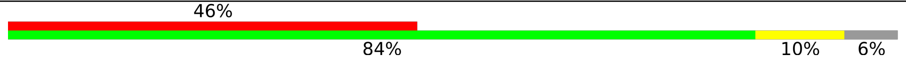
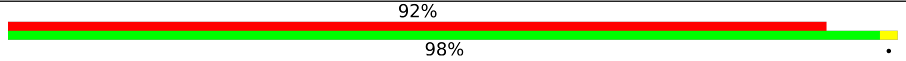
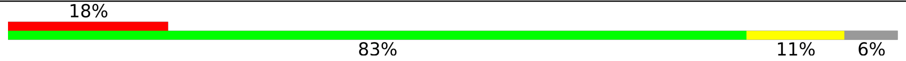
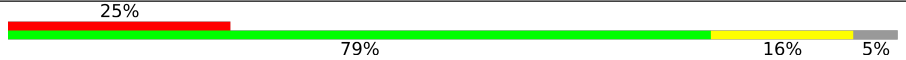
Mol	Chain	Length	Quality of chain
54	SF	128	
55	SG	475	
56	SH	373	
57	SI	1282	
58	SJ	244	
58	SK	244	
59	SL	198	
60	SM	291	
61	SP	2785	
62	SQ	756	
63	SR	143	
64	SS	771	
65	ST	632	
66	SU	472	
67	SW	252	
68	SX	177	
69	SY	253	
70	SZ	304	

2 Entry composition ⓘ

There are 75 unique types of molecules in this entry. The entry contains 245114 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	S		
4	L3	115	854	538	164	151	1	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	262	2076	1324	386	358	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	S		
11	LA	120	931	584	164	174	9	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	S		
17	LI	537	3889	2508	654	706	21	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 HEAT repeat-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LM	2005	15820	10259	2597	2883	81	0	0

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 4 homolog.

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

- Molecule 22 is a protein called Periodic tryptophan protein 2 homolog.

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

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 6 homolog.

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

- Molecule 24 is a protein called WD repeat-containing protein 3.

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

- Molecule 25 is a protein called Transducin beta-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LR	773	6015	3789	1079	1116	31	0	0

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 18 homolog.

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

- Molecule 27 is a protein called WD repeat-containing protein 36.

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

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

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

- Molecule 29 is a protein called WD repeat-containing protein 46.

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

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

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

- Molecule 31 is a RNA chain called 5’ETS rRNA.

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

- Molecule 32 is a protein called U3 small nucleolar ribonucleoprotein protein MPP10.

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

- Molecule 33 is a protein called Something about silencing protein 10.

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

- Molecule 34 is a protein called Neuroguidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	NC	94	779	469	160	147	3	0	0

- Molecule 35 is a protein called Nucleolar protein 7.

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

- Molecule 36 is a protein called Uncharacterized protein C1orf131.

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

- Molecule 37 is a protein called 40S ribosomal protein S13.

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

- Molecule 38 is a protein called 40S ribosomal protein S14.

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

- Molecule 39 is a protein called Nucleolar protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NH	1066	Total 8374	C 5345	N 1491	O 1506	S 32	0	0

- Molecule 40 is a protein called Ribosomal RNA-processing protein 7 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NI	234	Total 1840	C 1171	N 329	O 336	S 4	0	0

- Molecule 41 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NJ	827	Total 6526	C 4187	N 1126	O 1178	S 35	0	0
41	NK	815	Total 6419	C 4118	N 1109	O 1160	S 32	0	0

- Molecule 42 is a protein called 40S ribosomal protein S3a.

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

- Molecule 43 is a protein called Protein AATF.

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

- Molecule 44 is a protein called 40S ribosomal protein S15a.

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

- Molecule 45 is a protein called 40S ribosomal protein S27.

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

- Molecule 46 is a protein called RRP12-like protein.

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

- Molecule 47 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	NT	58	Total 470	C 295	N 89	O 79	S 7	0	0

- Molecule 48 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	NU	60	Total 495	C 314	N 98	O 81	S 2	0	0

- Molecule 49 is a protein called Nucleolar protein 10.

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

- Molecule 50 is a protein called KRR1 small subunit processome component homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	NY	274	2222	1422	391	400	9	0	0

- Molecule 51 is a protein called Nucleolar protein 56.

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

- Molecule 52 is a protein called Nucleolar protein 58.

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

- Molecule 53 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

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

- Molecule 54 is a protein called NHP2-like protein 1.

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

- Molecule 55 is a protein called U3 small nucleolar RNA-interacting protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SG	389	2884	1809	534	528	13	1	0

- Molecule 56 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 57 is a protein called Ribosome biogenesis protein BMS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SI	844	Total 6803	C 4351	N 1230	O 1188	S 34	0	0

- Molecule 58 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

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

- Molecule 59 is a protein called rRNA-processing protein FCF1 homolog.

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

- Molecule 60 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

- Molecule 61 is a protein called Small subunit processome component 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SP	1993	Total 16078	C 10412	N 2689	O 2897	S 80	0	0

- Molecule 62 is a protein called Deoxynucleotidyltransferase terminal-interacting protein 2.

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

- Molecule 63 is a protein called 40S ribosomal protein S23.

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

- Molecule 64 is a protein called U3 small nucleolar RNA-associated protein 14 homolog A.

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

- Molecule 65 is a protein called Nucleolar protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	ST	568	4170	2634	760	755	21	0	0

- Molecule 66 is a protein called Nucleolar complex protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SU	442	3154	2030	565	551	8	0	0

- Molecule 67 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	SW	180	1413	906	257	246	4	0	0

- Molecule 68 is a protein called Unassigned peptides.

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

- Molecule 69 is a protein called Probable U3 small nucleolar RNA-associated protein 11.

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

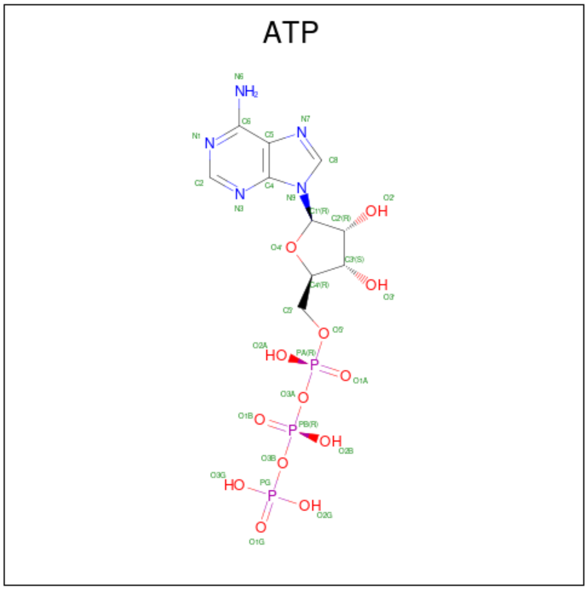
- Molecule 70 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	SZ	290	2222	1438	392	383	9	0	0

- Molecule 71 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 72 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

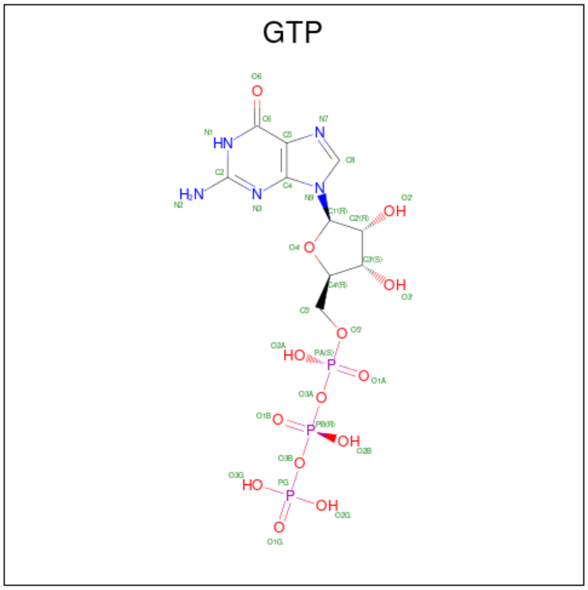


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
72	NH	1	31	10	5	13	3	0
72	NK	1	31	10	5	13	3	0

- Molecule 73 is ZINC ION (three-letter code: ZN) (formula: Zn).

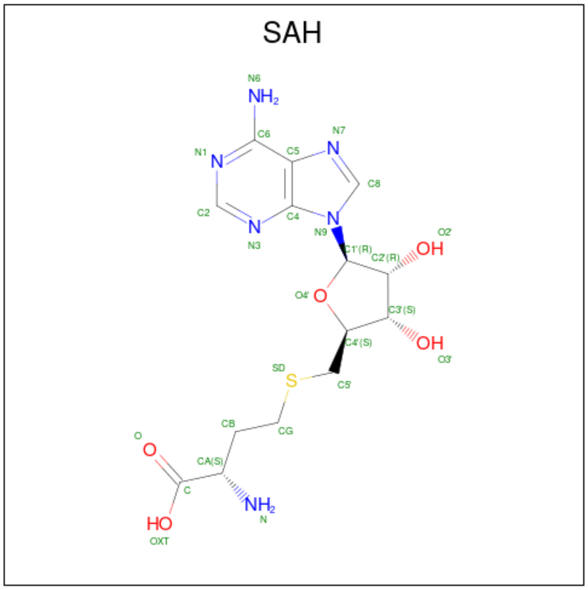
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
73	NQ	1	1	1	0
73	NT	1	Total 1	Zn 1	0
73	SL	1	Total 1	Zn 1	0

- Molecule 74 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 75 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

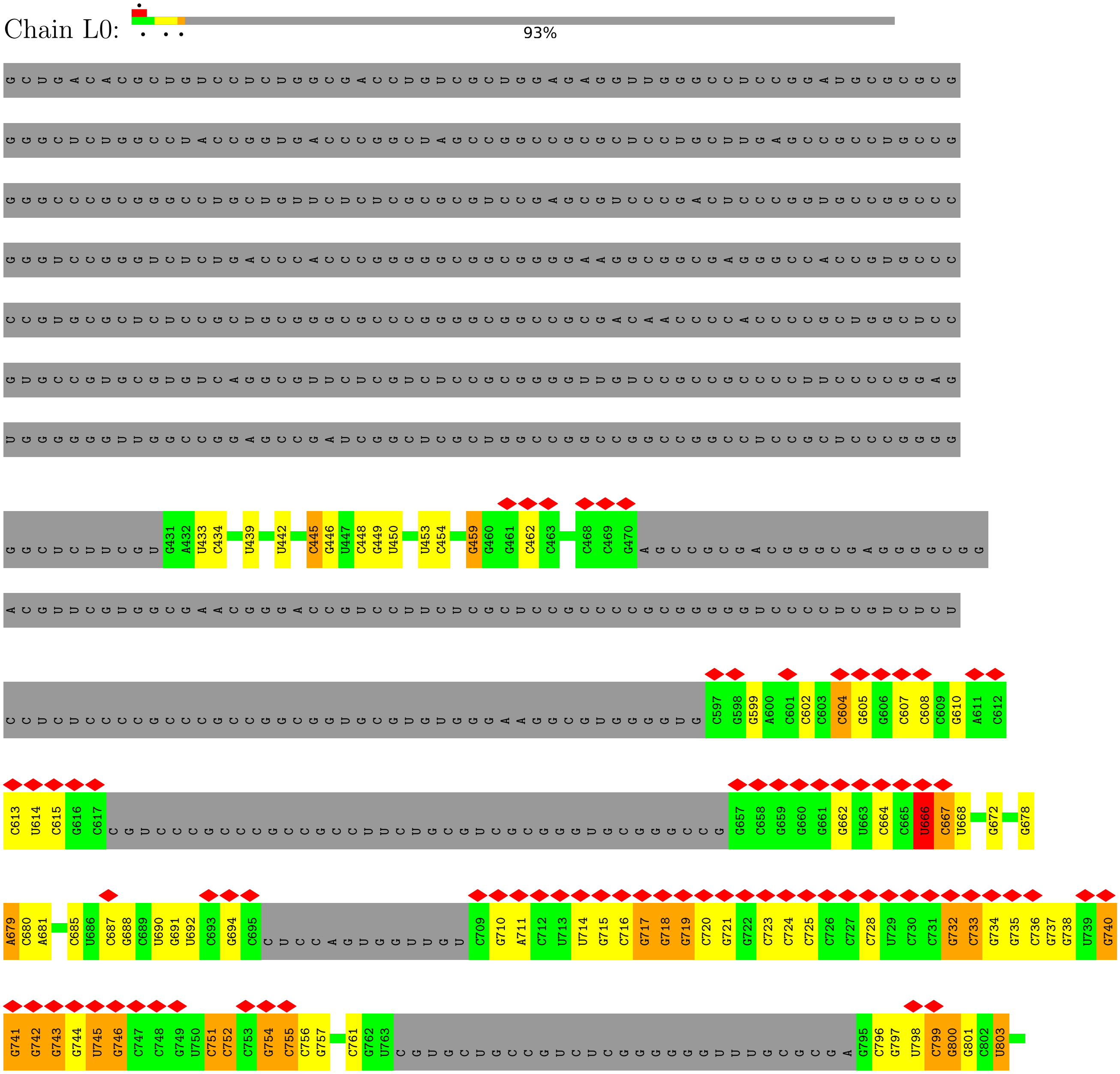


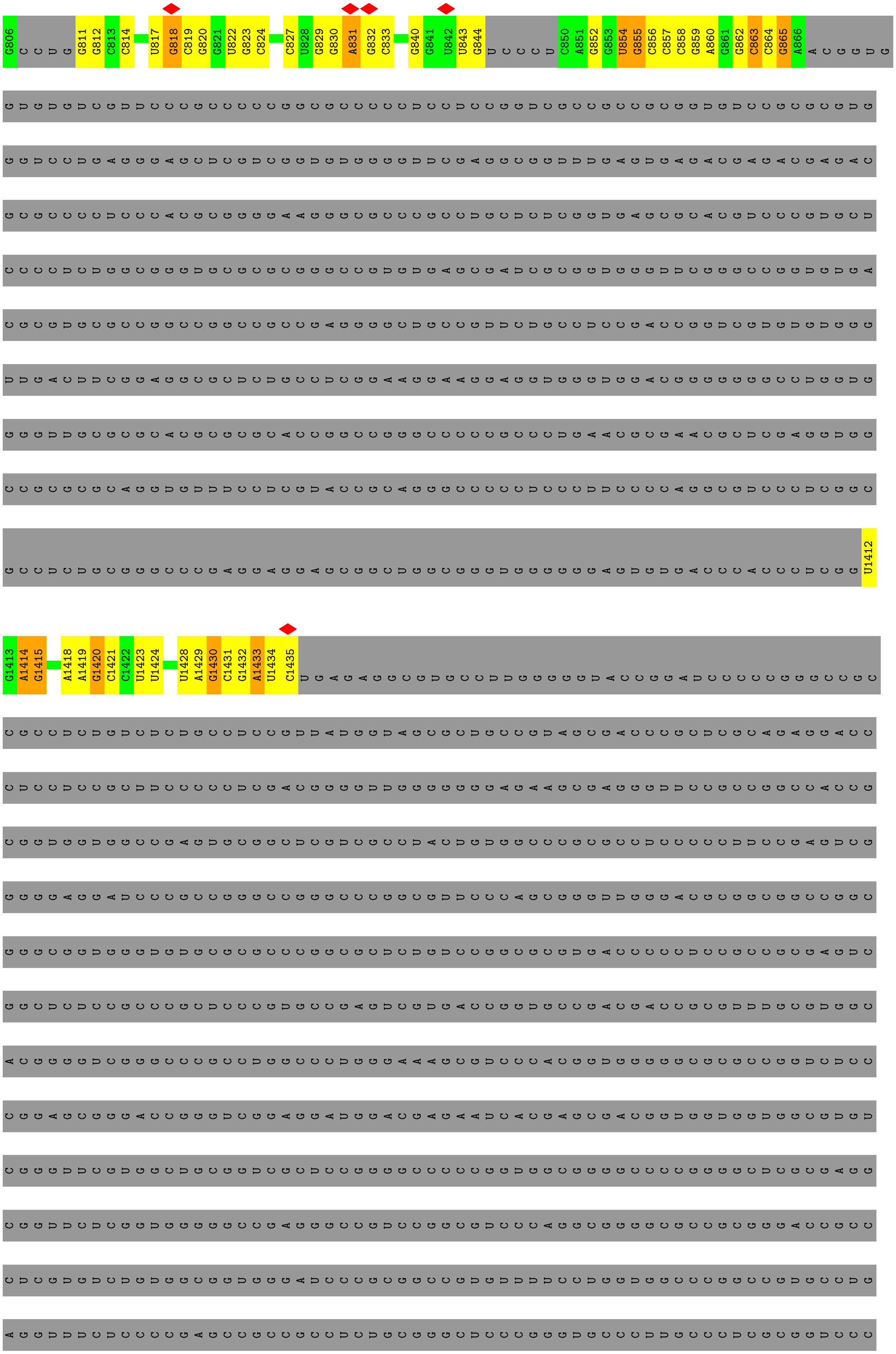
Mol	Chain	Residues	Atoms	AltConf
75	SJ	1	Total C N O S 26 14 6 5 1	0
75	SK	1	Total C N O S 26 14 6 5 1	0

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
U817
G818
C819
G820
G821
U822
G823
C824
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U828
G829
G830
A831
G832
C833
G840
G841
U842
U843
G844
C850
A851
G852
G853
U854
G855
C856
C857
C858
G859
A860
G861
G862
C863
C864
G865
A866
U1412
G1413
A1414
G1415
A1418
A1419
G1420
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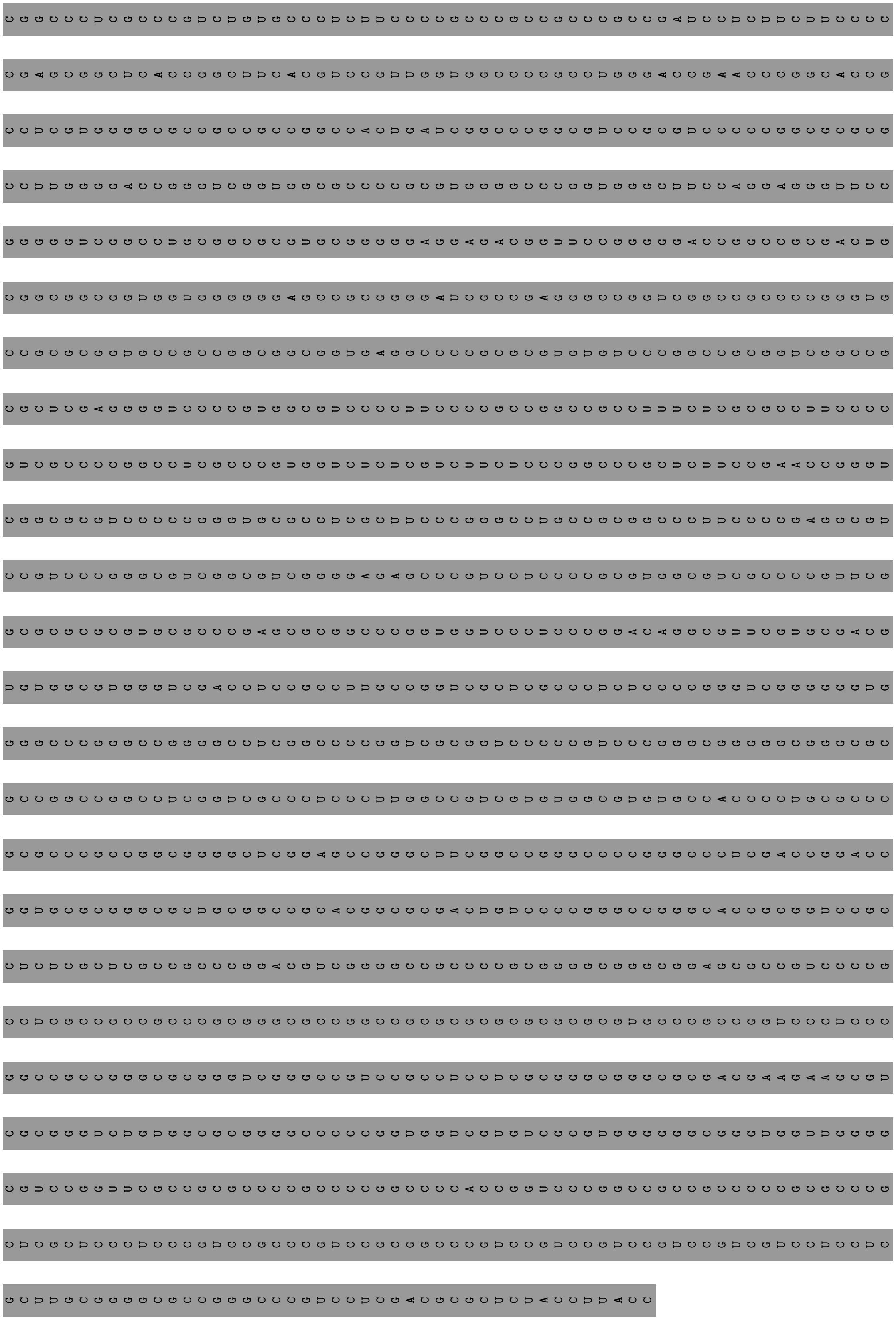
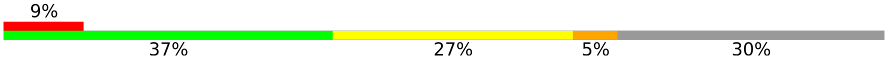
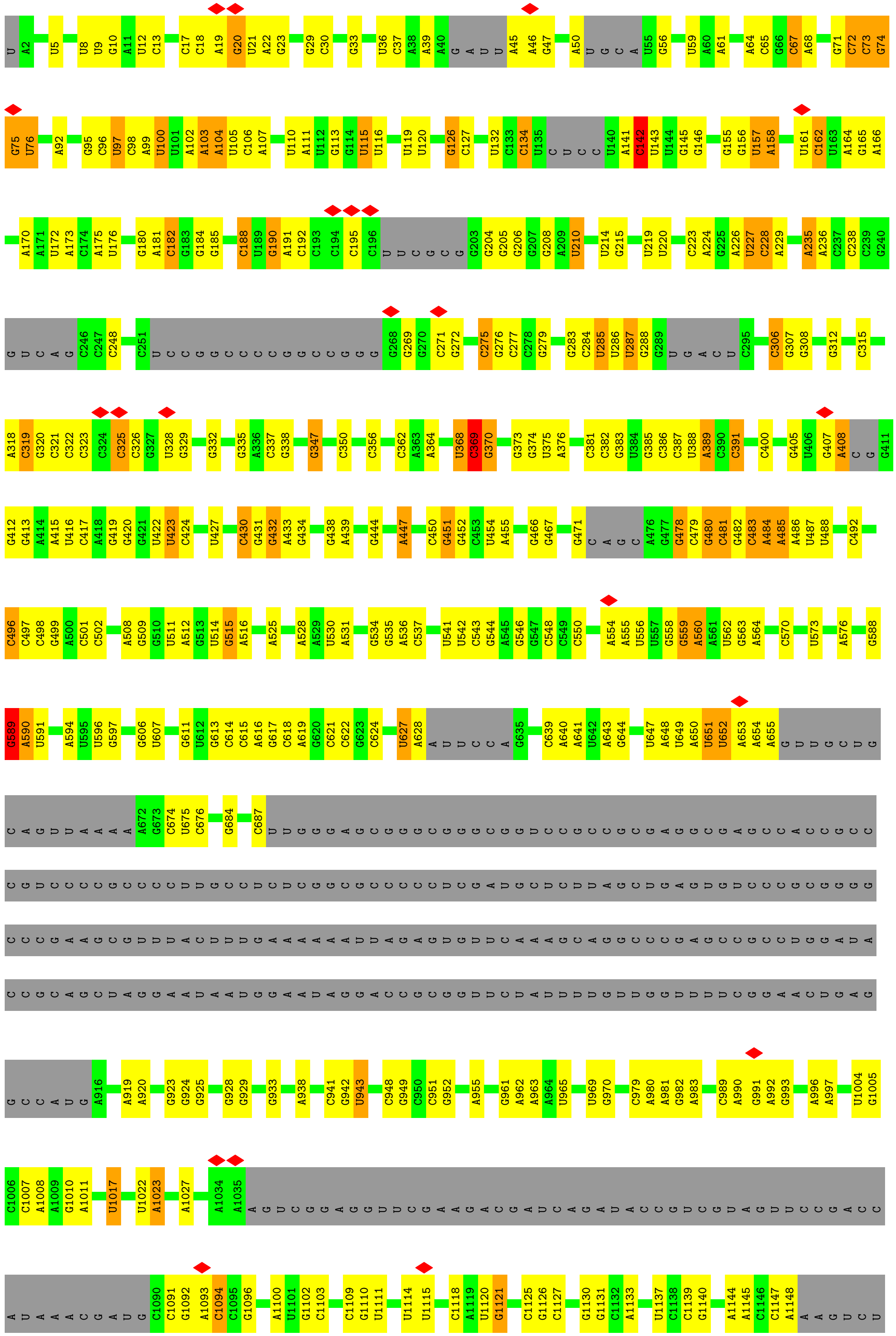
U1434
C1435

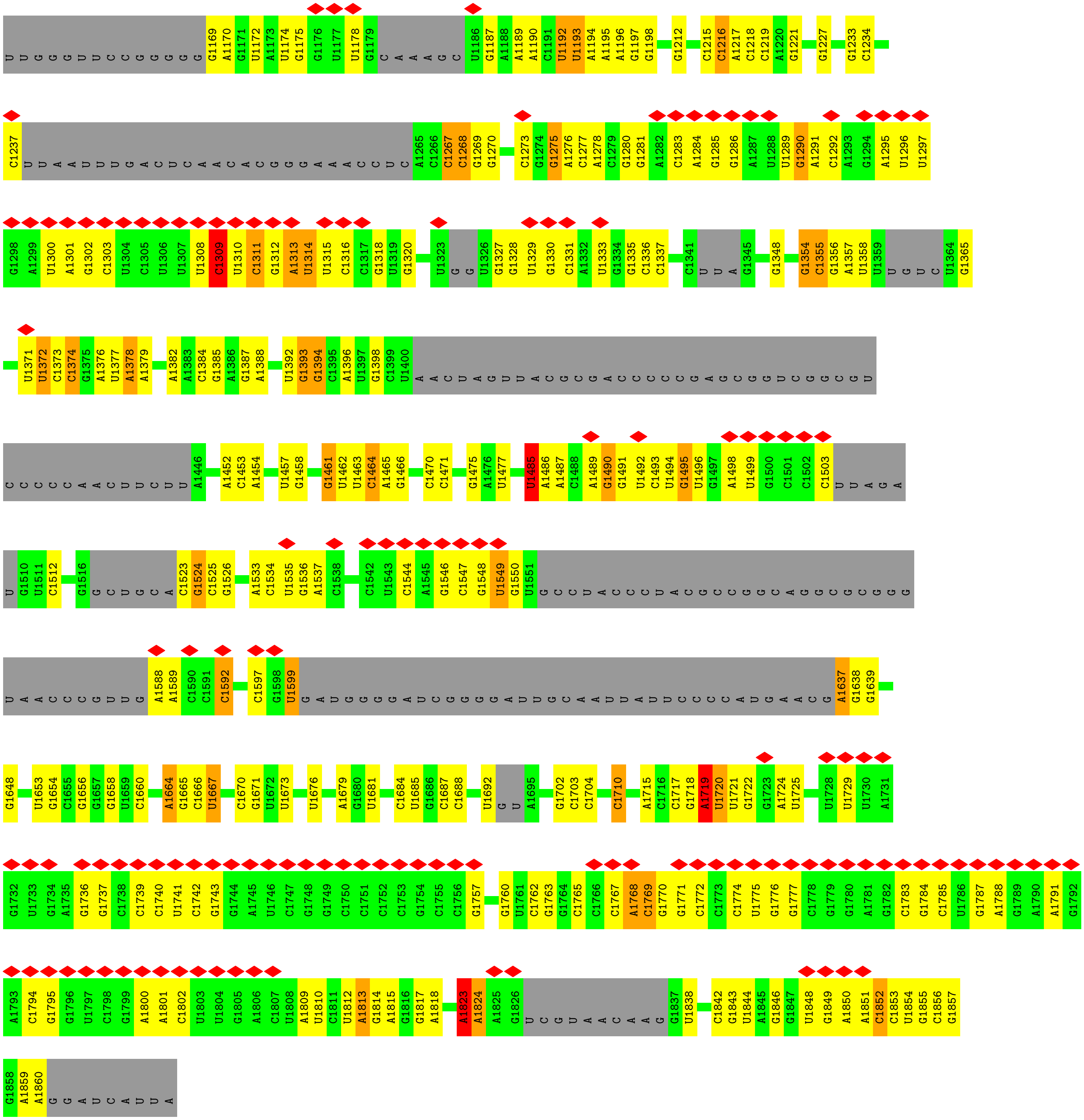


- Molecule 2: 18S rRNA

Chain L1:

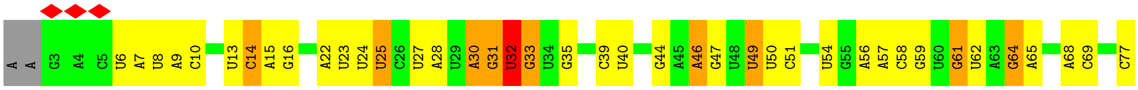


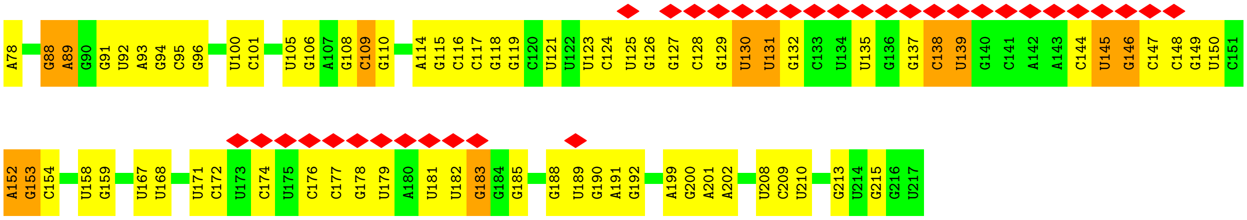

U A2 U5 U8 U9 G10 A11 U12 C13 C17 C18 A19 G20 U21 A22 G23 G29 C30 G33 U36 C37 A38 A39 A40 G A U U A45 A46 G47 A50 U G C A U55 G56 U59 A60 A61 A64 C65 G66 C67 A68 G71 C72 C73 G74
G75 U76 A92 G95 C96 U97 C98 A99 U100 U101 A102 A103 A104 U105 C106 A107 U110 A111 U112 G113 G114 U115 U116 U119 U120 G126 C127 U132 C133 C134 U135 C U C C U140 A141 C142 U143 U144 G145 G146 G155 G156 U157 A158 U161 C162 U163 A164 G165 A166
A170 A171 U172 A173 C174 A175 U176 G180 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 A235 A236 C237 C238 C239 G240
G U C A G C246 C247 C248 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 G279 G283 C284 U285 U286 U287 G288 G289 U G A C U C295 C306 G307 G308 G312 C315
A318 C319 G320 C321 C322 C323 C324 C325 C326 G327 U328 G329 G332 G335 A336 C337 G338 G347 C350 C356 C362 A363 A364 U368 C369 G370 G373 G374 U375 A376 C381 C382 G383 U384 G385 C386 C387 U388 A389 C390 C391 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 G438 A439 G444 A447 C450 G451 G452 C453 U454 A455 G466 G467 G471 C A G C A476 G477 G478 C479 G480 C481 G482 C483 A484 A485 A486 U487 U488 C492
C496 C497 C498 G499 A500 C501 C502 A508 G509 G510 U511 A512 G513 U514 G515 A516 A525 A528 A529 U530 A531 G534 G535 A536 C537 U541 U542 C543 G544 A545 G546 G547 C548 C549 C550 A554 A555 U556 U557 G558 G559 A560 A561 U562 G563 A564 C570 U573 A576 G588
G589 A590 U591 A594 U595 U596 G597 G606 U607 G611 U612 G613 C614 C615 A616 G617 C618 A619 G620 C621 C622 G623 C624 U627 A628 A U U C C A G635 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 C676 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 G C G A G G C G A G C C A C C G C C
C G U C 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 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 C A A A G C A G G C C C G A G C C G 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 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 G923 G924 G925 G928 G929 G933 A938 C941 G942 U943 C948 G949 C950 C951 G952 A955 G961 A962 A963 A964 U965 U969 G970 C979 A980 A981 G982 A983 C989 A990 G991 A992 G993 A996 A997 U1004 G1005
C1006 C1007 A1008 A1009 G1010 A1011 U1017 U1022 A1023 A1027 A1034 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 C1109 G1110 U1111 U1114 U1115 C1118 A1119 U1120 G1121 C1125 C1126 C1127 G1130 G1131 C1132 A1133 U1137 C1138 C1139 G1140 A1144 A1145 C1146 C1147 A1148 A A G U C U



- Molecule 3: U3 snoRNA

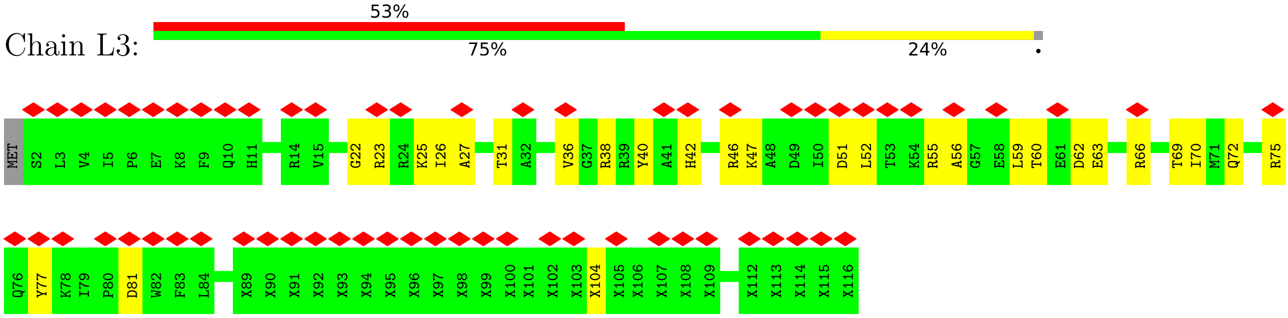
Chain L2:





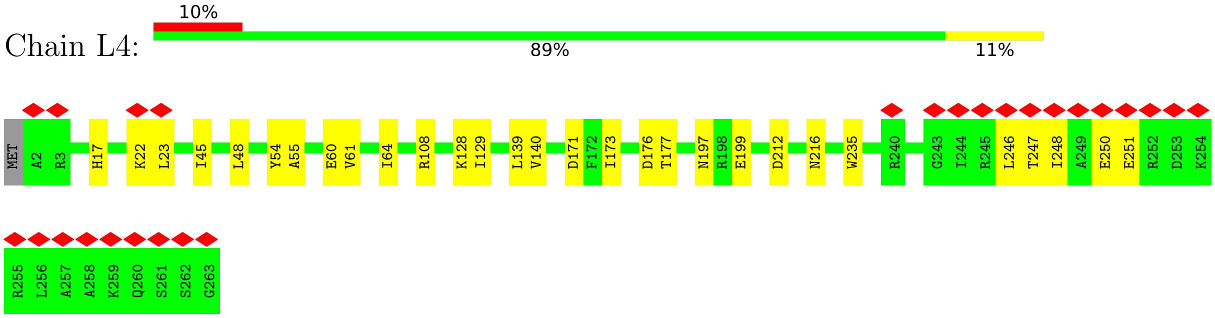
- Molecule 4: 40S ribosomal protein S18

Chain L3:



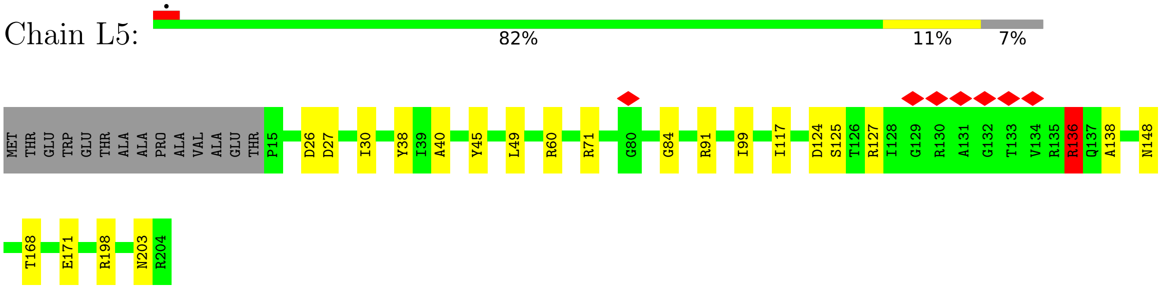
- Molecule 5: 40S ribosomal protein S4, X isoform

Chain L4:



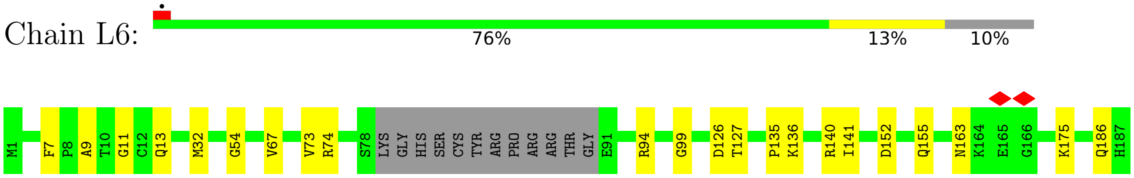
- Molecule 6: 40S ribosomal protein S5

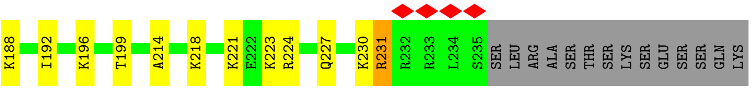
Chain L5:



- Molecule 7: 40S ribosomal protein S6

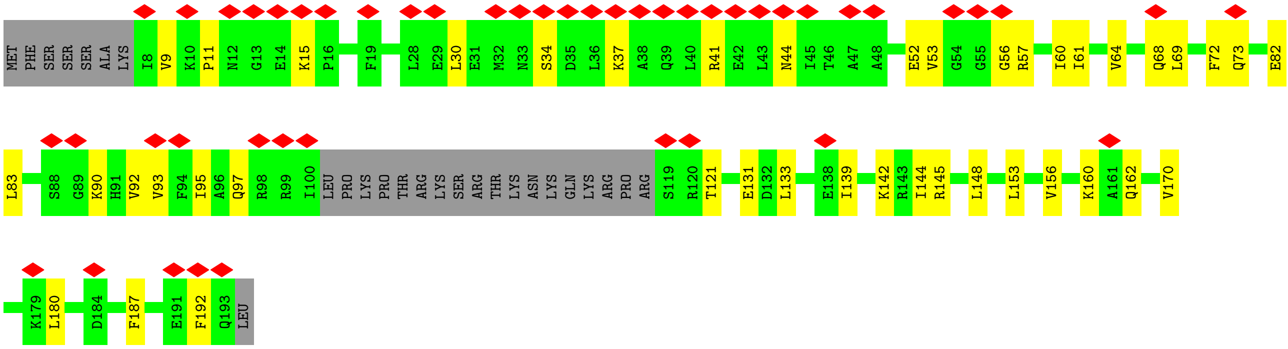
Chain L6:





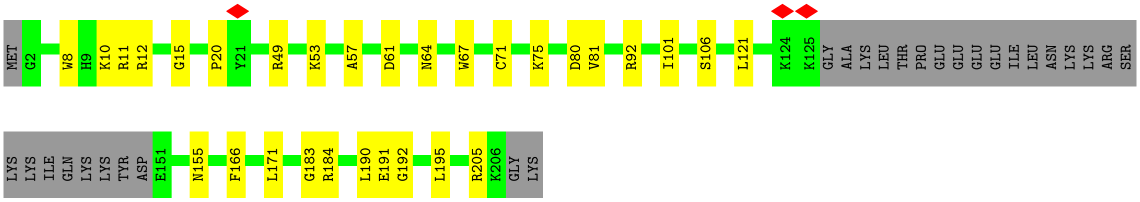
- Molecule 8: 40S ribosomal protein S7

Chain L7:



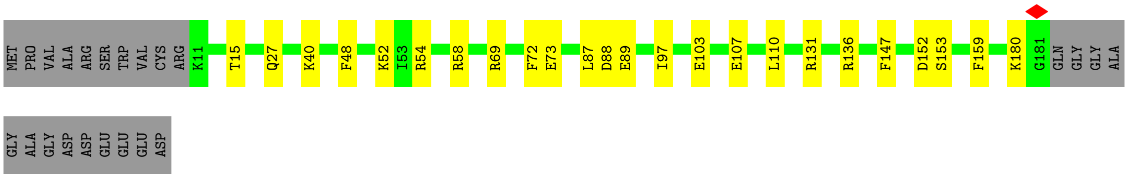
- Molecule 9: 40S ribosomal protein S8

Chain L8:



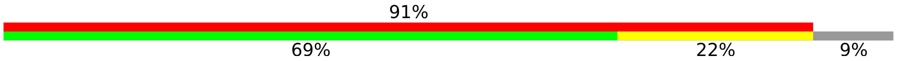
- Molecule 10: 40S ribosomal protein S9

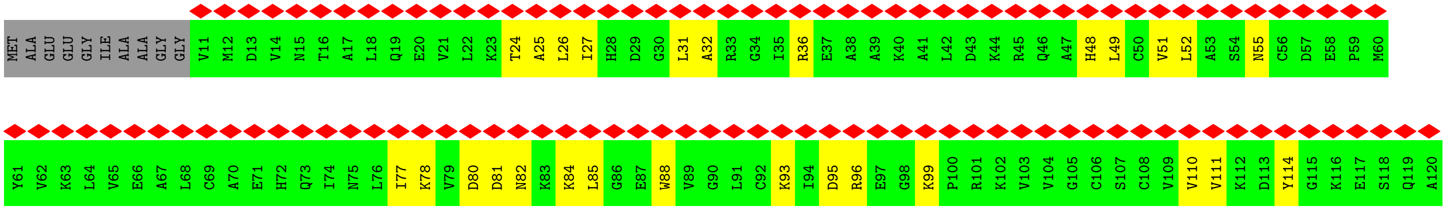
Chain L9:

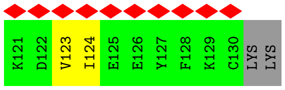


- Molecule 11: 40S ribosomal protein S12

Chain LA:

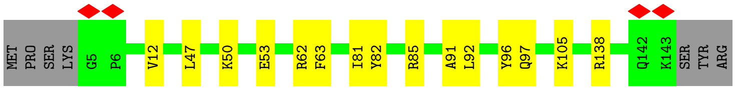






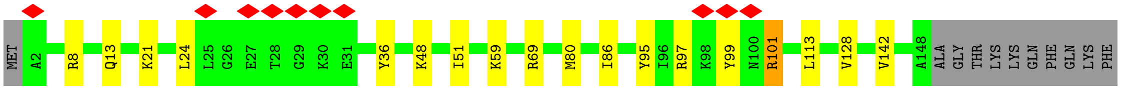
- Molecule 12: 40S ribosomal protein S16

Chain LC:



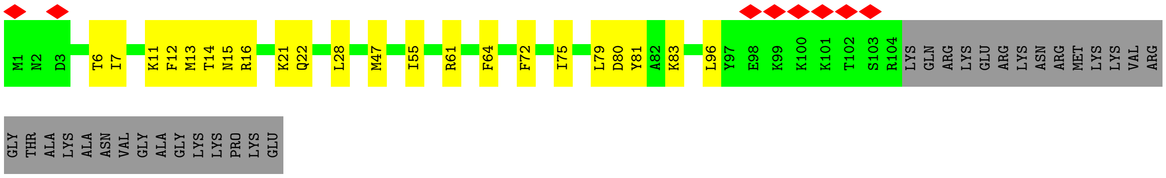
- Molecule 13: 40S ribosomal protein S11

Chain LD:



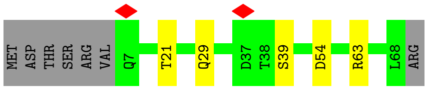
- Molecule 14: 40S ribosomal protein S24

Chain LF:



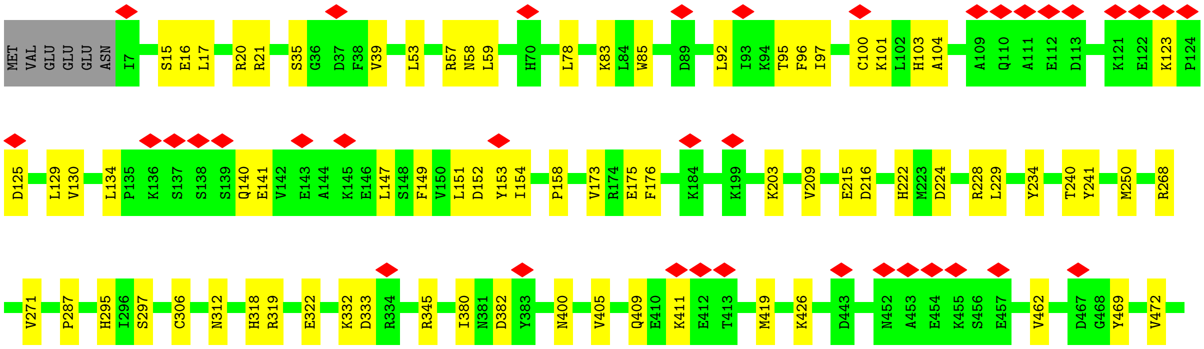
- Molecule 15: 40S ribosomal protein S28

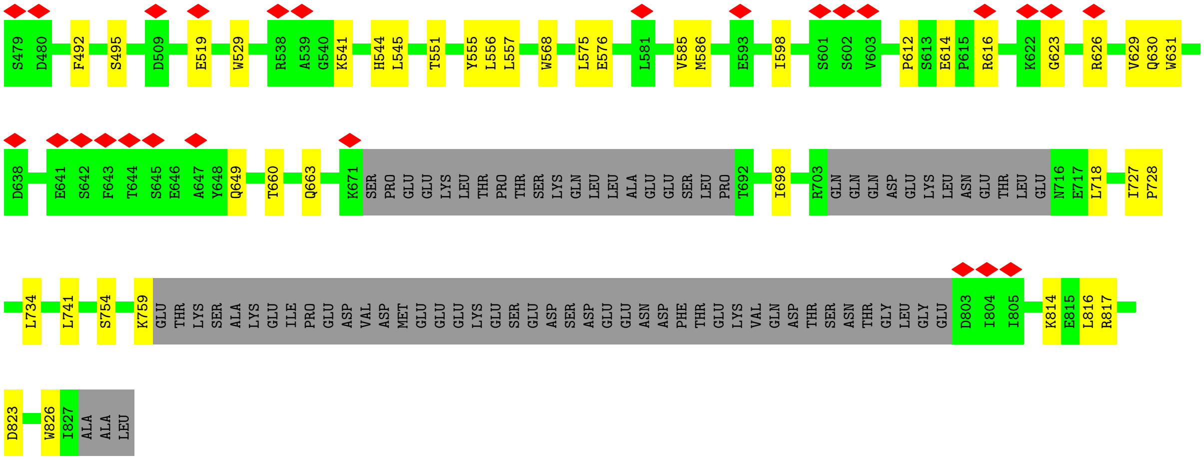
Chain LG:



- Molecule 16: WD repeat-containing protein 75

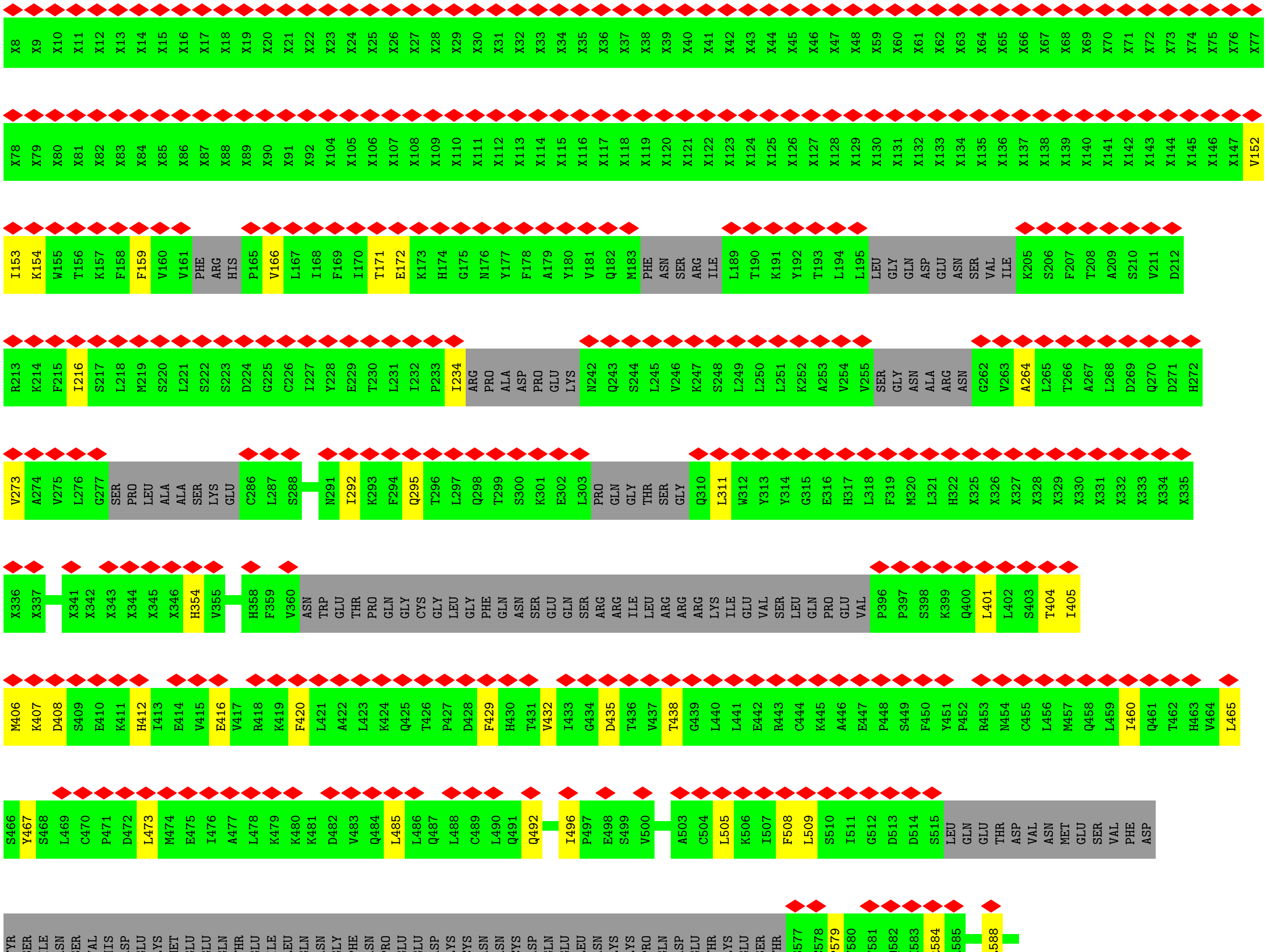
Chain LH:

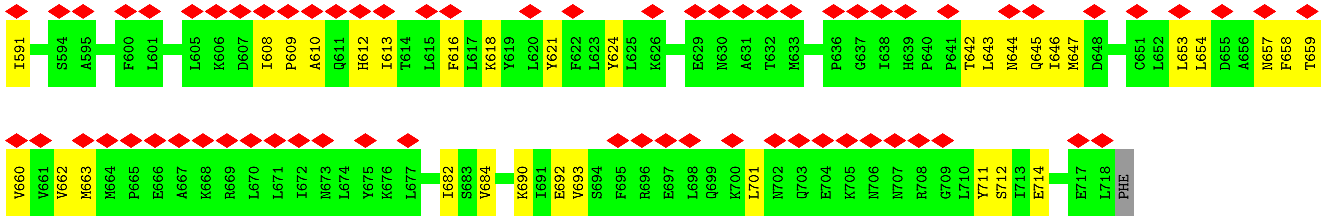




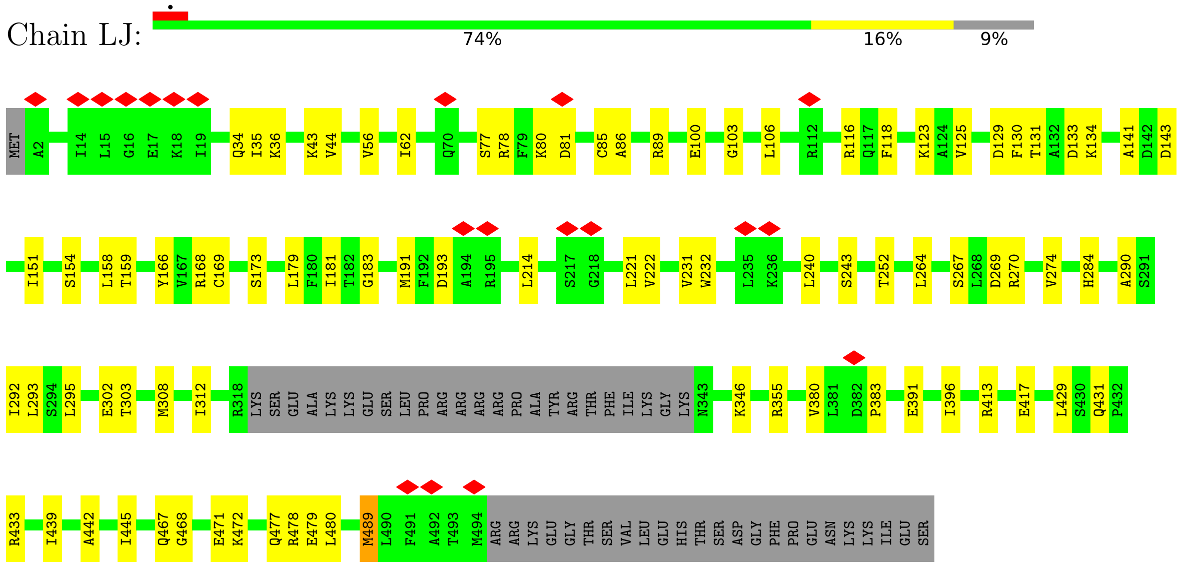
- Molecule 17: Nucleolar protein 11

Chain LI:

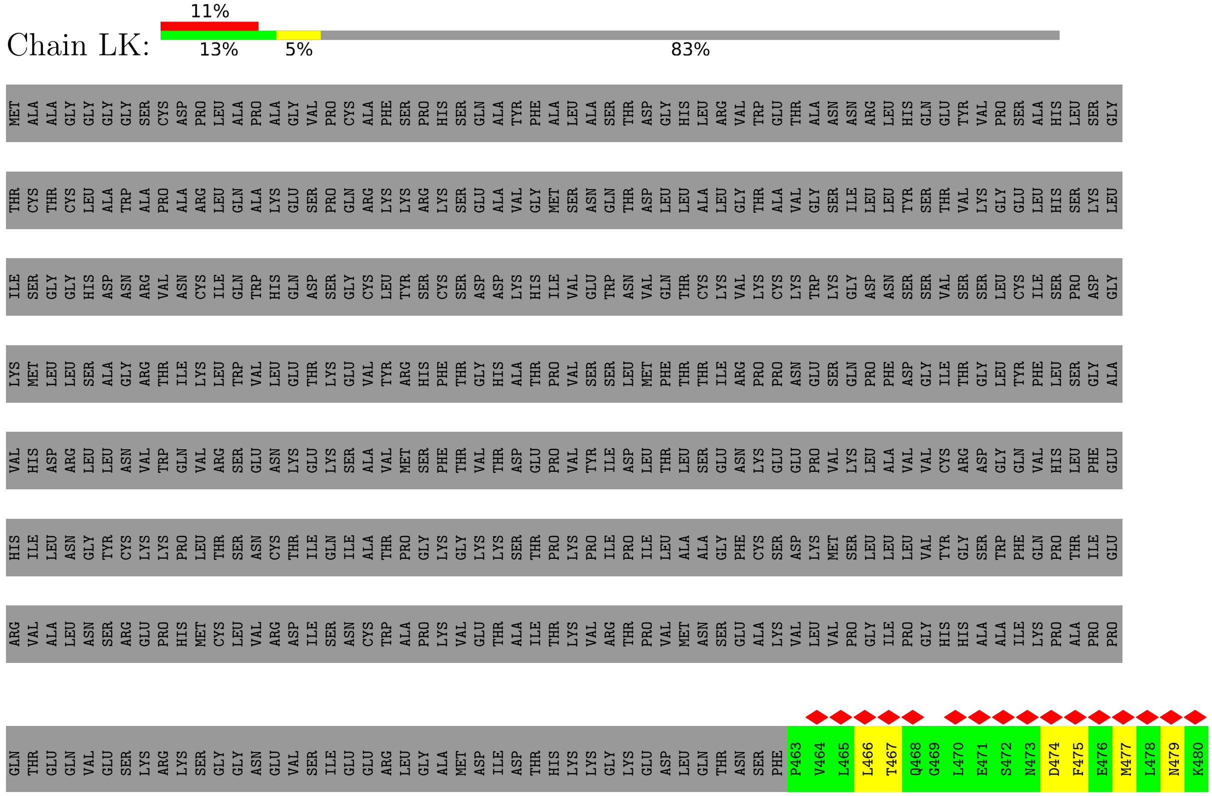


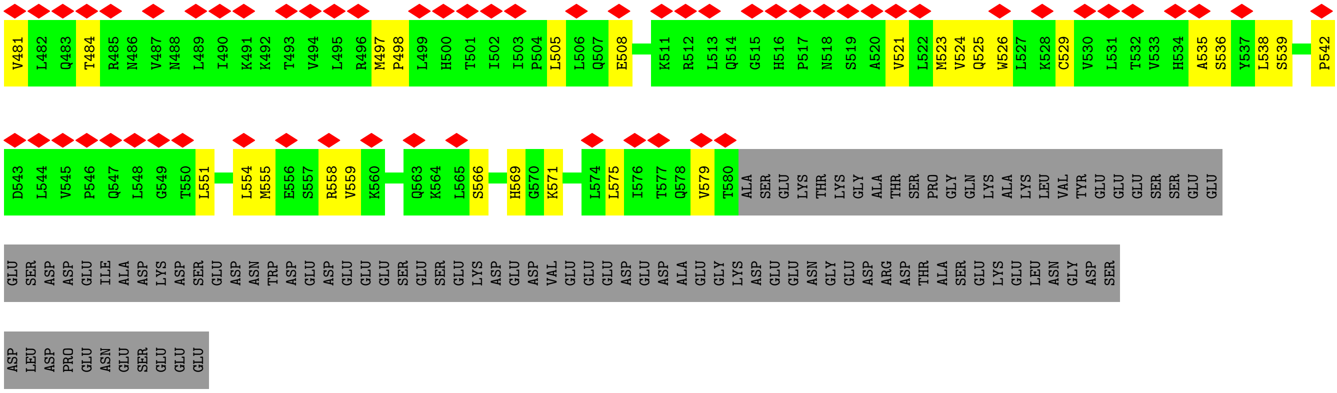


- Molecule 18: U3 small nucleolar RNA-associated protein 15 homolog



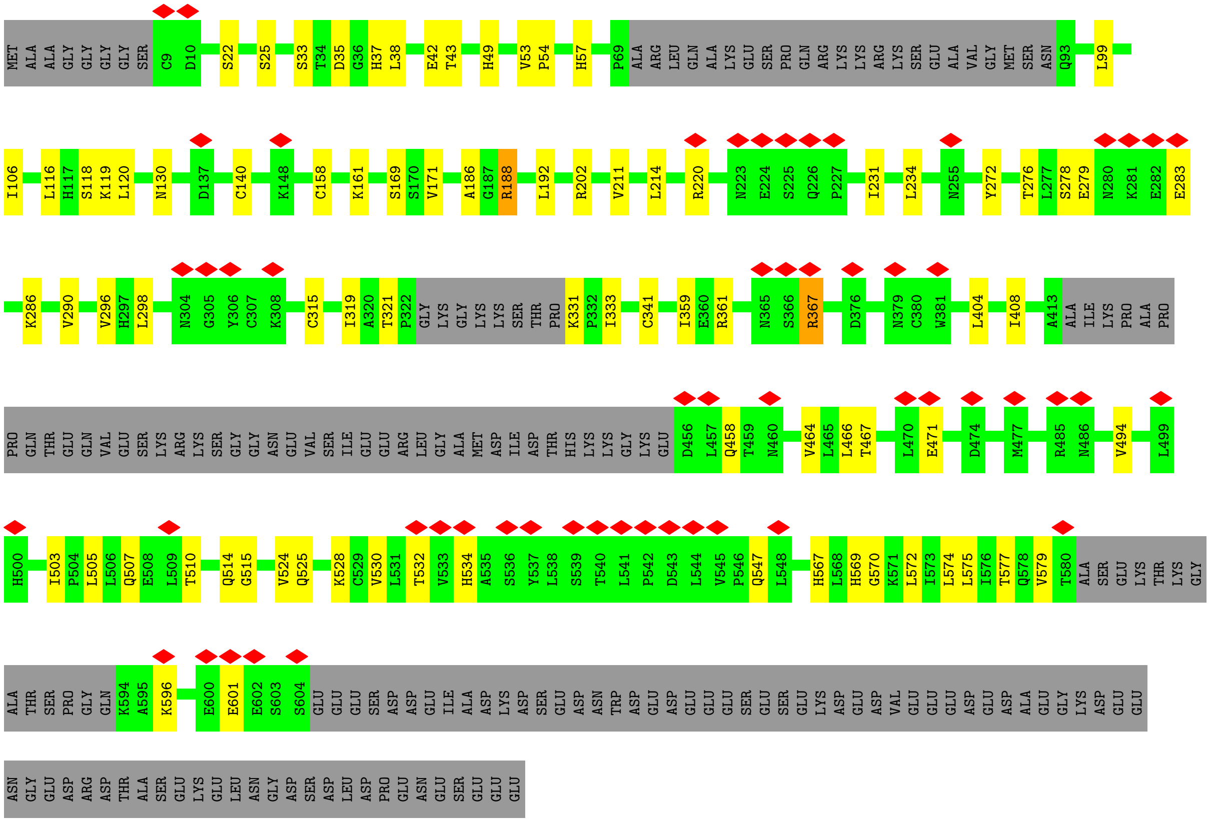
- Molecule 19: WD repeat-containing protein 43





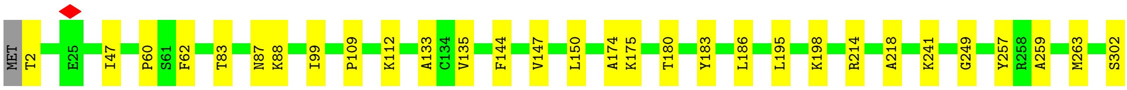
- Molecule 19: WD repeat-containing protein 43

