



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 9N6V / pdb_00009n6v
EMDB ID : EMD-49075
Title : SSU processome maturation and disassembly, State A
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 3.16 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

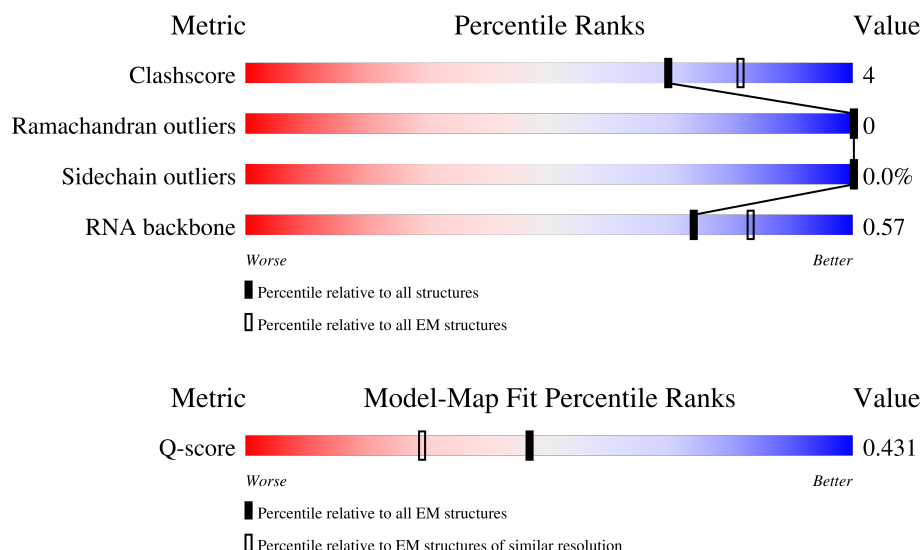
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.16 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14474 (2.66 - 3.66)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L0	700	5% 58% 15% 25%
2	L1	1808	6% 49% 13% 36%
3	L2	333	42% 9% 47%

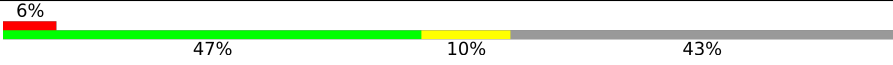
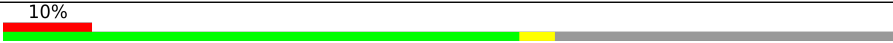
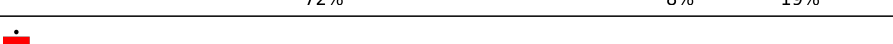
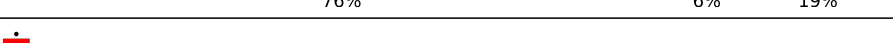
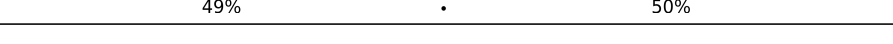
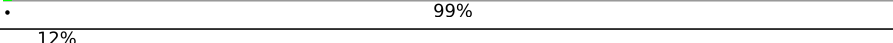
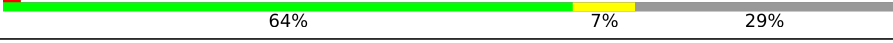
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L3	146	
5	L4	261	
6	L5	225	
7	L6	236	
8	L7	190	
9	L8	200	
10	L9	197	
11	LC	143	
12	LD	156	
13	LE	130	
14	LF	135	
15	LG	67	
16	LH	896	
17	LI	713	
18	LJ	513	
19	LK	575	
20	LL	643	
21	LM	1769	
22	LN	776	
23	LO	923	
24	LP	440	
25	LQ	943	
26	LR	817	
27	LS	594	
28	LT	939	

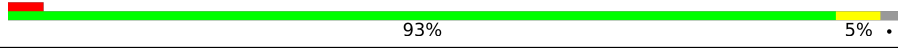
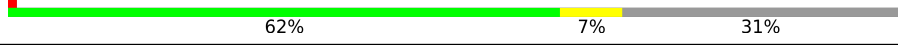
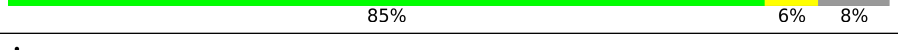
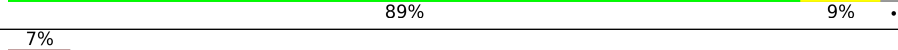
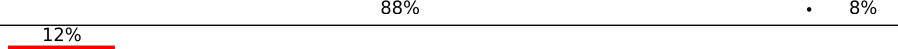
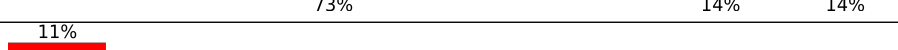
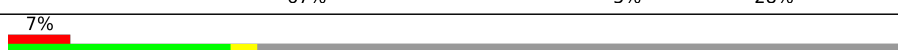
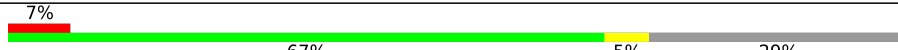
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LU	489	
30	LV	707	
31	LW	554	
32	LX	1056	
32	LY	1056	
33	LZ	183	
34	NA	593	
35	NB	610	
36	NC	357	
37	ND	214	
38	NE	346	
39	NF	151	
40	NG	137	
41	NH	1237	
42	NI	297	
43	NK	316	
44	NM	255	
45	NN	534	
46	NQ	82	
47	OA	1729	
48	SA	504	
49	SB	511	
50	SC	327	
50	SD	327	
51	SE	126	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
51	SF	126	
52	SG	573	
53	SH	367	
54	SI	1183	
55	SJ	252	
55	SK	252	
56	SL	189	
57	SM	290	
58	SN	274	
59	SP	2493	
60	SQ	217	
61	SR	145	
62	SS	899	
63	ST	810	
64	SU	552	
65	SV	206	
66	SW	274	
67	SY	250	
68	SZ	483	

2 Entry composition

There are 72 unique types of molecules in this entry. The entry contains 243904 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
1	L0	523	Total	C	N	O	P	0	0
			11158	4986	1978	3671	523		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	1149	Total	C	N	O	P	0	0
			24510	10958	4383	8020	1149		

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	175	Total	C	N	O	P	0	0
			3712	1661	649	1227	175		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	97	Total	C	N	O	S	0	0
			786	498	144	142	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L4	234	Total	C	N	O	S	0	0
			1866	1195	343	325	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	206	Total	C	N	O	S	0	0
			1635	1027	300	305	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	206	Total	C	N	O	S	0	0
			1653	1043	315	293	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	169	Total	C	N	O	S	0	0
			1347	869	230	248			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	171	Total	C	N	O	S	0	0
			1356	842	270	242	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	171	Total	C	N	O	S	0	0
			1388	879	268	240	1		

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	137	Total	C	N	O	S	0	0
			1112	714	212	183	3		

- Molecule 13 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	129	Total	C	N	O	S	0	0
			1022	650	188	181	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	LF	95	Total	C	N	O	0	0
			753	483	136	134		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	62	Total	C	N	O	S	0	0
			490	302	98	89	1		

- Molecule 16 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	808	Total	C	N	O	S	0	0
			6465	4123	1090	1233	19		

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	600	Total	C	N	O	S	0	0
			3792	2375	679	733	5		

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

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

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	132	Total	C	N	O	S	0	0
			1068	681	185	199	3		

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	504	Total	C	N	O	S	0	0
			3982	2522	679	768	13		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	1613	Total	C	N	O	S	0	0
			9380	5798	1748	1822	12		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	663	Total	C	N	O	S	0	0
			5263	3333	913	995	22		

- Molecule 23 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	LO	834	Total	C	N	O	P	S	0	0
			6639	4223	1140	1256	1	19		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	380	Total	C	N	O	S	0	0
			3220	2081	545	578	16		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	841	Total	C	N	O	S	0	0
			6707	4284	1125	1271	27		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	793	Total	C	N	O	S	0	0
			6207	3931	1044	1203	29		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	LS	480	Total	C	N	O	P	S	0	0
			3793	2402	666	715	1	9		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	873	Total	C	N	O	S	0	0
			6876	4363	1188	1303	22		

- Molecule 29 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	460	Total	C	N	O	S	0	0
			3756	2349	685	706	16		

- Molecule 30 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	405	Total	C	N	O	S	0	0
			3286	2083	567	626	10		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	535	Total	C	N	O	S	0	0
			4237	2656	762	807	12		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	852	Total	C	N	O	S	0	0
			6803	4350	1173	1254	26		
32	LY	846	Total	C	N	O	S	0	0
			6179	3918	1079	1165	17		

- Molecule 33 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LZ	181	Total	C	N	O	S	0	0
			1524	964	286	267	7		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NA	286	Total	C	N	O	S	0	0
			2075	1279	378	414	4		

- Molecule 35 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NB	267	Total	C	N	O	S	0	0
			1873	1156	360	356	1		

- Molecule 36 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NC	250	Total	C	N	O	S	0	0
			1693	1015	345	330	3		

- Molecule 37 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	ND	74	Total	C	N	O	0	0
			609	380	119	110		

- Molecule 38 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NE	215	Total	C	N	O	S	0	0
			1649	1021	327	298	3		

- Molecule 39 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NF	141	Total	C	N	O	S	0	0
			1135	725	214	194	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NG	119	Total	C	N	O	S	0	0
			875	541	166	165	3		

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NH	1077	Total	C	N	O	S	0	0
			8693	5650	1434	1585	24		

- Molecule 42 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NI	240	Total	C	N	O	S	0	0
			1953	1248	331	366	8		

- Molecule 43 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	NK	257	Total	C	N	O	S	0	0
			2107	1344	369	381	13		

- Molecule 44 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	NM	230	Total	C	N	O	S	0	0
			1838	1163	337	334	4		

- Molecule 45 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	NN	267	Total	C	N	O	S	0	0
			1481	909	280	292			

- Molecule 46 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 47 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	OA	13	Total	C	N	O	S	0	0
			96	63	14	19			

- Molecule 48 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SA	388	Total	C	N	O	S	0	0
			3056	1938	525	584	9		

- Molecule 49 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	436	Total	C	N	O	S	0	0
			3357	2116	574	657	10		

- Molecule 50 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	241	Total	C	N	O	S	0	0
			1871	1185	337	339	10		
50	SD	232	Total	C	N	O	S	0	0
			1817	1153	324	330	10		

- Molecule 51 is a protein called 13 kDa ribonucleoprotein-associated protein.

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

- Molecule 52 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	SG	453	Total	C	N	O	P	S	0	0
			3627	2302	633	681	1	10		

- Molecule 53 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 54 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SI	815	Total	C	N	O	S	0	0
			6616	4243	1167	1177	29		

- Molecule 55 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SJ	213	Total	C	N	O	S	0	0
			1678	1069	292	306	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SK	229	Total	C	N	O	S	0	0
			1793	1141	312	329	11		

- Molecule 56 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SL	173	Total	C	N	O	S	0	0
			1384	881	254	239	10		

- Molecule 57 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SN	253	Total	C	N	O	S	0	0
			2053	1313	364	368	8		

- Molecule 59 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SP	2156	Total	C	N	O	S	0	0
			17548	11328	2906	3254	60		

- Molecule 60 is a protein called rRNA-processing protein FCF2.

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

- Molecule 61 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 62 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SS	253	Total	C	N	O	S	0	0
			2102	1314	389	391	8		

- Molecule 63 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	ST	588	Total	C	N	O	S	0	0
			4482	2845	808	817	12		

- Molecule 64 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SU	534	Total	C	N	O	S	0	0
			4370	2845	709	802	14		

- Molecule 65 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SV	147	Total	C	N	O		0	0
			869	529	160	180			

- Molecule 66 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SW	199	Total	C	N	O	S	0	0
			1565	998	284	279	4		

- Molecule 67 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SY	233	Total	C	N	O	S	0	0
			1953	1218	379	349	7		

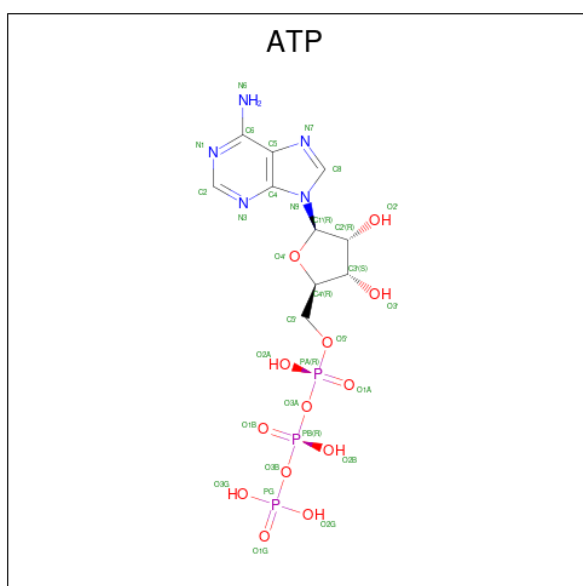
- Molecule 68 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SZ	259	Total	C	N	O		0	0
			1314	796	259	259			

- Molecule 69 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
69	L1	22	Total	Mg	0
			22	22	
69	L2	1	Total	Mg	0
			1	1	
69	NH	1	Total	Mg	0
			1	1	
69	SI	1	Total	Mg	0
			1	1	

- Molecule 70 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

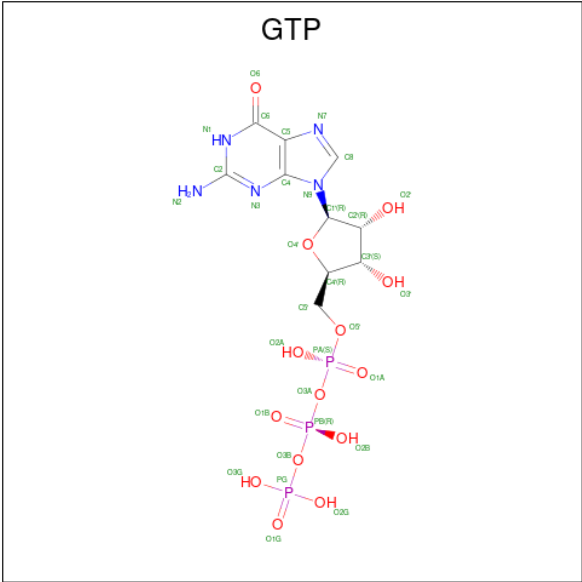


Mol	Chain	Residues	Atoms					AltConf
70	NH	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 71 is ZINC ION (CCD ID: ZN) (formula: Zn).

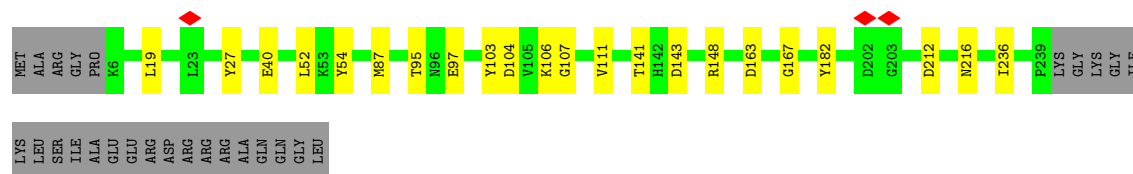
Mol	Chain	Residues	Atoms		AltConf
71	NQ	1	Total	Zn	0
			1	1	
71	SL	1	Total	Zn	0
			1	1	

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



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





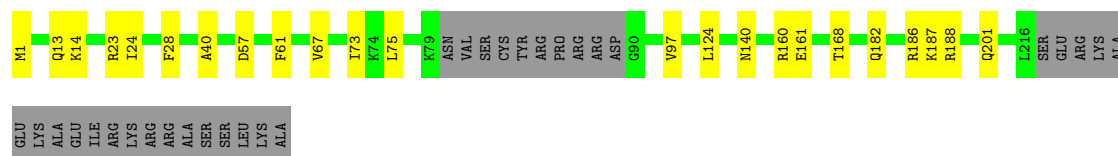
- Molecule 6: 40S ribosomal protein S5

Chain L5: 83% 8% 8%



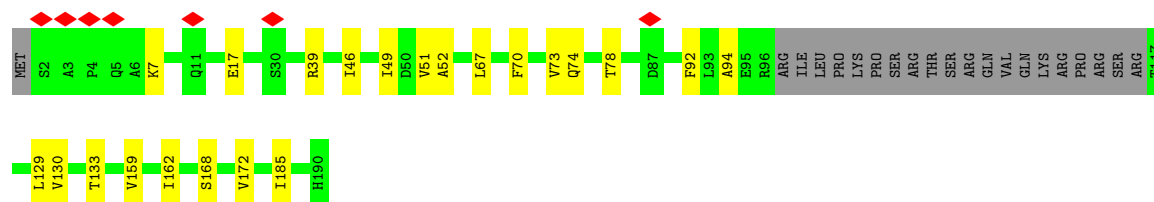
- Molecule 7: 40S ribosomal protein S6-A

Chain L6: 78% 10% 13%



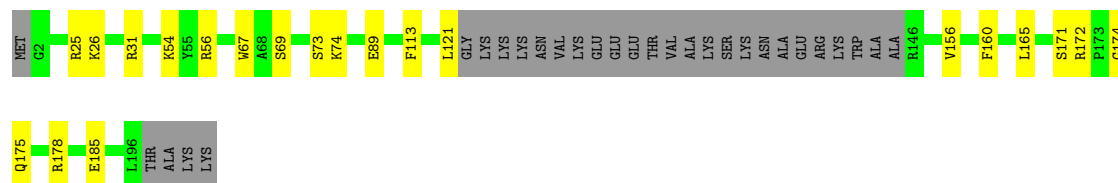
- Molecule 8: 40S ribosomal protein S7-A

Chain L7: 77% 12% 11%



- Molecule 9: 40S ribosomal protein S8-A

Chain L8: 75% 10% 14%



- Molecule 10: 40S ribosomal protein S9-A

Chain L9: 76% 11% 13%



ALA
ALA
ASP
GLU
GLU
ALA
ASP
GLU
ALA
ASP
GLU
GLU

- Molecule 11: 40S ribosomal protein S16-A

Chain LC:  77% 10% 13%

MET SER A3 E40 R45 V48 Y49 E50 F51 L52 L53 L54 D58 K59 F60 G72 R82 V97 D98 S101 L105 D120 K127 LYS PHE GLY LYS GLY ALA ARG SER ARG PHE GLN LYS SER TYR ARG

- Molecule 12: 40S ribosomal protein S11-A

Chain LD:  78% 10% 12%

MET SER THR GLU LEU THR V7 K29 L71 T72 G73 T78 K79 I84 R88 R103 N106 V111 I122 V123 T124 S132 R136 V139 V140 S143 ALA ALA ALA GLY LYS ALA ASN LYS GLN PHE ALA LYS PHE

- Molecule 13: 40S ribosomal protein S22-A

Chain LE:  91% 8% .

MET T2 A8 L11 N12 M15 H56 N70 W81 N92 L93 T105 S122 Y130

- Molecule 14: 40S ribosomal protein S24-A

Chain LF:  59% 12% 30%

MET SER A4 K11 P16 L17 N31 D38 E39 L40 L44 D53 N77 S78 V79 K83 E86 E87 T88 L91 G95 L96 A97 E98 LYS VAL GLU LYS ALA SER ARG GLN GLN ARG LYS GLN LYS LYS ASN ARG ASP LYS ILE PHE GLY THR GLY

LYS ARG LEU ALA LYS VAL ARG ALA ARG ASN ALA ASP

- Molecule 15: 40S ribosomal protein S28-A

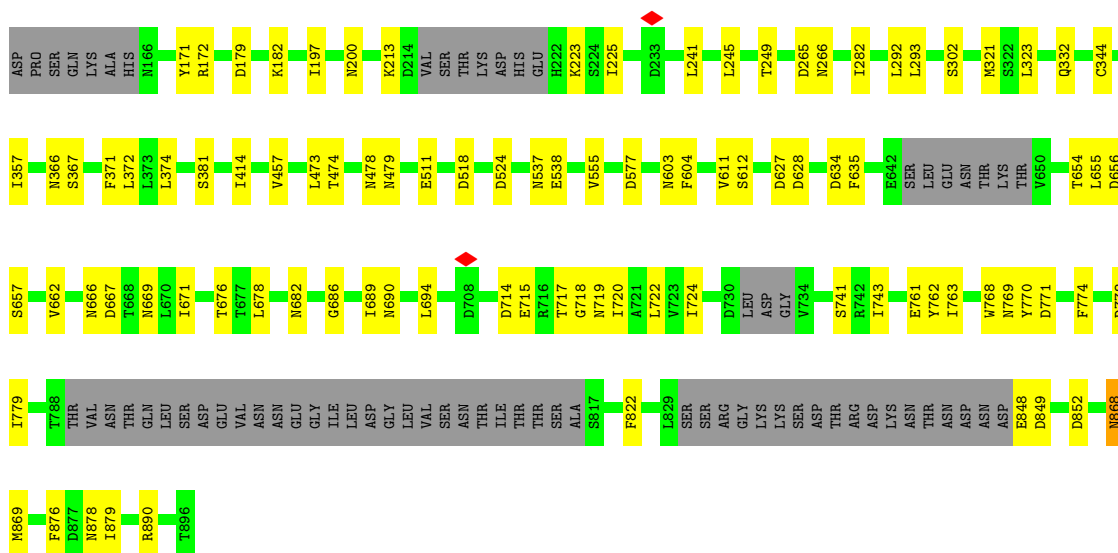
Chain LG:  82% 10% 7%

MET ASP ASN LYS THR P6 V12 V30 E58 R64 R65 L66 R67

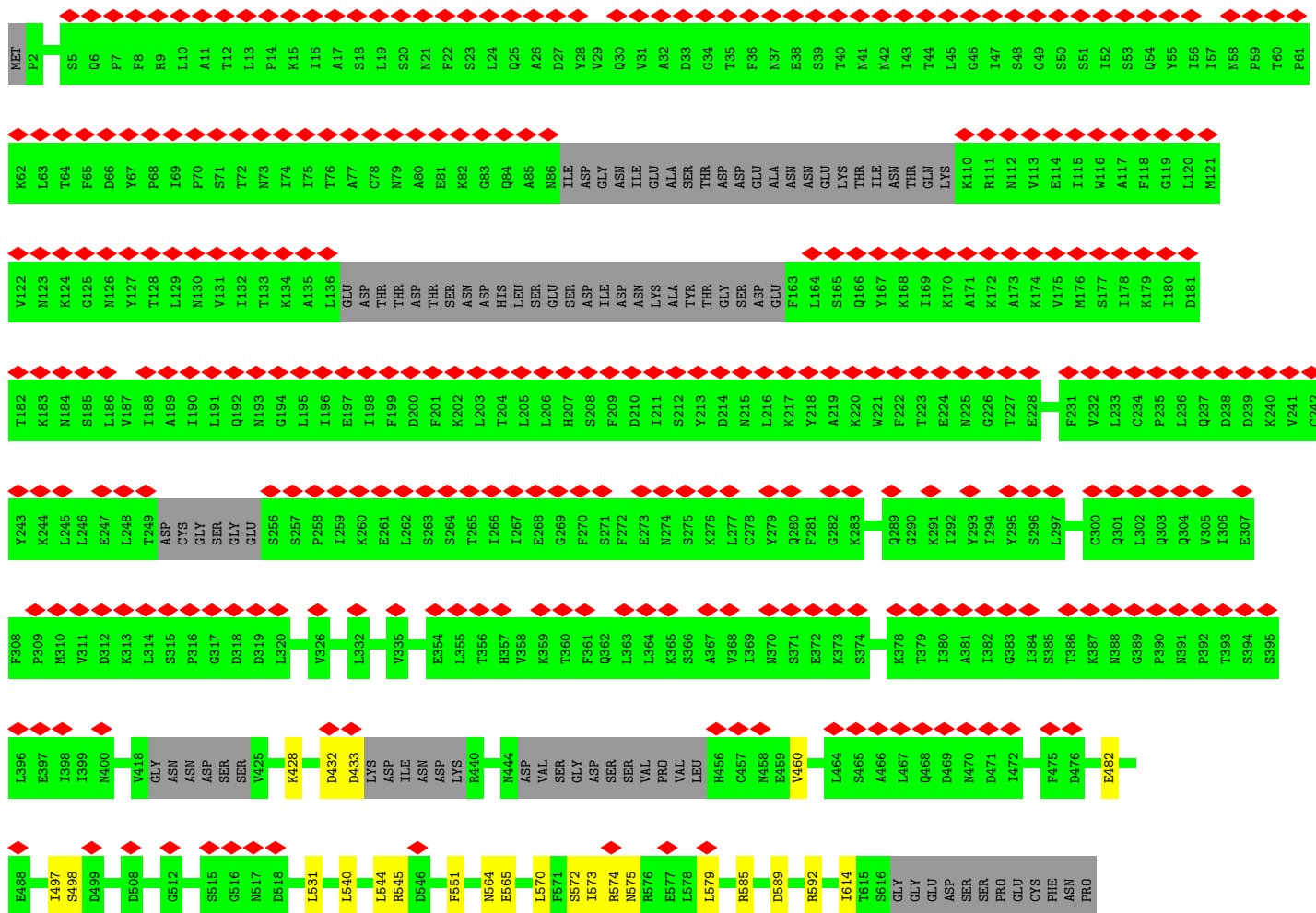
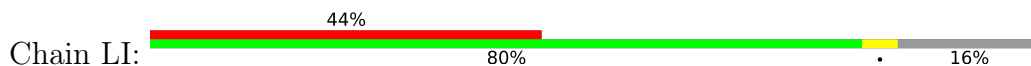
- Molecule 16: NET1-associated nuclear protein 1

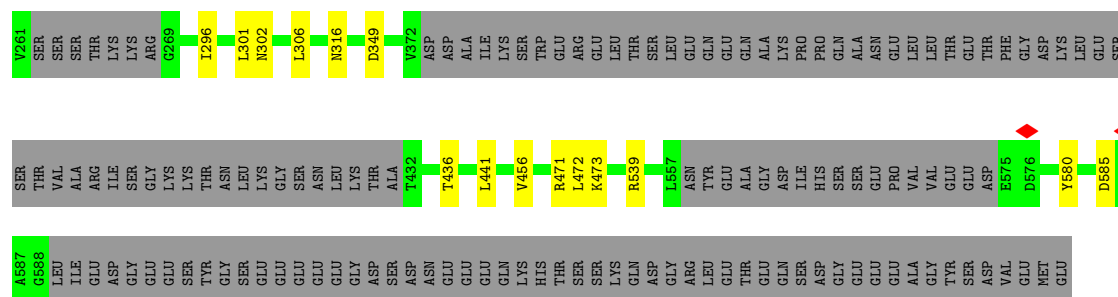
Chain LH:  77% 13% 10%

MET THR GLN SER LEU GLY ILE GLU Q9 S27 V28 T29 N71 S72 L73 L74 S75 S76 I77 F78 L79 GLN GLU GLU ASN N85 E86 V89 D95 I96 T97 V98 PRO GLN GLN GLU ASP A104 F110 T111 N112 N113 I117 L125 H131 E139 Y151 K158

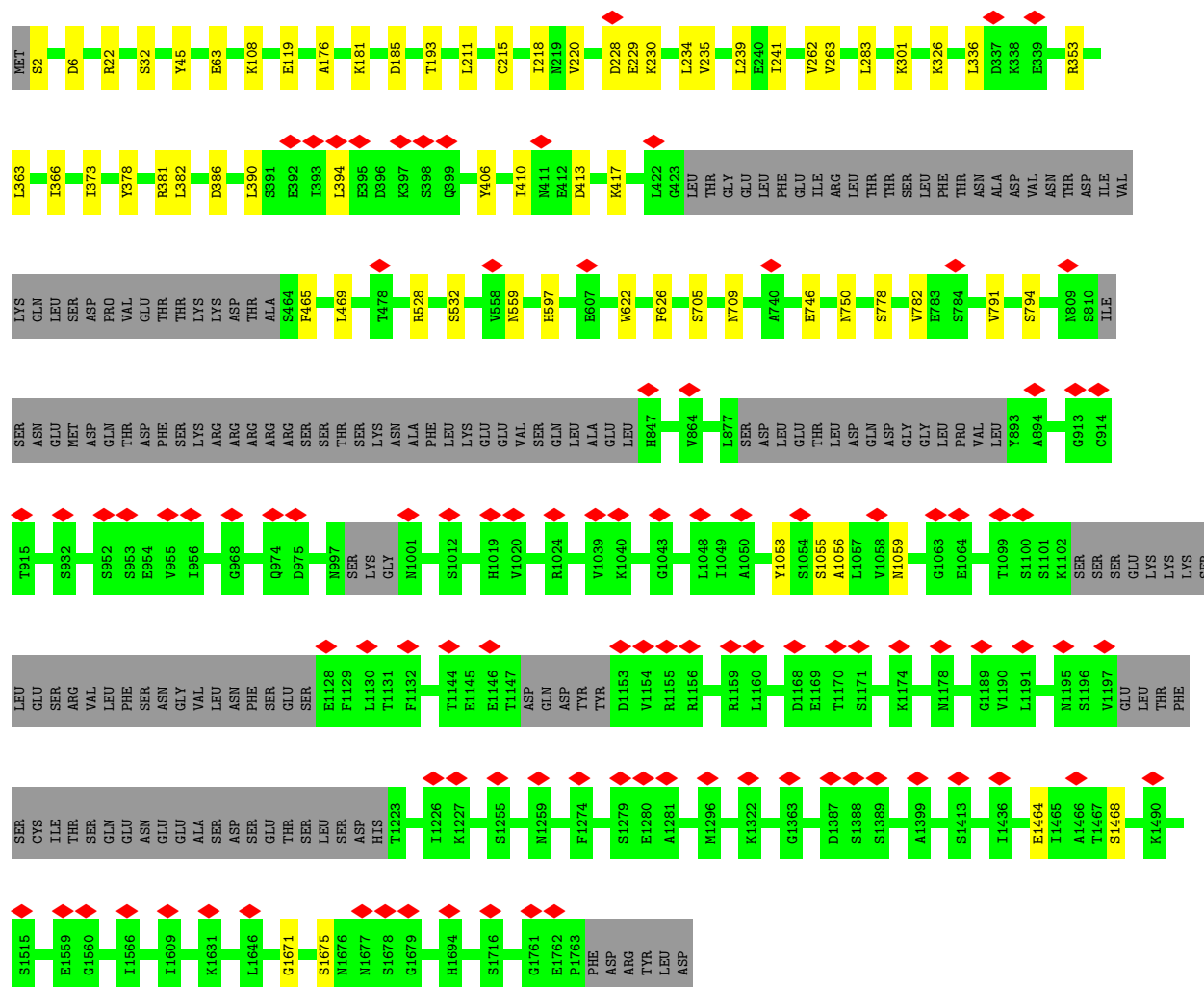
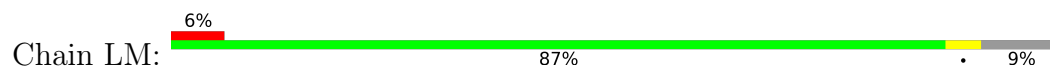


- Molecule 17: U3 small nucleolar RNA-associated protein 8

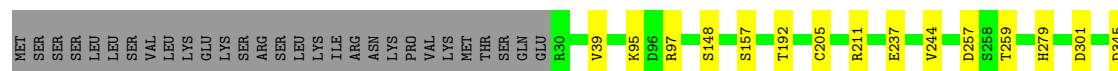
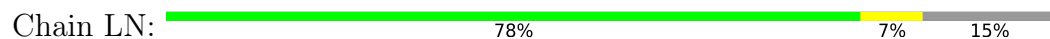




• Molecule 21: U3 small nucleolar RNA-associated protein 10

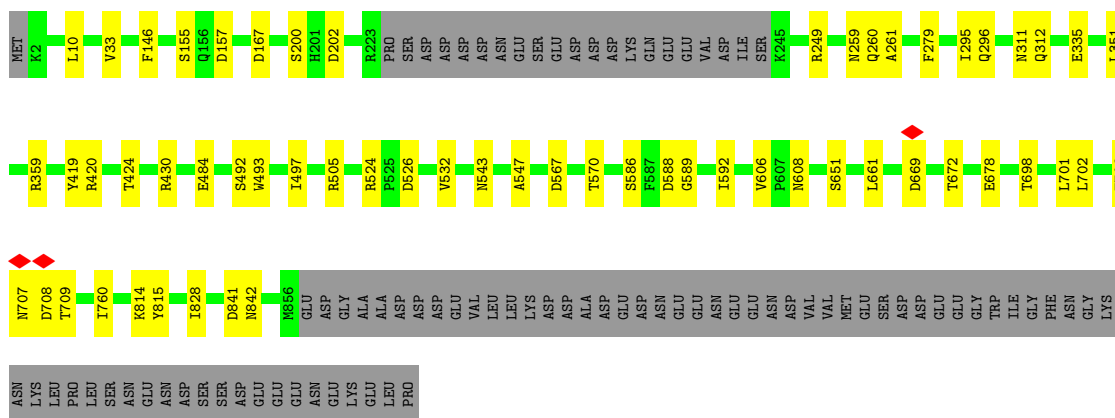


• Molecule 22: U3 small nucleolar RNA-associated protein 4



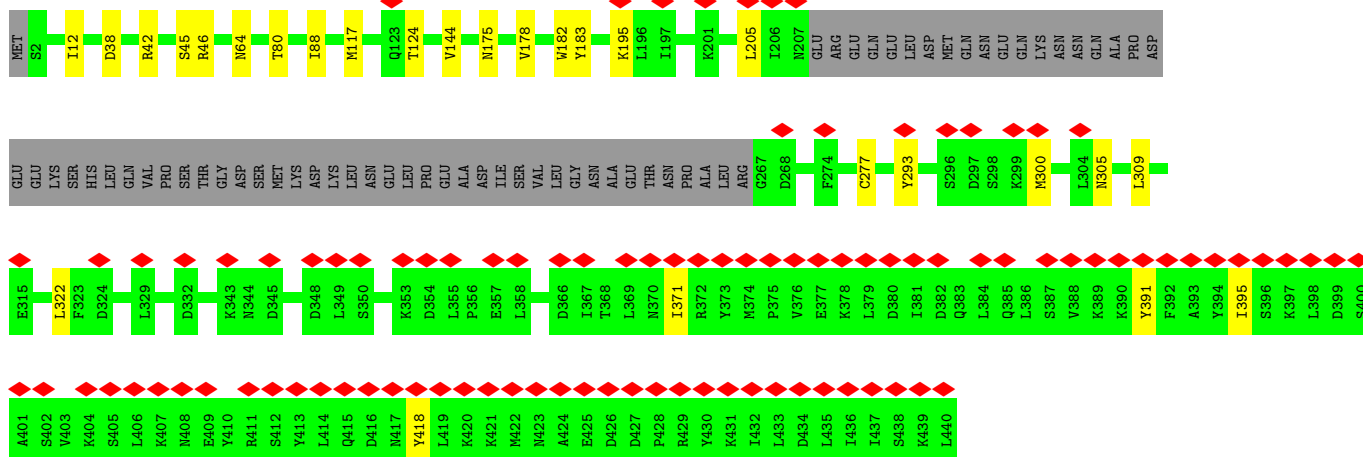
- Molecule 23: Periodic tryptophan protein 2

Chain LO:  84% 7% 10%



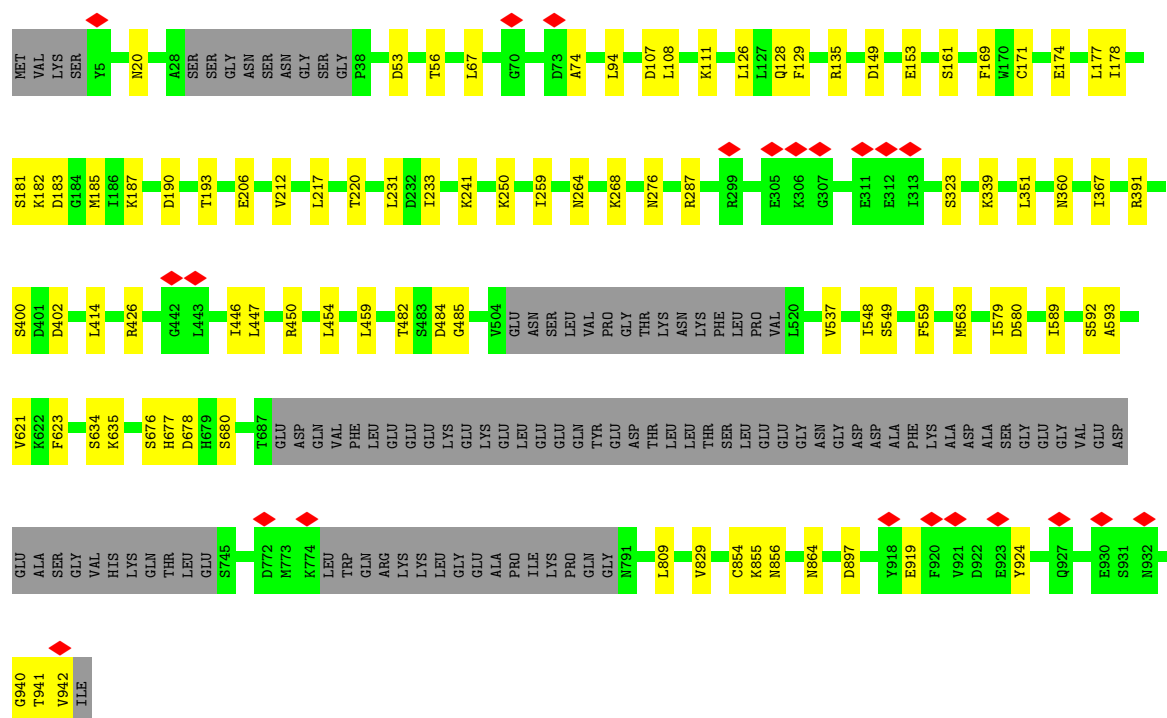
- Molecule 24: U3 small nucleolar RNA-associated protein 6

Chain LP: 

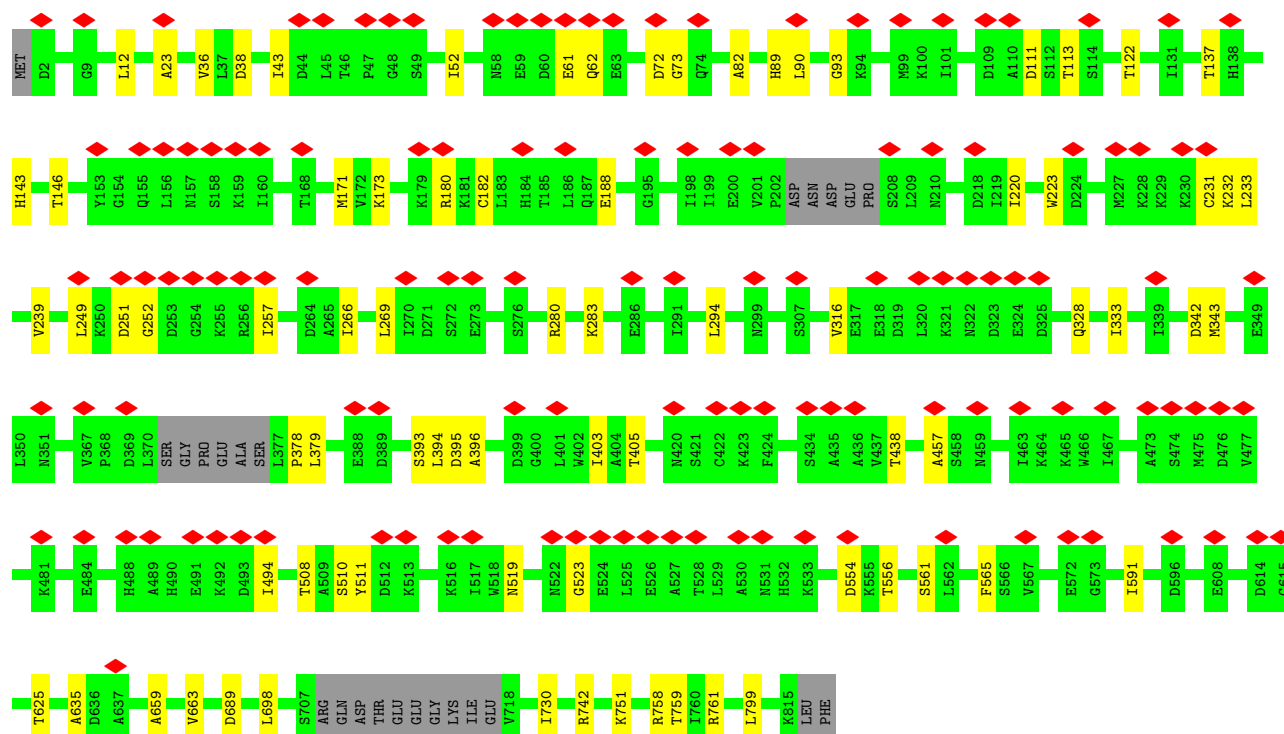


- Molecule 25: U3 small nucleolar RNA-associated protein 12

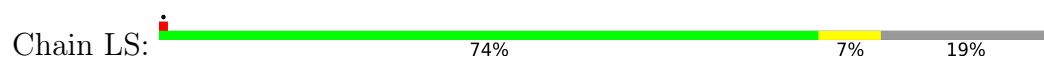
Chain LQ: 80% 9% 11%

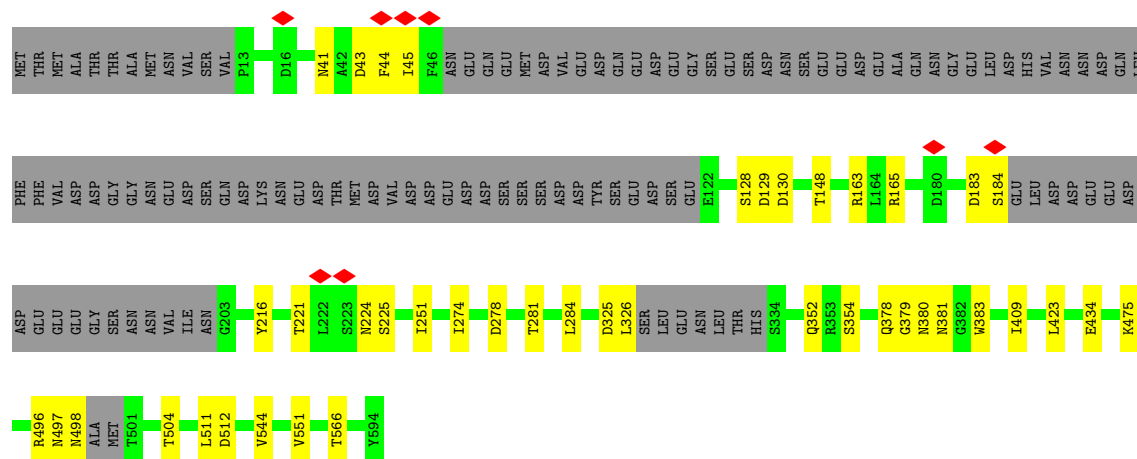


- Molecule 26: U3 small nucleolar RNA-associated protein 13



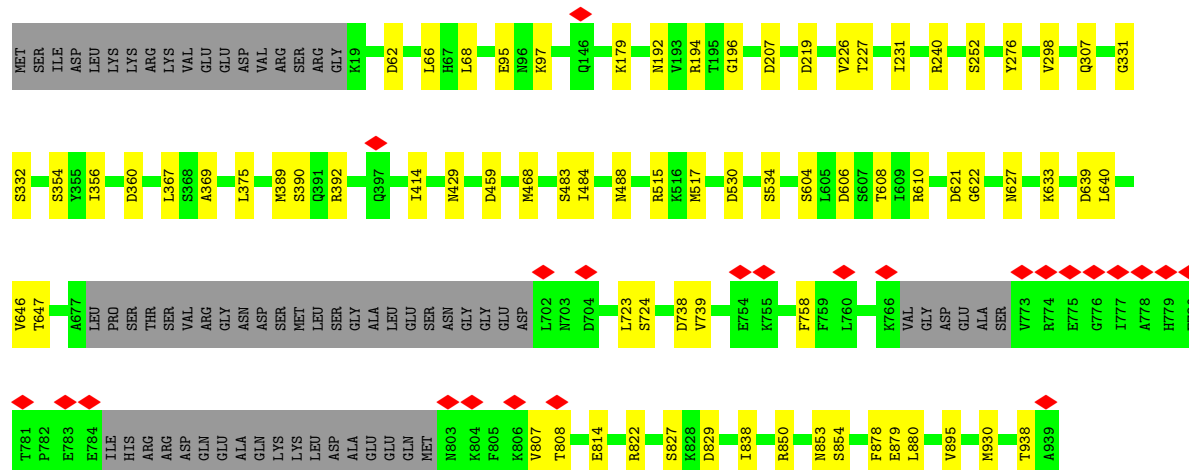
- Molecule 27: U3 small nucleolar RNA-associated protein 18





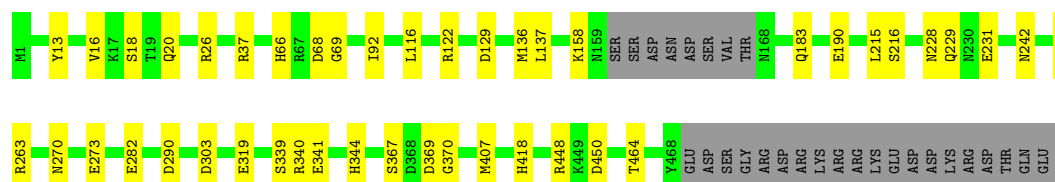
• Molecule 28: U3 small nucleolar RNA-associated protein 21

Chain LT: 85% 8% 7%



• Molecule 29: Protein SOF1

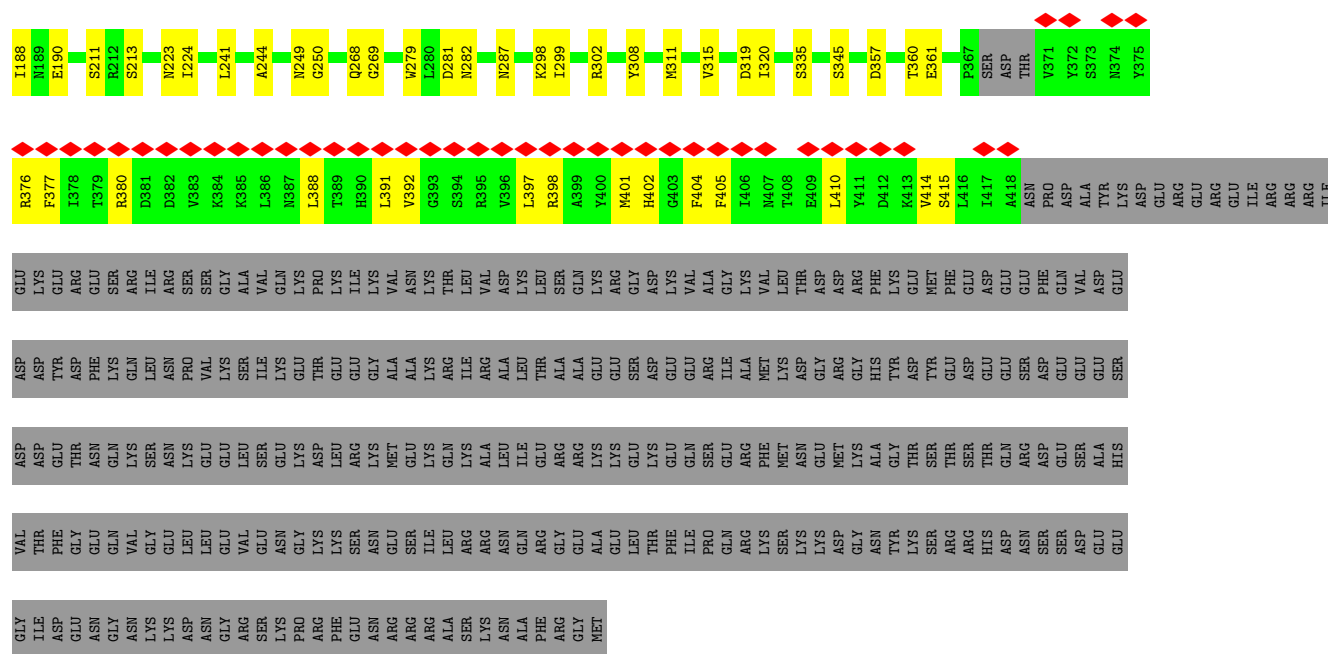
Chain LU: 85% 9% 6%



• Molecule 30: Ribosome biogenesis protein ENP2

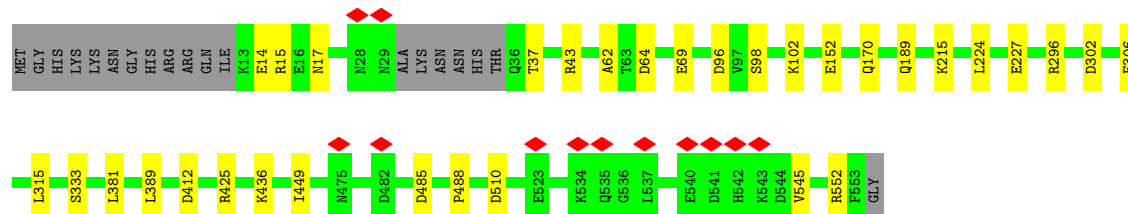
Chain LV: 6% 47% 10% 43%





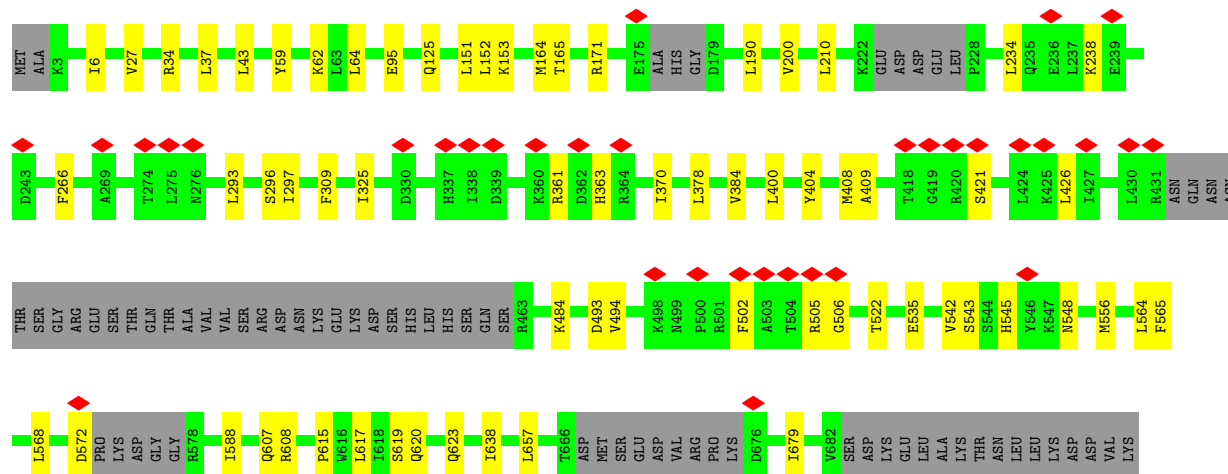
- Molecule 31: U3 small nucleolar RNA-associated protein 7

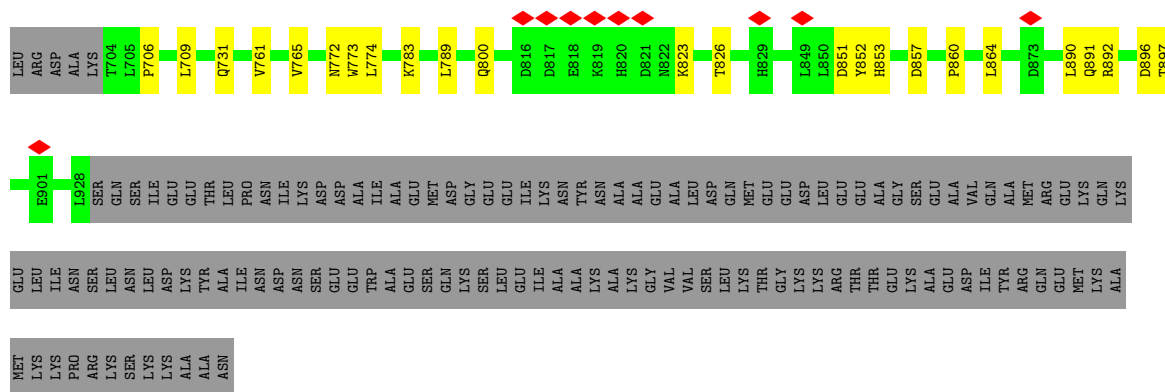
Chain LW: 91% 6%



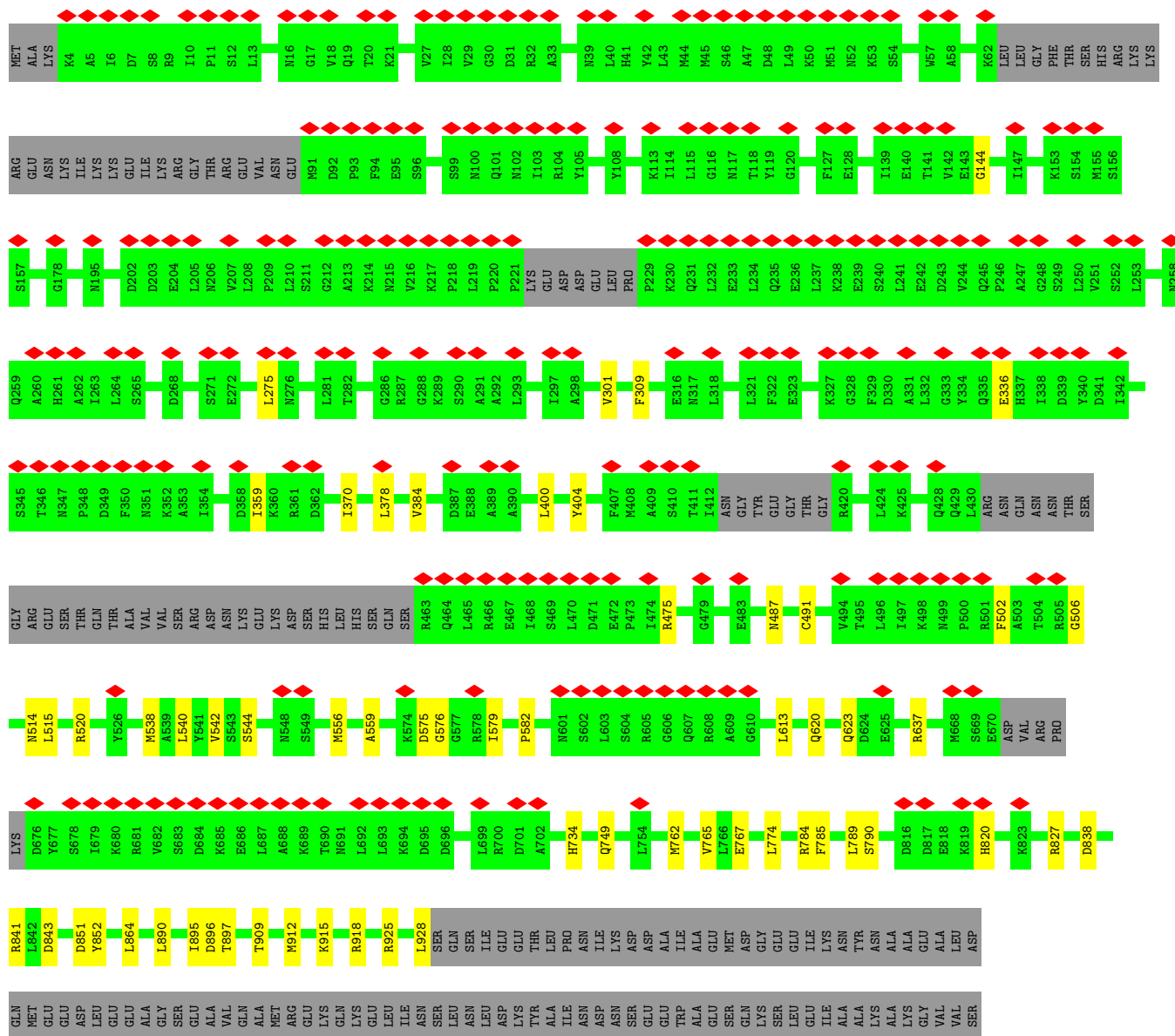
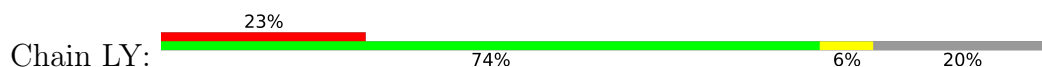
- Molecule 32: RNA cytidine acetyltransferase