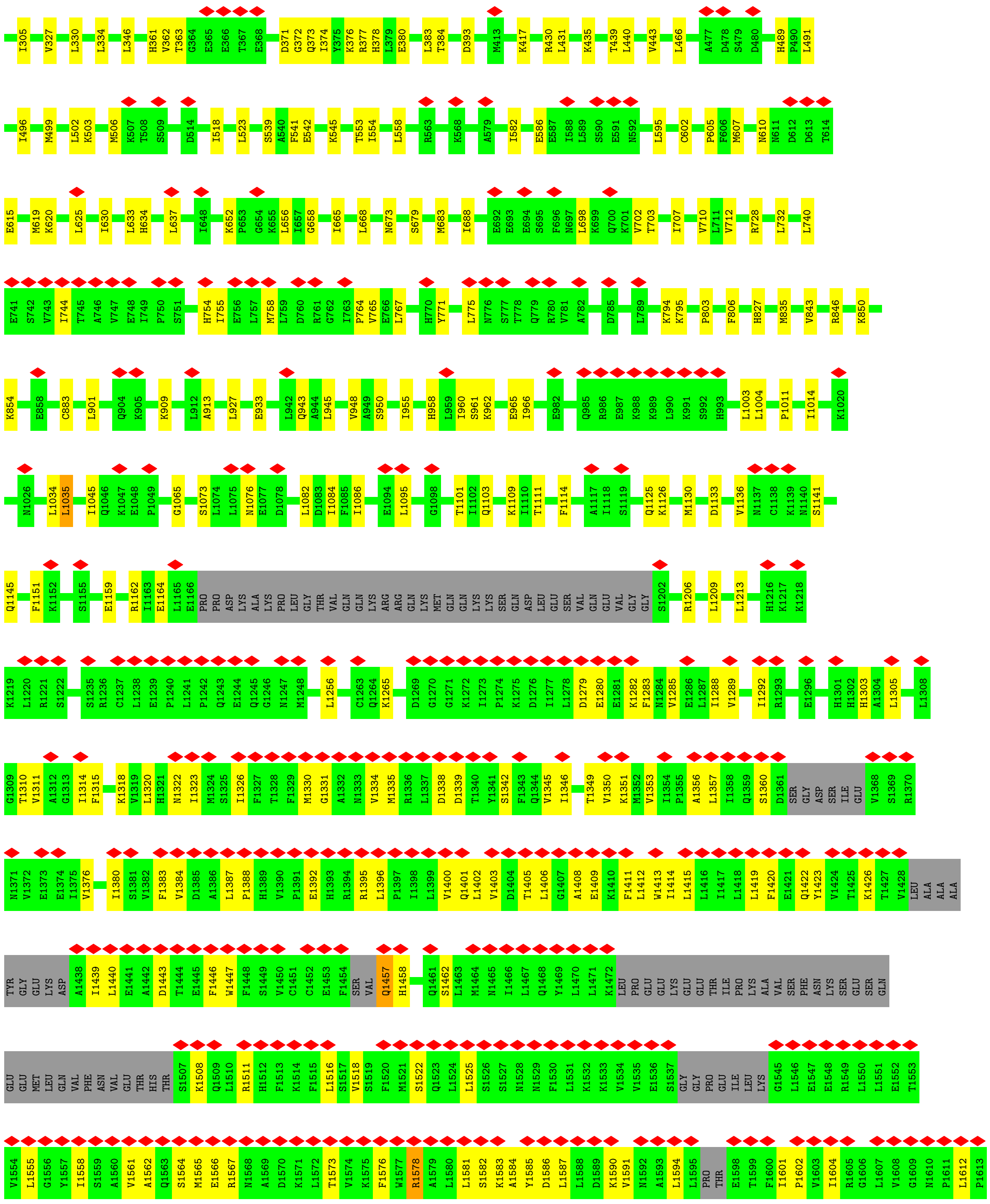
Chain LL:



- Molecule 20: HEAT repeat-containing protein 1

Chain LM:

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Q1145 F1151 K1152 S1155 E1159 R1162 I1163 E1164 L1165 E1166 PRO PRO ASP LYS ALA LYS PRO LEU GLY THR VAL GLN GLN LYS ARG ARG GLN LYS MET GLN GLN LYS LYS SER GLN ASP LEU GLU SER VAL GLN GLU VAL GLY GLY S1202 R1206 L1209 L1213 H1216 K1217 K1218
K1219 L1220 R1221 S1222 S1235 R1236 C1237 L1238 E1239 P1240 L1241 P1242 Q1243 E1244 Q1245 G1246 N1247 M1248 L1256 C1263 Q1264 K1265 D1269 G1270 G1271 K1272 I1273 P1274 K1275 D1276 I1277 L1278 D1279 E1280 E1281 K1282 F1283 N1284 V1285 E1286 L1287 I1288 V1289 I1292 R1293 E1296 H1301 H1302 H1303 A1304 L1305 L1308
G1309 T1310 V1311 A1312 G1313 I1314 F1315 K1318 V1319 L1320 H1321 N1322 I1323 M1324 S1325 I1326 F1327 T1328 F1329 M1330 G1331 A1332 N1333 V1334 M1335 R1336 L1337 D1338 D1339 T1340 Y1341 S1342 F1343 Q1344 V1345 I1346 T1349 V1350 K1351 M1352 V1353 I1354 P1355 A1356 L1357 I1358 Q1359 S1360 D1361 SER GLY ASP SER ILE GLU V1368 S1369 R1370
N1371 V1372 E1373 E1374 I1375 V1376 I1380 S1381 V1382 F1383 V1384 D1385 A1386 L1387 P1388 H1389 V1390 P1391 E1392 H1393 R1394 R1395 L1396 P1397 I1398 L1399 V1400 Q1401 L1402 V1403 D1404 T1405 L1406 G1407 A1408 E1409 K1410 F1411 L1412 W1413 I1414 L1415 L1416 I1417 L1418 L1419 F1420 E1421 Q1422 Y1423 V1424 T1425 K1426 T1427 V1428 LEU ALA ALA ALA
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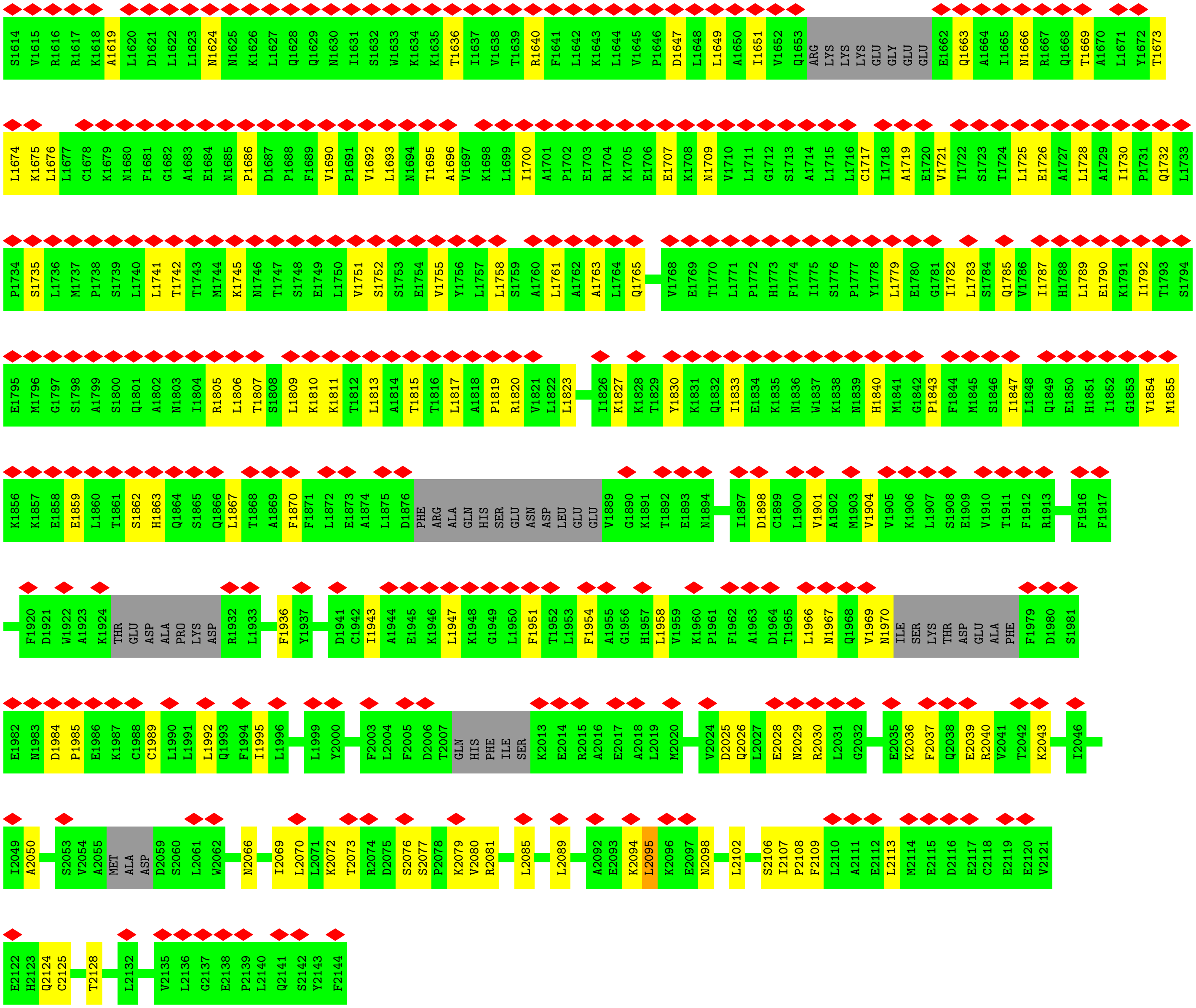
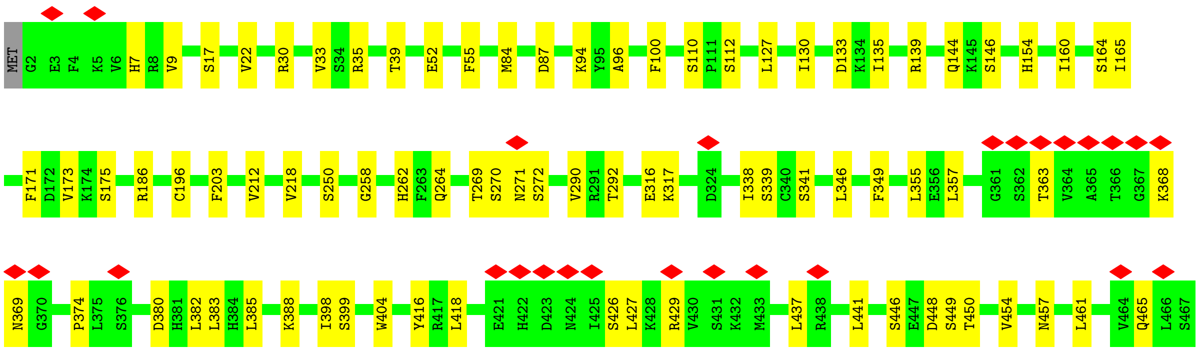
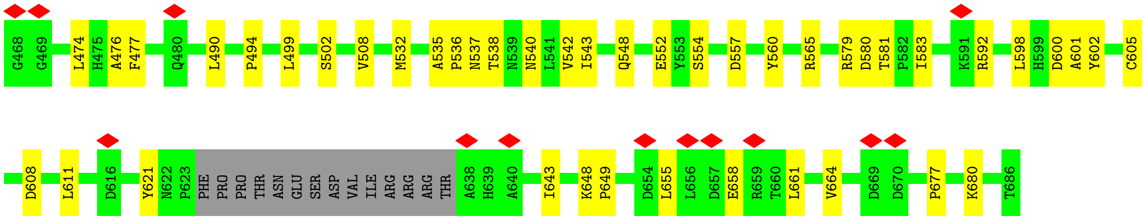
GLU GLU MET LEU GLN VAL PHE ASN VAL GLU THR HIS THR S1507 K1508 Q1509 L1510 R1511 H1512 F1513 K1514 F1515 L1516 S1517 V1518 S1519 F1520 M1521 S1522 Q1523 L1524 L1525 S1526 S1527 N1528 N1529 F1530 L1531 K1532 K1533 V1534 V1535 E1536 S1537 GLY GLY PRO GLU ILE LEU LYS G1545 L1546 E1547 E1548 R1549 L1550 L1551 E1552 T1553
V1554 L1555 G1556 Y1557 I1558 S1559 A1560 V1561 A1562 Q1563 S1564 M1565 E1566 R1567 N1568 A1569 D1570 K1571 L1572 T1573 V1574 K1575 F1576 W1577 R1578 A1579 L1580 L1581 S1582 K1583 A1584 Y1585 D1586 L1587 L1588 D1589 K1590 V1591 N1592 A1593 L1594 L1595 PRO THR E1598 T1599 F1600 I1601 P1602 V1603 I1604 R1605 G1606 L1607 V1608 G1609 N1610 P1611 L1612 P1613



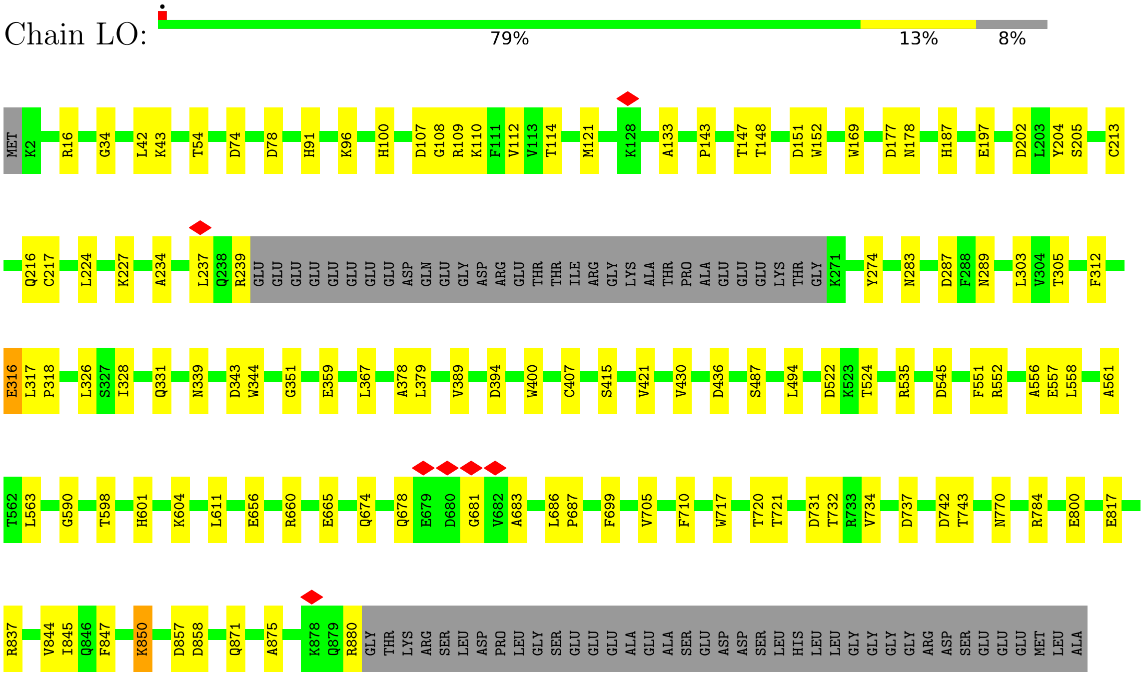
- Molecule 21: U3 small nucleolar RNA-associated protein 4 homolog

Chain LN:

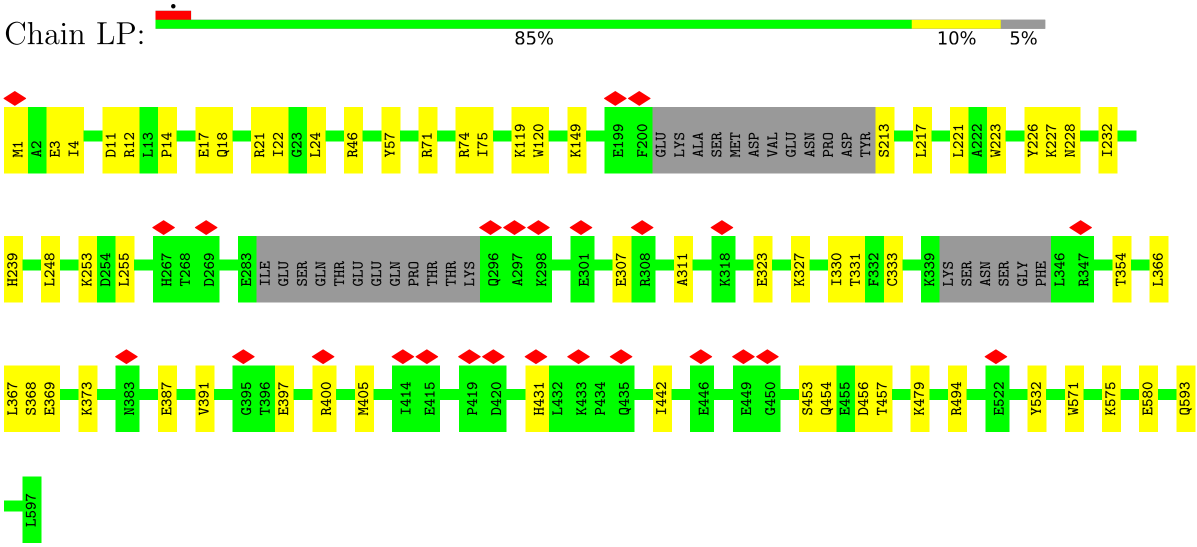




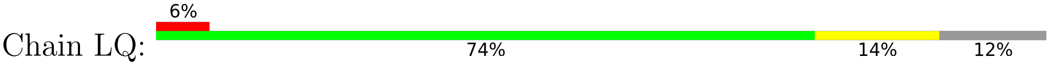
- Molecule 22: Periodic tryptophan protein 2 homolog

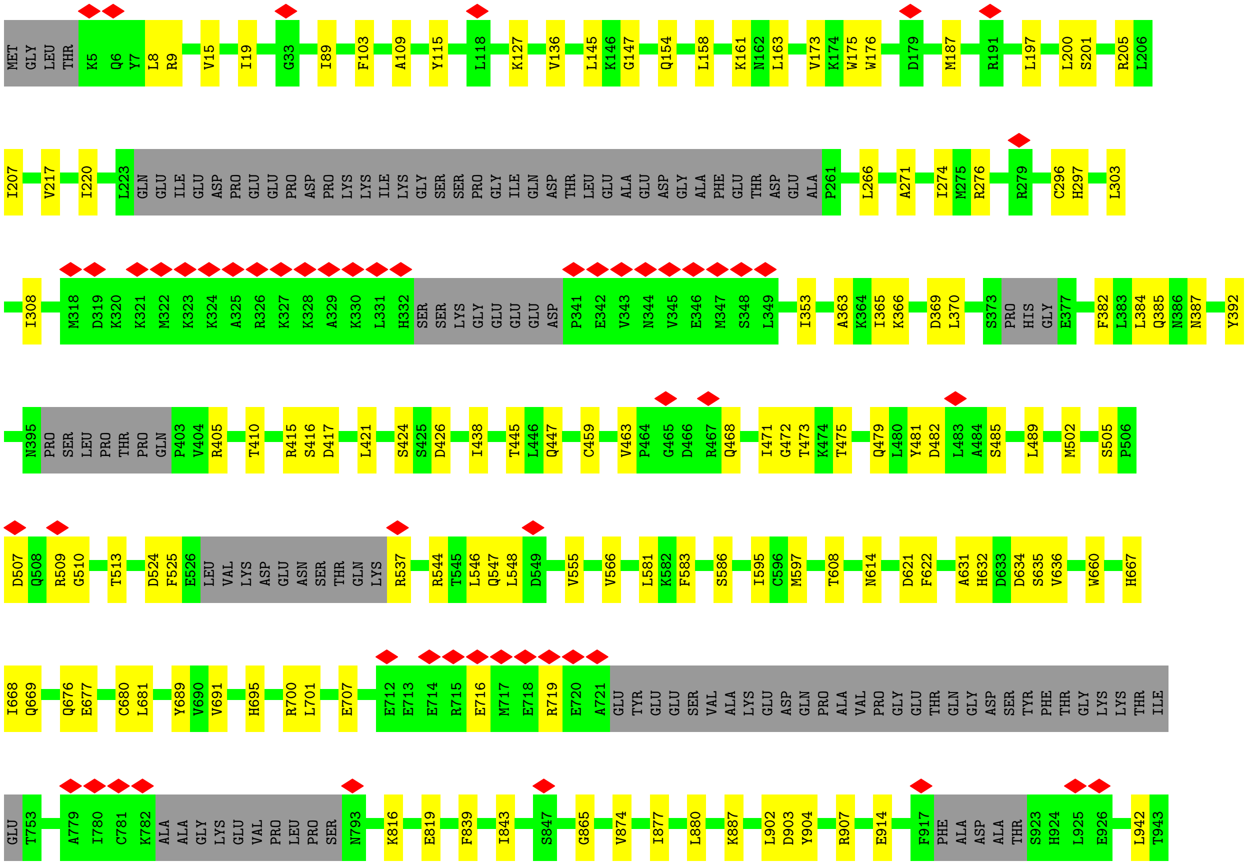


- Molecule 23: U3 small nucleolar RNA-associated protein 6 homolog



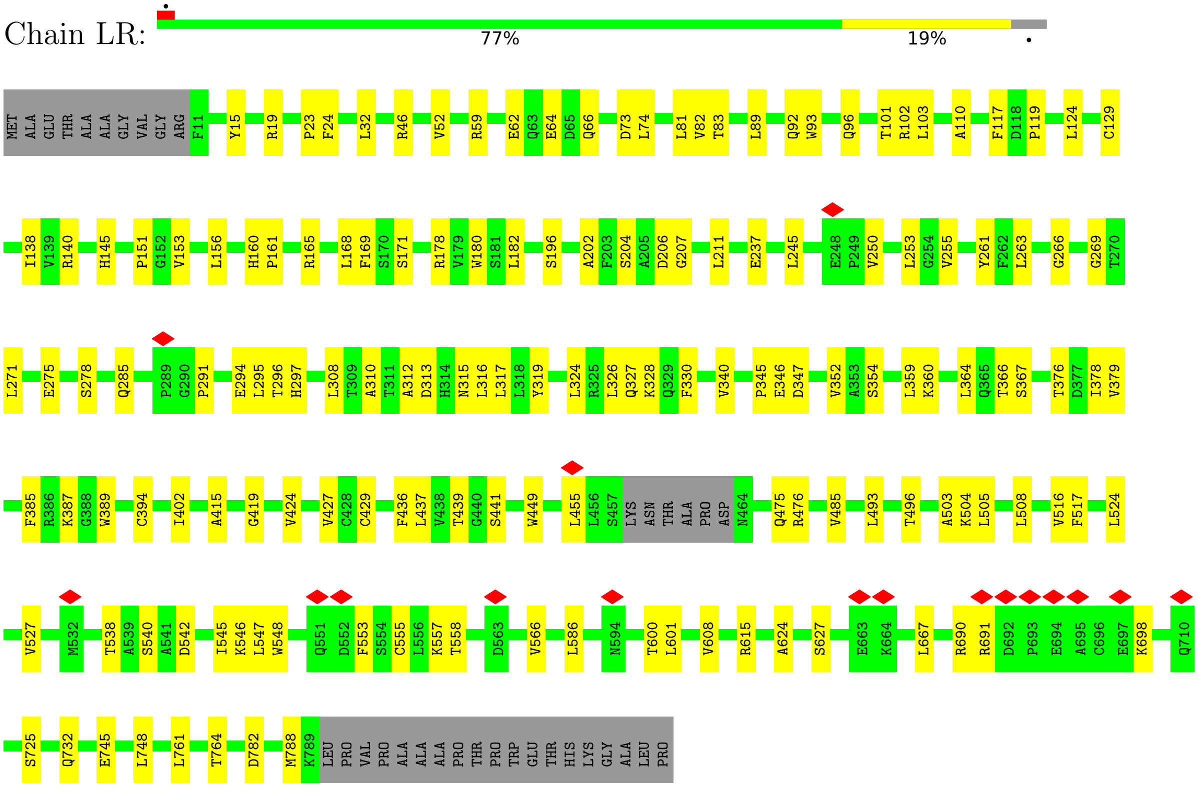
- Molecule 24: WD repeat-containing protein 3



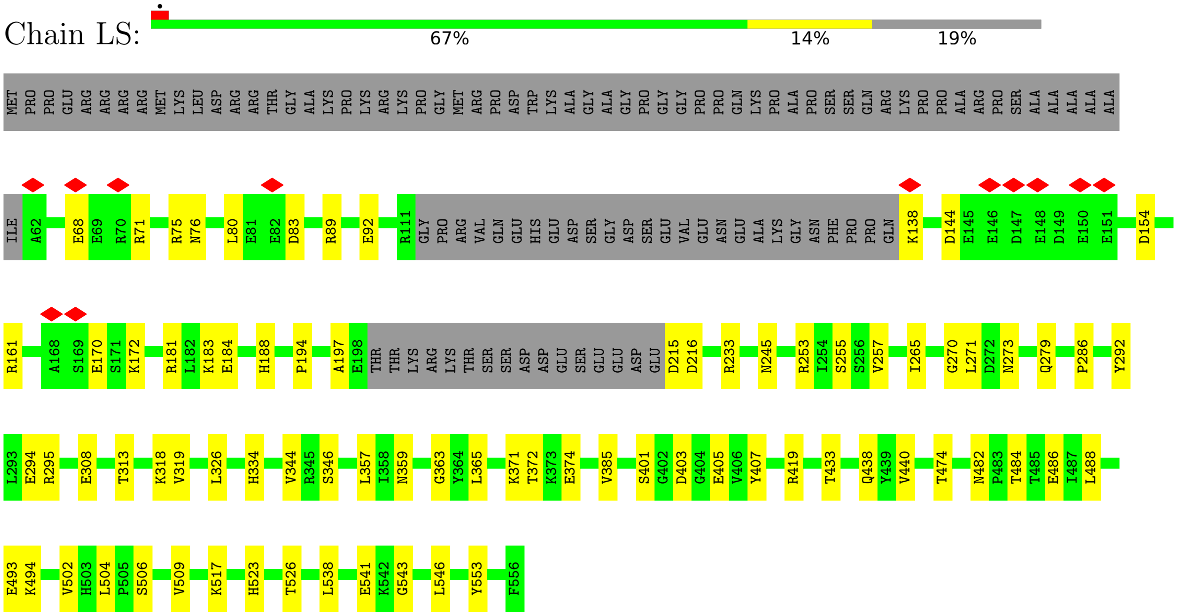


- Molecule 25: Transducin beta-like protein 3

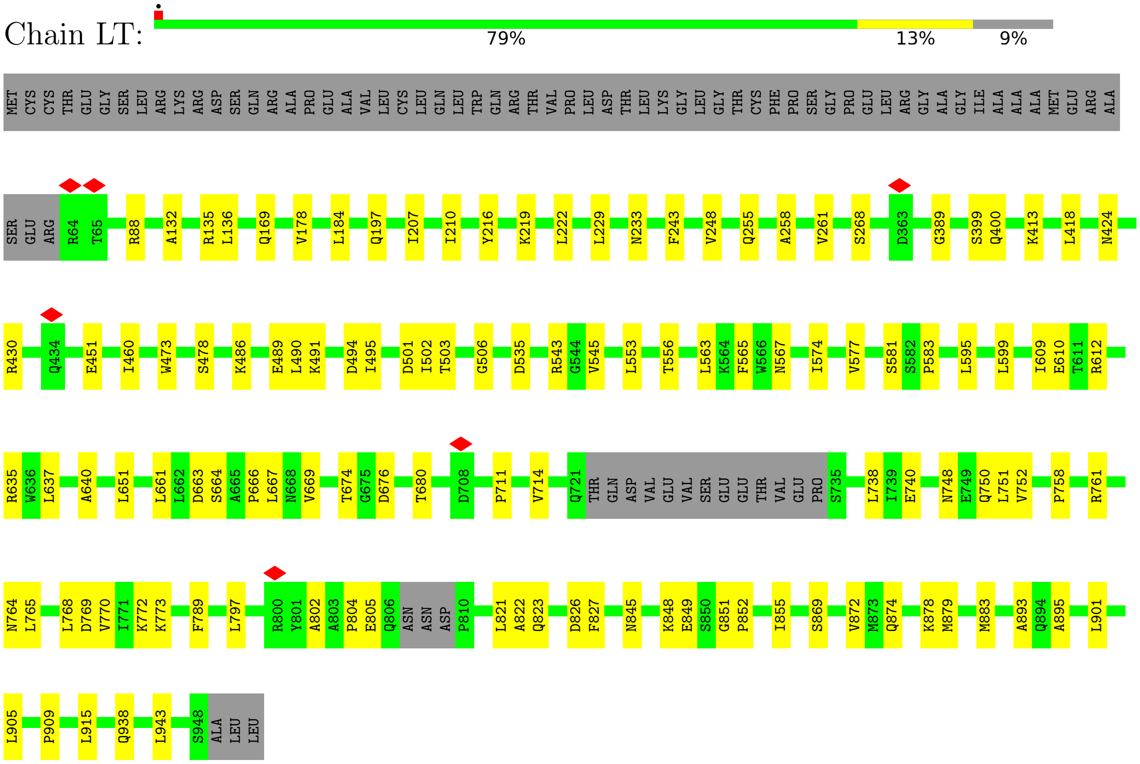
Chain LR:



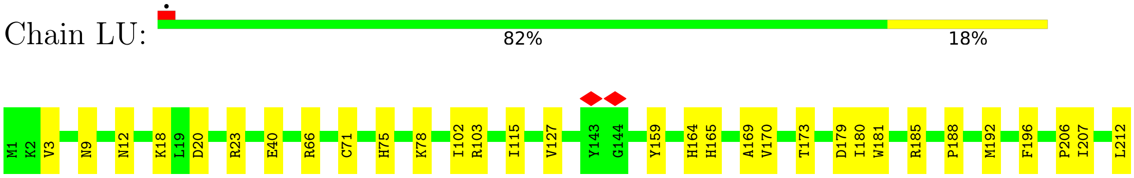
- Molecule 26: U3 small nucleolar RNA-associated protein 18 homolog

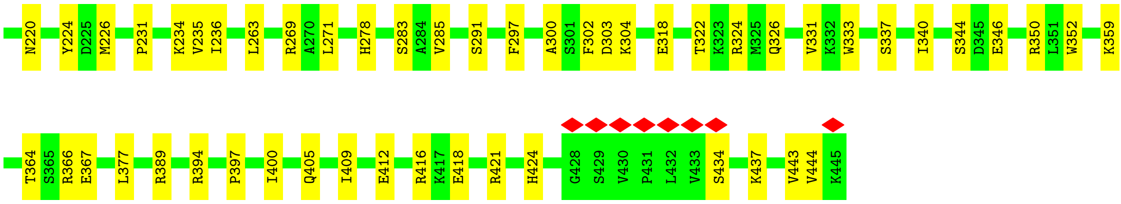


- Molecule 27: WD repeat-containing protein 36

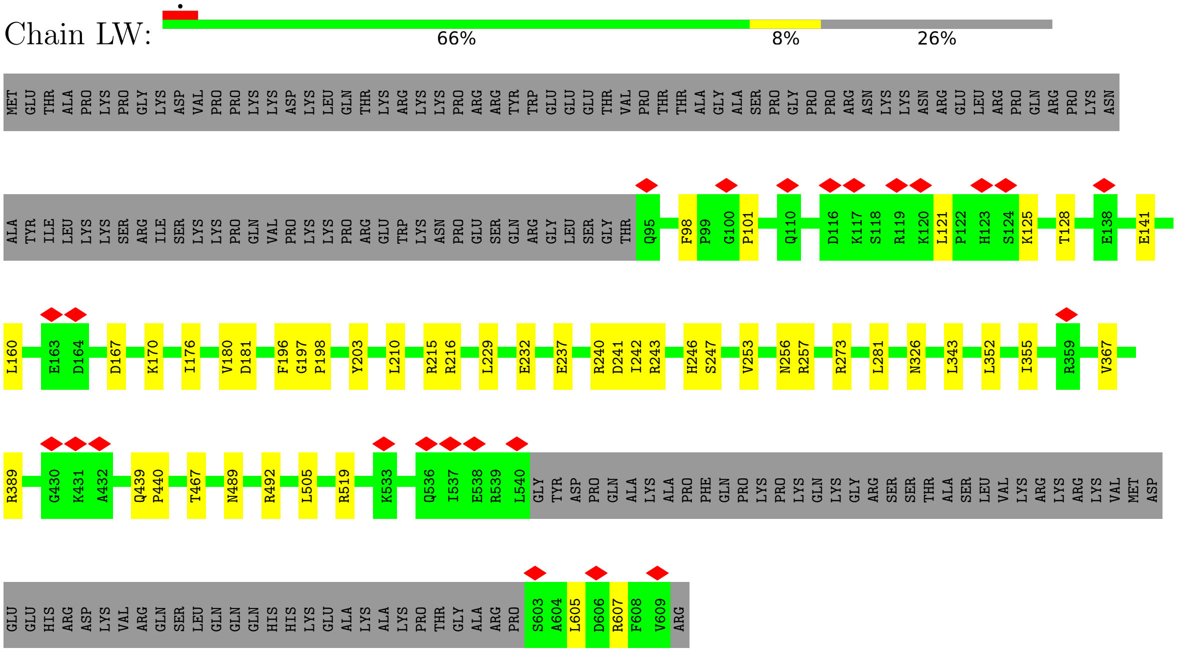


- Molecule 28: DDB1- and CUL4-associated factor 13

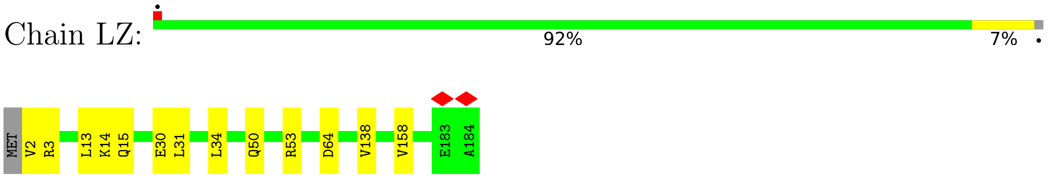




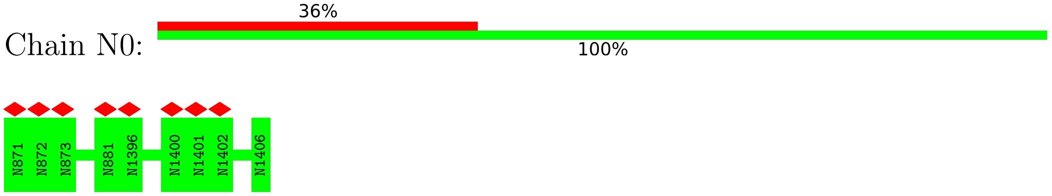
- Molecule 29: WD repeat-containing protein 46



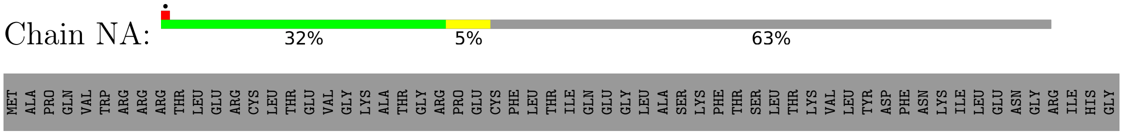
- Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP3

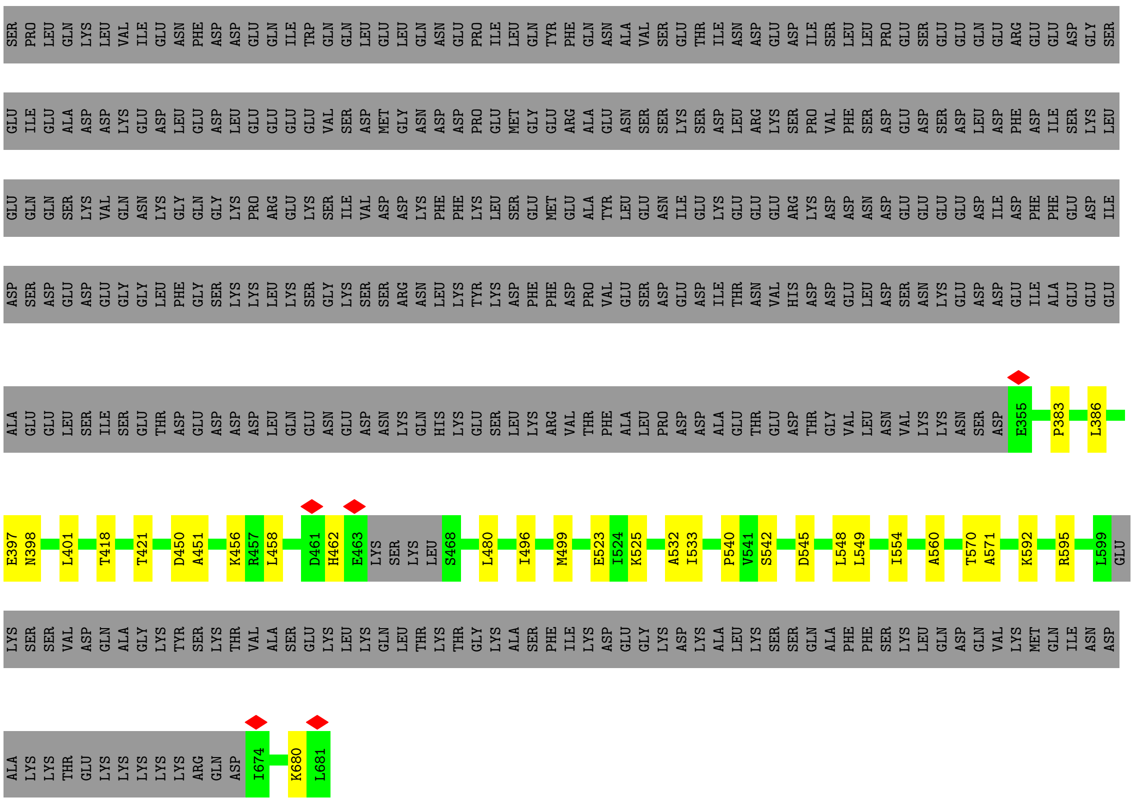


- Molecule 31: 5’ETS rRNA



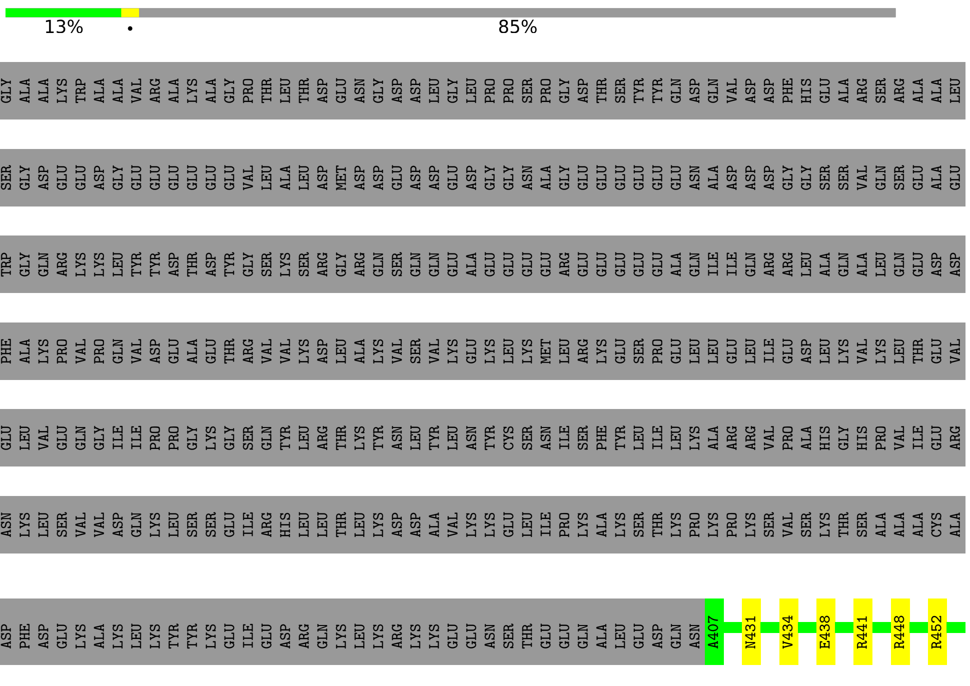
- Molecule 32: U3 small nucleolar ribonucleoprotein protein MPP10



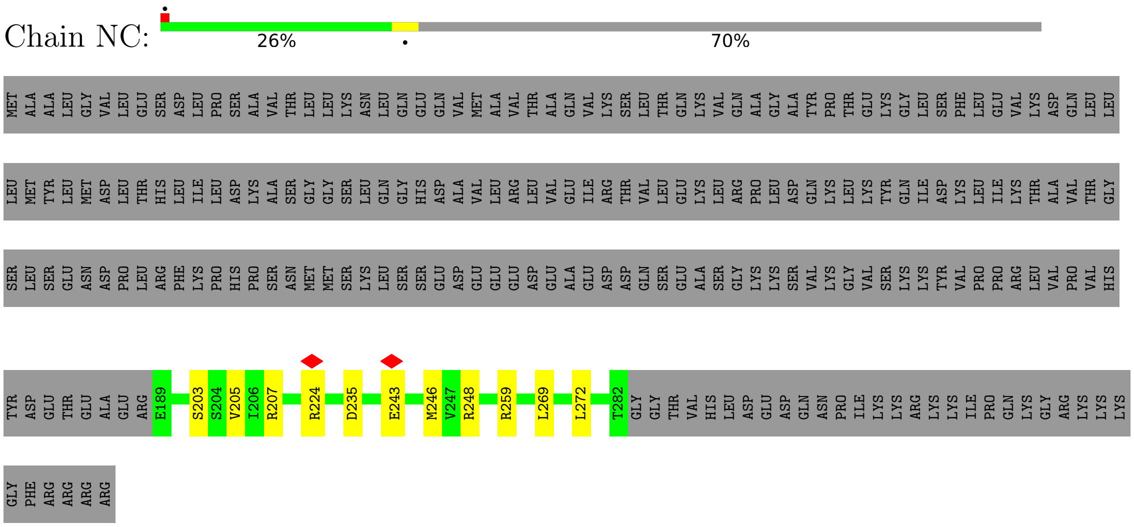


- Molecule 33: Something about silencing protein 10

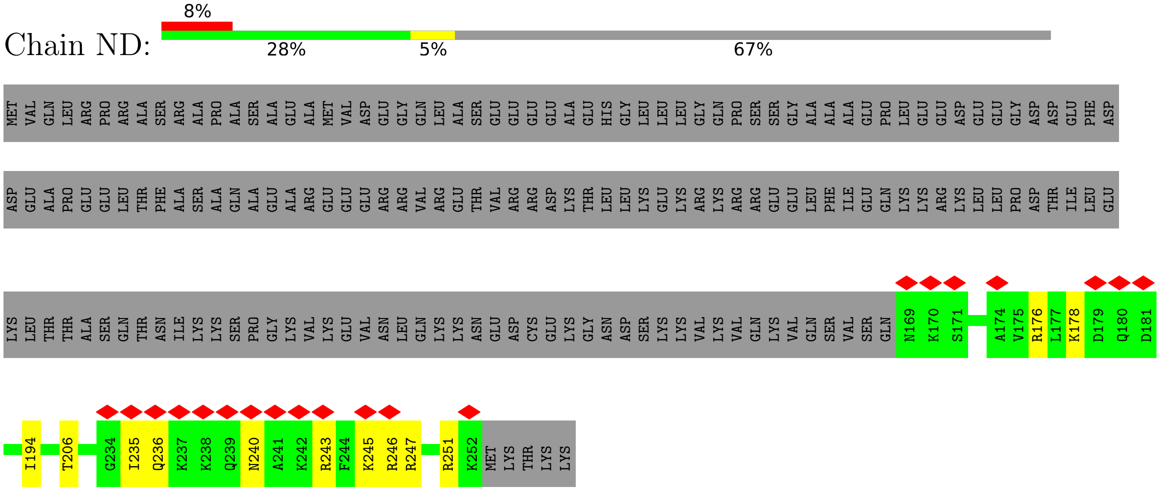
Chain NB:



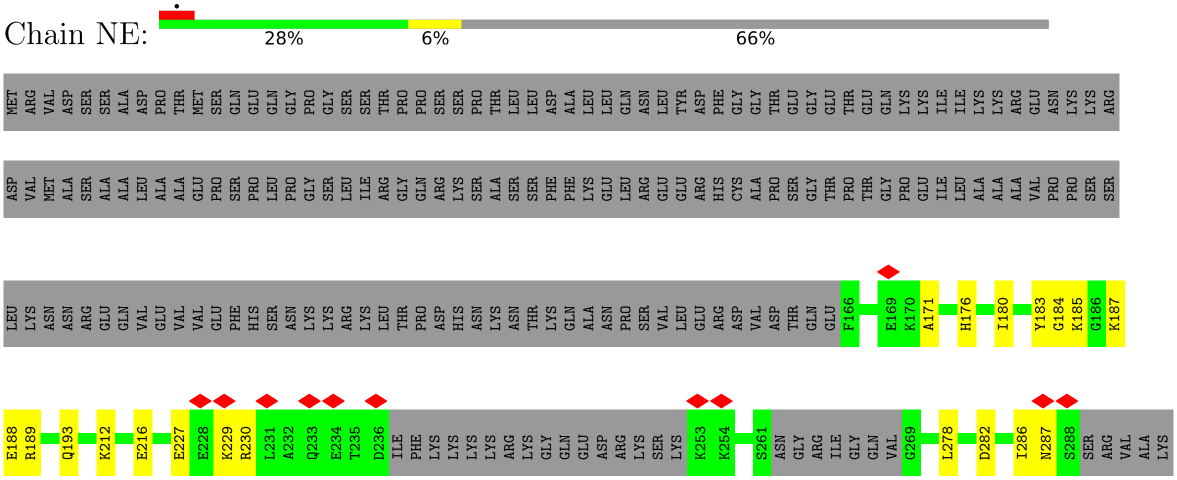
- Molecule 34: Neuroguidin



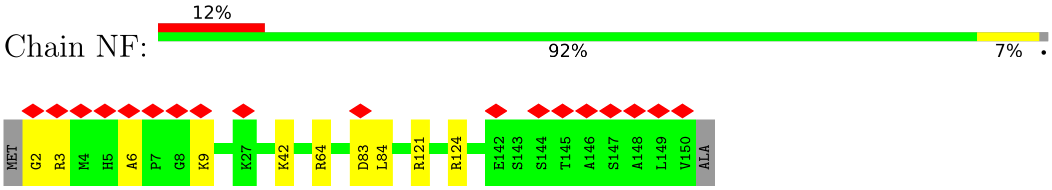
- Molecule 35: Nucleolar protein 7



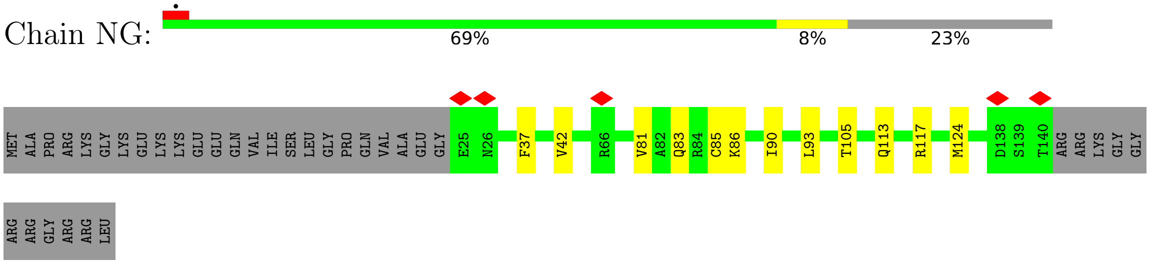
- Molecule 36: Uncharacterized protein C1orf131



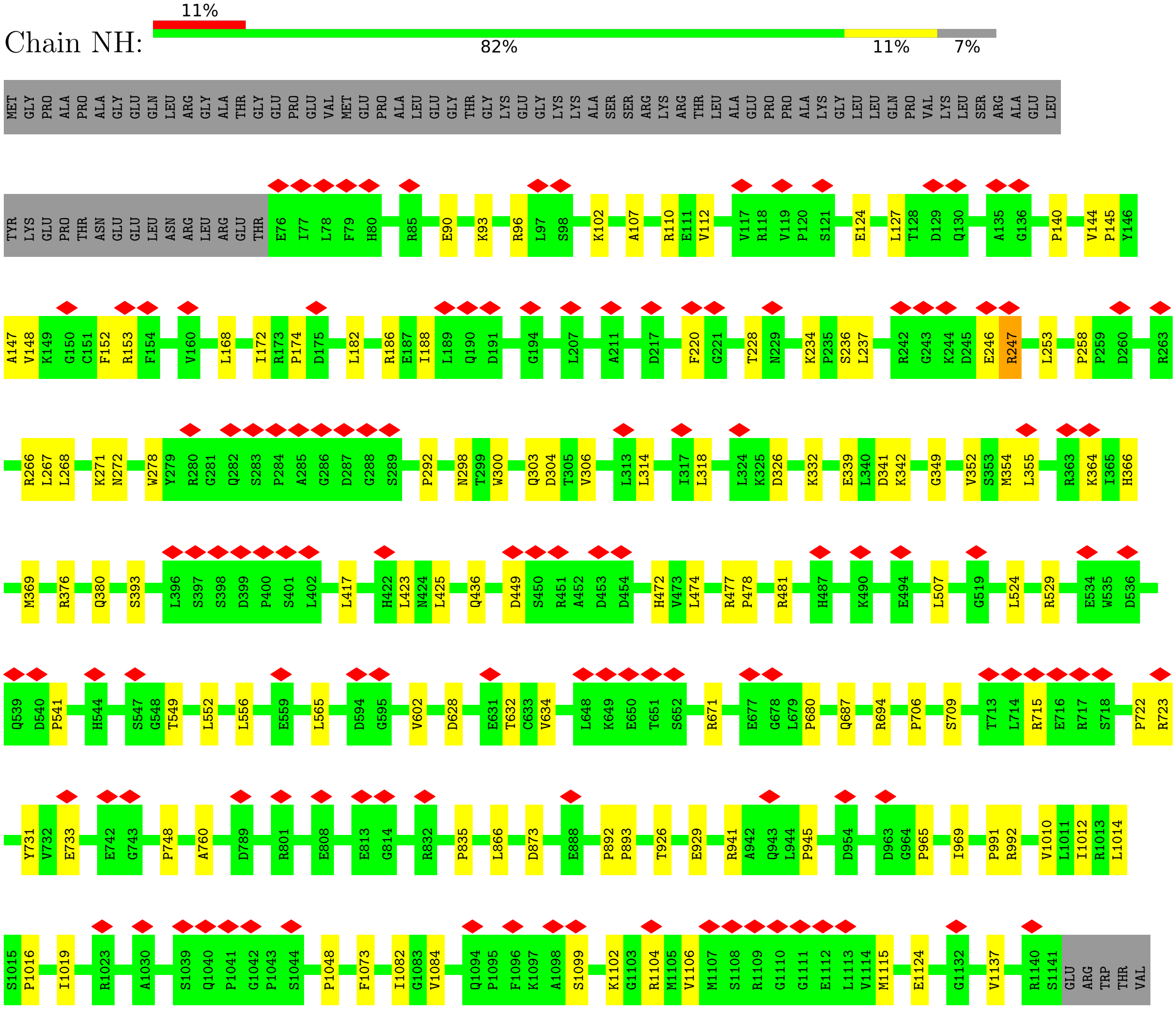
- Molecule 37: 40S ribosomal protein S13



- Molecule 38: 40S ribosomal protein S14

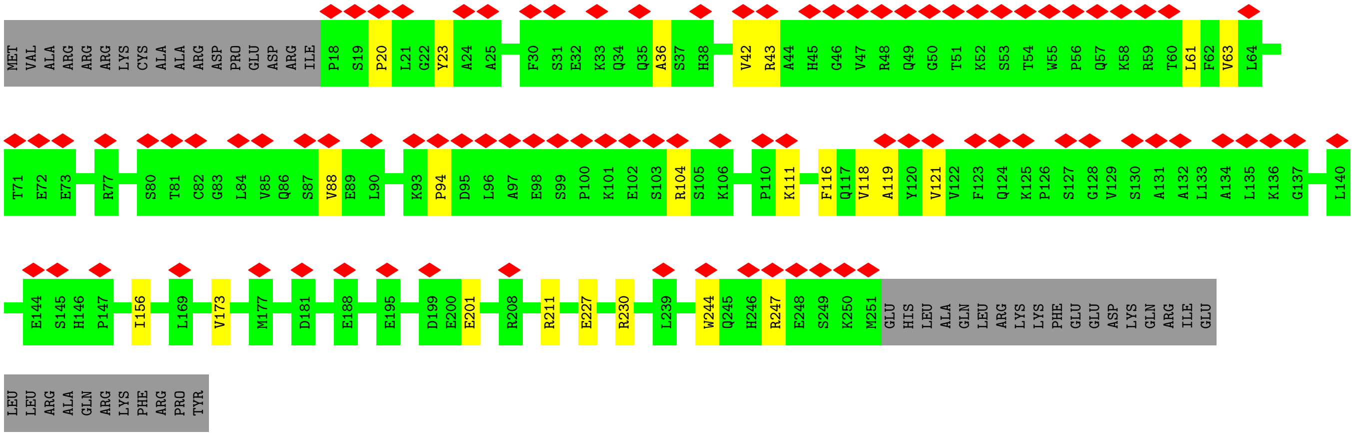


- Molecule 39: Nucleolar protein 6



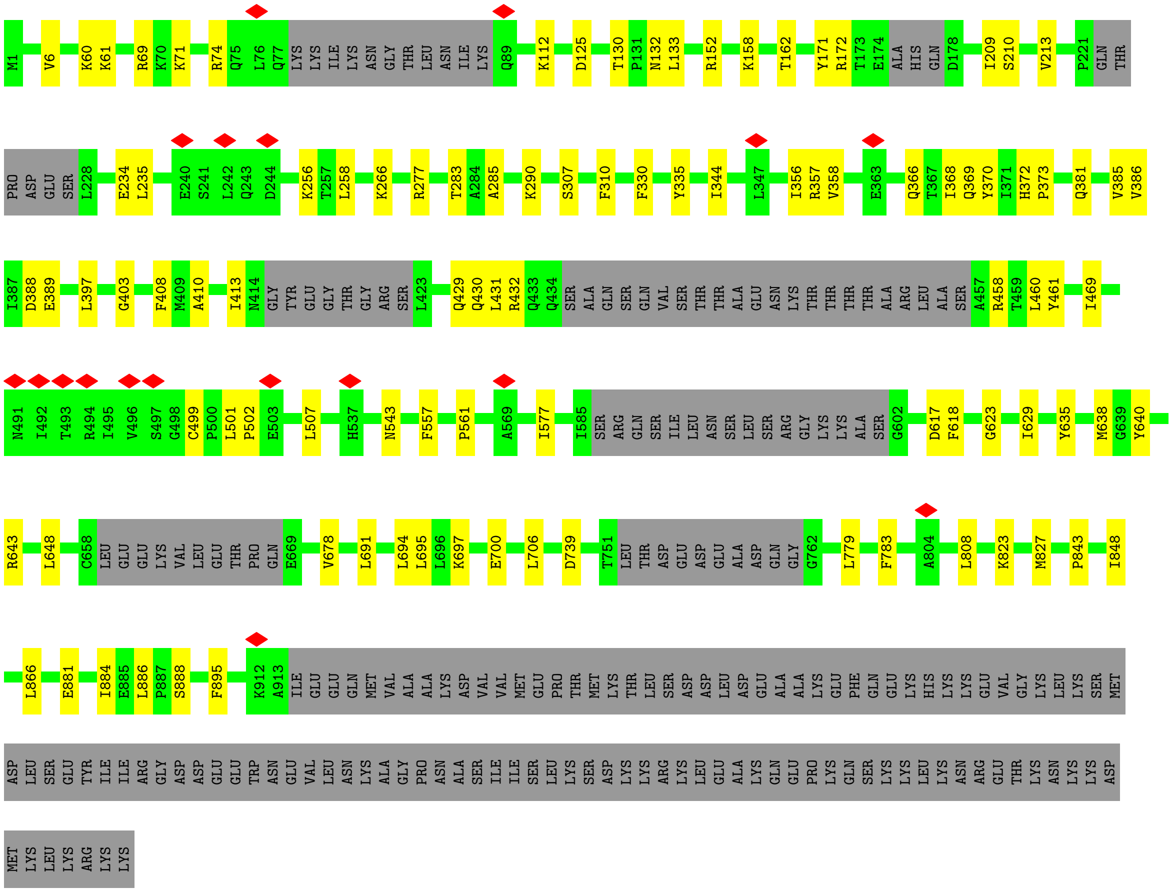
- Molecule 40: Ribosomal RNA-processing protein 7 homolog A

Chain NI:



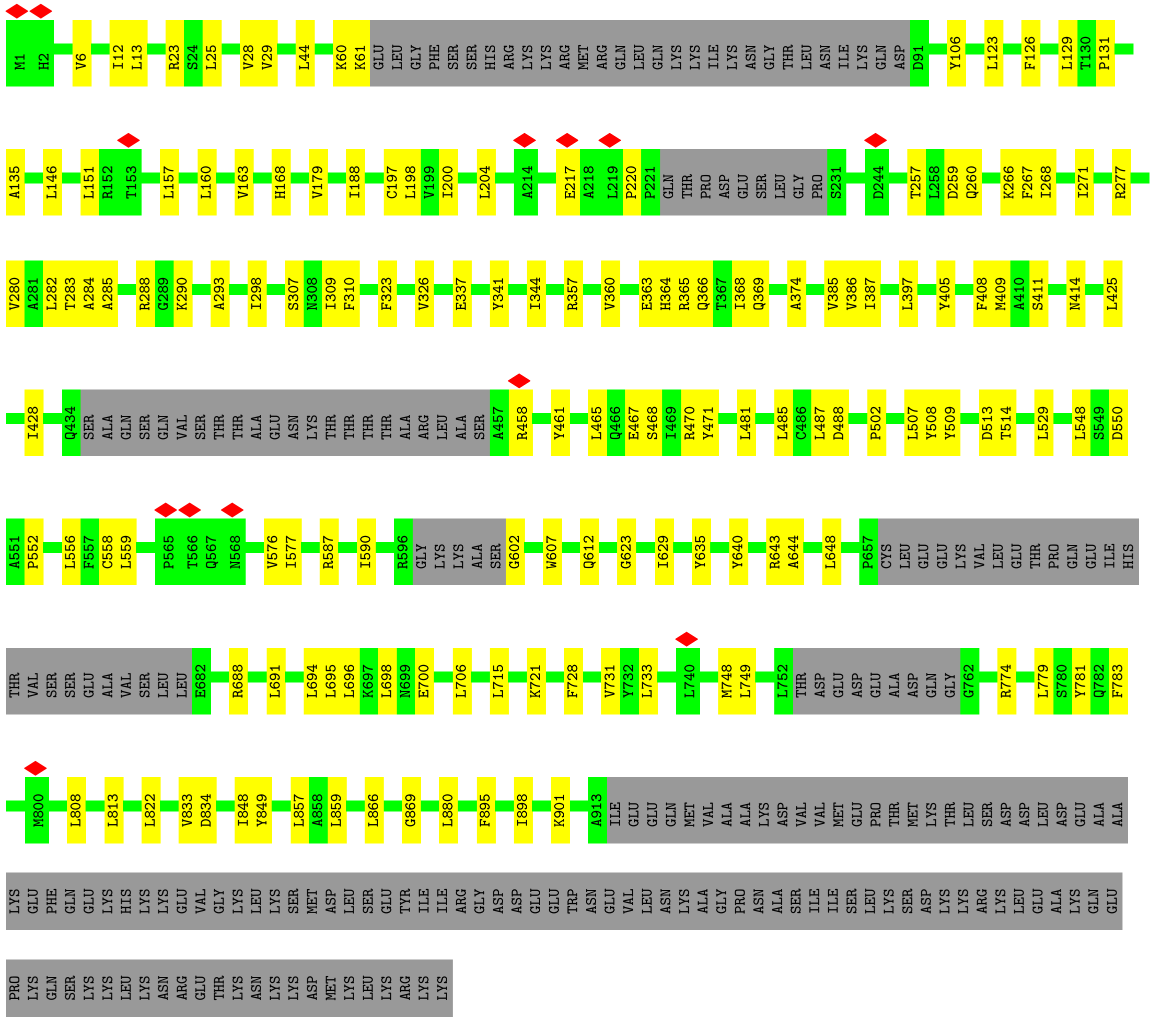
- Molecule 41: RNA cytidine acetyltransferase

Chain NJ:



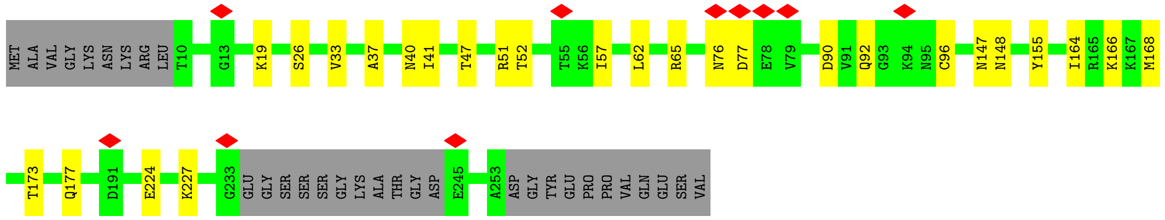
- Molecule 41: RNA cytidine acetyltransferase

Chain NK:



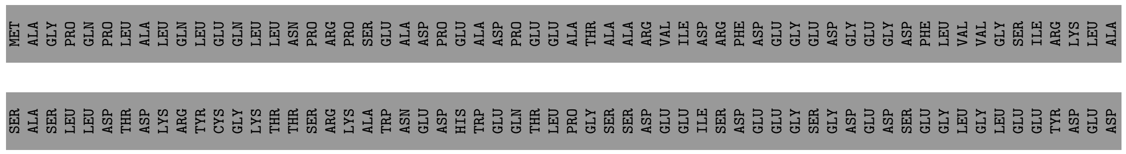
- Molecule 42: 40S ribosomal protein S3a

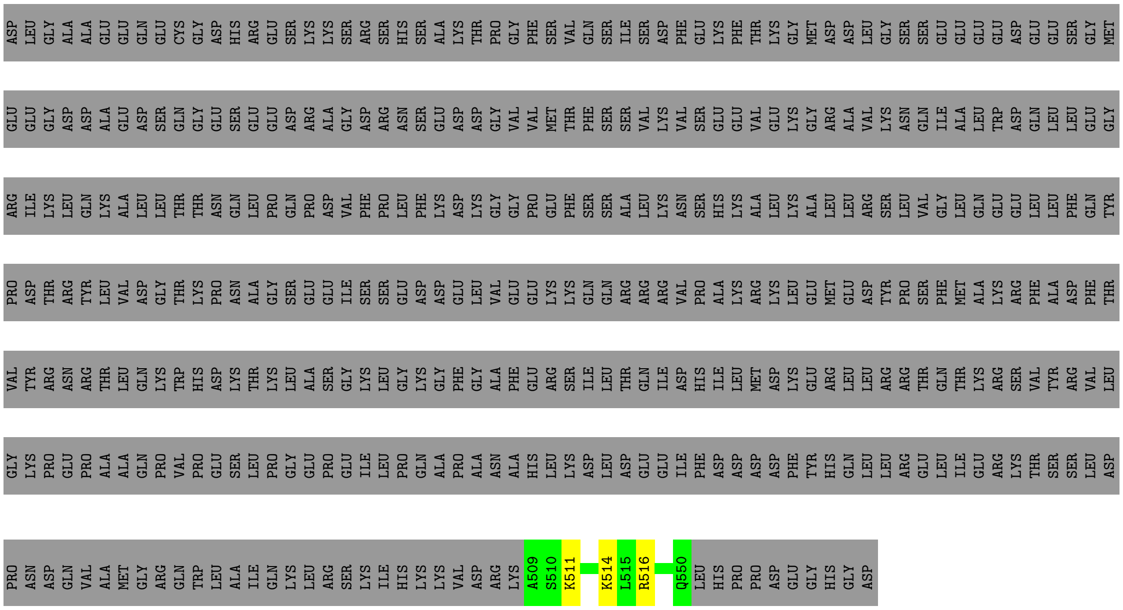
Chain NM:



- Molecule 43: Protein AATF

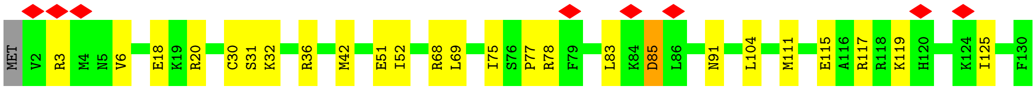
Chain NN:





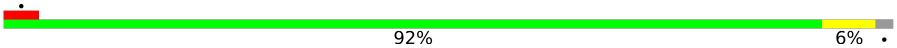
- Molecule 44: 40S ribosomal protein S15a

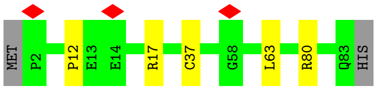
Chain NO:



- Molecule 45: 40S ribosomal protein S27

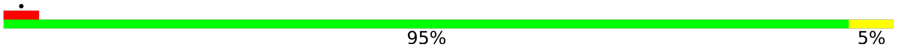
Chain NQ:

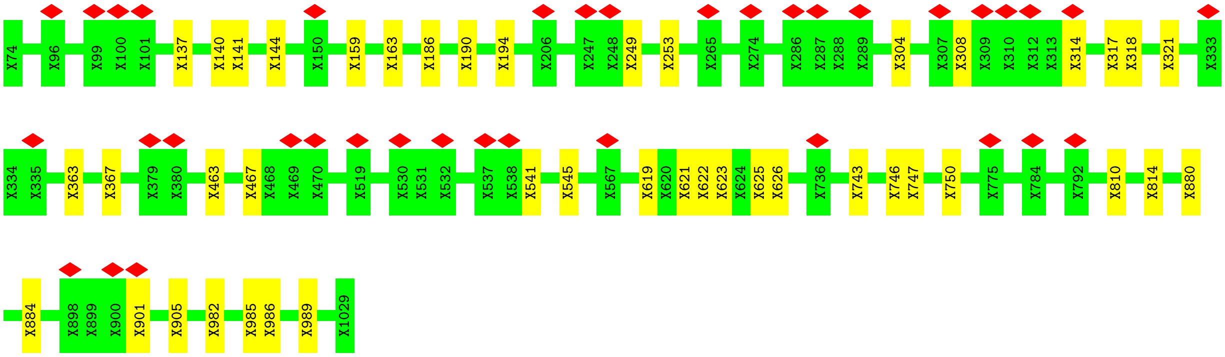




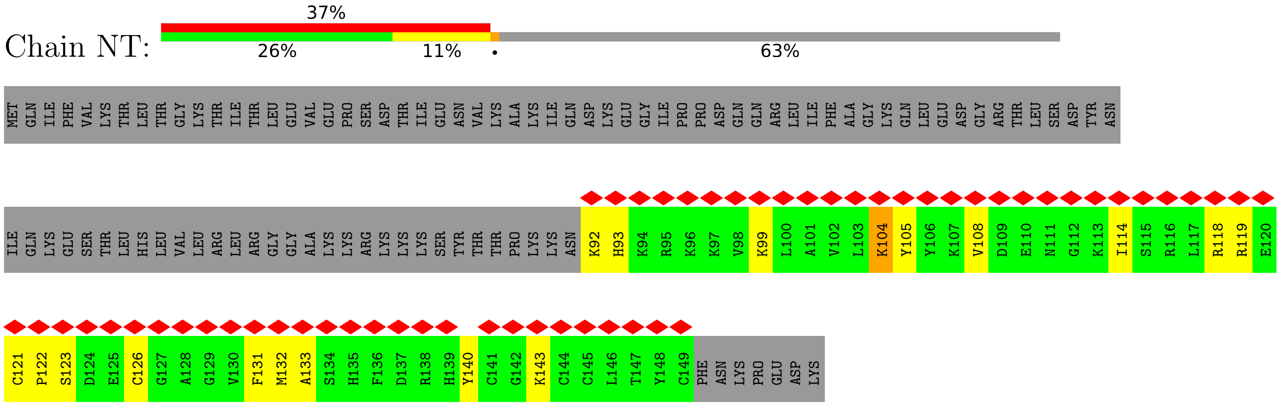
- Molecule 46: RRP12-like protein

Chain NR:

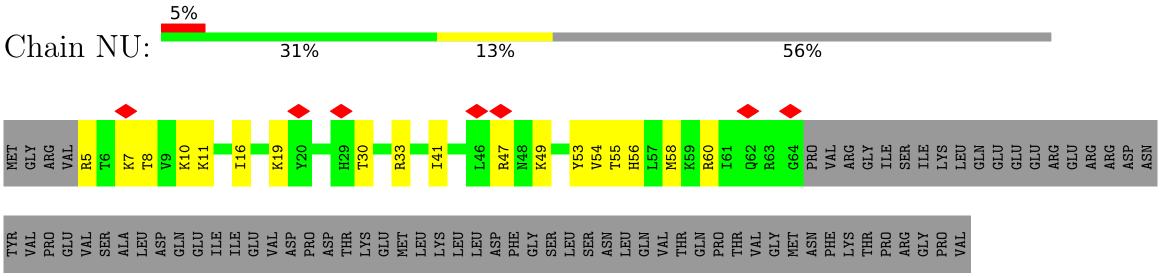




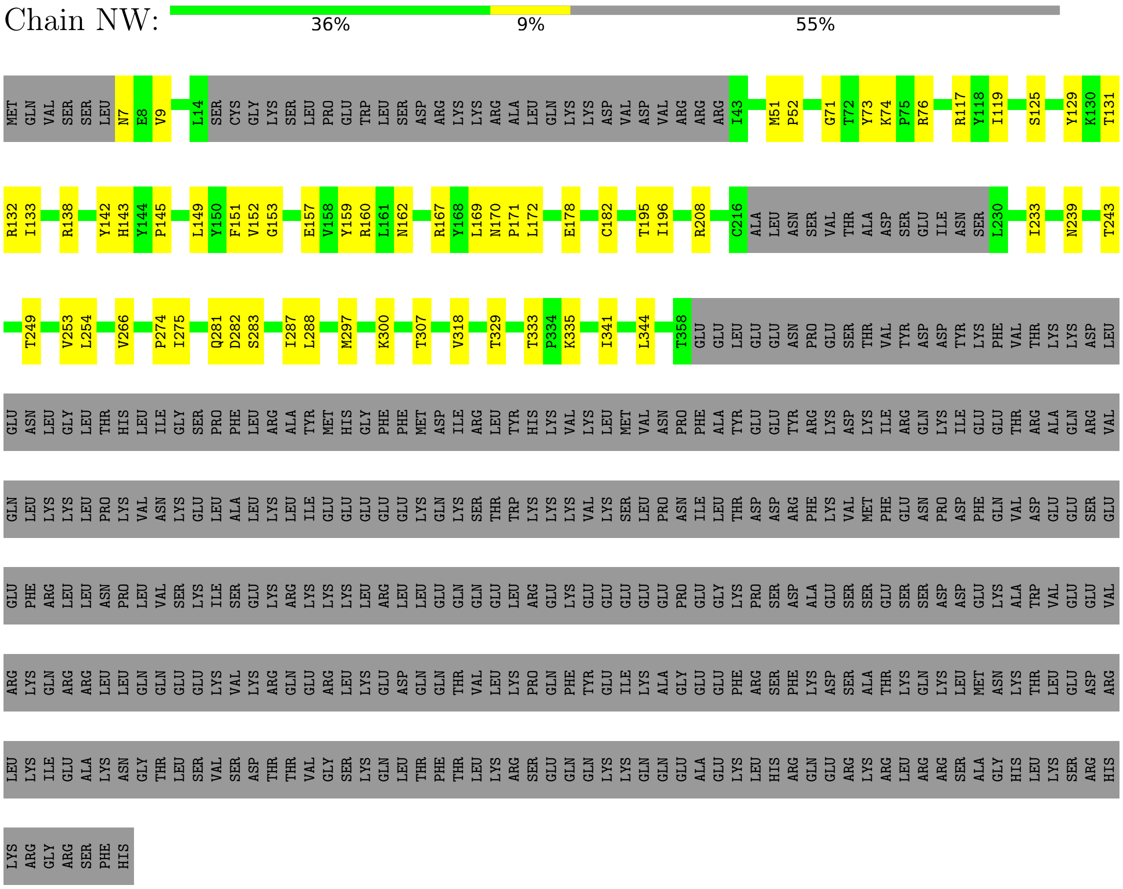
- Molecule 47: Ubiquitin-40S ribosomal protein S27a



- Molecule 48: 40S ribosomal protein S17

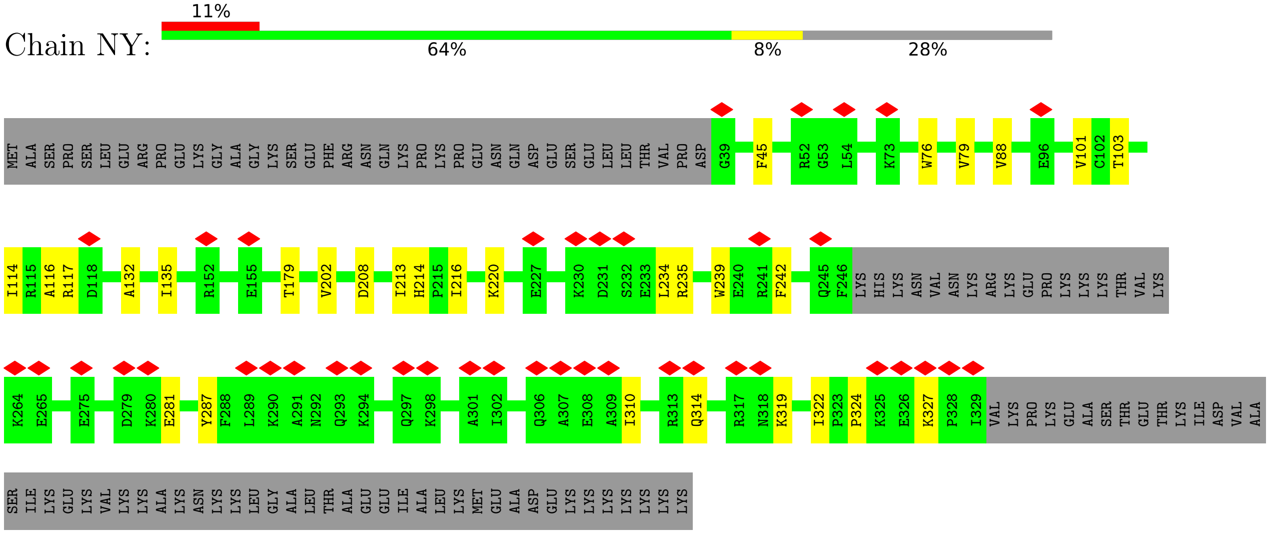


- Molecule 49: Nucleolar protein 10



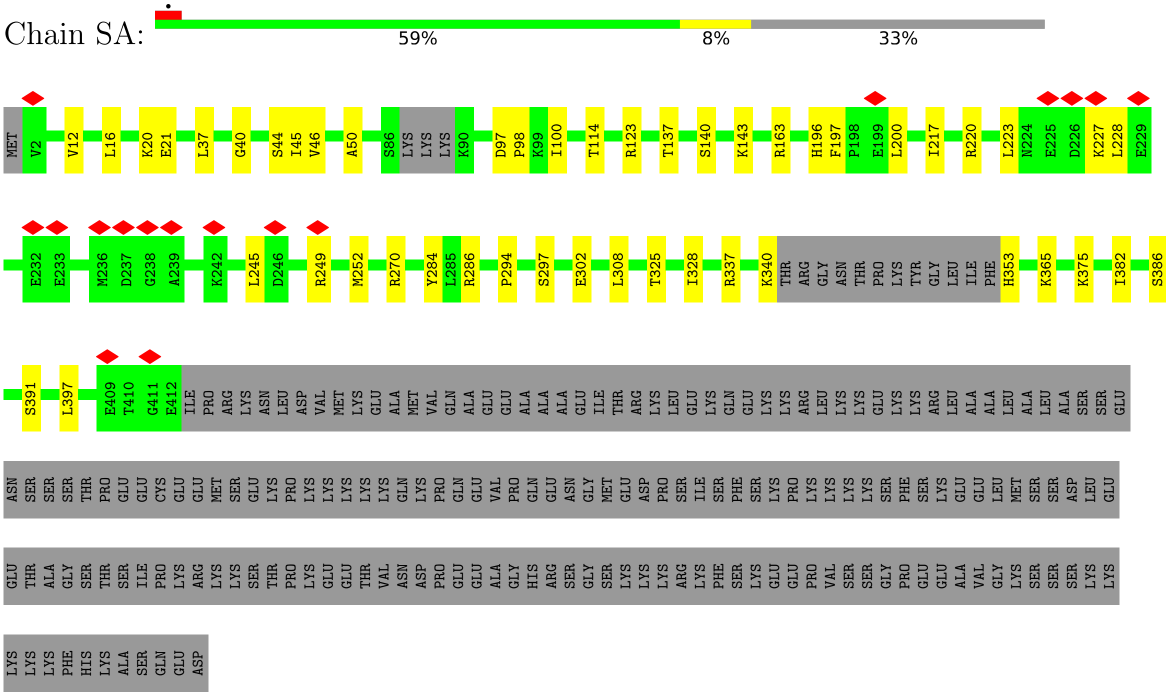
- Molecule 50: KRR1 small subunit processome component homolog

Chain NY:



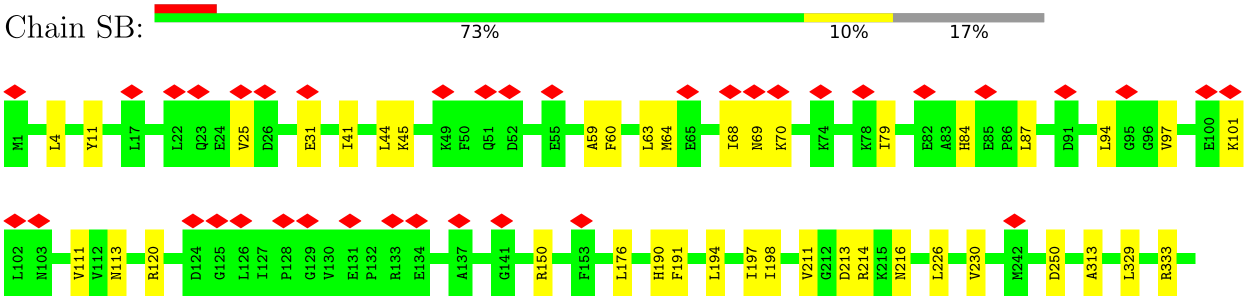
- Molecule 51: Nucleolar protein 56

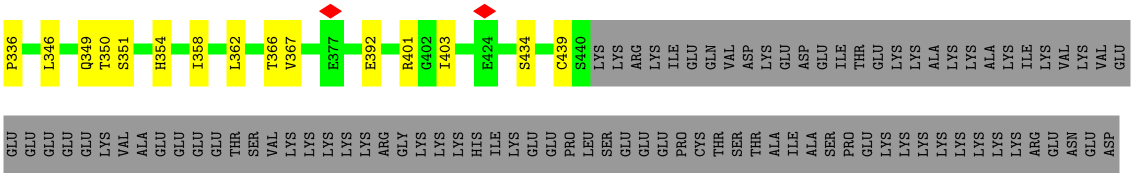
Chain SA:



- Molecule 52: Nucleolar protein 58

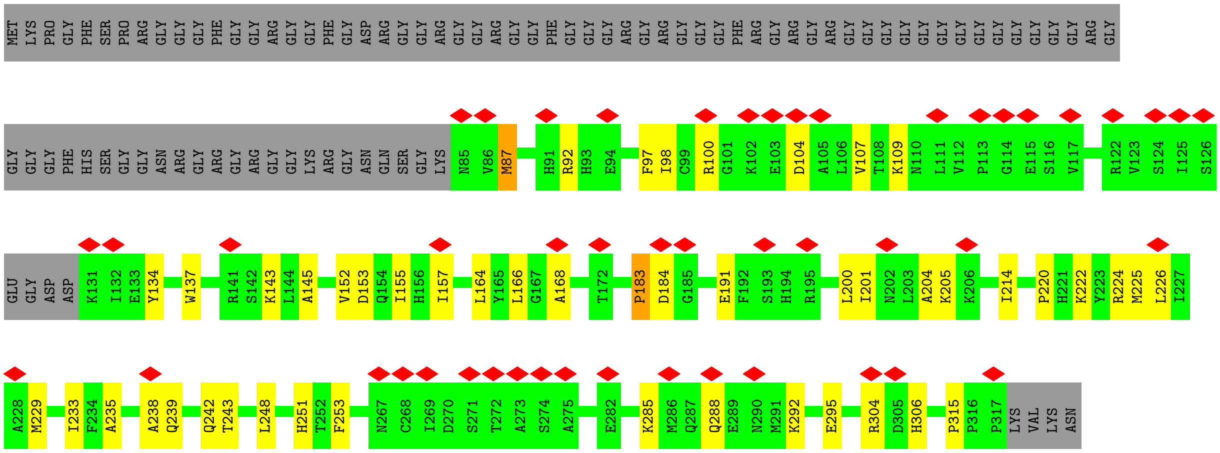
Chain SB:





- Molecule 53: rRNA 2’-O-methyltransferase fibrillarin

Chain SC:

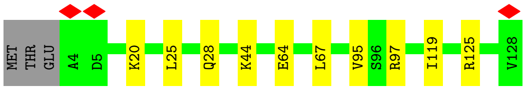


- Molecule 53: rRNA 2’-O-methyltransferase fibrillarin

Chain SD:

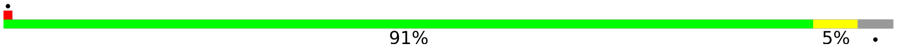
- Molecule 54: NHP2-like protein 1

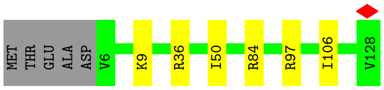
Chain SE:



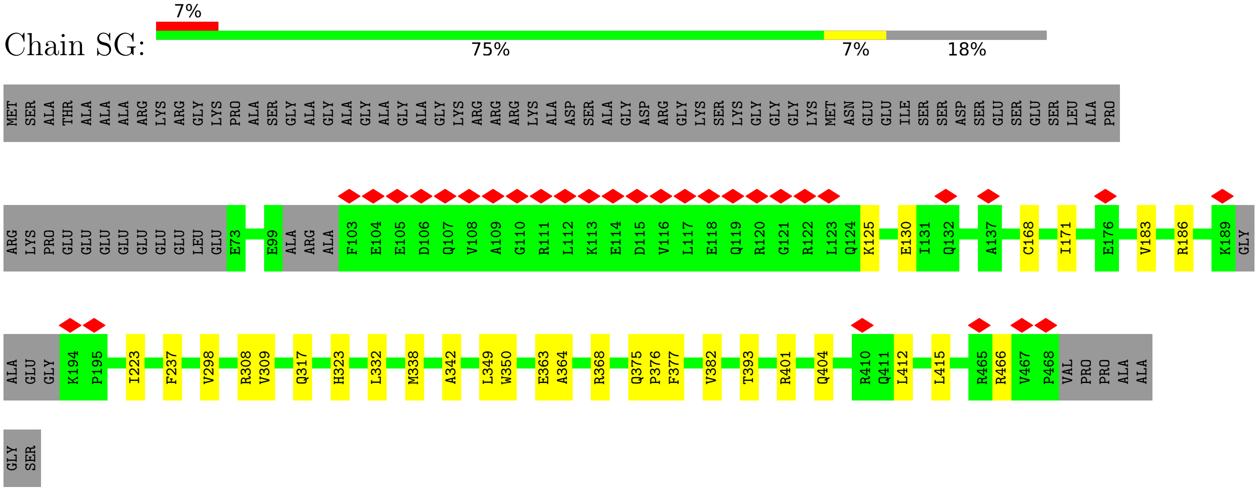
- Molecule 54: NHP2-like protein 1

Chain SF:

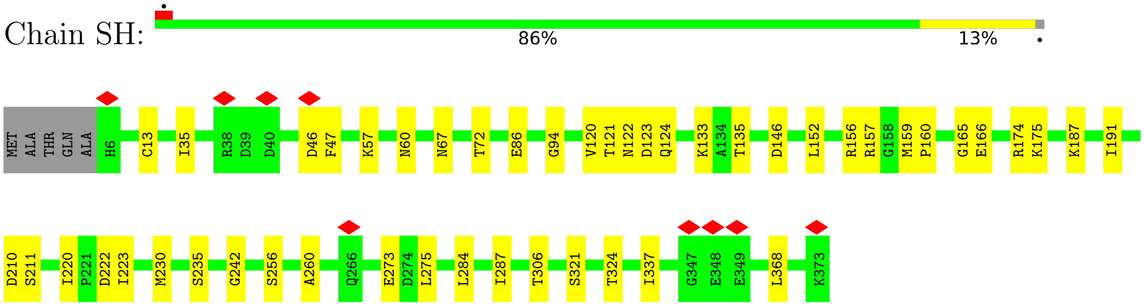




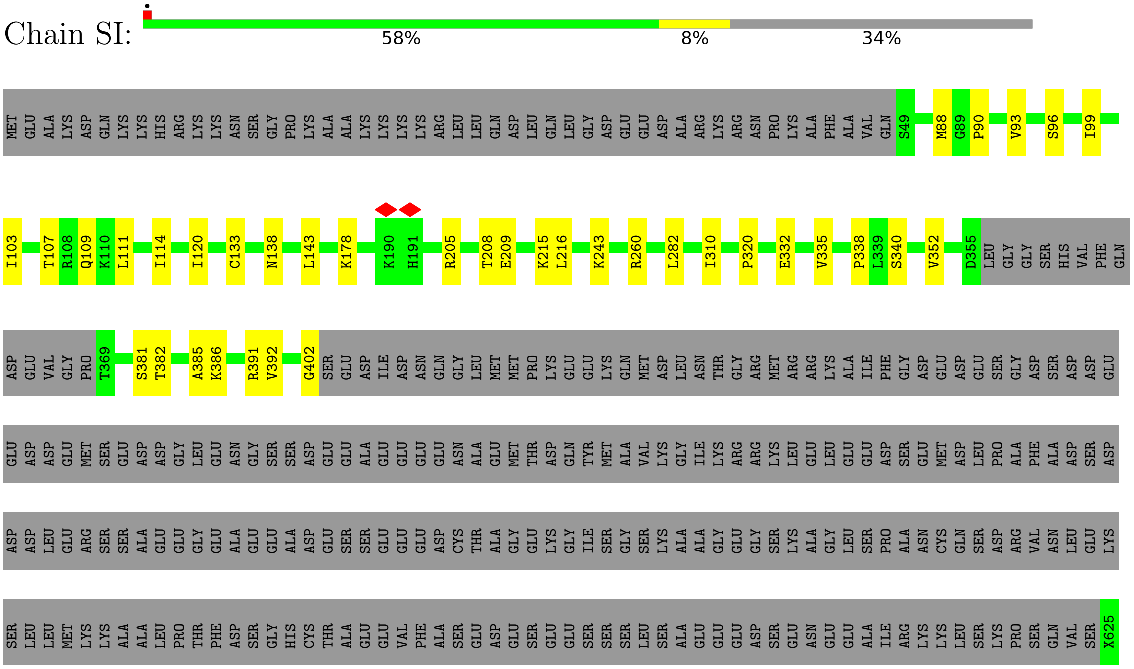
- Molecule 55: U3 small nucleolar RNA-interacting protein 2

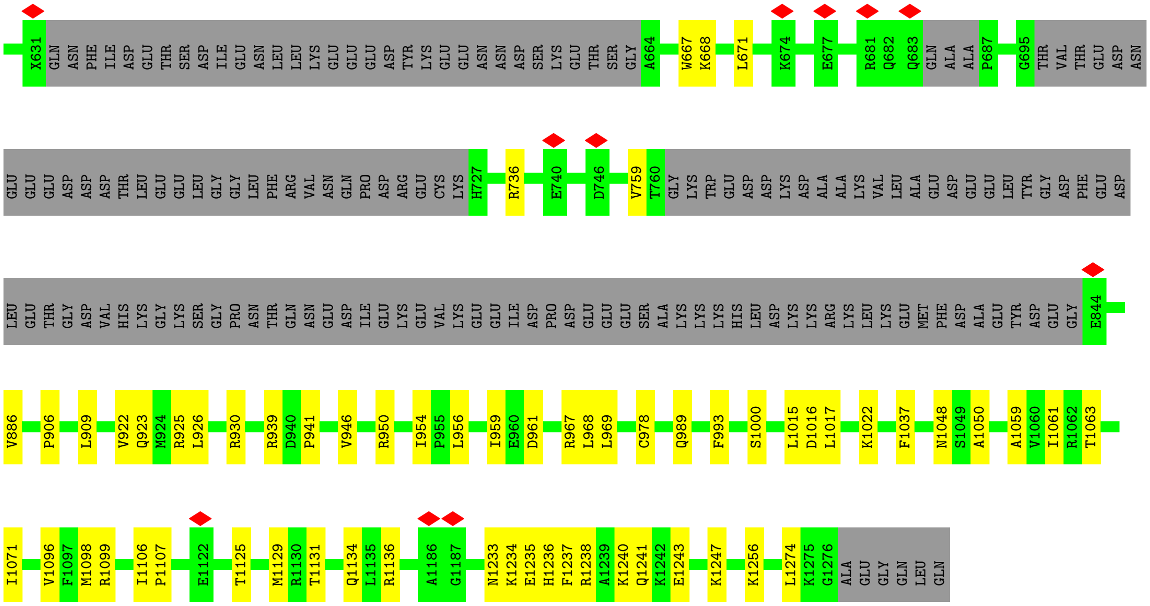


- Molecule 56: RNA 3'-terminal phosphate cyclase-like protein



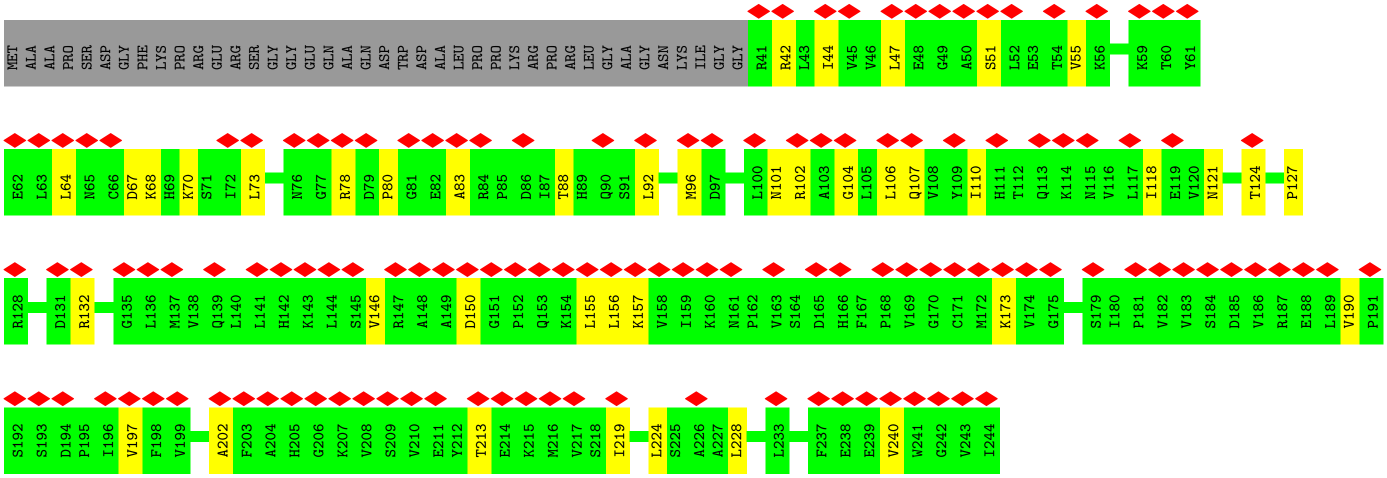
- Molecule 57: Ribosome biogenesis protein BMS1 homolog





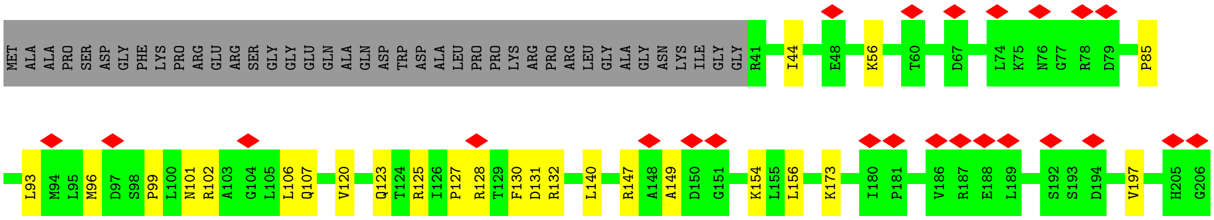
- Molecule 58: Ribosomal RNA small subunit methyltransferase NEP1

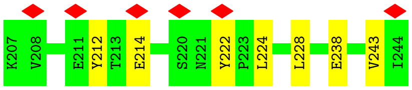
Chain SJ:



- Molecule 58: Ribosomal RNA small subunit methyltransferase NEP1

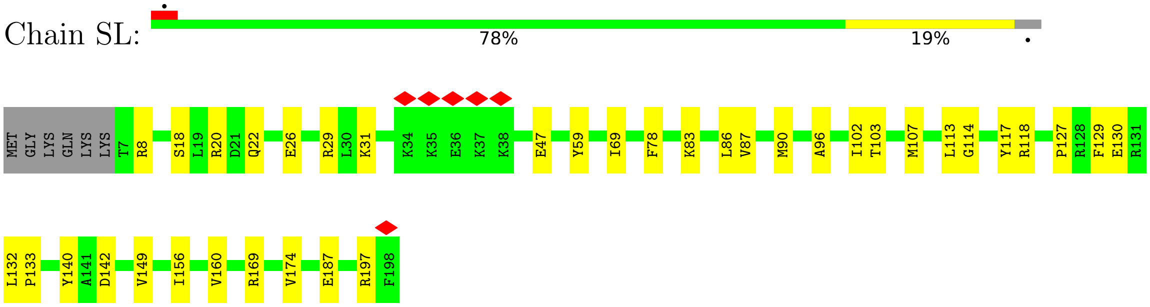
Chain SK:





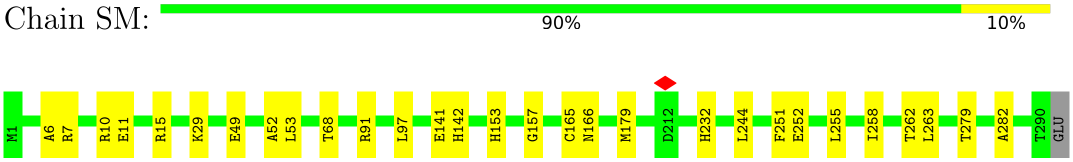
- Molecule 59: rRNA-processing protein FCF1 homolog

Chain SL:



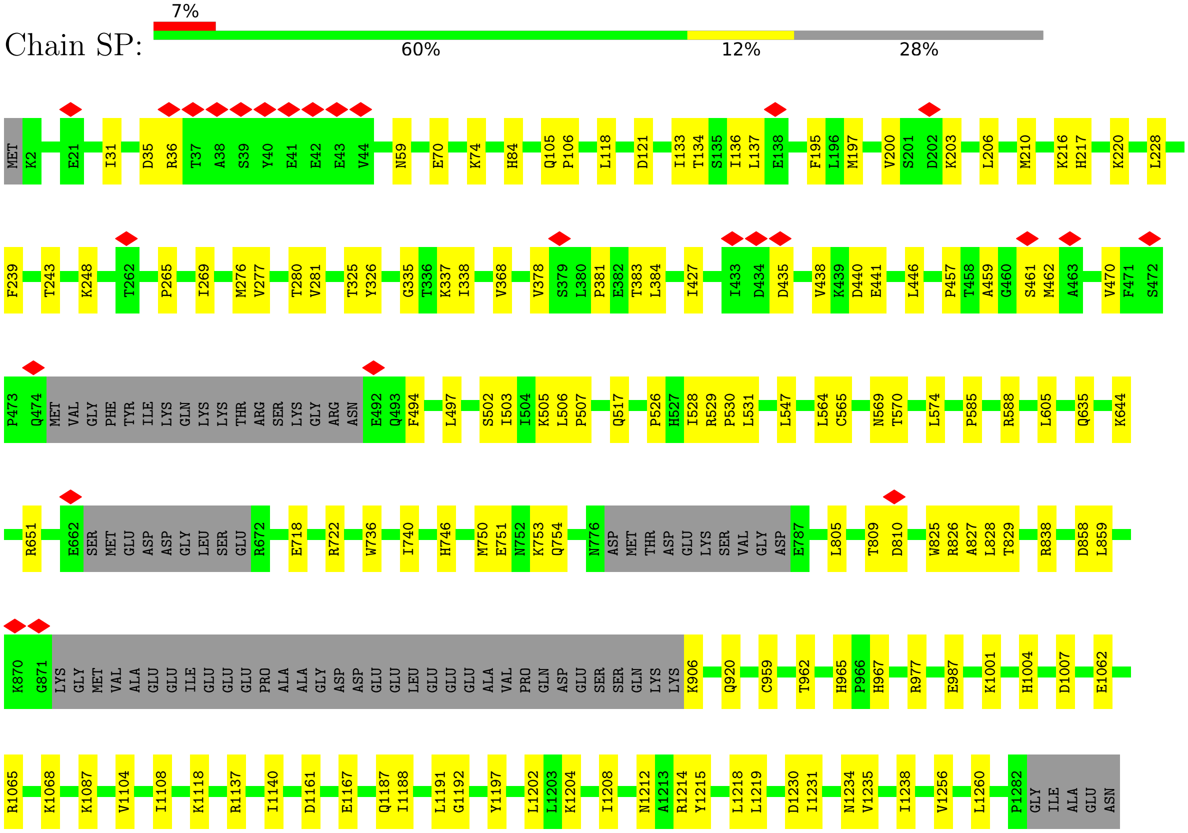
- Molecule 60: U3 small nucleolar ribonucleoprotein protein IMP4

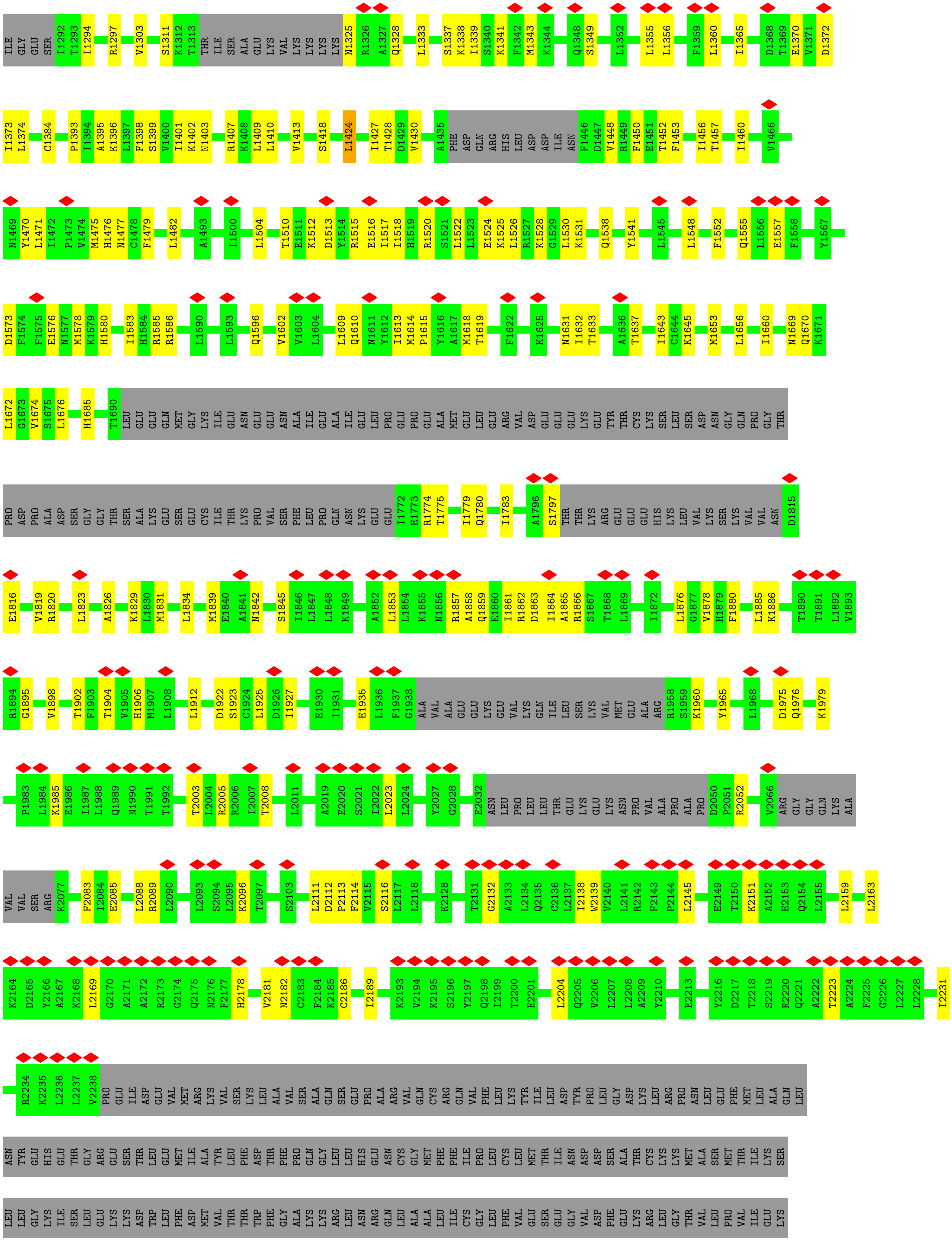
Chain SM:

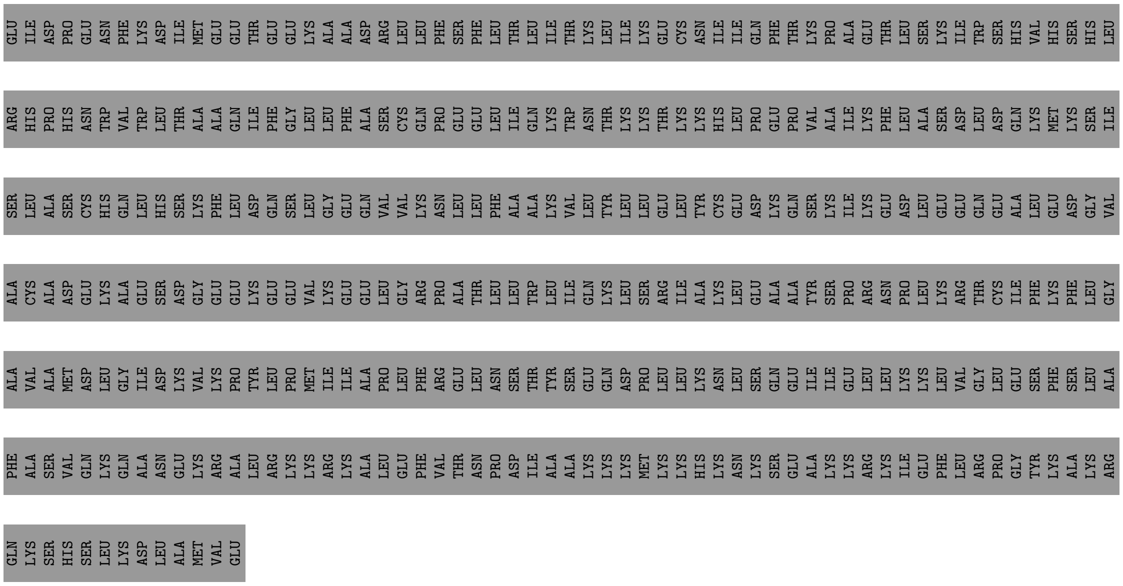


- Molecule 61: Small subunit processome component 20 homolog

Chain SP:

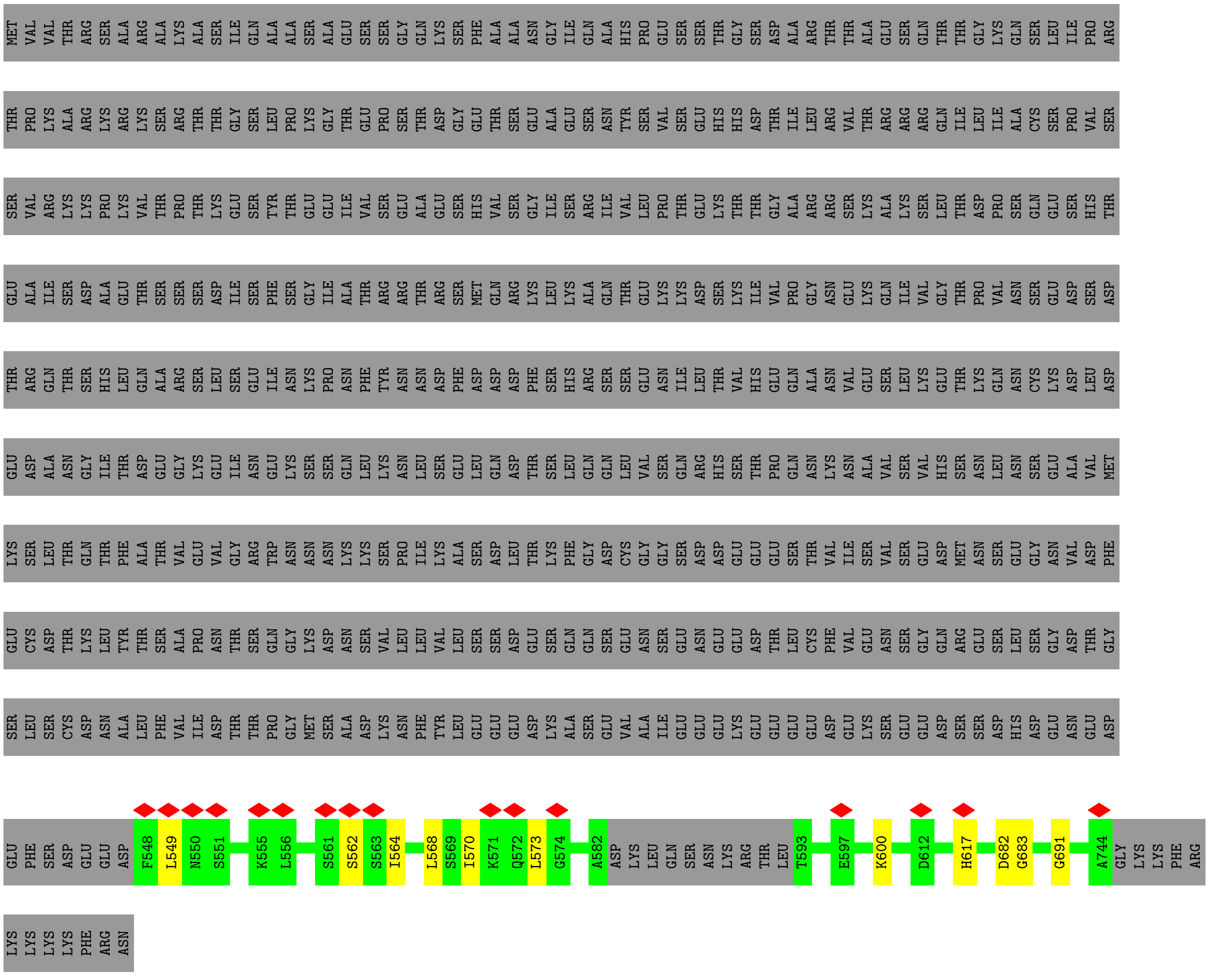



ILE GLY GLU SER I1292 T1293 I1294 R1297 V1303 S1311 K1312 T1313 THR ILE SER ALA GLU LYS VAL LYS LYS LYS LYS N1325 R1326 A1327 Q1328 L1333 S1337 K1338 I1339 S1340 K1341 F1342 M1343 K1344 Q1348 S1349 L1352 L1355 L1356 F1359 L1360 I1365 D1368 T1369 E1370 V1371 D1372
I1373 L1374 C1384 P1393 I1394 A1395 K1396 L1397 F1398 S1399 V1400 I1401 K1402 N1403 R1407 K1408 L1409 L1410 V1413 S1418 L1424 I1427 T1428 D1429 V1430 A1435 PHE ASP GLN ARG HIS LEU ASP ASP ILE ASN F1446 D1447 V1448 R1449 F1450 E1451 T1452 F1453 I1456 T1457 I1460 V1466
N1469 Y1470 L1471 I1472 P1473 V1474 M1475 H1476 N1477 C1478 F1479 L1482 A1493 I1500 L1504 T1510 E1511 K1512 D1513 Y1514 R1515 E1516 I1517 I1518 H1519 R1520 S1521 L1522 L1523 E1524 K1525 L1526 R1527 K1528 G1529 L1530 K1531 Q1538 Y1541 L1545 L1548 F1552 Q1555 L1556 E1557 F1558 Y1567
D1573 F1574 F1575 E1576 N1577 M1578 K1579 H1580 I1583 H1584 R1585 R1586 L1590 L1593 Q1596 V1602 V1603 L1604 L1609 Q1610 N1611 Y1612 I1613 M1614 P1615 Y1616 A1617 M1618 T1619 F1622 K1625 N1631 I1632 T1633 A1636 T1637 I1643 C1644 K1645 M1653 L1656 I1660 N1669 Q1670 K1671
L1672 G1673 V1674 S1675 L1676 H1685 T1690 LEU GLU GLU GLN MET GLY LYS ILE GLU ASN GLU GLU ASN ALA ILE GLU ALA ILE GLU LEU PRO GLU PRO GLU ALA MET GLU LEU GLU ARG VAL ASP GLU GLU GLU LYS GLU TYR THR CYS LYS SER LEU SER ASP ASN GLY GLN PRO GLY THR
PRO ASP PRO ALA ASP SER GLY GLY THR SER ALA LYS GLU SER GLU CYS ILE THR LYS PRO VAL SER PHE LEU PRO GLN ASN LYS GLU GLU I1772 E1773 R1774 T1775 I1779 Q1780 I1783 A1796 S1797 THR THR LYS ARG GLU GLU GLU HIS LYS LEU VAL LYS SER LYS VAL VAL ASN D1815
E1816 V1819 R1820 L1823 A1826 K1829 L1830 M1831 L1834 M1839 E1840 A1841 N1842 S1845 I1846 L1847 L1848 K1849 A1852 L1853 L1854 K1855 N1856 R1857 A1858 Q1859 E1860 I1861 R1862 D1863 I1864 A1865 R1866 S1867 T1868 L1869 I1872 L1876 G1877 V1878 H1879 F1880 L1885 K1886 T1890 T1891 L1892 V1893
R1894 G1895 V1898 T1902 F1903 T1904 V1905 H1906 M1907 L1908 L1912 D1922 S1923 C1924 L1925 D1926 I1927 E1930 I1931 E1935 L1936 F1937 G1938 ALA VAL ALA GLU GLU LYS GLU VAL LYS GLN ILE LEU SER LYS VAL MET GLU ALA ARG R1958 S1959 K1960 Y1965 L1968 D1975 Q1976 K1979
P1983 L1984 K1985 E1986 I1987 L1988 Q1989 N1990 T1991 T1992 T2003 L2004 R2005 R2006 I2007 T2008 L2011 A2019 E2020 S2021 I2022 L2023 L2024 Y2027 G2028 E2032 ASN LEU PRO LEU LEU THR GLU LYS GLU LYS ASN PRO VAL ALA PRO ALA PRO D2050 P2051 R2052 V2066 ARG GLY GLY GLN LYS ALA
VAL VAL SER ARG K2077 F2083 I2084 E2085 L2088 R2089 L2090 L2093 S2094 L2095 K2096 T2097 S2103 L2111 D2112 P2113 F2114 V2115 S2116 L2117 L2118 K2128 T2131 G2132 A2133 L2134 Q2135 C2136 L2137 I2138 W2139 V2140 L2141 R2142 F2143 P2144 L2145 E2149 T2150 K2151 A2152 E2153 Q2154 L2155 L2159 L2163
K2164 D2165 Y2166 A2167 K2168 L2169 G2170 A2171 A2172 R2173 G2174 Q2175 N2176 F2177 H2178 V2181 N2182 C2183 F2184 K2185 C2186 I2189 K2193 V2194 K2195 S2196 Y2197 Q2198 I2199 T2200 E2201 L2204 Q2205 V2206 L2207 L2208 A2209 Y2210 E2213 Y2216 D2217 T2218 S2219 R2220 Q2221 A2222 T2223 A2224 F2225 G2226 L2227 L2228 I2231
R2234 K2235 L2236 L2237 V2238 PRO GLU ILE ASP GLU VAL MET ARG LYS VAL SER LYS LEU ALA VAL SER ALA GLN SER GLU PRO ALA ARG VAL GLN CYS ARG GLN VAL PHE LEU LYS TYR ILE LEU ASP TYR PRO LEU GLY ASP LYS LEU ARG PRO ASN LEU GLU PHE MET LEU ALA GLN LEU
ASN TYR GLU HIS GLU THR GLY ARG GLU SER THR LEU GLU MET ILE ALA TYR LEU PHE ASP THR PHE PRO GLN GLY LEU LEU HIS GLU ASN CYS GLY MET PHE PHE ILE PRO LEU CYS LEU MET THR ILE ASN ASP ASP SER ALA THR CYS LYS LYS MET ALA SER MET THR ILE LYS SER
LEU LEU GLY LYS ILE SER LEU GLU LYS LYS ASP TRP LEU PHE ASP MET VAL THR THR TRP PHE GLY ALA LYS LYS ARG LEU ASN ARG GLN LEU ALA ALA LEU ILE CYS GLY LEU PHE VAL GLU SER GLY GLY VAL ASP PHE GLU LYS ARG LEU GLY THR VAL LEU PRO VAL ILE GLU LYS



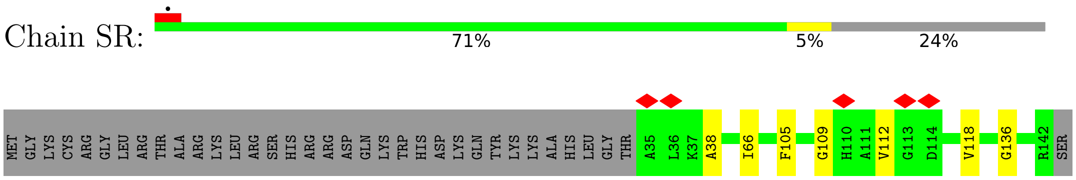
- Molecule 62: Deoxynucleotidyltransferase terminal-interacting protein 2

Chain SQ:



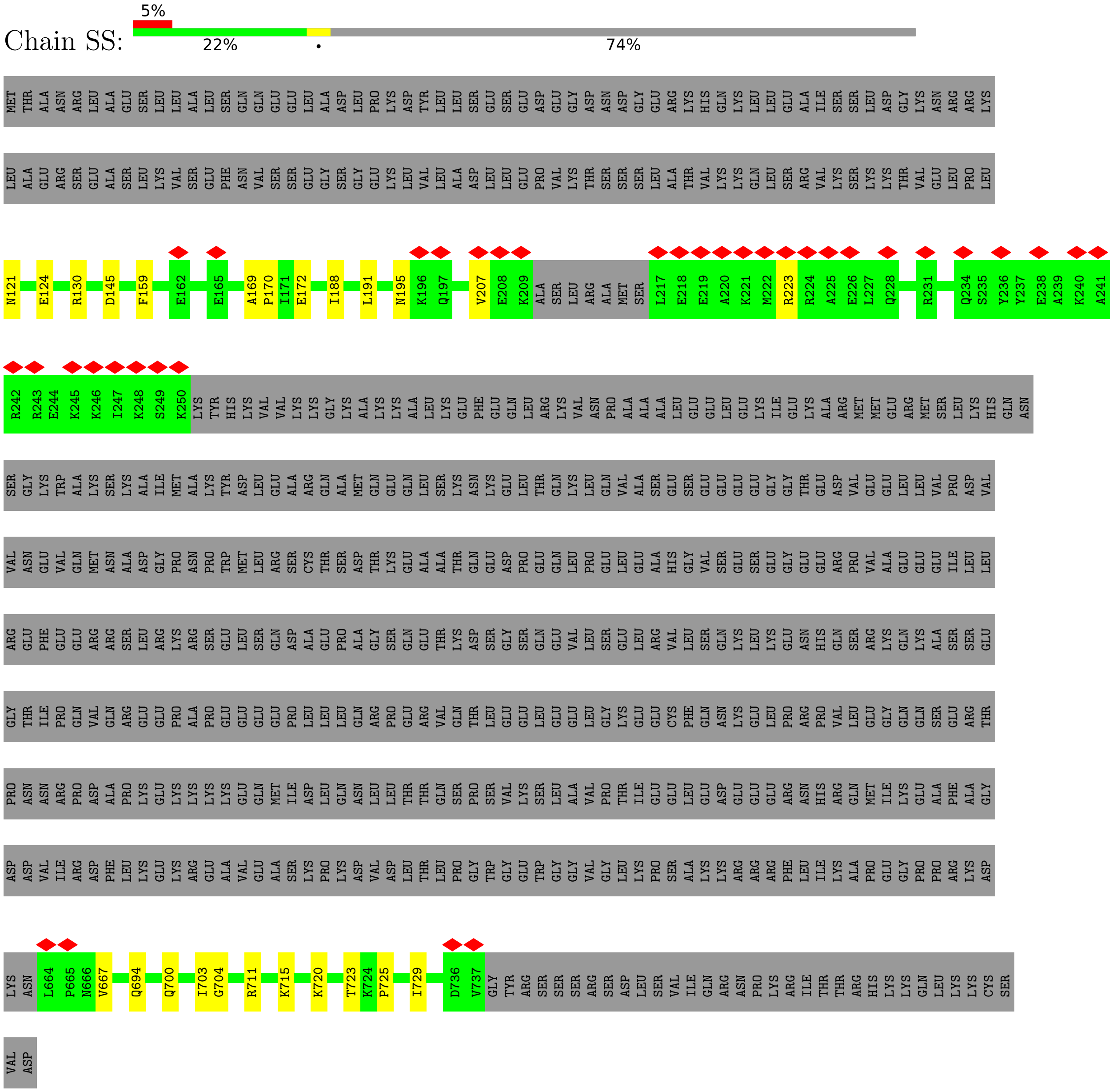
- Molecule 63: 40S ribosomal protein S23

Chain SR:



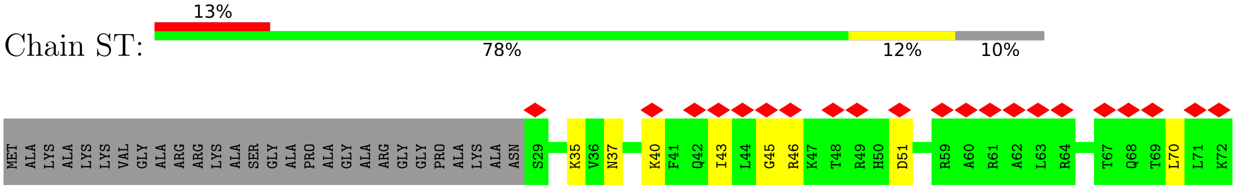
- Molecule 64: U3 small nucleolar RNA-associated protein 14 homolog A

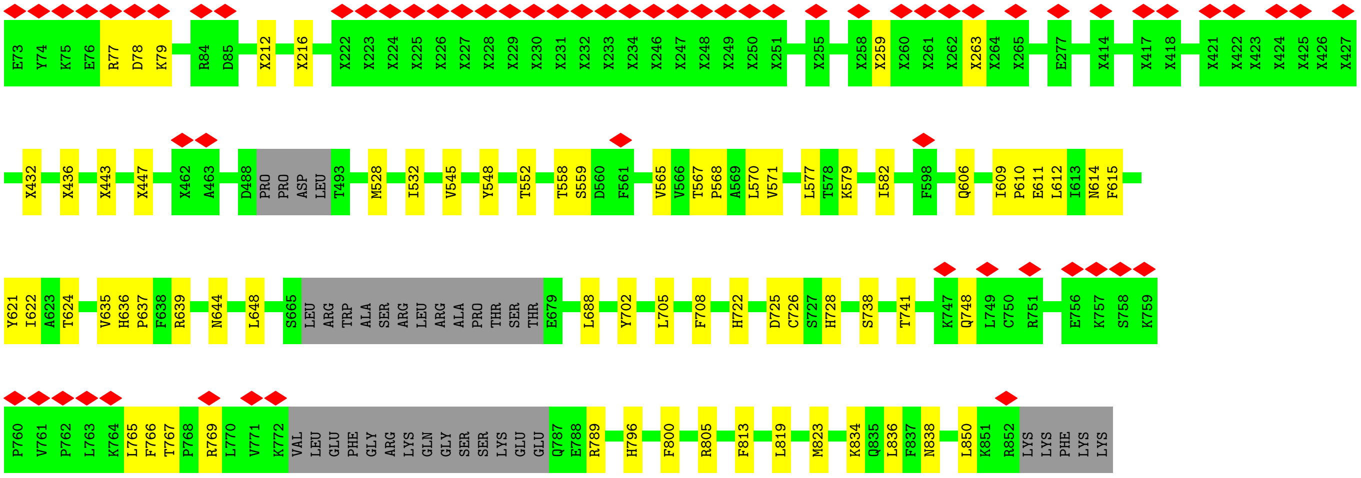
Chain SS:



- Molecule 65: Nucleolar protein 14

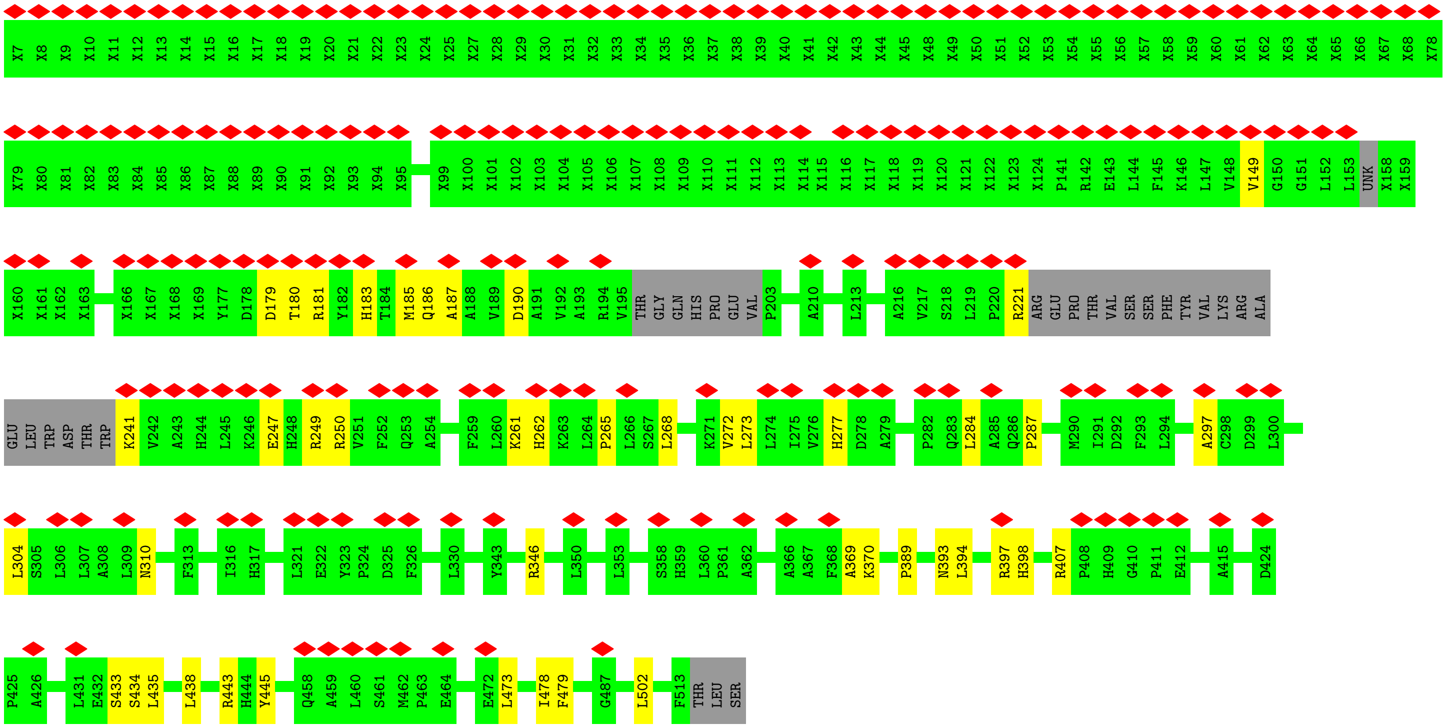
Chain ST:





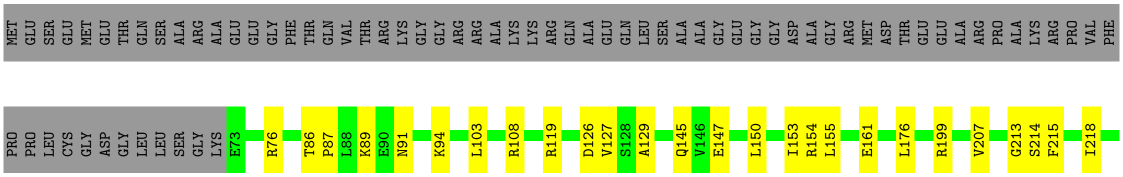
- Molecule 66: Nucleolar complex protein 4 homolog

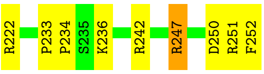
Chain SU:



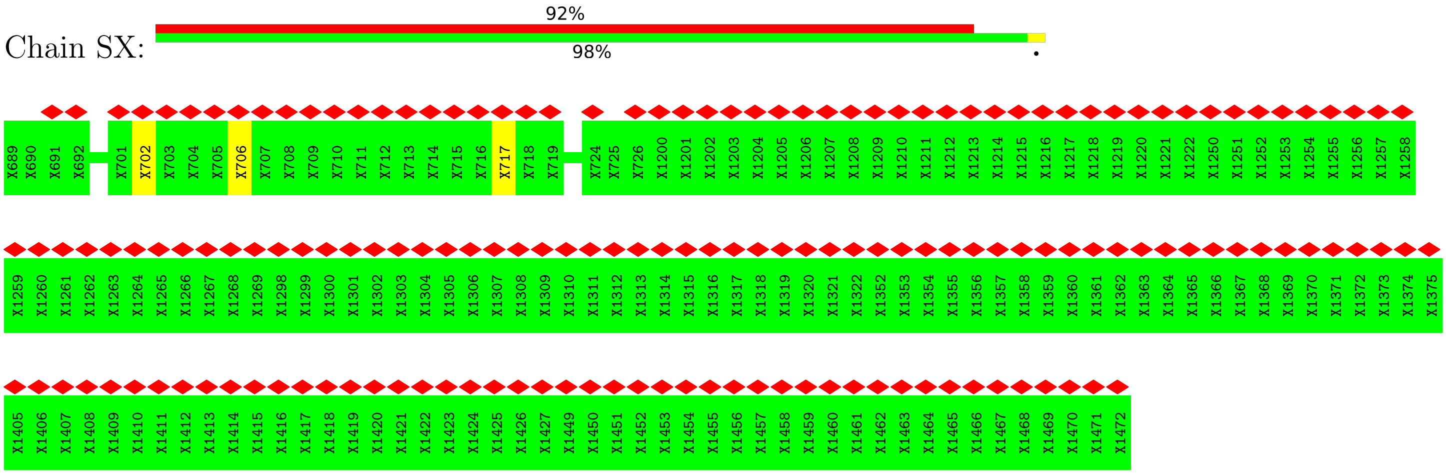
- Molecule 67: RNA-binding protein PNO1

Chain SW:

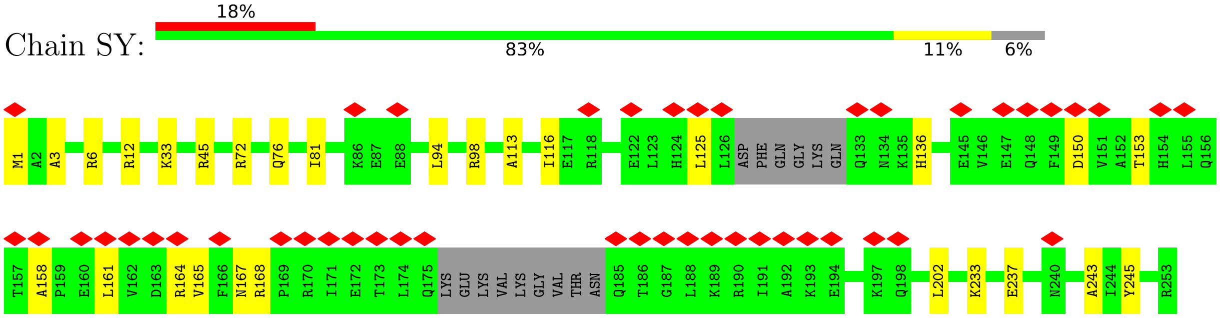




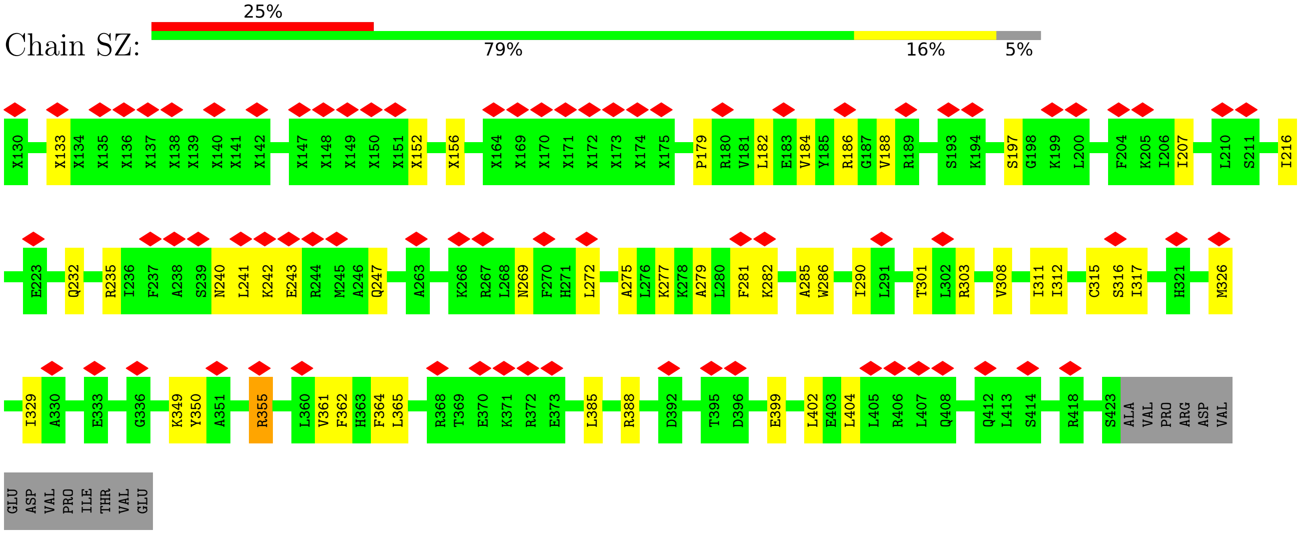
- Molecule 68: Unassigned peptides



- Molecule 69: Probable U3 small nucleolar RNA-associated protein 11



- Molecule 70: Bystin



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42142	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	20.935	Depositor
Minimum map value	-14.456	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.682	Depositor
Recommended contour level	2.68	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: ZN, MG, SAH, GTP, ATP