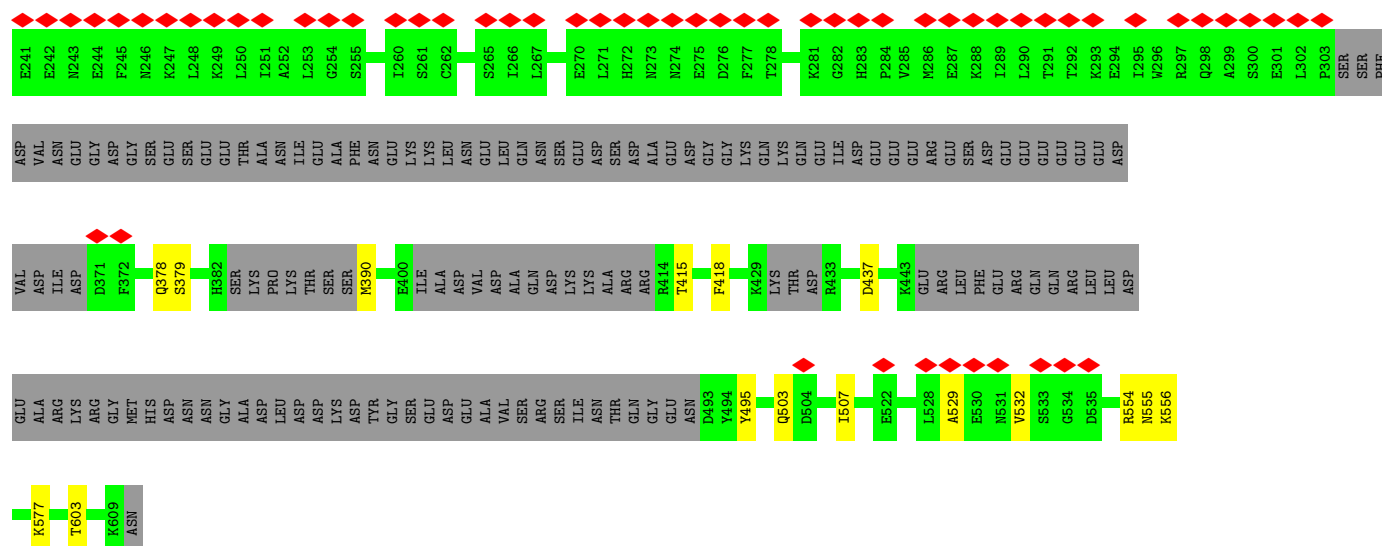
Chain LX: 72% 9% 19%



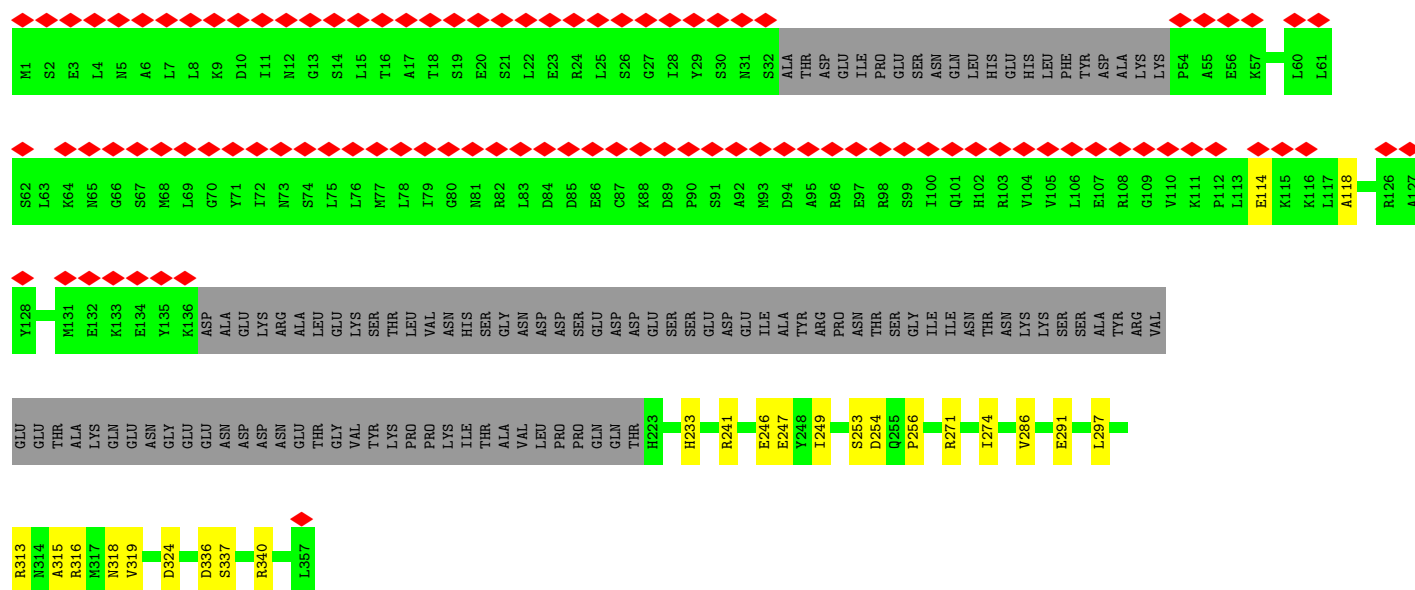


• Molecule 32: RNA cytidine acetyltransferase

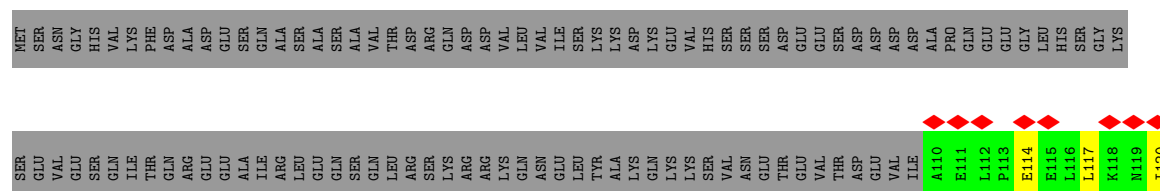


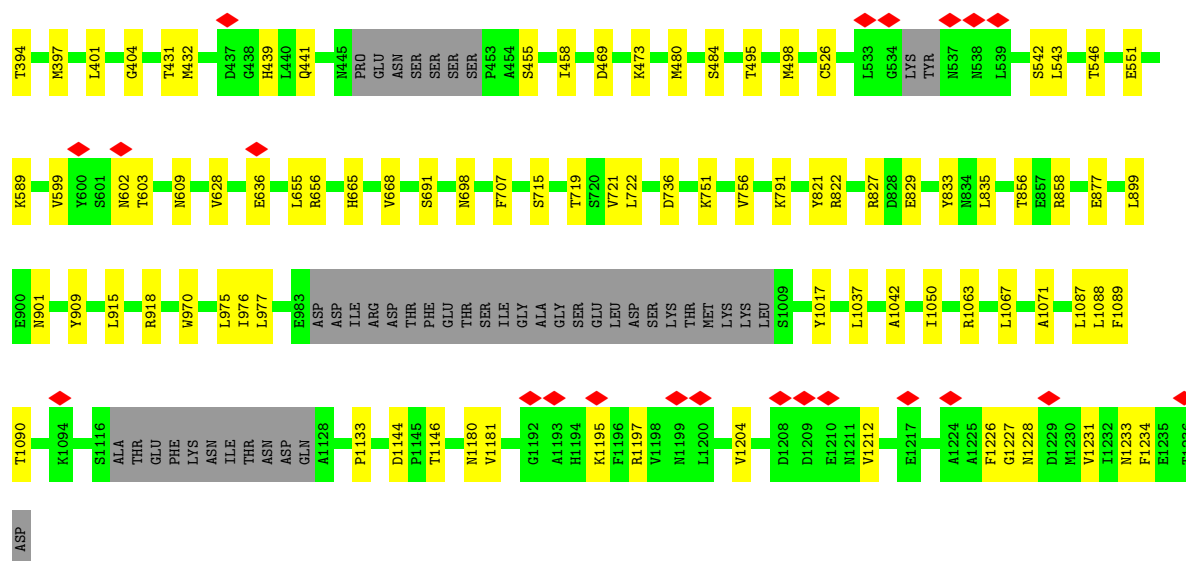


• Molecule 36: U3 small nucleolar ribonucleoprotein protein LCP5

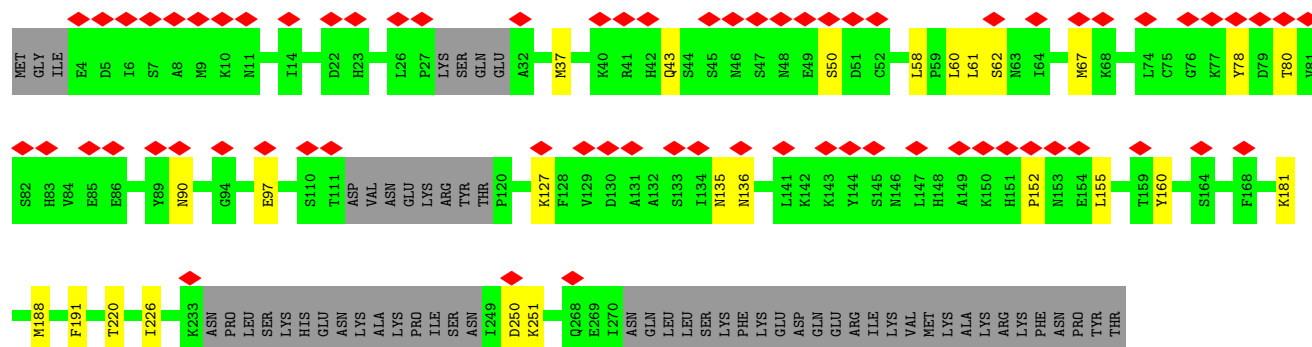
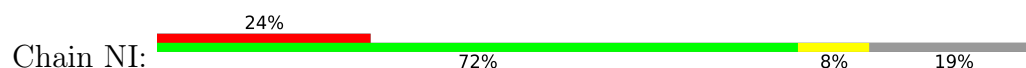


• Molecule 37: Bud site selection protein 21

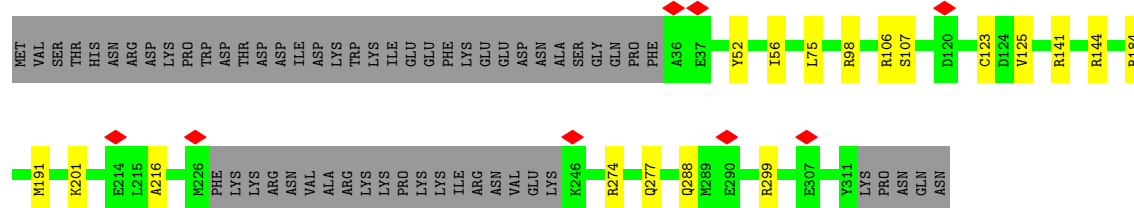
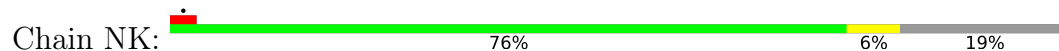




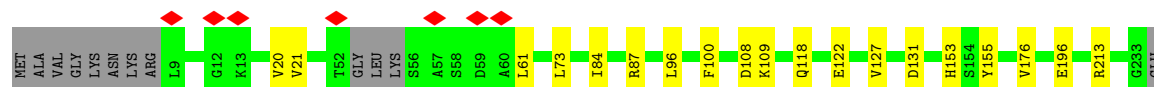
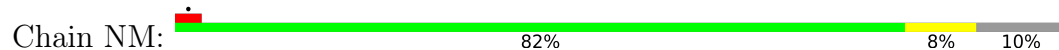
• Molecule 42: Ribosomal RNA-processing protein 7

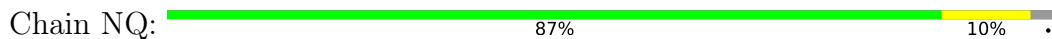


• Molecule 43: KRR1 small subunit processome component

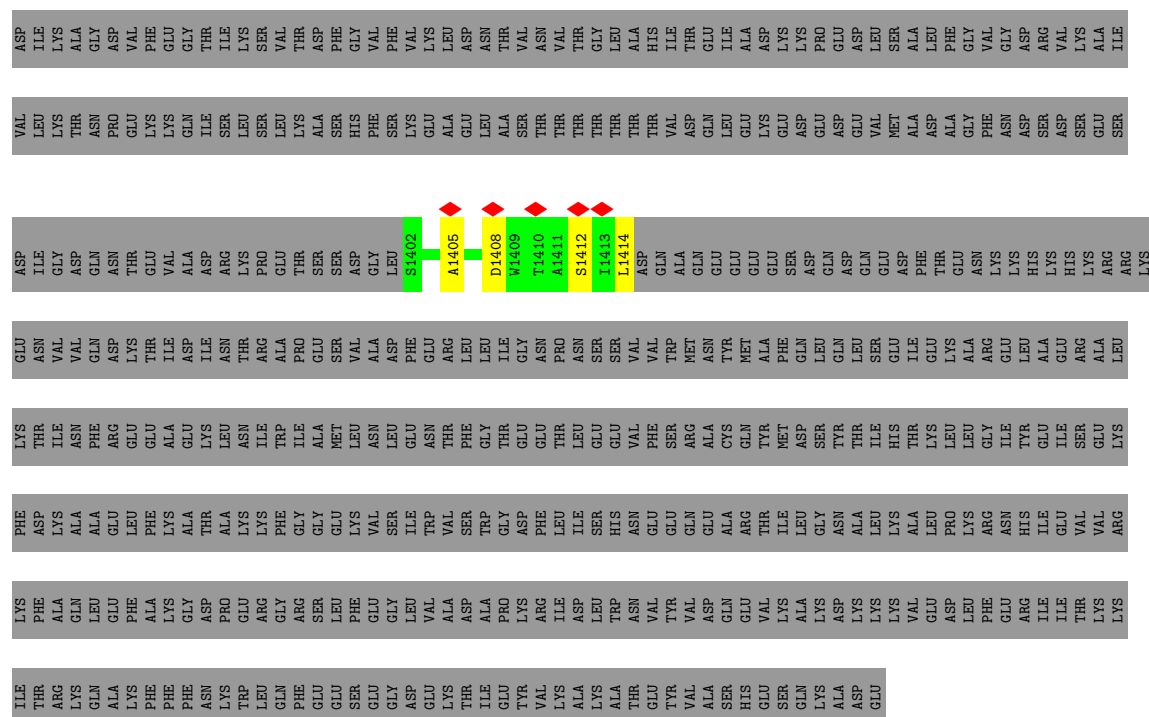


• Molecule 44: Small ribosomal subunit protein eS1A

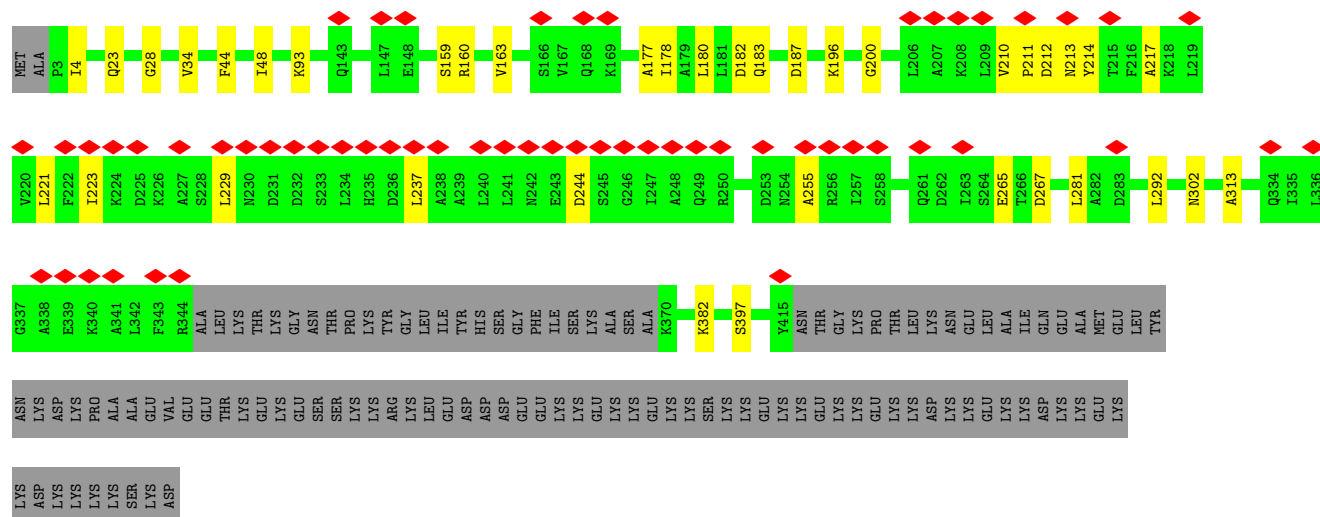




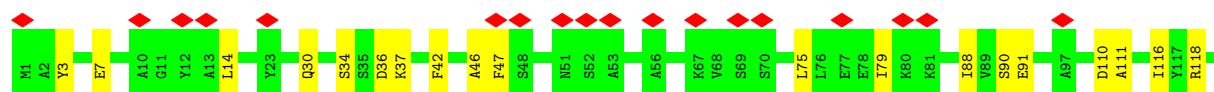
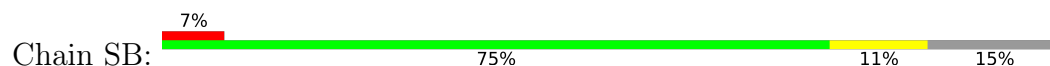


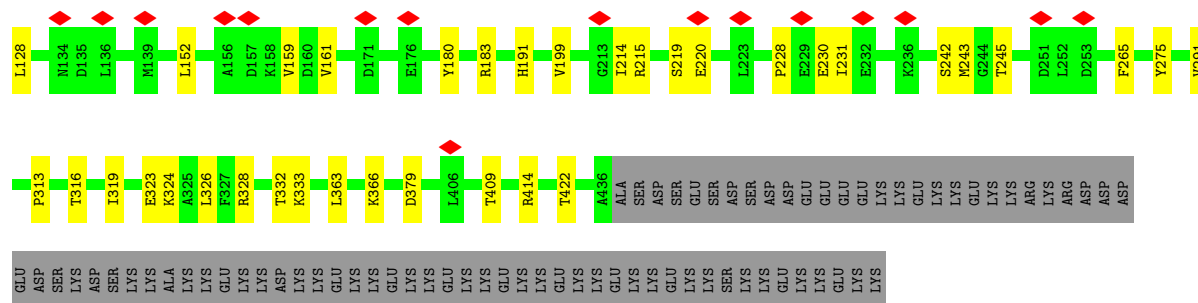


• Molecule 48: Nucleolar protein 56

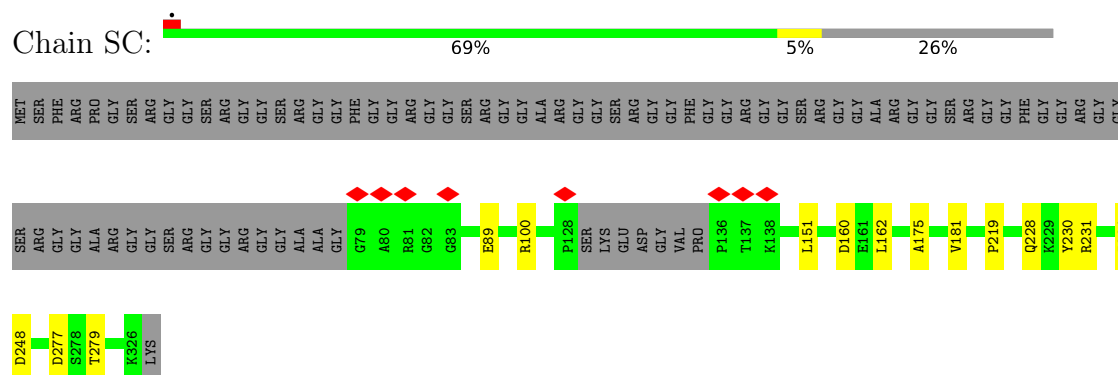


• Molecule 49: Nucleolar protein 58

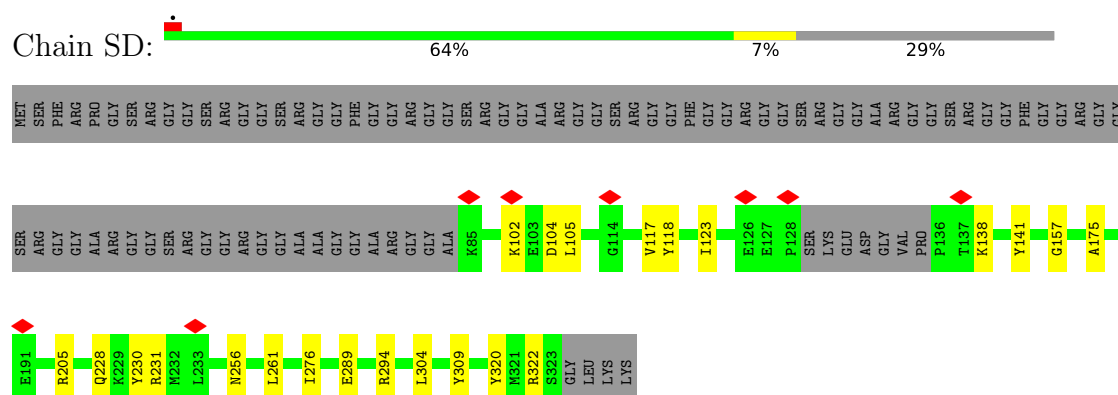




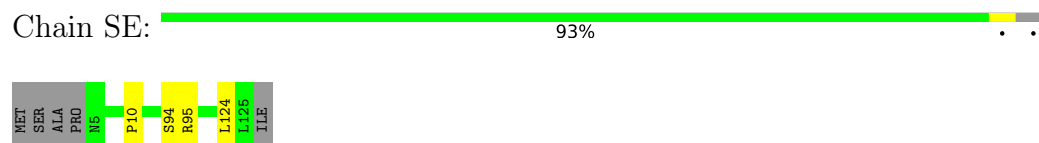
- Molecule 50: rRNA 2'-O-methyltransferase fibrillar



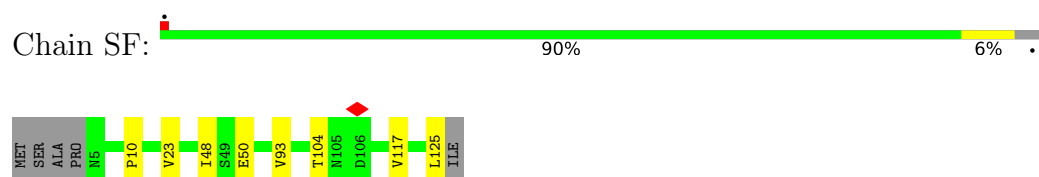
- Molecule 50: rRNA 2'-O-methyltransferase fibrillar



- Molecule 51: 13 kDa ribonucleoprotein-associated protein

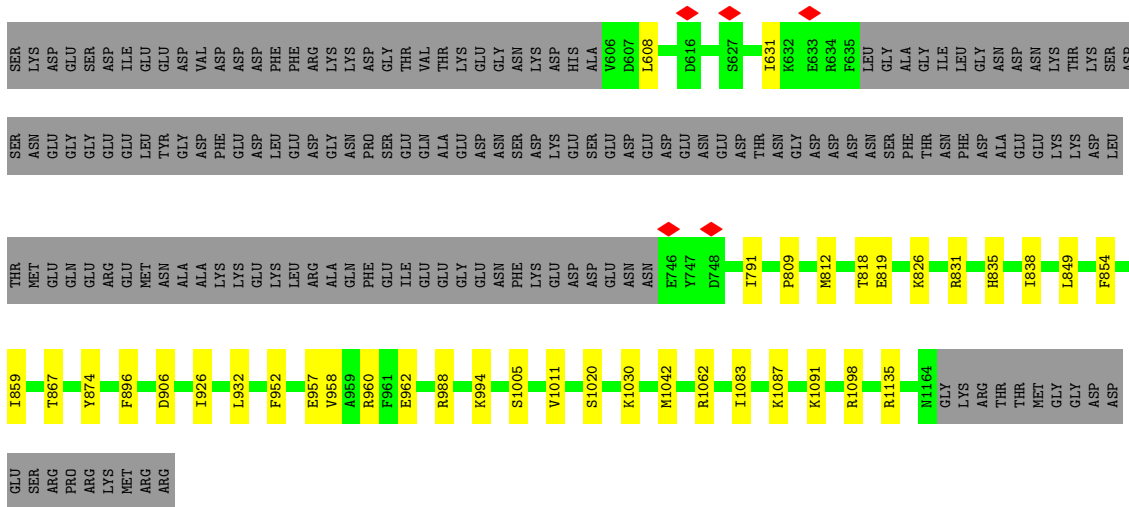


- Molecule 51: 13 kDa ribonucleoprotein-associated protein

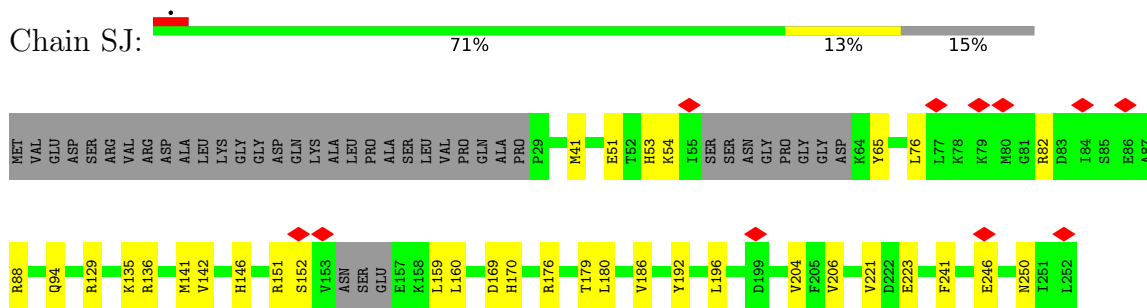


Chain SG: 71% 8% 21%

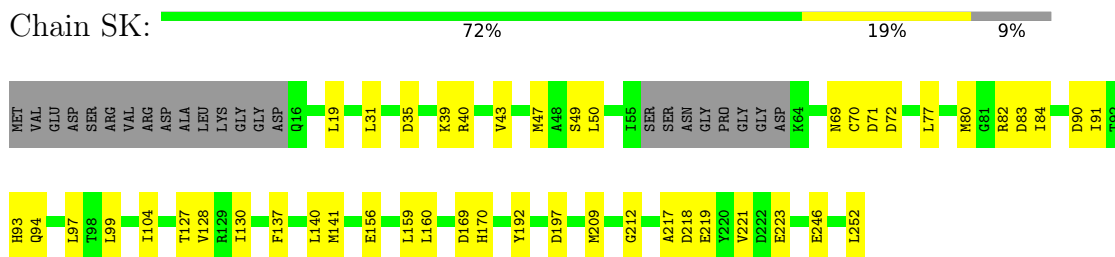




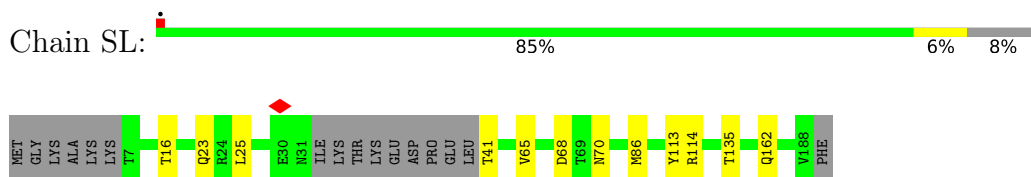
- Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1



- Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

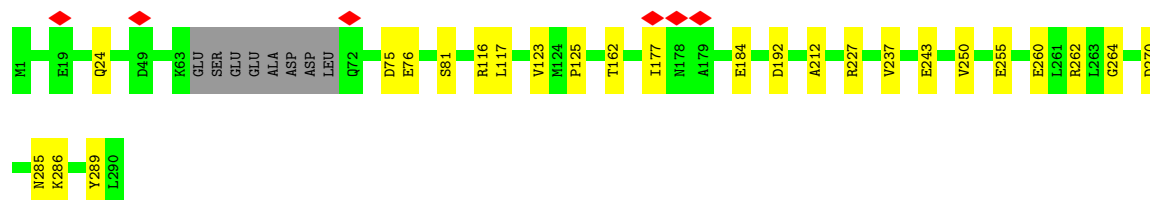


- Molecule 56: rRNA-processing protein FCF1

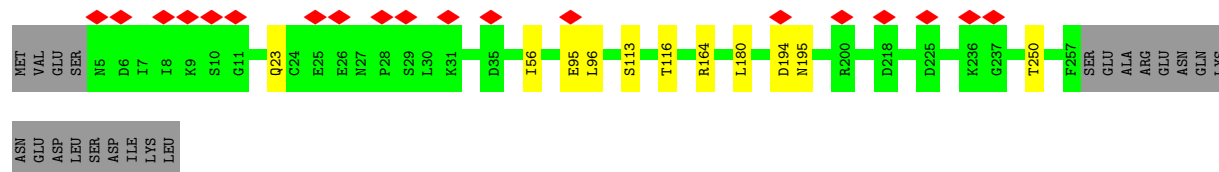
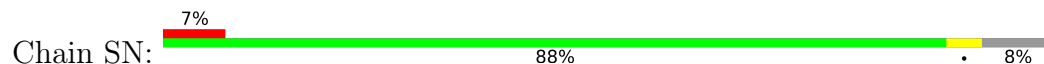


- Molecule 57: U3 small nucleolar ribonucleoprotein protein IMP4

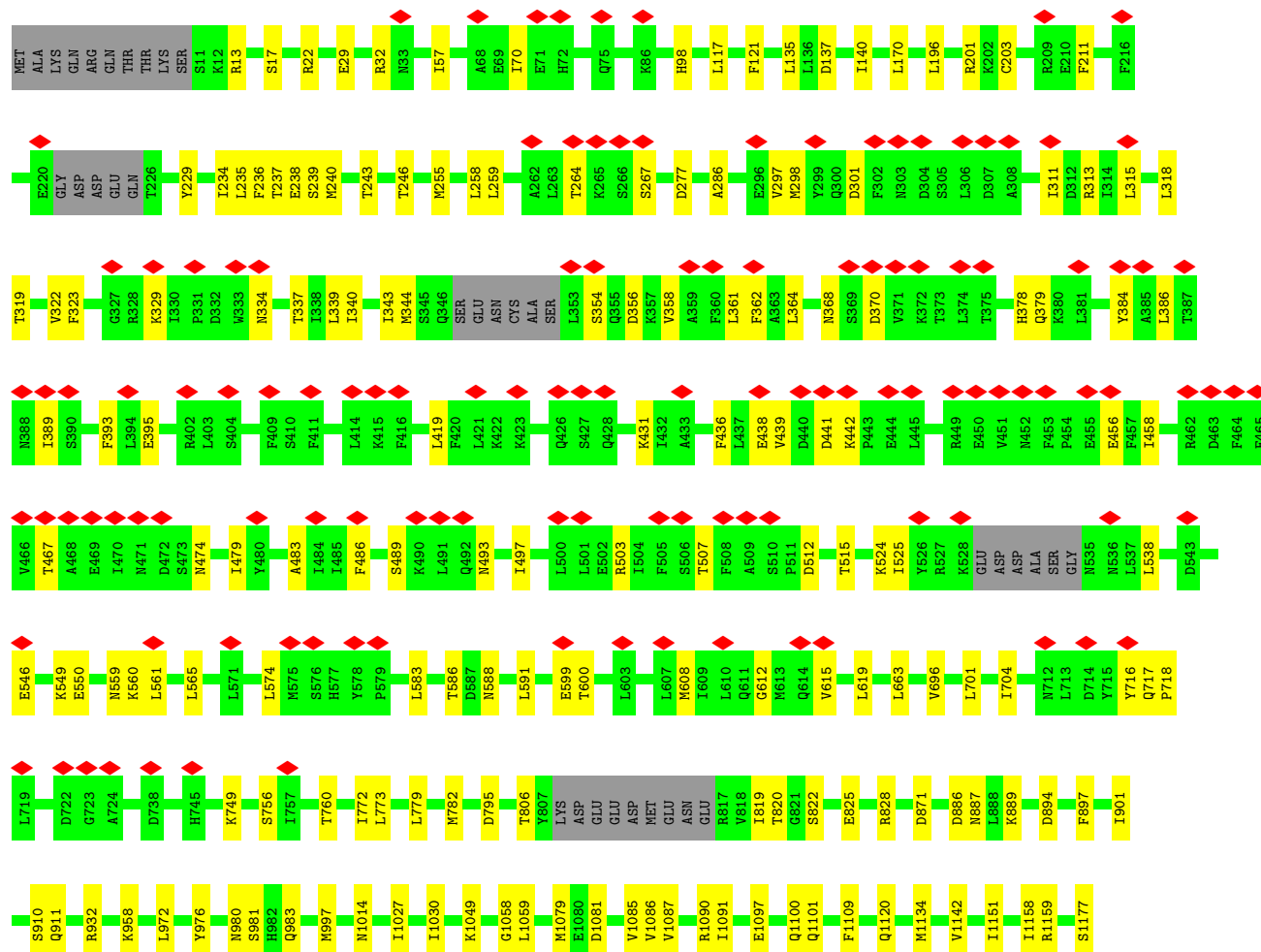
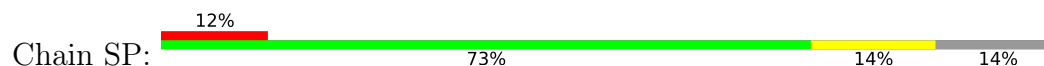