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	0.19	0/5739	0.85	2/8931 (0.0%)
2	L1	0.19	0/31039	0.85	66/48327 (0.1%)
3	L2	0.18	0/5130	0.81	5/7996 (0.1%)
4	L3	0.26	0/720	0.61	0/970
5	L4	0.25	0/2118	0.56	0/2849
6	L5	0.26	0/1523	0.56	2/2048 (0.1%)
7	L6	0.27	0/1830	0.59	0/2434
8	L7	0.29	0/1365	0.56	0/1830
9	L8	0.26	0/1500	0.57	0/2002
10	L9	0.25	0/1447	0.56	0/1930
11	LA	0.28	0/941	0.54	0/1264
12	LC	0.27	0/1115	0.56	0/1494
13	LD	0.26	0/1225	0.60	0/1640
14	LF	0.25	0/868	0.54	0/1159
15	LG	0.24	0/490	0.62	0/656
16	LH	0.25	0/6127	0.50	0/8292
17	LI	0.26	0/3245	0.48	0/4386
18	LJ	0.27	0/3788	0.56	2/5128 (0.0%)
19	LK	0.29	0/959	0.58	1/1302 (0.1%)
19	LL	0.24	0/4072	0.51	0/5539
20	LM	0.26	0/16110	0.50	3/21817 (0.0%)
21	LN	0.25	0/5438	0.51	1/7377 (0.0%)
22	LO	0.26	0/6835	0.55	0/9256
23	LP	0.25	0/4806	0.47	0/6455
24	LQ	0.24	0/6548	0.51	0/8839
25	LR	0.25	0/6141	0.53	0/8348
26	LS	0.25	0/3621	0.51	0/4876
27	LT	0.25	0/6907	0.50	0/9359
28	LU	0.24	0/3695	0.52	0/4986
29	LW	0.28	1/3594 (0.0%)	0.57	3/4867 (0.1%)
30	LZ	0.25	0/1560	0.56	0/2104
32	NA	0.26	0/2084	0.50	1/2789 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	NB	0.25	0/622	0.64	0/816
34	NC	0.24	0/788	0.57	0/1049
35	ND	0.25	0/708	0.54	0/947
36	NE	0.25	0/807	0.46	0/1069
37	NF	0.23	0/1226	0.49	0/1649
38	NG	0.25	0/873	0.52	0/1177
39	NH	0.25	0/8580	0.51	0/11685
40	NI	0.25	0/1887	0.52	0/2558
41	NJ	0.25	0/6652	0.50	0/9006
41	NK	0.25	0/6545	0.52	1/8867 (0.0%)
42	NM	0.24	0/1899	0.49	0/2533
43	NN	0.25	0/346	0.59	0/462
44	NO	0.27	0/1051	0.60	1/1406 (0.1%)
45	NQ	0.24	0/653	0.49	0/876
47	NT	0.28	0/479	0.69	1/635 (0.2%)
48	NU	0.25	0/501	0.55	0/667
49	NW	0.25	0/2556	0.54	0/3469
50	NY	0.25	0/2265	0.49	1/3045 (0.0%)
51	SA	0.24	0/3122	0.46	0/4208
52	SB	0.24	0/3491	0.48	0/4695
53	SC	0.29	0/1818	0.56	2/2463 (0.1%)
53	SD	0.24	0/1878	0.50	0/2540
54	SE	0.24	0/980	0.50	0/1323
54	SF	0.25	0/967	0.50	0/1305
55	SG	0.24	0/2941	0.51	0/3988
56	SH	0.24	0/2882	0.50	0/3887
57	SI	0.25	0/6917	0.49	0/9297
58	SJ	0.25	0/1609	0.53	0/2181
58	SK	0.25	0/1609	0.52	0/2181
59	SL	0.25	0/1619	0.53	0/2174
60	SM	0.25	0/2420	0.57	0/3264
61	SP	0.25	0/16393	0.49	2/22173 (0.0%)
62	SQ	0.25	0/1561	0.48	0/2083
63	SR	0.26	0/828	0.51	0/1110
64	SS	0.24	0/1663	0.50	0/2250
65	ST	0.27	0/3597	0.51	0/4836
66	SU	0.25	0/2634	0.52	1/3581 (0.0%)
67	SW	0.27	0/1436	0.59	0/1936
69	SY	0.24	0/2051	0.49	0/2723
70	SZ	0.25	0/2043	0.52	0/2763
All	All	0.24	1/245477 (0.0%)	0.59	95/340127 (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
6	L5	0	1
22	LO	0	1
67	SW	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LW	101	PRO	CG-CD	-7.89	1.24	1.50

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	LW	101	PRO	N-CD-CG	-10.97	86.75	103.20
2	L1	1453	C	N1-C2-O2	9.35	124.51	118.90
2	L1	1453	C	C2-N1-C1’	9.25	128.98	118.80
2	L1	1535	U	C2-N1-C1’	8.14	127.47	117.70
2	L1	1742	C	C2-N1-C1’	8.11	127.72	118.80
2	L1	1535	U	N1-C2-O2	7.93	128.35	122.80
2	L1	483	C	N1-C2-O2	7.77	123.56	118.90
53	SC	183	PRO	N-CD-CG	-7.76	91.56	103.20
2	L1	1453	C	N3-C2-O2	-7.58	116.59	121.90
2	L1	483	C	C2-N1-C1’	7.49	127.04	118.80
53	SC	183	PRO	CA-N-CD	-7.48	101.03	111.50
2	L1	369	C	N1-C2-O2	7.36	123.31	118.90
44	NO	85	ASP	CB-CG-OD1	7.30	124.87	118.30
2	L1	1535	U	N3-C2-O2	-7.27	117.11	122.20
20	LM	637	LEU	CA-CB-CG	7.27	132.01	115.30
2	L1	1742	C	N1-C2-O2	7.05	123.13	118.90
2	L1	100	U	C2-N1-C1’	6.94	126.03	117.70
66	SU	502	LEU	CA-CB-CG	6.88	131.13	115.30
19	LK	542	PRO	CA-N-CD	-6.87	101.88	111.50
3	L2	32	U	N1-C2-O2	6.73	127.51	122.80
2	L1	1218	C	N1-C2-O2	6.72	122.93	118.90
3	L2	32	U	C2-N1-C1’	6.67	125.71	117.70
2	L1	501	C	C2-N1-C1’	6.65	126.12	118.80
2	L1	501	C	N1-C2-O2	6.58	122.85	118.90
2	L1	589	G	P-O3’-C3’	6.44	127.42	119.70
2	L1	1453	C	C6-N1-C1’	-6.32	113.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	136	ARG	CB-CG-CD	6.29	127.95	111.60
2	L1	1453	C	C6-N1-C2	-6.26	117.79	120.30
2	L1	1022	U	C2-N1-C1'	6.25	125.20	117.70
2	L1	369	C	C2-N1-C1'	6.24	125.66	118.80
47	NT	122	PRO	CA-N-CD	-6.23	102.77	111.50
2	L1	369	C	N3-C2-O2	-6.18	117.57	121.90
2	L1	483	C	N3-C2-O2	-6.17	117.58	121.90
2	L1	1637	A	OP2-P-O3'	6.15	118.72	105.20
2	L1	1218	C	C2-N1-C1'	6.05	125.45	118.80
29	LW	101	PRO	CA-N-CD	-6.04	103.04	111.50
2	L1	481	C	C2-N1-C1'	6.00	125.40	118.80
32	NA	545	ASP	CB-CG-OD1	5.96	123.66	118.30
2	L1	1710	C	N1-C2-O2	5.88	122.43	118.90
2	L1	100	U	N1-C2-O2	5.86	126.90	122.80
3	L2	32	U	N3-C2-O2	-5.84	118.11	122.20
2	L1	481	C	N1-C2-O2	5.76	122.36	118.90
18	LJ	489	MET	CB-CG-SD	-5.75	95.16	112.40
2	L1	1802	C	N1-C2-O2	5.74	122.34	118.90
2	L1	1637	A	P-O3'-C3'	5.73	126.58	119.70
2	L1	1742	C	C6-N1-C2	-5.73	118.01	120.30
2	L1	188	C	N1-C2-O2	5.72	122.33	118.90
2	L1	1309	C	N1-C2-O2	5.70	122.32	118.90
50	NY	234	LEU	CA-CB-CG	5.68	128.37	115.30
2	L1	1742	C	N3-C2-O2	-5.68	117.92	121.90
3	L2	14	C	P-O3'-C3'	5.68	126.51	119.70
2	L1	188	C	C2-N1-C1'	5.68	125.05	118.80
2	L1	325	C	P-O3'-C3'	5.63	126.46	119.70
2	L1	1664	A	P-O3'-C3'	5.62	126.44	119.70
20	LM	1035	LEU	CA-CB-CG	5.61	128.19	115.30
2	L1	100	U	N3-C2-O2	-5.60	118.28	122.20
2	L1	1742	C	C6-N1-C1'	-5.60	114.08	120.80
2	L1	73	C	C2-N1-C1'	5.59	124.95	118.80
2	L1	1022	U	N1-C2-O2	5.54	126.68	122.80
61	SP	1161	ASP	CB-CG-OD2	5.52	123.27	118.30
2	L1	1314	U	C2-N1-C1'	5.49	124.28	117.70
21	LN	133	ASP	CB-CG-OD2	5.48	123.23	118.30
2	L1	423	U	P-O3'-C3'	5.42	126.21	119.70
20	LM	2095	LEU	CA-CB-CG	5.38	127.68	115.30
2	L1	423	U	OP1-P-O3'	5.38	117.04	105.20
2	L1	1523	C	N1-C2-O2	5.36	122.12	118.90
1	L0	666	U	OP2-P-O3'	5.35	116.96	105.20
41	NK	220	PRO	CA-N-CD	-5.34	104.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L1	451	G	N3-C4-C5	-5.32	125.94	128.60
2	L1	275	C	N1-C2-O2	5.30	122.08	118.90
2	L1	1547	C	N1-C2-O2	5.30	122.08	118.90
2	L1	1022	U	N3-C2-O2	-5.29	118.50	122.20
29	LW	101	PRO	CA-CB-CG	-5.28	93.96	104.00
2	L1	1218	C	N3-C2-O2	-5.26	118.22	121.90
3	L2	130	U	C2-N1-C1’	5.26	124.01	117.70
2	L1	483	C	C6-N1-C1’	-5.25	114.50	120.80
2	L1	1453	C	C5-C6-N1	5.22	123.61	121.00
2	L1	1535	U	C6-N1-C1’	-5.21	113.90	121.20
6	L5	136	ARG	CA-CB-CG	5.19	124.81	113.40
2	L1	142	C	N1-C2-O2	5.18	122.01	118.90
2	L1	1710	C	C2-N1-C1’	5.17	124.49	118.80
2	L1	1485	U	C2-N1-C1’	5.16	123.89	117.70
2	L1	1823	A	P-O3’-C3’	5.14	125.87	119.70
2	L1	1719	A	P-O3’-C3’	5.14	125.87	119.70
18	LJ	489	MET	CA-CB-CG	5.13	122.03	113.30
2	L1	965	U	N1-C2-O2	5.13	126.39	122.80
2	L1	391	C	C2-N1-C1’	5.13	124.44	118.80
2	L1	1802	C	C2-N1-C1’	5.12	124.43	118.80
2	L1	1464	C	N1-C2-O2	5.08	121.95	118.90
2	L1	284	C	N1-C2-O2	5.08	121.95	118.90
2	L1	1549	U	N3-C2-O2	-5.07	118.65	122.20
61	SP	1424	LEU	CA-CB-CG	5.06	126.94	115.30
2	L1	1461	G	C3’-C2’-C1’	5.02	105.52	101.50
1	L0	824	C	N1-C2-O2	5.02	121.91	118.90
2	L1	1549	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	L5	136	ARG	Sidechain
22	LO	316	GLU	Peptide
67	SW	247	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L0	5152	0	2630	49	0
2	L1	27777	0	14063	253	0
3	L2	4589	0	2306	44	0
4	L3	854	0	774	24	0
5	L4	2076	0	2177	17	0
6	L5	1501	0	1557	16	0
7	L6	1811	0	1974	22	0
8	L7	1346	0	1410	30	0
9	L8	1474	0	1542	21	0
10	L9	1425	0	1541	16	0
11	LA	931	0	961	18	0
12	LC	1098	0	1168	10	0
13	LD	1204	0	1274	11	0
14	LF	851	0	894	17	0
15	LG	488	0	514	4	0
16	LH	5987	0	5953	72	0
17	LI	3889	0	3464	54	0
18	LJ	3711	0	3758	65	0
19	LK	943	0	1023	25	0
19	LL	3982	0	4031	55	0
20	LM	15820	0	16318	272	0
21	LN	5299	0	5269	78	0
22	LO	6676	0	6579	74	0
23	LP	4705	0	4720	49	0
24	LQ	6438	0	6400	75	0
25	LR	6015	0	5981	90	0
26	LS	3560	0	3570	51	0
27	LT	6756	0	6768	80	0
28	LU	3611	0	3618	59	0
29	LW	3519	0	3518	33	0
30	LZ	1532	0	1553	10	0
31	N0	264	0	178	0	0
32	NA	2055	0	2135	21	0
33	NB	617	0	685	7	0
34	NC	779	0	788	10	0
35	ND	696	0	729	10	0
36	NE	799	0	854	11	0
37	NF	1202	0	1289	9	0
38	NG	861	0	871	8	0
39	NH	8374	0	8456	77	0
40	NI	1840	0	1812	18	0
41	NJ	6526	0	6599	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	NK	6419	0	6480	87	0
42	NM	1873	0	1968	17	0
43	NN	340	0	345	3	0
44	NO	1034	0	1080	18	0
45	NQ	640	0	661	5	0
46	NR	4305	0	945	22	0
47	NT	470	0	474	14	0
48	NU	495	0	541	10	0
49	NW	2498	0	2456	34	0
50	NY	2222	0	2310	16	0
51	SA	3077	0	3139	32	0
52	SB	3439	0	3559	42	0
53	SC	1781	0	1803	37	0
53	SD	1841	0	1867	14	0
54	SE	968	0	1017	7	0
54	SF	955	0	1008	5	0
55	SG	2884	0	2751	17	0
56	SH	2832	0	2937	28	0
57	SI	6803	0	6966	63	0
58	SJ	1579	0	1646	28	0
58	SK	1579	0	1646	24	0
59	SL	1586	0	1641	31	0
60	SM	2369	0	2376	18	0
61	SP	16078	0	16633	204	0
62	SQ	1533	0	1579	8	0
63	SR	816	0	871	5	0
64	SS	1626	0	1677	19	0
65	ST	4170	0	3804	56	0
66	SU	3154	0	2736	30	0
67	SW	1413	0	1489	26	0
68	SX	885	0	192	2	0
69	SY	2024	0	2148	19	0
70	SZ	2222	0	2142	32	0
71	L1	19	0	0	0	0
71	NH	1	0	0	0	0
71	SI	1	0	0	0	0
71	SL	1	0	0	0	0
72	NH	31	0	12	2	0
72	NK	31	0	12	1	0
73	NQ	1	0	0	0	0
73	NT	1	0	0	0	0
73	SL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	SI	32	0	12	0	0
75	SJ	26	0	19	3	0
75	SK	26	0	19	0	0
All	All	245114	0	224665	2570	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2570) 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)
20:LM:1457:GLN:HE21	20:LM:1457:GLN:N	1.53	1.06
28:LU:66:ARG:HH12	59:SL:127:PRO:HD3	1.40	0.84
27:LT:748:ASN:HB3	27:LT:751:LEU:HD23	1.60	0.83
21:LN:461:LEU:HB2	21:LN:477:PHE:HB2	1.63	0.81
61:SP:1430:VAL:HG12	61:SP:1477:ASN:HD21	1.45	0.80
61:SP:2085:GLU:HB3	61:SP:2089:ARG:HH12	1.46	0.79
18:LJ:179:LEU:HD12	18:LJ:193:ASP:HB2	1.65	0.78
2:L1:1396:A:O2'	2:L1:1398:G:N7	2.15	0.78
61:SP:1885:LEU:HB3	61:SP:1927:ILE:HG21	1.64	0.77
5:L4:248:ILE:HG22	5:L4:251:GLU:HG2	1.67	0.77
20:LM:605:PRO:HA	20:LM:703:THR:HG21	1.66	0.77
19:LL:276:THR:HB	19:LL:286:LYS:HB2	1.68	0.76
32:NA:383:PRO:HG2	32:NA:386:LEU:HD13	1.68	0.75
2:L1:164:A:H3'	2:L1:165:G:H21	1.51	0.75
8:L7:53:VAL:O	8:L7:57:ARG:HB2	1.86	0.75
4:L3:36:VAL:HG23	4:L3:40:TYR:HD2	1.52	0.75
2:L1:1354:G:N2	2:L1:1357:A:OP2	2.19	0.75
20:LM:843:VAL:HG22	20:LM:846:ARG:HH21	1.51	0.75
1:L0:1434:U:H5'	51:SA:44:SER:HA	1.68	0.74
2:L1:97:U:H3	2:L1:434:G:H1	1.32	0.74
20:LM:688:ILE:HG12	20:LM:732:LEU:HD11	1.68	0.74
19:LL:596:LYS:NZ	21:LN:380:ASP:OD2	2.21	0.74
2:L1:1392:U:H2'	2:L1:1393:G:H8	1.53	0.73
20:LM:1761:LEU:HB3	20:LM:1805:ARG:HH21	1.53	0.73
25:LR:732:GLN:HE22	25:LR:764:THR:HG23	1.54	0.72
24:LQ:668:ILE:HG22	24:LQ:669:GLN:HG3	1.72	0.72
49:NW:151:PHE:HB2	49:NW:159:TYR:HB2	1.72	0.72
51:SA:217:ILE:HG21	51:SA:223:LEU:HD12	1.71	0.72
1:L0:668:U:H5'	35:ND:247:ARG:HD2	1.71	0.72
23:LP:333:CYS:HB3	23:LP:354:THR:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:1457:GLN:N	20:LM:1457:GLN:NE2	2.34	0.71
21:LN:250:SER:HG	21:LN:262:HIS:HE2	1.38	0.71
5:L4:246:LEU:HD12	5:L4:247:THR:HG22	1.72	0.71
17:LI:608:ILE:HG23	17:LI:613:ILE:HD11	1.73	0.71
61:SP:565:CYS:HA	61:SP:605:LEU:HD12	1.72	0.71
4:L3:55:ARG:NH2	18:LJ:77:SER:O	2.24	0.70
19:LL:106:ILE:HB	19:LL:120:LEU:HB2	1.72	0.70
2:L1:368:U:OP2	43:NN:516:ARG:NH2	2.24	0.70
59:SL:69:ILE:HG22	59:SL:156:ILE:HB	1.72	0.70
17:LI:693:VAL:HB	19:LL:570:GLY:HA3	1.73	0.70
41:NK:160:LEU:HD23	41:NK:188:ILE:HD11	1.72	0.70
44:NO:91:ASN:O	59:SL:83:LYS:NZ	2.21	0.70
26:LS:68:GLU:HG2	26:LS:71:ARG:HH22	1.56	0.70
41:NK:779:LEU:HA	41:NK:783:PHE:HB2	1.74	0.69
22:LO:389:VAL:HG21	22:LO:430:VAL:HG21	1.74	0.69
25:LR:493:LEU:HD12	25:LR:505:LEU:HD11	1.73	0.69
41:NJ:283:THR:HG22	41:NJ:413:ILE:HD11	1.72	0.69
17:LI:657:ASN:HB3	17:LI:660:VAL:HB	1.73	0.69
25:LR:168:LEU:HB3	25:LR:180:TRP:HB2	1.74	0.69
26:LS:253:ARG:HH21	26:LS:271:LEU:HD21	1.58	0.69
56:SH:13:CYS:HB3	56:SH:35:ILE:HG23	1.73	0.69
2:L1:1130:G:N2	2:L1:1130:G:OP2	2.25	0.69
20:LM:1741:LEU:HD22	20:LM:1785:GLN:HG3	1.75	0.69
16:LH:21:ARG:HG2	16:LH:295:HIS:HB3	1.75	0.69
26:LS:371:LYS:HG3	26:LS:372:THR:HG23	1.74	0.69
1:L0:679:A:O2’	54:SE:28:GLN:NE2	2.26	0.68
61:SP:1191:LEU:HG	61:SP:1238:ILE:HD11	1.75	0.68
41:NK:284:ALA:HB3	41:NK:290:LYS:HD3	1.75	0.68
61:SP:1538:GLN:HE22	61:SP:1619:THR:HG21	1.58	0.68
61:SP:59:ASN:HD22	61:SP:106:PRO:HG2	1.58	0.68
4:L3:104:UNK:HA	65:ST:796:HIS:HD2	1.58	0.68
11:LA:80:ASP:OD1	11:LA:84:LYS:NZ	2.27	0.67
39:NH:393:SER:HA	39:NH:417:LEU:HB2	1.77	0.67
8:L7:57:ARG:HH22	8:L7:90:LYS:HA	1.58	0.67
61:SP:1609:LEU:HA	61:SP:1613:ILE:HD13	1.76	0.67
24:LQ:274:ILE:HG21	24:LQ:353:ILE:HD11	1.76	0.67
61:SP:1303:VAL:HG11	61:SP:1343:MET:HG3	1.77	0.67
61:SP:1826:ALA:HA	61:SP:1829:LYS:HE3	1.76	0.67
66:SU:407:ARG:NH2	66:SU:433:SER:O	2.28	0.67
70:SZ:182:LEU:HG	70:SZ:186:ARG:HH12	1.59	0.67
19:LL:298:LEU:HB2	19:LL:315:CYS:HB2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:1989:CYS:SG	20:LM:2040:ARG:NH2	2.67	0.67
21:LN:212:VAL:HG12	21:LN:218:VAL:HG22	1.77	0.67
2:L1:134:C:O2'	61:SP:906:LYS:NZ	2.28	0.67
16:LH:85:TRP:HE1	16:LH:92:LEU:HD13	1.60	0.67
19:LL:503:ILE:HG22	19:LL:507:GLN:HE22	1.60	0.67
53:SD:284:LYS:NZ	59:SL:130:GLU:OE1	2.28	0.67
25:LR:402:ILE:HG21	25:LR:455:LEU:HD21	1.77	0.67
49:NW:160:ARG:HD2	49:NW:172:LEU:HD23	1.76	0.67
44:NO:75:ILE:O	44:NO:78:ARG:NH1	2.27	0.67
58:SJ:96:MET:HA	58:SJ:101:ASN:HD22	1.60	0.67
61:SP:1260:LEU:HB3	61:SP:1338:LYS:HG3	1.75	0.67
6:L5:71:ARG:NH2	6:L5:148:ASN:OD1	2.28	0.66
23:LP:1:MET:SD	28:LU:366:ARG:NH2	2.68	0.66
41:NK:509:TYR:HB3	41:NK:696:LEU:HB2	1.77	0.66
2:L1:1192:U:H4'	2:L1:1193:U:H5'	1.77	0.66
6:L5:168:THR:OG1	6:L5:171:GLU:OE1	2.14	0.66
22:LO:880:ARG:HH22	27:LT:909:PRO:HB2	1.60	0.66
8:L7:148:LEU:HA	44:NO:42:MET:HE2	1.77	0.66
24:LQ:903:ASP:OD2	24:LQ:907:ARG:NH1	2.29	0.66
41:NK:309:ILE:HB	41:NK:368:ILE:HG22	1.78	0.66
49:NW:138:ARG:H	49:NW:153:GLY:HA2	1.61	0.66
2:L1:39:A:H61	2:L1:515:G:H1'	1.61	0.66
23:LP:149:LYS:NZ	62:SQ:564:ILE:O	2.29	0.66
41:NJ:277:ARG:HB3	41:NJ:458:ARG:HG2	1.75	0.66
61:SP:494:PHE:HB3	61:SP:497:LEU:HD13	1.78	0.66
9:L8:205:ARG:HH22	13:LD:8:ARG:HH21	1.44	0.66
20:LM:962:LYS:HB3	20:LM:965:GLU:HB2	1.76	0.66
59:SL:26:GLU:OE1	59:SL:29:ARG:NH1	2.28	0.66
17:LI:693:VAL:HG21	19:LL:567:HIS:HA	1.78	0.66
20:LM:688:ILE:HG23	20:LM:732:LEU:HD21	1.78	0.66
2:L1:1394:G:N2	2:L1:1475:G:O2'	2.26	0.66
39:NH:246:GLU:HG3	39:NH:247:ARG:HD3	1.77	0.66
41:NJ:501:LEU:HD11	41:NJ:638:MET:HG3	1.76	0.66
65:ST:708:PHE:HB3	65:ST:748:GLN:HE22	1.61	0.66
1:L0:1420:G:H1	3:L2:49:U:H3	1.42	0.66
10:L9:136:ARG:NH1	10:L9:159:PHE:O	2.29	0.66
19:LK:535:ALA:HB3	19:LL:577:THR:HG21	1.76	0.66
21:LN:494:PRO:HG2	21:LN:536:PRO:HA	1.76	0.66
52:SB:350:THR:HG21	52:SB:358:ILE:HG13	1.78	0.66
53:SD:195:ARG:NH2	54:SF:9:LYS:O	2.29	0.66
18:LJ:103:GLY:HA2	18:LJ:118:PHE:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:818:G:H5”	26:LS:517:LYS:HZ1	1.60	0.65
18:LJ:489:MET:HE2	19:LK:571:LYS:HA	1.78	0.65
61:SP:1530:LEU:HD13	61:SP:1615:PRO:HG3	1.79	0.65
2:L1:1736:G:H2’	2:L1:1737:G:H8	1.59	0.65
57:SI:178:LYS:NZ	57:SI:243:LYS:O	2.29	0.65
57:SI:1063:THR:HG22	57:SI:1096:VAL:HG12	1.76	0.65
16:LH:409:GLN:NE2	16:LH:411:LYS:O	2.29	0.65
61:SP:2204:LEU:HD23	61:SP:2231:ILE:HG13	1.76	0.65
18:LJ:181:ILE:HG21	18:LJ:221:LEU:HD11	1.77	0.65
39:NH:172:ILE:HG22	39:NH:174:PRO:HD2	1.79	0.65
20:LM:1765:GLN:NE2	20:LM:1805:ARG:O	2.30	0.65
41:NJ:310:PHE:HB2	41:NJ:385:VAL:HG22	1.79	0.65
1:L0:1414:A:N6	59:SL:18:SER:OG	2.29	0.65
2:L1:190:G:HO2’	61:SP:1197:TYR:HH	1.44	0.65
2:L1:508:A:H3’	2:L1:509:G:H8	1.62	0.65
12:LC:62:ARG:O	12:LC:96:TYR:OH	2.14	0.65
1:L0:852:G:N2	22:LO:287:ASP:O	2.30	0.64
20:LM:1863:HIS:HA	20:LM:1867:LEU:HB2	1.79	0.64
24:LQ:632:HIS:HD2	24:LQ:636:VAL:HG12	1.62	0.64
18:LJ:467:GLN:NE2	18:LJ:471:GLU:OE2	2.31	0.64
20:LM:610:ASN:H	20:LM:619:MET:HE1	1.61	0.64
27:LT:772:LYS:HG3	27:LT:773:LYS:HD2	1.78	0.64
60:SM:153:HIS:HB3	60:SM:157:GLY:HA3	1.79	0.64
22:LO:303:LEU:HB2	22:LO:317:LEU:HD11	1.79	0.64
51:SA:45:ILE:HG13	51:SA:46:VAL:HG23	1.78	0.64
67:SW:161:GLU:OE2	67:SW:222:ARG:NH1	2.30	0.64
18:LJ:264:LEU:HG	18:LJ:274:VAL:HG22	1.78	0.64
41:NK:386:VAL:HG22	41:NK:408:PHE:HB2	1.80	0.64
57:SI:90:PRO:HG2	57:SI:93:VAL:HB	1.78	0.64
70:SZ:308:VAL:HA	70:SZ:311:ILE:HD12	1.77	0.64
3:L2:159:G:OP2	54:SF:97:ARG:NH2	2.30	0.64
6:L5:124:ASP:OD1	6:L5:125:SER:N	2.30	0.64
56:SH:159:MET:HG3	56:SH:160:PRO:HD2	1.80	0.64
1:L0:858:C:OP2	30:LZ:53:ARG:NH2	2.28	0.64
2:L1:484:A:OP1	57:SI:215:LYS:NZ	2.30	0.64
5:L4:45:ILE:HG13	5:L4:61:VAL:HG21	1.79	0.64
25:LR:504:LYS:HG2	25:LR:516:VAL:HG12	1.80	0.64
23:LP:213:SER:OG	64:SS:195:ASN:ND2	2.30	0.64
3:L2:59:G:H5”	22:LO:598:THR:HG23	1.79	0.64
20:LM:652:LYS:O	20:LM:656:LEU:N	2.28	0.64
22:LO:857:ASP:OD1	22:LO:858:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:1125:GLN:NE2	20:LM:1164:GLU:OE2	2.31	0.63
28:LU:318:GLU:HG3	28:LU:394:ARG:HE	1.62	0.63
61:SP:1338:LYS:HD3	61:SP:1341:LYS:HZ3	1.64	0.63
20:LM:1004:LEU:HD12	20:LM:1034:LEU:HD21	1.80	0.63
2:L1:190:G:O2'	61:SP:1197:TYR:OH	2.16	0.63
4:L3:75:ARG:NH2	4:L3:81:ASP:OD2	2.29	0.63
10:L9:72:PHE:HB3	34:NC:205:VAL:HG11	1.80	0.63
23:LP:22:ILE:HD13	29:LW:98:PHE:HZ	1.62	0.63
28:LU:326:GLN:O	28:LU:344:SER:OG	2.17	0.63
40:NI:63:VAL:HB	40:NI:119:ALA:HB3	1.81	0.63
41:NJ:71:LYS:HA	41:NJ:74:ARG:HE	1.64	0.63
61:SP:1866:ARG:HG3	61:SP:1904:THR:HG23	1.80	0.63
65:ST:606:GLN:O	66:SU:443:ARG:NH2	2.31	0.63
2:L1:277:C:H5'	7:L6:231:ARG:HH21	1.63	0.63
16:LH:462:VAL:HG22	16:LH:472:VAL:HG22	1.80	0.63
16:LH:734:LEU:O	20:LM:175:LYS:NZ	2.32	0.63
20:LM:1289:VAL:HG22	20:LM:1326:ILE:HD11	1.81	0.63
41:NJ:285:ALA:HB2	41:NJ:413:ILE:HB	1.79	0.63
1:L0:715:G:H1	1:L0:755:C:H42	1.45	0.63
20:LM:554:ILE:HG21	20:LM:595:LEU:HD12	1.81	0.63
26:LS:363:GLY:HA2	26:LS:385:VAL:HG23	1.80	0.63
16:LH:823:ASP:O	16:LH:826:TRP:NE1	2.32	0.63
19:LL:186:ALA:HB1	19:LL:211:VAL:HB	1.79	0.63
39:NH:477:ARG:HD2	39:NH:992:ARG:HH21	1.64	0.63
48:NU:16:ILE:HA	48:NU:19:LYS:HZ2	1.63	0.63
2:L1:542:U:O2	57:SI:1234:LYS:NZ	2.31	0.63
41:NK:13:LEU:HD22	41:NK:198:LEU:HD13	1.81	0.63
48:NU:30:THR:HA	48:NU:33:ARG:HG2	1.81	0.63
1:L0:717:G:O6	1:L0:752:C:N4	2.32	0.62
39:NH:731:TYR:HE1	39:NH:733:GLU:HB2	1.64	0.62
3:L2:215:G:H4'	52:SB:401:ARG:HD2	1.79	0.62
28:LU:340:ILE:HB	28:LU:352:TRP:HB2	1.80	0.62
57:SI:143:LEU:HD21	57:SI:906:PRO:HG2	1.81	0.62
61:SP:1219:LEU:HA	61:SP:1231:ILE:HD11	1.81	0.62
61:SP:1820:ARG:HA	61:SP:1823:LEU:HD13	1.81	0.62
2:L1:1110:G:N7	40:NI:211:ARG:NH2	2.45	0.62
2:L1:1743:G:H1'	2:L1:1791:A:H61	1.64	0.62
17:LI:408:ASP:OD2	17:LI:412:HIS:ND1	2.31	0.62
17:LI:505:LEU:HD13	17:LI:591:ILE:HG21	1.81	0.62
22:LO:239:ARG:HD2	52:SB:439:CYS:HB2	1.81	0.62
61:SP:281:VAL:O	61:SP:337:LYS:NZ	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:44:VAL:HG22	18:LJ:56:VAL:HG22	1.82	0.62
21:LN:560:TYR:O	21:LN:565:ARG:NH1	2.33	0.62
6:L5:49:LEU:HD12	12:LC:50:LYS:HG2	1.82	0.62
7:L6:152:ASP:HB3	7:L6:155:GLN:HG3	1.82	0.62
19:LK:535:ALA:HA	19:LK:538:LEU:HD12	1.81	0.62
19:LL:494:VAL:HG21	19:LL:530:VAL:HG23	1.80	0.62
20:LM:1133:ASP:OD1	20:LM:1206:ARG:NH1	2.33	0.62
41:NK:290:LYS:NZ	41:NK:411:SER:O	2.33	0.62
2:L1:621:C:O4’	69:SY:12:ARG:NH2	2.32	0.62
16:LH:576:GLU:O	17:LI:354:HIS:N	2.32	0.62
29:LW:519:ARG:NH1	64:SS:700:GLN:OE1	2.33	0.62
65:ST:582:ILE:O	65:ST:644:ASN:ND2	2.32	0.62
28:LU:185:ARG:HA	61:SP:2169:LEU:HD22	1.80	0.62
20:LM:1331:GLY:O	20:LM:1335:MET:HB2	1.99	0.62
33:NB:448:ARG:O	33:NB:452:ARG:NH2	2.33	0.62
1:L0:604:C:H41	18:LJ:431:GLN:HB3	1.64	0.61
2:L1:1194:A:N6	24:LQ:614:ASN:OD1	2.33	0.61
61:SP:1475:MET:HB3	61:SP:1479:PHE:HE2	1.65	0.61
61:SP:1609:LEU:HD23	61:SP:1613:ILE:HD13	1.80	0.61
22:LO:151:ASP:OD1	22:LO:152:TRP:N	2.33	0.61
32:NA:523:GLU:OE2	32:NA:525:LYS:NZ	2.30	0.61
40:NI:201:GLU:O	45:NQ:80:ARG:NH1	2.33	0.61
20:LM:2:THR:N	22:LO:665:GLU:OE2	2.33	0.61
20:LM:542:GLU:O	20:LM:545:LYS:NZ	2.30	0.61
20:LM:688:ILE:HD13	20:LM:728:ARG:HB3	1.82	0.61
39:NH:706:PRO:HG3	39:NH:1048:PRO:HB3	1.82	0.61
65:ST:577:LEU:HD22	65:ST:611:GLU:HB3	1.82	0.61
70:SZ:275:ALA:O	70:SZ:279:ALA:N	2.33	0.61
20:LM:1602:PRO:HD3	20:LM:1640:ARG:HH12	1.64	0.61
23:LP:373:LYS:NZ	23:LP:405:MET:SD	2.68	0.61
60:SM:279:THR:HB	60:SM:282:ALA:HB2	1.83	0.61
23:LP:74:ARG:NH1	26:LS:83:ASP:O	2.32	0.61
2:L1:412:G:H1	2:L1:430:C:H42	1.46	0.61
16:LH:250:MET:SD	16:LH:268:ARG:NH2	2.73	0.61
27:LT:804:PRO:HD2	27:LT:805:GLU:H	1.65	0.61
57:SI:923:GLN:HB2	57:SI:1016:ASP:HB2	1.80	0.61
21:LN:186:ARG:HA	21:LN:196:CYS:HB2	1.82	0.61
18:LJ:413:ARG:HB3	18:LJ:417:GLU:HB2	1.82	0.61
24:LQ:438:ILE:HD11	24:LQ:471:ILE:HD13	1.82	0.61
2:L1:1702:G:OP2	2:L1:1702:G:N2	2.25	0.61
24:LQ:597:MET:HG2	24:LQ:608:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SP:70:GLU:O	61:SP:74:LYS:NZ	2.33	0.61
21:LN:357:LEU:HB3	21:LN:383:LEU:HB3	1.83	0.61
26:LS:488:LEU:HB2	26:LS:504:LEU:HD21	1.83	0.61
67:SW:247:ARG:NH2	67:SW:250:ASP:OD2	2.34	0.61
53:SC:152:VAL:HG11	53:SC:155:ILE:HD11	1.83	0.60
55:SG:364:ALA:O	55:SG:401:ARG:NH1	2.32	0.60
2:L1:1485:U:H3’	2:L1:1486:A:H8	1.67	0.60
20:LM:1761:LEU:HD21	20:LM:1806:LEU:HB2	1.83	0.60
20:LM:2107:ILE:HG13	20:LM:2108:PRO:HD3	1.82	0.60
22:LO:737:ASP:O	22:LO:770:ASN:ND2	2.25	0.60
25:LR:340:VAL:HG12	25:LR:352:VAL:HG12	1.83	0.60
39:NH:268:LEU:HB2	39:NH:271:LYS:HG2	1.82	0.60
49:NW:239:ASN:O	49:NW:243:THR:OG1	2.19	0.60
61:SP:326:TYR:HB3	61:SP:368:VAL:HG21	1.82	0.60
20:LM:430:ARG:NH1	20:LM:466:LEU:O	2.31	0.60
24:LQ:8:LEU:O	24:LQ:669:GLN:NE2	2.34	0.60
28:LU:346:GLU:OE2	28:LU:350:ARG:NH1	2.33	0.60
41:NJ:6:VAL:HB	57:SI:352:VAL:HB	1.82	0.60
47:NT:92:LYS:HG3	47:NT:93:HIS:H	1.66	0.60
61:SP:1859:GLN:OE1	61:SP:1862:ARG:NH2	2.29	0.60
1:L0:454:C:OP1	21:LN:680:LYS:NZ	2.35	0.60
16:LH:814:LYS:HG2	16:LH:817:ARG:HH21	1.67	0.60
20:LM:1164:GLU:OE1	20:LM:1206:ARG:NH2	2.35	0.60
25:LR:263:LEU:HD21	25:LR:271:LEU:HD22	1.83	0.60
54:SE:95:VAL:HG12	54:SE:97:ARG:H	1.66	0.60
21:LN:110:SER:OG	21:LN:112:SER:O	2.18	0.60
22:LO:710:PHE:HD1	22:LO:717:TRP:HB3	1.66	0.60
61:SP:825:TRP:HA	61:SP:828:LEU:HD12	1.82	0.60
63:SR:112:VAL:HG11	63:SR:118:VAL:HG21	1.83	0.60
28:LU:263:LEU:HD21	28:LU:285:VAL:HG11	1.82	0.60
30:LZ:138:VAL:HG22	30:LZ:158:VAL:HG12	1.82	0.60
41:NK:374:ALA:HA	41:NK:397:LEU:HD11	1.83	0.60
20:LM:658:GLY:HA3	20:LM:765:VAL:HG13	1.84	0.60
20:LM:1406:LEU:HD13	20:LM:1411:PHE:HB3	1.83	0.60
2:L1:369:C:H5	49:NW:132:ARG:HB2	1.66	0.60
2:L1:687:C:HO3’	8:L7:121:THR:HG1	1.42	0.60
51:SA:98:PRO:HA	51:SA:114:THR:HG21	1.84	0.60
61:SP:1294:ILE:HA	61:SP:1297:ARG:HD2	1.83	0.60
69:SY:237:GLU:HB3	69:SY:243:ALA:HB2	1.84	0.60
22:LO:331:GLN:HG3	22:LO:351:GLY:HA3	1.83	0.60
26:LS:154:ASP:HA	26:LS:172:LYS:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:634:HIS:NE2	20:LM:683:MET:SD	2.68	0.59
20:LM:1280:GLU:O	20:LM:1318:LYS:NZ	2.34	0.59
23:LP:226:TYR:OH	23:LP:239:HIS:NE2	2.34	0.59
25:LR:347:ASP:OD1	25:LR:615:ARG:NH1	2.35	0.59
50:NY:319:LYS:HA	50:NY:322:ILE:HD12	1.83	0.59
2:L1:286:U:H2’	2:L1:287:U:H4’	1.84	0.59
2:L1:1536:G:H2’	2:L1:1537:A:H8	1.66	0.59
19:LL:601:GLU:OE2	21:LN:429:ARG:NH1	2.34	0.59
20:LM:1045:ILE:HG23	20:LM:1095:LEU:HD21	1.84	0.59
25:LR:419:GLY:H	25:LR:449:TRP:HH2	1.49	0.59
57:SI:205:ARG:NH1	57:SI:208:THR:OG1	2.35	0.59
2:L1:454:U:H2’	2:L1:455:A:H8	1.66	0.59
2:L1:961:G:N2	50:NY:235:ARG:O	2.35	0.59
20:LM:1578:ARG:HH12	20:LM:1582:SER:HB3	1.66	0.59
64:SS:159:PHE:HB2	64:SS:723:THR:HG22	1.83	0.59
27:LT:229:LEU:HB2	27:LT:243:PHE:HB2	1.84	0.59
28:LU:206:PRO:HG2	28:LU:207:ILE:HD12	1.83	0.59
41:NK:507:LEU:HB3	41:NK:698:LEU:HD11	1.83	0.59
53:SC:243:THR:HG21	53:SC:285:LYS:HB3	1.84	0.59
57:SI:1106:ILE:HD12	57:SI:1107:PRO:HD2	1.84	0.59
60:SM:97:LEU:HD13	60:SM:141:GLU:HB3	1.83	0.59
61:SP:1457:THR:HA	61:SP:1460:ILE:HD12	1.85	0.59
61:SP:2181:VAL:HG22	61:SP:2223:THR:HG21	1.84	0.59
63:SR:105:PHE:HE2	63:SR:109:GLY:HA2	1.68	0.59
20:LM:2030:ARG:HH21	20:LM:2079:LYS:HB2	1.66	0.59
39:NH:760:ALA:HB2	40:NI:173:VAL:HG11	1.85	0.59
49:NW:318:VAL:HG23	49:NW:329:THR:HG22	1.84	0.59
57:SI:961:ASP:OD1	57:SI:967:ARG:NH1	2.36	0.59
25:LR:690:ARG:HB3	25:LR:691:ARG:HH21	1.68	0.59
41:NJ:779:LEU:HA	41:NJ:783:PHE:HB2	1.82	0.59
57:SI:382:THR:HG23	57:SI:385:ALA:H	1.67	0.59
58:SK:96:MET:HA	58:SK:101:ASN:HD22	1.68	0.59
61:SP:1360:LEU:HD23	61:SP:1365:ILE:HD11	1.85	0.59
65:ST:708:PHE:HB3	65:ST:748:GLN:NE2	2.18	0.59
1:L0:865:G:H1	1:L0:1412:U:H3	1.49	0.59
18:LJ:380:VAL:HG11	18:LJ:396:ILE:HG13	1.85	0.59
20:LM:1345:VAL:O	20:LM:1349:THR:OG1	2.16	0.59
20:LM:1674:LEU:HD13	20:LM:1692:VAL:HG13	1.83	0.59
20:LM:1707:GLU:HG3	20:LM:1709:ASN:H	1.67	0.59
22:LO:845:ILE:HG23	27:LT:943:LEU:HD22	1.85	0.59
25:LR:269:GLY:HA2	25:LR:295:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:NI:227:GLU:OE2	40:NI:230:ARG:NH2	2.35	0.59
52:SB:213:ASP:OD1	52:SB:214:ARG:N	2.36	0.59
8:L7:64:VAL:HB	8:L7:72:PHE:HE2	1.68	0.59
28:LU:235:VAL:HG21	28:LU:271:LEU:HB3	1.84	0.59
41:NJ:429:GLN:HA	41:NJ:432:ARG:HD2	1.85	0.59
41:NK:12:ILE:HD12	41:NK:217:GLU:HB3	1.84	0.59
61:SP:502:SER:HA	61:SP:505:LYS:HD2	1.85	0.59
20:LM:1351:LYS:HG3	20:LM:1401:GLN:HE21	1.68	0.59
20:LM:1901:VAL:HA	20:LM:1904:VAL:HG22	1.83	0.59
24:LQ:9:ARG:NH1	24:LQ:707:GLU:OE1	2.36	0.59
27:LT:88:ARG:HD3	27:LT:132:ALA:HB1	1.84	0.59
61:SP:1525:LYS:HG3	61:SP:1526:LEU:N	2.18	0.59
16:LH:15:SER:O	16:LH:312:ASN:ND2	2.36	0.59
29:LW:489:ASN:HB3	29:LW:492:ARG:HB3	1.84	0.59
2:L1:1512:C:H4’	70:SZ:197:SER:HB3	1.85	0.58
20:LM:1311:VAL:O	20:LM:1315:PHE:N	2.29	0.58
61:SP:2159:LEU:O	61:SP:2163:LEU:N	2.27	0.58
20:LM:1787:ILE:HG12	20:LM:1840:HIS:HB3	1.84	0.58
28:LU:12:ASN:O	28:LU:23:ARG:NH1	2.35	0.58
12:LC:82:TYR:HA	12:LC:85:ARG:HD3	1.84	0.58
41:NK:344:ILE:HD12	41:NK:357:ARG:HB3	1.85	0.58
3:L2:54:U:OP1	69:SY:72:ARG:NH2	2.35	0.58
13:LD:95:TYR:HE2	13:LD:97:ARG:HE	1.50	0.58
19:LK:536:SER:O	19:LK:539:SER:OG	2.19	0.58
30:LZ:64:ASP:O	36:NE:185:LYS:NZ	2.26	0.58
2:L1:102:A:OP2	2:L1:408:A:N6	2.37	0.58
2:L1:1762:C:H2’	2:L1:1763:G:C8	2.38	0.58
20:LM:1566:GLU:HG2	20:LM:1612:LEU:HD21	1.85	0.58
39:NH:474:LEU:HD23	39:NH:552:LEU:HD12	1.84	0.58
58:SJ:110:ILE:HB	58:SJ:118:ILE:HB	1.86	0.58
61:SP:2116:SER:HB2	61:SP:2151:LYS:HE2	1.84	0.58
2:L1:1004:U:H2’	2:L1:1005:G:H8	1.68	0.58
14:LF:14:THR:HG23	14:LF:21:LYS:HG2	1.85	0.58
21:LN:146:SER:OG	21:LN:164:SER:OG	2.21	0.58
24:LQ:158:LEU:HD12	24:LQ:163:LEU:HB2	1.86	0.58
26:LS:401:SER:OG	26:LS:403:ASP:OD1	2.22	0.58
41:NK:514:THR:HG21	41:NK:694:LEU:HA	1.85	0.58
6:L5:138:ALA:HB3	15:LG:63:ARG:HH12	1.69	0.58
10:L9:103:GLU:O	10:L9:107:GLU:HG2	2.04	0.58
16:LH:15:SER:OG	16:LH:35:SER:OG	2.20	0.58
41:NJ:290:LYS:NZ	41:NJ:388:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NK:123:LEU:HD23	41:NK:129:LEU:HD21	1.86	0.58
53:SC:225:MET:N	53:SC:225:MET:SD	2.74	0.58
57:SI:103:ILE:HG21	57:SI:111:LEU:HD12	1.86	0.58
47:NT:105:TYR:HD2	47:NT:131:PHE:HD2	1.50	0.58
20:LM:384:THR:HA	20:LM:435:LYS:HE3	1.85	0.58
20:LM:2030:ARG:NH2	20:LM:2077:SER:OG	2.37	0.58
39:NH:268:LEU:O	39:NH:298:ASN:ND2	2.37	0.58
16:LH:333:ASP:O	16:LH:663:GLN:NE2	2.37	0.58
18:LJ:222:VAL:HG12	18:LJ:231:VAL:HG22	1.86	0.58
20:LM:1413:TRP:HB3	20:LM:1462:SER:HA	1.85	0.58
20:LM:2076:SER:O	20:LM:2081:ARG:NH2	2.34	0.58
21:LN:22:VAL:H	21:LN:292:THR:HG21	1.68	0.58
61:SP:531:LEU:HD21	61:SP:574:LEU:HD22	1.85	0.58
1:L0:812:G:OP2	1:L0:812:G:N2	2.28	0.57
17:LI:509:LEU:HB3	17:LI:612:HIS:HD2	1.69	0.57
39:NH:474:LEU:HD11	39:NH:634:VAL:HG13	1.86	0.57
70:SZ:133:UNK:HA	70:SZ:303:ARG:HH12	1.69	0.57
16:LH:555:TYR:HE1	16:LH:576:GLU:HG3	1.69	0.57
24:LQ:555:VAL:HG12	24:LQ:566:VAL:HG12	1.85	0.57
26:LS:144:ASP:OD1	27:LT:233:ASN:ND2	2.37	0.57
28:LU:263:LEU:HB2	28:LU:278:HIS:HB2	1.86	0.57
39:NH:354:MET:HG3	39:NH:425:LEU:HD21	1.86	0.57
41:NK:310:PHE:HB2	41:NK:385:VAL:HG22	1.86	0.57
41:NK:808:LEU:HD12	41:NK:848:ILE:HG21	1.86	0.57
49:NW:162:ASN:HB2	49:NW:169:LEU:HG	1.86	0.57
61:SP:197:MET:O	61:SP:203:LYS:NZ	2.37	0.57
61:SP:1517:ILE:HG13	61:SP:1518:ILE:HG12	1.86	0.57
2:L1:319:C:H2’	2:L1:320:G:C8	2.39	0.57
4:L3:22:GLY:HA2	4:L3:56:ALA:HB3	1.87	0.57
20:LM:1807:THR:HA	20:LM:1810:LYS:HD3	1.85	0.57
41:NK:470:ARG:NH2	72:NK:1101:ATP:O3’	2.37	0.57
20:LM:2073:THR:HB	20:LM:2113:LEU:HD11	1.87	0.57
26:LS:255:SER:H	26:LS:270:GLY:HA2	1.68	0.57
36:NE:227:GLU:HA	36:NE:230:ARG:HH11	1.68	0.57
41:NK:307:SER:HA	41:NK:366:GLN:HG2	1.84	0.57
61:SP:277:VAL:HG21	61:SP:325:THR:HG23	1.87	0.57
2:L1:67:C:H41	7:L6:163:ASN:HA	1.70	0.57
2:L1:1392:U:H2’	2:L1:1393:G:C8	2.35	0.57
23:LP:221:LEU:HD11	64:SS:188:ILE:HG23	1.86	0.57
27:LT:553:LEU:HD11	27:LT:565:PHE:HB3	1.87	0.57
52:SB:197:ILE:HG23	52:SB:198:ILE:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SH:306:THR:HG22	56:SH:337:ILE:HD13	1.86	0.57
16:LH:623:GLY:HA2	16:LH:626:ARG:HH22	1.69	0.57
18:LJ:477:GLN:HA	18:LJ:480:LEU:HD12	1.86	0.57
19:LL:404:LEU:HA	19:LL:408:ILE:HD11	1.86	0.57
28:LU:333:TRP:HE1	28:LU:337:SER:HA	1.69	0.57
41:NJ:507:LEU:HD11	41:NJ:557:PHE:HB3	1.87	0.57
18:LJ:36:LYS:HA	18:LJ:312:ILE:HG22	1.87	0.57
19:LL:42:GLU:OE2	19:LL:49:HIS:ND1	2.37	0.57
20:LM:1636:THR:O	20:LM:1640:ARG:HG3	2.05	0.57
61:SP:1853:LEU:HD23	61:SP:1865:ALA:HB2	1.86	0.57
5:L4:17:HIS:HB2	5:L4:108:ARG:HG3	1.86	0.57
20:LM:1967:ASN:HA	20:LM:1970:ASN:HD22	1.69	0.57
27:LT:772:LYS:HD3	67:SW:247:ARG:NH1	2.18	0.57
10:L9:15:THR:O	59:SL:197:ARG:NH1	2.34	0.57
19:LL:33:SER:OG	19:LL:35:ASP:OD1	2.20	0.57
20:LM:1690:VAL:HG21	20:LM:1728:LEU:HD22	1.85	0.57
21:LN:341:SER:HB3	21:LN:346:LEU:HB2	1.86	0.57
57:SI:1061:ILE:HG22	57:SI:1098:MET:HB3	1.86	0.57
69:SY:158:ALA:HB3	69:SY:161:LEU:HD13	1.86	0.57
2:L1:1525:C:H2'	2:L1:1526:G:H8	1.70	0.57
2:L1:1856:C:O3'	25:LR:140:ARG:NH2	2.38	0.57
19:LK:554:LEU:O	19:LK:558:ARG:HG2	2.05	0.57
26:LS:257:VAL:H	26:LS:526:THR:HG21	1.70	0.57
26:LS:502:VAL:HG22	26:LS:509:VAL:HG22	1.86	0.57
52:SB:4:LEU:HB2	52:SB:87:LEU:HD11	1.85	0.57
58:SK:128:ARG:H	58:SK:132:ARG:HH21	1.52	0.57
65:ST:609:ILE:HD13	65:ST:612:LEU:HB2	1.86	0.57
4:L3:60:THR:OG1	4:L3:62:ASP:OD1	2.21	0.56
7:L6:192:ILE:HG22	7:L6:196:LYS:HE3	1.86	0.56
21:LN:465:GLN:HB2	21:LN:474:LEU:HD21	1.85	0.56
41:NK:259:ASP:OD1	41:NK:260:GLN:N	2.38	0.56
58:SJ:42:ARG:HE	58:SJ:107:GLN:HB2	1.70	0.56
59:SL:103:THR:HG22	59:SL:132:LEU:HD11	1.87	0.56
2:L1:103:A:H4'	2:L1:104:A:C8	2.40	0.56
2:L1:925:G:OP1	37:NF:121:ARG:NH1	2.37	0.56
2:L1:1589:A:H1'	2:L1:1654:G:H4'	1.87	0.56
2:L1:1679:A:OP1	6:L5:60:ARG:NH2	2.38	0.56
18:LJ:181:ILE:HG13	18:LJ:191:MET:HG3	1.86	0.56
20:LM:1111:THR:H	20:LM:1114:PHE:HB3	1.70	0.56
20:LM:1819:PRO:HG3	20:LM:1855:MET:HG3	1.87	0.56
25:LR:503:ALA:HB3	25:LR:517:PHE:HB2	1.86	0.56

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
58:SJ:47:LEU:HD12	58:SJ:202:ALA:HB2	1.87	0.56
61:SP:335:GLY:HA3	61:SP:378:VAL:HB	1.87	0.56
2:L1:647:U:H2’	2:L1:648:A:H8	1.70	0.56
2:L1:1297:U:N3	2:L1:1300:U:OP2	2.36	0.56
3:L2:56:A:H2’	3:L2:57:A:C8	2.40	0.56
3:L2:210:U:OP2	54:SE:44:LYS:NZ	2.34	0.56
14:LF:61:ARG:HG2	34:NC:248:ARG:HH12	1.70	0.56
17:LI:509:LEU:HD23	17:LI:612:HIS:HB3	1.88	0.56
18:LJ:355:ARG:HH21	26:LS:295:ARG:HG3	1.69	0.56
22:LO:784:ARG:HD3	27:LT:751:LEU:HD21	1.85	0.56
41:NJ:577:ILE:HG22	41:NJ:629:ILE:HG13	1.87	0.56
41:NK:857:LEU:HD12	41:NK:901:LYS:HB3	1.88	0.56
50:NY:76:TRP:HA	50:NY:79:VAL:HG12	1.88	0.56
51:SA:16:LEU:HB3	51:SA:50:ALA:HB3	1.87	0.56
51:SA:37:LEU:HD11	53:SD:256:ASN:HD22	1.69	0.56
61:SP:967:HIS:ND1	61:SP:1007:ASP:OD2	2.38	0.56
61:SP:1427:ILE:HG13	61:SP:1470:TYR:HD1	1.69	0.56
19:LL:503:ILE:O	19:LL:507:GLN:NE2	2.38	0.56
28:LU:102:ILE:HG22	28:LU:103:ARG:HG3	1.86	0.56
61:SP:959:CYS:O	61:SP:962:THR:OG1	2.22	0.56
20:LM:1086:ILE:HD12	20:LM:1130:MET:HG3	1.87	0.56
21:LN:535:ALA:HB3	21:LN:540:ASN:H	1.69	0.56
24:LQ:546:LEU:HD12	24:LQ:581:LEU:HG	1.85	0.56
25:LR:275:GLU:HG3	25:LR:278:SER:H	1.69	0.56
29:LW:505:LEU:HB3	30:LZ:13:LEU:HD11	1.88	0.56
32:NA:533:ILE:HD12	32:NA:542:SER:HB2	1.88	0.56
36:NE:287:ASN:ND2	44:NO:85:ASP:OD2	2.36	0.56
58:SJ:146:VAL:HB	58:SJ:156:LEU:HB2	1.85	0.56
12:LC:12:VAL:HG21	12:LC:91:ALA:HA	1.86	0.56
15:LG:21:THR:HG22	15:LG:29:GLN:HG3	1.88	0.56
18:LJ:106:LEU:HD12	18:LJ:116:ARG:HB2	1.87	0.56
19:LL:220:ARG:NH2	19:LL:279:GLU:O	2.37	0.56
27:LT:169:GLN:HB2	27:LT:210:ILE:HD12	1.86	0.56
16:LH:16:GLU:OE1	16:LH:332:LYS:NZ	2.38	0.56
19:LK:474:ASP:HB3	19:LK:477:MET:HG2	1.87	0.56
20:LM:1511:ARG:HG2	20:LM:1583:LYS:HE3	1.88	0.56
49:NW:281:GLN:HE22	49:NW:283:SER:HB2	1.70	0.56
61:SP:547:LEU:HB3	61:SP:564:LEU:HD12	1.88	0.56
2:L1:389:A:OP1	49:NW:117:ARG:NH1	2.37	0.56
2:L1:923:G:OP1	37:NF:2:GLY:N	2.39	0.56
3:L2:131:U:O4	3:L2:138:C:N4	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L8:11:ARG:NH1	9:L8:15:GLY:O	2.36	0.56
24:LQ:173:VAL:HB	24:LQ:187:MET:HB2	1.88	0.56
27:LT:821:LEU:O	27:LT:823:GLN:NE2	2.38	0.56
58:SJ:96:MET:SD	58:SJ:101:ASN:ND2	2.79	0.56
61:SP:506:LEU:HD12	61:SP:507:PRO:HD2	1.87	0.56
2:L1:925:G:H1	2:L1:1017:U:H3	1.53	0.56
2:L1:1311:C:H2'	2:L1:1312:G:C8	2.41	0.56
2:L1:1717:C:H2'	2:L1:1718:G:C8	2.41	0.56
18:LJ:116:ARG:NH1	18:LJ:154:SER:OG	2.39	0.56
20:LM:1751:VAL:HG11	20:LM:1792:ILE:HG12	1.86	0.56
25:LR:436:PHE:HZ	25:LR:508:LEU:HD21	1.70	0.56
57:SI:205:ARG:NH1	57:SI:209:GLU:OE2	2.39	0.56
57:SI:954:ILE:HG22	57:SI:1106:ILE:HD11	1.88	0.56
61:SP:526:PRO:HG3	61:SP:570:THR:HG23	1.87	0.56
61:SP:2111:LEU:HB3	61:SP:2145:LEU:HD21	1.87	0.56
20:LM:1402:LEU:HD23	20:LM:1415:LEU:HD13	1.87	0.56
24:LQ:15:VAL:HG22	24:LQ:700:ARG:HG2	1.88	0.56
53:SC:98:ILE:HG23	53:SC:100:ARG:HH12	1.71	0.56
59:SL:169:ARG:NH1	59:SL:187:GLU:OE1	2.39	0.56
3:L2:95:C:H2'	3:L2:96:G:H8	1.71	0.55
8:L7:93:VAL:HG21	8:L7:133:LEU:HD12	1.88	0.55
16:LH:405:VAL:HG22	16:LH:419:MET:HG3	1.87	0.55
20:LM:1280:GLU:HB3	20:LM:1318:LYS:HD2	1.89	0.55
21:LN:144:GLN:O	54:SE:125:ARG:NH2	2.39	0.55
56:SH:60:ASN:ND2	65:ST:79:LYS:O	2.40	0.55
59:SL:149:VAL:HG13	59:SL:174:VAL:HG21	1.88	0.55
61:SP:1530:LEU:HD12	61:SP:1531:LYS:HE3	1.88	0.55
2:L1:981:A:H2'	2:L1:982:G:C8	2.41	0.55
17:LI:153:ILE:HA	17:LI:171:THR:HG22	1.88	0.55
20:LM:1356:ALA:O	20:LM:1360:SER:HB3	2.05	0.55
27:LT:797:LEU:H	67:SW:251:ARG:HG2	1.71	0.55
28:LU:212:LEU:HB2	28:LU:224:TYR:HB2	1.88	0.55
51:SA:163:ARG:NH1	51:SA:386:SER:O	2.33	0.55
2:L1:126:G:H8	7:L6:199:THR:HG21	1.71	0.55
2:L1:170:A:OP2	7:L6:140:ARG:NH1	2.40	0.55
2:L1:1813:A:H2'	2:L1:1814:G:C8	2.40	0.55
18:LJ:35:ILE:O	18:LJ:312:ILE:HA	2.06	0.55
18:LJ:116:ARG:NH1	18:LJ:151:ILE:O	2.39	0.55
20:LM:1663:GLN:HB2	20:LM:1666:ASN:HD22	1.70	0.55
21:LN:154:HIS:HD2	21:LN:203:PHE:HE2	1.54	0.55
27:LT:389:GLY:HA2	27:LT:451:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:NB:473:LYS:HE2	59:SL:47:GLU:HG2	1.89	0.55
40:NI:94:PRO:HA	40:NI:118:VAL:HG21	1.88	0.55
59:SL:22:GLN:HA	59:SL:29:ARG:HE	1.71	0.55
61:SP:1669:ASN:HB3	61:SP:1672:LEU:HB3	1.87	0.55
66:SU:389:PRO:O	66:SU:393:ASN:ND2	2.39	0.55
18:LJ:89:ARG:NH1	18:LJ:134:LYS:O	2.39	0.55
51:SA:217:ILE:HG22	51:SA:227:LYS:HE3	1.88	0.55
56:SH:133:LYS:NZ	56:SH:152:LEU:O	2.37	0.55
61:SP:1167:GLU:O	61:SP:1214:ARG:NH1	2.40	0.55
61:SP:1311:SER:HB3	61:SP:1355:LEU:HD21	1.89	0.55
70:SZ:286:TRP:HH2	70:SZ:312:ILE:HG13	1.70	0.55
2:L1:1378:A:OP2	2:L1:1379:A:O2’	2.22	0.55
16:LH:380:ILE:HG22	16:LH:382:ASP:H	1.71	0.55
16:LH:718:LEU:HB2	26:LS:438:GLN:HE22	1.71	0.55
20:LM:615:GLU:O	20:LM:620:LYS:NZ	2.40	0.55
28:LU:173:THR:OG1	28:LU:181:TRP:NE1	2.40	0.55
39:NH:1124:GLU:HG2	40:NI:36:ALA:HB3	1.89	0.55
49:NW:288:LEU:HG	49:NW:297:MET:HG2	1.89	0.55
57:SI:941:PRO:HG3	57:SI:1129:MET:HG2	1.87	0.55
65:ST:43:ILE:HB	65:ST:46:ARG:HG2	1.88	0.55
6:L5:198:ARG:NH2	58:SK:214:GLU:OE2	2.39	0.55
20:LM:503:LYS:O	20:LM:506:MET:HB3	2.06	0.55
27:LT:501:ASP:OD1	27:LT:502:ILE:N	2.39	0.55
51:SA:375:LYS:HD3	51:SA:397:LEU:HD22	1.88	0.55
2:L1:613:G:N7	69:SY:45:ARG:NH2	2.43	0.55
20:LM:1334:VAL:O	20:LM:1338:ASP:N	2.40	0.55
24:LQ:502:MET:HG2	24:LQ:513:THR:HG22	1.88	0.55
40:NI:244:TRP:HA	40:NI:247:ARG:HG2	1.88	0.55
55:SG:332:LEU:HD23	55:SG:338:MET:HB3	1.87	0.55
60:SM:15:ARG:NH2	60:SM:68:THR:OG1	2.39	0.55
16:LH:698:ILE:HG22	26:LS:265:ILE:HD11	1.88	0.55
20:LM:1843:PRO:O	20:LM:1847:ILE:HG12	2.06	0.55
22:LO:731:ASP:HB3	22:LO:734:VAL:HG23	1.89	0.55
2:L1:1127:C:H4’	45:NQ:17:ARG:HH11	1.72	0.55
16:LH:59:LEU:HB3	16:LH:78:LEU:HD12	1.87	0.55
18:LJ:267:SER:OG	18:LJ:269:ASP:OD1	2.24	0.55
19:LL:278:SER:HB2	19:LL:283:GLU:HB3	1.89	0.55
20:LM:1419:LEU:HD22	20:LM:1447:TRP:HE1	1.72	0.55
21:LN:418:LEU:HA	21:LN:426:SER:O	2.06	0.55
25:LR:196:SER:HG	42:NM:51:ARG:HH21	1.52	0.55
51:SA:12:VAL:HG21	51:SA:137:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:173:LYS:HD2	58:SK:212:TYR:HD2	1.72	0.55
20:LM:1145:GLN:NE2	52:SB:84:HIS:O	2.40	0.54
22:LO:817:GLU:HG2	27:LT:752:VAL:HB	1.88	0.54
39:NH:1099:SER:O	39:NH:1102:LYS:NZ	2.40	0.54
41:NJ:356:ILE:HG23	41:NJ:370:TYR:HB3	1.88	0.54
41:NK:298:ILE:HD11	41:NK:386:VAL:HG21	1.89	0.54
57:SI:1059:ALA:HB3	57:SI:1071:ILE:HD12	1.89	0.54
2:L1:1702:G:O2'	32:NA:560:ALA:O	2.24	0.54
4:L3:38:ARG:O	4:L3:42:HIS:ND1	2.29	0.54
55:SG:223:ILE:HB	55:SG:237:PHE:HB2	1.89	0.54
61:SP:1645:LYS:HD3	61:SP:1685:HIS:HB3	1.89	0.54
61:SP:1857:ARG:O	61:SP:1862:ARG:NH1	2.40	0.54
16:LH:519:GLU:HA	16:LH:541:LYS:HA	1.89	0.54
39:NH:90:GLU:HA	39:NH:93:LYS:HD3	1.87	0.54
39:NH:941:ARG:NH1	39:NH:945:PRO:O	2.36	0.54
2:L1:447:A:OP1	9:L8:49:ARG:NH1	2.39	0.54
58:SK:140:LEU:HD22	58:SK:156:LEU:HD13	1.90	0.54
66:SU:435:LEU:HB3	66:SU:438:LEU:HD23	1.90	0.54
2:L1:649:U:H2'	2:L1:650:A:C8	2.43	0.54
20:LM:1392:GLU:HA	20:LM:1395:ARG:HB2	1.88	0.54
21:LN:17:SER:O	21:LN:35:ARG:NH1	2.40	0.54
21:LN:621:TYR:HB2	21:LN:643:ILE:HD11	1.90	0.54
25:LR:204:SER:OG	25:LR:206:ASP:O	2.25	0.54
41:NJ:697:LYS:HB2	41:NJ:700:GLU:HG3	1.89	0.54
49:NW:152:VAL:HG21	49:NW:182:CYS:HB3	1.90	0.54
61:SP:1418:SER:HB3	61:SP:1428:THR:HG21	1.88	0.54
2:L1:1524:G:H21	65:ST:37:ASN:HD21	1.54	0.54
18:LJ:252:THR:H	18:LJ:267:SER:HA	1.71	0.54
46:NR:186:UNK:O	46:NR:190:UNK:N	2.41	0.54
47:NT:119:ARG:HG3	47:NT:132:MET:HG3	1.89	0.54
70:SZ:365:LEU:HA	70:SZ:404:LEU:HD21	1.90	0.54
4:L3:23:ARG:HH22	18:LJ:80:LYS:HA	1.72	0.54
20:LM:374:ILE:HG13	20:LM:378:HIS:CE1	2.43	0.54
20:LM:1408:ALA:HA	20:LM:1411:PHE:HB2	1.90	0.54
21:LN:448:ASP:OD2	21:LN:450:THR:OG1	2.22	0.54
24:LQ:363:ALA:HB3	24:LQ:384:LEU:HD13	1.89	0.54
41:NJ:344:ILE:HD12	41:NJ:357:ARG:HG2	1.89	0.54
53:SC:220:PRO:HG3	53:SC:248:LEU:HB3	1.88	0.54
61:SP:239:PHE:HB3	61:SP:243:THR:HG21	1.89	0.54
2:L1:370:G:O2'	9:L8:10:LYS:NZ	2.36	0.54
16:LH:123:LYS:NZ	16:LH:125:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:83:THR:O	20:LM:87:ASN:ND2	2.41	0.54
21:LN:127:LEU:HB3	21:LN:139:ARG:HG2	1.89	0.54
22:LO:187:HIS:NE2	22:LO:205:SER:OG	2.29	0.54
24:LQ:621:ASP:OD1	24:LQ:622:PHE:N	2.41	0.54
25:LR:15:TYR:HB2	25:LR:601:LEU:HD21	1.90	0.54
39:NH:722:PRO:HG2	40:NI:156:ILE:HG12	1.90	0.54
41:NJ:158:LYS:HB2	41:NJ:678:VAL:HG21	1.89	0.54
41:NJ:431:LEU:HB3	41:NJ:460:LEU:HD13	1.90	0.54
58:SJ:121:ASN:HB3	58:SJ:124:THR:HG23	1.90	0.54
20:LM:1351:LYS:HA	20:LM:1405:THR:HG21	1.89	0.54
24:LQ:421:LEU:HD21	24:LQ:691:VAL:HG12	1.89	0.54
26:LS:538:LEU:HD23	26:LS:546:LEU:HD12	1.89	0.54
61:SP:1482:LEU:HD13	61:SP:1541:TYR:HE1	1.72	0.54
2:L1:1762:C:H2'	2:L1:1763:G:H8	1.73	0.54
20:LM:47:ILE:HG12	62:SQ:600:LYS:HG3	1.90	0.54
20:LM:1011:PRO:HD2	20:LM:1014:ILE:HD12	1.90	0.54
24:LQ:595:ILE:HG23	32:NA:680:LYS:HD2	1.90	0.54
25:LR:129:CYS:HA	25:LR:153:VAL:HG23	1.90	0.54
28:LU:359:LYS:NZ	28:LU:367:GLU:OE2	2.41	0.54
17:LI:682:ILE:HG13	19:LK:569:HIS:CD2	2.43	0.53
20:LM:1320:LEU:O	20:LM:1323:ILE:HG22	2.07	0.53
21:LN:548:GLN:OE1	21:LN:579:ARG:NH2	2.41	0.53
51:SA:382:ILE:O	51:SA:386:SER:OG	2.22	0.53
20:LM:1827:LYS:HE2	20:LM:1870:PHE:HB2	1.90	0.53
25:LR:424:VAL:HG12	25:LR:441:SER:HB2	1.90	0.53
26:LS:184:GLU:O	26:LS:188:HIS:ND1	2.41	0.53
26:LS:215:ASP:OD1	26:LS:216:ASP:N	2.40	0.53
61:SP:1303:VAL:HG13	61:SP:1339:ILE:HG23	1.90	0.53
14:LF:6:THR:HB	14:LF:28:LEU:HB2	1.91	0.53
49:NW:9:VAL:HG21	49:NW:307:THR:HB	1.91	0.53
61:SP:585:PRO:HG2	61:SP:588:ARG:HD3	1.89	0.53
65:ST:570:LEU:HD21	66:SU:445:TYR:HD2	1.74	0.53
17:LI:642:THR:OG1	17:LI:644:ASN:OD1	2.17	0.53
20:LM:707:ILE:HA	20:LM:710:VAL:HG22	1.91	0.53
20:LM:1693:LEU:HB2	20:LM:1721:VAL:HG11	1.90	0.53
24:LQ:509:ARG:NH2	24:LQ:525:PHE:O	2.41	0.53
41:NK:280:VAL:HG22	41:NK:461:TYR:HD2	1.73	0.53
70:SZ:207:ILE:HD12	70:SZ:216:ILE:HG21	1.90	0.53
2:L1:1856:C:H2'	2:L1:1857:G:C8	2.44	0.53
4:L3:46:ARG:HH22	4:L3:52:LEU:HG	1.73	0.53
18:LJ:302:GLU:OE1	18:LJ:303:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:334:LEU:HD21	20:LM:346:LEU:HD23	1.91	0.53
22:LO:732:THR:O	27:LT:635:ARG:NH2	2.38	0.53
40:NI:42:VAL:HB	40:NI:61:LEU:HD11	1.90	0.53
41:NK:468:SER:OG	41:NK:471:TYR:O	2.25	0.53
61:SP:1187:GLN:HB2	61:SP:1202:LEU:HD13	1.89	0.53
65:ST:767:THR:HG21	68:SX:717:UNK:HA	1.91	0.53
2:L1:1457:U:H2’	2:L1:1458:G:H8	1.72	0.53
8:L7:44:ASN:OD1	8:L7:68:GLN:NE2	2.42	0.53
18:LJ:391:GLU:OE2	18:LJ:433:ARG:NH1	2.42	0.53
18:LJ:479:GLU:HB3	19:LL:524:VAL:HG11	1.90	0.53
20:LM:83:THR:HA	29:LW:181:ASP:HA	1.89	0.53
25:LR:540:SER:OG	25:LR:542:ASP:OD1	2.24	0.53
29:LW:273:ARG:NH2	30:LZ:30:GLU:OE2	2.41	0.53
32:NA:458:LEU:O	32:NA:462:HIS:ND1	2.41	0.53
32:NA:549:LEU:HB3	32:NA:554:ILE:HD11	1.91	0.53
56:SH:187:LYS:HD3	57:SI:759:VAL:HA	1.90	0.53
57:SI:956:LEU:HG	57:SI:1106:ILE:HD13	1.89	0.53
65:ST:635:VAL:HG23	65:ST:637:PRO:HD2	1.90	0.53
3:L2:46:A:H2’	3:L2:47:G:H8	1.73	0.53
20:LM:901:LEU:HD22	20:LM:945:LEU:HD21	1.91	0.53
20:LM:2070:LEU:O	20:LM:2073:THR:OG1	2.20	0.53
24:LQ:297:HIS:CE1	24:LQ:365:ILE:HB	2.44	0.53
47:NT:104:LYS:HZ2	47:NT:118:ARG:HE	1.55	0.53
49:NW:195:THR:H	49:NW:233:ILE:HD12	1.73	0.53
56:SH:321:SER:HB2	56:SH:324:THR:HG23	1.91	0.53
58:SK:127:PRO:HB3	58:SK:132:ARG:HG3	1.90	0.53
61:SP:1512:LYS:HA	61:SP:1515:ARG:HH21	1.74	0.53
65:ST:51:ASP:OD1	65:ST:51:ASP:N	2.41	0.53
2:L1:1120:U:H5’	2:L1:1121:G:H5’	1.91	0.53
8:L7:69:LEU:O	8:L7:73:GLN:HG2	2.09	0.53
20:LM:1350:VAL:HB	20:LM:1401:GLN:HE22	1.74	0.53
25:LR:82:VAL:HG22	25:LR:92:GLN:HG3	1.90	0.53
27:LT:764:ASN:ND2	32:NA:540:PRO:O	2.40	0.53
39:NH:687:GLN:HB3	39:NH:835:PRO:HB3	1.89	0.53
58:SJ:173:LYS:HB2	58:SJ:213:THR:HA	1.90	0.53
65:ST:725:ASP:OD1	65:ST:726:CYS:N	2.42	0.53
1:L0:667:C:H5	35:ND:246:ARG:HG2	1.73	0.53
2:L1:546:G:H5’	33:NB:472:VAL:HG11	1.91	0.53
2:L1:1702:G:H1	25:LR:725:SER:HG	1.57	0.53
14:LF:61:ARG:HG2	34:NC:248:ARG:NH1	2.23	0.53
27:LT:135:ARG:HB2	27:LT:136:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:ND:178:LYS:HA	35:ND:178:LYS:HE3	1.91	0.53
61:SP:2178:HIS:O	61:SP:2182:ASN:ND2	2.41	0.53
1:L0:1431:C:H2'	1:L0:1432:G:H8	1.74	0.53
19:LL:321:THR:HG1	19:LL:331:LYS:N	2.07	0.53
20:LM:2025:ASP:O	20:LM:2029:ASN:N	2.42	0.53
21:LN:537:ASN:OD1	21:LN:538:THR:N	2.42	0.53
61:SP:1068:LYS:HE3	61:SP:1118:LYS:HD2	1.91	0.53
4:L3:70:ILE:HA	4:L3:77:TYR:CE2	2.43	0.52
16:LH:175:GLU:HG3	16:LH:176:PHE:H	1.73	0.52
33:NB:431:ASN:HB3	33:NB:434:VAL:HG22	1.90	0.52
37:NF:3:ARG:HB2	37:NF:6:ALA:HB3	1.90	0.52
61:SP:826:ARG:O	61:SP:829:THR:OG1	2.27	0.52
1:L0:817:U:OP1	27:LT:424:ASN:ND2	2.38	0.52
3:L2:152:A:O2'	3:L2:153:G:OP1	2.27	0.52
16:LH:53:LEU:HD23	16:LH:85:TRP:CE3	2.44	0.52
18:LJ:169:CYS:O	18:LJ:183:GLY:N	2.42	0.52
20:LM:542:GLU:HB3	20:LM:582:ILE:HD11	1.91	0.52
20:LM:1392:GLU:HA	20:LM:1395:ARG:HE	1.74	0.52
20:LM:1649:LEU:HB3	20:LM:1695:THR:HG21	1.90	0.52
24:LQ:479:GLN:OE1	24:LQ:481:TYR:OH	2.24	0.52
25:LR:546:LYS:HG2	25:LR:558:THR:HG22	1.91	0.52
27:LT:874:GLN:O	27:LT:878:LYS:HG3	2.09	0.52
2:L1:45:A:N1	2:L1:480:G:O2'	2.40	0.52
5:L4:48:LEU:HD23	5:L4:61:VAL:HG13	1.90	0.52
20:LM:1419:LEU:HD13	20:LM:1447:TRP:CD1	2.44	0.52
23:LP:307:GLU:O	23:LP:311:ALA:N	2.38	0.52
24:LQ:220:ILE:HD11	24:LQ:266:LEU:HD22	1.90	0.52
41:NJ:381:GLN:NE2	41:NK:369:GLN:OE1	2.42	0.52
51:SA:140:SER:HB3	51:SA:143:LYS:HE2	1.91	0.52
2:L1:559:G:O2'	2:L1:560:A:O5'	2.27	0.52
14:LF:11:LYS:HE3	34:NC:243:GLU:HB3	1.91	0.52
18:LJ:129:ASP:OD2	18:LJ:130:PHE:N	2.43	0.52
20:LM:1159:GLU:OE2	20:LM:1162:ARG:NH2	2.42	0.52
24:LQ:147:GLY:HA3	24:LQ:176:TRP:HH2	1.74	0.52
25:LR:83:THR:HG1	25:LR:93:TRP:HE1	1.56	0.52
42:NM:26:SER:O	42:NM:51:ARG:NH1	2.43	0.52
50:NY:281:GLU:HG2	50:NY:287:TYR:HB2	1.92	0.52
61:SP:1337:SER:O	61:SP:1341:LYS:NZ	2.41	0.52
2:L1:948:C:H2'	2:L1:949:G:H8	1.75	0.52
19:LL:290:VAL:HG22	19:LL:296:VAL:HG22	1.91	0.52
20:LM:1035:LEU:HD12	20:LM:1084:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LR:424:VAL:HA	25:LR:441:SER:HA	1.91	0.52
61:SP:718:GLU:OE2	61:SP:722:ARG:NE	2.41	0.52
61:SP:1583:ILE:HA	61:SP:1586:ARG:HE	1.74	0.52
66:SU:473:LEU:HD13	66:SU:478:ILE:HD11	1.92	0.52
70:SZ:247:GLN:HG2	70:SZ:285:ALA:HA	1.90	0.52
20:LM:1305:LEU:HD21	20:LM:1345:VAL:HG13	1.92	0.52
20:LM:1936:PHE:HE2	20:LM:1958:LEU:HD21	1.75	0.52
23:LP:369:GLU:HG2	23:LP:373:LYS:HE2	1.91	0.52
25:LR:402:ILE:HD11	25:LR:437:LEU:HD11	1.91	0.52
27:LT:883:MET:HE2	27:LT:893:ALA:HB2	1.90	0.52
41:NK:277:ARG:NH1	41:NK:405:TYR:O	2.43	0.52
45:NQ:37:CYS:HB3	45:NQ:63:LEU:HD21	1.92	0.52
61:SP:1399:SER:HB2	61:SP:1476:HIS:HB3	1.92	0.52
20:LM:909:LYS:HB3	20:LM:948:VAL:HG21	1.91	0.52
20:LM:1732:GLN:OE1	20:LM:1735:SER:OG	2.28	0.52
32:NA:386:LEU:HD23	57:SI:939:ARG:HH12	1.74	0.52
41:NK:731:VAL:HG11	41:NK:749:LEU:HD12	1.92	0.52
61:SP:1374:LEU:HD22	61:SP:1413:VAL:HG21	1.92	0.52
20:LM:383:LEU:HB3	20:LM:431:LEU:HD22	1.92	0.52
53:SC:107:VAL:HB	53:SC:134:TYR:HB3	1.92	0.52
2:L1:1718:G:HO2'	2:L1:1719:A:H8	1.57	0.52
20:LM:133:ALA:HB1	20:LM:195:LEU:HD13	1.92	0.52
21:LN:583:ILE:HG12	21:LN:598:LEU:HD12	1.92	0.52
51:SA:297:SER:HB2	51:SA:302:GLU:HG3	1.91	0.52
61:SP:1780:GLN:HG3	61:SP:1834:LEU:HG	1.90	0.52
17:LI:154:LYS:HD3	17:LI:172:GLU:HB3	1.92	0.52
22:LO:487:SER:HB2	22:LO:494:LEU:HD21	1.91	0.52
53:SD:179:ASP:OD1	53:SD:207:ARG:NH1	2.35	0.52
1:L0:710:G:H2'	1:L0:711:A:H8	1.75	0.51
2:L1:1227:G:OP1	65:ST:40:LYS:NZ	2.35	0.51
3:L2:77:C:H2'	3:L2:78:A:H8	1.75	0.51
20:LM:1403:VAL:HB	20:LM:1415:LEU:HD22	1.91	0.51
25:LR:46:ARG:HG2	25:LR:62:GLU:HB2	1.91	0.51
26:LS:255:SER:O	26:LS:526:THR:OG1	2.28	0.51
52:SB:25:VAL:HB	52:SB:111:VAL:HG12	1.92	0.51
1:L0:757:G:H1	1:L0:803:U:H3	1.56	0.51
20:LM:60:PRO:O	20:LM:62:PHE:N	2.43	0.51
20:LM:1984:ASP:OD1	20:LM:1985:PRO:HD3	2.10	0.51
24:LQ:489:LEU:HD12	24:LQ:537:ARG:HH11	1.75	0.51
61:SP:335:GLY:HA2	61:SP:338:ILE:HD12	1.92	0.51
62:SQ:549:LEU:HD13	62:SQ:570:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:530:U:H2’	2:L1:531:A:H8	1.75	0.51
2:L1:1787:G:H2’	2:L1:1788:A:C8	2.45	0.51
8:L7:145:ARG:NE	44:NO:51:GLU:OE1	2.43	0.51
13:LD:99:TYR:HB2	13:LD:101:ARG:HD2	1.91	0.51
19:LL:464:VAL:HA	19:LL:467:THR:HG22	1.91	0.51
19:LL:507:GLN:OE1	19:LL:547:GLN:NE2	2.43	0.51
28:LU:224:TYR:HA	28:LU:231:PRO:HA	1.90	0.51
38:NG:83:GLN:HA	38:NG:86:LYS:NZ	2.26	0.51
39:NH:96:ARG:NH2	39:NH:326:ASP:OD1	2.43	0.51
52:SB:31:GLU:HB3	52:SB:41:ILE:HG13	1.92	0.51
70:SZ:315:CYS:SG	70:SZ:316:SER:N	2.83	0.51
7:L6:136:LYS:NZ	7:L6:175:LYS:O	2.39	0.51
18:LJ:34:GLN:HE21	18:LJ:312:ILE:HD12	1.76	0.51
20:LM:1721:VAL:O	20:LM:1725:LEU:N	2.40	0.51
27:LT:761:ARG:NH2	27:LT:849:GLU:O	2.43	0.51
39:NH:549:THR:HG21	39:NH:991:PRO:HG2	1.92	0.51
39:NH:866:LEU:HB3	39:NH:1073:PHE:HB3	1.91	0.51
39:NH:1106:VAL:HG21	40:NI:20:PRO:HD3	1.92	0.51
41:NK:728:PHE:HB3	41:NK:748:MET:HB3	1.92	0.51
51:SA:97:ASP:HB3	51:SA:100:ILE:HG22	1.92	0.51
51:SA:196:HIS:O	51:SA:220:ARG:NH1	2.44	0.51
2:L1:928:G:H2’	2:L1:929:G:C8	2.45	0.51
2:L1:1275:G:C6	70:SZ:277:LYS:HE3	2.46	0.51
4:L3:62:ASP:OD1	4:L3:63:GLU:N	2.43	0.51
18:LJ:468:GLY:O	18:LJ:472:LYS:HG3	2.09	0.51
21:LN:9:VAL:HB	21:LN:664:VAL:HA	1.92	0.51
39:NH:481:ARG:NH2	39:NH:628:ASP:O	2.41	0.51
57:SI:668:LYS:HA	57:SI:671:LEU:HG	1.93	0.51
58:SJ:73:LEU:HD12	58:SJ:78:ARG:HG3	1.92	0.51
60:SM:262:THR:HG22	60:SM:263:LEU:HD23	1.92	0.51
2:L1:1457:U:H2’	2:L1:1458:G:C8	2.46	0.51
8:L7:9:VAL:HG12	8:L7:11:PRO:HD3	1.91	0.51
21:LN:100:PHE:HZ	53:SC:288:GLN:HG3	1.75	0.51
25:LR:124:LEU:HB2	25:LR:138:ILE:HD11	1.93	0.51
25:LR:285:GLN:NE2	25:LR:319:TYR:OH	2.43	0.51
55:SG:298:VAL:HG12	55:SG:309:VAL:HG22	1.93	0.51
61:SP:1614:MET:HB3	61:SP:1618:MET:HG2	1.92	0.51
1:L0:830:G:H3’	1:L0:831:A:H5”	1.93	0.51
2:L1:1310:U:H4’	47:NT:143:LYS:HD3	1.91	0.51
2:L1:1546:G:O2’	2:L1:1670:C:O2’	2.23	0.51
13:LD:113:LEU:HD23	13:LD:142:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LK:505:LEU:O	19:LK:508:GLU:HG3	2.10	0.51
20:LM:1686:PRO:HB2	20:LM:1725:LEU:HD21	1.93	0.51
52:SB:211:VAL:HG13	52:SB:216:ASN:HB2	1.92	0.51
56:SH:230:MET:O	56:SH:235:SER:OG	2.27	0.51
61:SP:459:ALA:HB3	61:SP:462:MET:HG3	1.93	0.51
1:L0:666:U:H4'	1:L0:667:C:OP2	2.08	0.51
1:L0:1423:U:H2'	1:L0:1424:U:C6	2.46	0.51
2:L1:573:U:N3	2:L1:576:A:OP2	2.37	0.51
16:LH:53:LEU:HD23	16:LH:85:TRP:HE3	1.76	0.51
20:LM:1586:ASP:O	20:LM:1590:LYS:N	2.44	0.51
41:NK:135:ALA:HA	41:NK:481:LEU:HD21	1.92	0.51
53:SC:166:LEU:HB2	53:SC:235:ALA:HA	1.93	0.51
61:SP:1333:LEU:HD21	61:SP:1372:ASP:HB3	1.93	0.51
61:SP:1779:ILE:O	61:SP:1783:ILE:HG12	2.10	0.51
65:ST:443:UNK:O	65:ST:447:UNK:N	2.44	0.51
67:SW:150:LEU:HD12	67:SW:153:ILE:HD12	1.92	0.51
2:L1:1007:C:H2'	2:L1:1008:A:C8	2.45	0.51
2:L1:1597:C:H5"	4:L3:25:LYS:HD2	1.93	0.51
8:L7:144:ILE:HB	44:NO:52:ILE:HB	1.92	0.51
17:LI:644:ASN:OD1	17:LI:645:GLN:N	2.44	0.51
18:LJ:292:ILE:HA	18:LJ:308:MET:HE2	1.93	0.51
26:LS:433:THR:HG22	26:LS:440:VAL:HG22	1.91	0.51
28:LU:269:ARG:NH1	64:SS:145:ASP:OD1	2.38	0.51
28:LU:377:LEU:HD23	64:SS:703:ILE:HD11	1.93	0.51
29:LW:607:ARG:HH22	39:NH:748:PRO:HG3	1.75	0.51
39:NH:376:ARG:NH2	39:NH:449:ASP:OD1	2.44	0.51
48:NU:41:ILE:HG21	48:NU:47:ARG:HB2	1.93	0.51
61:SP:1573:ASP:OD1	61:SP:1576:GLU:N	2.40	0.51
2:L1:1118:C:O2'	42:NM:166:LYS:NZ	2.35	0.51
17:LI:692:GLU:HG3	19:LK:559:VAL:HG21	1.92	0.51
20:LM:955:ILE:HD13	20:LM:1003:LEU:HD21	1.92	0.51
20:LM:1256:LEU:HD22	20:LM:1303:HIS:HB3	1.93	0.51
22:LO:178:ASN:HD21	22:LO:224:LEU:HA	1.74	0.51
24:LQ:547:GLN:NE2	24:LQ:548:LEU:O	2.43	0.51
27:LT:503:THR:HG23	27:LT:506:GLY:H	1.76	0.51
56:SH:135:THR:HG21	56:SH:256:SER:HB3	1.93	0.51
56:SH:146:ASP:O	56:SH:174:ARG:NH2	2.44	0.51
70:SZ:399:GLU:HA	70:SZ:402:LEU:HD13	1.93	0.51
22:LO:100:HIS:ND1	22:LO:148:THR:O	2.44	0.50
25:LR:359:LEU:HD21	25:LR:379:VAL:HG11	1.93	0.50
25:LR:667:LEU:HD11	25:LR:698:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LS:75:ARG:NH2	26:LS:76:ASN:OD1	2.44	0.50
39:NH:694:ARG:NH2	39:NH:873:ASP:OD2	2.43	0.50
41:NJ:808:LEU:HD11	41:NJ:848:ILE:HG21	1.93	0.50
41:NK:502:PRO:HA	41:NK:643:ARG:HD3	1.93	0.50
66:SU:370:LYS:NZ	66:SU:434:SER:O	2.34	0.50
2:L1:674:C:H2'	2:L1:675:U:C6	2.46	0.50
2:L1:1842:C:H2'	2:L1:1843:G:C8	2.45	0.50
17:LI:654:LEU:HG	19:LK:575:LEU:HD11	1.93	0.50
41:NJ:60:LYS:HG3	41:NJ:61:LYS:HG3	1.91	0.50
58:SJ:127:PRO:HB3	58:SJ:132:ARG:HE	1.76	0.50
61:SP:1576:GLU:OE1	61:SP:1585:ARG:NH2	2.45	0.50
61:SP:1583:ILE:HG22	61:SP:1632:ILE:HD11	1.92	0.50
67:SW:233:PRO:HG2	67:SW:236:LYS:HE3	1.92	0.50
19:LL:37:HIS:HD1	19:LL:53:VAL:HG22	1.75	0.50
24:LQ:276:ARG:NE	24:LQ:296:CYS:SG	2.80	0.50
27:LT:640:ALA:HB1	27:LT:666:PRO:HG2	1.93	0.50
27:LT:748:ASN:ND2	27:LT:750:GLN:OE1	2.44	0.50
52:SB:60:PHE:O	52:SB:64:MET:HG2	2.11	0.50
2:L1:103:A:O4'	2:L1:356:C:N4	2.43	0.50
2:L1:1216:C:H42	60:SM:179:MET:HB2	1.76	0.50
2:L1:1599:U:OP2	18:LJ:78:ARG:NH2	2.45	0.50
24:LQ:303:LEU:HD13	24:LQ:382:PHE:HE2	1.77	0.50
26:LS:161:ARG:NH2	52:SB:434:SER:O	2.41	0.50
41:NJ:694:LEU:HG	41:NJ:695:LEU:HD12	1.92	0.50
41:NK:363:GLU:HG2	41:NK:364:HIS:ND1	2.27	0.50
44:NO:83:LEU:HD11	44:NO:117:ARG:HA	1.94	0.50
46:NR:743:UNK:O	46:NR:747:UNK:N	2.44	0.50
53:SD:125:ILE:HD13	62:SQ:691:GLY:HA3	1.92	0.50
56:SH:122:ASN:OD1	56:SH:157:ARG:NH1	2.44	0.50
67:SW:145:GLN:NE2	67:SW:147:GLU:OE1	2.40	0.50
11:LA:81:ASP:OD1	11:LA:84:LYS:NZ	2.36	0.50
19:LK:475:PHE:O	19:LK:479:ASN:ND2	2.44	0.50
26:LS:170:GLU:OE1	26:LS:181:ARG:NH1	2.41	0.50
39:NH:182:LEU:HD11	39:NH:253:LEU:HD12	1.93	0.50
41:NJ:635:TYR:HB3	41:NJ:640:TYR:HE2	1.76	0.50
44:NO:18:GLU:HG2	44:NO:69:LEU:HB3	1.91	0.50
2:L1:374:G:OP1	13:LD:59:LYS:NZ	2.45	0.50
5:L4:197:ASN:ND2	5:L4:199:GLU:OE2	2.43	0.50
7:L6:223:LYS:O	7:L6:227:GLN:HG2	2.11	0.50
16:LH:129:LEU:HB3	16:LH:151:LEU:HB2	1.94	0.50
19:LK:477:MET:O	19:LK:481:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:1966:LEU:O	20:LM:1970:ASN:ND2	2.45	0.50
27:LT:758:PRO:HD2	27:LT:761:ARG:HD2	1.93	0.50
61:SP:1104:VAL:HG13	61:SP:1108:ILE:HD11	1.93	0.50
64:SS:121:ASN:N	64:SS:124:GLU:OE2	2.44	0.50
65:ST:577:LEU:HD21	65:ST:615:PHE:HB2	1.94	0.50
2:L1:166:A:H1'	7:L6:13:GLN:HE21	1.77	0.50
17:LI:643:LEU:HA	17:LI:646:ILE:HD12	1.92	0.50
19:LL:466:LEU:HD11	19:LL:505:LEU:HD21	1.93	0.50
20:LM:1289:VAL:HG13	20:LM:1326:ILE:HG12	1.93	0.50
21:LN:542:VAL:HG12	21:LN:552:GLU:HG3	1.93	0.50
24:LQ:89:ILE:HB	24:LQ:103:PHE:HB2	1.94	0.50
24:LQ:843:ILE:O	24:LQ:887:LYS:NZ	2.41	0.50
25:LR:202:ALA:HB3	25:LR:211:LEU:HB3	1.93	0.50
41:NJ:357:ARG:HD2	41:NJ:369:GLN:HG2	1.93	0.50
65:ST:688:LEU:HD11	65:ST:722:HIS:HE1	1.77	0.50
18:LJ:383:PRO:HG2	35:ND:251:ARG:HH12	1.77	0.50
20:LM:1555:LEU:HA	20:LM:1558:ILE:HG12	1.93	0.50
22:LO:216:GLN:NE2	22:LO:217:CYS:O	2.45	0.50
24:LQ:158:LEU:HD11	24:LQ:175:TRP:HZ3	1.75	0.50
25:LR:547:LEU:HD12	25:LR:557:LYS:HB2	1.94	0.50
38:NG:117:ARG:HH11	50:NY:45:PHE:HB2	1.77	0.50
41:NJ:403:GLY:O	41:NJ:458:ARG:NH1	2.44	0.50
41:NK:357:ARG:HD2	41:NK:369:GLN:HB2	1.92	0.50
46:NR:622:UNK:O	46:NR:626:UNK:N	2.45	0.50
49:NW:287:ILE:HD11	49:NW:300:LYS:HG3	1.94	0.50
51:SA:340:LYS:HD2	51:SA:353:HIS:HB2	1.94	0.50
57:SI:1243:GLU:O	57:SI:1247:LYS:N	2.39	0.50
58:SK:173:LYS:HG2	58:SK:197:VAL:HB	1.94	0.50
60:SM:7:ARG:NH1	60:SM:11:GLU:OE2	2.45	0.50
61:SP:826:ARG:NH1	61:SP:920:GLN:OE1	2.43	0.50
67:SW:126:ASP:OD2	67:SW:127:VAL:N	2.45	0.50
2:L1:444:G:N2	2:L1:447:A:OP2	2.44	0.50
4:L3:47:LYS:HE3	4:L3:77:TYR:HB3	1.92	0.50
9:L8:67:TRP:NE1	9:L8:191:GLU:OE2	2.40	0.50
20:LM:1823:LEU:O	20:LM:1827:LYS:HG2	2.12	0.50
21:LN:87:ASP:HB2	21:LN:94:LYS:HG3	1.94	0.50
27:LT:661:LEU:HD23	27:LT:714:VAL:HG12	1.94	0.50
44:NO:68:ARG:HA	59:SL:118:ARG:HH22	1.77	0.50
57:SI:120:ILE:HG22	57:SI:335:VAL:HG22	1.94	0.50
3:L2:137:G:N2	3:L2:139:U:O2'	2.43	0.49
11:LA:49:LEU:HB3	11:LA:111:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:618:LYS:HZ3	17:LI:621:TYR:HD2	1.58	0.49
24:LQ:874:VAL:HG22	25:LR:788:MET:HG2	1.92	0.49
25:LR:64:GLU:O	25:LR:66:GLN:NE2	2.45	0.49
44:NO:104:LEU:HD23	44:NO:125:ILE:HA	1.94	0.49
61:SP:1476:HIS:HA	61:SP:1479:PHE:HD2	1.77	0.49
61:SP:2085:GLU:HA	61:SP:2088:LEU:HD12	1.94	0.49
18:LJ:471:GLU:OE2	19:LL:569:HIS:NE2	2.45	0.49
20:LM:489:HIS:CE1	20:LM:491:LEU:HB2	2.47	0.49
20:LM:2070:LEU:HD21	20:LM:2106:SER:HA	1.94	0.49
25:LR:385:PHE:CE1	25:LR:429:CYS:HB3	2.47	0.49
41:NK:529:LEU:HD11	41:NK:576:VAL:HG21	1.92	0.49
41:NK:577:ILE:HG22	41:NK:629:ILE:HG13	1.93	0.49
52:SB:113:ASN:ND2	53:SC:251:HIS:CE1	2.80	0.49
55:SG:404:GLN:HB2	55:SG:415:LEU:HD21	1.95	0.49
16:LH:83:LYS:HG2	16:LH:95:THR:HG23	1.95	0.49
18:LJ:131:THR:OG1	18:LJ:133:ASP:OD1	2.23	0.49
20:LM:541:PHE:HZ	20:LM:553:THR:HG22	1.76	0.49
20:LM:1065:GLY:HA2	20:LM:1109:LYS:HE2	1.92	0.49
24:LQ:19:ILE:HB	24:LQ:387:ASN:HB2	1.94	0.49
27:LT:822:ALA:HB3	67:SW:215:PHE:HZ	1.77	0.49
28:LU:300:ALA:HB2	28:LU:331:VAL:HG23	1.93	0.49
32:NA:496:ILE:HA	32:NA:499:MET:HG2	1.93	0.49
38:NG:37:PHE:HE2	38:NG:105:THR:HG21	1.76	0.49
61:SP:1188:ILE:HG12	61:SP:1231:ILE:HG22	1.94	0.49
61:SP:1393:PRO:HA	61:SP:1396:LYS:HG2	1.94	0.49
61:SP:2023:LEU:HD22	61:SP:2114:PHE:HE2	1.77	0.49
70:SZ:362:PHE:HA	70:SZ:365:LEU:HG	1.94	0.49
8:L7:160:LYS:O	8:L7:162:GLN:N	2.45	0.49
16:LH:318:HIS:NE2	16:LH:322:GLU:HB3	2.28	0.49
20:LM:361:HIS:CG	20:LM:372:GLY:HA3	2.47	0.49
20:LM:1859:GLU:O	20:LM:1862:SER:HB3	2.12	0.49
20:LM:2028:GLU:HG2	20:LM:2072:LYS:HD2	1.93	0.49
24:LQ:583:PHE:HZ	24:LQ:586:SER:HB2	1.77	0.49
28:LU:434:SER:HB3	28:LU:437:LYS:HG2	1.93	0.49
41:NK:485:LEU:HB2	41:NK:487:LEU:HG	1.95	0.49
9:L8:57:ALA:HB2	9:L8:183:GLY:HA2	1.95	0.49
21:LN:127:LEU:HD23	21:LN:139:ARG:HD3	1.93	0.49
22:LO:16:ARG:HB3	22:LO:34:GLY:H	1.77	0.49
23:LP:21:ARG:HH21	29:LW:98:PHE:HD2	1.61	0.49
27:LT:418:LEU:HD22	27:LT:478:SER:HA	1.94	0.49
41:NJ:235:LEU:HD13	41:NJ:258:LEU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SJ:55:VAL:HG11	58:SJ:64:LEU:HD13	1.94	0.49
62:SQ:568:LEU:HD23	62:SQ:573:LEU:HD21	1.94	0.49
1:L0:740:G:H3’	1:L0:741:G:H5”	1.95	0.49
2:L1:141:A:H4’	2:L1:142:C:H5’	1.95	0.49
2:L1:454:U:H2’	2:L1:455:A:C8	2.45	0.49
2:L1:941:C:H2’	2:L1:942:G:H8	1.77	0.49
2:L1:1673:U:O2’	6:L5:84:GLY:O	2.24	0.49
4:L3:23:ARG:NH1	18:LJ:80:LYS:O	2.46	0.49
20:LM:1581:LEU:HB3	20:LM:1585:TYR:CE2	2.47	0.49
20:LM:2085:LEU:HD21	20:LM:2125:CYS:HA	1.93	0.49
23:LP:442:ILE:HD12	23:LP:479:LYS:HD2	1.95	0.49
24:LQ:510:GLY:HA2	24:LQ:524:ASP:HA	1.94	0.49
39:NH:1102:LYS:HB3	40:NI:116:PHE:HD2	1.78	0.49
41:NK:61:LYS:HA	41:NK:106:TYR:HE2	1.78	0.49
46:NR:619:UNK:O	46:NR:623:UNK:N	2.45	0.49
48:NU:7:LYS:HA	48:NU:10:LYS:HG2	1.94	0.49
70:SZ:286:TRP:CD1	70:SZ:290:ILE:HD13	2.47	0.49
2:L1:1842:C:H2’	2:L1:1843:G:H8	1.77	0.49
3:L2:46:A:H2’	3:L2:47:G:C8	2.47	0.49
16:LH:17:LEU:N	16:LH:312:ASN:OD1	2.44	0.49
16:LH:629:VAL:HG22	16:LH:660:THR:HG22	1.93	0.49
20:LM:1141:SER:HA	52:SB:84:HIS:HB3	1.93	0.49
22:LO:710:PHE:CD1	22:LO:717:TRP:HB3	2.47	0.49
25:LR:119:PRO:HG3	25:LR:161:PRO:HA	1.93	0.49
25:LR:316:LEU:HB2	25:LR:330:PHE:HB2	1.94	0.49
28:LU:173:THR:HG1	28:LU:181:TRP:HE1	1.59	0.49
39:NH:147:ALA:O	39:NH:278:TRP:NE1	2.37	0.49
58:SK:123:GLN:HB3	65:ST:766:PHE:HD2	1.78	0.49
70:SZ:317:ILE:O	70:SZ:350:TYR:OH	2.24	0.49
1:L0:817:U:OP2	27:LT:430:ARG:NH2	2.46	0.49
19:LL:192:LEU:HB3	19:LL:202:ARG:HB2	1.94	0.49
20:LM:1136:VAL:HG12	20:LM:1209:LEU:HD12	1.95	0.49
28:LU:412:GLU:HG3	28:LU:416:ARG:HH12	1.78	0.49
39:NH:234:LYS:NZ	39:NH:304:ASP:OD1	2.35	0.49
39:NH:671:ARG:HH12	42:NM:37:ALA:HB1	1.78	0.49
39:NH:926:THR:HG22	39:NH:929:GLU:HG3	1.93	0.49
41:NJ:577:ILE:HD12	41:NJ:648:LEU:HD11	1.95	0.49
42:NM:47:THR:OG1	42:NM:65:ARG:NH1	2.46	0.49
46:NR:982:UNK:O	46:NR:986:UNK:N	2.46	0.49
52:SB:64:MET:HE2	53:SC:222:LYS:HA	1.95	0.49
61:SP:1349:SER:HB3	61:SP:1384:CYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SP:1448:VAL:O	61:SP:1452:THR:OG1	2.28	0.49
61:SP:1475:MET:HB3	61:SP:1479:PHE:CE2	2.47	0.49
66:SU:149:VAL:HG11	66:SU:187:ALA:HB1	1.94	0.49
20:LM:1601:ILE:HA	20:LM:1604:ILE:HG22	1.95	0.49
22:LO:344:TRP:NE1	22:LO:359:GLU:OE1	2.39	0.49
25:LR:378:ILE:HD11	42:NM:19:LYS:HG2	1.95	0.49
42:NM:90:ASP:OD2	42:NM:92:GLN:NE2	2.45	0.49
44:NO:3:ARG:HD3	44:NO:6:VAL:HG12	1.94	0.49
46:NR:314:UNK:O	46:NR:318:UNK:N	2.46	0.49
49:NW:51:MET:HG2	49:NW:71:GLY:HA3	1.93	0.49
51:SA:284:TYR:OH	52:SB:250:ASP:OD1	2.27	0.49
56:SH:175:LYS:NZ	57:SI:989:GLN:OE1	2.46	0.49
65:ST:834:LYS:O	65:ST:838:ASN:ND2	2.41	0.49
66:SU:369:ALA:HB2	66:SU:394:LEU:HD23	1.94	0.49
67:SW:91:ASN:HA	67:SW:94:LYS:HE2	1.94	0.49
2:L1:641:A:OP1	10:L9:40:LYS:NZ	2.42	0.49
4:L3:47:LYS:HG3	4:L3:70:ILE:HD13	1.95	0.49
14:LF:72:PHE:HE2	34:NC:248:ARG:HE	1.60	0.49
16:LH:727:ILE:HD13	16:LH:754:SER:HB3	1.93	0.49
19:LL:458:GLN:HE22	66:SU:262:HIS:HB3	1.78	0.49
20:LM:1073:SER:HA	20:LM:1076:ASN:HD22	1.77	0.49
23:LP:46:ARG:HD2	28:LU:20:ASP:HA	1.94	0.49
24:LQ:676:GLN:HB3	24:LQ:695:HIS:HB3	1.94	0.49
25:LR:545:ILE:HD11	25:LR:566:VAL:HG21	1.94	0.49
38:NG:93:LEU:HG	38:NG:124:MET:HE2	1.94	0.49
41:NJ:386:VAL:HG22	41:NJ:408:PHE:HB2	1.95	0.49
49:NW:51:MET:HG3	49:NW:52:PRO:HD2	1.95	0.49
53:SD:97:PHE:HB2	53:SD:107:VAL:HG23	1.95	0.49
56:SH:57:LYS:NZ	56:SH:86:GLU:O	2.45	0.49
2:L1:1234:C:O2	65:ST:35:LYS:NZ	2.45	0.48
2:L1:1787:G:H2’	2:L1:1788:A:H8	1.77	0.48
3:L2:61:G:OP2	22:LO:660:ARG:NH1	2.40	0.48
7:L6:67:VAL:HG13	7:L6:99:GLY:HA2	1.95	0.48
14:LF:83:LYS:HE2	14:LF:96:LEU:HD12	1.95	0.48
17:LI:584:ARG:O	17:LI:588:LEU:HG	2.12	0.48
21:LN:605:CYS:HB2	21:LN:643:ILE:HG22	1.94	0.48
23:LP:119:LYS:HG2	23:LP:120:TRP:CD1	2.48	0.48
24:LQ:877:ILE:HA	24:LQ:880:LEU:HB2	1.94	0.48
25:LR:250:VAL:H	25:LR:255:VAL:HB	1.77	0.48
29:LW:326:ASN:HA	29:LW:367:VAL:HG21	1.95	0.48
39:NH:127:LEU:HB2	39:NH:148:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:NM:147:ASN:OD1	42:NM:148:ASN:N	2.46	0.48
58:SJ:42:ARG:NH1	58:SJ:104:GLY:O	2.46	0.48
61:SP:1674:VAL:HG21	61:SP:1819:VAL:HB	1.93	0.48
1:L0:604:C:H42	18:LJ:433:ARG:HE	1.61	0.48
2:L1:1536:G:H2'	2:L1:1537:A:C8	2.46	0.48
23:LP:24:LEU:HD22	23:LP:71:ARG:HB3	1.94	0.48
37:NF:2:GLY:HA2	37:NF:9:LYS:HG2	1.94	0.48
39:NH:127:LEU:HD23	39:NH:152:PHE:HB2	1.94	0.48
41:NK:29:VAL:HG12	41:NK:151:LEU:HD12	1.95	0.48
58:SJ:73:LEU:HD21	58:SJ:80:PRO:HA	1.95	0.48
59:SL:20:ARG:HH12	59:SL:31:LYS:HB3	1.78	0.48
65:ST:432:UNK:O	65:ST:436:UNK:N	2.46	0.48
66:SU:179:ASP:O	66:SU:183:HIS:ND1	2.41	0.48
4:L3:46:ARG:HH12	4:L3:52:LEU:HD11	1.76	0.48
11:LA:26:LEU:HB2	11:LA:31:LEU:HD13	1.95	0.48
11:LA:52:LEU:HD11	11:LA:78:LYS:HG3	1.95	0.48
20:LM:1342:SER:O	20:LM:1346:ILE:HG12	2.13	0.48
20:LM:1966:LEU:HD21	20:LM:1995:ILE:HG21	1.96	0.48
21:LN:579:ARG:NE	21:LN:600:ASP:OD2	2.45	0.48
23:LP:221:LEU:HD13	64:SS:191:LEU:HD23	1.95	0.48
25:LR:527:VAL:HG22	25:LR:538:THR:HG22	1.94	0.48
28:LU:75:HIS:HD2	28:LU:78:LYS:H	1.61	0.48
36:NE:189:ARG:O	36:NE:193:GLN:HG2	2.12	0.48
61:SP:805:LEU:O	61:SP:809:THR:OG1	2.28	0.48
61:SP:1902:THR:HG21	61:SP:1935:GLU:HB2	1.95	0.48
65:ST:545:VAL:HA	65:ST:548:TYR:HD1	1.78	0.48
2:L1:1139:C:H2'	2:L1:1140:G:H8	1.78	0.48
2:L1:1859:A:H2'	2:L1:1860:A:C8	2.48	0.48
16:LH:345:ARG:NH2	16:LH:400:ASN:OD1	2.46	0.48
20:LM:1719:ALA:HB2	20:LM:1763:ALA:HA	1.94	0.48
25:LR:394:CYS:HB2	25:LR:424:VAL:HG23	1.96	0.48
27:LT:674:THR:OG1	27:LT:676:ASP:OD1	2.31	0.48
50:NY:88:VAL:HG23	50:NY:103:THR:HA	1.94	0.48
58:SK:238:GLU:HB3	58:SK:243:VAL:HB	1.96	0.48
60:SM:232:HIS:HB3	60:SM:244:LEU:HD22	1.95	0.48
5:L4:22:LYS:HG3	5:L4:23:LEU:HG	1.96	0.48
20:LM:109:PRO:HA	20:LM:112:LYS:HD3	1.95	0.48
20:LM:174:ALA:HB2	52:SB:403:ILE:HG22	1.96	0.48
20:LM:764:PRO:HG2	20:LM:767:LEU:HB2	1.94	0.48
20:LM:1409:GLU:HA	20:LM:1458:HIS:CD2	2.49	0.48
20:LM:1815:THR:HG22	20:LM:1854:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LT:543:ARG:NH1	27:LT:583:PRO:O	2.46	0.48
40:NI:20:PRO:HG2	40:NI:23:TYR:HB2	1.94	0.48
58:SJ:190:VAL:HG11	58:SJ:240:VAL:HG21	1.96	0.48
58:SK:93:LEU:HD11	58:SK:128:ARG:HG3	1.96	0.48
61:SP:1524:GLU:HG3	61:SP:1528:LYS:HZ1	1.79	0.48
1:L0:459:G:H22	35:ND:245:LYS:NZ	2.12	0.48
2:L1:104:A:OP1	9:L8:12:ARG:NE	2.46	0.48
5:L4:129:ILE:HD11	5:L4:139:LEU:HD12	1.94	0.48
16:LH:97:ILE:HD11	16:LH:141:GLU:HG3	1.94	0.48
18:LJ:125:VAL:HA	18:LJ:141:ALA:HA	1.94	0.48
23:LP:223:TRP:HB2	23:LP:255:LEU:HD11	1.94	0.48
25:LR:297:HIS:HB2	25:LR:310:ALA:HB3	1.95	0.48
27:LT:789:PHE:O	67:SW:199:ARG:NH2	2.36	0.48
44:NO:75:ILE:HG22	44:NO:77:PRO:HD2	1.96	0.48
60:SM:29:LYS:HA	60:SM:53:LEU:HD23	1.96	0.48
61:SP:967:HIS:HA	61:SP:1004:HIS:HD2	1.78	0.48
61:SP:1479:PHE:CD1	61:SP:1525:LYS:HD3	2.49	0.48
64:SS:207:VAL:HG21	64:SS:223:ARG:HH22	1.79	0.48
66:SU:179:ASP:OD1	66:SU:180:THR:N	2.47	0.48
5:L4:128:LYS:HB3	5:L4:140:VAL:HB	1.95	0.48
10:L9:54:ARG:NH2	59:SL:96:ALA:HB2	2.29	0.48
14:LF:14:THR:HG22	14:LF:16:ARG:HE	1.79	0.48
20:LM:1376:VAL:HG21	20:LM:1411:PHE:HD1	1.79	0.48
20:LM:1387:LEU:O	20:LM:1395:ARG:NH1	2.44	0.48
22:LO:674:GLN:HA	22:LO:699:PHE:CZ	2.48	0.48
24:LQ:217:VAL:HG13	24:LQ:271:ALA:HB3	1.95	0.48
24:LQ:410:THR:OG1	24:LQ:415:ARG:NH1	2.47	0.48
27:LT:769:ASP:OD1	27:LT:770:VAL:N	2.47	0.48
28:LU:235:VAL:HG22	28:LU:443:VAL:HG22	1.95	0.48
32:NA:450:ASP:OD1	32:NA:451:ALA:N	2.45	0.48
47:NT:108:VAL:HG22	47:NT:114:ILE:HG12	1.95	0.48
2:L1:210:U:OP2	61:SP:1137:ARG:NH2	2.47	0.48
2:L1:597:G:H5”	69:SY:1:MET:HG3	1.96	0.48
12:LC:53:GLU:OE1	12:LC:85:ARG:NH2	2.33	0.48
18:LJ:81:ASP:HB3	18:LJ:100:GLU:HG2	1.96	0.48
18:LJ:181:ILE:HD13	18:LJ:214:LEU:HD11	1.96	0.48
20:LM:374:ILE:HD12	20:LM:377:ARG:HE	1.79	0.48
21:LN:418:LEU:HB3	21:LN:427:LEU:HD23	1.96	0.48
28:LU:322:THR:HG22	28:LU:324:ARG:H	1.79	0.48
41:NK:513:ASP:OD1	41:NK:514:THR:N	2.46	0.48
53:SC:168:ALA:N	53:SC:191:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SD:107:VAL:HG12	53:SD:136:ALA:HA	1.96	0.48
56:SH:220:ILE:HG22	56:SH:222:ASP:H	1.79	0.48
61:SP:1192:GLY:HA2	61:SP:1238:ILE:HG12	1.96	0.48
66:SU:221:ARG:O	66:SU:249:ARG:NH2	2.47	0.48
17:LI:684:VAL:HG23	19:LK:524:VAL:HG21	1.95	0.48
20:LM:1558:ILE:HA	20:LM:1561:VAL:HG12	1.95	0.48
24:LQ:109:ALA:HB3	24:LQ:127:LYS:HD2	1.96	0.48
26:LS:482:ASN:OD1	26:LS:484:THR:OG1	2.29	0.48
35:ND:176:ARG:HG2	35:ND:178:LYS:H	1.79	0.48
41:NK:360:VAL:HG23	41:NK:366:GLN:HB2	1.95	0.48
67:SW:176:LEU:HD21	67:SW:207:VAL:HG12	1.94	0.48
1:L0:827:C:C4	27:LT:413:LYS:HA	2.48	0.48
2:L1:382:C:H2'	2:L1:383:G:H8	1.78	0.48
3:L2:32:U:O2'	3:L2:33:G:O5'	2.28	0.48
3:L2:135:U:H3	3:L2:138:C:P	2.37	0.48
3:L2:139:U:OP2	20:LM:1752:SER:OG	2.19	0.48
18:LJ:166:TYR:HB3	18:LJ:168:ARG:HD2	1.96	0.48
20:LM:1693:LEU:HD21	20:LM:1732:GLN:HG2	1.96	0.48
39:NH:366:HIS:H	39:NH:369:MET:HE3	1.79	0.48
55:SG:308:ARG:NH1	55:SG:317:GLN:OE1	2.36	0.48
1:L0:811:G:C8	27:LT:486:LYS:HD2	2.49	0.47
2:L1:106:C:H2'	2:L1:107:A:H8	1.79	0.47
2:L1:1125:C:H2'	2:L1:1126:G:H8	1.79	0.47
7:L6:126:ASP:OD1	7:L6:127:THR:N	2.47	0.47
16:LH:173:VAL:HG21	16:LH:209:VAL:HB	1.96	0.47
16:LH:544:HIS:HB3	16:LH:586:MET:HE2	1.95	0.47
17:LI:435:ASP:O	17:LI:438:THR:OG1	2.24	0.47
21:LN:581:THR:HG21	21:LN:601:ALA:HB3	1.96	0.47
40:NI:88:VAL:HG12	40:NI:121:VAL:HG23	1.96	0.47
41:NJ:691:LEU:HD21	57:SI:392:VAL:HA	1.95	0.47
42:NM:33:VAL:HA	42:NM:96:CYS:HB2	1.95	0.47
58:SJ:219:ILE:HG12	75:SJ:301:SAH:N1	2.29	0.47
2:L1:219:U:H1'	9:L8:184:ARG:HD2	1.95	0.47
2:L1:1280:G:H2'	2:L1:1281:G:H8	1.79	0.47
8:L7:61:ILE:HG23	8:L7:95:ILE:HD13	1.95	0.47
9:L8:155:ASN:O	13:LD:21:LYS:NZ	2.44	0.47
20:LM:2095:LEU:HD12	20:LM:2098:ASN:HB2	1.96	0.47
39:NH:124:GLU:OE2	39:NH:153:ARG:NH1	2.45	0.47
65:ST:77:ARG:HD3	65:ST:77:ARG:HA	1.72	0.47
2:L1:924:G:OP2	37:NF:3:ARG:NH2	2.42	0.47
3:L2:6:U:H2'	3:L2:7:A:C8	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L9:88:ASP:OD1	10:L9:89:GLU:N	2.48	0.47
17:LI:152:VAL:O	17:LI:152:VAL:HG12	2.15	0.47
20:LM:1565:MET:HG3	20:LM:1581:LEU:HD11	1.95	0.47
24:LQ:366:LYS:HE2	24:LQ:385:GLN:HG3	1.97	0.47
39:NH:477:ARG:NH2	39:NH:632:THR:O	2.47	0.47
46:NR:190:UNK:O	46:NR:194:UNK:N	2.48	0.47
50:NY:132:ALA:O	50:NY:135:ILE:HG12	2.13	0.47
53:SD:100:ARG:NH1	53:SD:104:ASP:OD1	2.46	0.47
66:SU:265:PRO:HD2	66:SU:268:LEU:HD12	1.96	0.47
2:L1:919:A:OP2	37:NF:64:ARG:NH2	2.45	0.47
2:L1:1280:G:H2’	2:L1:1281:G:C8	2.50	0.47
3:L2:93:A:H2’	3:L2:94:G:C8	2.50	0.47
10:L9:48:PHE:CE2	10:L9:52:LYS:HE2	2.49	0.47
10:L9:152:ASP:OD2	10:L9:153:SER:N	2.47	0.47
20:LM:1742:THR:HG23	20:LM:1745:LYS:HE3	1.95	0.47
22:LO:177:ASP:HB2	22:LO:227:LYS:HA	1.96	0.47
27:LT:789:PHE:C	67:SW:199:ARG:HH22	2.17	0.47
41:NK:277:ARG:NE	41:NK:458:ARG:HG2	2.28	0.47
52:SB:120:ARG:HG2	53:SC:229:MET:SD	2.54	0.47
58:SJ:44:ILE:HG13	58:SJ:107:GLN:HB3	1.96	0.47
58:SJ:67:ASP:OD2	58:SJ:68:LYS:N	2.47	0.47
70:SZ:326:MET:HA	70:SZ:329:ILE:HG22	1.97	0.47
70:SZ:364:PHE:HE2	70:SZ:385:LEU:HD22	1.80	0.47
2:L1:433:A:H2’	2:L1:434:G:C8	2.49	0.47
2:L1:511:U:H2’	2:L1:512:A:C8	2.49	0.47
7:L6:74:ARG:HB3	7:L6:94:ARG:HG2	1.96	0.47
17:LI:273:VAL:HB	17:LI:292:ILE:HD11	1.96	0.47
18:LJ:43:LYS:HD3	18:LJ:85:CYS:HA	1.97	0.47
18:LJ:123:LYS:HE2	18:LJ:143:ASP:HB3	1.96	0.47
18:LJ:181:ILE:HD13	18:LJ:214:LEU:HD21	1.96	0.47
20:LM:607:MET:SD	20:LM:625:LEU:HD23	2.55	0.47
20:LM:1813:LEU:HA	20:LM:1817:LEU:HD13	1.96	0.47
21:LN:250:SER:OG	21:LN:262:HIS:NE2	2.30	0.47
26:LS:493:GLU:O	26:LS:523:HIS:ND1	2.48	0.47
39:NH:332:LYS:HD3	39:NH:349:GLY:HA3	1.96	0.47
41:NJ:130:THR:HG23	41:NJ:133:LEU:H	1.80	0.47
41:NK:257:THR:HG21	41:NK:467:GLU:HB2	1.97	0.47
53:SC:87:MET:N	53:SC:87:MET:SD	2.87	0.47
57:SI:282:LEU:HD13	57:SI:909:LEU:HD11	1.95	0.47
57:SI:926:LEU:O	57:SI:978:CYS:N	2.46	0.47
58:SK:125:ARG:NH2	65:ST:765:LEU:O	2.47	0.47