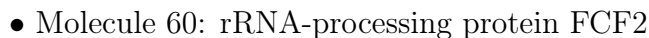


- Molecule 58: Ribosome biogenesis protein UTP30

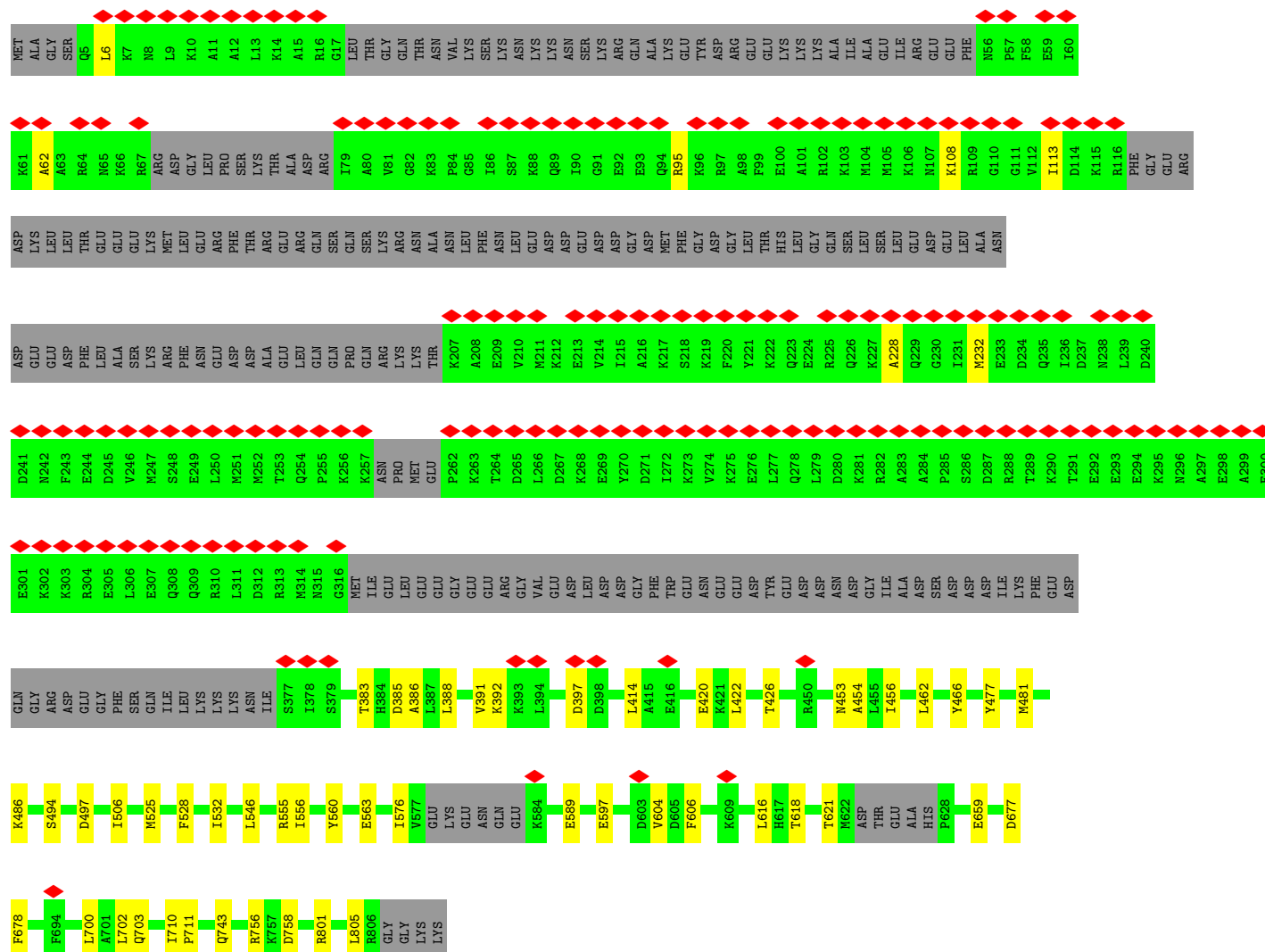


- Molecule 59: U3 small nucleolar RNA-associated protein 20

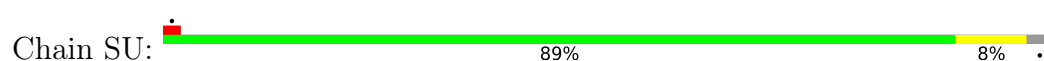




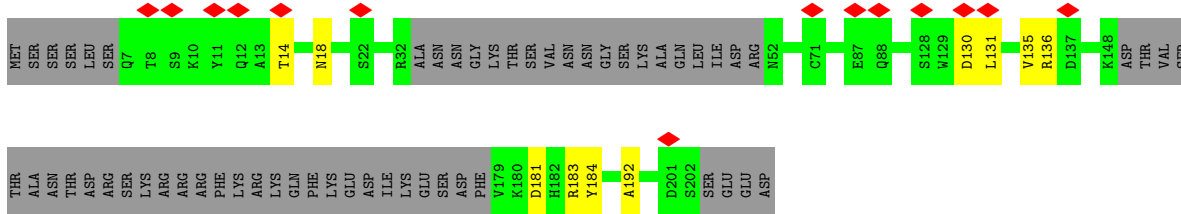
- Molecule 63: Nucleolar complex protein 14



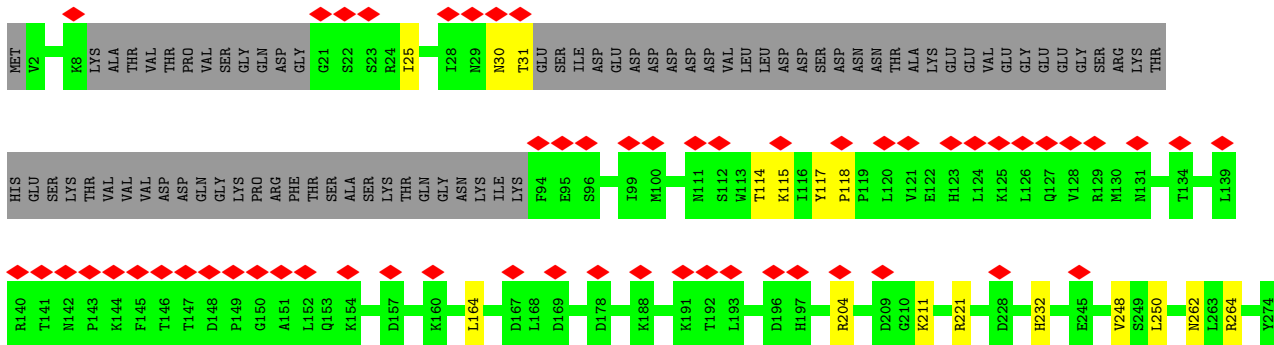
- Molecule 64: Nucleolar complex protein 4



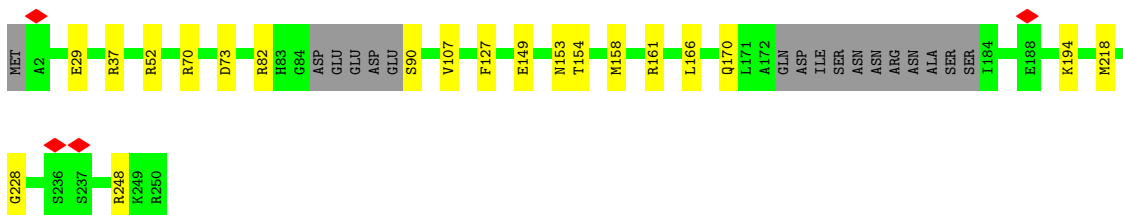
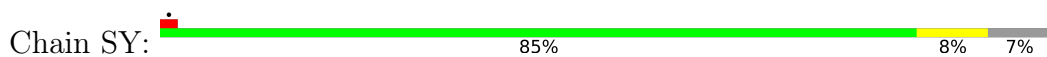
- Molecule 65: Regulator of rDNA transcription protein 14



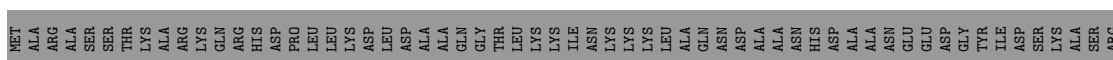
- Molecule 66: Pre-rRNA-processing protein PNO1

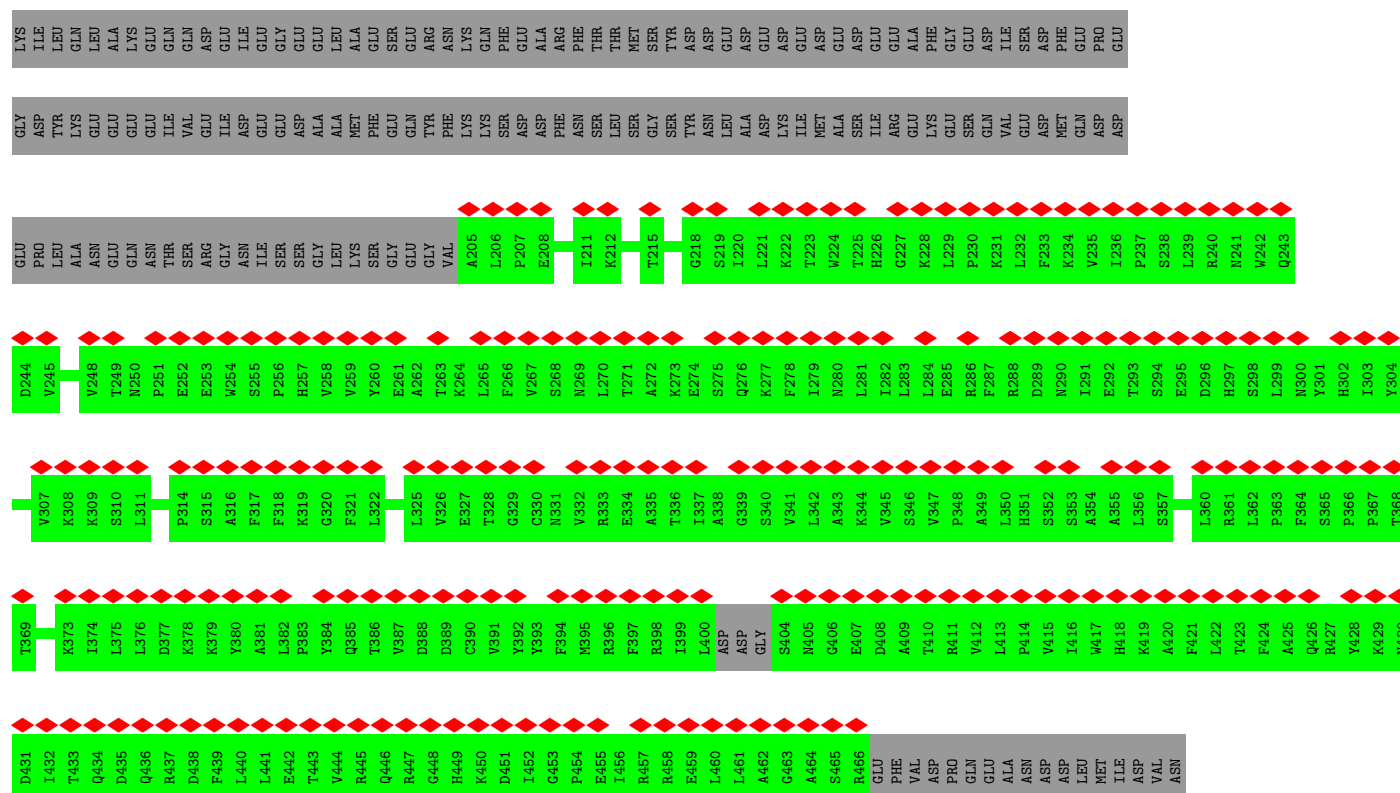


- Molecule 67: U3 small nucleolar RNA-associated protein 11



- Molecule 68: Essential nuclear protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.228	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.128	Depositor
Map value standard deviation	0.212	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	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, ATP, MG, SEP, GTP

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	0.10	0/12478	0.24	0/19437
2	L1	0.10	0/27400	0.26	0/42643
3	L2	0.10	0/4143	0.22	0/6440
4	L3	0.12	0/794	0.27	0/1069
5	L4	0.12	0/1906	0.31	0/2572
6	L5	0.12	0/1655	0.31	0/2237
7	L6	0.14	0/1674	0.31	0/2236
8	L7	0.14	0/1369	0.35	0/1846
9	L8	0.13	0/1379	0.31	0/1844
10	L9	0.12	0/1410	0.29	0/1888
11	LC	0.14	0/990	0.32	0/1335
12	LD	0.17	0/1138	0.35	0/1533
13	LE	0.14	0/1039	0.32	0/1395
14	LF	0.16	0/766	0.38	0/1030
15	LG	0.12	0/492	0.31	0/659
16	LH	0.14	0/6592	0.35	0/8924
17	LI	0.12	0/3835	0.32	0/5263
18	LJ	0.13	0/3993	0.31	0/5413
19	LK	0.11	0/1085	0.27	0/1463
20	LL	0.12	0/4052	0.30	0/5501
21	LM	0.13	0/9462	0.32	0/13078
22	LN	0.13	0/5359	0.30	0/7255
23	LO	0.13	0/6773	0.29	0/9164
24	LP	0.11	0/3288	0.26	0/4419
25	LQ	0.11	0/6837	0.28	0/9227
26	LR	0.12	0/6313	0.29	0/8551
27	LS	0.13	0/3866	0.29	0/5239
28	LT	0.12	0/7015	0.29	0/9479
29	LU	0.13	0/3835	0.29	0/5162
30	LV	0.14	0/3360	0.32	0/4549
31	LW	0.13	0/4321	0.31	1/5832 (0.0%)
32	LX	0.12	0/6936	0.30	0/9371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LY	0.13	0/6292	0.31	0/8556
33	LZ	0.11	0/1553	0.28	0/2089
34	NA	0.11	0/2090	0.28	0/2817
35	NB	0.12	0/1891	0.29	0/2541
36	NC	0.13	0/1708	0.32	0/2303
37	ND	0.13	0/613	0.31	0/811
38	NE	0.12	0/1662	0.28	0/2212
39	NF	0.11	0/1158	0.27	0/1559
40	NG	0.13	0/886	0.29	0/1194
41	NH	0.12	0/8899	0.28	0/12035
42	NI	0.13	0/1994	0.31	0/2684
43	NK	0.11	0/2144	0.28	0/2880
44	NM	0.11	0/1862	0.28	0/2494
45	NN	0.09	0/1491	0.25	0/2063
46	NQ	0.11	0/605	0.28	0/817
47	OA	0.11	0/98	0.28	0/133
48	SA	0.24	1/3104 (0.0%)	0.39	3/4181 (0.1%)
49	SB	0.12	0/3396	0.30	0/4576
50	SC	0.12	0/1906	0.29	0/2570
50	SD	0.13	0/1852	0.29	0/2500
51	SE	0.13	0/928	0.30	0/1262
51	SF	0.12	0/928	0.31	0/1262
52	SG	0.12	0/3686	0.28	0/4959
53	SH	0.12	0/2832	0.32	0/3825
54	SI	0.13	0/6758	0.31	0/9093
55	SJ	0.14	0/1703	0.32	0/2295
55	SK	0.13	0/1822	0.30	0/2462
56	SL	0.12	0/1406	0.28	0/1890
57	SM	0.12	0/2337	0.27	0/3148
58	SN	0.13	0/2088	0.32	0/2808
59	SP	0.13	0/17901	0.31	0/24216
60	SQ	0.13	0/1156	0.34	0/1536
61	SR	0.13	0/804	0.31	0/1074
62	SS	0.14	0/2139	0.39	2/2872 (0.1%)
63	ST	0.12	0/4549	0.29	0/6126
64	SU	0.11	0/4480	0.28	0/6073
65	SV	0.11	0/875	0.28	0/1206
66	SW	0.12	0/1591	0.28	0/2143
67	SY	0.11	0/1978	0.27	0/2616
68	SZ	0.14	0/1326	0.29	0/1859
All	All	0.12	1/252046 (0.0%)	0.29	6/349794 (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
36	NC	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	SA	211	PRO	CG-CD	-10.14	1.16	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	SA	211	PRO	N-CD-CG	-12.49	84.46	103.20
48	SA	211	PRO	CA-N-CD	-10.14	97.81	112.00
48	SA	211	PRO	CA-CB-CG	-6.22	92.68	104.50
31	LW	488	PRO	CA-N-CD	-5.34	104.52	112.00
62	SS	313	PHE	CA-C-N	-5.26	113.26	119.84
62	SS	313	PHE	C-N-CA	-5.26	113.26	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	NC	313	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	11158	0	5609	31	0
2	L1	24510	0	12366	109	0
3	L2	3712	0	1882	20	0
4	L3	786	0	823	3	0
5	L4	1866	0	1935	15	0
6	L5	1635	0	1697	14	0
7	L6	1653	0	1750	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L7	1347	0	1406	16	0
9	L8	1356	0	1377	18	0
10	L9	1388	0	1467	15	0
11	LC	973	0	1029	12	0
12	LD	1112	0	1179	10	0
13	LE	1022	0	1060	8	0
14	LF	753	0	778	12	0
15	LG	490	0	529	4	0
16	LH	6465	0	6415	81	0
17	LI	3792	0	2859	20	0
18	LJ	3911	0	3906	31	0
19	LK	1068	0	1120	7	0
20	LL	3982	0	3983	31	0
21	LM	9380	0	6279	39	0
22	LN	5263	0	5270	32	0
23	LO	6639	0	6524	41	0
24	LP	3220	0	3272	22	0
25	LQ	6707	0	6738	53	0
26	LR	6207	0	6247	56	0
27	LS	3793	0	3770	28	0
28	LT	6876	0	6853	50	0
29	LU	3756	0	3708	30	0
30	LV	3286	0	3208	51	0
31	LW	4237	0	4239	22	0
32	LX	6803	0	6928	57	0
32	LY	6179	0	5745	41	0
33	LZ	1524	0	1567	13	0
34	NA	2075	0	1915	23	0
35	NB	1873	0	1638	14	0
36	NC	1693	0	1368	19	0
37	ND	609	0	671	5	0
38	NE	1649	0	1669	13	0
39	NF	1135	0	1197	5	0
40	NG	875	0	905	6	0
41	NH	8693	0	8806	83	0
42	NI	1953	0	1933	16	0
43	NK	2107	0	2184	13	0
44	NM	1838	0	1933	16	0
45	NN	1481	0	866	6	0
46	NQ	595	0	609	5	0
47	OA	96	0	90	4	0
48	SA	3056	0	3083	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	SB	3357	0	3471	45	0
50	SC	1871	0	1916	10	0
50	SD	1817	0	1857	18	0
51	SE	916	0	964	3	0
51	SF	916	0	964	5	0
52	SG	3627	0	3626	34	0
53	SH	2781	0	2878	15	0
54	SI	6616	0	6793	66	0
55	SJ	1678	0	1756	22	0
55	SK	1793	0	1874	32	0
56	SL	1384	0	1464	10	0
57	SM	2296	0	2325	18	0
58	SN	2053	0	2168	11	0
59	SP	17548	0	17805	233	0
60	SQ	1137	0	1188	12	0
61	SR	792	0	847	4	0
62	SS	2102	0	2120	31	0
63	ST	4482	0	4360	47	0
64	SU	4370	0	4365	34	0
65	SV	869	0	554	7	0
66	SW	1565	0	1647	11	0
67	SY	1953	0	2050	18	0
68	SZ	1314	0	649	0	0
69	L1	22	0	0	0	0
69	L2	1	0	0	0	0
69	NH	1	0	0	0	0
69	SI	1	0	0	0	0
70	NH	31	0	12	1	0
71	NQ	1	0	0	0	0
71	SL	1	0	0	0	0
72	SI	32	0	12	0	0
All	All	243904	0	220050	1652	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 4.