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
61:SP:200:VAL:HG21	61:SP:206:LEU:HD22	1.95	0.47
61:SP:858:ASP:OD1	61:SP:859:LEU:N	2.47	0.47
61:SP:1552:PHE:HB3	61:SP:1555:GLN:HG2	1.94	0.47
1:L0:1414:A:H5’	1:L0:1415:G:H5”	1.95	0.47
3:L2:64:G:H2’	3:L2:65:A:C8	2.49	0.47
7:L6:67:VAL:HG21	7:L6:73:VAL:HG21	1.97	0.47
8:L7:52:GLU:OE2	8:L7:56:GLY:N	2.42	0.47
14:LF:64:PHE:HB3	34:NC:224:ARG:HH22	1.80	0.47
16:LH:130:VAL:HG12	16:LH:149:PHE:HA	1.96	0.47
20:LM:702:VAL:HG12	20:LM:771:TYR:HE2	1.80	0.47
24:LQ:482:ASP:OD1	24:LQ:489:LEU:HD21	2.14	0.47
27:LT:663:ASP:OD1	27:LT:664:SER:N	2.48	0.47
28:LU:220:ASN:HB3	28:LU:236:ILE:HG12	1.95	0.47
29:LW:605:LEU:HB3	39:NH:680:PRO:HG2	1.96	0.47
39:NH:341:ASP:OD1	39:NH:341:ASP:N	2.48	0.47
41:NJ:210:SER:HB2	41:NJ:213:VAL:HG13	1.96	0.47
41:NJ:358:VAL:HB	41:NJ:368:ILE:HB	1.96	0.47
41:NK:602:GLY:HA2	41:NK:607:TRP:HE1	1.79	0.47
61:SP:1256:VAL:O	61:SP:1260:LEU:HG	2.15	0.47
2:L1:375:U:H2’	2:L1:376:A:C8	2.50	0.47
2:L1:650:A:H2’	2:L1:651:U:O4’	2.15	0.47
2:L1:996:A:H2’	2:L1:997:A:C8	2.49	0.47
2:L1:1592:C:H5”	6:L5:91:ARG:HH12	1.80	0.47
7:L6:214:ALA:O	7:L6:218:LYS:HG3	2.14	0.47
8:L7:131:GLU:HG3	8:L7:139:ILE:HD12	1.97	0.47
14:LF:7:ILE:HD12	14:LF:47:MET:HE1	1.97	0.47
17:LI:658:PHE:CZ	18:LJ:489:MET:HB3	2.50	0.47
20:LM:758:MET:HA	20:LM:794:LYS:HD2	1.96	0.47
20:LM:1101:THR:HG22	20:LM:1103:GLN:H	1.80	0.47
20:LM:1525:LEU:HD22	20:LM:1594:LEU:HB3	1.96	0.47
24:LQ:392:TYR:OH	24:LQ:405:ARG:NH2	2.43	0.47
25:LR:586:LEU:HD12	25:LR:600:THR:HG22	1.95	0.47
41:NJ:499:CYS:SG	41:NJ:561:PRO:HB3	2.54	0.47
41:NK:44:LEU:HD22	41:NK:146:LEU:HG	1.97	0.47
41:NK:696:LEU:HD12	41:NK:700:GLU:HB2	1.96	0.47
49:NW:253:VAL:HG22	49:NW:275:ILE:HD13	1.97	0.47
52:SB:45:LYS:HE2	52:SB:79:ILE:HG23	1.96	0.47
52:SB:97:VAL:HG13	52:SB:101:LYS:NZ	2.29	0.47
57:SI:946:VAL:HG22	57:SI:993:PHE:HB2	1.97	0.47
58:SJ:101:ASN:HB2	58:SJ:106:LEU:HD12	1.97	0.47
58:SJ:127:PRO:HB3	58:SJ:132:ARG:NE	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:99:PRO:HA	58:SK:102:ARG:HB2	1.96	0.47
61:SP:134:THR:HA	61:SP:137:LEU:HD13	1.96	0.47
61:SP:1583:ILE:HA	61:SP:1586:ARG:HH21	1.80	0.47
65:ST:259:UNK:HA	70:SZ:355:ARG:HH21	1.79	0.47
65:ST:621:TYR:O	65:ST:624:THR:OG1	2.30	0.47
11:LA:85:LEU:HA	11:LA:88:TRP:HD1	1.79	0.47
20:LM:186:LEU:HB3	20:LM:241:LYS:HE3	1.97	0.47
20:LM:374:ILE:O	20:LM:378:HIS:ND1	2.36	0.47
20:LM:1726:GLU:O	20:LM:1730:ILE:HG13	2.15	0.47
22:LO:871:GLN:O	22:LO:875:ALA:N	2.48	0.47
23:LP:248:LEU:HD21	62:SQ:562:SER:HB3	1.97	0.47
25:LR:101:THR:HG23	25:LR:102:ARG:HG2	1.97	0.47
28:LU:291:SER:HA	28:LU:333:TRP:CD1	2.50	0.47
41:NK:715:LEU:HD22	41:NK:733:LEU:HD11	1.96	0.47
61:SP:1001:LYS:HD2	61:SP:1004:HIS:CE1	2.50	0.47
61:SP:1522:LEU:HD21	61:SP:1548:LEU:HD11	1.96	0.47
61:SP:1975:ASP:OD1	61:SP:1975:ASP:N	2.46	0.47
2:L1:1588:A:H2'	2:L1:1589:A:C8	2.49	0.47
9:L8:8:TRP:CZ3	9:L8:20:PRO:HB3	2.50	0.47
17:LI:401:LEU:HD11	17:LI:420:PHE:CG	2.49	0.47
18:LJ:429:LEU:HD11	18:LJ:439:ILE:HG13	1.97	0.47
20:LM:1649:LEU:HD21	20:LM:1692:VAL:HG22	1.96	0.47
21:LN:399:SER:HB3	21:LN:404:TRP:HB2	1.97	0.47
25:LR:117:PHE:CE1	25:LR:124:LEU:HD12	2.50	0.47
25:LR:313:ASP:O	25:LR:315:ASN:N	2.46	0.47
25:LR:485:VAL:HG12	25:LR:496:THR:HG22	1.97	0.47
25:LR:782:ASP:OD2	27:LT:938:GLN:NE2	2.47	0.47
27:LT:768:LEU:C	27:LT:772:LYS:HZ2	2.18	0.47
36:NE:184:GLY:O	36:NE:188:GLU:N	2.41	0.47
50:NY:114:ILE:HG23	50:NY:117:ARG:HH12	1.80	0.47
57:SI:959:ILE:HB	57:SI:969:LEU:HD11	1.97	0.47
61:SP:133:ILE:HA	61:SP:136:ILE:HD12	1.97	0.47
2:L1:485:A:N6	57:SI:216:LEU:O	2.48	0.47
2:L1:1470:C:H2'	2:L1:1471:C:H6	1.79	0.47
3:L2:105:U:OP1	51:SA:337:ARG:NH1	2.47	0.47
16:LH:20:ARG:NH2	16:LH:103:HIS:O	2.48	0.47
17:LI:662:VAL:HG13	19:LK:579:VAL:HG22	1.96	0.47
19:LL:494:VAL:HG22	19:LL:534:HIS:CD2	2.49	0.47
20:LM:843:VAL:HG22	20:LM:846:ARG:NH2	2.26	0.47
20:LM:2070:LEU:HD23	20:LM:2109:PHE:CD2	2.50	0.47
22:LO:312:PHE:HE1	22:LO:328:ILE:HD11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LT:494:ASP:OD1	27:LT:495:ILE:N	2.48	0.47
41:NK:179:VAL:HG12	41:NK:552:PRO:HD3	1.95	0.47
57:SI:1050:ALA:HB3	65:ST:800:PHE:HZ	1.80	0.47
65:ST:259:UNK:O	65:ST:263:UNK:N	2.48	0.47
1:L0:719:G:N2	1:L0:751:C:N3	2.63	0.46
2:L1:387:C:OP2	9:L8:10:LYS:NZ	2.48	0.46
2:L1:649:U:H2'	2:L1:650:A:H8	1.79	0.46
2:L1:1237:C:H42	65:ST:805:ARG:HH22	1.62	0.46
19:LL:116:LEU:HD21	19:LL:119:LYS:HG3	1.96	0.46
19:LL:169:SER:OG	19:LL:188:ARG:NH1	2.37	0.46
28:LU:179:ASP:HB3	28:LU:188:PRO:HB3	1.97	0.46
28:LU:364:THR:HG23	28:LU:367:GLU:H	1.80	0.46
29:LW:241:ASP:OD1	29:LW:242:ILE:N	2.48	0.46
41:NK:387:ILE:HB	41:NK:409:MET:HG2	1.98	0.46
46:NR:901:UNK:O	46:NR:905:UNK:N	2.49	0.46
60:SM:49:GLU:HG2	60:SM:52:ALA:HB3	1.96	0.46
1:L0:1433:A:N7	51:SA:40:GLY:HA3	2.30	0.46
2:L1:388:U:H2'	2:L1:389:A:H8	1.80	0.46
2:L1:562:U:H2'	2:L1:563:G:C8	2.50	0.46
2:L1:617:G:H2'	2:L1:618:C:C6	2.51	0.46
2:L1:1823:A:H4'	2:L1:1824:A:O5'	2.14	0.46
3:L2:8:U:H2'	3:L2:9:A:C8	2.50	0.46
7:L6:7:PHE:CE2	7:L6:9:ALA:HB3	2.50	0.46
19:LL:38:LEU:HD22	19:LL:99:LEU:HD21	1.96	0.46
20:LM:2036:LYS:HZ2	20:LM:2040:ARG:HB2	1.79	0.46
20:LM:2089:LEU:HD12	20:LM:2128:THR:HA	1.98	0.46
21:LN:441:LEU:HG	21:LN:457:ASN:HA	1.97	0.46
21:LN:532:MET:HG2	21:LN:543:ILE:HG12	1.97	0.46
41:NK:268:ILE:HD13	41:NK:271:ILE:HD12	1.96	0.46
44:NO:111:MET:HE3	44:NO:115:GLU:HG3	1.97	0.46
50:NY:208:ASP:OD1	50:NY:213:ILE:HB	2.15	0.46
53:SD:246:VAL:HG11	53:SD:262:ILE:HD11	1.97	0.46
56:SH:211:SER:OG	56:SH:273:GLU:OE2	2.33	0.46
61:SP:528:ILE:HG22	61:SP:530:PRO:HD2	1.98	0.46
64:SS:159:PHE:HB3	64:SS:729:ILE:HG12	1.97	0.46
2:L1:1221:G:O2'	2:L1:1676:U:O2	2.33	0.46
3:L2:49:U:H2'	3:L2:50:U:C6	2.50	0.46
6:L5:38:TYR:OH	15:LG:54:ASP:OD1	2.30	0.46
11:LA:123:VAL:HG13	11:LA:124:ILE:HD12	1.97	0.46
16:LH:585:VAL:HB	16:LH:598:ILE:HB	1.97	0.46
19:LK:467:THR:HG21	19:LK:498:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LP:323:GLU:HG3	23:LP:366:LEU:HB3	1.96	0.46
61:SP:1409:LEU:O	61:SP:1413:VAL:HG23	2.15	0.46
2:L1:1004:U:H2'	2:L1:1005:G:C8	2.49	0.46
17:LI:610:ALA:HA	17:LI:613:ILE:HD13	1.97	0.46
21:LN:437:LEU:HD22	21:LN:454:VAL:HG11	1.97	0.46
21:LN:446:SER:OG	21:LN:448:ASP:O	2.31	0.46
23:LP:226:TYR:HH	23:LP:239:HIS:CD2	2.33	0.46
23:LP:253:LYS:O	23:LP:253:LYS:HD2	2.16	0.46
23:LP:330:ILE:HD13	23:LP:367:LEU:HD11	1.98	0.46
26:LS:233:ARG:NH1	26:LS:506:SER:OG	2.48	0.46
29:LW:241:ASP:OD2	29:LW:281:LEU:N	2.43	0.46
39:NH:237:LEU:HB3	39:NH:253:LEU:HB2	1.97	0.46
39:NH:1104:ARG:HD3	39:NH:1115:MET:HB3	1.97	0.46
41:NK:813:LEU:HD11	41:NK:822:LEU:HD21	1.97	0.46
52:SB:190:HIS:NE2	52:SB:213:ASP:OD1	2.45	0.46
61:SP:216:LYS:HD3	61:SP:216:LYS:HA	1.73	0.46
61:SP:1398:PHE:HD2	61:SP:1410:LEU:HD21	1.80	0.46
2:L1:942:G:H2'	2:L1:943:U:C6	2.50	0.46
17:LI:467:TYR:HB2	17:LI:496:ILE:HD13	1.97	0.46
20:LM:440:LEU:HA	20:LM:443:VAL:HG12	1.96	0.46
20:LM:1741:LEU:HD21	20:LM:1782:ILE:HG22	1.98	0.46
22:LO:522:ASP:OD1	22:LO:524:THR:OG1	2.27	0.46
22:LO:844:VAL:O	22:LO:847:PHE:HB3	2.15	0.46
23:LP:453:SER:OG	23:LP:456:ASP:OD2	2.33	0.46
24:LQ:424:SER:OG	24:LQ:426:ASP:O	2.28	0.46
25:LR:24:PHE:HZ	25:LR:330:PHE:HB3	1.81	0.46
39:NH:1010:VAL:HB	39:NH:1084:VAL:HB	1.97	0.46
40:NI:104:ARG:HG2	40:NI:111:LYS:NZ	2.30	0.46
41:NJ:823:LYS:O	41:NJ:827:MET:HG2	2.15	0.46
41:NJ:881:GLU:HG3	41:NJ:888:SER:HB2	1.97	0.46
42:NM:173:THR:O	42:NM:177:GLN:HG2	2.16	0.46
58:SJ:224:LEU:HD22	58:SJ:228:LEU:HD22	1.98	0.46
61:SP:1670:GLN:HG3	61:SP:1819:VAL:HG21	1.98	0.46
1:L0:1429:A:H2'	1:L0:1430:G:C8	2.51	0.46
2:L1:75:G:H1'	2:L1:76:U:H2'	1.97	0.46
18:LJ:252:THR:HG21	18:LJ:293:LEU:HA	1.98	0.46
21:LN:368:LYS:HD2	21:LN:369:ASN:H	1.81	0.46
23:LP:11:ASP:OD2	64:SS:711:ARG:NH2	2.48	0.46
27:LT:610:GLU:O	27:LT:612:ARG:NH1	2.48	0.46
27:LT:768:LEU:HD21	27:LT:852:PRO:HB2	1.96	0.46
39:NH:306:VAL:HG11	39:NH:423:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SA:21:GLU:HB2	64:SS:725:PRO:HG2	1.97	0.46
60:SM:255:LEU:HD21	60:SM:258:ILE:HD11	1.98	0.46
61:SP:1797:SER:O	61:SP:1820:ARG:NH1	2.48	0.46
61:SP:1861:ILE:HA	61:SP:1864:ILE:HG22	1.97	0.46
70:SZ:152:UNK:O	70:SZ:156:UNK:N	2.49	0.46
2:L1:1653:U:H3	2:L1:1671:G:H1	1.63	0.46
3:L2:59:G:N3	59:SL:8:ARG:NH1	2.63	0.46
7:L6:227:GLN:O	7:L6:230:LYS:HG2	2.15	0.46
8:L7:82:GLU:OE2	8:L7:83:LEU:HD22	2.14	0.46
16:LH:229:LEU:O	16:LH:241:TYR:HA	2.15	0.46
19:LL:467:THR:O	19:LL:471:GLU:HG2	2.16	0.46
20:LM:214:ARG:NE	23:LP:593:GLN:O	2.45	0.46
22:LO:545:ASP:HB3	22:LO:563:LEU:HB2	1.98	0.46
25:LR:52:VAL:O	25:LR:328:LYS:HE2	2.14	0.46
33:NB:438:GLU:OE2	33:NB:441:ARG:NH2	2.42	0.46
55:SG:338:MET:HG2	55:SG:350:TRP:HB2	1.97	0.46
56:SH:210:ASP:N	56:SH:210:ASP:OD1	2.49	0.46
61:SP:1167:GLU:OE1	61:SP:1212:ASN:ND2	2.48	0.46
61:SP:1842:ASN:OD1	61:SP:1845:SER:OG	2.33	0.46
70:SZ:269:ASN:HB2	70:SZ:272:LEU:HD12	1.97	0.46
70:SZ:282:LYS:HD3	70:SZ:282:LYS:HA	1.80	0.46
2:L1:432:G:H2’	2:L1:433:A:C8	2.51	0.46
2:L1:615:C:H2’	2:L1:616:A:C8	2.50	0.46
2:L1:1739:C:H2’	2:L1:1740:C:H6	1.81	0.46
3:L2:57:A:H2’	3:L2:58:C:C6	2.50	0.46
10:L9:69:ARG:O	10:L9:73:GLU:HG2	2.16	0.46
18:LJ:355:ARG:N	26:LS:294:GLU:OE1	2.46	0.46
20:LM:362:VAL:HG12	20:LM:363:THR:HG23	1.98	0.46
22:LO:197:GLU:OE2	22:LO:204:TYR:OH	2.16	0.46
22:LO:400:TRP:HA	22:LO:407:CYS:HA	1.96	0.46
38:NG:85:CYS:HB3	38:NG:90:ILE:HB	1.97	0.46
41:NK:694:LEU:HG	41:NK:695:LEU:HG	1.97	0.46
52:SB:191:PHE:CD2	52:SB:194:LEU:HB2	2.51	0.46
52:SB:351:SER:OG	52:SB:354:HIS:ND1	2.43	0.46
53:SC:183:PRO:HD2	53:SC:184:ASP:H	1.80	0.46
57:SI:96:SER:HA	57:SI:99:ILE:HD12	1.98	0.46
67:SW:214:SER:O	67:SW:218:ILE:HG12	2.16	0.46
1:L0:718:G:N2	1:L0:752:C:N3	2.64	0.46
9:L8:92:ARG:HH12	49:NW:138:ARG:NE	2.14	0.46
11:LA:32:ALA:HB3	11:LA:110:VAL:HB	1.98	0.46
13:LD:128:VAL:HG12	13:LD:142:VAL:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:509:LEU:HB3	17:LI:612:HIS:CD2	2.48	0.46
20:LM:803:PRO:HG2	20:LM:806:PHE:HB2	1.97	0.46
20:LM:1584:ALA:O	20:LM:1587:LEU:HB3	2.16	0.46
22:LO:74:ASP:OD1	22:LO:78:ASP:N	2.49	0.46
23:LP:575:LYS:HD3	52:SB:349:GLN:HB3	1.98	0.46
39:NH:352:VAL:HA	39:NH:355:LEU:HB2	1.98	0.46
39:NH:715:ARG:HH11	39:NH:715:ARG:HA	1.81	0.46
41:NJ:162:THR:HG21	41:NJ:171:TYR:HB2	1.97	0.46
41:NK:323:PHE:HA	41:NK:326:VAL:HG12	1.98	0.46
61:SP:1633:THR:O	61:SP:1637:THR:OG1	2.23	0.46
61:SP:1863:ASP:OD1	61:SP:1866:ARG:NH1	2.47	0.46
65:ST:622:ILE:HG22	65:ST:648:LEU:H	1.81	0.46
65:ST:819:LEU:O	65:ST:823:MET:HG2	2.16	0.46
9:L8:67:TRP:O	9:L8:71:CYS:N	2.48	0.46
16:LH:104:ALA:HB2	16:LH:158:PRO:HG3	1.98	0.46
17:LI:579:PRO:HG3	17:LI:618:LYS:HG3	1.98	0.46
20:LM:1779:LEU:O	20:LM:1783:LEU:HG	2.16	0.46
20:LM:2029:ASN:O	20:LM:2037:PHE:HE2	1.99	0.46
21:LN:490:LEU:HD22	21:LN:499:LEU:HD11	1.97	0.46
25:LR:427:VAL:HG12	25:LR:439:THR:HG22	1.98	0.46
27:LT:802:ALA:HB2	27:LT:826:ASP:HB3	1.98	0.46
41:NJ:307:SER:HA	41:NJ:366:GLN:HG2	1.97	0.46
47:NT:123:SER:HB2	47:NT:126:CYS:HB2	1.98	0.46
51:SA:294:PRO:HB2	51:SA:391:SER:HB3	1.97	0.46
59:SL:86:LEU:O	59:SL:90:MET:HG3	2.16	0.46
59:SL:87:VAL:HA	59:SL:90:MET:HE2	1.98	0.46
69:SY:76:GLN:HB2	69:SY:81:ILE:HD13	1.97	0.46
2:L1:1169:G:O6	57:SI:1256:LYS:NZ	2.32	0.45
2:L1:1309:C:OP1	47:NT:104:LYS:NZ	2.47	0.45
19:LL:341:CYS:SG	19:LL:361:ARG:NH1	2.89	0.45
20:LM:1330:MET:O	20:LM:1334:VAL:HG22	2.16	0.45
22:LO:552:ARG:NH1	22:LO:557:GLU:OE1	2.50	0.45
24:LQ:816:LYS:HB3	24:LQ:819:GLU:HG2	1.97	0.45
25:LR:110:ALA:HB1	25:LR:129:CYS:HB2	1.98	0.45
42:NM:76:ASN:OD1	42:NM:77:ASP:N	2.49	0.45
42:NM:164:ILE:O	42:NM:168:MET:HG3	2.17	0.45
61:SP:381:PRO:HG2	61:SP:384:LEU:HD23	1.98	0.45
61:SP:753:LYS:HD3	61:SP:838:ARG:HH12	1.81	0.45
61:SP:1513:ASP:O	61:SP:1517:ILE:HG12	2.16	0.45
61:SP:1965:TYR:CE2	61:SP:2003:THR:HG23	2.51	0.45
69:SY:165:VAL:HG23	69:SY:168:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:445:C:H5”	26:LS:318:LYS:HD2	1.98	0.45
1:L0:857:C:OP1	30:LZ:50:GLN:NE2	2.50	0.45
2:L1:1687:C:H2’	2:L1:1688:C:H6	1.81	0.45
8:L7:60:ILE:HD13	8:L7:92:VAL:HG22	1.98	0.45
8:L7:192:PHE:HZ	45:NQ:12:PRO:HA	1.81	0.45
19:LL:231:ILE:HD12	19:LL:234:LEU:HD12	1.97	0.45
20:LM:384:THR:HG22	20:LM:431:LEU:HD11	1.97	0.45
20:LM:927:LEU:HD22	20:LM:966:ILE:HG21	1.98	0.45
20:LM:1322:ASN:O	20:LM:1326:ILE:HG13	2.17	0.45
20:LM:1811:LYS:HE2	20:LM:1815:THR:HG21	1.98	0.45
23:LP:71:ARG:NH2	26:LS:92:GLU:OE1	2.40	0.45
24:LQ:689:TYR:HB3	24:LQ:701:LEU:HD11	1.98	0.45
25:LR:387:LYS:HG3	25:LR:389:TRP:H	1.81	0.45
53:SC:225:MET:HG2	53:SC:226:LEU:HD22	1.98	0.45
61:SP:1775:THR:O	61:SP:1779:ILE:HG12	2.16	0.45
2:L1:1094:C:H4’	44:NO:20:ARG:NH2	2.32	0.45
3:L2:176:C:H2’	3:L2:177:C:C6	2.52	0.45
16:LH:568:TRP:HA	16:LH:575:LEU:HA	1.98	0.45
19:LK:521:VAL:O	19:LK:524:VAL:HB	2.16	0.45
22:LO:343:ASP:OD2	67:SW:251:ARG:HD2	2.16	0.45
27:LT:489:GLU:HG3	27:LT:490:LEU:HD22	1.98	0.45
27:LT:661:LEU:HB2	27:LT:711:PRO:HG2	1.98	0.45
29:LW:125:LYS:HB2	29:LW:128:THR:HG23	1.98	0.45
29:LW:439:GLN:HG3	29:LW:440:PRO:HD2	1.98	0.45
41:NJ:623:GLY:HA2	41:NJ:706:LEU:HG	1.98	0.45
43:NN:514:LYS:HA	43:NN:514:LYS:HD3	1.66	0.45
49:NW:333:THR:HG22	49:NW:335:LYS:H	1.80	0.45
52:SB:313:ALA:HA	52:SB:367:VAL:HG11	1.97	0.45
53:SD:284:LYS:HE3	59:SL:132:LEU:HA	1.98	0.45
61:SP:1504:LEU:HD13	61:SP:1517:ILE:HD12	1.99	0.45
61:SP:1653:MET:HA	61:SP:1656:LEU:HD12	1.97	0.45
2:L1:115:U:O2’	2:L1:381:C:O2	2.23	0.45
2:L1:478:G:H2’	2:L1:479:C:C6	2.52	0.45
2:L1:1292:C:H1’	47:NT:140:TYR:CE1	2.51	0.45
17:LI:711:TYR:OH	21:LN:7:HIS:ND1	2.49	0.45
19:LK:481:VAL:O	19:LK:484:THR:HG23	2.17	0.45
20:LM:259:ALA:O	20:LM:263:MET:HG3	2.17	0.45
20:LM:668:LEU:HD12	20:LM:710:VAL:HG11	1.97	0.45
20:LM:1624:ASN:OD1	20:LM:1676:LEU:HD12	2.17	0.45
22:LO:107:ASP:OD1	22:LO:108:GLY:N	2.50	0.45
27:LT:765:LEU:HD12	27:LT:895:ALA:HB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:NH:339:GLU:O	39:NH:529:ARG:NH2	2.48	0.45
49:NW:341:ILE:HG22	49:NW:344:LEU:H	1.82	0.45
59:SL:102:ILE:HG21	59:SL:107:MET:HE2	1.98	0.45
61:SP:1555:GLN:HE21	61:SP:1557:GLU:HB3	1.81	0.45
61:SP:1886:LYS:NZ	61:SP:1927:ILE:HD11	2.30	0.45
61:SP:2138:ILE:HD11	61:SP:2182:ASN:HB3	1.98	0.45
2:L1:157:U:O2'	2:L1:158:A:OP1	2.33	0.45
2:L1:1010:G:H2'	2:L1:1011:A:H8	1.82	0.45
8:L7:170:VAL:HG13	8:L7:187:PHE:HB2	1.98	0.45
10:L9:87:LEU:HD11	10:L9:97:ILE:HG12	1.99	0.45
17:LI:508:PHE:O	17:LI:584:ARG:NH1	2.49	0.45
18:LJ:489:MET:CE	19:LK:571:LYS:HA	2.46	0.45
20:LM:740:LEU:O	20:LM:744:ILE:HG12	2.16	0.45
21:LN:30:ARG:NH1	21:LN:52:GLU:OE2	2.49	0.45
22:LO:316:GLU:OE1	22:LO:318:PRO:HD2	2.17	0.45
25:LR:745:GLU:HA	25:LR:748:LEU:HD12	1.98	0.45
39:NH:436:GLN:HG2	39:NH:524:LEU:HD21	1.98	0.45
41:NK:160:LEU:HD12	41:NK:163:VAL:HG21	1.99	0.45
44:NO:30:CYS:SG	44:NO:31:SER:N	2.90	0.45
57:SI:107:THR:HG23	57:SI:109:GLN:H	1.82	0.45
1:L0:863:C:N3	60:SM:11:GLU:HG2	2.32	0.45
2:L1:227:U:H4'	2:L1:228:C:O5'	2.16	0.45
2:L1:1311:C:H4'	70:SZ:241:LEU:HD11	1.99	0.45
25:LR:165:ARG:HH22	25:LR:207:GLY:HA3	1.82	0.45
25:LR:475:GLN:NE2	25:LR:476:ARG:O	2.49	0.45
29:LW:121:LEU:HD13	64:SS:694:GLN:HG2	1.98	0.45
39:NH:234:LYS:HE2	39:NH:300:TRP:HB3	1.98	0.45
41:NJ:112:LYS:HB3	41:NJ:112:LYS:HE3	1.85	0.45
58:SK:101:ASN:HB2	58:SK:106:LEU:HD23	1.99	0.45
61:SP:1215:TYR:HA	61:SP:1218:LEU:HD13	1.98	0.45
2:L1:478:G:H2'	2:L1:479:C:H6	1.82	0.45
13:LD:48:LYS:O	13:LD:51:ILE:N	2.50	0.45
16:LH:630:GLN:HG3	16:LH:631:TRP:CD1	2.52	0.45
17:LI:159:PHE:CE1	17:LI:166:VAL:HB	2.52	0.45
18:LJ:346:LYS:HB2	26:LS:292:TYR:CE2	2.51	0.45
19:LK:497:MET:HG3	19:LK:498:PRO:HD2	1.98	0.45
19:LK:525:GLN:NE2	19:LK:529:CYS:SG	2.89	0.45
19:LL:22:SER:OG	19:LL:25:SER:O	2.21	0.45
20:LM:417:LYS:HA	20:LM:417:LYS:HD3	1.73	0.45
20:LM:502:LEU:O	20:LM:506:MET:N	2.45	0.45
23:LP:46:ARG:NH1	28:LU:20:ASP:OD1	2.43	0.45

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
61:SP:1230:ASP:O	61:SP:1234:ASN:ND2	2.49	0.45
61:SP:1424:LEU:HB2	61:SP:1427:ILE:HD13	1.99	0.45
61:SP:1450:PHE:HA	61:SP:1453:PHE:CD2	2.52	0.45
2:L1:110:U:H2’	2:L1:111:A:C8	2.52	0.45
2:L1:639:C:H2’	2:L1:640:A:H8	1.82	0.45
2:L1:1373:C:H2’	2:L1:1374:C:C6	2.52	0.45
5:L4:55:ALA:HB1	5:L4:60:GLU:HG3	1.99	0.45
5:L4:171:ASP:OD1	5:L4:171:ASP:N	2.49	0.45
8:L7:61:ILE:HD13	8:L7:180:LEU:HD11	1.99	0.45
16:LH:319:ARG:HG2	26:LS:374:GLU:HG2	1.99	0.45
17:LI:460:ILE:HG12	17:LI:465:LEU:HD23	1.99	0.45
17:LI:712:SER:OG	17:LI:714:GLU:OE2	2.34	0.45
20:LM:1966:LEU:HD22	20:LM:2026:GLN:HG3	1.99	0.45
21:LN:258:GLY:HA2	21:LN:290:VAL:HG23	1.98	0.45
24:LQ:463:VAL:HG11	24:LQ:468:GLN:HB2	1.98	0.45
24:LQ:473:THR:OG1	24:LQ:475:THR:O	2.23	0.45
27:LT:563:LEU:HB3	27:LT:577:VAL:HB	1.99	0.45
29:LW:242:ILE:HD13	29:LW:253:VAL:HG12	1.99	0.45
30:LZ:14:LYS:O	30:LZ:15:GLN:HG2	2.16	0.45
39:NH:1016:PRO:HA	39:NH:1019:ILE:HD12	1.99	0.45
46:NR:159:UNK:O	46:NR:163:UNK:N	2.50	0.45
61:SP:470:VAL:HG22	61:SP:529:ARG:HG3	1.99	0.45
61:SP:1783:ILE:HG13	61:SP:1834:LEU:HD21	1.99	0.45
66:SU:181:ARG:O	66:SU:185:MET:HG2	2.15	0.45
2:L1:36:U:H2’	2:L1:37:C:C6	2.51	0.45
2:L1:191:A:N6	2:L1:208:G:O2’	2.48	0.45
2:L1:1844:U:H3	2:L1:1855:G:H1	1.65	0.45
2:L1:1852:C:H2’	2:L1:1853:C:C6	2.52	0.45
3:L2:31:G:H5”	3:L2:32:U:C2	2.52	0.45
16:LH:39:VAL:O	16:LH:53:LEU:HB2	2.17	0.45
17:LI:460:ILE:HG22	17:LI:492:GLN:HG3	1.99	0.45
18:LJ:478:ARG:NH1	18:LJ:479:GLU:OE2	2.50	0.45
20:LM:327:VAL:HG23	20:LM:330:LEU:HB2	1.97	0.45
21:LN:160:ILE:HB	21:LN:171:PHE:HB2	1.98	0.45
22:LO:601:HIS:HA	22:LO:604:LYS:HD3	1.99	0.45
23:LP:18:GLN:O	23:LP:22:ILE:HG12	2.16	0.45
23:LP:75:ILE:HD11	26:LS:80:LEU:HG	1.99	0.45
25:LR:253:LEU:HD21	25:LR:324:LEU:HD13	1.98	0.45
25:LR:436:PHE:CZ	25:LR:508:LEU:HD21	2.51	0.45
27:LT:216:TYR:HB3	27:LT:219:LYS:HB2	1.97	0.45
27:LT:535:ASP:OD1	27:LT:535:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NK:266:LYS:HE3	41:NK:461:TYR:CG	2.52	0.45
48:NU:56:HIS:O	48:NU:60:ARG:HG2	2.17	0.45
49:NW:178:GLU:HB3	49:NW:196:ILE:HB	1.99	0.45
56:SH:94:GLY:HA2	56:SH:120:VAL:HG13	1.98	0.45
61:SP:427:ILE:HG21	61:SP:446:LEU:HD21	1.99	0.45
61:SP:1452:THR:O	61:SP:1456:ILE:HG12	2.16	0.45
65:ST:610:PRO:HD2	66:SU:445:TYR:HE1	1.81	0.45
65:ST:636:HIS:O	65:ST:639:ARG:NH1	2.50	0.45
2:L1:980:A:H2'	2:L1:981:A:C8	2.52	0.45
3:L2:30:A:O2'	3:L2:32:U:O4	2.30	0.45
19:LL:43:THR:HG23	19:LL:359:ILE:HG21	1.98	0.45
20:LM:1647:ASP:O	20:LM:1651:ILE:HG12	2.17	0.45
21:LN:461:LEU:O	21:LN:476:ALA:HA	2.17	0.45
27:LT:595:LEU:HB2	27:LT:609:ILE:HD11	1.99	0.45
35:ND:240:ASN:HA	35:ND:243:ARG:HH21	1.82	0.45
40:NI:23:TYR:HE1	40:NI:43:ARG:HD3	1.82	0.45
46:NR:621:UNK:O	46:NR:625:UNK:N	2.50	0.45
56:SH:284:LEU:HA	56:SH:287:ILE:HD12	1.99	0.45
56:SH:368:LEU:O	57:SI:989:GLN:NE2	2.45	0.45
61:SP:644:LYS:NZ	61:SP:810:ASP:O	2.42	0.45
62:SQ:682:ASP:OD1	62:SQ:683:GLY:N	2.50	0.45
2:L1:219:U:H2'	2:L1:220:U:C6	2.52	0.44
2:L1:618:C:H2'	2:L1:619:A:O4'	2.18	0.44
16:LH:816:LEU:HB3	20:LM:933:GLU:HG2	1.97	0.44
19:LL:130:ASN:ND2	19:LL:171:VAL:O	2.47	0.44
23:LP:3:GLU:HG2	23:LP:4:ILE:HD12	1.99	0.44
23:LP:22:ILE:HD13	29:LW:98:PHE:CZ	2.49	0.44
25:LR:32:LEU:HG	25:LR:308:LEU:HD22	1.99	0.44
25:LR:151:PRO:HD3	25:LR:178:ARG:HH21	1.82	0.44
29:LW:229:LEU:HD21	29:LW:232:GLU:HB2	1.99	0.44
41:NK:28:VAL:HG12	41:NK:200:ILE:HG13	1.98	0.44
41:NK:284:ALA:HB2	41:NK:465:LEU:H	1.82	0.44
49:NW:167:ARG:HD3	50:NY:324:PRO:HG3	2.00	0.44
53:SC:92:ARG:HH11	69:SY:168:ARG:HG3	1.82	0.44
58:SJ:190:VAL:HG11	58:SJ:240:VAL:HG11	2.00	0.44
1:L0:751:C:H2'	1:L0:752:C:C6	2.52	0.44
17:LI:406:MET:SD	17:LI:407:LYS:HG2	2.57	0.44
20:LM:135:VAL:HG22	20:LM:144:PHE:HD1	1.83	0.44
20:LM:1830:TYR:O	20:LM:1833:ILE:HG22	2.16	0.44
22:LO:217:CYS:HB3	22:LO:274:TYR:CE1	2.53	0.44
23:LP:213:SER:O	23:LP:217:LEU:HD23	2.17	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
25:LR:291:PRO:HD3	25:LR:376:THR:HG22	1.99	0.44
25:LR:294:GLU:HB2	25:LR:312:ALA:HB2	2.00	0.44
26:LS:319:VAL:HA	26:LS:334:HIS:HA	1.98	0.44
27:LT:851:GLY:O	27:LT:855:ILE:HG12	2.17	0.44
41:NJ:866:LEU:HD21	41:NJ:895:PHE:HB2	1.99	0.44
57:SI:88:MET:HB3	57:SI:133:CYS:HB3	1.98	0.44
58:SK:44:ILE:HB	58:SK:197:VAL:HG22	1.99	0.44
65:ST:571:VAL:HG11	66:SU:479:PHE:HB2	1.99	0.44
69:SY:33:LYS:HA	69:SY:33:LYS:HD3	1.86	0.44
2:L1:119:U:H2’	2:L1:120:U:H6	1.83	0.44
3:L2:89:A:H5’	52:SB:336:PRO:HB3	1.99	0.44
20:LM:1383:PHE:O	20:LM:1387:LEU:HG	2.18	0.44
20:LM:1422:GLN:O	20:LM:1426:LYS:HG2	2.17	0.44
20:LM:1573:THR:O	20:LM:1576:PHE:HB3	2.18	0.44
20:LM:1669:THR:O	20:LM:1673:THR:HG23	2.16	0.44
20:LM:1992:LEU:HD23	20:LM:1992:LEU:HA	1.88	0.44
24:LQ:660:TRP:CZ3	24:LQ:667:HIS:HB2	2.51	0.44
25:LR:81:LEU:O	25:LR:93:TRP:N	2.41	0.44
26:LS:346:SER:OG	26:LS:359:ASN:OD1	2.32	0.44
29:LW:243:ARG:HD3	29:LW:243:ARG:HA	1.82	0.44
34:NC:235:ASP:OD1	34:NC:259:ARG:NE	2.50	0.44
39:NH:186:ARG:HG2	39:NH:258:PRO:HG2	1.99	0.44
39:NH:892:PRO:HA	39:NH:893:PRO:HD3	1.89	0.44
41:NK:623:GLY:HA2	41:NK:706:LEU:HG	1.98	0.44
49:NW:282:ASP:OD1	49:NW:283:SER:N	2.49	0.44
56:SH:124:GLN:NE2	56:SH:260:ALA:O	2.42	0.44
58:SK:131:ASP:OD1	58:SK:132:ARG:N	2.49	0.44
61:SP:1399:SER:O	61:SP:1402:LYS:NZ	2.41	0.44
70:SZ:240:ASN:O	70:SZ:242:LYS:HG3	2.17	0.44
2:L1:103:A:H4’	2:L1:104:A:H8	1.81	0.44
2:L1:223:C:H2’	2:L1:224:A:H8	1.81	0.44
2:L1:498:C:H2’	2:L1:499:G:C8	2.53	0.44
2:L1:1355:C:H2’	2:L1:1356:G:O4’	2.17	0.44
9:L8:101:ILE:HD12	9:L8:190:LEU:HD11	1.99	0.44
16:LH:469:TYR:HD1	16:LH:495:SER:HB3	1.82	0.44
20:LM:1604:ILE:HD11	20:LM:1619:ALA:HA	1.98	0.44
20:LM:1951:PHE:HE1	20:LM:1954:PHE:HB2	1.82	0.44
21:LN:554:SER:HB3	21:LN:557:ASP:HB2	1.99	0.44
22:LO:54:THR:HG21	22:LO:74:ASP:HB3	2.00	0.44
22:LO:339:ASN:ND2	22:LO:343:ASP:OD1	2.39	0.44
39:NH:709:SER:O	39:NH:723:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NJ:256:LYS:HD3	41:NJ:469:ILE:HG23	1.99	0.44
41:NK:131:PRO:HB3	41:NK:485:LEU:HD22	1.98	0.44
41:NK:425:LEU:HA	41:NK:428:ILE:HG22	2.00	0.44
57:SI:310:ILE:HD11	57:SI:886:VAL:HB	1.99	0.44
58:SJ:88:THR:O	58:SJ:92:LEU:HG	2.18	0.44
58:SK:56:LYS:O	65:ST:45:GLY:HA3	2.18	0.44
63:SR:66:ILE:HG23	65:ST:836:LEU:HD23	1.97	0.44
1:L0:799:C:O2'	1:L0:800:G:OP2	2.31	0.44
2:L1:337:C:H2'	2:L1:338:G:C8	2.52	0.44
19:LL:575:LEU:O	19:LL:579:VAL:HG23	2.18	0.44
20:LM:1288:ILE:O	20:LM:1292:ILE:HG13	2.18	0.44
20:LM:1810:LYS:HE3	20:LM:1847:ILE:HD11	2.00	0.44
27:LT:460:ILE:HB	27:LT:473:TRP:HB2	1.99	0.44
27:LT:567:ASN:ND2	27:LT:574:ILE:HD11	2.33	0.44
29:LW:197:GLY:HA3	29:LW:215:ARG:HB3	2.00	0.44
29:LW:246:HIS:CG	29:LW:247:SER:H	2.35	0.44
39:NH:364:LYS:HE3	39:NH:364:LYS:HB3	1.81	0.44
41:NK:341:TYR:HB3	41:NK:360:VAL:HG12	1.99	0.44
41:NK:548:LEU:HD21	41:NK:556:LEU:HD11	2.00	0.44
42:NM:40:ASN:OD1	42:NM:41:ILE:N	2.51	0.44
47:NT:104:LYS:HD3	47:NT:118:ARG:HH21	1.82	0.44
47:NT:133:ALA:HB3	47:NT:140:TYR:HB3	1.99	0.44
53:SC:224:ARG:HA	53:SC:253:PHE:CZ	2.53	0.44
60:SM:6:ALA:HB1	60:SM:10:ARG:HH12	1.82	0.44
61:SP:1656:LEU:O	61:SP:1660:ILE:HD12	2.18	0.44
2:L1:558:G:H2'	2:L1:559:G:C8	2.53	0.44
3:L2:144:C:H3'	3:L2:145:U:C5'	2.48	0.44
5:L4:48:LEU:HD21	5:L4:64:ILE:HG21	2.00	0.44
5:L4:248:ILE:HG23	5:L4:250:GLU:H	1.83	0.44
20:LM:586:GLU:HA	20:LM:633:LEU:HD11	2.00	0.44
20:LM:754:HIS:CD2	20:LM:755:ILE:HG23	2.52	0.44
20:LM:1423:TYR:OH	20:LM:1440:LEU:HG	2.17	0.44
26:LS:313:THR:OG1	26:LS:344:VAL:O	2.35	0.44
26:LS:405:GLU:HG2	26:LS:407:TYR:HE1	1.83	0.44
27:LT:826:ASP:OD1	27:LT:827:PHE:N	2.50	0.44
27:LT:869:SER:HB3	27:LT:872:VAL:HG23	2.00	0.44
28:LU:234:LYS:HB3	28:LU:444:VAL:HB	2.00	0.44
32:NA:532:ALA:HA	32:NA:548:LEU:HD13	2.00	0.44
35:ND:235:ILE:HG23	35:ND:236:GLN:HG2	1.99	0.44
39:NH:965:PRO:HA	39:NH:969:ILE:HD11	2.00	0.44
41:NK:721:LYS:HE2	41:NK:721:LYS:HB3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SA:123:ARG:NH2	53:SD:254:LEU:O	2.51	0.44
53:SC:164:LEU:HB3	53:SC:233:ILE:HG12	1.99	0.44
54:SE:64:GLU:HA	54:SE:67:LEU:HG	1.99	0.44
55:SG:171:ILE:HG12	55:SG:183:VAL:HG22	2.00	0.44
61:SP:217:HIS:HB2	61:SP:220:LYS:HE2	1.99	0.44
61:SP:1578:MET:HA	61:SP:1586:ARG:HG3	2.00	0.44
65:ST:528:MET:O	65:ST:532:ILE:HG13	2.17	0.44
70:SZ:232:GLN:OE1	70:SZ:235:ARG:NE	2.43	0.44
2:L1:1312:G:O6	11:LA:36:ARG:NH1	2.51	0.44
17:LI:429:PHE:O	17:LI:432:VAL:HB	2.17	0.44
18:LJ:232:TRP:CH2	18:LJ:240:LEU:HD12	2.52	0.44
20:LM:180:THR:HA	20:LM:183:TYR:CE2	2.53	0.44
20:LM:1696:ALA:O	20:LM:1700:ILE:HG12	2.17	0.44
20:LM:1806:LEU:O	20:LM:1809:LEU:HG	2.18	0.44
22:LO:234:ALA:HA	22:LO:237:LEU:HG	2.00	0.44
23:LP:24:LEU:O	23:LP:71:ARG:NH1	2.48	0.44
23:LP:397:GLU:HA	23:LP:400:ARG:HH22	1.83	0.44
24:LQ:145:LEU:HD12	24:LQ:176:TRP:CE3	2.53	0.44
24:LQ:904:TYR:CD1	27:LT:905:LEU:HD22	2.52	0.44
29:LW:237:GLU:OE1	29:LW:257:ARG:N	2.47	0.44
39:NH:272:ASN:ND2	39:NH:292:PRO:O	2.51	0.44
39:NH:1014:LEU:HD11	39:NH:1082:ILE:HG13	1.98	0.44
56:SH:242:GLY:HA2	56:SH:275:LEU:HD21	2.00	0.44
61:SP:1137:ARG:HA	61:SP:1140:ILE:HG12	2.00	0.44
67:SW:103:LEU:HB3	67:SW:129:ALA:HB1	2.00	0.44
1:L0:817:U:H4'	26:LS:517:LYS:HG2	1.99	0.44
2:L1:640:A:H2'	2:L1:641:A:C8	2.52	0.44
2:L1:1125:C:H2'	2:L1:1126:G:C8	2.53	0.44
11:LA:99:LYS:HE2	11:LA:99:LYS:HB3	1.75	0.44
17:LI:404:THR:HG21	17:LI:416:GLU:HG3	1.99	0.44
20:LM:1400:VAL:HG22	20:LM:1446:PHE:CZ	2.53	0.44
21:LN:130:ILE:HG12	21:LN:135:ILE:HG22	1.99	0.44
22:LO:109:ARG:HG3	22:LO:110:LYS:HG3	2.00	0.44
24:LQ:505:SER:OG	24:LQ:507:ASP:OD1	2.22	0.44
25:LR:73:ASP:OD2	25:LR:74:LEU:N	2.51	0.44
25:LR:402:ILE:HB	25:LR:415:ALA:HB3	1.99	0.44
27:LT:258:ALA:HB3	27:LT:261:VAL:HB	2.00	0.44
28:LU:66:ARG:NH1	59:SL:127:PRO:HD3	2.21	0.44
28:LU:180:ILE:HD13	28:LU:226:MET:HG3	1.99	0.44
29:LW:196:PHE:HA	29:LW:216:ARG:HH11	1.81	0.44
32:NA:480:LEU:HD13	32:NA:523:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NK:577:ILE:HD12	41:NK:648:LEU:HD22	1.99	0.44
46:NR:363:UNK:O	46:NR:367:UNK:N	2.50	0.44
50:NY:179:THR:HG21	50:NY:202:VAL:HG23	1.99	0.44
53:SC:104:ASP:O	69:SY:125:LEU:HD13	2.18	0.44
53:SD:284:LYS:HE3	59:SL:133:PRO:HD3	1.98	0.44
57:SI:1237:PHE:O	57:SI:1241:GLN:HG2	2.18	0.44
58:SJ:96:MET:HA	58:SJ:101:ASN:ND2	2.31	0.44
61:SP:210:MET:HE1	61:SP:228:LEU:HD21	2.00	0.44
66:SU:261:LYS:HE3	66:SU:261:LYS:HB2	1.86	0.44
2:L1:615:C:H2'	2:L1:616:A:H8	1.82	0.44
16:LH:222:HIS:CE1	16:LH:228:ARG:HH11	2.36	0.44
20:LM:1663:GLN:HB2	20:LM:1666:ASN:ND2	2.33	0.44
21:LN:271:ASN:OD1	21:LN:272:SER:N	2.51	0.44
39:NH:112:VAL:HG22	39:NH:220:PHE:HE1	1.83	0.44
41:NK:365:ARG:HG3	57:SI:667:TRP:CD1	2.52	0.44
46:NR:140:UNK:O	46:NR:144:UNK:N	2.51	0.44
48:NU:5:ARG:HH11	48:NU:53:TYR:HD1	1.65	0.44
49:NW:74:LYS:O	49:NW:76:ARG:HG3	2.18	0.44
52:SB:150:ARG:NE	53:SC:214:ILE:O	2.51	0.44
55:SG:323:HIS:CE1	55:SG:342:ALA:HB2	2.53	0.44
61:SP:248:LYS:HA	61:SP:248:LYS:HD3	1.74	0.44
61:SP:740:ILE:HD12	61:SP:827:ALA:HB2	2.00	0.44
61:SP:1516:GLU:HA	61:SP:1520:ARG:HG2	2.00	0.44
66:SU:247:GLU:CD	66:SU:250:ARG:HH12	2.21	0.44
67:SW:108:ARG:CZ	67:SW:119:ARG:HH22	2.31	0.44
1:L0:854:U:H4'	1:L0:855:G:O5'	2.17	0.43
2:L1:1109:C:H1'	28:LU:424:HIS:O	2.18	0.43
2:L1:1284:A:H4'	2:L1:1285:G:H5"	1.99	0.43
2:L1:1854:U:H2'	2:L1:1855:G:H8	1.82	0.43
17:LI:692:GLU:HG2	19:LK:555:MET:HB3	2.00	0.43
22:LO:96:LYS:HD2	22:LO:96:LYS:HA	1.86	0.43
26:LS:273:ASN:HB2	26:LS:292:TYR:CE1	2.53	0.43
28:LU:3:VAL:HG22	29:LW:160:LEU:HD13	1.99	0.43
36:NE:212:LYS:O	36:NE:216:GLU:HG2	2.18	0.43
41:NJ:132:ASN:HD21	41:NJ:543:ASN:HB2	1.81	0.43
56:SH:67:ASN:HB2	56:SH:72:THR:HG22	1.99	0.43
56:SH:123:ASP:OD1	56:SH:124:GLN:N	2.48	0.43
57:SI:381:SER:HB2	57:SI:386:LYS:HE3	2.00	0.43
61:SP:1398:PHE:CD2	61:SP:1410:LEU:HD21	2.53	0.43
66:SU:397:ARG:HG3	66:SU:398:HIS:ND1	2.32	0.43
2:L1:306:C:O2	9:L8:53:LYS:NZ	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:589:G:HO2'	2:L1:590:A:P	2.40	0.43
8:L7:64:VAL:O	8:L7:97:GLN:N	2.49	0.43
11:LA:24:THR:O	11:LA:27:ILE:HG22	2.18	0.43
12:LC:47:LEU:O	12:LC:50:LYS:HB2	2.18	0.43
12:LC:97:GLN:HB2	12:LC:105:LYS:HG3	1.99	0.43
18:LJ:270:ARG:HG2	18:LJ:290:ALA:C	2.39	0.43
20:LM:2066:ASN:HD22	20:LM:2102:LEU:HB3	1.82	0.43
22:LO:847:PHE:O	22:LO:850:LYS:HG3	2.18	0.43
23:LP:494:ARG:NH1	23:LP:532:TYR:OH	2.42	0.43
24:LQ:482:ASP:HB2	24:LQ:485:SER:HB2	2.00	0.43
25:LR:524:LEU:HA	25:LR:540:SER:HA	1.99	0.43
26:LS:245:ASN:ND2	26:LS:543:GLY:O	2.47	0.43
41:NJ:209:ILE:O	57:SI:382:THR:OG1	2.36	0.43
42:NM:224:GLU:OE1	42:NM:227:LYS:N	2.50	0.43
46:NR:746:UNK:O	46:NR:750:UNK:N	2.51	0.43
56:SH:124:GLN:O	57:SI:736:ARG:NH1	2.51	0.43
59:SL:86:LEU:HD23	59:SL:129:PHE:CZ	2.53	0.43
61:SP:31:ILE:HD11	61:SP:195:PHE:HB2	2.01	0.43
61:SP:1235:VAL:HA	61:SP:1238:ILE:HD12	1.99	0.43
61:SP:2088:LEU:HD13	61:SP:2132:GLY:HA3	2.00	0.43
2:L1:145:G:H2'	2:L1:146:G:C8	2.53	0.43
2:L1:979:C:H2'	2:L1:980:A:H8	1.82	0.43
4:L3:36:VAL:HG23	4:L3:40:TYR:CD2	2.41	0.43
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.51	0.43
8:L7:37:LYS:HG2	8:L7:41:ARG:HG3	2.00	0.43
11:LA:55:ASN:OD1	11:LA:81:ASP:HA	2.18	0.43
12:LC:138:ARG:HG3	22:LO:535:ARG:HG2	2.00	0.43
16:LH:318:HIS:HE2	16:LH:322:GLU:HB3	1.83	0.43
20:LM:302:SER:HA	20:LM:305:ILE:HD12	1.99	0.43
20:LM:1323:ILE:HD12	20:LM:1353:VAL:HG21	2.00	0.43
24:LQ:369:ASP:OD1	24:LQ:370:LEU:N	2.52	0.43
26:LS:407:TYR:CD1	26:LS:419:ARG:HG2	2.54	0.43
39:NH:140:PRO:HA	39:NH:541:PRO:HG3	2.00	0.43
41:NJ:290:LYS:HD3	41:NJ:410:ALA:HB1	2.00	0.43
48:NU:8:THR:HA	48:NU:11:LYS:NZ	2.33	0.43
58:SJ:44:ILE:HB	58:SJ:197:VAL:HG22	2.00	0.43
58:SJ:102:ARG:NH2	58:SK:222:TYR:OH	2.51	0.43
61:SP:1670:GLN:HG2	61:SP:1816:GLU:HG3	2.00	0.43
61:SP:1976:GLN:NE2	61:SP:1979:LYS:HD2	2.33	0.43
2:L1:1336:C:H2'	2:L1:1337:C:C6	2.53	0.43
2:L1:1794:C:H2'	2:L1:1795:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L9:54:ARG:HH21	59:SL:96:ALA:HB2	1.84	0.43
16:LH:557:LEU:HD11	16:LH:612:PRO:HB3	2.00	0.43
23:LP:227:LYS:HE3	23:LP:227:LYS:HB3	1.76	0.43
24:LQ:902:LEU:HD23	25:LR:761:LEU:HD22	2.01	0.43
27:LT:845:ASN:O	27:LT:848:LYS:HG2	2.19	0.43
28:LU:283:SER:HB3	28:LU:302:PHE:HB3	2.01	0.43
28:LU:418:GLU:OE1	28:LU:421:ARG:NH1	2.51	0.43
40:NI:42:VAL:HG12	40:NI:63:VAL:HG13	2.00	0.43
58:SJ:150:ASP:OD1	58:SJ:150:ASP:N	2.52	0.43
61:SP:118:LEU:HB3	61:SP:121:ASP:HB2	2.00	0.43
61:SP:276:MET:O	61:SP:280:THR:OG1	2.33	0.43
61:SP:457:PRO:HD2	61:SP:569:ASN:HD21	1.82	0.43
65:ST:565:VAL:C	65:ST:568:PRO:HD2	2.39	0.43
2:L1:318:A:H61	7:L6:186:GLN:HE22	1.67	0.43
2:L1:989:C:OP2	42:NM:155:TYR:OH	2.26	0.43
3:L2:88:G:O6	52:SB:333:ARG:NH1	2.51	0.43
6:L5:30:ILE:HG23	6:L5:117:ILE:HD11	2.01	0.43
8:L7:153:LEU:HD21	28:LU:196:PHE:CD2	2.54	0.43
20:LM:363:THR:HG22	20:LM:417:LYS:HD2	2.00	0.43
20:LM:1790:GLU:OE1	20:LM:1806:LEU:HD22	2.18	0.43
26:LS:486:GLU:OE1	26:LS:553:TYR:OH	2.31	0.43
46:NR:810:UNK:O	46:NR:814:UNK:N	2.51	0.43
61:SP:2186:CYS:HA	61:SP:2189:ILE:HD12	2.00	0.43
3:L2:50:U:H2’	3:L2:51:C:C6	2.54	0.43
4:L3:23:ARG:NH2	18:LJ:80:LYS:HA	2.34	0.43
16:LH:614:GLU:HG3	16:LH:616:ARG:HG2	2.00	0.43
18:LJ:264:LEU:HB3	18:LJ:295:LEU:HD21	1.99	0.43
22:LO:590:GLY:HA2	22:LO:656:GLU:HA	2.00	0.43
24:LQ:200:LEU:HD22	24:LQ:308:ILE:HD13	2.00	0.43
28:LU:180:ILE:HD12	28:LU:192:MET:HE3	2.01	0.43
41:NK:508:TYR:N	41:NK:558:CYS:O	2.51	0.43
48:NU:55:THR:HA	48:NU:58:MET:HB3	1.99	0.43
57:SI:956:LEU:HD22	57:SI:968:LEU:HD11	2.00	0.43
61:SP:977:ARG:NH1	61:SP:987:GLU:OE1	2.49	0.43
8:L7:30:LEU:O	8:L7:34:SER:HB3	2.18	0.43
8:L7:64:VAL:HB	8:L7:72:PHE:CE2	2.51	0.43
9:L8:61:ASP:OD2	9:L8:61:ASP:N	2.52	0.43
16:LH:345:ARG:HE	16:LH:426:LYS:NZ	2.16	0.43
17:LI:509:LEU:HD21	17:LI:616:PHE:HB2	2.01	0.43
17:LI:690:LYS:O	19:LL:569:HIS:ND1	2.50	0.43
20:LM:373:GLN:HA	20:LM:376:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:502:LEU:HD11	20:LM:518:ILE:HG12	2.01	0.43
20:LM:1518:VAL:HB	20:LM:1590:LYS:HD3	2.00	0.43
20:LM:1587:LEU:O	20:LM:1591:VAL:N	2.51	0.43
21:LN:363:THR:OG1	21:LN:374:PRO:O	2.37	0.43
21:LN:404:TRP:HE1	21:LN:449:SER:HB2	1.83	0.43
21:LN:502:SER:HB3	21:LN:508:VAL:HG22	2.01	0.43
25:LR:317:LEU:HD12	25:LR:326:LEU:HD11	2.01	0.43
25:LR:517:PHE:HE1	25:LR:553:PHE:HA	1.84	0.43
27:LT:248:VAL:HG11	27:LT:268:SER:H	1.84	0.43
38:NG:83:GLN:HA	38:NG:86:LYS:HZ3	1.83	0.43
39:NH:267:LEU:HD22	39:NH:298:ASN:HA	2.01	0.43
39:NH:477:ARG:HB2	39:NH:478:PRO:HD3	2.01	0.43
40:NI:63:VAL:O	40:NI:119:ALA:N	2.39	0.43
61:SP:1631:ASN:OD1	61:SP:1632:ILE:HD12	2.19	0.43
61:SP:1985:LYS:HG3	61:SP:2083:PHE:HE2	1.83	0.43
2:L1:285:U:H2'	2:L1:286:U:C6	2.54	0.43
2:L1:1387:G:H3'	2:L1:1388:A:H8	1.84	0.43
5:L4:54:TYR:O	14:LF:15:ASN:ND2	2.52	0.43
5:L4:176:ASP:OD1	5:L4:177:THR:N	2.51	0.43
9:L8:64:ASN:HA	9:L8:75:LYS:HA	2.01	0.43
9:L8:80:ASP:OD2	9:L8:81:VAL:N	2.52	0.43
19:LL:118:SER:HG	19:LL:158:CYS:HG	1.66	0.43
20:LM:249:GLY:HA2	20:LM:257:TYR:CE2	2.54	0.43
25:LR:524:LEU:HD23	25:LR:538:THR:HB	2.01	0.43
28:LU:9:ASN:HB2	28:LU:12:ASN:ND2	2.33	0.43
28:LU:164:HIS:CE1	28:LU:169:ALA:HA	2.54	0.43
29:LW:355:ILE:HG13	64:SS:667:VAL:HG13	2.00	0.43
41:NJ:330:PHE:HA	41:NJ:335:TYR:HD2	1.84	0.43
41:NK:285:ALA:HB3	41:NK:288:ARG:HE	1.84	0.43
41:NK:587:ARG:O	41:NK:590:ILE:HG22	2.19	0.43
50:NY:239:TRP:HA	50:NY:242:PHE:HD2	1.84	0.43
55:SG:349:LEU:HD11	55:SG:412:LEU:HD13	2.00	0.43
60:SM:97:LEU:HD22	60:SM:141:GLU:HG2	2.01	0.43
61:SP:635:GLN:HE21	61:SP:722:ARG:HE	1.65	0.43
61:SP:1204:LYS:O	61:SP:1208:ILE:HG12	2.19	0.43
66:SU:186:GLN:NE2	66:SU:190:ASP:OD1	2.51	0.43
66:SU:241:LYS:HB2	66:SU:247:GLU:HG3	2.00	0.43
12:LC:63:PHE:CZ	12:LC:92:LEU:HD22	2.54	0.43
16:LH:57:ARG:HD3	16:LH:57:ARG:HA	1.81	0.43
17:LI:658:PHE:HZ	18:LJ:489:MET:HB3	1.84	0.43
20:LM:558:LEU:HD11	20:LM:602:CYS:HB2	2.01	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
26:LS:183:LYS:HB2	26:LS:183:LYS:HE2	1.82	0.43
26:LS:279:GLN:HB3	26:LS:286:PRO:HD2	2.00	0.43
29:LW:343:LEU:O	29:LW:352:LEU:N	2.44	0.43
48:NU:54:VAL:O	48:NU:58:MET:N	2.43	0.43
49:NW:119:ILE:HD11	49:NW:133:ILE:HB	2.01	0.43
50:NY:101:VAL:HG21	50:NY:116:ALA:HB1	2.01	0.43
59:SL:113:LEU:HB3	59:SL:117:TYR:CD1	2.53	0.43
66:SU:277:HIS:CE1	66:SU:346:ARG:HH22	2.36	0.43
66:SU:310:ASN:HD22	66:SU:346:ARG:NH2	2.17	0.43
69:SY:116:ILE:HG23	69:SY:202:LEU:HD11	2.01	0.43
2:L1:175:A:H2’	2:L1:176:U:C6	2.54	0.43
2:L1:219:U:H2’	2:L1:220:U:H6	1.84	0.43
2:L1:1289:U:H2’	2:L1:1290:G:C8	2.54	0.43
2:L1:1670:C:OP2	60:SM:91:ARG:NH1	2.52	0.43
7:L6:188:LYS:O	7:L6:192:ILE:HG12	2.19	0.43
9:L8:192:GLY:O	9:L8:195:LEU:N	2.51	0.43
10:L9:131:ARG:HA	10:L9:131:ARG:HD2	1.80	0.43
16:LH:152:ASP:OD1	16:LH:153:TYR:N	2.50	0.43
18:LJ:173:SER:OG	18:LJ:179:LEU:HB3	2.19	0.43
22:LO:705:VAL:HA	22:LO:721:THR:HG22	2.00	0.43
23:LP:12:ARG:NH2	23:LP:57:TYR:OH	2.52	0.43
23:LP:580:GLU:OE2	23:LP:580:GLU:N	2.42	0.43
24:LQ:680:CYS:SG	24:LQ:681:LEU:N	2.92	0.43
26:LS:357:LEU:HD11	26:LS:365:LEU:HB3	2.00	0.43
27:LT:491:LYS:HE2	27:LT:491:LYS:HB2	1.82	0.43
28:LU:234:LYS:HD2	28:LU:444:VAL:HG21	2.00	0.43
37:NF:83:ASP:OD1	37:NF:84:LEU:N	2.52	0.43
41:NJ:388:ASP:OD1	41:NJ:389:GLU:N	2.51	0.43
41:NK:612:GLN:HB3	41:NK:774:ARG:HH12	1.83	0.43
42:NM:52:THR:HG23	42:NM:57:ILE:HA	2.01	0.43
49:NW:143:HIS:CD2	49:NW:145:PRO:HD2	2.54	0.43
53:SC:155:ILE:HG22	53:SC:157:ILE:HG12	2.01	0.43
58:SJ:51:SER:OG	58:SJ:83:ALA:HA	2.19	0.43
58:SJ:124:THR:HG22	58:SJ:155:LEU:HB3	2.01	0.43
61:SP:1637:THR:HG23	61:SP:1676:LEU:HD23	2.01	0.43
64:SS:720:LYS:HE3	64:SS:720:LYS:HB3	1.92	0.43
65:ST:738:SER:O	65:ST:741:THR:OG1	2.29	0.43
66:SU:284:LEU:HD23	66:SU:287:PRO:HA	2.00	0.43
66:SU:297:ALA:HB1	66:SU:304:LEU:HD21	2.00	0.43
2:L1:980:A:H2’	2:L1:981:A:H8	1.84	0.42
2:L1:1384:C:H2’	2:L1:1385:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1687:C:H2'	2:L1:1688:C:C6	2.54	0.42
8:L7:142:LYS:HE2	8:L7:156:VAL:HG22	2.00	0.42
14:LF:13:MET:SD	14:LF:22:GLN:NE2	2.85	0.42
14:LF:55:ILE:HG13	14:LF:75:ILE:HD13	2.01	0.42
17:LI:624:TYR:HE1	17:LI:647:MET:HE2	1.84	0.42
17:LI:682:ILE:HD11	19:LK:566:SER:HA	2.01	0.42
20:LM:1334:VAL:HB	20:LM:1339:ASP:HB3	2.01	0.42
20:LM:1396:LEU:O	20:LM:1400:VAL:HG23	2.19	0.42
21:LN:100:PHE:CZ	53:SC:288:GLN:HG3	2.53	0.42
24:LQ:445:THR:HG22	24:LQ:447:GLN:OE1	2.18	0.42
25:LR:345:PRO:HG2	25:LR:346:GLU:OE1	2.19	0.42
27:LT:207:ILE:HG12	27:LT:222:LEU:HD22	2.00	0.42
29:LW:198:PRO:HB3	29:LW:467:THR:HG22	2.01	0.42
39:NH:266:ARG:HD2	39:NH:266:ARG:HA	1.83	0.42
47:NT:99:LYS:HB2	47:NT:99:LYS:HE2	1.84	0.42
53:SC:97:PHE:CE1	53:SC:109:LYS:HE3	2.54	0.42
54:SF:36:ARG:HA	54:SF:36:ARG:HD2	1.81	0.42
61:SP:1398:PHE:HA	61:SP:1401:ILE:HG22	2.01	0.42
61:SP:1895:GLY:O	61:SP:1898:VAL:HG22	2.19	0.42
3:L2:178:G:H1'	3:L2:183:G:C2	2.54	0.42
4:L3:26:ILE:HD12	4:L3:59:LEU:HD11	2.00	0.42
14:LF:12:PHE:HZ	14:LF:21:LYS:HD3	1.83	0.42
16:LH:130:VAL:HG21	16:LH:147:LEU:HD12	2.00	0.42
16:LH:297:SER:HB2	16:LH:306:CYS:SG	2.59	0.42
20:LM:1755:VAL:O	20:LM:1758:LEU:HG	2.18	0.42
20:LM:2085:LEU:HD23	20:LM:2124:GLN:HG3	2.01	0.42
21:LN:602:TYR:HA	21:LN:648:LYS:O	2.19	0.42
22:LO:742:ASP:OD1	22:LO:743:THR:N	2.51	0.42
23:LP:400:ARG:HG2	23:LP:431:HIS:HB3	2.02	0.42
28:LU:127:VAL:HG11	28:LU:159:TYR:HB2	2.01	0.42
30:LZ:2:VAL:HG23	30:LZ:3:ARG:H	1.84	0.42
52:SB:59:ALA:HA	52:SB:69:ASN:OD1	2.19	0.42
52:SB:64:MET:CE	53:SC:222:LYS:HA	2.48	0.42
54:SF:50:ILE:HA	54:SF:106:ILE:HD12	2.01	0.42
55:SG:382:VAL:HG12	55:SG:393:THR:HG22	2.01	0.42
65:ST:548:TYR:O	65:ST:552:THR:HG23	2.19	0.42
2:L1:375:U:H2'	2:L1:376:A:H8	1.82	0.42
2:L1:993:G:OP1	2:L1:1131:G:N2	2.48	0.42
2:L1:1091:C:H2'	2:L1:1092:G:C8	2.54	0.42
2:L1:1387:G:C2	2:L1:1388:A:H1'	2.54	0.42
3:L2:9:A:H2'	3:L2:10:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L2:25:U:O4	28:LU:389:ARG:NH1	2.52	0.42
4:L3:66:ARG:O	4:L3:70:ILE:HG13	2.18	0.42
11:LA:51:VAL:HG22	11:LA:77:ILE:HG22	2.02	0.42
14:LF:72:PHE:HB3	34:NC:246:MET:HE2	2.02	0.42
20:LM:99:ILE:HD11	20:LM:198:LYS:HE3	2.02	0.42
20:LM:1420:PHE:HB3	20:LM:1516:LEU:HD21	2.01	0.42
21:LN:39:THR:HA	21:LN:55:PHE:O	2.19	0.42
22:LO:202:ASP:OD1	22:LO:216:GLN:HA	2.20	0.42
25:LR:354:SER:OG	25:LR:360:LYS:NZ	2.52	0.42
39:NH:376:ARG:O	39:NH:380:GLN:HG3	2.19	0.42
41:NK:267:PHE:HZ	41:NK:282:LEU:HD11	1.84	0.42
46:NR:304:UNK:O	46:NR:308:UNK:N	2.52	0.42
47:NT:104:LYS:HE3	47:NT:105:TYR:CE1	2.54	0.42
49:NW:249:THR:HA	49:NW:274:PRO:HB3	2.01	0.42
53:SC:295:GLU:OE2	69:SY:136:HIS:NE2	2.52	0.42
54:SF:84:ARG:HB2	55:SG:375:GLN:HE21	1.84	0.42
56:SH:46:ASP:OD1	56:SH:47:PHE:N	2.52	0.42
56:SH:156:ARG:HG2	56:SH:166:GLU:HB3	2.01	0.42
3:L2:40:U:H5'	28:LU:18:LYS:HE3	2.01	0.42
8:L7:153:LEU:HD21	28:LU:196:PHE:HD2	1.84	0.42
16:LH:545:LEU:HD11	16:LH:556:LEU:HD21	2.01	0.42
17:LI:609:PRO:HB2	17:LI:612:HIS:ND1	2.34	0.42
18:LJ:240:LEU:HD21	18:LJ:243:SER:HB2	2.01	0.42
20:LM:1522:SER:HA	20:LM:1594:LEU:HD11	2.00	0.42
25:LR:237:GLU:OE1	25:LR:266:GLY:HA3	2.18	0.42
27:LT:210:ILE:HG22	27:LT:222:LEU:HD23	2.01	0.42
27:LT:901:LEU:O	27:LT:905:LEU:HB2	2.19	0.42
38:NG:42:VAL:HG13	38:NG:81:VAL:HG21	2.00	0.42
47:NT:121:CYS:HB3	47:NT:126:CYS:HB3	2.02	0.42
48:NU:5:ARG:HG2	48:NU:49:LYS:NZ	2.35	0.42
49:NW:73:TYR:O	49:NW:76:ARG:NH1	2.52	0.42
53:SC:239:GLN:O	53:SC:242:GLN:HG3	2.19	0.42
57:SI:930:ARG:NH1	63:SR:136:GLY:O	2.47	0.42
61:SP:383:THR:HG23	61:SP:384:LEU:HD22	2.01	0.42
61:SP:461:SER:H	61:SP:651:ARG:HH21	1.68	0.42
61:SP:1325:ASN:HD21	61:SP:1328:GLN:HG3	1.84	0.42
69:SY:164:ARG:HH21	69:SY:167:ASN:HB3	1.84	0.42
70:SZ:349:LYS:HB3	70:SZ:388:ARG:HD3	2.01	0.42
1:L0:856:C:H2'	1:L0:857:C:C6	2.54	0.42
2:L1:19:A:O2'	2:L1:20:G:O4'	2.37	0.42
11:LA:80:ASP:OD1	11:LA:80:ASP:N	2.53	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
19:LL:510:THR:O	19:LL:514:GLN:NE2	2.43	0.42
20:LM:698:LEU:HB2	20:LM:775:LEU:HD22	2.01	0.42
20:LM:1508:LYS:HA	20:LM:1511:ARG:HE	1.84	0.42
20:LM:1789:LEU:HA	20:LM:1792:ILE:HG22	2.00	0.42
21:LN:404:TRP:NE1	21:LN:449:SER:HB2	2.35	0.42
22:LO:800:GLU:OE2	22:LO:837:ARG:NH2	2.39	0.42
24:LQ:544:ARG:HD2	24:LQ:544:ARG:HA	1.83	0.42
24:LQ:839:PHE:O	24:LQ:843:ILE:HG12	2.20	0.42
37:NF:42:LYS:HD2	37:NF:42:LYS:HA	1.76	0.42
39:NH:153:ARG:HE	39:NH:188:ILE:HG22	1.85	0.42
39:NH:303:GLN:HG3	72:NH:3000:ATP:C2	2.55	0.42
41:NJ:125:ASP:OD1	41:NJ:152:ARG:NH2	2.52	0.42
41:NJ:266:LYS:HD2	41:NJ:461:TYR:CG	2.54	0.42
41:NJ:617:ASP:OD1	41:NJ:618:PHE:N	2.52	0.42
41:NK:280:VAL:HA	41:NK:461:TYR:HB2	2.01	0.42
41:NK:859:LEU:HD22	41:NK:898:ILE:HG12	2.01	0.42
51:SA:249:ARG:HA	51:SA:249:ARG:HD3	1.92	0.42
65:ST:702:TYR:HB3	65:ST:705:LEU:HD12	2.01	0.42
2:L1:74:G:H1’	2:L1:76:U:OP1	2.20	0.42
2:L1:639:C:H2’	2:L1:640:A:C8	2.54	0.42
2:L1:1373:C:H2’	2:L1:1374:C:H6	1.85	0.42
6:L5:99:ILE:HD13	6:L5:171:GLU:HG3	2.00	0.42
8:L7:192:PHE:CZ	45:NQ:12:PRO:HA	2.55	0.42
11:LA:95:ASP:OD1	11:LA:95:ASP:N	2.53	0.42
16:LH:96:PHE:CE1	16:LH:134:LEU:HB3	2.55	0.42
16:LH:271:VAL:HG13	16:LH:287:PRO:HA	2.02	0.42
17:LI:401:LEU:O	17:LI:405:ILE:HG13	2.19	0.42
20:LM:1265:LYS:HE2	20:LM:1265:LYS:HB3	1.76	0.42
21:LN:580:ASP:N	21:LN:580:ASP:OD1	2.52	0.42
23:LP:14:PRO:HA	23:LP:17:GLU:HG2	2.02	0.42
25:LR:160:HIS:HB2	25:LR:169:PHE:HE2	1.84	0.42
27:LT:669:VAL:HG23	27:LT:680:THR:HG22	2.02	0.42
28:LU:71:CYS:HB3	28:LU:115:ILE:HG22	2.01	0.42
36:NE:176:HIS:CE1	36:NE:180:ILE:HD11	2.55	0.42
39:NH:228:THR:HB	39:NH:236:SER:HB3	2.01	0.42
53:SC:137:TRP:CE2	53:SC:145:ALA:HB2	2.55	0.42
55:SG:168:CYS:HB2	55:SG:186:ARG:HB2	2.01	0.42
61:SP:746:HIS:O	61:SP:750:MET:HG2	2.19	0.42
65:ST:212:UNK:O	65:ST:216:UNK:N	2.52	0.42
67:SW:213:GLY:N	67:SW:218:ILE:HD11	2.34	0.42
2:L1:675:U:H2’	2:L1:676:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:951:C:H2'	2:L1:952:G:H8	1.84	0.42
20:LM:913:ALA:O	20:LM:950:SER:OG	2.25	0.42
20:LM:1283:PHE:HE2	20:LM:1285:VAL:HG22	1.83	0.42
20:LM:1562:ALA:HB1	20:LM:1612:LEU:HD12	2.02	0.42
20:LM:1966:LEU:O	20:LM:2026:GLN:NE2	2.51	0.42
20:LM:2036:LYS:NZ	20:LM:2040:ARG:HB2	2.34	0.42
20:LM:2066:ASN:ND2	20:LM:2102:LEU:HB3	2.35	0.42
21:LN:677:PRO:HB3	35:ND:206:THR:O	2.19	0.42
22:LO:91:HIS:ND1	22:LO:133:ALA:HB2	2.34	0.42
24:LQ:154:GLN:HG2	24:LQ:197:LEU:HB3	2.02	0.42
26:LS:474:THR:HG21	26:LS:494:LYS:HB2	2.02	0.42
30:LZ:31:LEU:HD23	30:LZ:34:LEU:HD12	2.01	0.42
39:NH:102:LYS:HE3	39:NH:102:LYS:HB2	1.90	0.42
41:NK:635:TYR:HB3	41:NK:640:TYR:HE2	1.85	0.42
52:SB:194:LEU:HD12	52:SB:194:LEU:HA	1.93	0.42
53:SC:97:PHE:HB2	53:SC:107:VAL:HG23	2.02	0.42
55:SG:363:GLU:HG2	55:SG:376:PRO:HB3	2.01	0.42
57:SI:1235:GLU:HG3	57:SI:1238:ARG:HH21	1.84	0.42
58:SK:85:PRO:HG2	58:SK:130:PHE:HZ	1.84	0.42
61:SP:435:ASP:HB3	61:SP:438:VAL:HG12	2.01	0.42
61:SP:1610:GLN:HA	61:SP:1614:MET:CE	2.50	0.42
61:SP:1906:HIS:HB2	61:SP:1960:LYS:HB3	2.01	0.42
3:L2:46:A:O2'	59:SL:22:GLN:NE2	2.51	0.42
6:L5:26:ASP:OD1	6:L5:27:ASP:N	2.52	0.42
13:LD:80:MET:HA	13:LD:86:ILE:HG22	2.01	0.42
19:LL:272:TYR:HB3	19:LL:290:VAL:HB	2.01	0.42
19:LL:319:ILE:HG22	19:LL:333:ILE:HD12	2.01	0.42
20:LM:610:ASN:ND2	20:LM:702:VAL:HG21	2.35	0.42
20:LM:943:GLN:HG2	20:LM:960:ILE:HG23	2.02	0.42
20:LM:1279:ASP:HB3	20:LM:1282:LYS:HE2	2.02	0.42
20:LM:1376:VAL:O	20:LM:1380:ILE:HG12	2.19	0.42
21:LN:608:ASP:OD2	21:LN:611:LEU:N	2.50	0.42
24:LQ:201:SER:HB3	24:LQ:205:ARG:HG3	2.02	0.42
25:LR:19:ARG:NE	25:LR:364:LEU:O	2.41	0.42
34:NC:203:SER:O	34:NC:207:ARG:HG3	2.20	0.42
46:NR:317:UNK:O	46:NR:321:UNK:N	2.52	0.42
52:SB:63:LEU:O	52:SB:94:LEU:HD21	2.19	0.42
52:SB:346:LEU:HD12	52:SB:362:LEU:HD13	2.02	0.42
52:SB:362:LEU:O	52:SB:366:THR:OG1	2.24	0.42
69:SY:233:LYS:HG2	69:SY:245:TYR:HE1	1.84	0.42
2:L1:1219:C:OP1	6:L5:127:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:27:ALA:O	4:L3:31:THR:HG23	2.20	0.42
16:LH:529:TRP:CE3	16:LH:529:TRP:HA	2.55	0.42
16:LH:741:LEU:HD23	20:LM:218:ALA:HB1	2.01	0.42
19:LK:466:LEU:HD13	19:LK:481:VAL:HG11	2.01	0.42
20:LM:2069:ILE:O	20:LM:2073:THR:HG23	2.20	0.42
22:LO:552:ARG:HH21	22:LO:556:ALA:HB3	1.85	0.42
24:LQ:631:ALA:HA	24:LQ:660:TRP:CZ2	2.54	0.42
27:LT:667:LEU:HD23	27:LT:667:LEU:HA	1.87	0.42
28:LU:283:SER:HB2	28:LU:303:ASP:H	1.85	0.42
36:NE:282:ASP:O	36:NE:286:ILE:HG13	2.20	0.42
46:NR:880:UNK:O	46:NR:884:UNK:N	2.53	0.42
53:SC:292:LYS:HE2	53:SC:315:PRO:HG3	2.02	0.42
61:SP:751:GLU:OE1	61:SP:754:GLN:N	2.46	0.42
61:SP:1471:LEU:O	61:SP:1475:MET:HG2	2.19	0.42
61:SP:1580:HIS:CG	61:SP:1585:ARG:HD3	2.55	0.42
61:SP:1831:MET:HE2	61:SP:1839:MET:HA	2.01	0.42
1:L0:453:U:H2’	1:L0:454:C:C6	2.55	0.42
2:L1:1667:U:H5’	60:SM:142:HIS:HA	2.00	0.42
11:LA:82:ASN:HA	11:LA:85:LEU:HD12	2.02	0.42
22:LO:674:GLN:O	22:LO:678:GLN:HG2	2.20	0.42
23:LP:571:TRP:HZ3	52:SB:392:GLU:HG2	1.84	0.42
25:LR:89:LEU:HD22	25:LR:103:LEU:HD21	2.01	0.42
27:LT:637:LEU:HB2	27:LT:651:LEU:HD11	2.02	0.42
29:LW:141:GLU:HG2	64:SS:715:LYS:HE2	2.02	0.42
36:NE:278:LEU:HB2	44:NO:77:PRO:HG2	2.01	0.42
41:NK:414:ASN:HB2	41:NK:488:ASP:HA	2.01	0.42
53:SC:92:ARG:NH2	53:SC:153:ASP:OD1	2.52	0.42
53:SC:304:ARG:O	53:SC:306:HIS:ND1	2.47	0.42
55:SG:125:LYS:H	55:SG:125:LYS:HD2	1.83	0.42
57:SI:1236:HIS:O	57:SI:1240:LYS:HG2	2.20	0.42
58:SK:224:LEU:HD23	58:SK:228:LEU:HG	2.00	0.42
59:SL:140:TYR:CZ	59:SL:142:ASP:HB2	2.55	0.42
64:SS:169:ALA:HA	64:SS:170:PRO:HD3	1.86	0.42
67:SW:86:THR:OG1	67:SW:87:PRO:HD3	2.20	0.42
2:L1:29:G:H2’	2:L1:30:C:C6	2.55	0.41
2:L1:607:U:OP1	57:SI:1099:ARG:NH1	2.53	0.41
2:L1:1102:G:H2’	2:L1:1103:C:C6	2.55	0.41
17:LI:701:LEU:HD21	19:LL:574:LEU:HG	2.01	0.41
20:LM:850:LYS:O	20:LM:854:LYS:HG2	2.20	0.41
21:LN:592:ARG:NH2	21:LN:658:GLU:OE2	2.53	0.41
22:LO:42:LEU:HD11	22:LO:367:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LO:112:VAL:HG22	22:LO:121:MET:HG3	2.02	0.41
22:LO:681:GLY:O	22:LO:683:ALA:N	2.49	0.41
24:LQ:459:CYS:O	24:LQ:472:GLY:N	2.47	0.41
27:LT:769:ASP:HA	27:LT:772:LYS:NZ	2.35	0.41
29:LW:240:ARG:NH2	29:LW:256:ASN:OD1	2.53	0.41
57:SI:260:ARG:HD3	57:SI:338:PRO:HB2	2.01	0.41
57:SI:1274:LEU:HA	57:SI:1274:LEU:HD12	1.87	0.41
59:SL:78:PHE:CD1	59:SL:160:VAL:HG21	2.55	0.41
61:SP:1395:ALA:HA	61:SP:1398:PHE:CE2	2.55	0.41
65:ST:579:LYS:O	65:ST:579:LYS:HG2	2.20	0.41
67:SW:89:LYS:HD3	67:SW:89:LYS:HA	1.89	0.41
67:SW:154:ARG:HG3	67:SW:155:LEU:HD12	2.02	0.41
2:L1:1267:C:H2'	2:L1:1268:C:C6	2.55	0.41
2:L1:1269:G:H2'	2:L1:1270:G:C8	2.54	0.41
2:L1:1495:G:OP1	70:SZ:301:THR:OG1	2.26	0.41
3:L2:109:C:N4	33:NB:457:GLU:HG2	2.36	0.41
3:L2:145:U:O2'	3:L2:146:G:OP2	2.31	0.41
8:L7:15:LYS:HE2	8:L7:15:LYS:HB3	1.79	0.41
9:L8:106:SER:HB3	9:L8:171:LEU:HG	2.02	0.41
16:LH:240:THR:HG21	21:LN:264:GLN:HE22	1.85	0.41
17:LI:216:ILE:HD11	17:LI:234:ILE:HG13	2.01	0.41
19:LL:528:LYS:O	19:LL:532:THR:OG1	2.10	0.41
19:LL:601:GLU:OE1	21:LN:416:TYR:OH	2.26	0.41
20:LM:374:ILE:HD12	20:LM:374:ILE:HA	1.94	0.41
20:LM:630:ILE:HD12	20:LM:630:ILE:H	1.86	0.41
24:LQ:115:TYR:HE1	24:LQ:136:VAL:HG21	1.86	0.41
24:LQ:207:ILE:HG13	24:LQ:217:VAL:HG23	2.01	0.41
28:LU:304:LYS:HG2	28:LU:326:GLN:HA	2.01	0.41
28:LU:397:PRO:HD2	28:LU:400:ILE:HD12	2.02	0.41
28:LU:405:GLN:O	28:LU:409:ILE:HG12	2.20	0.41
35:ND:194:ILE:HD12	35:ND:194:ILE:HA	1.88	0.41
41:NK:157:LEU:HB3	41:NK:188:ILE:HD13	2.02	0.41
44:NO:32:LYS:O	44:NO:36:ARG:HG3	2.21	0.41
52:SB:351:SER:HB3	62:SQ:617:HIS:CG	2.55	0.41
57:SI:922:VAL:HG22	57:SI:1017:LEU:HD23	2.02	0.41
57:SI:1131:THR:HG22	57:SI:1134:GLN:HG3	2.01	0.41
58:SK:149:ALA:HB2	65:ST:769:ARG:HA	2.01	0.41
61:SP:736:TRP:O	61:SP:740:ILE:HG12	2.20	0.41
1:L0:742:G:H3'	1:L0:743:G:H8	1.85	0.41
1:L0:858:C:P	30:LZ:53:ARG:HH22	2.43	0.41
2:L1:941:C:H2'	2:L1:942:G:C8	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:221:LYS:HD2	7:L6:224:ARG:HH11	1.85	0.41
18:LJ:442:ALA:HA	18:LJ:445:ILE:HG12	2.02	0.41
19:LL:169:SER:HG	19:LL:188:ARG:HH12	1.66	0.41
20:LM:1082:LEU:HD21	20:LM:1126:LYS:HD3	2.01	0.41
20:LM:1601:ILE:O	20:LM:1604:ILE:HG22	2.20	0.41
22:LO:114:THR:HB	22:LO:147:THR:OG1	2.20	0.41
22:LO:143:PRO:HG3	22:LO:169:TRP:CD1	2.55	0.41
22:LO:283:ASN:HD21	22:LO:289:ASN:HB3	1.84	0.41
23:LP:368:SER:OG	23:LP:369:GLU:N	2.53	0.41
24:LQ:716:GLU:HA	24:LQ:719:ARG:HD2	2.02	0.41
25:LR:156:LEU:HB3	25:LR:171:SER:HB3	2.01	0.41
27:LT:399:SER:OG	27:LT:400:GLN:N	2.54	0.41
27:LT:879:MET:O	27:LT:883:MET:HG3	2.21	0.41
34:NC:269:LEU:HD22	34:NC:272:LEU:HD11	2.02	0.41
36:NE:183:TYR:HB3	36:NE:187:LYS:HB2	2.02	0.41
39:NH:472:HIS:CE1	39:NH:556:LEU:HD11	2.55	0.41
53:SC:238:ALA:H	53:SC:242:GLN:HE21	1.68	0.41
54:SE:25:LEU:HD22	54:SE:119:ILE:HG13	2.02	0.41
61:SP:1356:LEU:HG	61:SP:1373:ILE:HG23	2.01	0.41
65:ST:558:THR:OG1	65:ST:559:SER:N	2.52	0.41
65:ST:570:LEU:HD11	66:SU:445:TYR:HB2	2.01	0.41
66:SU:261:LYS:HG2	66:SU:262:HIS:HD2	1.85	0.41
2:L1:1314:U:O2'	70:SZ:281:PHE:O	2.32	0.41
19:LL:596:LYS:HZ1	21:LN:382:LEU:HA	1.86	0.41
20:LM:523:LEU:HD23	20:LM:523:LEU:HA	1.88	0.41
20:LM:539:SER:O	20:LM:542:GLU:HG3	2.21	0.41
20:LM:1898:ASP:HA	20:LM:1901:VAL:HG22	2.02	0.41
21:LN:22:VAL:HG12	21:LN:33:VAL:HG22	2.02	0.41
21:LN:338:ILE:HG12	21:LN:349:PHE:CD1	2.55	0.41
22:LO:561:ALA:HB2	22:LO:611:LEU:HD11	2.01	0.41
25:LR:59:ARG:NH2	25:LR:96:GLN:O	2.53	0.41
28:LU:326:GLN:HE22	59:SL:114:GLY:HA2	1.85	0.41
29:LW:176:ILE:O	29:LW:180:VAL:HG23	2.20	0.41
41:NK:283:THR:HG22	41:NK:411:SER:HB2	2.02	0.41
41:NK:337:GLU:HA	41:NK:341:TYR:CZ	2.55	0.41
42:NM:62:LEU:HD12	42:NM:62:LEU:HA	1.92	0.41
51:SA:252:MET:HB3	53:SC:205:LYS:HG2	2.02	0.41
53:SC:200:LEU:O	53:SC:204:ALA:N	2.48	0.41
54:SE:20:LYS:HA	54:SE:20:LYS:HD2	1.91	0.41
55:SG:368:ARG:HB3	55:SG:377:PHE:CZ	2.55	0.41
56:SH:191:ILE:HB	56:SH:223:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SI:391:ARG:HA	57:SI:402:GLY:HA3	2.02	0.41
57:SI:925:ARG:HB2	57:SI:1015:LEU:HD11	2.03	0.41
58:SK:173:LYS:HD2	58:SK:212:TYR:CD2	2.55	0.41
61:SP:74:LYS:HD2	61:SP:84:HIS:HB3	2.01	0.41
61:SP:1524:GLU:HG3	61:SP:1528:LYS:NZ	2.35	0.41
61:SP:1878:VAL:HG12	61:SP:1912:LEU:HD13	2.02	0.41
65:ST:726:CYS:SG	65:ST:728:HIS:NE2	2.92	0.41
69:SY:3:ALA:HA	69:SY:6:ARG:HE	1.85	0.41
2:L1:71:G:H2’	2:L1:72:C:O4’	2.20	0.41
2:L1:438:G:N2	49:NW:125:SER:OG	2.53	0.41
2:L1:1740:C:H2’	2:L1:1741:U:H6	1.85	0.41
6:L5:40:ALA:HB1	6:L5:45:TYR:CG	2.56	0.41
12:LC:81:ILE:O	12:LC:85:ARG:HG3	2.21	0.41
19:LL:54:PRO:HG2	19:LL:57:HIS:HB3	2.02	0.41
20:LM:665:ILE:HA	20:LM:710:VAL:HG12	2.03	0.41
22:LO:379:LEU:HD22	22:LO:720:THR:HG23	2.02	0.41
24:LQ:9:ARG:HA	24:LQ:669:GLN:NE2	2.35	0.41
25:LR:245:LEU:HD12	25:LR:261:TYR:HB3	2.02	0.41
26:LS:253:ARG:HB3	26:LS:271:LEU:HG	2.02	0.41
32:NA:418:THR:HG22	32:NA:421:THR:HG23	2.03	0.41
39:NH:425:LEU:HD12	72:NH:3000:ATP:N1	2.35	0.41
46:NR:249:UNK:O	46:NR:253:UNK:N	2.53	0.41
52:SB:11:TYR:HE1	52:SB:63:LEU:HD11	1.85	0.41
53:SD:312:VAL:HG13	53:SD:315:PRO:HG3	2.02	0.41
57:SI:320:PRO:HB3	57:SI:332:GLU:OE1	2.19	0.41
57:SI:1022:LYS:NZ	65:ST:78:ASP:OD2	2.53	0.41
58:SK:147:ARG:HG2	58:SK:154:LYS:HD3	2.02	0.41
59:SL:132:LEU:HA	59:SL:133:PRO:HD3	1.90	0.41
60:SM:165:CYS:HB2	60:SM:252:GLU:HB2	2.01	0.41
1:L0:614:U:H2’	1:L0:615:C:C6	2.55	0.41
2:L1:373:G:H2’	2:L1:374:G:H8	1.85	0.41
2:L1:496:C:H2’	2:L1:497:C:H6	1.86	0.41
2:L1:979:C:H2’	2:L1:980:A:C8	2.56	0.41
2:L1:1702:G:N1	25:LR:725:SER:OG	2.51	0.41
14:LF:80:ASP:OD1	14:LF:81:TYR:N	2.52	0.41
16:LH:129:LEU:HB2	16:LH:154:ILE:HD13	2.03	0.41
18:LJ:158:LEU:HD23	18:LJ:159:THR:N	2.36	0.41
20:LM:496:ILE:HA	20:LM:499:MET:HE2	2.02	0.41
20:LM:794:LYS:HB3	20:LM:794:LYS:HE3	1.89	0.41
20:LM:827:HIS:CD2	20:LM:883:CYS:HB3	2.56	0.41
20:LM:958:HIS:O	20:LM:961:SER:OG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LM:1387:LEU:HD23	20:LM:1395:ARG:HD2	2.01	0.41
21:LN:316:GLU:HG2	21:LN:317:LYS:HG3	2.03	0.41
41:NJ:172:ARG:HE	41:NJ:172:ARG:HB3	1.76	0.41
41:NJ:884:ILE:HG22	41:NJ:886:LEU:H	1.85	0.41
41:NK:849:TYR:CZ	41:NK:859:LEU:HD12	2.55	0.41
52:SB:329:LEU:HD23	52:SB:329:LEU:HA	1.89	0.41
61:SP:965:HIS:CD2	61:SP:967:HIS:H	2.39	0.41
61:SP:1370:GLU:CD	61:SP:1403:ASN:HD22	2.23	0.41
63:SR:38:ALA:O	65:ST:850:LEU:HD23	2.21	0.41
2:L1:1091:C:H2'	2:L1:1092:G:H8	1.86	0.41
2:L1:1313:A:H4'	2:L1:1314:U:O4'	2.20	0.41
3:L2:100:U:H2'	3:L2:101:C:H6	1.85	0.41
3:L2:121:U:H1'	3:L2:153:G:N2	2.35	0.41
11:LA:25:ALA:HB3	11:LA:31:LEU:HD12	2.03	0.41
14:LF:79:LEU:HG	14:LF:83:LYS:HE3	2.01	0.41
15:LG:39:SER:HB3	24:LQ:865:GLY:HA3	2.03	0.41
16:LH:58:ASN:HD22	16:LH:78:LEU:HB2	1.85	0.41
16:LH:271:VAL:HG22	16:LH:287:PRO:HA	2.02	0.41
16:LH:551:THR:HB	17:LI:295:GLN:HE21	1.86	0.41
19:LL:367:ARG:H	19:LL:367:ARG:HD3	1.85	0.41
20:LM:1408:ALA:HB1	20:LM:1412:LEU:HB2	2.02	0.41
20:LM:1969:VAL:HG12	20:LM:2029:ASN:HD21	1.84	0.41
22:LO:43:LYS:HG3	67:SW:252:PHE:CE2	2.56	0.41
22:LO:551:PHE:CE1	22:LO:558:LEU:HD12	2.56	0.41
25:LR:608:VAL:HA	25:LR:624:ALA:HA	2.02	0.41
27:LT:255:GLN:NE2	27:LT:261:VAL:O	2.54	0.41
27:LT:797:LEU:HB2	67:SW:251:ARG:NE	2.35	0.41
32:NA:398:ASN:HB3	32:NA:401:LEU:HD12	2.02	0.41
49:NW:142:TYR:HD1	49:NW:149:LEU:HB2	1.85	0.41
49:NW:254:LEU:HG	49:NW:266:VAL:HG12	2.02	0.41
75:SJ:301:SAH:H8	75:SJ:301:SAH:SD	2.61	0.41
61:SP:1510:THR:HG23	61:SP:1513:ASP:H	1.86	0.41
61:SP:1876:LEU:HB3	61:SP:1880:PHE:CD2	2.55	0.41
61:SP:2096:LYS:HB2	61:SP:2139:TRP:CZ3	2.55	0.41
69:SY:94:LEU:HG	69:SY:98:ARG:HE	1.84	0.41
70:SZ:361:VAL:HG12	70:SZ:365:LEU:HD23	2.02	0.41
1:L0:745:U:O2'	1:L0:746:G:H5"	2.20	0.41
1:L0:754:G:H2'	1:L0:755:C:C5	2.55	0.41
2:L1:110:U:H2'	2:L1:111:A:H8	1.86	0.41
2:L1:1296:U:H2'	2:L1:1297:U:O4'	2.21	0.41
2:L1:1768:A:H2'	2:L1:1769:C:H4'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:25:LYS:HA	4:L3:55:ARG:HA	2.02	0.41
7:L6:32:MET:SD	7:L6:54:GLY:HA2	2.61	0.41
13:LD:24:LEU:HD23	13:LD:24:LEU:HA	1.91	0.41
17:LI:473:LEU:HD21	17:LI:485:LEU:HD21	2.03	0.41
20:LM:380:GLU:O	20:LM:384:THR:HG23	2.20	0.41
20:LM:1310:THR:O	20:LM:1314:ILE:HG12	2.20	0.41
20:LM:2030:ARG:NH2	20:LM:2080:VAL:HG13	2.35	0.41
21:LN:269:THR:OG1	21:LN:271:ASN:OD1	2.29	0.41
22:LO:305:THR:O	22:LO:312:PHE:HA	2.21	0.41
24:LQ:416:SER:OG	24:LQ:417:ASP:N	2.53	0.41
26:LS:194:PRO:HG2	26:LS:197:ALA:HB2	2.03	0.41
27:LT:545:VAL:HG12	27:LT:556:THR:HG22	2.03	0.41
28:LU:75:HIS:HD2	28:LU:78:LYS:N	2.19	0.41
28:LU:263:LEU:HD13	28:LU:297:PHE:HE1	1.86	0.41
32:NA:592:LYS:HA	32:NA:595:ARG:NH1	2.35	0.41
41:NJ:502:PRO:HA	41:NJ:643:ARG:HD3	2.02	0.41
41:NK:833:VAL:HG23	41:NK:834:ASP:OD1	2.20	0.41
52:SB:44:LEU:HD23	52:SB:44:LEU:HA	1.80	0.41
75:SJ:301:SAH:HG2	75:SJ:301:SAH:H3’	2.03	0.41
2:L1:22:A:H61	2:L1:652:U:H3	1.68	0.41
2:L1:61:A:HO2’	2:L1:315:C:HO2’	1.65	0.41
2:L1:1233:G:H2’	2:L1:1234:C:C6	2.56	0.41
3:L2:106:G:N2	3:L2:167:U:OP2	2.45	0.41
7:L6:7:PHE:O	7:L6:11:GLY:N	2.53	0.41
7:L6:135:PRO:HG2	7:L6:141:ILE:HG12	2.03	0.41
9:L8:121:LEU:HD21	9:L8:166:PHE:CG	2.55	0.41
10:L9:110:LEU:HB2	10:L9:147:PHE:HB3	2.01	0.41
13:LD:13:GLN:NE2	13:LD:36:TYR:HB3	2.36	0.41
16:LH:203:LYS:H	16:LH:224:ASP:HB3	1.85	0.41
18:LJ:479:GLU:OE1	19:LL:525:GLN:NE2	2.54	0.41
19:LL:140:CYS:SG	19:LL:161:LYS:NZ	2.70	0.41
20:LM:147:VAL:HA	20:LM:150:LEU:HD12	2.03	0.41
20:LM:679:SER:O	20:LM:683:MET:HG2	2.20	0.41
20:LM:1151:PHE:CE2	20:LM:1213:LEU:HB3	2.56	0.41
20:LM:1384:VAL:O	20:LM:1388:PRO:HD3	2.20	0.41
20:LM:1555:LEU:HD23	20:LM:1558:ILE:HD11	2.02	0.41
20:LM:1675:LYS:HG3	20:LM:1717:CYS:SG	2.61	0.41
20:LM:2039:GLU:HB3	20:LM:2043:LYS:HZ1	1.86	0.41
20:LM:2050:ALA:HB1	20:LM:2094:LYS:HG3	2.02	0.41
20:LM:2077:SER:O	20:LM:2081:ARG:HG3	2.21	0.41
21:LN:139:ARG:NH2	21:LN:173:VAL:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LN:165:ILE:H	21:LN:165:ILE:HD12	1.86	0.41
21:LN:339:SER:HB2	21:LN:398:ILE:HG22	2.03	0.41
21:LN:388:LYS:HE2	21:LN:388:LYS:HB2	1.78	0.41
22:LO:312:PHE:CE1	22:LO:326:LEU:HB2	2.55	0.41
22:LO:415:SER:OG	22:LO:436:ASP:OD1	2.27	0.41
23:LP:454:GLN:O	23:LP:457:THR:OG1	2.31	0.41
25:LR:23:PRO:HG3	25:LR:627:SER:OG	2.21	0.41
27:LT:178:VAL:HG22	27:LT:184:LEU:HD12	2.03	0.41
27:LT:738:LEU:HD13	27:LT:740:GLU:HG3	2.02	0.41
27:LT:770:VAL:HG12	32:NA:533:ILE:HB	2.02	0.41
27:LT:909:PRO:HA	27:LT:915:LEU:HD21	2.02	0.41
28:LU:40:GLU:OE2	64:SS:704:GLY:N	2.54	0.41
28:LU:165:HIS:N	28:LU:170:VAL:O	2.43	0.41
29:LW:167:ASP:HB3	29:LW:170:LYS:HE2	2.03	0.41
33:NB:465:LEU:HD12	53:SD:103:GLU:OE2	2.21	0.41
39:NH:107:ALA:HA	39:NH:110:ARG:HE	1.86	0.41
39:NH:314:LEU:HD12	39:NH:318:LEU:HD13	2.03	0.41
39:NH:507:LEU:HD23	39:NH:507:LEU:HA	1.90	0.41
41:NJ:234:GLU:HB2	41:NJ:258:LEU:HD22	2.03	0.41
41:NJ:843:PRO:HD3	41:NK:781:TYR:OH	2.20	0.41
41:NK:6:VAL:HG12	41:NK:204:LEU:HG	2.03	0.41
41:NK:25:LEU:HD23	41:NK:197:CYS:SG	2.61	0.41
41:NK:688:ARG:O	41:NK:691:LEU:HD22	2.21	0.41
41:NK:866:LEU:HD21	41:NK:895:PHE:HB2	2.02	0.41
44:NO:119:LYS:HA	44:NO:119:LYS:HD3	1.84	0.41
46:NR:541:UNK:O	46:NR:545:UNK:N	2.54	0.41
51:SA:197:PHE:CD2	51:SA:200:LEU:HB2	2.56	0.41
51:SA:365:LYS:HB2	51:SA:365:LYS:HE2	1.83	0.41
53:SC:201:ILE:HG22	53:SC:205:LYS:HE3	2.03	0.41
55:SG:130:GLU:OE1	55:SG:466:ARG:NH2	2.54	0.41
57:SI:1000:SER:HB2	57:SI:1125:THR:HA	2.03	0.41
61:SP:1609:LEU:HD22	61:SP:1643:ILE:HD12	2.03	0.41
61:SP:1925:LEU:HD23	61:SP:1976:GLN:HE21	1.85	0.41
61:SP:2005:ARG:O	61:SP:2008:THR:OG1	2.31	0.41
61:SP:2112:ASP:HB3	61:SP:2113:PRO:HD3	2.02	0.41
67:SW:251:ARG:HD3	67:SW:251:ARG:O	2.21	0.41
2:L1:530:U:H2'	2:L1:531:A:C8	2.55	0.41
2:L1:596:U:H2'	2:L1:597:G:C8	2.56	0.41
2:L1:1336:C:H2'	2:L1:1337:C:H6	1.85	0.41
2:L1:1658:G:H2'	57:SI:1037:PHE:HB3	2.02	0.41
2:L1:1814:G:H2'	2:L1:1815:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:51:ASP:OD1	4:L3:51:ASP:N	2.53	0.41
16:LH:100:CYS:SG	16:LH:101:LYS:N	2.94	0.41
17:LI:616:PHE:HD2	17:LI:653:LEU:HD11	1.86	0.41
18:LJ:467:GLN:HA	19:LL:572:LEU:HD13	2.03	0.41
20:LM:1564:SER:O	20:LM:1567:ARG:HG2	2.21	0.41
20:LM:1741:LEU:HD23	20:LM:1741:LEU:HA	1.92	0.41
21:LN:84:MET:HG2	21:LN:96:ALA:HB2	2.04	0.41
22:LO:378:ALA:HB1	22:LO:421:VAL:HG22	2.02	0.41
22:LO:686:LEU:HD12	22:LO:687:PRO:HD2	2.03	0.41
23:LP:327:LYS:HA	23:LP:330:ILE:HG12	2.03	0.41
24:LQ:634:ASP:OD1	24:LQ:635:SER:N	2.46	0.41
29:LW:203:TYR:CE1	29:LW:210:LEU:HD12	2.56	0.41
39:NH:342:LYS:HA	39:NH:342:LYS:HD2	1.78	0.41
46:NR:463:UNK:O	46:NR:467:UNK:N	2.54	0.41
49:NW:170:ASN:HA	49:NW:171:PRO:HD3	1.95	0.41
51:SA:286:ARG:NH1	51:SA:302:GLU:OE1	2.54	0.41
51:SA:325:THR:HA	51:SA:328:ILE:HD12	2.03	0.41
52:SB:226:LEU:HD21	52:SB:230:VAL:HG12	2.03	0.41
57:SI:138:ASN:HB3	57:SI:950:ARG:HH12	1.86	0.41
58:SK:107:GLN:NE2	58:SK:120:VAL:O	2.53	0.41
60:SM:166:ASN:O	60:SM:251:PHE:HA	2.20	0.41
61:SP:105:GLN:HB3	61:SP:106:PRO:HD3	2.02	0.41
61:SP:1858:ALA:HB3	61:SP:1861:ILE:HG12	2.03	0.41
65:ST:567:THR:OG1	65:ST:568:PRO:HD3	2.20	0.41
65:ST:570:LEU:HD21	66:SU:445:TYR:CD2	2.55	0.41
65:ST:614:ASN:HB3	65:ST:635:VAL:HG21	2.02	0.41
66:SU:272:VAL:HG13	66:SU:273:LEU:HD12	2.02	0.41
2:L1:115:U:H2’	2:L1:116:U:C6	2.56	0.40
2:L1:181:A:H2’	2:L1:182:C:C6	2.56	0.40
2:L1:543:C:OP2	57:SI:1233:ASN:ND2	2.53	0.40
2:L1:627:U:OP1	57:SI:1136:ARG:NH2	2.41	0.40
3:L2:177:C:H2’	3:L2:178:G:O4’	2.21	0.40
18:LJ:274:VAL:HB	18:LJ:284:HIS:HB3	2.02	0.40
21:LN:648:LYS:HB2	21:LN:649:PRO:HD3	2.03	0.40
23:LP:228:ASN:O	23:LP:232:ILE:HG12	2.21	0.40
24:LQ:161:LYS:HE3	24:LQ:161:LYS:HB3	1.89	0.40
24:LQ:942:LEU:HD21	32:NA:451:ALA:HB2	2.03	0.40
25:LR:296:THR:HG23	25:LR:297:HIS:ND1	2.36	0.40
25:LR:366:THR:O	25:LR:367:SER:OG	2.30	0.40
27:LT:581:SER:HB3	27:LT:599:LEU:HB3	2.02	0.40
36:NE:171:ALA:HB1	50:NY:220:LYS:HG3	2.02	0.40