All (1652) 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)
59:SP:297:VAL:HG13	59:SP:298:MET:HE2	1.49	0.91
8:L7:67:LEU:HD22	8:L7:94:ALA:HB2	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:958:LYS:NZ	59:SP:1014:ASN:O	2.11	0.84
7:L6:161:GLU:OE2	7:L6:168:THR:OG1	1.96	0.83
59:SP:615:VAL:HG13	59:SP:619:LEU:HD23	1.59	0.82
11:LC:98:ASP:OD2	28:LT:488:ASN:ND2	2.13	0.82
31:LW:552:ARG:NH2	41:NH:791:LYS:O	2.13	0.82
35:NB:495:TYR:HD1	58:SN:23:GLN:HE21	1.27	0.81
59:SP:474:ASN:OD1	59:SP:716:TYR:OH	1.98	0.81
54:SI:137:LEU:HD13	54:SI:230:MET:HE1	1.60	0.80
2:L1:1618:C:OP2	23:LO:505:ARG:NH2	2.13	0.80
29:LU:367:SER:OG	29:LU:369:ASP:OD1	1.99	0.80
2:L1:904:G:N2	43:NK:216:ALA:O	2.14	0.80
6:L5:145:ASP:OD2	6:L5:146:THR:N	2.14	0.80
16:LH:524:ASP:OD2	20:LL:539:ARG:NH2	2.15	0.80
2:L1:932:U:OP2	44:NH:155:TYR:OH	1.99	0.80
2:L1:1638:G:OP2	26:LR:751:LYS:NZ	2.15	0.79
32:LX:783:LYS:NZ	32:LY:838:ASP:OD2	2.14	0.79
49:SB:7:GLU:OE2	50:SD:231:ARG:NE	2.16	0.79
59:SP:264:THR:O	59:SP:313:ARG:NH1	2.16	0.79
13:LE:81:VAL:O	13:LE:122:SER:OG	2.00	0.79
27:LS:165:ARG:NH2	28:LT:219:ASP:OD2	2.16	0.78
32:LX:620:GLN:O	32:LX:623:GLN:NE2	2.15	0.78
30:LV:376:ARG:NH1	30:LV:377:PHE:O	2.17	0.78
59:SP:354:SER:OG	59:SP:356:ASP:OD1	2.01	0.78
59:SP:1420:VAL:HG12	59:SP:1424:MET:HE1	1.66	0.77
55:SJ:151:ARG:NH1	55:SJ:152:SER:O	2.17	0.77
59:SP:1436:ASP:OD2	59:SP:1480:SER:OG	2.01	0.77
32:LY:620:GLN:O	32:LY:623:GLN:NE2	2.18	0.77
1:L0:296:C:O2'	28:LT:68:LEU:O	2.03	0.76
10:L9:65:LYS:NZ	52:SG:57:GLU:O	2.19	0.76
20:LL:153:ILE:HG22	20:LL:163:LEU:HD22	1.66	0.76
2:L1:561:G:OP2	57:SM:286:LYS:NZ	2.18	0.76
2:L1:1124:A:OP2	38:NE:112:LYS:NZ	2.18	0.76
32:LX:400:LEU:O	32:LX:404:TYR:OH	2.02	0.76
24:LP:117:MET:HE3	24:LP:124:THR:HG21	1.66	0.76
36:NC:340:ARG:NH2	52:SG:53:GLU:OE2	2.18	0.76
31:LW:17:ASN:ND2	31:LW:64:ASP:OD2	2.19	0.75
2:L1:545:A:O2'	2:L1:594:A:N6	2.19	0.75
59:SP:871:ASP:OD1	59:SP:889:LYS:NZ	2.19	0.75
55:SJ:94:GLN:OE1	55:SK:94:GLN:NE2	2.20	0.75
55:SJ:142:VAL:O	55:SJ:146:HIS:ND1	2.14	0.75
59:SP:286:ALA:O	59:SP:329:LYS:NZ	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LV:224:ILE:O	30:LV:415:SER:OG	2.02	0.74
52:SG:401:SER:OG	52:SG:418:ASP:OD2	2.05	0.74
59:SP:1966:PHE:O	59:SP:1970:THR:OG1	2.05	0.74
44:NH:122:GLU:OE2	44:NH:213:ARG:NH1	2.20	0.74
41:NH:145:SER:OG	41:NH:148:GLU:OE1	2.05	0.74
63:ST:525:MET:HE1	63:ST:546:LEU:HD22	1.70	0.74
18:LJ:258:LEU:HD21	18:LJ:272:LEU:HD11	1.70	0.74
3:L2:82:G:OP1	49:SB:366:LYS:NZ	2.20	0.74
32:LX:165:THR:O	54:SI:410:LYS:NZ	2.20	0.74
54:SI:962:GLU:OE1	63:ST:756:ARG:NH1	2.20	0.74
59:SP:717:GLN:NE2	59:SP:718:PRO:O	2.21	0.74
63:ST:703:GLN:NE2	64:SU:484:PHE:O	2.21	0.74
2:L1:340:U:OP1	30:LV:136:ARG:NH1	2.20	0.73
2:L1:1162:C:OP1	6:L5:148:ARG:NH2	2.21	0.73
59:SP:243:THR:HG1	59:SP:246:THR:HG1	1.33	0.73
27:LS:380:ASN:OD1	27:LS:381:ASN:N	2.22	0.73
2:L1:1609:U:O2'	6:L5:105:GLY:O	2.05	0.73
20:LL:436:THR:OG1	64:SU:297:ASP:OD2	2.05	0.73
31:LW:96:ASP:OD2	31:LW:98:SER:OG	2.05	0.73
25:LQ:287:ARG:NH1	25:LQ:323:SER:O	2.22	0.73
2:L1:352:A:OP1	12:LD:103:ARG:NH2	2.22	0.73
22:LN:469:LEU:O	22:LN:473:THR:OG1	2.04	0.73
54:SI:826:LYS:HE2	54:SI:926:ILE:HD13	1.71	0.73
60:SQ:180:ASP:O	60:SQ:184:ASN:ND2	2.22	0.72
3:L2:64:A:OP2	28:LT:392:ARG:NH1	2.22	0.72
30:LV:361:GLU:OE1	32:LY:915:LYS:NZ	2.21	0.72
5:L4:103:TYR:O	5:L4:182:TYR:OH	2.08	0.72
41:NH:431:THR:OG1	41:NH:432:MET:SD	2.48	0.72
20:LL:580:TYR:OH	20:LL:585:ASP:OD2	2.07	0.72
36:NC:336:ASP:OD1	36:NC:337:SER:N	2.23	0.72
39:NF:48:SER:OG	39:NF:86:GLU:OE1	2.04	0.72
1:L0:551:A:O2'	62:SS:381:ARG:NH2	2.23	0.71
17:LI:592:ARG:HE	17:LI:640:LEU:HD21	1.55	0.71
23:LO:484:GLU:OE2	23:LO:815:TYR:OH	2.08	0.71
49:SB:30:GLN:O	49:SB:37:LYS:NZ	2.23	0.71
59:SP:2031:HIS:O	59:SP:2036:ARG:NH1	2.23	0.71
2:L1:59:C:O4'	2:L1:452:A:O2'	2.07	0.71
41:NH:833:TYR:OH	42:NI:97:GLU:OE2	2.05	0.71
16:LH:27:SER:OG	16:LH:171:TYR:OH	2.09	0.71
29:LU:122:ARG:NH2	29:LU:190:GLU:O	2.24	0.71
52:SG:235:HIS:ND1	52:SG:257:ASP:OD2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LY:400:LEU:O	32:LY:404:TYR:OH	2.05	0.71
2:L1:163:G:OP2	2:L1:163:G:N2	2.19	0.71
48:SA:159:SER:OG	50:SC:219:PRO:O	2.08	0.71
59:SP:243:THR:OG1	59:SP:246:THR:OG1	2.09	0.71
59:SP:1090:ARG:NH2	59:SP:1097:GLU:OE2	2.23	0.71
2:L1:331:A:OP1	9:L8:56:ARG:NH1	2.24	0.70
1:L0:247:U:OP1	67:SY:82:ARG:NH1	2.24	0.70
19:LK:412:THR:OG1	19:LK:415:GLU:OE1	2.09	0.70
41:NH:707:PHE:O	41:NH:918:ARG:NH1	2.25	0.70
32:LY:827:ARG:NH2	32:LY:928:LEU:O	2.25	0.70
54:SI:791:ILE:HD12	54:SI:812:MET:HE1	1.72	0.70
59:SP:1142:VAL:O	59:SP:1188:LYS:NZ	2.20	0.70
30:LV:269:GLY:O	30:LV:376:ARG:NH1	2.24	0.70
21:LM:185:ASP:OD1	49:SB:414:ARG:NH2	2.24	0.70
1:L0:333:G:O6	33:LZ:25:GLN:NE2	2.23	0.70
38:NE:164:LEU:HD11	38:NE:213:MET:HE3	1.74	0.70
2:L1:192:U:H3	2:L1:193:U:HO2'	1.38	0.70
10:L9:82:ARG:NH2	36:NC:247:GLU:OE2	2.25	0.70
27:LS:41:ASN:ND2	27:LS:43:ASP:OD2	2.25	0.70
43:NK:274:ARG:NH1	43:NK:277:GLN:OE1	2.25	0.70
22:LN:345:ASP:OD2	22:LN:360:SER:OG	2.10	0.69
22:LN:682:THR:OG1	22:LN:684:GLU:OE1	2.09	0.69
8:L7:7:LYS:NZ	8:L7:39:ARG:O	2.25	0.69
24:LP:38:ASP:OD1	24:LP:42:ARG:NH2	2.25	0.69
2:L1:330:G:OP2	9:L8:172:ARG:NH1	2.25	0.69
2:L1:1627:U:O3'	34:NA:538:LYS:NZ	2.25	0.69
21:LM:413:ASP:OD2	21:LM:417:LYS:NZ	2.25	0.69
2:L1:1189:A:N6	55:SK:71:ASP:OD1	2.24	0.69
64:SU:85:GLU:O	64:SU:89:ASN:ND2	2.25	0.69
32:LX:789:LEU:HD22	32:LX:891:GLN:HE22	1.57	0.69
2:L1:385:A:OP1	9:L8:25:ARG:NH2	2.26	0.69
26:LR:220:ILE:HD12	26:LR:239:VAL:HG11	1.74	0.69
8:L7:133:THR:HG21	8:L7:162:ILE:HG21	1.74	0.69
18:LJ:375:HIS:NE2	18:LJ:377:ASP:OD2	2.26	0.69
29:LU:92:ILE:HD12	29:LU:136:MET:HE3	1.74	0.69
22:LN:541:ALA:HB2	22:LN:555:LEU:HD11	1.75	0.68
41:NH:1144:ASP:OD2	41:NH:1146:THR:HG22	1.92	0.68
55:SK:39:LYS:NZ	55:SK:197:ASP:O	2.25	0.68
24:LP:144:VAL:HG11	24:LP:178:VAL:HG21	1.75	0.68
53:SH:60:THR:O	63:ST:108:LYS:NZ	2.27	0.68
52:SG:546:GLU:OE2	52:SG:551:ARG:NH1	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:583:LEU:O	59:SP:586:THR:OG1	2.10	0.68
23:LO:359:ARG:NH1	34:NA:484:MET:SD	2.66	0.68
65:SV:130:ASP:OD1	67:SY:161:ARG:NH1	2.27	0.68
52:SG:55:GLU:OE2	59:SP:1780:ARG:NH2	2.27	0.68
25:LQ:482:THR:OG1	25:LQ:484:ASP:OD1	2.09	0.68
55:SJ:135:LYS:NZ	55:SK:72:ASP:OD1	2.25	0.68
59:SP:749:LYS:O	59:SP:756:SER:OG	2.07	0.68
1:L0:337:G:OP1	38:NE:209:ARG:NH2	2.27	0.68
13:LE:93:LEU:HD22	38:NE:311:VAL:HG21	1.76	0.68
21:LM:32:SER:OG	21:LM:119:GLU:OE2	2.10	0.68
59:SP:489:SER:OG	59:SP:493:ASN:OD1	2.13	0.68
2:L1:416:A:N1	32:LX:59:TYR:OH	2.26	0.67
5:L4:40:GLU:OE2	5:L4:103:TYR:OH	2.12	0.67
22:LN:424:ASP:OD2	22:LN:444:ARG:NH2	2.27	0.67
49:SB:34:SER:OG	49:SB:36:ASP:OD1	2.09	0.67
2:L1:320:U:OP1	43:NK:299:ARG:NH2	2.28	0.67
55:SJ:51:GLU:OE1	55:SJ:82:ARG:NH1	2.27	0.67
2:L1:200:A:O2'	59:SP:1101:GLN:NE2	2.27	0.67
66:SW:204:ARG:NH1	66:SW:250:LEU:O	2.27	0.67
20:LL:185:PRO:O	20:LL:215:TYR:OH	2.09	0.67
23:LO:419:TYR:OH	34:NA:484:MET:HE2	1.95	0.67
25:LQ:20:ASN:OD1	25:LQ:339:LYS:NZ	2.28	0.67
32:LY:538:MET:HE1	32:LY:556:MET:HE1	1.78	0.67
28:LT:604:SER:OG	28:LT:606:ASP:OD1	2.13	0.66
54:SI:1062:ARG:NH2	67:SY:29:GLU:OE2	2.27	0.66
21:LM:22:ARG:NH2	29:LU:20:GLN:O	2.28	0.66
11:LC:50:GLU:OE1	11:LC:82:ARG:NH2	2.28	0.66
25:LQ:919:GLU:OE1	66:SW:264:ARG:NH1	2.29	0.66
32:LX:823:LYS:NZ	32:LX:826:THR:HG23	2.11	0.66
50:SD:309:TYR:OH	67:SY:127:PHE:O	2.09	0.66
54:SI:230:MET:HE3	54:SI:232:PHE:HE2	1.59	0.66
2:L1:563:U:OP2	57:SM:289:TYR:OH	2.12	0.66
27:LS:278:ASP:OD2	27:LS:281:THR:OG1	2.12	0.66
34:NA:335:ARG:NH2	54:SI:957:GLU:OE1	2.28	0.66
59:SP:559:ASN:ND2	59:SP:599:GLU:OE1	2.28	0.66
28:LT:207:ASP:OD2	28:LT:227:THR:OG1	2.13	0.66
32:LX:309:PHE:HB2	32:LX:384:VAL:HG22	1.77	0.66
59:SP:1476:LEU:HB2	59:SP:1481:ILE:HD11	1.78	0.66
10:L9:106:GLU:OE1	10:L9:115:LYS:NZ	2.22	0.66
23:LO:430:ARG:NH1	34:NA:459:LYS:O	2.28	0.66
59:SP:981:SER:O	59:SP:983:GLN:NE2	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SA:397:SER:OG	52:SG:453:GLY:O	2.11	0.65
5:L4:19:LEU:HD23	5:L4:19:LEU:O	1.96	0.65
59:SP:1261:ILE:HD12	59:SP:1291:LEU:HD22	1.77	0.65
49:SB:14:LEU:HD23	49:SB:79:ILE:HD12	1.78	0.65
59:SP:1159:ARG:HA	59:SP:1208:MET:HE1	1.78	0.65
5:L4:148:ARG:NH2	7:L6:201:GLN:OE1	2.30	0.65
50:SD:102:LYS:O	67:SY:194:LYS:NZ	2.24	0.65
28:LT:808:THR:HG22	28:LT:853:ASN:HB2	1.78	0.65
28:LT:827:SER:OG	28:LT:829:ASP:OD1	2.08	0.65
48:SA:177:ALA:HB3	48:SA:292:LEU:HD13	1.79	0.65
59:SP:378:HIS:NE2	59:SP:379:GLN:OE1	2.29	0.65
25:LQ:897:ASP:OD2	26:LR:758:ARG:NH1	2.29	0.64
30:LV:268:GLN:O	30:LV:298:LYS:NZ	2.27	0.64
16:LH:457:VAL:HG12	16:LH:473:LEU:HD11	1.79	0.64
16:LH:714:ASP:OD1	16:LH:715:GLU:N	2.30	0.64
54:SI:193:ARG:NH1	54:SI:197:GLU:OE1	2.30	0.64
25:LQ:897:ASP:OD1	26:LR:761:ARG:NH1	2.31	0.64
59:SP:608:MET:O	59:SP:612:GLY:N	2.30	0.64
9:L8:69:SER:OG	9:L8:185:GLU:OE1	2.11	0.64
37:ND:182:SER:O	50:SD:294:ARG:NH2	2.30	0.64
2:L1:1657:U:OP1	2:L1:1658:G:O2'	2.14	0.64
2:L1:967:A:OP2	39:NF:124:ARG:NH2	2.30	0.64
27:LS:352:GLN:NE2	27:LS:354:SER:O	2.31	0.64
42:NI:37:MET:HE3	42:NI:58:LEU:HD13	1.80	0.64
17:LI:585:ARG:NE	17:LI:589:ASP:OD2	2.31	0.64
56:SL:68:ASP:OD2	56:SL:70:ASN:ND2	2.30	0.64
19:LK:394:HIS:ND1	19:LK:405:ASP:OD2	2.31	0.64
20:LL:51:LEU:HD22	20:LL:88:TYR:CD1	2.33	0.64
32:LX:823:LYS:HZ1	32:LX:826:THR:HG23	1.62	0.64
59:SP:588:ASN:ND2	59:SP:600:THR:OG1	2.30	0.64
2:L1:182:A:OP2	59:SP:1049:LYS:NZ	2.31	0.64
30:LV:357:ASP:OD1	32:LY:912:MET:HE3	1.98	0.64
32:LY:309:PHE:HB2	32:LY:384:VAL:HG22	1.80	0.64
59:SP:1991:ASN:OD1	59:SP:2030:ASN:ND2	2.31	0.64
50:SC:277:ASP:OD2	50:SC:279:THR:OG1	2.14	0.63
48:SA:4:ILE:O	48:SA:23:GLN:NE2	2.31	0.63
52:SG:52:GLU:N	52:SG:52:GLU:OE1	2.31	0.63
7:L6:182:GLN:OE1	7:L6:186:ARG:NH2	2.31	0.63
28:LT:95:GLU:OE2	28:LT:97:LYS:NZ	2.30	0.63
14:LF:11:LYS:NZ	36:NC:291:GLU:O	2.32	0.63
21:LM:193:THR:OG1	21:LM:241:ILE:HD11	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LS:221:THR:OG1	27:LS:224:ASN:ND2	2.31	0.63
64:SU:174:ASN:OD1	64:SU:176:ILE:HG22	1.98	0.63
2:L1:1132:A:O3'	53:SH:231:ARG:NH1	2.31	0.63
34:NA:345:LEU:HD21	54:SI:932:LEU:HD23	1.80	0.63
49:SB:319:ILE:HD12	49:SB:326:LEU:HD22	1.81	0.63
7:L6:67:VAL:HG21	7:L6:73:ILE:HD11	1.80	0.63
26:LR:188:GLU:OE1	26:LR:188:GLU:N	2.32	0.63
34:NA:341:LEU:O	54:SI:960:ARG:NH1	2.30	0.63
54:SI:549:ILE:HD13	54:SI:567:TRP:NE1	2.14	0.63
59:SP:524:LYS:O	59:SP:560:LYS:NZ	2.20	0.63
54:SI:831:ARG:NH1	54:SI:835:HIS:O	2.32	0.62
16:LH:868:ASN:C	16:LH:868:ASN:HD22	2.06	0.62
34:NA:344:GLU:OE1	54:SI:960:ARG:NH2	2.32	0.62
52:SG:409:ASP:OD1	52:SG:410:ASP:N	2.32	0.62
1:L0:505:G:OP1	48:SA:93:LYS:NZ	2.33	0.62
2:L1:959:U:OP2	46:NQ:20:LYS:NZ	2.32	0.62
17:LI:570:LEU:HD21	17:LI:637:LEU:HD21	1.80	0.62
28:LT:226:VAL:HG13	28:LT:227:THR:HG23	1.81	0.62
30:LV:319:ASP:OD1	30:LV:320:ILE:N	2.33	0.62
41:NH:1195:LYS:O	41:NH:1197:ARG:NE	2.31	0.62
59:SP:1952:SER:OG	59:SP:1995:ARG:NH1	2.31	0.62
2:L1:512:A:O2'	10:L9:133:HIS:NE2	2.22	0.62
23:LO:608:ASN:OD1	28:LT:515:ARG:NH2	2.33	0.62
31:LW:189:GLN:OE1	31:LW:224:LEU:HD22	2.00	0.62
61:SR:46:SER:OG	61:SR:48:HIS:O	2.17	0.62
54:SI:230:MET:HE3	54:SI:232:PHE:CE2	2.33	0.62
57:SM:243:GLU:OE1	57:SM:243:GLU:N	2.33	0.62
59:SP:2136:LYS:O	59:SP:2140:ILE:HD12	2.00	0.62
2:L1:315:A:O2'	43:NK:288:GLN:OE1	2.18	0.62
2:L1:1482:C:O2'	11:LC:72:GLY:O	2.08	0.62
52:SG:234:GLY:O	52:SG:259:LYS:NZ	2.32	0.62
59:SP:259:LEU:HD22	59:SP:298:MET:SD	2.40	0.62
2:L1:1045:C:OP1	44:NM:153:HIS:NE2	2.29	0.62
2:L1:1752:U:OP1	34:NA:522:ARG:NH1	2.33	0.62
51:SF:50:GLU:OE1	51:SF:104:THR:HG22	2.00	0.62
49:SB:328:ARG:O	49:SB:332:THR:HG22	2.00	0.61
55:SK:156:GLU:OE1	55:SK:156:GLU:N	2.33	0.61
2:L1:51:A:N3	54:SI:344:ARG:N	2.48	0.61
32:LX:772:ASN:OD1	32:LX:773:TRP:N	2.33	0.61
59:SP:386:LEU:HD13	59:SP:419:LEU:HD22	1.81	0.61
59:SP:976:TYR:O	59:SP:980:ASN:ND2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:254:C:OP2	65:SV:184:TYR:OH	2.18	0.61
16:LH:682:ASN:CG	16:LH:689:ILE:HD11	2.25	0.61
21:LM:528:ARG:O	21:LM:532:SER:N	2.31	0.61
34:NA:520:LEU:O	34:NA:525:LYS:NZ	2.32	0.61
2:L1:66:U:O2	7:L6:160:ARG:NE	2.32	0.61
8:L7:74:GLN:O	8:L7:78:THR:HG23	2.01	0.61
17:LI:670:GLU:OE2	18:LJ:499:LYS:NZ	2.32	0.61
20:LL:441:LEU:HD13	20:LL:456:VAL:HG11	1.81	0.61
27:LS:216:TYR:OH	28:LT:276:TYR:OH	2.19	0.61
59:SP:239:SER:OG	59:SP:240:MET:SD	2.59	0.61
44:NM:73:LEU:HD22	44:NM:84:ILE:HD11	1.81	0.61
55:SK:35:ASP:O	55:SK:40:ARG:NH2	2.33	0.61
2:L1:861:U:O2'	13:LE:56:HIS:O	2.18	0.61
22:LN:385:ASN:ND2	22:LN:387:GLU:O	2.34	0.61
16:LH:741:SER:OG	16:LH:761:GLU:O	2.15	0.61
30:LV:308:TYR:OH	30:LV:345:SER:OG	2.14	0.61
35:NB:437:ASP:O	55:SJ:88:ARG:NH1	2.32	0.61
66:SW:164:LEU:HD22	66:SW:232:HIS:CE1	2.36	0.61
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.33	0.61
22:LN:681:ILE:HG22	22:LN:683:ASP:H	1.65	0.61
48:SA:302:ASN:ND2	48:SA:397:SER:O	2.34	0.61
49:SB:215:ARG:NH1	49:SB:242:SER:OG	2.33	0.61
59:SP:117:LEU:O	59:SP:121:PHE:N	2.34	0.61
1:L0:272:A:O2'	67:SY:228:GLY:O	2.17	0.61
33:LZ:20:GLU:OE1	56:SL:25:LEU:HD22	2.01	0.61
57:SM:116:ARG:NH1	57:SM:117:LEU:O	2.34	0.61
8:L7:168:SER:O	8:L7:172:VAL:HG23	2.01	0.61
32:LX:494:VAL:HG22	32:LX:535:GLU:OE2	2.00	0.61
34:NA:319:VAL:HG21	54:SI:1042:MET:HE1	1.82	0.61
56:SL:65:VAL:HG11	56:SL:86:MET:HE2	1.82	0.61
59:SP:1182:LEU:HD22	59:SP:1223:SER:HB2	1.81	0.61
6:L5:94:THR:HG22	6:L5:114:ILE:HG13	1.81	0.60
63:ST:422:LEU:O	63:ST:426:THR:HG23	2.00	0.60
1:L0:320:A:OP1	23:LO:249:ARG:NH1	2.34	0.60
11:LC:50:GLU:O	11:LC:54:LEU:HD23	2.01	0.60
32:LX:864:LEU:HD22	32:LX:890:LEU:HD21	1.82	0.60
41:NH:132:TYR:HD1	41:NH:183:ILE:HG21	1.66	0.60
41:NH:899:LEU:HD11	41:NH:909:TYR:CE2	2.37	0.60
54:SI:849:LEU:HD12	54:SI:854:PHE:HZ	1.66	0.60
5:L4:95:THR:HG22	14:LF:16:PRO:HG2	1.83	0.60
17:LI:614:ILE:HG13	17:LI:638:LEU:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SD:104:ASP:C	50:SD:105:LEU:HD12	2.26	0.60
54:SI:994:LYS:O	67:SY:37:ARG:NH2	2.33	0.60
16:LH:852:ASP:OD1	27:LS:475:LYS:NZ	2.29	0.60
23:LO:669:ASP:O	23:LO:672:THR:OG1	2.18	0.60
59:SP:389:ILE:O	59:SP:393:PHE:N	2.35	0.60
22:LN:540:ILE:HG21	22:LN:596:MET:HE1	1.82	0.60
59:SP:1454:VAL:HG21	59:SP:1488:MET:HE3	1.83	0.60
3:L2:30:A:N6	29:LU:341:GLU:OE2	2.34	0.60
28:LT:850:ARG:NH2	66:SW:262:ASN:OD1	2.34	0.60
34:NA:383:ARG:NH2	57:SM:212:ALA:O	2.35	0.60
55:SJ:53:HIS:CE1	55:SJ:76:LEU:HD23	2.37	0.60
23:LO:335:GLU:OE1	25:LQ:924:TYR:OH	2.16	0.60
25:LQ:94:LEU:HB2	25:LQ:108:LEU:HD21	1.83	0.60
25:LQ:128:GLN:NE2	25:LQ:129:PHE:O	2.34	0.60
58:SN:56:ILE:HD12	65:SV:192:ALA:HA	1.84	0.60
2:L1:67:A:O2'	2:L1:69:G:OP1	2.20	0.60
32:LX:588:ILE:HD11	32:LX:657:LEU:HD11	1.84	0.60
36:NC:256:PRO:HB2	52:SG:357:LEU:HD22	1.83	0.60
41:NH:172:THR:HG22	41:NH:172:THR:O	2.02	0.60
41:NH:599:VAL:HG11	41:NH:609:ASN:ND2	2.17	0.60
64:SU:378:SER:OG	64:SU:456:THR:OG1	2.18	0.60
28:LT:758:PHE:O	66:SW:221:ARG:NH2	2.35	0.59
59:SP:1085:VAL:HG23	59:SP:1086:VAL:HG23	1.84	0.59
16:LH:139:GLU:OE2	16:LH:172:ARG:NH1	2.35	0.59
59:SP:1922:ILE:CD1	59:SP:1965:ALA:HB1	2.32	0.59
16:LH:682:ASN:O	16:LH:686:GLY:N	2.35	0.59
26:LR:343:MET:HE2	26:LR:635:ALA:HB2	1.84	0.59
41:NH:721:VAL:HG23	41:NH:722:LEU:HD12	1.83	0.59
41:NH:829:GLU:N	41:NH:829:GLU:OE1	2.35	0.59
63:ST:426:THR:HG21	63:ST:466:TYR:HB2	1.84	0.59
14:LF:88:THR:OG1	59:SP:13:ARG:NH1	2.35	0.59
20:LL:302:ASN:ND2	20:LL:316:ASN:OD1	2.35	0.59
28:LT:307:GLN:NE2	49:SB:422:THR:O	2.35	0.59
54:SI:246:ALA:HB2	54:SI:271:ILE:HD11	1.84	0.59
3:L2:256:G:OP1	48:SA:382:LYS:NZ	2.36	0.59
21:LM:235:VAL:HG13	21:LM:239:LEU:HD12	1.85	0.59
31:LW:37:THR:O	31:LW:43:ARG:NH2	2.35	0.59
2:L1:1169:G:N1	2:L1:1575:G:OP2	2.34	0.59
18:LJ:100:ASP:OD2	18:LJ:101:ALA:N	2.36	0.59
30:LV:38:LYS:O	30:LV:44:GLN:NE2	2.36	0.59
41:NH:822:ARG:NH2	41:NH:1133:PRO:O	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:267:SER:O	59:SP:313:ARG:NH2	2.34	0.59
63:ST:563:GLU:N	63:ST:563:GLU:OE1	2.36	0.59
16:LH:878:ASN:OD1	16:LH:890:ARG:NH1	2.36	0.59
17:LI:575:ASN:O	17:LI:579:LEU:HD23	2.03	0.59
52:SG:235:HIS:CD2	52:SG:261:ILE:HD12	2.37	0.59
54:SI:952:PHE:CD2	54:SI:958:VAL:HG22	2.37	0.59
22:LN:237:GLU:OE2	37:ND:208:ARG:NE	2.36	0.59
48:SA:267:ASP:OD1	49:SB:275:TYR:OH	2.17	0.59
7:L6:24:ILE:HG22	7:L6:28:PHE:CE1	2.38	0.58
32:LX:27:VAL:HG13	32:LX:152:LEU:HD13	1.85	0.58
8:L7:129:LEU:HD21	8:L7:172:VAL:HG11	1.86	0.58
41:NH:369:TRP:HE1	41:NH:495:THR:HG21	1.67	0.58
44:NM:87:ARG:NH1	44:NM:100:PHE:O	2.34	0.58
59:SP:1387:ALA:O	59:SP:1391:ILE:HD12	2.03	0.58
32:LX:43:LEU:HD21	54:SI:371:VAL:HG21	1.86	0.58
41:NH:132:TYR:CD1	41:NH:183:ILE:HG21	2.38	0.58
43:NK:141:ARG:NH1	43:NK:191:MET:O	2.36	0.58
59:SP:438:GLU:OE2	59:SP:760:THR:OG1	2.16	0.58
28:LT:930:MET:HE2	28:LT:930:MET:HA	1.86	0.58
32:LX:502:PHE:O	32:LX:506:GLY:N	2.36	0.58
41:NH:313:ASN:OD1	41:NH:314:CYS:N	2.36	0.58
59:SP:234:ILE:O	59:SP:237:THR:HG22	2.04	0.58
59:SP:1355:ILE:HD12	59:SP:1417:TYR:CZ	2.39	0.58
64:SU:155:LEU:O	64:SU:218:LYS:NZ	2.37	0.58
48:SA:187:ASP:OD2	49:SB:180:TYR:OH	2.19	0.58
53:SH:161:LEU:HD23	53:SH:237:LYS:HB3	1.85	0.58
55:SK:169:ASP:OD1	55:SK:170:HIS:N	2.36	0.58
59:SP:1087:VAL:O	59:SP:1091:ILE:HG23	2.04	0.58
16:LH:879:ILE:HD12	21:LM:215:CYS:SG	2.44	0.58
34:NA:426:LEU:HD11	34:NA:430:LEU:HD23	1.85	0.58
23:LO:146:PHE:N	23:LO:167:ASP:OD2	2.36	0.58
35:NB:378:GLN:NE2	35:NB:379:SER:O	2.36	0.58
24:LP:182:TRP:CG	24:LP:277:CYS:HG	2.21	0.58
16:LH:669:ASN:ND2	16:LH:682:ASN:OD1	2.36	0.58
44:NM:61:LEU:HD13	44:NM:96:LEU:HD21	1.85	0.58
54:SI:85:LEU:HD22	54:SI:141:LEU:HD21	1.86	0.58
62:SS:357:ASP:OD1	62:SS:358:SER:N	2.36	0.58
20:LL:90:VAL:HG13	20:LL:91:LEU:HD22	1.86	0.58
48:SA:281:LEU:HD11	49:SB:265:PHE:CZ	2.39	0.58
16:LH:179:ASP:OD2	16:LH:182:LYS:NZ	2.29	0.57
41:NH:1063:ARG:NH1	47:OA:1405:ALA:O	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:334:ASN:O	59:SP:337:THR:OG1	2.18	0.57