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
38:NG:113:GLN:HE21	38:NG:117:ARG:HH21	1.67	0.40
41:NJ:372:HIS:CG	41:NJ:373:PRO:HD2	2.56	0.40
41:NJ:739:ASP:OD1	41:NJ:739:ASP:N	2.53	0.40
41:NK:168:HIS:NE2	41:NK:550:ASP:OD2	2.52	0.40
49:NW:129:TYR:CE2	49:NW:131:THR:HB	2.56	0.40
50:NY:214:HIS:CE1	50:NY:216:ILE:HG12	2.56	0.40
51:SA:20:LYS:HB3	51:SA:20:LYS:HE2	1.72	0.40
61:SP:35:ASP:OD1	61:SP:35:ASP:N	2.45	0.40
61:SP:1925:LEU:HD22	61:SP:1976:GLN:HG3	2.02	0.40
65:ST:70:LEU:HD12	65:ST:813:PHE:CD2	2.57	0.40
65:ST:579:LYS:HE3	65:ST:579:LYS:HB3	1.87	0.40
70:SZ:240:ASN:O	70:SZ:241:LEU:HG	2.21	0.40
2:L1:12:U:H2’	2:L1:13:C:H6	1.86	0.40
2:L1:235:A:C4	2:L1:236:A:C8	3.09	0.40
2:L1:370:G:N7	43:NN:511:LYS:HE3	2.36	0.40
2:L1:1490:G:H2’	2:L1:1490:G:N3	2.36	0.40
5:L4:173:ILE:HD11	5:L4:235:TRP:CD2	2.56	0.40
17:LI:264:ALA:HB3	17:LI:311:LEU:HD13	2.03	0.40
18:LJ:62:ILE:HD13	18:LJ:86:ALA:HB2	2.04	0.40
20:LM:371:ASP:O	20:LM:374:ILE:HG22	2.21	0.40
20:LM:712:VAL:HG12	20:LM:795:LYS:HD2	2.02	0.40
20:LM:1819:PRO:O	20:LM:1823:LEU:HG	2.20	0.40
24:LQ:914:GLU:OE2	67:SW:242:ARG:NH2	2.54	0.40
32:NA:456:LYS:HE2	32:NA:456:LYS:HB2	1.85	0.40
39:NH:144:VAL:HB	39:NH:145:PRO:HD3	2.03	0.40
41:NJ:397:LEU:HD12	41:NJ:397:LEU:HA	1.94	0.40
41:NK:559:LEU:HD23	41:NK:644:ALA:HB2	2.02	0.40
41:NK:587:ARG:HG2	41:NK:587:ARG:HH11	1.86	0.40
46:NR:137:UNK:O	46:NR:141:UNK:N	2.54	0.40
46:NR:985:UNK:O	46:NR:989:UNK:N	2.55	0.40
53:SC:143:LYS:HZ1	53:SC:306:HIS:HD2	1.67	0.40
57:SI:114:ILE:HA	57:SI:340:SER:OG	2.21	0.40
61:SP:503:ILE:HD13	61:SP:517:GLN:HB3	2.02	0.40
61:SP:1596:GLN:HB3	61:SP:1602:VAL:HG12	2.03	0.40
70:SZ:243:GLU:O	70:SZ:247:GLN:HG3	2.21	0.40
1:L0:732:G:O2’	1:L0:733:C:OP1	2.34	0.40
2:L1:1023:A:OP2	37:NF:124:ARG:NH1	2.55	0.40
2:L1:1736:G:H2’	2:L1:1737:G:C8	2.49	0.40
10:L9:180:LYS:HE2	10:L9:180:LYS:HB3	1.69	0.40
11:LA:48:HIS:CE1	11:LA:114:TYR:HB2	2.55	0.40
16:LH:333:ASP:N	16:LH:663:GLN:HE22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:727:ILE:HA	16:LH:728:PRO:HD3	1.97	0.40
19:LK:523:MET:O	19:LK:526:TRP:HB2	2.22	0.40
20:LM:393:ASP:HB3	20:LM:439:THR:HG21	2.03	0.40
20:LM:1320:LEU:HD11	20:LM:1357:LEU:HD11	2.02	0.40
20:LM:1423:TYR:HE1	20:LM:1439:ILE:HB	1.85	0.40
22:LO:394:ASP:N	22:LO:394:ASP:OD1	2.54	0.40
23:LP:330:ILE:HG13	23:LP:331:THR:N	2.36	0.40
23:LP:387:GLU:O	23:LP:391:VAL:HG23	2.21	0.40
25:LR:145:HIS:CE1	25:LR:182:LEU:HD12	2.57	0.40
25:LR:548:TRP:CZ3	25:LR:555:CYS:HB2	2.57	0.40
26:LS:138:LYS:HD3	26:LS:138:LYS:HA	1.87	0.40
26:LS:253:ARG:HG2	26:LS:541:GLU:HA	2.04	0.40
29:LW:389:ARG:HD3	29:LW:389:ARG:HA	1.78	0.40
32:NA:570:THR:OG1	32:NA:571:ALA:N	2.53	0.40
39:NH:565:LEU:HG	39:NH:602:VAL:HG22	2.03	0.40
51:SA:228:LEU:HD22	51:SA:245:LEU:HD13	2.02	0.40
51:SA:270:ARG:HA	51:SA:270:ARG:HH11	1.85	0.40
61:SP:1583:ILE:HD12	61:SP:1583:ILE:H	1.85	0.40
61:SP:1922:ASP:OD1	61:SP:1923:SER:N	2.54	0.40
69:SY:113:ALA:HA	69:SY:116:ILE:HD12	2.04	0.40
70:SZ:184:VAL:O	70:SZ:188:VAL:HG23	2.22	0.40
1:L0:604:C:H3’	19:LL:515:GLY:HA2	2.03	0.40
2:L1:276:G:H2’	2:L1:277:C:C6	2.56	0.40
2:L1:536:A:H3’	2:L1:537:C:H6	1.86	0.40
2:L1:962:A:H2’	2:L1:963:A:O4’	2.21	0.40
2:L1:1719:A:H2’	2:L1:1720:U:O4’	2.22	0.40
6:L5:136:ARG:HG3	6:L5:203:ASN:OD1	2.20	0.40
8:L7:44:ASN:H	8:L7:68:GLN:HE22	1.70	0.40
16:LH:215:GLU:HG2	16:LH:216:ASP:N	2.37	0.40
16:LH:472:VAL:HB	16:LH:492:PHE:HB3	2.03	0.40
17:LI:659:THR:O	17:LI:663:MET:HG2	2.21	0.40
20:LM:489:HIS:HE1	20:LM:491:LEU:HB2	1.85	0.40
20:LM:1414:ILE:H	20:LM:1414:ILE:HG13	1.78	0.40
20:LM:1742:THR:O	20:LM:1745:LYS:HG2	2.21	0.40
21:LN:355:LEU:HB2	21:LN:385:LEU:HG	2.03	0.40
24:LQ:677:GLU:OE2	24:LQ:677:GLU:N	2.52	0.40
25:LR:327:GLN:OE1	25:LR:327:GLN:N	2.54	0.40
26:LS:308:GLU:HB3	26:LS:326:LEU:HD23	2.04	0.40
32:NA:397:GLU:HA	57:SI:1048:ASN:ND2	2.36	0.40
41:NK:869:GLY:HA3	41:NK:880:LEU:HD11	2.03	0.40
49:NW:157:GLU:OE2	49:NW:171:PRO:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SB:68:ILE:HD12	52:SB:101:LYS:HE3	2.04	0.40
53:SC:183:PRO:HD2	53:SC:184:ASP:N	2.37	0.40
58:SK:99:PRO:HB2	58:SK:238:GLU:OE1	2.22	0.40
61:SP:440:ASP:OD1	61:SP:441:GLU:N	2.55	0.40
61:SP:1062:GLU:OE2	61:SP:1065:ARG:NE	2.52	0.40
61:SP:1403:ASN:O	61:SP:1407:ARG:HG2	2.22	0.40
67:SW:233:PRO:HA	67:SW:234:PRO:HD3	1.96	0.40
68:SX:702:UNK:O	68:SX:706:UNK:N	2.55	0.40
69:SY:150:ASP:HB3	69:SY:153:THR:HB	2.02	0.40
2:L1:116:U:H3	2:L1:347:G:H1	1.69	0.40
2:L1:156:G:H1	2:L1:162:C:H42	1.69	0.40
2:L1:382:C:H2'	2:L1:383:G:C8	2.55	0.40
2:L1:589:G:O2'	2:L1:590:A:O5'	2.32	0.40
2:L1:1010:G:H2'	2:L1:1011:A:C8	2.56	0.40
2:L1:1290:G:H2'	2:L1:1291:A:C8	2.56	0.40
2:L1:1372:U:H2'	2:L1:1373:C:C6	2.55	0.40
4:L3:69:THR:O	4:L3:72:GLN:HG2	2.21	0.40
10:L9:27:GLN:HG3	59:SL:59:TYR:CZ	2.57	0.40
16:LH:234:TYR:CE1	21:LN:270:SER:HB2	2.56	0.40
19:LK:551:LEU:O	19:LK:555:MET:HG3	2.22	0.40
19:LL:214:LEU:HD23	19:LL:214:LEU:HA	1.97	0.40
20:LM:88:LYS:HB3	20:LM:88:LYS:HE3	1.90	0.40
20:LM:835:MET:HE3	20:LM:835:MET:HB3	1.76	0.40
20:LM:1443:ASP:HB3	20:LM:1447:TRP:CZ2	2.56	0.40
20:LM:1943:ILE:HG23	20:LM:1947:LEU:HD13	2.03	0.40
21:LN:655:LEU:HD23	21:LN:661:LEU:HG	2.04	0.40
22:LO:205:SER:OG	22:LO:213:CYS:HB3	2.20	0.40
39:NH:168:LEU:HD23	39:NH:168:LEU:HA	1.92	0.40
39:NH:1012:ILE:HD12	39:NH:1137:VAL:HG22	2.03	0.40
41:NK:126:PHE:CD2	41:NK:160:LEU:HD11	2.56	0.40
41:NK:260:GLN:HG3	41:NK:293:ALA:HB2	2.03	0.40
50:NY:310:ILE:O	50:NY:314:GLN:HG2	2.21	0.40
51:SA:308:LEU:HD23	51:SA:308:LEU:HA	1.90	0.40
52:SB:176:LEU:HD12	52:SB:176:LEU:HA	1.96	0.40
56:SH:121:THR:HG23	56:SH:165:GLY:HA3	2.03	0.40
61:SP:265:PRO:O	61:SP:269:ILE:HG13	2.21	0.40
61:SP:1456:ILE:O	61:SP:1460:ILE:HG13	2.21	0.40
64:SS:170:PRO:O	64:SS:172:GLU:N	2.46	0.40
70:SZ:179:PRO:O	70:SZ:182:LEU:HB3	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%)	84 (99%)	1 (1%)	0	100	100
5	L4	260/263 (99%)	259 (100%)	1 (0%)	0	100	100
6	L5	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
7	L6	219/249 (88%)	218 (100%)	1 (0%)	0	100	100
8	L7	164/194 (84%)	160 (98%)	4 (2%)	0	100	100
9	L8	176/208 (85%)	174 (99%)	2 (1%)	0	100	100
10	L9	169/194 (87%)	168 (99%)	1 (1%)	0	100	100
11	LA	118/132 (89%)	111 (94%)	7 (6%)	0	100	100
12	LC	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
13	LD	145/158 (92%)	141 (97%)	4 (3%)	0	100	100
14	LF	102/133 (77%)	102 (100%)	0	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	374/678 (55%)	370 (99%)	4 (1%)	0	100	100
18	LJ	465/518 (90%)	448 (96%)	17 (4%)	0	100	100
19	LK	116/677 (17%)	113 (97%)	3 (3%)	0	100	100
19	LL	500/677 (74%)	483 (97%)	17 (3%)	0	100	100
20	LM	1977/2144 (92%)	1933 (98%)	44 (2%)	0	100	100
21	LN	667/686 (97%)	647 (97%)	19 (3%)	1 (0%)	51	83
22	LO	844/919 (92%)	826 (98%)	18 (2%)	0	100	100
23	LP	559/597 (94%)	556 (100%)	3 (0%)	0	100	100
24	LQ	810/943 (86%)	792 (98%)	18 (2%)	0	100	100
25	LR	769/808 (95%)	748 (97%)	21 (3%)	0	100	100
26	LS	447/556 (80%)	440 (98%)	7 (2%)	0	100	100
27	LT	863/951 (91%)	847 (98%)	16 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	LU	443/445 (100%)	435 (98%)	8 (2%)	0	100	100
29	LW	449/610 (74%)	436 (97%)	13 (3%)	0	100	100
30	LZ	181/184 (98%)	179 (99%)	2 (1%)	0	100	100
32	NA	243/681 (36%)	242 (100%)	1 (0%)	0	100	100
33	NB	71/479 (15%)	69 (97%)	2 (3%)	0	100	100
34	NC	92/315 (29%)	90 (98%)	2 (2%)	0	100	100
35	ND	82/257 (32%)	81 (99%)	1 (1%)	0	100	100
36	NE	94/293 (32%)	94 (100%)	0	0	100	100
37	NF	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
38	NG	114/151 (76%)	113 (99%)	1 (1%)	0	100	100
39	NH	1064/1146 (93%)	1044 (98%)	20 (2%)	0	100	100
40	NI	232/280 (83%)	229 (99%)	3 (1%)	0	100	100
41	NJ	809/1025 (79%)	783 (97%)	26 (3%)	0	100	100
41	NK	801/1025 (78%)	782 (98%)	19 (2%)	0	100	100
42	NM	229/264 (87%)	226 (99%)	3 (1%)	0	100	100
43	NN	40/560 (7%)	39 (98%)	1 (2%)	0	100	100
44	NO	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
45	NQ	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
47	NT	56/156 (36%)	55 (98%)	1 (2%)	0	100	100
48	NU	58/135 (43%)	57 (98%)	1 (2%)	0	100	100
49	NW	305/688 (44%)	293 (96%)	12 (4%)	0	100	100
50	NY	270/381 (71%)	270 (100%)	0	0	100	100
51	SA	390/594 (66%)	388 (100%)	2 (0%)	0	100	100
52	SB	438/529 (83%)	437 (100%)	1 (0%)	0	100	100
53	SC	225/321 (70%)	219 (97%)	6 (3%)	0	100	100
53	SD	233/321 (73%)	227 (97%)	6 (3%)	0	100	100
54	SE	123/128 (96%)	122 (99%)	1 (1%)	0	100	100
54	SF	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
55	SG	383/475 (81%)	374 (98%)	9 (2%)	0	100	100
56	SH	366/373 (98%)	362 (99%)	4 (1%)	0	100	100
57	SI	825/1282 (64%)	812 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	SJ	202/244 (83%)	200 (99%)	2 (1%)	0	100	100
58	SK	202/244 (83%)	200 (99%)	2 (1%)	0	100	100
59	SL	190/198 (96%)	186 (98%)	4 (2%)	0	100	100
60	SM	288/291 (99%)	280 (97%)	8 (3%)	0	100	100
61	SP	1967/2785 (71%)	1933 (98%)	34 (2%)	0	100	100
62	SQ	183/756 (24%)	182 (100%)	1 (0%)	0	100	100
63	SR	106/143 (74%)	104 (98%)	2 (2%)	0	100	100
64	SS	191/771 (25%)	187 (98%)	4 (2%)	0	100	100
65	ST	432/632 (68%)	424 (98%)	8 (2%)	0	100	100
66	SU	316/472 (67%)	311 (98%)	5 (2%)	0	100	100
67	SW	178/252 (71%)	175 (98%)	3 (2%)	0	100	100
69	SY	232/253 (92%)	230 (99%)	2 (1%)	0	100	100
70	SZ	244/304 (80%)	237 (97%)	7 (3%)	0	100	100
All	All	24774/33986 (73%)	24292 (98%)	481 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	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	
4	L3	76/77 (99%)	76 (100%)	0	100	100
5	L4	224/225 (100%)	224 (100%)	0	100	100
6	L5	160/170 (94%)	160 (100%)	0	100	100
7	L6	195/218 (89%)	194 (100%)	1 (0%)	88	95
8	L7	149/174 (86%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L8	155/180 (86%)	155 (100%)	0	100	100
10	L9	152/168 (90%)	151 (99%)	1 (1%)	84	93
11	LA	102/108 (94%)	100 (98%)	2 (2%)	55	79
12	LC	114/121 (94%)	114 (100%)	0	100	100
13	LD	133/142 (94%)	131 (98%)	2 (2%)	65	84
14	LF	92/115 (80%)	92 (100%)	0	100	100
15	LG	55/62 (89%)	55 (100%)	0	100	100
16	LH	670/748 (90%)	667 (100%)	3 (0%)	91	97
17	LI	368/497 (74%)	368 (100%)	0	100	100
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	97
20	LM	1783/1943 (92%)	1779 (100%)	4 (0%)	93	98
21	LN	582/597 (98%)	582 (100%)	0	100	100
22	LO	726/783 (93%)	725 (100%)	1 (0%)	93	98
23	LP	499/527 (95%)	499 (100%)	0	100	100
24	LQ	690/828 (83%)	690 (100%)	0	100	100
25	LR	648/672 (96%)	648 (100%)	0	100	100
26	LS	393/476 (83%)	392 (100%)	1 (0%)	92	97
27	LT	744/823 (90%)	743 (100%)	1 (0%)	93	98
28	LU	399/399 (100%)	399 (100%)	0	100	100
29	LW	373/512 (73%)	373 (100%)	0	100	100
30	LZ	166/167 (99%)	166 (100%)	0	100	100
32	NA	229/626 (37%)	229 (100%)	0	100	100
33	NB	63/413 (15%)	63 (100%)	0	100	100
34	NC	87/282 (31%)	87 (100%)	0	100	100
35	ND	72/222 (32%)	72 (100%)	0	100	100
36	NE	86/253 (34%)	85 (99%)	1 (1%)	71	87
37	NF	130/131 (99%)	130 (100%)	0	100	100
38	NG	92/119 (77%)	92 (100%)	0	100	100
39	NH	917/984 (93%)	916 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	NI	193/246 (78%)	193 (100%)	0	100	100
41	NJ	707/899 (79%)	705 (100%)	2 (0%)	92	97
41	NK	692/899 (77%)	690 (100%)	2 (0%)	92	97
42	NM	207/231 (90%)	207 (100%)	0	100	100
43	NN	37/484 (8%)	37 (100%)	0	100	100
44	NO	112/113 (99%)	112 (100%)	0	100	100
45	NQ	74/76 (97%)	74 (100%)	0	100	100
47	NT	51/140 (36%)	50 (98%)	1 (2%)	55	79
48	NU	53/122 (43%)	53 (100%)	0	100	100
49	NW	282/635 (44%)	280 (99%)	2 (1%)	84	93
50	NY	245/340 (72%)	244 (100%)	1 (0%)	91	97
51	SA	334/511 (65%)	334 (100%)	0	100	100
52	SB	372/455 (82%)	371 (100%)	1 (0%)	92	97
53	SC	192/234 (82%)	191 (100%)	1 (0%)	88	95
53	SD	198/234 (85%)	198 (100%)	0	100	100
54	SE	108/111 (97%)	108 (100%)	0	100	100
54	SF	107/111 (96%)	107 (100%)	0	100	100
55	SG	287/382 (75%)	287 (100%)	0	100	100
56	SH	315/318 (99%)	315 (100%)	0	100	100
57	SI	738/1114 (66%)	738 (100%)	0	100	100
58	SJ	181/209 (87%)	179 (99%)	2 (1%)	73	88
58	SK	181/209 (87%)	181 (100%)	0	100	100
59	SL	177/182 (97%)	177 (100%)	0	100	100
60	SM	253/254 (100%)	253 (100%)	0	100	100
61	SP	1822/2522 (72%)	1818 (100%)	4 (0%)	93	98
62	SQ	165/676 (24%)	165 (100%)	0	100	100
63	SR	85/115 (74%)	85 (100%)	0	100	100
64	SS	177/686 (26%)	176 (99%)	1 (1%)	86	94
65	ST	389/439 (89%)	388 (100%)	1 (0%)	92	97
66	SU	269/303 (89%)	269 (100%)	0	100	100
67	SW	152/208 (73%)	151 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	SY	219/232 (94%)	219 (100%)	0	100	100
70	SZ	214/227 (94%)	213 (100%)	1 (0%)	88	95
All	All	21892/29323 (75%)	21852 (100%)	40 (0%)	93	98

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	L6	231	ARG
10	L9	58	ARG
11	LA	93	LYS
11	LA	96	ARG
13	LD	69	ARG
13	LD	101	ARG
16	LH	140	GLN
16	LH	649	GLN
16	LH	759	LYS
19	LL	188	ARG
19	LL	367	ARG
20	LM	673	ASN
20	LM	1457	GLN
20	LM	1578	ARG
20	LM	1820	ARG
22	LO	850	LYS
26	LS	89	ARG
27	LT	197	GLN
36	NE	229	LYS
39	NH	247	ARG
41	NJ	69	ARG
41	NJ	430	GLN
41	NK	23	ARG
41	NK	60	LYS
47	NT	104	LYS
49	NW	7	ASN
49	NW	208	ARG
50	NY	327	LYS
52	SB	70	LYS
53	SC	87	MET
58	SJ	70	LYS
58	SJ	157	LYS
61	SP	36	ARG
61	SP	1087	LYS

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Mol	Chain	Res	Type
61	SP	1774	ARG
61	SP	2052	ARG
64	SS	130	ARG
65	ST	789	ARG
67	SW	76	ARG
70	SZ	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
8	L7	162	GLN
19	LL	458	GLN
19	LL	507	GLN
19	LL	547	GLN
20	LM	373	GLN
20	LM	489	HIS
20	LM	1125	GLN
20	LM	1401	GLN
20	LM	1666	ASN
20	LM	1765	GLN
20	LM	1970	ASN
23	LP	267	HIS
24	LQ	632	HIS
28	LU	75	HIS
28	LU	176	GLN
35	ND	236	GLN
41	NK	372	HIS
41	NK	543	ASN
41	NK	831	ASN
52	SB	113	ASN
53	SC	251	HIS
54	SE	28	GLN
58	SJ	101	ASN
61	SP	635	GLN
61	SP	1403	ASN
61	SP	1538	GLN
61	SP	1976	GLN
61	SP	2182	ASN
64	SS	195	ASN
65	ST	37	ASN
65	ST	722	HIS
65	ST	748	GLN

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Mol	Chain	Res	Type
65	ST	796	HIS
66	SU	262	HIS
66	SU	310	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	234/3617 (6%)	101 (43%)	6 (2%)
2	L1	1275/1869 (68%)	346 (27%)	23 (1%)
3	L2	214/217 (98%)	80 (37%)	4 (1%)
31	N0	0/22	-	-
All	All	1723/5725 (30%)	527 (30%)	33 (1%)

All (527) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	434	C
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	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

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Mol	Chain	Res	Type
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
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	738	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

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Mol	Chain	Res	Type
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	840	G
1	L0	843	U
1	L0	844	G
1	L0	855	G
1	L0	859	G
1	L0	860	A
1	L0	862	G
1	L0	863	C
1	L0	864	C
1	L0	865	G
1	L0	1414	A
1	L0	1415	G
1	L0	1418	A
1	L0	1419	A
1	L0	1420	G
1	L0	1421	C
1	L0	1428	U
1	L0	1430	G
1	L0	1433	A
1	L0	1435	C
2	L1	5	U
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

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Mol	Chain	Res	Type
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	59	U
2	L1	64	A
2	L1	65	C
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	95	G
2	L1	96	C
2	L1	97	U
2	L1	98	C
2	L1	99	A
2	L1	100	U
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	155	G
2	L1	158	A
2	L1	161	U
2	L1	162	C
2	L1	172	U
2	L1	173	A
2	L1	180	G
2	L1	182	C

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Mol	Chain	Res	Type
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	235	A
2	L1	238	C
2	L1	248	C
2	L1	269	G
2	L1	271	C
2	L1	272	G
2	L1	275	C
2	L1	279	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	332	G
2	L1	335	G

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Mol	Chain	Res	Type
2	L1	347	G
2	L1	350	C
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	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
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	432	G
2	L1	439	A
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

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Mol	Chain	Res	Type
2	L1	487	U
2	L1	488	U
2	L1	492	C
2	L1	496	C
2	L1	502	C
2	L1	514	U
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	559	G
2	L1	560	A
2	L1	564	A
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	627	U
2	L1	628	A
2	L1	643	A
2	L1	644	G
2	L1	651	U
2	L1	652	U
2	L1	653	A
2	L1	654	A
2	L1	655	A
2	L1	684	G

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Mol	Chain	Res	Type
2	L1	920	A
2	L1	933	G
2	L1	938	A
2	L1	943	U
2	L1	955	A
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
2	L1	1144	A
2	L1	1145	A
2	L1	1147	C
2	L1	1148	A
2	L1	1170	A
2	L1	1172	U
2	L1	1174	U
2	L1	1175	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	1198	G
2	L1	1212	G

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Mol	Chain	Res	Type
2	L1	1215	C
2	L1	1216	C
2	L1	1217	A
2	L1	1267	C
2	L1	1268	C
2	L1	1273	C
2	L1	1275	G
2	L1	1276	A
2	L1	1277	C
2	L1	1278	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	1311	C
2	L1	1313	A
2	L1	1315	U
2	L1	1316	C
2	L1	1318	G
2	L1	1320	G
2	L1	1327	G
2	L1	1328	G
2	L1	1329	U
2	L1	1330	G
2	L1	1331	C
2	L1	1333	U
2	L1	1335	G
2	L1	1348	G
2	L1	1354	G
2	L1	1355	C
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

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Mol	Chain	Res	Type
2	L1	1378	A
2	L1	1382	A
2	L1	1394	G
2	L1	1452	A
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	1485	U
2	L1	1487	A
2	L1	1489	A
2	L1	1490	G
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	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
2	L1	1638	G
2	L1	1639	G
2	L1	1648	G
2	L1	1656	G
2	L1	1660	C
2	L1	1664	A
2	L1	1665	G
2	L1	1666	C