59:SP:806:THR:HG1	59:SP:820:THR:HG1	1.47	0.57
59:SP:2030:ASN:OD1	59:SP:2031:HIS:N	2.36	0.57
1:L0:326:C:O2'	1:L0:327:A:OP1	2.21	0.57
16:LH:518:ASP:OD2	18:LJ:428:ARG:NH2	2.37	0.57
16:LH:769:ASN:OD1	16:LH:770:TYR:N	2.37	0.57
30:LV:30:ALA:O	30:LV:34:LYS:N	2.37	0.57
32:LX:617:LEU:CD2	32:LX:761:VAL:HG21	2.35	0.57
41:NH:188:SER:N	70:NH:1300:ATP:O2B	2.37	0.57
59:SP:2157:PHE:CE1	62:SS:250:VAL:HG21	2.38	0.57
64:SU:10:ASP:OD2	64:SU:14:ARG:NH2	2.37	0.57
21:LM:1464:GLU:O	21:LM:1468:SER:N	2.38	0.57
54:SI:244:MET:CG	54:SI:812:MET:HE2	2.34	0.57
59:SP:311:ILE:HD11	59:SP:343:ILE:HB	1.86	0.57
59:SP:1298:LEU:O	59:SP:1298:LEU:HD23	2.05	0.57
32:LY:843:ASP:OD1	32:LY:925:ARG:NH2	2.36	0.57
42:NI:50:SER:O	42:NI:127:LYS:NZ	2.37	0.57
59:SP:319:THR:HG22	59:SP:361:LEU:HB2	1.87	0.57
2:L1:168:A:OP1	7:L6:140:ASN:ND2	2.38	0.57
2:L1:188:A:N6	2:L1:197:A:O2'	2.38	0.57
17:LI:540:LEU:O	17:LI:544:LEU:HD13	2.04	0.57
27:LS:43:ASP:OD2	27:LS:44:PHE:N	2.38	0.57
49:SB:333:LYS:NZ	54:SI:1098:ARG:O	2.37	0.57
11:LC:45:ARG:O	11:LC:48:VAL:HG12	2.04	0.57
30:LV:148:LYS:NZ	30:LV:190:GLU:OE1	2.29	0.57
41:NH:751:LYS:NZ	44:NH:196:GLU:OE1	2.36	0.57
41:NH:1037:LEU:HD22	41:NH:1050:ILE:HG22	1.86	0.57
49:SB:14:LEU:HD13	49:SB:75:LEU:HD23	1.87	0.57
55:SK:137:PHE:CE1	55:SK:141:MET:HE3	2.39	0.57
23:LO:592:ILE:HD12	23:LO:606:VAL:HG22	1.87	0.57
52:SG:245:SER:OG	52:SG:247:ASP:OD1	2.21	0.57
59:SP:315:LEU:O	59:SP:319:THR:HG23	2.05	0.57
59:SP:1606:ILE:HG21	59:SP:1650:LEU:HD12	1.86	0.57
25:LQ:161:SER:OG	25:LQ:187:LYS:NZ	2.30	0.57
25:LQ:171:CYS:HB2	25:LQ:177:LEU:HD13	1.87	0.57
59:SP:1247:LEU:O	59:SP:1251:VAL:HG22	2.05	0.57
23:LO:706:THR:HG22	23:LO:706:THR:O	2.04	0.56
26:LR:333:ILE:HG23	26:LR:379:LEU:HB3	1.87	0.56
45:NN:182:GLN:O	45:NN:186:PHE:N	2.36	0.56
2:L1:346:G:O5'	12:LD:79:LYS:NZ	2.30	0.56
29:LU:258:ILE:HG22	29:LU:464:THR:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:789:LEU:HD22	32:LX:891:GLN:NE2	2.20	0.56
41:NH:602:ASN:OD1	41:NH:603:THR:N	2.39	0.56
41:NH:628:VAL:HG12	41:NH:668:VAL:HG22	1.87	0.56
59:SP:486:PHE:CD2	59:SP:525:ILE:HG21	2.39	0.56
62:SS:244:LEU:HD21	62:SS:263:LEU:HD13	1.87	0.56
2:L1:1767:G:OP1	66:SW:211:LYS:NZ	2.24	0.56
17:LI:632:THR:HB	19:LK:492:ILE:HD13	1.87	0.56
31:LW:152:GLU:OE1	31:LW:170:GLN:NE2	2.38	0.56
32:LX:545:HIS:NE2	32:LX:638:ILE:O	2.37	0.56
36:NC:249:ILE:O	36:NC:253:SER:N	2.39	0.56
48:SA:265:GLU:N	48:SA:265:GLU:OE1	2.38	0.56
54:SI:400:LEU:O	54:SI:403:VAL:HG12	2.05	0.56
24:LP:305:ASN:O	24:LP:309:LEU:HD23	2.05	0.56
27:LS:148:THR:OG1	27:LS:163:ARG:NH2	2.39	0.56
59:SP:2101:SER:OG	62:SS:262:LEU:HD12	2.04	0.56
59:SP:2207:TYR:O	59:SP:2211:ASN:ND2	2.36	0.56
14:LF:86:GLU:O	59:SP:13:ARG:NH2	2.38	0.56
30:LV:223:ASN:OD1	30:LV:224:ILE:HD12	2.06	0.56
32:LY:144:GLY:N	32:LY:475:ARG:O	2.38	0.56
42:NI:188:MET:O	42:NI:191:PHE:N	2.37	0.56
1:L0:125:G:OP1	64:SU:145:ASN:ND2	2.38	0.56
59:SP:1281:ARG:NH2	59:SP:1309:ASN:OD1	2.39	0.56
64:SU:166:VAL:HG21	64:SU:173:GLU:HG2	1.87	0.56
2:L1:447:U:O2'	5:L4:27:TYR:O	2.24	0.56
8:L7:17:GLU:HG3	8:L7:46:ILE:HG22	1.87	0.56
24:LP:64:ASN:HB2	24:LP:88:ILE:HG21	1.88	0.56
52:SG:522:THR:OG1	52:SG:542:SER:OG	2.22	0.56
2:L1:931:C:O2'	44:NM:118:GLN:O	2.23	0.56
16:LH:778:ASP:OD1	16:LH:779:ILE:N	2.38	0.56
21:LM:746:GLU:O	21:LM:750:ASN:N	2.38	0.56
28:LT:723:LEU:HD22	28:LT:879:GLU:HG2	1.86	0.56
54:SI:124:ASP:OD1	54:SI:126:ASN:N	2.39	0.56
59:SP:1384:LEU:O	59:SP:1388:SER:N	2.38	0.56
3:L2:79:G:O2'	3:L2:328:A:N1	2.32	0.56
21:LM:218:ILE:HD12	21:LM:263:VAL:HG21	1.88	0.56
55:SJ:169:ASP:OD1	55:SJ:170:HIS:N	2.39	0.56
63:ST:525:MET:HE1	63:ST:546:LEU:CD2	2.36	0.56
65:SV:131:LEU:O	65:SV:136:ARG:NH1	2.38	0.56
6:L5:25:LEU:HD12	6:L5:29:ILE:HD13	1.86	0.56
13:LE:11:LEU:O	13:LE:15:ASN:ND2	2.39	0.56
16:LH:71:ASN:HD22	16:LH:125:LEU:HD21	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:96:ILE:HD12	16:LH:96:ILE:H	1.71	0.56
22:LN:532:ASN:OD1	22:LN:546:GLY:N	2.39	0.56
25:LQ:400:SER:OG	25:LQ:402:ASP:OD1	2.20	0.56
32:LX:565:PHE:CE1	32:LX:588:ILE:HD12	2.41	0.56
32:LY:575:ASP:OD1	32:LY:576:GLY:N	2.39	0.56
59:SP:1640:CYS:HB3	59:SP:1680:THR:HG21	1.88	0.56
57:SM:270:ASP:OD1	67:SY:52:ARG:NH2	2.39	0.55
8:L7:70:PHE:O	8:L7:74:GLN:N	2.39	0.55
24:LP:205:LEU:HD22	60:SQ:52:PHE:CZ	2.41	0.55
59:SP:436:PHE:HA	59:SP:439:VAL:HG22	1.89	0.55
2:L1:1637:C:OP1	25:LQ:855:LYS:NZ	2.40	0.55
25:LQ:135:ARG:NH1	25:LQ:174:GLU:OE2	2.39	0.55
25:LQ:414:LEU:HD12	25:LQ:447:LEU:HD11	1.86	0.55
27:LS:504:THR:HG23	27:LS:504:THR:O	2.07	0.55
36:NC:286:VAL:HG13	36:NC:297:LEU:HD21	1.88	0.55
64:SU:378:SER:OG	64:SU:453:PRO:O	2.24	0.55
2:L1:284:G:N7	7:L6:188:ARG:NH1	2.54	0.55
2:L1:524:U:N3	2:L1:527:A:OP2	2.40	0.55
16:LH:457:VAL:HG12	16:LH:473:LEU:CD1	2.36	0.55
26:LR:173:LYS:NZ	26:LR:182:CYS:SG	2.71	0.55
54:SI:217:ASP:OD1	54:SI:218:ARG:N	2.40	0.55
59:SP:1418:VAL:HG21	59:SP:1455:ASN:HD21	1.71	0.55
9:L8:56:ARG:NH1	9:L8:174:GLY:O	2.40	0.55
19:LK:415:GLU:OE1	19:LK:415:GLU:N	2.40	0.55
51:SE:94:SER:OG	67:SY:248:ARG:NH1	2.40	0.55
52:SG:318:LEU:HD11	52:SG:351:ILE:HD12	1.89	0.55
59:SP:1277:GLU:OE2	59:SP:1277:GLU:N	2.35	0.55
64:SU:181:THR:HG22	64:SU:222:LEU:HD12	1.87	0.55
49:SB:230:GLU:HG2	49:SB:231:ILE:HD12	1.88	0.55
52:SG:522:THR:HG1	52:SG:542:SER:HG	1.54	0.55
16:LH:690:ASN:OD1	17:LI:428:LYS:NZ	2.40	0.55
23:LO:841:ASP:OD1	23:LO:842:ASN:N	2.39	0.55
36:NC:241:ARG:NE	36:NC:246:GLU:OE2	2.40	0.55
41:NH:542:SER:O	41:NH:546:THR:HG23	2.06	0.55
2:L1:1159:C:N4	57:SM:184:GLU:OE2	2.39	0.55
18:LJ:118:LEU:HD11	18:LJ:157:ALA:CB	2.37	0.55
21:LM:2:SER:OG	21:LM:6:ASP:OD2	2.21	0.55
26:LR:249:LEU:N	26:LR:257:ILE:O	2.38	0.55
26:LR:561:SER:O	26:LR:565:PHE:N	2.40	0.55
59:SP:1642:VAL:HG12	59:SP:1650:LEU:HD21	1.89	0.55
63:ST:560:TYR:OH	64:SU:388:LEU:O	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SH:337:VAL:N	54:SI:554:TYR:OH	2.40	0.55
59:SP:456:GLU:N	59:SP:456:GLU:OE2	2.40	0.55
59:SP:1189:LEU:HD11	59:SP:1198:PHE:CE2	2.42	0.55
59:SP:1277:GLU:OE2	59:SP:1280:LEU:HD12	2.07	0.55
25:LQ:181:SER:OG	25:LQ:183:ASP:OD1	2.24	0.55
29:LU:407:MET:HE2	29:LU:407:MET:HA	1.89	0.55
30:LV:147:ASN:OD1	30:LV:149:VAL:N	2.40	0.55
41:NH:203:ILE:HB	41:NH:292:ILE:HD13	1.89	0.55
48:SA:217:ALA:O	48:SA:221:LEU:HD23	2.07	0.55
55:SK:77:LEU:HD23	55:SK:84:ILE:HG22	1.89	0.55
59:SP:886:ASP:OD1	59:SP:887:ASN:N	2.40	0.55
63:ST:95:ARG:NH1	63:ST:758:ASP:OD2	2.40	0.55
2:L1:454:U:OP1	2:L1:455:C:N4	2.40	0.54
23:LO:708:ASP:OD1	23:LO:709:THR:N	2.40	0.54
32:LX:293:LEU:HD11	32:LX:409:ALA:HB2	1.87	0.54
41:NH:215:GLU:OE1	41:NH:227:LYS:NZ	2.40	0.54
2:L1:1657:U:OP2	25:LQ:450:ARG:NH2	2.37	0.54
23:LO:311:ASN:OD1	23:LO:312:GLN:N	2.40	0.54
35:NB:529:ALA:O	35:NB:532:VAL:HG22	2.07	0.54
64:SU:504:ASP:OD2	64:SU:505:SER:N	2.40	0.54
18:LJ:312:ALA:HB3	18:LJ:316:ARG:HH11	1.71	0.54
25:LQ:185:MET:HE1	26:LR:663:VAL:HG21	1.89	0.54
26:LR:111:ASP:OD2	26:LR:113:THR:OG1	2.24	0.54
33:LZ:65:PRO:HD3	38:NE:203:ILE:HG22	1.89	0.54
59:SP:897:PHE:CZ	59:SP:901:ILE:HD11	2.42	0.54
59:SP:1979:LEU:HD22	59:SP:2013:LEU:CD1	2.36	0.54
62:SS:313:PHE:CE2	62:SS:883:ILE:HG23	2.42	0.54
3:L2:245:U:O4	3:L2:246:A:N6	2.41	0.54
16:LH:474:THR:HG22	16:LH:511:GLU:CD	2.32	0.54
42:NI:250:ASP:OD1	42:NI:251:LYS:N	2.41	0.54
64:SU:154:ALA:O	64:SU:157:SER:OG	2.25	0.54
20:LL:74:VAL:HG13	20:LL:90:VAL:HG12	1.89	0.54
23:LO:814:LYS:NZ	28:LT:938:THR:O	2.34	0.54
28:LT:367:LEU:HD21	28:LT:389:MET:HE1	1.89	0.54
32:LX:731:GLN:NE2	32:LX:800:GLN:OE1	2.39	0.54
32:LY:502:PHE:O	32:LY:506:GLY:N	2.38	0.54
55:SJ:179:THR:HG23	55:SJ:221:VAL:HG21	1.89	0.54
59:SP:1369:HIS:HA	59:SP:1372:MET:HE2	1.90	0.54
59:SP:2119:ARG:NH1	62:SS:227:TYR:O	2.41	0.54
3:L2:332:G:H21	16:LH:869:MET:CE	2.21	0.54
20:LL:2:ASP:OD1	20:LL:3:SER:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LP:300:MET:HE2	49:SB:214:ILE:HD11	1.90	0.54
25:LQ:53:ASP:OD2	25:LQ:56:THR:OG1	2.26	0.54
28:LT:814:GLU:OE1	28:LT:822:ARG:NH1	2.40	0.54
32:LY:544:SER:O	32:LY:637:ARG:NH2	2.41	0.54
59:SP:1643:LEU:HB2	59:SP:1654:VAL:HG11	1.88	0.54
62:SS:387:MET:HE1	62:SS:395:ARG:HD2	1.89	0.54
63:ST:700:LEU:HD11	63:ST:702:LEU:HD21	1.89	0.54
2:L1:547:U:OP2	35:NB:554:ARG:NH2	2.41	0.54
2:L1:1584:G:N2	2:L1:1611:A:OP2	2.24	0.54
16:LH:656:ASP:OD1	16:LH:657:SER:N	2.41	0.54
23:LO:586:SER:OG	23:LO:588:ASP:OD1	2.17	0.54
42:NI:62:SER:O	42:NI:90:ASN:ND2	2.41	0.54
59:SP:588:ASN:HB3	59:SP:600:THR:HG21	1.89	0.54
32:LX:408:MET:HE1	32:LX:426:LEU:HD21	1.89	0.54
55:SJ:141:MET:N	55:SJ:141:MET:HE2	2.23	0.54
18:LJ:42:VAL:HG23	18:LJ:42:VAL:O	2.08	0.54
23:LO:259:ASN:OD1	23:LO:260:GLN:N	2.41	0.54
30:LV:392:VAL:HA	30:LV:397:LEU:HD22	1.89	0.54
32:LX:62:LYS:O	32:LX:125:GLN:NE2	2.38	0.54
53:SH:362:THR:HG21	54:SI:818:THR:HG21	1.89	0.54
55:SK:77:LEU:HD11	55:SK:82:ARG:HB2	1.90	0.54
64:SU:196:GLN:OE1	64:SU:260:ASN:ND2	2.38	0.54
40:NG:93:THR:HG21	43:NK:123:CYS:O	2.07	0.54
2:L1:1516:A:H62	58:SN:116:THR:HG23	1.73	0.53
30:LV:161:GLU:OE2	30:LV:177:LYS:NZ	2.40	0.53
59:SP:1220:LEU:HD22	59:SP:1250:ILE:HD12	1.90	0.53
2:L1:524:U:O2'	2:L1:527:A:N6	2.37	0.53
21:LM:283:LEU:O	21:LM:326:LYS:NZ	2.38	0.53
34:NA:367:ASP:OD1	34:NA:370:ARG:NH2	2.41	0.53
49:SB:152:LEU:HD13	50:SD:205:ARG:HG2	1.90	0.53
2:L1:1028:C:OP2	43:NK:144:ARG:NH2	2.41	0.53
21:LM:778:SER:O	21:LM:782:VAL:N	2.41	0.53
29:LU:26:ARG:NH2	62:SS:867:GLN:O	2.40	0.53
30:LV:397:LEU:HD21	30:LV:404:PHE:CD2	2.43	0.53
41:NH:1226:PHE:CZ	42:NI:60:LEU:HD21	2.43	0.53
52:SG:70:TYR:CE2	52:SG:74:LEU:HD11	2.43	0.53
55:SK:31:LEU:HD23	55:SK:40:ARG:HD3	1.89	0.53
1:L0:546:G:O6	1:L0:591:U:O2	2.27	0.53
2:L1:1231:U:HO2'	2:L1:1258:U:HO2'	1.49	0.53
26:LR:62:GLN:OE1	26:LR:82:ALA:HB2	2.08	0.53
59:SP:229:TYR:OH	59:SP:277:ASP:OD2	2.25	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:1706:LYS:O	59:SP:1760:ASN:ND2	2.41	0.53
59:SP:2111:PHE:O	62:SS:231:SER:OG	2.20	0.53
64:SU:130:GLU:OE1	64:SU:147:THR:OG1	2.15	0.53
1:L0:452:A:H1'	54:SI:1083:ILE:HG22	1.90	0.53
18:LJ:432:TYR:O	18:LJ:470:TYR:OH	2.24	0.53
42:NI:135:ASN:OD1	42:NI:136:ASN:N	2.41	0.53
48:SA:196:LYS:O	48:SA:200:GLY:N	2.42	0.53
50:SD:157:GLY:HA3	50:SD:304:LEU:HD21	1.91	0.53
59:SP:1613:ALA:HB1	59:SP:1639:ILE:HD11	1.89	0.53
21:LM:45:TYR:CE2	29:LU:16:VAL:HG11	2.44	0.53
21:LM:353:ARG:NH1	21:LM:386:ASP:OD2	2.41	0.53
29:LU:263:ARG:NH2	29:LU:282:GLU:OE1	2.41	0.53
59:SP:772:ILE:HG23	59:SP:773:LEU:HD22	1.91	0.53
59:SP:1332:ILE:HG23	59:SP:1373:LYS:HE3	1.90	0.53
64:SU:522:GLU:N	64:SU:522:GLU:OE1	2.42	0.53
29:LU:26:ARG:NH1	31:LW:412:ASP:OD2	2.42	0.53
30:LV:211:SER:OG	30:LV:213:SER:OG	2.19	0.53
32:LX:853:HIS:O	32:LY:749:GLN:NE2	2.40	0.53
55:SJ:176:ARG:HE	55:SJ:196:LEU:HD11	1.74	0.53
59:SP:467:THR:HG23	59:SP:467:THR:O	2.09	0.53
2:L1:-7:A:N6	29:LU:290:ASP:OD2	2.42	0.53
16:LH:848:GLU:OE2	21:LM:381:ARG:NH2	2.42	0.53
26:LR:38:ASP:OD1	26:LR:61:GLU:N	2.42	0.53
29:LU:116:LEU:HD12	29:LU:137:LEU:O	2.09	0.53
29:LU:242:ASN:OD1	29:LU:263:ARG:N	2.42	0.53
32:LX:164:MET:HE3	32:LX:190:LEU:HD11	1.91	0.53
41:NH:655:LEU:HD13	41:NH:665:HIS:CD2	2.43	0.53
41:NH:976:ILE:HD11	41:NH:1017:TYR:CE1	2.44	0.53
49:SB:110:ASP:OD1	49:SB:111:ALA:N	2.42	0.53
16:LH:627:ASP:OD1	16:LH:628:ASP:N	2.42	0.53
16:LH:743:ILE:HD11	16:LH:763:ILE:HD12	1.91	0.53
20:LL:112:LEU:HD11	20:LL:131:LEU:HD11	1.90	0.53
32:LY:542:VAL:HG12	32:LY:542:VAL:O	2.09	0.53
34:NA:384:ARG:NH1	57:SM:81:SER:O	2.40	0.53
38:NE:107:VAL:HG23	38:NE:107:VAL:O	2.07	0.53
59:SP:704:ILE:HD11	59:SP:782:MET:SD	2.49	0.53
2:L1:1682:U:O2	2:L1:1720:G:N2	2.42	0.53
9:L8:89:GLU:N	9:L8:89:GLU:OE2	2.42	0.53
26:LR:438:THR:HG21	26:LR:494:ILE:O	2.08	0.53
30:LV:152:ASP:OD1	30:LV:166:ASN:ND2	2.42	0.53
3:L2:39:C:O2'	29:LU:18:SER:O	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:43:THR:O	18:LJ:304:SER:OG	2.27	0.52
55:SK:93:HIS:O	55:SK:97:LEU:HD23	2.09	0.52
16:LH:321:MET:HE3	16:LH:323:LEU:CD1	2.39	0.52
23:LO:351:LEU:HD22	23:LO:701:LEU:HD11	1.92	0.52
54:SI:141:LEU:HD23	54:SI:170:VAL:HB	1.91	0.52
55:SK:192:TYR:OH	55:SK:223:GLU:OE2	2.24	0.52
64:SU:450:GLU:OE2	64:SU:451:SER:N	2.42	0.52
2:L1:1192:C:N3	55:SJ:136:ARG:NH1	2.58	0.52
59:SP:1030:ILE:HD11	59:SP:1058:GLY:HA3	1.90	0.52
2:L1:207:U:O2	9:L8:178:ARG:NH2	2.41	0.52
27:LS:352:GLN:NE2	27:LS:378:GLN:O	2.40	0.52
40:NG:117:ASP:OD2	43:NK:98:ARG:NH1	2.42	0.52
41:NH:136:GLN:O	41:NH:180:LYS:NZ	2.43	0.52
48:SA:182:ASP:OD1	48:SA:183:GLN:N	2.42	0.52
52:SG:134:ARG:NH2	52:SG:535:GLU:OE1	2.42	0.52
59:SP:538:LEU:HD22	59:SP:574:LEU:HD23	1.90	0.52
59:SP:1918:LEU:O	59:SP:1922:ILE:HG23	2.09	0.52
59:SP:2144:TYR:HE2	62:SS:256:VAL:HG11	1.74	0.52
26:LR:137:THR:O	26:LR:180:ARG:NH2	2.42	0.52
26:LR:280:ARG:NH1	41:NH:636:GLU:OE2	2.41	0.52
26:LR:342:ASP:OD1	26:LR:343:MET:N	2.43	0.52
28:LT:354:SER:N	28:LT:369:ALA:O	2.40	0.52
30:LV:152:ASP:OD2	30:LV:164:ARG:NH1	2.42	0.52
67:SY:154:THR:OG1	67:SY:166:LEU:O	2.26	0.52
20:LL:197:ILE:HD11	20:LL:203:ILE:HB	1.91	0.52
25:LQ:854:CYS:HB3	26:LR:799:LEU:HD12	1.92	0.52
30:LV:388:LEU:HD22	30:LV:391:LEU:CD1	2.40	0.52
30:LV:398:ARG:O	30:LV:405:PHE:N	2.43	0.52
53:SH:289:VAL:O	53:SH:317:GLN:NE2	2.40	0.52
53:SH:314:ASN:OD1	53:SH:315:LYS:N	2.42	0.52
59:SP:1633:PRO:O	59:SP:1637:THR:HG23	2.10	0.52
25:LQ:426:ARG:NE	25:LQ:459:LEU:O	2.43	0.52
27:LS:511:LEU:HD13	27:LS:544:VAL:HG21	1.92	0.52
35:NB:555:ASN:OD1	35:NB:556:LYS:N	2.42	0.52
62:SS:223:GLU:OE1	62:SS:223:GLU:N	2.43	0.52
64:SU:166:VAL:HG21	64:SU:173:GLU:CG	2.40	0.52
1:L0:262:U:OP2	58:SN:164:ARG:NH2	2.43	0.52
4:L3:45:LEU:HD13	58:SN:95:GLU:HG3	1.92	0.52
20:LL:51:LEU:HD22	20:LL:88:TYR:CE1	2.45	0.52
41:NH:736:ASP:OD2	41:NH:821:TYR:OH	2.26	0.52
49:SB:219:SER:OG	49:SB:220:GLU:OE1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SM:123:VAL:HG12	57:SM:125:PRO:HD2	1.92	0.52
63:ST:576:ILE:HG22	63:ST:576:ILE:O	2.09	0.52
2:L1:1460:A:OP1	63:ST:743:GLN:NE2	2.41	0.52
16:LH:29:THR:O	16:LH:200:ASN:ND2	2.43	0.52
23:LO:295:ILE:HG22	23:LO:296:GLN:HG3	1.91	0.52
26:LR:742:ARG:NH1	34:NA:506:GLU:OE1	2.38	0.52
40:NG:48:VAL:HG21	40:NG:53:ASP:HB2	1.92	0.52
49:SB:159:VAL:HG12	49:SB:161:VAL:HG22	1.90	0.52
59:SP:1217:ARG:HG2	59:SP:1250:ILE:HD11	1.92	0.52
59:SP:2144:TYR:O	59:SP:2147:ALA:N	2.43	0.52
62:SS:357:ASP:O	62:SS:358:SER:OG	2.24	0.52
25:LQ:360:ASN:O	25:LQ:391:ARG:NH2	2.43	0.52
59:SP:1414:GLN:O	59:SP:1418:VAL:HG23	2.10	0.52
62:SS:371:GLU:OE1	62:SS:371:GLU:N	2.41	0.52
1:L0:156:U:O2'	1:L0:157:U:O5'	2.29	0.51
2:L1:85:A:N3	2:L1:148:A:O2'	2.38	0.51
16:LH:112:ASN:OD1	16:LH:113:ASN:N	2.43	0.51
26:LR:122:THR:HA	26:LR:146:THR:HG23	1.92	0.51
32:LX:505:ARG:NH1	32:LX:572:ASP:OD2	2.43	0.51
52:SG:318:LEU:HD11	52:SG:351:ILE:CD1	2.40	0.51
54:SI:126:ASN:OD1	54:SI:1020:SER:OG	2.28	0.51
55:SK:77:LEU:HA	55:SK:80:MET:HE2	1.91	0.51
2:L1:348:U:OP1	12:LD:106:ASN:ND2	2.42	0.51
2:L1:501:U:OP1	35:NB:577:LYS:NZ	2.32	0.51
49:SB:228:PRO:HD2	49:SB:231:ILE:HD13	1.92	0.51
55:SK:217:ALA:O	55:SK:221:VAL:HG12	2.11	0.51
62:SS:247:MET:HE2	62:SS:247:MET:N	2.25	0.51
10:L9:94:ASP:OD1	10:L9:95:TYR:N	2.43	0.51
25:LQ:233:ILE:O	25:LQ:241:LYS:NZ	2.38	0.51
32:LY:336:GLU:OE2	32:LY:336:GLU:N	2.43	0.51
63:ST:420:GLU:N	63:ST:420:GLU:OE1	2.42	0.51
30:LV:380:ARG:NE	30:LV:402:HIS:O	2.42	0.51
32:LY:370:ILE:HD13	32:LY:378:LEU:HD21	1.93	0.51
35:NB:390:MET:HE1	63:ST:486:LYS:O	2.11	0.51
59:SP:2007:VAL:HG11	59:SP:2045:GLN:HG3	1.91	0.51
2:L1:1655:A:N1	2:L1:1745:G:O6	2.43	0.51
13:LE:8:ALA:O	13:LE:12:ASN:ND2	2.42	0.51
16:LH:197:ILE:HD11	16:LH:213:LYS:HG3	1.92	0.51
26:LR:393:SER:OG	26:LR:394:LEU:N	2.43	0.51
27:LS:130:ASP:OD2	28:LT:179:LYS:NZ	2.43	0.51
28:LT:367:LEU:HD21	28:LT:389:MET:CE	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:484:LYS:NZ	32:LX:493:ASP:OD2	2.43	0.51
55:SK:43:VAL:HG11	55:SK:99:LEU:HD11	1.93	0.51
1:L0:552:G:O4'	62:SS:381:ARG:NH2	2.44	0.51
17:LI:564:ASN:OD1	17:LI:565:GLU:N	2.43	0.51
22:LN:39:VAL:HG22	22:LN:402:TRP:CZ3	2.45	0.51
22:LN:192:THR:HG23	22:LN:244:VAL:HG22	1.93	0.51
22:LN:540:ILE:HG21	22:LN:596:MET:CE	2.40	0.51
23:LO:200:SER:OG	23:LO:202:ASP:OD1	2.22	0.51
31:LW:302:ASP:O	31:LW:306:PHE:N	2.44	0.51
44:NM:244:VAL:O	44:NM:244:VAL:HG13	2.09	0.51
64:SU:117:LEU:HD23	64:SU:176:ILE:HD12	1.91	0.51
6:L5:136:ALA:O	6:L5:140:THR:HG22	2.10	0.51
16:LH:724:ILE:HG21	16:LH:762:TYR:CD1	2.46	0.51
26:LR:457:ALA:HB1	26:LR:494:ILE:HG21	1.92	0.51
32:LX:494:VAL:HG22	32:LX:535:GLU:CD	2.36	0.51
41:NH:177:ASN:OD1	41:NH:178:TYR:N	2.44	0.51
41:NH:827:ARG:NH1	41:NH:835:LEU:O	2.44	0.51
52:SG:157:LEU:HD11	52:SG:189:THR:HB	1.92	0.51
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.28	0.51
16:LH:302:SER:OG	16:LH:344:CYS:N	2.44	0.51
26:LR:251:ASP:OD1	26:LR:252:GLY:N	2.43	0.51
32:LY:540:LEU:HD11	32:LY:582:PRO:O	2.11	0.51
32:LY:851:ASP:OD1	32:LY:852:TYR:N	2.43	0.51
43:NK:106:ARG:O	43:NK:107:SER:OG	2.25	0.51
48:SA:213:ASN:OD1	48:SA:214:TYR:N	2.44	0.51
60:SQ:56:GLU:HG3	62:SS:382:LEU:HD13	1.93	0.51
2:L1:630:A:N6	2:L1:969:C:O2'	2.44	0.51
2:L1:1670:G:O2'	2:L1:1731:A:N6	2.41	0.51
18:LJ:500:GLU:O	18:LJ:504:ILE:HD12	2.10	0.51
34:NA:454:VAL:HG12	34:NA:454:VAL:O	2.11	0.51
43:NK:52:TYR:CE1	43:NK:56:ILE:HD13	2.46	0.51
48:SA:160:ARG:NH1	49:SB:243:MET:O	2.42	0.51
59:SP:1697:ILE:HG22	59:SP:1701:MET:HE2	1.93	0.51
62:SS:390:GLU:N	62:SS:390:GLU:OE1	2.42	0.51
2:L1:472:U:H4'	36:NC:316:ARG:NH2	2.26	0.51
3:L2:90:C:O2'	3:L2:91:C:OP1	2.22	0.51
28:LT:192:ASN:O	28:LT:196:GLY:N	2.42	0.51
37:ND:117:LEU:HD13	64:SU:22:LYS:HA	1.92	0.51
59:SP:1079:MET:HE1	59:SP:1120:GLN:HB3	1.93	0.51
59:SP:1387:ALA:O	59:SP:1390:SER:N	2.44	0.51
59:SP:1482:SER:HB3	59:SP:1518:MET:HE1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:23:ARG:NE	7:L6:40:ALA:O	2.44	0.50
20:LL:210:ARG:NH1	20:LL:228:ALA:O	2.44	0.50
32:LX:200:VAL:HG21	32:LX:210:LEU:HD11	1.93	0.50
49:SB:90:SER:OG	49:SB:91:GLU:OE1	2.09	0.50
59:SP:240:MET:SD	59:SP:255:MET:HE3	2.51	0.50
59:SP:389:ILE:O	59:SP:389:ILE:HG22	2.11	0.50