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Mol	Chain	Res	Type
2	L1	1667	U
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	1765	C
2	L1	1767	C
2	L1	1768	A
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
2	L1	1812	U
2	L1	1813	A
2	L1	1818	A
2	L1	1824	A
2	L1	1838	U
2	L1	1846	G
2	L1	1848	U
2	L1	1849	G
2	L1	1850	A

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Mol	Chain	Res	Type
2	L1	1851	A
2	L1	1852	C
3	L2	13	U
3	L2	14	C
3	L2	15	A
3	L2	16	G
3	L2	22	A
3	L2	23	U
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	39	C
3	L2	44	G
3	L2	46	A
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	92	U
3	L2	108	G
3	L2	109	C
3	L2	110	G
3	L2	114	A
3	L2	115	G
3	L2	116	C
3	L2	117	C
3	L2	118	G
3	L2	119	G
3	L2	123	U
3	L2	124	C
3	L2	125	U

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Mol	Chain	Res	Type
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	152	A
3	L2	153	G
3	L2	154	C
3	L2	158	U
3	L2	168	U
3	L2	171	U
3	L2	172	C
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
3	L2	208	U
3	L2	209	C
3	L2	213	G

All (33) 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	450	C
2	L1	466	G
2	L1	487	U
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 $\lvert Z\rvert > 2$ 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
74	GTP	SI	2001	71	26,34,34	1.13	2 (7%)	32,54,54	1.54	6 (18%)
72	ATP	NK	1101	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
72	ATP	NH	3000	71	26,33,33	0.58	0	31,52,52	0.81	2 (6%)
75	SAH	SK	301	-	24,28,28	1.19	3 (12%)	25,40,40	1.71	5 (20%)
75	SAH	SJ	301	-	24,28,28	1.20	3 (12%)	25,40,40	1.70	5 (20%)

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	GTP	SI	2001	71	-	7/18/38/38	0/3/3/3
72	ATP	NK	1101	-	-	7/18/38/38	0/3/3/3
72	ATP	NH	3000	71	-	6/18/38/38	0/3/3/3
75	SAH	SK	301	-	-	9/11/31/31	0/3/3/3
75	SAH	SJ	301	-	-	3/11/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	SI	2001	GTP	C5-C6	-4.16	1.39	1.47
75	SJ	301	SAH	C2-N3	3.92	1.38	1.32
75	SK	301	SAH	C2-N3	3.86	1.38	1.32
75	SK	301	SAH	C2-N1	2.47	1.38	1.33
75	SJ	301	SAH	C2-N1	2.45	1.38	1.33
74	SI	2001	GTP	C2-N3	2.15	1.38	1.33
75	SK	301	SAH	OXT-C	-2.12	1.23	1.30
75	SJ	301	SAH	OXT-C	-2.12	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	SK	301	SAH	N3-C2-N1	-5.40	120.25	128.68
75	SJ	301	SAH	N3-C2-N1	-5.39	120.25	128.68
74	SI	2001	GTP	PB-O3B-PG	-3.57	120.57	132.83
75	SK	301	SAH	C5'-SD-CG	-3.42	92.02	102.27
75	SJ	301	SAH	C5'-SD-CG	-3.31	92.33	102.27
74	SI	2001	GTP	C8-N7-C5	3.15	108.99	102.99
74	SI	2001	GTP	C3'-C2'-C1'	3.13	105.69	100.98
74	SI	2001	GTP	C5-C6-N1	3.07	119.38	113.95
75	SJ	301	SAH	C3'-C2'-C1'	2.85	105.27	100.98
75	SK	301	SAH	C3'-C2'-C1'	2.77	105.15	100.98
74	SI	2001	GTP	C2-N1-C6	-2.76	120.02	125.10
75	SK	301	SAH	OXT-C-O	-2.69	117.99	124.09
74	SI	2001	GTP	PA-O3A-PB	-2.69	123.60	132.83
75	SJ	301	SAH	OXT-C-O	-2.64	118.09	124.09
72	NK	1101	ATP	C5-C6-N6	2.31	123.87	120.35
72	NH	3000	ATP	C5-C6-N6	2.30	123.85	120.35
75	SK	301	SAH	OXT-C-CA	2.24	121.02	113.38
75	SJ	301	SAH	OXT-C-CA	2.24	121.00	113.38
72	NK	1101	ATP	PB-O3B-PG	2.07	139.95	132.83
72	NH	3000	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

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

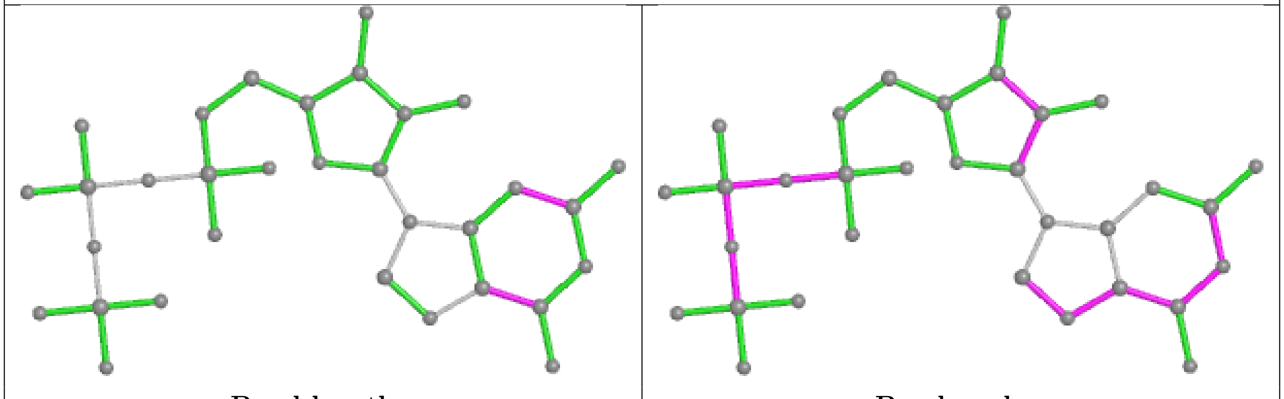
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	NK	1101	ATP	1	0
72	NH	3000	ATP	2	0
75	SJ	301	SAH	3	0

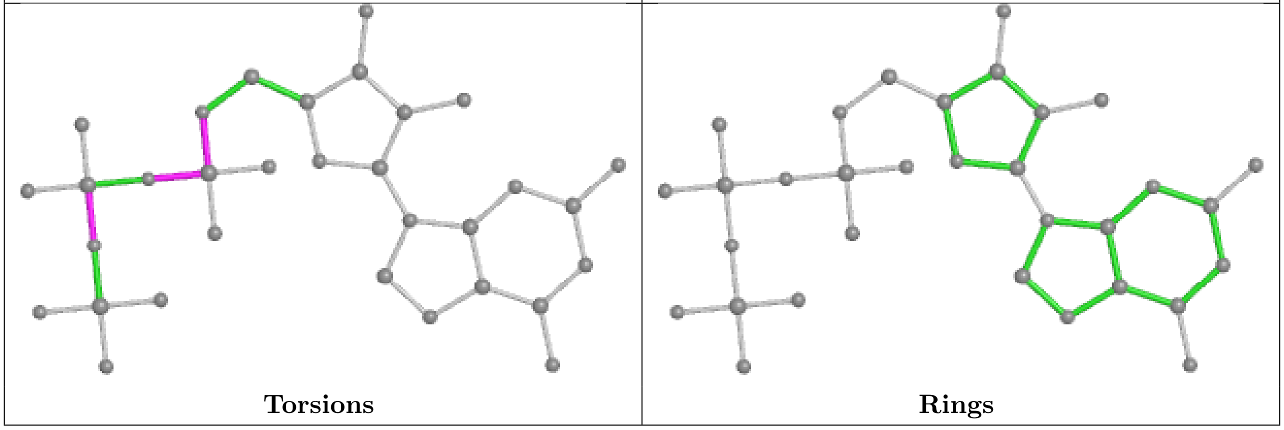
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GTP SI 2001



Bond lengths

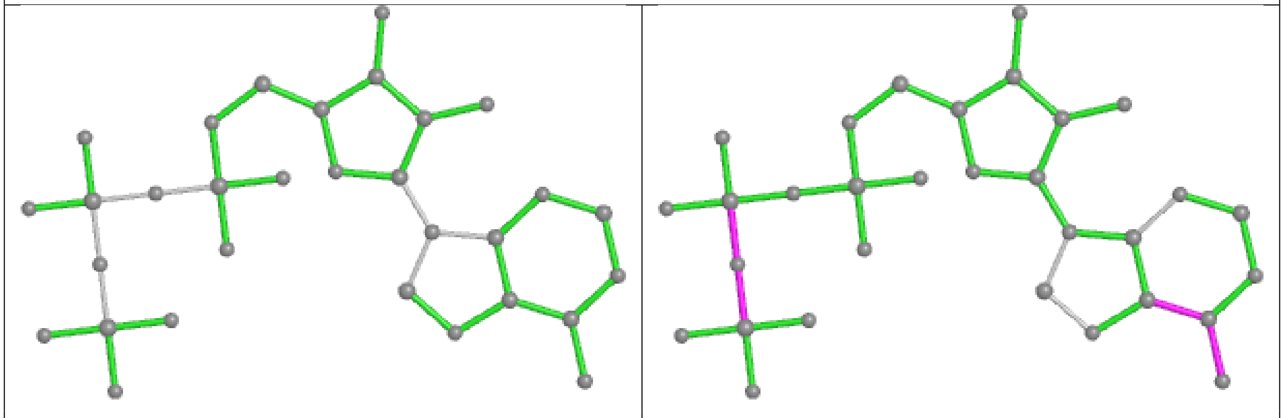
Bond angles



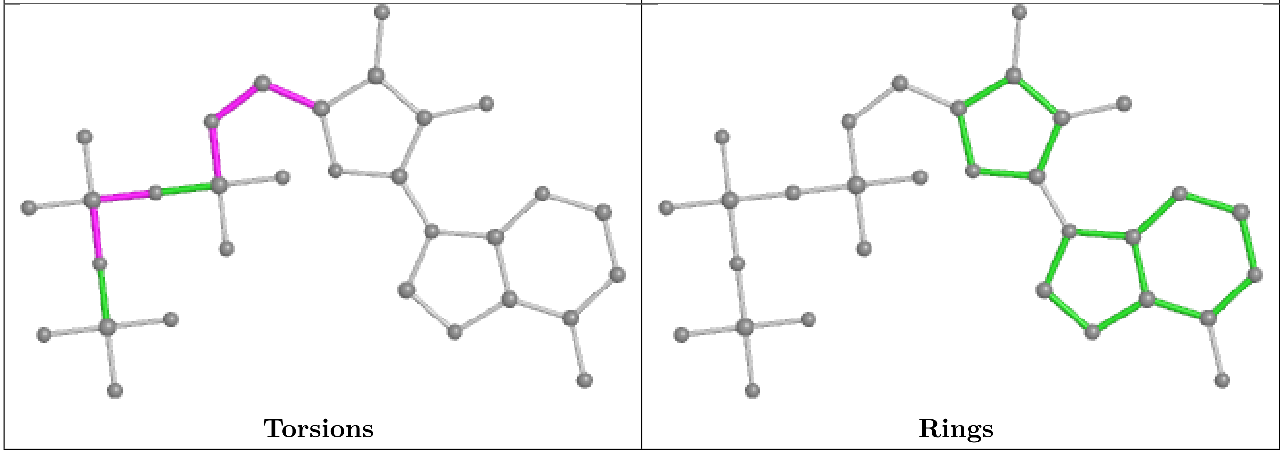
Torsions

Rings

Ligand ATP NK 1101

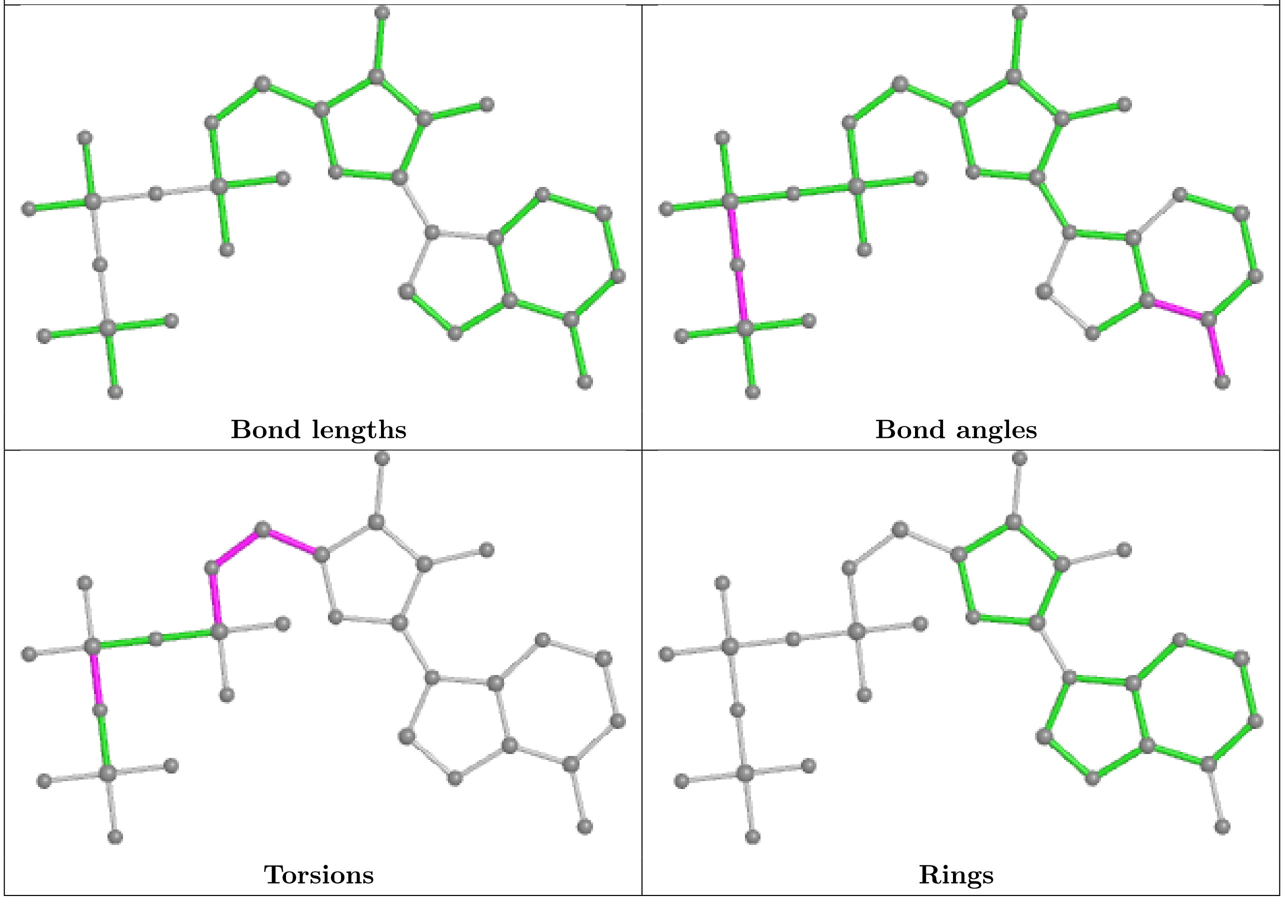


Bond lengths **Bond angles**



Torsions **Rings**

Ligand ATP NH 3000



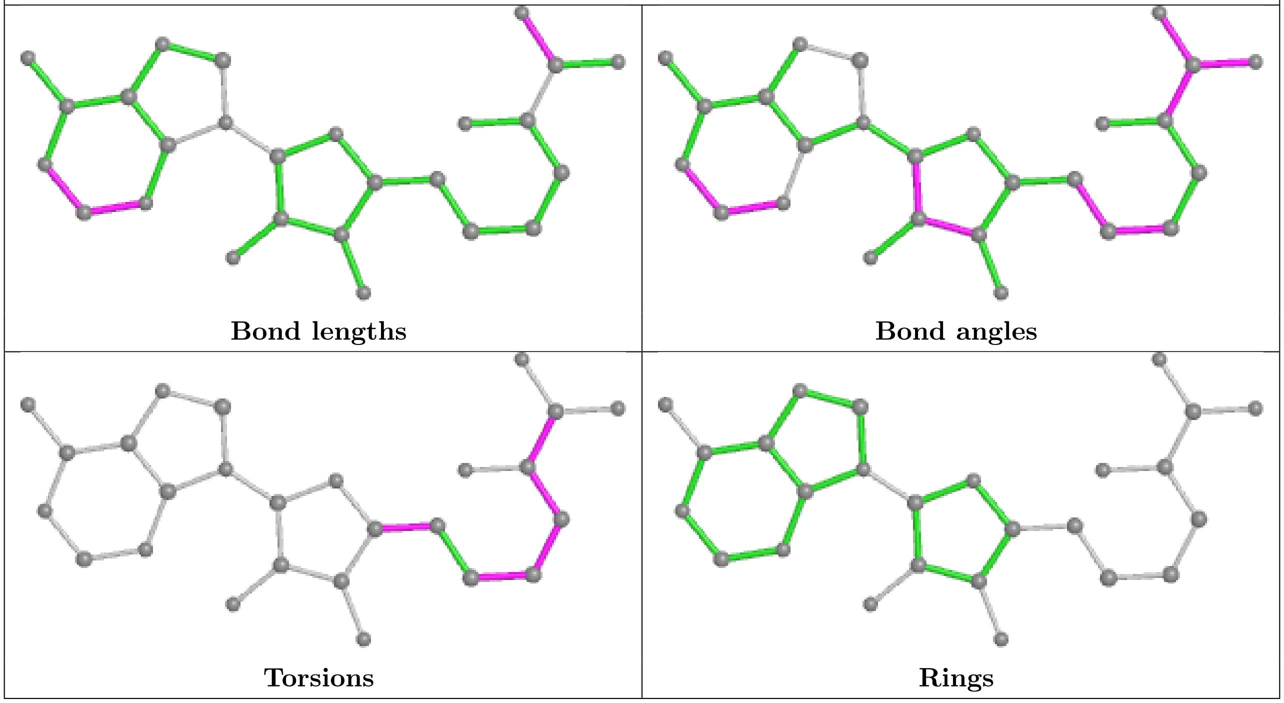
Bond lengths

Bond angles

Torsions

Rings

Ligand SAH SK 301



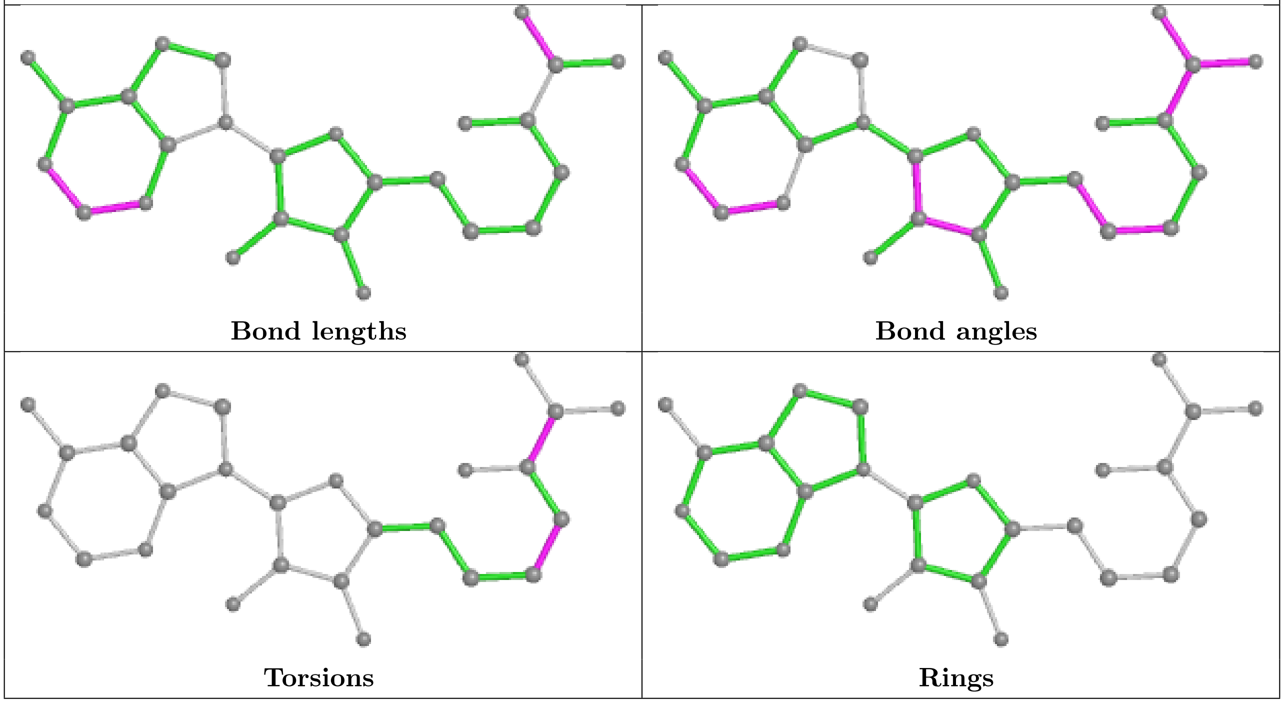
Bond lengths

Bond angles

Torsions

Rings

Ligand SAH SJ 301



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
46	NR	41
68	SX	6
17	LI	5
66	SU	5
65	ST	3
31	N0	1
70	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	185.51
1	ST	298:LEU	C	414:UNK	N	52.49
1	SX	1269:UNK	C	1298:UNK	N	38.16
1	ST	86:LYS	C	186:UNK	N	37.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SX	1427:UNK	C	1449:UNK	N	35.74
1	SX	1375:UNK	C	1405:UNK	N	33.56
1	LI	48:UNK	C	59:UNK	N	26.45
1	ST	234:UNK	C	246:UNK	N	22.17
1	LI	92:UNK	C	104:UNK	N	18.16
1	SX	1322:UNK	C	1352:UNK	N	17.59
1	NR	567:UNK	C	571:UNK	N	16.63
1	NR	310:UNK	C	312:UNK	N	16.61
1	NR	803:UNK	C	807:UNK	N	16.44
1	SX	1222:UNK	C	1250:UNK	N	15.85
1	NR	131:UNK	C	134:UNK	N	15.65
1	N0	881:N	O3'	1396:N	P	15.50
1	LI	346:UNK	C	354:HIS	N	15.48
1	NR	358:UNK	C	361:UNK	N	15.11
1	NR	450:UNK	C	452:UNK	N	14.79
1	NR	976:UNK	C	980:UNK	N	14.36
1	NR	915:UNK	C	919:UNK	N	13.77
1	NR	496:UNK	C	498:UNK	N	13.11
1	NR	101:UNK	C	112:UNK	N	13.01
1	NR	647:UNK	C	651:UNK	N	12.81
1	NR	953:UNK	C	957:UNK	N	12.49
1	NR	613:UNK	C	616:UNK	N	12.32
1	NR	517:UNK	C	519:UNK	N	12.19
1	SU	68:UNK	C	78:UNK	N	12.19
1	LI	147:UNK	C	152:VAL	N	12.09
1	NR	688:UNK	C	692:UNK	N	12.06
1	NR	475:UNK	C	477:UNK	N	11.96
1	NR	426:UNK	C	428:UNK	N	11.89
1	NR	221:UNK	C	225:UNK	N	11.77
1	NR	870:UNK	C	874:UNK	N	11.74
1	NR	995:UNK	C	999:UNK	N	11.59
1	NR	335:UNK	C	339:UNK	N	11.11
1	NR	672:UNK	C	674:UNK	N	11.07
1	NR	713:UNK	C	717:UNK	N	10.68
1	NR	846:UNK	C	850:UNK	N	10.28
1	NR	934:UNK	C	936:UNK	N	10.24
1	NR	894:UNK	C	898:UNK	N	10.23
1	SZ	164:UNK	C	169:UNK	N	10.07
1	NR	631:UNK	C	633:UNK	N	9.93
1	NR	780:UNK	C	784:UNK	N	9.87
1	NR	590:UNK	C	592:UNK	N	9.00
1	NR	538:UNK	C	541:UNK	N	8.70

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	NR	824:UNK	C	828:UNK	N	8.69
1	NR	550:UNK	C	555:UNK	N	8.55
1	SU	169:UNK	C	177:TYR	N	8.34
1	SU	25:UNK	C	27:UNK	N	7.92
1	NR	1008:UNK	C	1010:UNK	N	7.73
1	NR	243:UNK	C	246:UNK	N	7.72
1	NR	262:UNK	C	264:UNK	N	7.28
1	NR	756:UNK	C	760:UNK	N	7.03
1	NR	734:UNK	C	736:UNK	N	6.94
1	NR	381:UNK	C	383:UNK	N	5.74
1	SU	45:UNK	C	48:UNK	N	5.53
1	NR	200:UNK	C	204:UNK	N	5.43
1	LI	322:HIS	C	325:UNK	N	5.34
1	SU	124:UNK	C	141:PRO	N	4.96
1	NR	289:UNK	C	291:UNK	N	4.86
1	NR	404:UNK	C	407:UNK	N	3.63

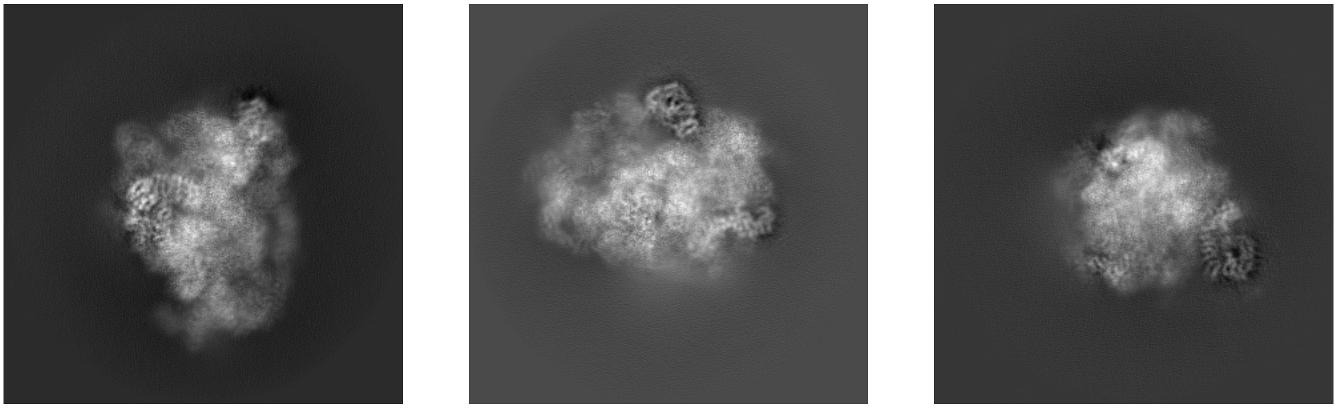
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23936. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

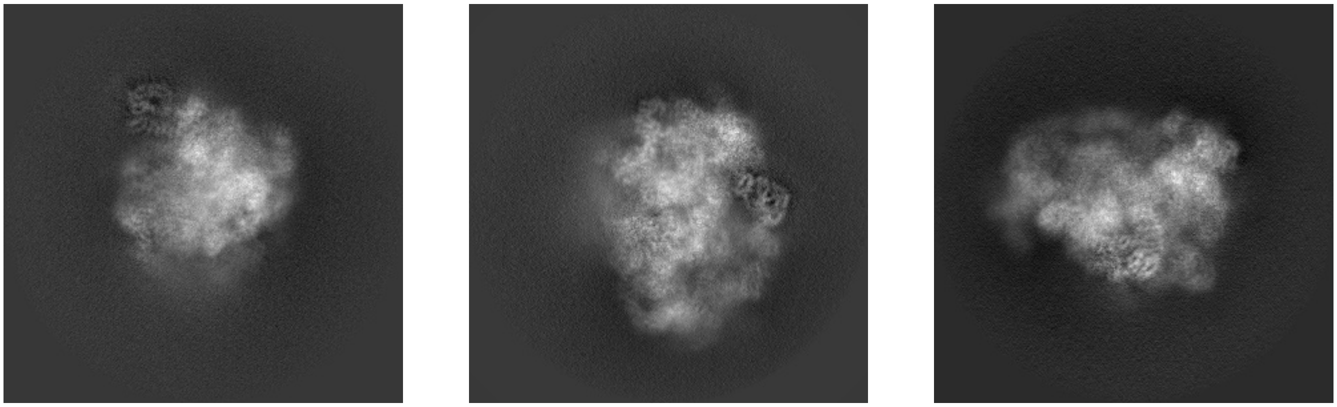
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

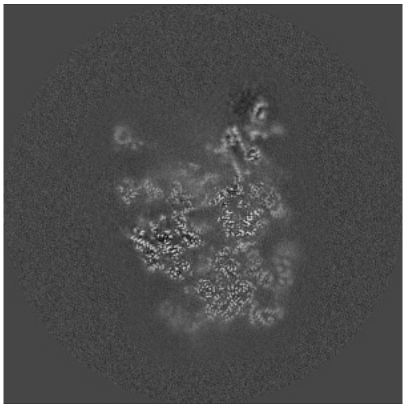


X Y Z

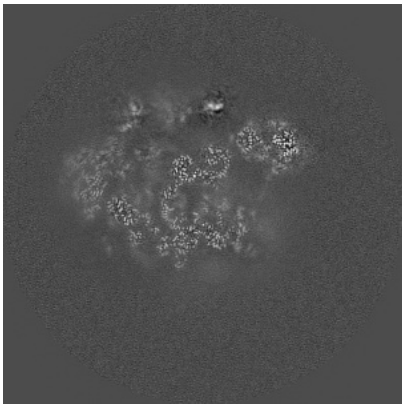
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

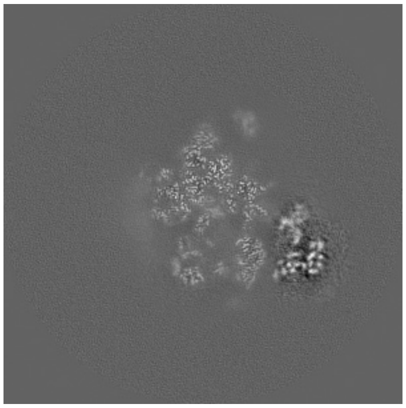
6.2.1 Primary map



X Index: 280

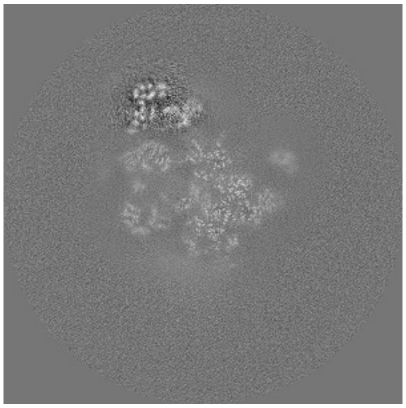


Y Index: 280

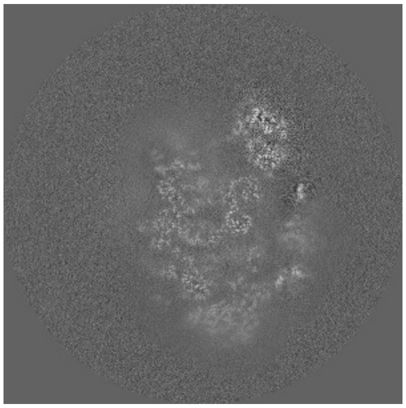


Z Index: 280

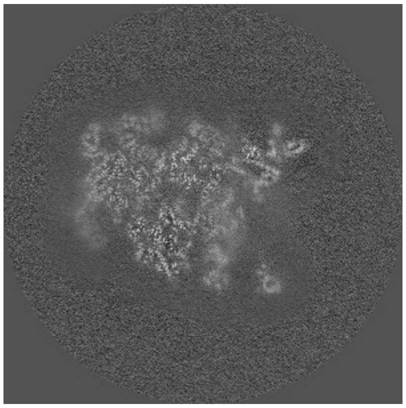
6.2.2 Raw map



X Index: 280



Y Index: 280

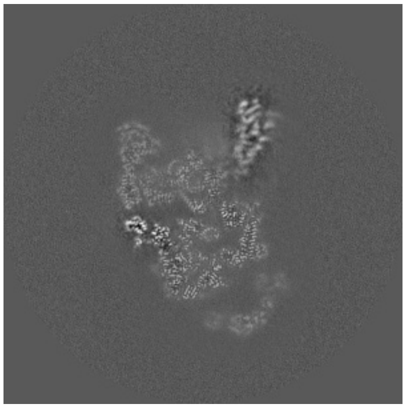


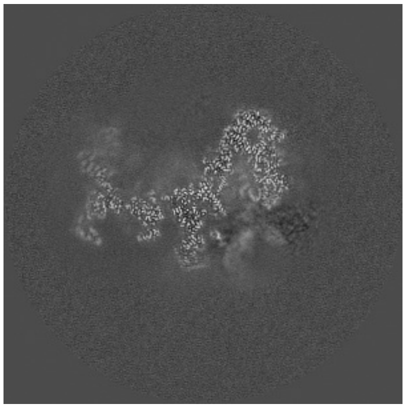
Z Index: 280

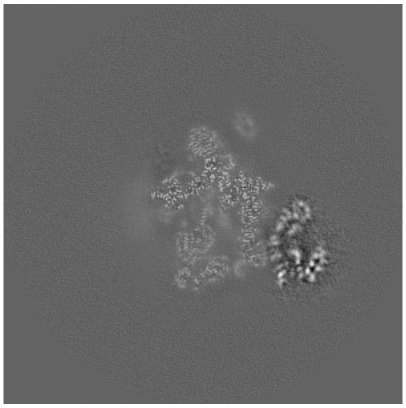
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

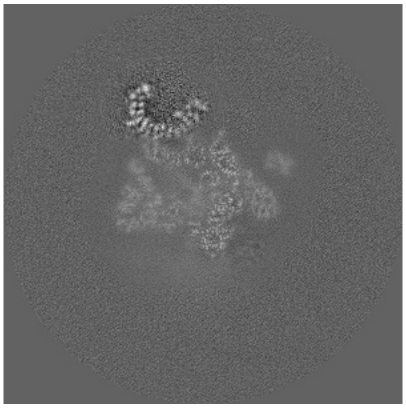
6.3.1 Primary map

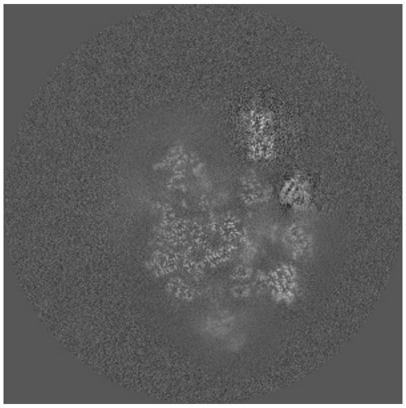

X Index: 254

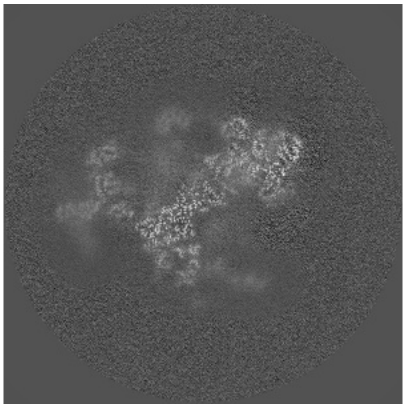

Y Index: 318


Z Index: 291

6.3.2 Raw map


X Index: 298


Y Index: 261


Z Index: 320

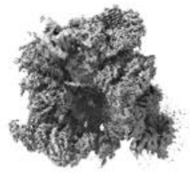
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X

Y

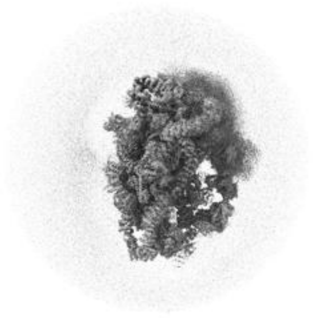


Z

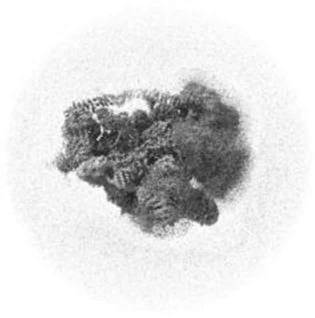
The images above show the 3D surface view of the map at the recommended contour level 2.68. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

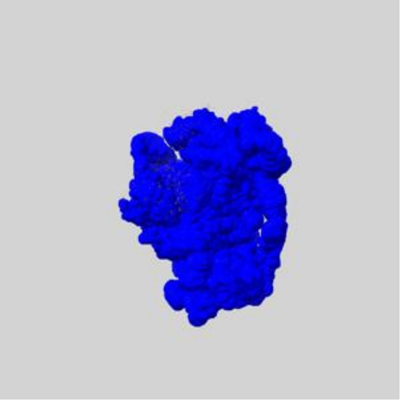
6.5 Mask visualisation

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

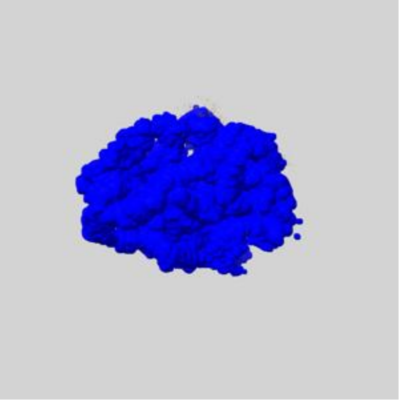
A mask typically either:

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

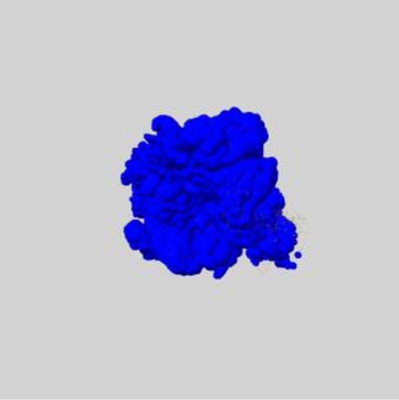
6.5.1 emd_23936_msk_1.map



X



Y

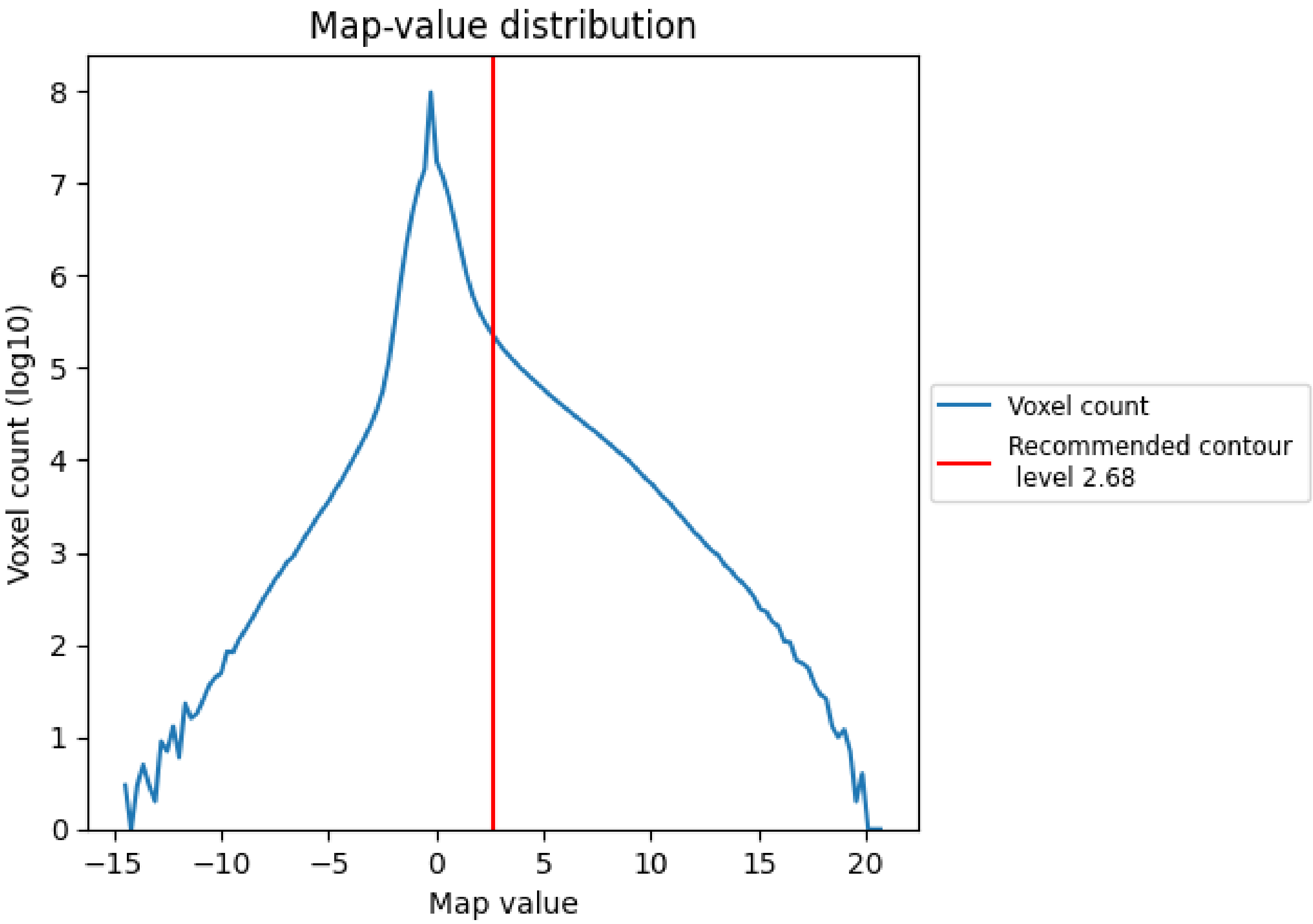


Z

7 Map analysis ⓘ

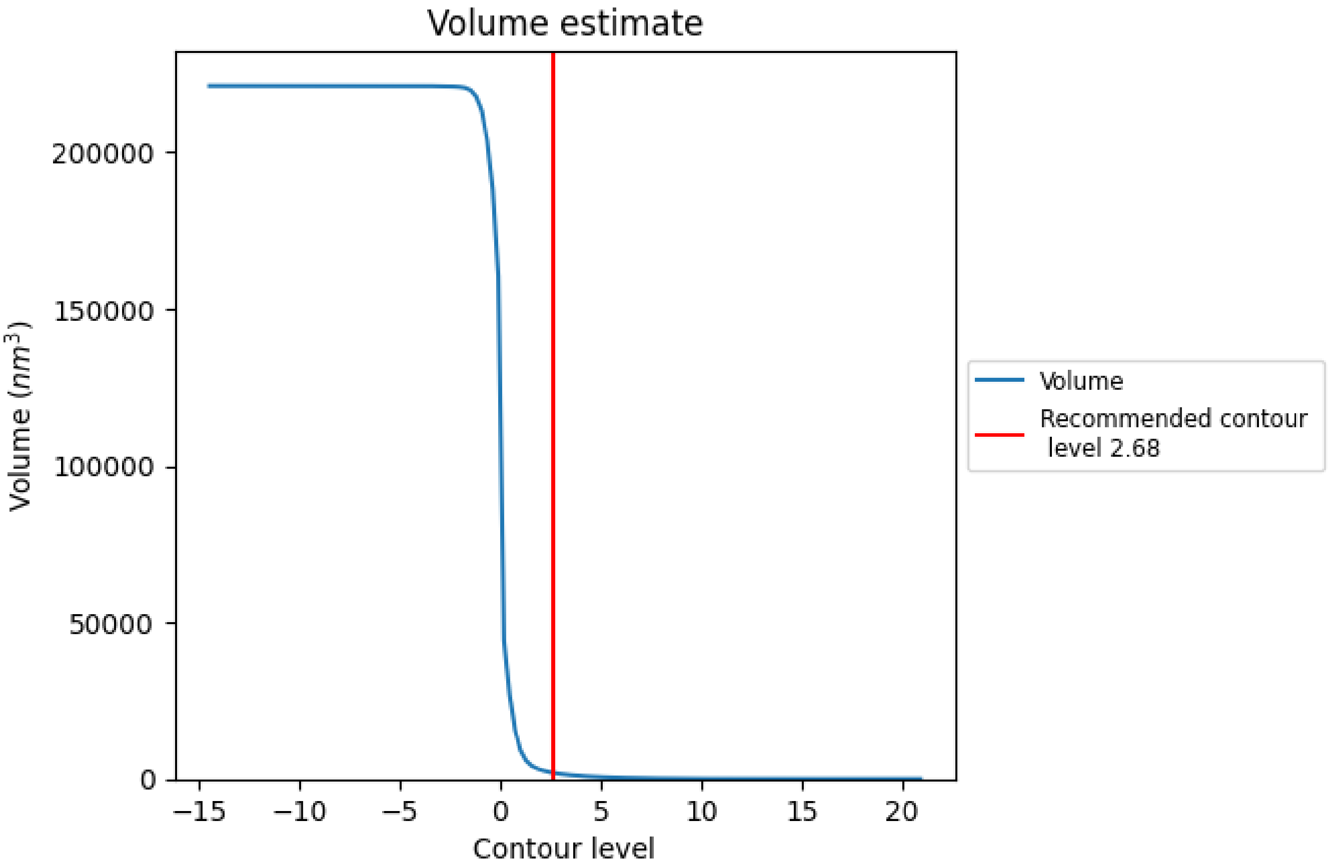
This section contains the results of statistical analysis of the map.

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.

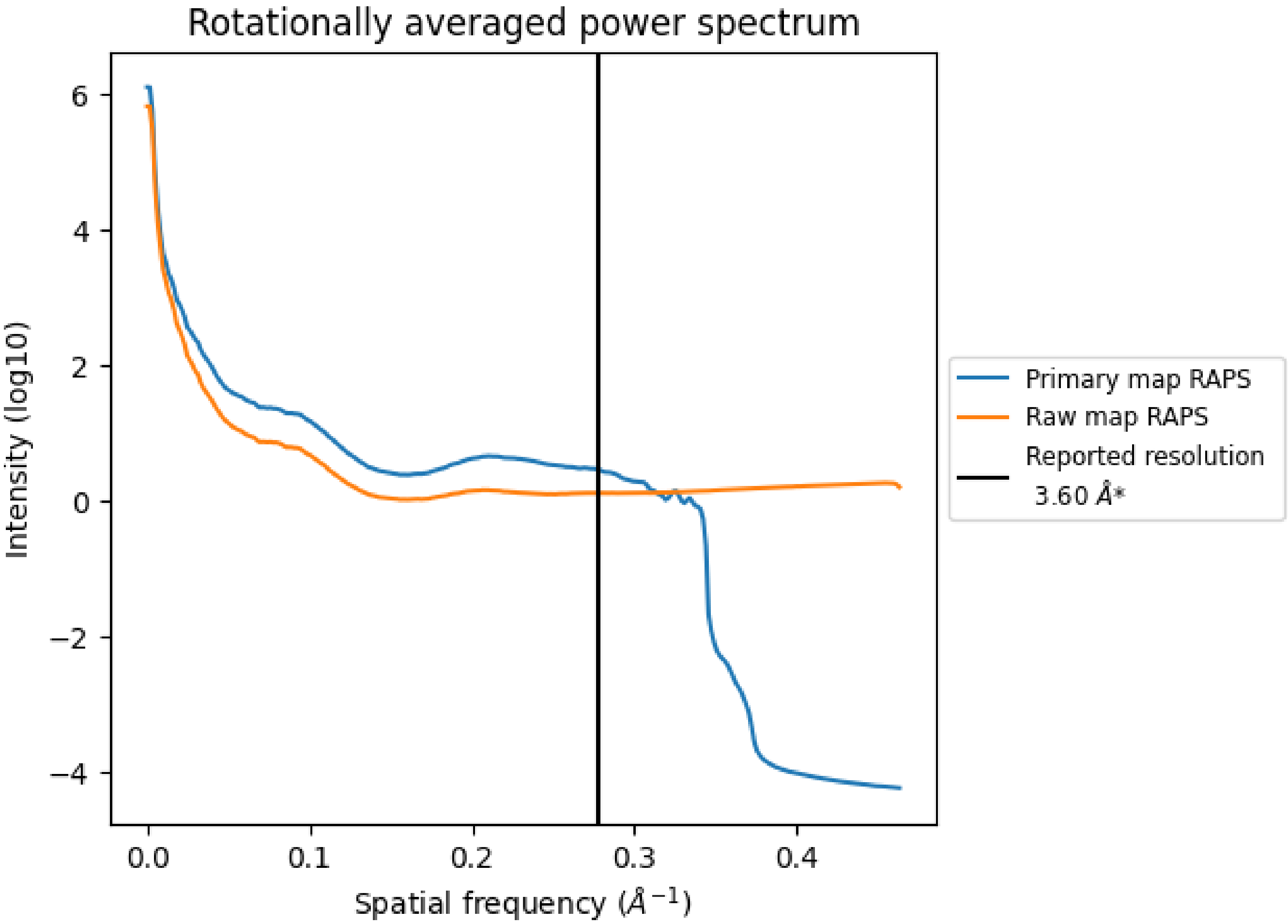
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1931 nm^3; this corresponds to an approximate mass of 1744 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 ⓘ

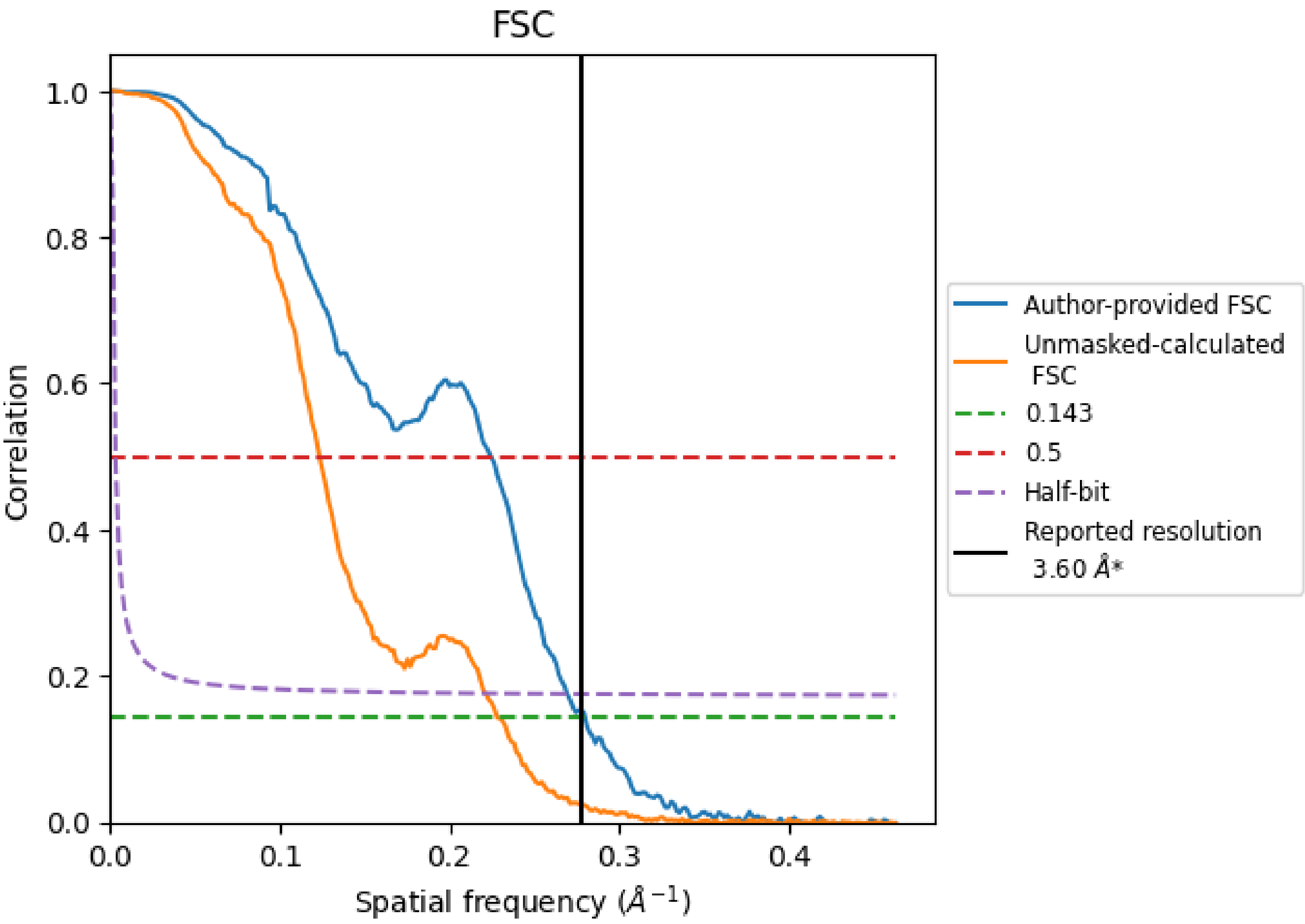


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates ⓘ

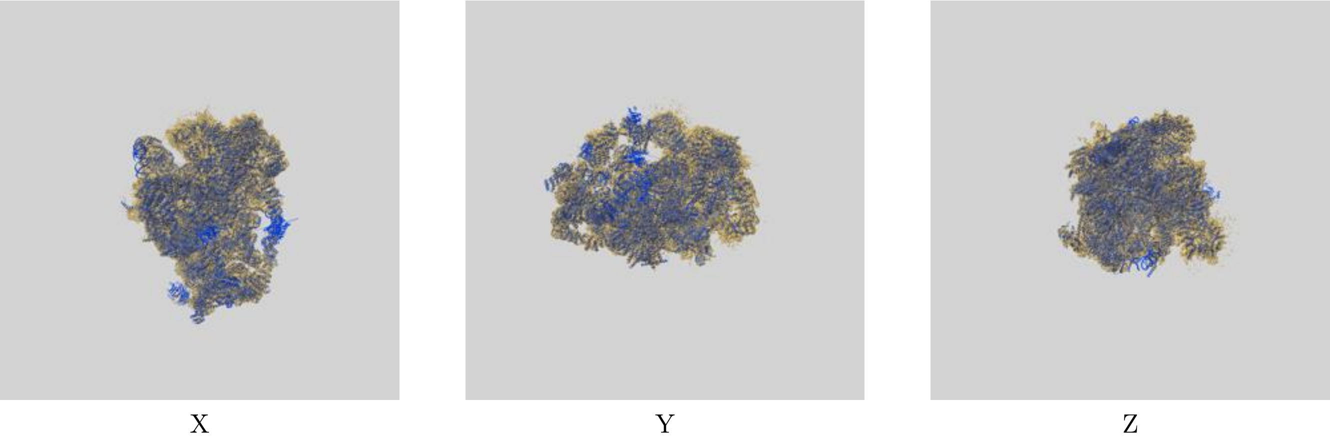
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.46	3.71
Unmasked-calculated*	4.38	8.10	4.52

*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 4.38 differs from the reported value 3.6 by more than 10 %

9 Map-model fit ⓘ

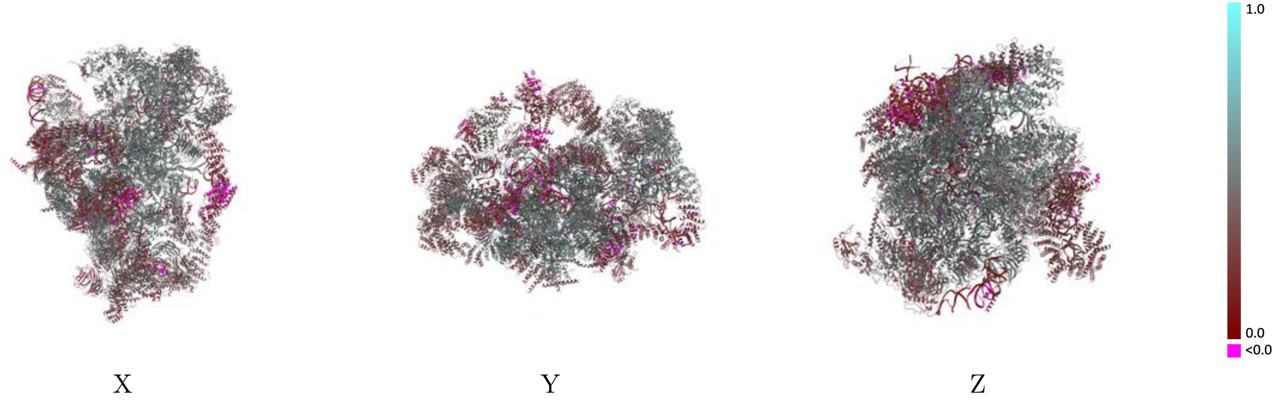
This section contains information regarding the fit between EMDB map EMD-23936 and PDB model 7MQ8. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay ⓘ



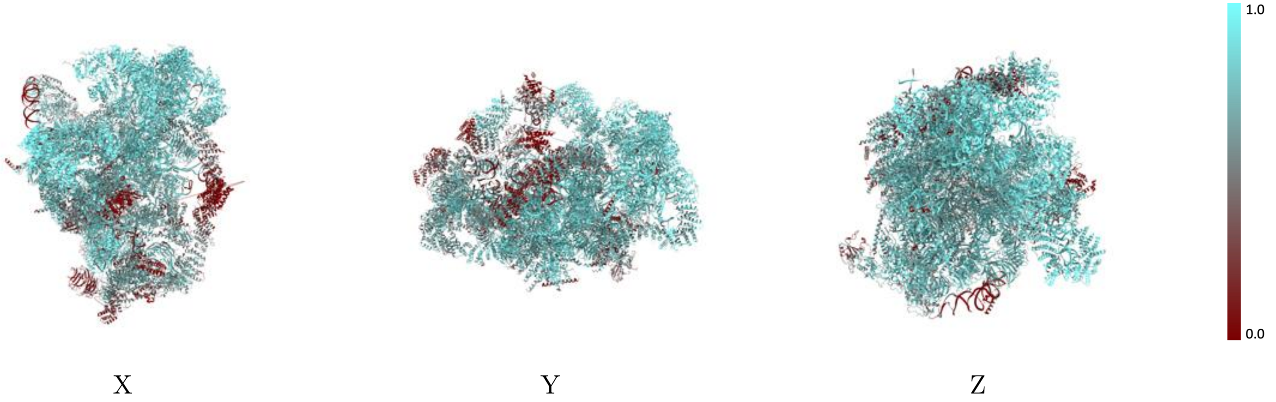
The images above show the 3D surface view of the map at the recommended contour level 2.68 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



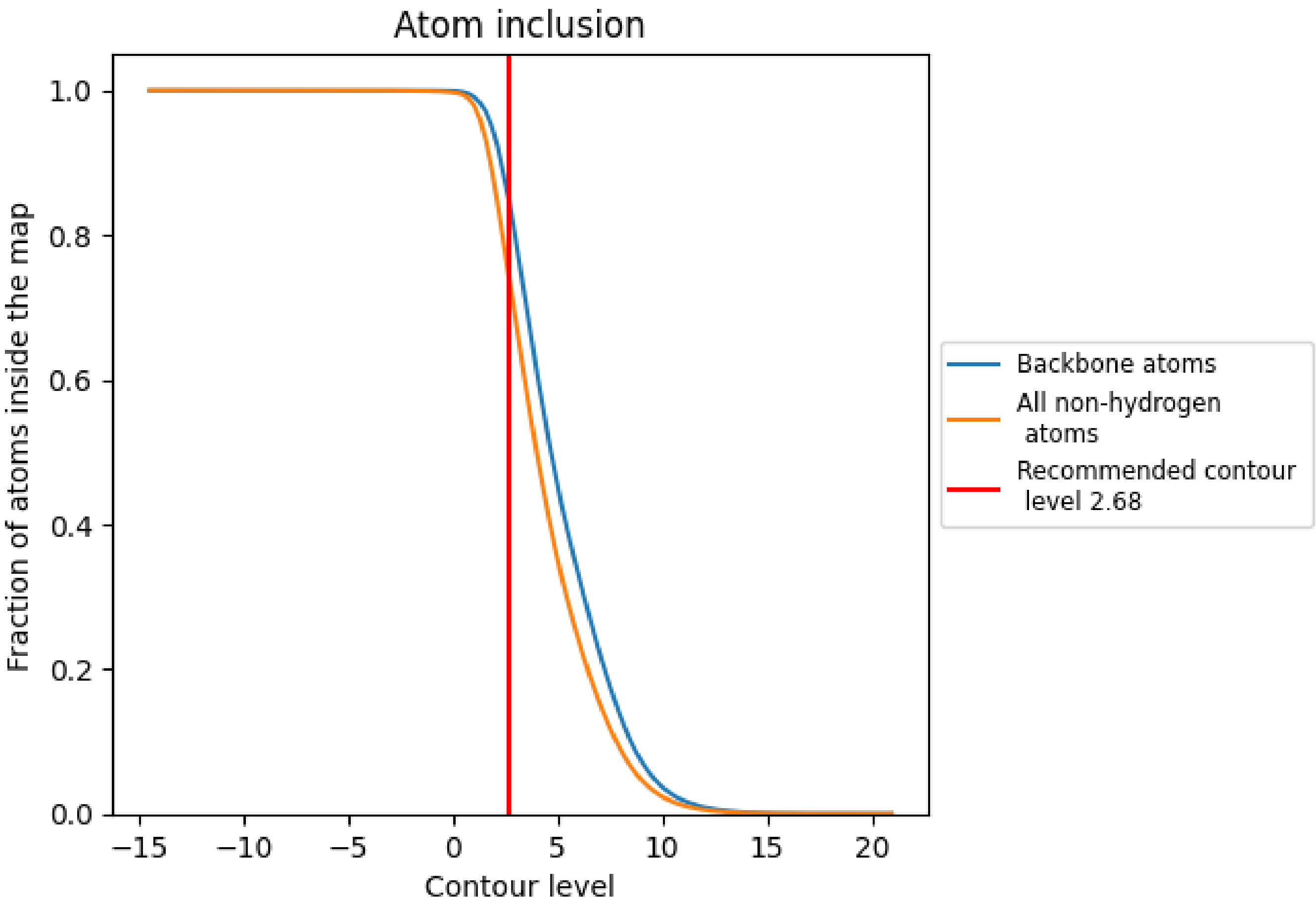
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (2.68).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.68) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.4170
L0	0.5928	0.3800
L1	0.8243	0.3850
L2	0.7871	0.4060
L3	0.3730	0.3330
L4	0.8267	0.4270
L5	0.8644	0.5070
L6	0.8726	0.4700
L7	0.5343	0.3320
L8	0.9090	0.4960
L9	0.9007	0.5360
LA	0.0022	0.0770
LC	0.8592	0.5180
LD	0.8340	0.4070
LF	0.8154	0.4490
LG	0.8574	0.5030
LH	0.7380	0.4450
LI	0.1925	0.2410
LJ	0.7516	0.4570
LK	0.3240	0.3190
LL	0.7275	0.4550
LM	0.5094	0.2910
LN	0.7617	0.4500
LO	0.8737	0.5190
LP	0.7729	0.4530
LQ	0.7595	0.4540
LR	0.7838	0.4430
LS	0.8284	0.5170
LT	0.8667	0.5220
LU	0.8528	0.5120
LW	0.8219	0.5080
LZ	0.8780	0.5340
N0	0.5303	0.3920
NA	0.7893	0.4960
NB	0.9142	0.5630

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Chain	Atom inclusion	Q-score
NC	0.7543	0.4330
ND	0.6012	0.4040
NE	0.6565	0.4580
NF	0.6801	0.4240
NG	0.7666	0.4680
NH	0.6655	0.3730
NI	0.4705	0.3110
NJ	0.8628	0.4660
NK	0.8895	0.4630
NM	0.7034	0.4540
NN	0.8550	0.4880
NO	0.7099	0.4780
NQ	0.7711	0.5090
NR	0.9115	0.2750
NT	0.0350	0.1220
NU	0.7071	0.2240
NW	0.8851	0.4900
NY	0.6540	0.4250
SA	0.8384	0.4900
SB	0.7290	0.4540
SC	0.6166	0.3780
SD	0.9279	0.5620
SE	0.8615	0.5220
SF	0.8798	0.5270
SG	0.7847	0.4290
SH	0.8555	0.5200
SI	0.8631	0.5100
SJ	0.3445	0.2800
SK	0.5872	0.4270
SL	0.8709	0.5300
SM	0.8863	0.5350
SP	0.7814	0.3450
SQ	0.7577	0.4580
SR	0.8755	0.5290
SS	0.6782	0.4560
ST	0.7307	0.3820
SU	0.4610	0.3320
SW	0.8379	0.3510
SX	0.0814	0.0890
SY	0.6789	0.4100
SZ	0.5934	0.2680