59:SP:395:GLU:OE1	59:SP:431:LYS:NZ	2.35	0.50
59:SP:1612:ILE:HG22	59:SP:1616:LEU:HD23	1.93	0.50
65:SV:131:LEU:HD21	65:SV:135:VAL:HB	1.93	0.50
3:L2:64:A:OP1	28:LT:390:SER:OG	2.10	0.50
22:LN:205:CYS:SG	22:LN:211:ARG:NH1	2.84	0.50
36:NC:256:PRO:CB	52:SG:357:LEU:HD22	2.41	0.50
59:SP:663:LEU:HD12	59:SP:696:VAL:HG22	1.92	0.50
8:L7:78:THR:HG22	8:L7:92:PHE:HE1	1.77	0.50
21:LM:228:ASP:OD1	21:LM:229:GLU:N	2.44	0.50
22:LN:279:HIS:HD1	22:LN:301:ASP:CG	2.19	0.50
40:NG:30:VAL:HG11	40:NG:71:CYS:SG	2.51	0.50
59:SP:29:GLU:OE1	59:SP:32:ARG:N	2.40	0.50
29:LU:37:ARG:NH1	31:LW:449:ILE:O	2.44	0.50
52:SG:185:LEU:HD13	52:SG:527:VAL:HG11	1.93	0.50
52:SG:227:GLU:OE2	52:SG:279:ARG:N	2.44	0.50
59:SP:1258:TRP:CZ2	59:SP:1342:LEU:HD13	2.47	0.50
63:ST:604:VAL:HG21	63:ST:606:PHE:CZ	2.45	0.50
2:L1:332:U:OP1	9:L8:31:ARG:NH1	2.40	0.50
23:LO:497:ILE:CD1	23:LO:532:VAL:HG11	2.40	0.50
55:SJ:204:VAL:HG21	55:SJ:241:PHE:CE2	2.46	0.50
16:LH:245:LEU:HD22	16:LH:249:THR:HG21	1.94	0.50
27:LS:325:ASP:OD1	27:LS:326:LEU:N	2.44	0.50
27:LS:497:ASN:OD1	27:LS:498:ASN:N	2.44	0.50
50:SC:228:GLN:O	50:SC:231:ARG:NH1	2.43	0.50
59:SP:779:LEU:HA	59:SP:782:MET:HE3	1.92	0.50
59:SP:1158:ILE:O	59:SP:1208:MET:HE1	2.12	0.50
59:SP:1436:ASP:OD1	59:SP:1437:MET:N	2.44	0.50
67:SY:158:MET:HA	67:SY:158:MET:HE3	1.94	0.50
30:LV:153:LEU:N	30:LV:165:LEU:O	2.39	0.50
30:LV:388:LEU:HD22	30:LV:391:LEU:HD12	1.93	0.50
30:LV:401:MET:HE2	59:SP:911:GLN:HA	1.93	0.50
52:SG:327:ASP:OD1	52:SG:328:ILE:N	2.45	0.50
59:SP:894:ASP:OD1	59:SP:932:ARG:NH2	2.42	0.50
5:L4:104:ASP:OD1	5:L4:107:GLY:N	2.45	0.50
26:LR:494:ILE:HD11	26:LR:508:THR:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SB:191:HIS:ND1	49:SB:245:THR:O	2.44	0.50
54:SI:819:GLU:OE1	54:SI:819:GLU:N	2.45	0.50
59:SP:441:ASP:OD1	59:SP:442:LYS:N	2.45	0.50
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.45	0.50
16:LH:478:ASN:OD1	16:LH:479:ASN:N	2.42	0.50
21:LM:465:PHE:O	21:LM:469:LEU:N	2.40	0.50
30:LV:103:ASP:OD1	30:LV:104:PHE:N	2.45	0.50
33:LZ:137:ARG:NH1	33:LZ:162:ASP:OD1	2.45	0.50
48:SA:177:ALA:CB	48:SA:292:LEU:HD13	2.41	0.50
59:SP:1645:SER:HB3	59:SP:1650:LEU:HD22	1.93	0.50
1:L0:247:U:O4	54:SI:1091:LYS:NZ	2.45	0.49
2:L1:1204:A:O2'	2:L1:1208:A:N3	2.42	0.49
3:L2:91:C:OP1	49:SB:324:LYS:NZ	2.38	0.49
16:LH:77:ILE:HD13	16:LH:117:ILE:HD11	1.94	0.49
17:LI:570:LEU:HD12	17:LI:579:LEU:HD13	1.93	0.49
35:NB:503:GLN:O	35:NB:507:ILE:HD12	2.12	0.49
59:SP:2012:MET:HE2	59:SP:2012:MET:HA	1.92	0.49
22:LN:441:VAL:HG22	22:LN:450:VAL:HG22	1.94	0.49
59:SP:588:ASN:OD1	59:SP:591:LEU:HD12	2.12	0.49
1:L0:268:G:N2	67:SY:90:SER:OG	2.45	0.49
16:LH:720:ILE:HD12	16:LH:774:PHE:CD2	2.47	0.49
26:LR:73:GLY:O	26:LR:90:LEU:HD12	2.12	0.49
29:LU:228:ASN:OD1	29:LU:229:GLN:N	2.45	0.49
30:LV:361:GLU:OE2	32:LY:918:ARG:NH1	2.45	0.49
48:SA:281:LEU:HD11	49:SB:265:PHE:HZ	1.77	0.49
52:SG:417:SER:OG	52:SG:418:ASP:N	2.45	0.49
57:SM:260:GLU:OE2	57:SM:262:ARG:NH1	2.45	0.49
59:SP:1081:ASP:O	59:SP:1085:VAL:HG22	2.11	0.49
59:SP:1880:ILE:O	59:SP:1884:ARG:NH2	2.44	0.49
2:L1:1223:A:O2'	63:ST:414:LEU:O	2.31	0.49
24:LP:183:TYR:CZ	24:LP:322:LEU:HD13	2.47	0.49
28:LT:627:ASN:OD1	28:LT:647:THR:OG1	2.29	0.49
46:NQ:67:THR:OG1	46:NQ:70:LYS:O	2.30	0.49
59:SP:1191:ASP:OD1	59:SP:1193:ASN:N	2.45	0.49
5:L4:54:TYR:CD2	14:LF:17:LEU:HD13	2.48	0.49
22:LN:257:ASP:OD1	22:LN:259:THR:OG1	2.26	0.49
22:LN:564:ALA:HB2	22:LN:594:PHE:CE1	2.47	0.49
23:LO:524:ARG:NH1	23:LO:526:ASP:OD2	2.44	0.49
32:LX:522:THR:HG21	32:LX:706:PRO:O	2.13	0.49
54:SI:838:ILE:HD12	54:SI:874:TYR:HB3	1.93	0.49
57:SM:237:VAL:HG13	57:SM:250:VAL:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SY:158:MET:HE1	67:SY:161:ARG:HE	1.76	0.49
1:L0:120:C:O2'	64:SU:137:GLU:OE2	2.10	0.49
3:L2:24:U:O2'	3:L2:25:U:OP2	2.30	0.49
25:LQ:220:THR:HG23	25:LQ:259:ILE:HD11	1.94	0.49
59:SP:1134:MET:SD	59:SP:1177:SER:OG	2.66	0.49
54:SI:906:ASP:OD1	54:SI:1030:LYS:NZ	2.45	0.49
59:SP:1027:ILE:CG2	59:SP:1085:VAL:HG21	2.43	0.49
8:L7:17:GLU:CG	8:L7:46:ILE:HG22	2.43	0.49
16:LH:876:PHE:CD2	21:LM:176:ALA:HB1	2.48	0.49
20:LL:72:ASP:OD1	20:LL:73:THR:N	2.44	0.49
20:LL:471:ARG:NH1	64:SU:297:ASP:OD1	2.44	0.49
38:NE:164:LEU:HD11	38:NE:213:MET:CE	2.42	0.49
44:NM:20:VAL:HG23	44:NM:21:VAL:HG23	1.93	0.49
59:SP:70:ILE:O	59:SP:70:ILE:HG22	2.11	0.49
59:SP:1989:ASP:OD1	59:SP:1995:ARG:NE	2.39	0.49
63:ST:456:ILE:HD13	64:SU:529:VAL:HG21	1.93	0.49
64:SU:99:LYS:NZ	64:SU:147:THR:HG23	2.28	0.49
9:L8:67:TRP:NE1	9:L8:185:GLU:OE2	2.41	0.49
16:LH:71:ASN:O	16:LH:75:SER:OG	2.30	0.49
16:LH:381:SER:OG	20:LL:349:ASP:OD2	2.11	0.49
16:LH:822:PHE:CD1	20:LL:91:LEU:HD21	2.48	0.49
25:LQ:414:LEU:CD1	25:LQ:447:LEU:HD11	2.43	0.49
29:LU:344:HIS:NE2	29:LU:418:HIS:O	2.45	0.49
30:LV:281:ASP:OD1	30:LV:282:ASN:N	2.45	0.49
44:NM:61:LEU:HD13	44:NM:96:LEU:CD2	2.43	0.49
54:SI:952:PHE:HD2	54:SI:958:VAL:HG22	1.77	0.49
55:SK:69:ASN:OD1	55:SK:70:CYS:N	2.46	0.49
1:L0:168:G:H22	1:L0:227:U:H3	1.61	0.49
3:L2:324:U:N3	49:SB:323:GLU:OE2	2.46	0.49
30:LV:299:ILE:HD11	30:LV:311:MET:CE	2.43	0.49
59:SP:550:GLU:OE1	59:SP:591:LEU:HD11	2.13	0.49
16:LH:612:SER:HB3	16:LH:662:VAL:HG12	1.95	0.48
31:LW:296:ARG:NH1	31:LW:315:LEU:O	2.45	0.48
32:LY:864:LEU:HD22	32:LY:890:LEU:HD21	1.94	0.48
55:SK:140:LEU:HD21	55:SK:160:LEU:HD12	1.95	0.48
59:SP:1295:VAL:HG12	59:SP:1297:GLU:H	1.78	0.48
63:ST:494:SER:N	63:ST:497:ASP:OD2	2.45	0.48
2:L1:37:U:O2'	36:NC:271:ARG:NH2	2.45	0.48
16:LH:71:ASN:OD1	16:LH:73:LEU:N	2.43	0.48
50:SC:89:GLU:OE2	50:SC:100:ARG:NE	2.42	0.48
2:L1:1057:U:O4	41:NH:791:LYS:NZ	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L2:24:U:O4	31:LW:436:LYS:NZ	2.46	0.48
28:LT:854:SER:HB2	28:LT:895:VAL:HG21	1.95	0.48
48:SA:223:ILE:HD11	48:SA:237:LEU:HD22	1.95	0.48
63:ST:113:ILE:HG23	63:ST:113:ILE:O	2.13	0.48
16:LH:849:ASP:OD2	27:LS:475:LYS:NZ	2.41	0.48
16:LH:879:ILE:HD11	21:LM:211:LEU:C	2.38	0.48
41:NH:756:VAL:HG12	41:NH:756:VAL:O	2.14	0.48
48:SA:178:ILE:HD11	48:SA:313:ALA:HB3	1.96	0.48
59:SP:255:MET:HB3	59:SP:298:MET:HE3	1.94	0.48
62:SS:319:THR:HG23	62:SS:319:THR:O	2.13	0.48
2:L1:-7:A:O2'	2:L1:-6:A:O5'	2.31	0.48
18:LJ:168:THR:OG1	18:LJ:190:ASP:OD1	2.23	0.48
25:LQ:559:PHE:O	25:LQ:563:MET:N	2.46	0.48
32:LX:370:ILE:CD1	32:LX:378:LEU:HD21	2.44	0.48
34:NA:473:THR:OG1	34:NA:487:ALA:O	2.30	0.48
41:NH:656:ARG:NH2	44:NM:241:GLY:O	2.47	0.48
44:NM:108:ASP:OD1	44:NM:109:LYS:N	2.46	0.48
59:SP:370:ASP:OD1	59:SP:370:ASP:N	2.47	0.48
59:SP:1651:ARG:NH1	59:SP:1744:GLU:OE1	2.46	0.48
18:LJ:238:ASP:O	18:LJ:242:ASN:N	2.46	0.48
23:LO:707:ASN:OD1	23:LO:708:ASP:N	2.47	0.48
28:LT:367:LEU:HD22	28:LT:375:LEU:HD21	1.94	0.48
29:LU:66:HIS:N	29:LU:370:GLY:O	2.44	0.48
32:LX:851:ASP:OD1	32:LX:852:TYR:N	2.44	0.48
33:LZ:34:ARG:NH2	56:SL:16:THR:O	2.47	0.48
38:NE:196:VAL:HG23	38:NE:196:VAL:O	2.14	0.48
1:L0:326:C:HO2'	1:L0:327:A:P	2.37	0.48
1:L0:354:G:N1	31:LW:485:ASP:O	2.44	0.48
24:LP:178:VAL:O	24:LP:178:VAL:HG23	2.14	0.48
30:LV:147:ASN:HD22	30:LV:188:ILE:HD11	1.79	0.48
57:SM:75:ASP:OD1	57:SM:76:GLU:N	2.47	0.48
63:ST:388:LEU:O	63:ST:392:LYS:N	2.46	0.48
7:L6:57:ASP:OD1	7:L6:61:PHE:N	2.47	0.48
49:SB:46:ALA:HB1	49:SB:75:LEU:HD11	1.96	0.48
59:SP:1189:LEU:HD22	59:SP:1194:SER:HB3	1.95	0.48
16:LH:265:ASP:OD1	16:LH:266:ASN:N	2.45	0.48
23:LO:33:VAL:HG23	23:LO:33:VAL:O	2.13	0.48
41:NH:975:LEU:HD11	41:NH:977:LEU:HD21	1.96	0.48
48:SA:28:GLY:O	48:SA:34:VAL:HG21	2.13	0.48
62:SS:260:ALA:O	62:SS:264:LYS:NZ	2.46	0.48
7:L6:1:MET:HE3	7:L6:24:ILE:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:127:THR:HG23	18:LJ:142:THR:HG23	1.96	0.48
18:LJ:386:ARG:HD2	18:LJ:413:LEU:HD21	1.96	0.48
26:LR:12:LEU:HD11	26:LR:378:PRO:HG2	1.96	0.48
42:NI:43:GLN:OE1	42:NI:43:GLN:N	2.47	0.48
51:SF:48:ILE:C	51:SF:104:THR:HG23	2.38	0.48
56:SL:41:THR:HG23	56:SL:41:THR:O	2.14	0.48
59:SP:512:ASP:O	59:SP:515:THR:OG1	2.27	0.48
63:ST:391:VAL:O	63:ST:391:VAL:HG12	2.14	0.48
63:ST:659:GLU:N	63:ST:659:GLU:OE1	2.45	0.48
16:LH:96:ILE:HG23	16:LH:151:TYR:CZ	2.49	0.47
18:LJ:304:SER:O	18:LJ:321:GLY:N	2.43	0.47
25:LQ:212:VAL:HG22	25:LQ:217:LEU:HD12	1.96	0.47
25:LQ:351:LEU:O	25:LQ:367:ILE:N	2.42	0.47
26:LR:223:TRP:NE1	26:LR:233:LEU:HD13	2.28	0.47
27:LS:379:GLY:N	27:LS:383:TRP:O	2.39	0.47
27:LS:434:GLU:OE2	27:LS:496:ARG:NH1	2.45	0.47
32:LX:37:LEU:HD21	32:LX:151:LEU:HD21	1.96	0.47
32:LY:767:GLU:N	32:LY:767:GLU:OE1	2.47	0.47
59:SP:255:MET:CE	59:SP:258:LEU:HD12	2.44	0.47
59:SP:1603:ASP:O	59:SP:1606:ILE:HG22	2.13	0.47
55:SJ:192:TYR:OH	55:SJ:223:GLU:OE2	2.27	0.47
55:SK:104:ILE:N	55:SK:246:GLU:OE2	2.46	0.47
9:L8:156:VAL:HG12	9:L8:160:PHE:CE2	2.49	0.47
16:LH:666:ASN:OD1	16:LH:667:ASP:N	2.45	0.47
31:LW:545:VAL:HG21	42:NI:181:LYS:HB3	1.96	0.47
32:LX:164:MET:HE1	32:LX:171:ARG:HE	1.80	0.47
32:LX:896:ASP:OD1	32:LX:897:THR:N	2.47	0.47
50:SD:117:VAL:HG23	50:SD:118:TYR:CD2	2.48	0.47
59:SP:1680:THR:HG23	59:SP:1681:LEU:HG	1.95	0.47
62:SS:793:GLU:OE1	62:SS:793:GLU:N	2.48	0.47
6:L5:140:THR:HG23	6:L5:171:ALA:HB1	1.96	0.47
10:L9:138:LYS:NZ	52:SG:354:GLU:OE1	2.46	0.47
16:LH:366:ASN:OD1	16:LH:367:SER:N	2.48	0.47
20:LL:472:LEU:HD23	20:LL:473:LYS:O	2.15	0.47
16:LH:577:ASP:O	16:LH:611:VAL:HG21	2.14	0.47
20:LL:111:ASP:OD1	20:LL:112:LEU:N	2.46	0.47
23:LO:10:LEU:HD13	23:LO:702:LEU:HD23	1.95	0.47
24:LP:300:MET:HE2	49:SB:214:ILE:CD1	2.44	0.47
28:LT:62:ASP:O	28:LT:66:LEU:N	2.43	0.47
51:SE:10:PRO:HB2	51:SE:124:LEU:HD21	1.96	0.47
55:SK:47:MET:HA	55:SK:47:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:332:U:OP2	9:L8:54:LYS:NZ	2.36	0.47
2:L1:396:G:O6	9:L8:26:LYS:NZ	2.33	0.47
13:LE:70:ASN:OD1	56:SL:114:ARG:NH1	2.47	0.47
18:LJ:412:GLU:O	18:LJ:416:THR:HG23	2.14	0.47
55:SK:97:LEU:HD22	55:SK:130:ILE:HD11	1.96	0.47
59:SP:137:ASP:O	59:SP:140:ILE:HG22	2.14	0.47
59:SP:497:ILE:HD11	59:SP:525:ILE:HG22	1.96	0.47
59:SP:503:ARG:O	59:SP:507:THR:OG1	2.23	0.47
59:SP:1030:ILE:HG21	59:SP:1086:VAL:HG22	1.96	0.47
59:SP:1518:MET:O	59:SP:1573:SER:N	2.44	0.47
16:LH:678:LEU:HD23	16:LH:694:LEU:HD11	1.96	0.47
16:LH:768:TRP:NE1	16:LH:771:ASP:O	2.47	0.47
24:LP:45:SER:OG	24:LP:46:ARG:N	2.46	0.47
28:LT:738:ASP:OD1	28:LT:739:VAL:N	2.46	0.47
41:NH:282:ASP:OD1	41:NH:283:TYR:N	2.48	0.47
57:SM:162:THR:OG1	57:SM:264:GLY:O	2.27	0.47
59:SP:322:VAL:O	59:SP:368:ASN:ND2	2.47	0.47
63:ST:385:ASP:OD1	63:ST:386:ALA:N	2.47	0.47
63:ST:618:THR:O	63:ST:621:THR:OG1	2.22	0.47
9:L8:156:VAL:HG12	9:L8:160:PHE:HE2	1.79	0.47
28:LT:608:THR:OG1	28:LT:610:ARG:NH1	2.48	0.47
29:LU:231:GLU:OE2	29:LU:250:ARG:NH1	2.46	0.47
41:NH:439:HIS:NE2	41:NH:458:ILE:HD13	2.30	0.47
42:NI:152:PRO:HA	42:NI:155:LEU:HD23	1.97	0.47
54:SI:849:LEU:HD23	54:SI:896:PHE:HB3	1.96	0.47
55:SJ:54:LYS:HB2	55:SJ:65:TYR:CD1	2.50	0.47
2:L1:495:C:O5'	54:SI:1135:ARG:NH2	2.47	0.47
7:L6:1:MET:HE3	7:L6:24:ILE:CG2	2.45	0.47
25:LQ:829:VAL:HG21	25:LQ:864:ASN:HD21	1.80	0.47
26:LR:143:HIS:CE1	26:LR:171:MET:HE2	2.50	0.47
32:LY:370:ILE:CD1	32:LY:378:LEU:HD21	2.45	0.47
41:NH:551:GLU:OE1	41:NH:551:GLU:N	2.45	0.47
41:NH:915:LEU:HD21	41:NH:1089:PHE:HZ	1.80	0.47
14:LF:91:LEU:O	14:LF:95:GLY:N	2.47	0.47
16:LH:717:THR:HG23	16:LH:718:GLY:N	2.31	0.47
30:LV:223:ASN:ND2	45:NN:429:ALA:O	2.47	0.47
30:LV:357:ASP:O	30:LV:360:THR:HG23	2.15	0.47
33:LZ:29:ASP:OD1	33:LZ:30:THR:N	2.48	0.47
41:NH:369:TRP:NE1	41:NH:495:THR:HG21	2.29	0.47
60:SQ:113:MET:HE3	60:SQ:113:MET:HA	1.97	0.47
4:L3:45:LEU:HD11	4:L3:49:LYS:HE3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LD:73:GLY:O	12:LD:122:ILE:HD12	2.15	0.46
15:LG:65:ARG:O	15:LG:67:ARG:NH1	2.48	0.46
16:LH:89:VAL:HG22	16:LH:110:PHE:O	2.15	0.46
18:LJ:53:HIS:NE2	18:LJ:311:THR:O	2.48	0.46
21:LM:336:LEU:HD12	21:LM:373:ILE:HB	1.97	0.46
21:LM:410:ILE:O	21:LM:410:ILE:HG23	2.15	0.46
27:LS:45:ILE:H	27:LS:45:ILE:HD12	1.80	0.46
53:SH:131:GLU:OE1	53:SH:131:GLU:N	2.47	0.46
55:SK:127:THR:HG23	63:ST:711:PRO:O	2.14	0.46
57:SM:177:ILE:HG12	63:ST:62:ALA:HB3	1.97	0.46
59:SP:546:GLU:O	59:SP:549:LYS:NZ	2.48	0.46
2:L1:139:C:OP2	7:L6:187:LYS:NZ	2.47	0.46
24:LP:80:THR:HG23	24:LP:80:THR:O	2.16	0.46
26:LR:343:MET:CE	26:LR:635:ALA:HB2	2.45	0.46
36:NC:274:ILE:HD12	36:NC:274:ILE:H	1.80	0.46
55:SK:49:SER:C	55:SK:50:LEU:HD12	2.40	0.46
2:L1:-6:A:OP1	62:SS:307:ARG:NH2	2.48	0.46
6:L5:90:ILE:O	6:L5:94:THR:HG23	2.14	0.46
20:LL:5:VAL:HG23	20:LL:306:LEU:HD11	1.97	0.46
28:LT:639:ASP:OD1	28:LT:640:LEU:N	2.48	0.46
32:LY:765:VAL:HG23	32:LY:774:LEU:HD22	1.98	0.46
41:NH:1233:ASN:OD1	41:NH:1234:PHE:N	2.48	0.46
50:SD:320:TYR:OH	50:SD:322:ARG:NH1	2.49	0.46
54:SI:392:GLU:OE1	54:SI:392:GLU:N	2.48	0.46
55:SK:90:ASP:OD1	55:SK:91:ILE:N	2.48	0.46
56:SL:135:THR:O	56:SL:135:THR:HG22	2.15	0.46
65:SV:181:ASP:OD2	65:SV:183:ARG:NH2	2.46	0.46
10:L9:56:ALA:O	10:L9:60:LEU:HD23	2.16	0.46
26:LR:394:LEU:HD11	26:LR:403:ILE:CG2	2.45	0.46
27:LS:129:ASP:OD1	28:LT:194:ARG:NH2	2.45	0.46
32:LX:860:PRO:O	32:LX:864:LEU:HD23	2.15	0.46
42:NI:60:LEU:HD23	42:NI:61:LEU:HB2	1.97	0.46
50:SD:228:GLN:O	50:SD:231:ARG:NH1	2.43	0.46
59:SP:201:ARG:NH2	59:SP:238:GLU:O	2.47	0.46
2:L1:896:U:O2	40:NG:41:ARG:NH1	2.42	0.46
11:LC:97:VAL:HG12	11:LC:98:ASP:H	1.79	0.46
17:LI:460:VAL:HG22	17:LI:482:GLU:CD	2.39	0.46
26:LR:249:LEU:HD21	26:LR:316:VAL:HG11	1.97	0.46
31:LW:14:GLU:OE1	31:LW:14:GLU:N	2.49	0.46
41:NH:1063:ARG:CZ	41:NH:1067:LEU:HD21	2.46	0.46
52:SG:454:GLU:OE1	52:SG:459:LEU:HD23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SI:791:ILE:CD1	54:SI:812:MET:HE1	2.44	0.46
5:L4:87:MET:HE1	5:L4:236:ILE:HD13	1.98	0.46
17:LI:497:ILE:HG22	17:LI:497:ILE:O	2.15	0.46
21:LM:390:LEU:O	21:LM:394:LEU:N	2.47	0.46
38:NE:152:ASP:OD2	43:NK:201:LYS:NZ	2.34	0.46
59:SP:17:SER:O	59:SP:22:ARG:NH2	2.46	0.46
59:SP:825:GLU:OE2	59:SP:828:ARG:NH1	2.49	0.46
9:L8:73:SER:O	9:L8:74:LYS:NZ	2.38	0.46
14:LF:83:LYS:CE	14:LF:96:LEU:HD12	2.45	0.46
25:LQ:446:ILE:HD11	25:LQ:454:LEU:HD21	1.98	0.46
29:LU:68:ASP:OD1	29:LU:69:GLY:N	2.43	0.46
30:LV:58:ALA:HB3	30:LV:76:THR:HG21	1.97	0.46
49:SB:3:TYR:O	49:SB:88:ILE:N	2.45	0.46
52:SG:158:THR:HG21	52:SG:240:LEU:HA	1.97	0.46
57:SM:255:GLU:N	57:SM:255:GLU:OE1	2.49	0.46
59:SP:1642:VAL:CG1	59:SP:1650:LEU:HD21	2.45	0.46
63:ST:506:ILE:HD11	64:SU:529:VAL:HG22	1.97	0.46
65:SV:14:THR:O	65:SV:18:ASN:N	2.41	0.46
2:L1:18:C:O4'	56:SL:162:GLN:NE2	2.49	0.46
16:LH:374:LEU:HD23	16:LH:381:SER:HA	1.97	0.46
24:LP:183:TYR:OH	24:LP:322:LEU:HD13	2.16	0.46
24:LP:195:LYS:NZ	62:SS:385:GLU:O	2.49	0.46
26:LR:266:ILE:HD11	26:LR:283:LYS:HB2	1.98	0.46
26:LR:510:SER:OG	26:LR:511:TYR:N	2.49	0.46
41:NH:526:CYS:O	41:NH:698:ASN:ND2	2.49	0.46
59:SP:356:ASP:OD1	59:SP:356:ASP:N	2.49	0.46
59:SP:1482:SER:CB	59:SP:1518:MET:HE1	2.46	0.46
63:ST:597:GLU:N	63:ST:597:GLU:OE1	2.48	0.46
5:L4:95:THR:OG1	5:L4:97:GLU:OE1	2.29	0.46
15:LG:58:GLU:OE1	15:LG:58:GLU:N	2.49	0.46
17:LI:498:SER:HB3	17:LI:531:LEU:HD12	1.96	0.46
18:LJ:404:ALA:HB2	18:LJ:417:VAL:HG11	1.98	0.46
21:LM:559:ASN:N	21:LM:597:HIS:O	2.45	0.46
21:LM:1053:TYR:O	21:LM:1056:ALA:N	2.49	0.46
29:LU:13:TYR:OH	31:LW:69:GLU:OE1	2.34	0.46
41:NH:397:MET:O	41:NH:401:LEU:HD23	2.15	0.46
52:SG:164:GLN:NE2	52:SG:528:GLU:O	2.49	0.46
59:SP:1441:LEU:HD21	59:SP:1451:PHE:CE2	2.50	0.46
60:SQ:121:LEU:HD23	60:SQ:143:VAL:HG13	1.98	0.46
2:L1:875:G:O2'	2:L1:877:G:OP2	2.25	0.46
3:L2:115:G:O2'	3:L2:257:A:N3	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L4:163:ASP:O	5:L4:167:GLY:N	2.46	0.46
18:LJ:302:VAL:HG22	18:LJ:322:LEU:CD2	2.46	0.46
32:LY:378:LEU:HD22	32:LY:384:VAL:HG21	1.97	0.46
49:SB:42:PHE:CZ	49:SB:116:ILE:HG23	2.51	0.46
54:SI:298:VAL:HG13	54:SI:791:ILE:HG23	1.97	0.46
59:SP:1261:ILE:CD1	59:SP:1291:LEU:HD22	2.44	0.46
59:SP:1459:LEU:HD21	59:SP:1499:ARG:NH2	2.31	0.46
59:SP:1612:ILE:HG22	59:SP:1616:LEU:CD2	2.46	0.46
11:LC:58:ASP:OD1	11:LC:59:LYS:N	2.49	0.45
27:LS:224:ASN:OD1	27:LS:225:SER:N	2.49	0.45
30:LV:388:LEU:HD21	30:LV:414:VAL:HG21	1.98	0.45
31:LW:510:ASP:OD1	43:NK:75:LEU:HD12	2.16	0.45
32:LX:421:SER:OG	32:LX:543:SER:O	2.32	0.45
37:ND:120:ILE:HD11	64:SU:21:ARG:HD2	1.97	0.45
59:SP:170:LEU:HD22	59:SP:203:CYS:SG	2.56	0.45
15:LG:12:VAL:HG22	15:LG:30:VAL:HG12	1.99	0.45
16:LH:868:ASN:C	16:LH:868:ASN:ND2	2.70	0.45
21:LM:1055:SER:O	21:LM:1059:ASN:N	2.42	0.45
22:LN:434:SER:OG	22:LN:436:ASP:OD1	2.22	0.45
32:LX:34:ARG:NH1	32:LX:64:LEU:O	2.49	0.45
53:SH:342:VAL:HG22	53:SH:349:ASP:O	2.16	0.45
59:SP:1310:SER:OG	59:SP:1323:ARG:NH2	2.49	0.45
63:ST:481:MET:HE1	63:ST:497:ASP:OD1	2.17	0.45
63:ST:710:ILE:H	63:ST:710:ILE:HD12	1.82	0.45
64:SU:384:ALA:O	64:SU:387:THR:OG1	2.34	0.45
8:L7:73:VAL:HG22	8:L7:73:VAL:O	2.16	0.45
16:LH:197:ILE:HD11	16:LH:213:LYS:CG	2.47	0.45
30:LV:315:VAL:HG21	30:LV:335:SER:HB3	1.98	0.45
32:LY:896:ASP:OD1	32:LY:897:THR:N	2.49	0.45
35:NB:495:TYR:HE2	58:SN:250:THR:HG22	1.82	0.45
38:NE:239:ARG:NH1	38:NE:286:ARG:O	2.50	0.45
47:OA:1408:ASP:OD2	47:OA:1412:SER:N	2.49	0.45
49:SB:7:GLU:N	49:SB:7:GLU:OE1	2.49	0.45
52:SG:235:HIS:NE2	52:SG:261:ILE:HD12	2.31	0.45
54:SI:99:ASN:OD1	54:SI:100:ASP:N	2.50	0.45
17:LI:432:ASP:OD1	17:LI:433:ASP:N	2.48	0.45
22:LN:389:ARG:NH2	22:LN:405:GLY:O	2.46	0.45
22:LN:487:VAL:HG21	22:LN:555:LEU:HD21	1.98	0.45
30:LV:410:LEU:O	30:LV:414:VAL:HG23	2.16	0.45
32:LY:514:ASN:OD1	32:LY:515:LEU:N	2.48	0.45
41:NH:856:THR:HG22	41:NH:858:ARG:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SD:117:VAL:HG23	50:SD:118:TYR:HD2	1.82	0.45
59:SP:1445:ASP:O	59:SP:1449:ASP:N	2.46	0.45
59:SP:1670:LEU:HD13	59:SP:1701:MET:HE1	1.97	0.45
64:SU:57:MET:HE2	64:SU:57:MET:HA	1.97	0.45
2:L1:1164:G:O2'	2:L1:1612:U:O2	2.32	0.45
6:L5:118:LEU:HD22	6:L5:129:PRO:HB2	1.98	0.45
22:LN:95:LYS:O	22:LN:97:ARG:NH1	2.47	0.45
26:LR:395:ASP:OD1	26:LR:396:ALA:N	2.50	0.45
27:LS:544:VAL:HG22	27:LS:551:VAL:HG22	1.98	0.45
28:LT:838:ILE:HD12	28:LT:880:LEU:HD22	1.99	0.45
29:LU:319:GLU:OE2	29:LU:340:ARG:NE	2.48	0.45
41:NH:388:PHE:CD2	41:NH:480:MET:HE3	2.52	0.45
55:SK:128:VAL:CA	55:SK:159:LEU:HD12	2.46	0.45
59:SP:1151:ILE:HG21	59:SP:1198:PHE:CD1	2.51	0.45
2:L1:1779:U:N3	2:L1:1781:A:OP2	2.48	0.45
10:L9:146:PHE:CZ	36:NC:274:ILE:HD11	2.51	0.45
22:LN:363:SER:O	22:LN:367:GLY:N	2.45	0.45
23:LO:420:ARG:NH1	34:NA:494:GLU:OE2	2.49	0.45
23:LO:661:LEU:HD22	33:LZ:50:ILE:HD11	1.97	0.45
29:LU:215:LEU:O	29:LU:216:SER:OG	2.29	0.45
41:NH:835:LEU:HD23	41:NH:835:LEU:H	1.82	0.45
53:SH:19:LEU:HD22	54:SI:608:LEU:HD12	1.98	0.45
59:SP:318:LEU:HD11	59:SP:339:LEU:HD23	1.99	0.45
12:LD:124:THR:O	12:LD:140:VAL:HG12	2.16	0.45
14:LF:53:ASP:HB3	14:LF:79:VAL:HG13	1.99	0.45
21:LM:406:TYR:O	21:LM:410:ILE:HG22	2.17	0.45
27:LS:183:ASP:O	27:LS:184:SER:OG	2.30	0.45
30:LV:138:PRO:CG	45:NN:464:LEU:HD13	2.47	0.45
32:LX:171:ARG:CG	32:LX:679:ILE:HG21	2.47	0.45
32:LX:171:ARG:HG2	32:LX:679:ILE:HG21	1.99	0.45
32:LY:820:HIS:O	32:LY:820:HIS:ND1	2.46	0.45
47:OA:1408:ASP:OD2	47:OA:1412:SER:OG	2.25	0.45
59:SP:2157:PHE:HE1	62:SS:250:VAL:HG21	1.78	0.45
2:L1:1516:A:H62	58:SN:116:THR:CG2	2.29	0.45
17:LI:573:ILE:O	17:LI:579:LEU:HD21	2.16	0.45
41:NH:270:ILE:HD13	41:NH:294:LEU:HD23	1.99	0.45
59:SP:1456:HIS:O	59:SP:1462:ARG:NE	2.50	0.45
63:ST:453:ASN:OD1	63:ST:454:ALA:N	2.49	0.45
2:L1:1600:A:OP2	54:SI:988:ARG:NH1	2.47	0.45
10:L9:157:ASP:OD1	52:SG:280:ARG:NH2	2.49	0.45
11:LC:98:ASP:OD1	11:LC:101:SER:OG	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:96:ILE:HG23	16:LH:151:TYR:CE2	2.52	0.45
26:LR:72:ASP:OD1	26:LR:73:GLY:N	2.49	0.45
26:LR:220:ILE:CD1	26:LR:239:VAL:HG11	2.46	0.45
28:LT:646:VAL:HG13	28:LT:647:THR:HG23	1.98	0.45
44:NM:127:VAL:HG13	44:NM:176:VAL:HG11	1.99	0.45
48:SA:180:LEU:HD22	49:SB:183:ARG:NE	2.32	0.45
53:SH:47:ASP:OD1	53:SH:48:TYR:N	2.50	0.45
54:SI:407:ILE:HG22	54:SI:411:PHE:HE2	1.82	0.45
59:SP:1245:LYS:NZ	59:SP:1283:SER:OG	2.49	0.45
60:SQ:102:ASP:OD1	60:SQ:103:TRP:N	2.48	0.45
2:L1:151:G:N3	7:L6:13:GLN:NE2	2.61	0.45
2:L1:1528:U:OP1	6:L5:112:ARG:NH2	2.48	0.45
10:L9:79:ARG:NH1	36:NC:324:ASP:O	2.48	0.45
17:LI:650:LEU:HD23	19:LK:506:LEU:HD13	1.99	0.45
19:LK:459:LEU:HD23	19:LK:467:LEU:HD11	1.98	0.45
22:LN:148:SER:OG	22:LN:157:SER:OG	2.34	0.45
28:LT:621:ASP:OD1	28:LT:622:GLY:N	2.50	0.45
42:NI:60:LEU:HD22	42:NI:160:TYR:OH	2.16	0.45
48:SA:180:LEU:HD13	49:SB:183:ARG:HH21	1.82	0.45
49:SB:291:VAL:HG12	49:SB:363:LEU:HD21	1.98	0.45
51:SF:23:VAL:HG21	51:SF:117:VAL:HG21	1.99	0.45
54:SI:220:ILE:HD13	54:SI:223:LEU:HD12	1.99	0.45
59:SP:701:LEU:HD21	59:SP:795:ASP:HB3	1.99	0.45
59:SP:1397:ILE:O	59:SP:1401:ASN:ND2	2.49	0.45
59:SP:1548:ILE:O	59:SP:1552:SER:OG	2.28	0.45
67:SY:107:VAL:HG21	67:SY:218:MET:CE	2.46	0.45
6:L5:25:LEU:HD12	6:L5:29:ILE:CD1	2.48	0.44
18:LJ:319:VAL:HG22	18:LJ:329:ILE:CD1	2.46	0.44
22:LN:441:VAL:HG21	22:LN:486:ILE:HD13	1.99	0.44
23:LO:588:ASP:OD1	23:LO:589:GLY:N	2.50	0.44
30:LV:44:GLN:OE1	30:LV:44:GLN:N	2.48	0.44
30:LV:180:THR:HG22	30:LV:181:GLU:N	2.32	0.44
33:LZ:44:TYR:CD2	33:LZ:103:VAL:HG11	2.51	0.44
49:SB:118:ARG:NH2	50:SD:261:LEU:O	2.45	0.44
6:L5:186:ASN:OD1	6:L5:187:ILE:N	2.50	0.44
10:L9:85:VAL:HG21	10:L9:104:PHE:CD2	2.52	0.44
25:LQ:676:SER:OG	25:LQ:677:HIS:N	2.51	0.44
29:LU:303:ASP:OD2	29:LU:339:SER:N	2.44	0.44
41:NH:599:VAL:HG11	41:NH:609:ASN:HD22	1.82	0.44
5:L4:52:LEU:HD21	5:L4:111:VAL:HG11	1.98	0.44
23:LO:430:ARG:HA	23:LO:430:ARG:NE	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:567:ASP:OD1	33:LZ:144:ASN:ND2	2.50	0.44
25:LQ:107:ASP:O	25:LQ:111:LYS:N	2.50	0.44
26:LR:438:THR:HG21	26:LR:494:ILE:HG23	1.99	0.44
46:NQ:59:CYS:O	46:NQ:60:SER:OG	2.27	0.44
51:SF:10:PRO:HG3	51:SF:125:LEU:HD23	1.99	0.44
59:SP:1239:ASP:OD1	59:SP:1240:THR:N	2.48	0.44
59:SP:1616:LEU:HB3	59:SP:1635:ILE:HD13	1.98	0.44
59:SP:2130:LEU:HB3	59:SP:2172:ILE:HD11	2.00	0.44
62:SS:374:ARG:HA	62:SS:377:THR:HG23	1.98	0.44
2:L1:1492:A:OP1	60:SQ:210:LYS:NZ	2.34	0.44
18:LJ:31:THR:HG23	18:LJ:32:SER:N	2.33	0.44
22:LN:453:LEU:HD23	22:LN:462:VAL:HG12	1.99	0.44
41:NH:1037:LEU:CD2	41:NH:1050:ILE:HG22	2.47	0.44
50:SC:175:ALA:HB1	50:SC:181:VAL:HG21	1.98	0.44
54:SI:1087:LYS:NZ	67:SY:73:ASP:OD2	2.43	0.44
59:SP:1534:LEU:HD22	59:SP:1541:MET:SD	2.57	0.44
59:SP:1979:LEU:HD22	59:SP:2013:LEU:HD11	1.98	0.44
59:SP:2121:MET:HE3	59:SP:2125:LEU:CD1	2.47	0.44
64:SU:145:ASN:OD1	64:SU:146:LYS:N	2.50	0.44
12:LD:78:THR:HA	12:LD:84:ILE:HG22	1.99	0.44
18:LJ:45:ILE:HD13	18:LJ:319:VAL:HG12	1.98	0.44
20:LL:225:VAL:HG23	20:LL:225:VAL:O	2.18	0.44
21:LM:262:VAL:HG13	21:LM:301:LYS:HG2	1.99	0.44
25:LQ:537:VAL:HG12	25:LQ:548:ILE:HG13	1.98	0.44
29:LU:129:ASP:OD2	29:LU:158:LYS:NZ	2.50	0.44
32:LX:607:GLN:NE2	32:LX:608:ARG:O	2.50	0.44
35:NB:231:ALA:HB3	35:NB:232:PRO:HD3	2.00	0.44
41:NH:589:LYS:O	41:NH:609:ASN:ND2	2.46	0.44
41:NH:1180:ASN:OD1	41:NH:1181:VAL:N	2.50	0.44
59:SP:340:ILE:HD11	59:SP:362:PHE:HE1	1.82	0.44
59:SP:486:PHE:HD2	59:SP:525:ILE:HG21	1.81	0.44
63:ST:228:ALA:O	63:ST:232:MET:N	2.47	0.44
2:L1:1651:A:N3	25:LQ:182:LYS:NZ	2.65	0.44
16:LH:86:GLU:OE2	16:LH:113:ASN:ND2	2.51	0.44
21:LM:363:LEU:HD23	21:LM:366:ILE:HD12	1.99	0.44
24:LP:391:TYR:CE2	24:LP:395:ILE:HD11	2.52	0.44
25:LQ:250:LYS:NZ	25:LQ:276:ASN:OD1	2.46	0.44
25:LQ:549:SER:HB3	25:LQ:579:ILE:HD11	1.98	0.44
26:LR:220:ILE:HD12	26:LR:239:VAL:CG1	2.46	0.44
30:LV:79:PRO:O	30:LV:97:THR:N	2.49	0.44
32:LX:95:GLU:OE1	32:LX:95:GLU:N	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:568:LEU:HD11	32:LX:709:LEU:HD22	2.00	0.44
41:NH:543:LEU:HD13	41:NH:691:SER:HB3	1.98	0.44
2:L1:511:A:OP2	10:L9:176:ASN:ND2	2.44	0.44
16:LH:537:ASN:OD1	16:LH:538:GLU:N	2.51	0.44
24:LP:371:ILE:O	24:LP:418:TYR:OH	2.36	0.44
28:LT:429:ASN:O	28:LT:468:MET:HE1	2.17	0.44
41:NH:495:THR:HG22	41:NH:498:MET:HE3	2.00	0.44
59:SP:1030:ILE:HD12	59:SP:1059:LEU:HD22	2.00	0.44
1:L0:467:A:N1	1:L0:468:A:N6	2.65	0.44
2:L1:1632:C:N4	25:LQ:940:GLY:O	2.51	0.44
21:LM:622:TRP:O	21:LM:626:PHE:N	2.37	0.44
28:LT:807:VAL:HG13	66:SW:248:VAL:HG11	2.00	0.44
32:LX:266:PHE:HD2	32:LX:296:SER:HG	1.64	0.44
58:SN:113:SER:O	58:SN:116:THR:OG1	2.28	0.44
1:L0:474:A:OP2	31:LW:425:ARG:NH2	2.49	0.44
3:L2:59:G:H5'	23:LO:570:THR:HG23	1.99	0.44
11:LC:40:GLU:OE2	11:LC:45:ARG:NH2	2.51	0.44
11:LC:101:SER:O	11:LC:105:LEU:HD13	2.18	0.44
16:LH:656:ASP:OD2	16:LH:676:THR:OG1	2.36	0.44
20:LL:255:ILE:HD11	20:LL:301:LEU:HD13	2.00	0.44
26:LR:36:VAL:O	26:LR:36:VAL:HG13	2.18	0.44
26:LR:554:ASP:OD1	26:LR:556:THR:OG1	2.34	0.44
27:LS:274:ILE:O	27:LS:284:LEU:HD12	2.17	0.44
30:LV:244:ALA:HB2	30:LV:279:TRP:CZ2	2.53	0.44
32:LX:234:LEU:HD21	32:LX:238:LYS:HE3	1.99	0.44
50:SC:234:ILE:HG22	50:SC:235:GLY:O	2.18	0.44
59:SP:196:LEU:HG	59:SP:235:LEU:HD11	2.00	0.44
59:SP:550:GLU:OE1	59:SP:591:LEU:HD21	2.18	0.44
59:SP:2148:TRP:NE1	62:SS:247:MET:SD	2.85	0.44
63:ST:426:THR:HG22	63:ST:462:LEU:HB3	1.99	0.44
2:L1:187:G:O2'	59:SP:1100:GLN:NE2	2.51	0.43
2:L1:501:U:O2'	2:L1:502:U:OP2	2.28	0.43
8:L7:159:VAL:HG23	8:L7:185:ILE:HG21	1.99	0.43
11:LC:52:LEU:HD23	11:LC:60:PHE:CZ	2.52	0.43
25:LQ:67:LEU:HD11	25:LQ:74:ALA:HA	2.00	0.43
32:LY:487:ASN:O	32:LY:491:CYS:N	2.50	0.43
32:LY:520:ARG:NH1	32:LY:559:ALA:O	2.51	0.43
33:LZ:173:TYR:OH	67:SY:70:ARG:NH2	2.45	0.43
50:SD:276:ILE:HD13	50:SD:289:GLU:OE2	2.18	0.43
59:SP:344:MET:HE3	59:SP:384:TYR:HB3	2.00	0.43
59:SP:1352:LEU:HD23	59:SP:1355:ILE:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:1605:THR:O	59:SP:1609:ARG:NE	2.49	0.43
2:L1:93:A:H62	2:L1:396:G:H21	1.66	0.43
2:L1:936:G:OP1	2:L1:1074:G:N2	2.35	0.43
3:L2:80:U:OP2	51:SE:95:ARG:NE	2.48	0.43
21:LM:791:VAL:O	21:LM:794:SER:N	2.51	0.43
24:LP:205:LEU:HD22	60:SQ:52:PHE:HZ	1.83	0.43
46:NQ:18:LYS:O	46:NQ:29:ARG:NH2	2.52	0.43
49:SB:91:GLU:OE2	50:SD:228:GLN:NE2	2.51	0.43
59:SP:1636:LEU:HD23	59:SP:1639:ILE:HD12	2.00	0.43
59:SP:2023:THR:HA	59:SP:2026:ILE:HG22	2.00	0.43
66:SW:25:ILE:HD12	66:SW:25:ILE:H	1.83	0.43
1:L0:332:U:OP1	33:LZ:49:ARG:NH2	2.50	0.43
6:L5:27:THR:O	6:L5:29:ILE:HD12	2.18	0.43
18:LJ:467:LEU:HD21	18:LJ:484:MET:SD	2.59	0.43
23:LO:678:GLU:O	23:LO:698:THR:HG21	2.18	0.43
25:LQ:592:SER:OG	25:LQ:593:ALA:N	2.51	0.43
32:LX:361:ARG:O	32:LX:363:HIS:N	2.49	0.43
41:NH:146:LEU:HB2	41:NH:172:THR:HG21	2.01	0.43
51:SF:93:VAL:O	52:SG:552:TRP:NE1	2.50	0.43
59:SP:1418:VAL:HG21	59:SP:1455:ASN:ND2	2.32	0.43
63:ST:6:LEU:C	63:ST:6:LEU:HD23	2.43	0.43
10:L9:63:ASP:OD1	10:L9:64:GLU:N	2.51	0.43
13:LE:105:THR:HG23	13:LE:105:THR:O	2.18	0.43
17:LI:647:LEU:HD21	19:LK:505:MET:HE3	1.99	0.43
23:LO:828:ILE:HB	28:LT:930:MET:HE3	1.99	0.43
25:LQ:484:ASP:OD1	25:LQ:485:GLY:N	2.51	0.43
25:LQ:580:ASP:OD2	25:LQ:623:PHE:N	2.47	0.43
25:LQ:809:LEU:HD22	25:LQ:856:ASN:ND2	2.34	0.43
28:LT:252:SER:OG	28:LT:298:VAL:O	2.22	0.43
30:LV:244:ALA:HB2	30:LV:279:TRP:HZ2	1.84	0.43
31:LW:215:LYS:NZ	31:LW:227:GLU:OE1	2.51	0.43
50:SC:151:LEU:HD11	50:SC:162:LEU:HD11	2.01	0.43
54:SI:137:LEU:HD22	54:SI:230:MET:HE1	2.01	0.43
55:SJ:192:TYR:O	55:SJ:196:LEU:HD23	2.19	0.43
59:SP:1457:ILE:HD12	59:SP:1457:ILE:H	1.83	0.43
62:SS:387:MET:HE2	62:SS:392:ARG:HA	2.00	0.43
66:SW:30:ASN:OD1	66:SW:31:THR:N	2.50	0.43
16:LH:282:ILE:HD13	16:LH:293:LEU:HD13	2.00	0.43
20:LL:167:SER:O	20:LL:191:VAL:HG23	2.18	0.43
23:LO:543:ASN:O	23:LO:547:ALA:N	2.47	0.43
26:LR:659:ALA:O	26:LR:663:VAL:HG23	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SI:114:ARG:NH1	54:SI:306:ASP:OD2	2.52	0.43
55:SK:31:LEU:HD23	55:SK:40:ARG:CG	2.49	0.43
59:SP:1087:VAL:HG13	59:SP:1109:PHE:CZ	2.53	0.43
59:SP:1436:ASP:CG	59:SP:1437:MET:HE2	2.44	0.43
59:SP:1896:ILE:HG23	59:SP:1933:ILE:HG21	2.00	0.43
62:SS:313:PHE:CZ	62:SS:883:ILE:HG23	2.54	0.43
1:L0:338:A:O2'	1:L0:340:U:O4	2.34	0.43
7:L6:14:LYS:N	7:L6:124:LEU:HD21	2.34	0.43
7:L6:75:LEU:HD12	7:L6:97:VAL:CG2	2.49	0.43
10:L9:20:GLU:OE2	10:L9:22:SER:OG	2.36	0.43
22:LN:476:LYS:C	22:LN:477:LEU:HD12	2.44	0.43
26:LR:698:LEU:HD13	26:LR:759:THR:HG21	2.00	0.43
28:LT:723:LEU:HD23	28:LT:878:PHE:CE1	2.53	0.43
36:NC:315:ALA:O	36:NC:318:ASN:N	2.50	0.43
55:SJ:180:LEU:HD12	55:SJ:206:VAL:HG22	2.00	0.43
59:SP:1560:ARG:NH2	59:SP:1621:LEU:O	2.51	0.43
9:L8:160:PHE:CE1	9:L8:165:LEU:HD11	2.54	0.43
17:LI:572:SER:O	17:LI:574:ARG:NH1	2.44	0.43
22:LN:479:LYS:HB3	22:LN:536:VAL:HG12	2.01	0.43
22:LN:481:ILE:HD11	22:LN:555:LEU:HD23	2.00	0.43
23:LO:155:SER:OG	23:LO:157:ASP:OD1	2.31	0.43
24:LP:293:TYR:OH	48:SA:160:ARG:NE	2.42	0.43
32:LX:615:PRO:O	32:LX:619:SER:OG	2.30	0.43
41:NH:970:TRP:CE2	47:OA:1414:LEU:HD11	2.54	0.43
53:SH:19:LEU:HD21	53:SH:325:LEU:HD12	2.00	0.43
59:SP:170:LEU:HD23	59:SP:211:PHE:CG	2.54	0.43
25:LQ:264:ASN:O	25:LQ:268:LYS:N	2.52	0.43
42:NI:67:MET:HE3	42:NI:67:MET:HA	1.99	0.43
42:NI:78:TYR:O	42:NI:80:THR:HG23	2.19	0.43
59:SP:259:LEU:HD23	59:SP:301:ASP:HB2	1.99	0.43
59:SP:458:ILE:HD12	59:SP:489:SER:HB3	2.01	0.43
59:SP:2098:LEU:CD2	62:SS:262:LEU:HD11	2.48	0.43
59:SP:2230:ASP:OD1	59:SP:2231:ILE:N	2.51	0.43
61:SR:65:ASN:N	61:SR:90:ASP:OD2	2.43	0.43
63:ST:525:MET:CE	63:ST:546:LEU:HD22	2.45	0.43
2:L1:1680:G:H21	2:L1:1681:A:N6	2.17	0.43
2:L1:1681:A:N6	2:L1:1720:G:C6	2.87	0.43
7:L6:75:LEU:HD23	30:LV:90:SER:HB2	2.01	0.43
14:LF:77:ASN:ND2	59:SP:57:ILE:HG23	2.34	0.43
32:LY:275:LEU:O	32:LY:404:TYR:N	2.52	0.43
36:NC:114:GLU:O	36:NC:118:ALA:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:NI:220:THR:HG21	42:NI:226:ILE:HD11	2.01	0.43
59:SP:1478:ASP:OD1	59:SP:1478:ASP:N	2.51	0.43
60:SQ:172:THR:HG22	60:SQ:173:ILE:N	2.34	0.43
2:L1:1193:A:N1	55:SJ:129:ARG:NE	2.67	0.43
7:L6:67:VAL:CG2	7:L6:73:ILE:HD11	2.48	0.43
11:LC:97:VAL:HG12	11:LC:98:ASP:N	2.33	0.43
16:LH:671:ILE:HD13	16:LH:719:ASN:ND2	2.33	0.43
16:LH:722:LEU:HD11	16:LH:763:ILE:CG2	2.49	0.43
25:LQ:190:ASP:OD2	25:LQ:193:THR:OG1	2.27	0.43
27:LS:251:ILE:O	27:LS:566:THR:HG23	2.19	0.43
38:NE:303:GLU:OE2	56:SL:113:TYR:OH	2.37	0.43
59:SP:1547:LEU:O	59:SP:1551:LEU:N	2.46	0.43
63:ST:700:LEU:HD11	63:ST:702:LEU:CD2	2.49	0.43
2:L1:170:U:N3	2:L1:289:U:O2'	2.52	0.42
9:L8:172:ARG:HE	9:L8:175:GLN:HG3	1.84	0.42
16:LH:73:LEU:HD21	16:LH:131:HIS:HB2	2.01	0.42
16:LH:555:VAL:O	16:LH:555:VAL:HG13	2.18	0.42
26:LR:269:LEU:HD11	26:LR:316:VAL:HG13	2.00	0.42
32:LX:6:ILE:HG13	54:SI:373:ILE:HD12	1.99	0.42
32:LX:378:LEU:HD22	32:LX:384:VAL:HG21	2.01	0.42
38:NE:103:SER:OG	38:NE:105:VAL:HG12	2.19	0.42
41:NH:203:ILE:HD11	41:NH:290:PHE:CD2	2.54	0.42
41:NH:270:ILE:CD1	41:NH:294:LEU:HD23	2.49	0.42
26:LR:438:THR:CG2	26:LR:494:ILE:HG23	2.49	0.42
28:LT:231:ILE:HG23	28:LT:240:ARG:HG3	2.01	0.42
28:LT:356:ILE:O	28:LT:633:LYS:NZ	2.52	0.42
28:LT:360:ASP:OD1	28:LT:360:ASP:N	2.51	0.42
30:LV:109:ASP:OD1	30:LV:110:ASP:N	2.52	0.42
32:LX:542:VAL:HG13	32:LX:548:ASN:HD21	1.83	0.42
41:NH:495:THR:HG22	41:NH:498:MET:CE	2.49	0.42
48:SA:210:VAL:O	48:SA:212:ASP:N	2.52	0.42
59:SP:236:PHE:O	59:SP:239:SER:OG	2.32	0.42
60:SQ:112:ASN:OD1	60:SQ:113:MET:N	2.52	0.42
63:ST:477:TYR:O	63:ST:481:MET:N	2.45	0.42
2:L1:578:U:N3	54:SI:838:ILE:HD11	2.34	0.42
12:LD:132:SER:O	12:LD:136:ARG:NH1	2.51	0.42
16:LH:414:ILE:HD12	16:LH:414:ILE:H	1.84	0.42
18:LJ:125:HIS:NE2	55:SK:19:LEU:O	2.51	0.42
18:LJ:177:ILE:HD13	18:LJ:239:LEU:HD11	2.01	0.42
35:NB:603:THR:HG21	50:SC:160:ASP:HA	2.01	0.42
50:SC:230:TYR:CD2	50:SC:234:ILE:HD12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SH:280:LEU:HD22	54:SI:631:ILE:HD11	2.01	0.42
54:SI:557:ASN:OD1	54:SI:558:ILE:N	2.51	0.42
55:SK:83:ASP:OD1	55:SK:83:ASP:N	2.53	0.42
59:SP:1182:LEU:C	59:SP:1182:LEU:HD23	2.44	0.42
59:SP:1341:GLU:OE1	59:SP:1341:GLU:N	2.45	0.42
64:SU:99:LYS:HZ3	64:SU:147:THR:HG23	1.84	0.42
16:LH:292:LEU:C	16:LH:293:LEU:HD12	2.44	0.42
25:LQ:126:LEU:HD23	25:LQ:169:PHE:CD2	2.54	0.42
28:LT:459:ASP:OD2	28:LT:483:SER:OG	2.32	0.42
30:LV:287:ASN:OD1	30:LV:302:ARG:NH2	2.47	0.42
34:NA:352:LYS:NZ	57:SM:285:ASN:O	2.49	0.42
41:NH:715:SER:O	41:NH:719:THR:HG23	2.20	0.42
41:NH:901:ASN:ND2	44:NM:131:ASP:OD1	2.52	0.42
41:NH:1226:PHE:O	41:NH:1228:ASN:ND2	2.52	0.42
55:SJ:159:LEU:C	55:SJ:160:LEU:HD12	2.43	0.42
63:ST:677:ASP:OD1	63:ST:678:PHE:N	2.52	0.42
8:L7:129:LEU:HD21	8:L7:172:VAL:CG1	2.49	0.42
16:LH:225:ILE:HD11	16:LH:241:LEU:HD13	2.00	0.42
26:LR:519:ASN:O	26:LR:523:GLY:N	2.49	0.42
27:LS:512:ASP:OD1	27:LS:512:ASP:N	2.52	0.42
29:LU:183:GLN:O	29:LU:183:GLN:NE2	2.51	0.42
30:LV:249:ASN:OD1	30:LV:250:GLY:N	2.53	0.42
53:SH:333:PHE:CD1	53:SH:357:ILE:HD13	2.54	0.42
67:SY:170:GLN:OE1	67:SY:170:GLN:N	2.50	0.42
20:LL:248:THR:OG1	20:LL:252:SER:O	2.38	0.42
24:LP:144:VAL:CG1	24:LP:178:VAL:HG21	2.48	0.42
39:NF:87:ASP:OD1	39:NF:87:ASP:N	2.51	0.42
40:NG:27:PHE:HD1	40:NG:43:THR:HG23	1.84	0.42
41:NH:1071:ALA:HB1	41:NH:1088:LEU:HD11	2.02	0.42
41:NH:1204:VAL:HG21	41:NH:1212:VAL:HG21	2.02	0.42
59:SP:98:HIS:HD2	59:SP:135:LEU:HD13	1.85	0.42
59:SP:386:LEU:CD1	59:SP:419:LEU:HD22	2.48	0.42
59:SP:1951:THR:HG21	59:SP:1989:ASP:OD2	2.19	0.42
59:SP:2239:LEU:HD11	59:SP:2254:VAL:HG21	2.02	0.42
63:ST:506:ILE:CD1	64:SU:529:VAL:HG22	2.49	0.42
63:ST:616:LEU:HD21	64:SU:530:PHE:HE2	1.84	0.42
1:L0:394:U:OP1	33:LZ:108:ARG:NH2	2.52	0.42
14:LF:83:LYS:HE3	14:LF:96:LEU:HD12	2.01	0.42
15:LG:64:ARG:O	15:LG:66:LEU:HD12	2.19	0.42
20:LL:95:VAL:HG13	20:LL:95:VAL:O	2.19	0.42
20:LL:160:VAL:HG23	20:LL:160:VAL:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:678:ASP:OD1	25:LQ:680:SER:OG	2.28	0.42
26:LR:12:LEU:HD11	26:LR:378:PRO:CG	2.49	0.42
59:SP:1454:VAL:HG21	59:SP:1488:MET:CE	2.49	0.42
2:L1:1680:G:H21	2:L1:1681:A:H61	1.67	0.42
16:LH:654:THR:C	16:LH:655:LEU:HD22	2.45	0.42
18:LJ:284:PHE:CE2	18:LJ:292:VAL:HG22	2.54	0.42
26:LR:43:ILE:HG22	26:LR:52:ILE:HG12	2.01	0.42
28:LT:530:ASP:O	28:LT:534:SER:N	2.53	0.42
32:LX:892:ARG:NH1	32:LY:790:SER:OG	2.53	0.42
32:LY:378:LEU:HD22	32:LY:384:VAL:CG2	2.49	0.42
50:SD:175:ALA:HB1	50:SD:181:VAL:HG21	2.01	0.42
59:SP:358:VAL:HB	59:SP:389:ILE:HD11	2.01	0.42
59:SP:1217:ARG:CG	59:SP:1250:ILE:HD11	2.50	0.42
63:ST:555:ARG:HG3	63:ST:556:ILE:HG13	2.02	0.42
3:L2:332:G:H21	16:LH:869:MET:HE3	1.85	0.42
13:LE:92:ASN:HB3	38:NE:311:VAL:HG22	2.02	0.42
34:NA:319:VAL:HG21	54:SI:1042:MET:CE	2.47	0.42
41:NH:257:SER:O	41:NH:267:ILE:N	2.44	0.42
41:NH:349:LEU:HD22	41:NH:394:THR:HG22	2.01	0.42
50:SC:248:ASP:OD1	50:SC:248:ASP:N	2.48	0.42
55:SK:209:MET:HE1	55:SK:212:GLY:O	2.20	0.42
16:LH:95:ASP:OD2	16:LH:97:THR:OG1	2.36	0.42
31:LW:15:ARG:CZ	31:LW:62:ALA:HB2	2.50	0.42
35:NB:415:THR:HG23	35:NB:418:PHE:H	1.85	0.42
41:NH:388:PHE:CE2	41:NH:480:MET:HE3	2.55	0.42
46:NQ:56:CYS:O	46:NQ:60:SER:N	2.50	0.42
49:SB:379:ASP:OD1	49:SB:379:ASP:N	2.53	0.42
52:SG:159:CYS:SG	52:SG:160:ILE:N	2.93	0.42
55:SK:93:HIS:NE2	55:SK:97:LEU:HD21	2.35	0.42
59:SP:1670:LEU:HD23	59:SP:1713:SER:OG	2.19	0.42
59:SP:1763:LEU:N	59:SP:1805:ASP:OD2	2.53	0.42
21:LM:220:VAL:HG12	21:LM:234:LEU:HD21	2.02	0.41
23:LO:760:ILE:H	23:LO:760:ILE:HD12	1.85	0.41
24:LP:12:ILE:HG21	31:LW:62:ALA:HB1	2.02	0.41
28:LT:375:LEU:HD12	28:LT:414:ILE:CD1	2.49	0.41
34:NA:345:LEU:HD23	54:SI:1005:SER:OG	2.20	0.41
54:SI:407:ILE:HG22	54:SI:411:PHE:CE2	2.55	0.41
55:SJ:186:VAL:HG11	55:SK:252:LEU:HD21	2.02	0.41
55:SK:218:ASP:OD1	55:SK:219:GLU:N	2.53	0.41
63:ST:397:ASP:OD1	63:ST:397:ASP:N	2.49	0.41
63:ST:801:ARG:O	63:ST:805:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:871:G:H2'	2:L1:872:G:C8	2.55	0.41
18:LJ:141:ALA:HB2	18:LJ:176:PHE:HZ	1.85	0.41
23:LO:261:ALA:HB1	23:LO:279:PHE:HB3	2.02	0.41
23:LO:492:SER:OG	23:LO:493:TRP:N	2.54	0.41
26:LR:89:HIS:O	26:LR:93:GLY:N	2.48	0.41
41:NH:1087:LEU:HA	41:NH:1090:THR:HG22	2.03	0.41
49:SB:313:PRO:HG2	49:SB:316:THR:HG23	2.02	0.41
54:SI:867:THR:HG22	61:SR:62:LYS:NZ	2.35	0.41
59:SP:479:ILE:O	59:SP:483:ALA:N	2.53	0.41
59:SP:1811:ILE:HD12	59:SP:1879:VAL:HG21	2.02	0.41
59:SP:1987:LEU:HD13	59:SP:2019:ILE:CD1	2.49	0.41
2:L1:1533:C:H2'	2:L1:1534:G:O4'	2.20	0.41
2:L1:1681:A:H2'	2:L1:1682:U:O4'	2.19	0.41
6:L5:23:VAL:O	6:L5:23:VAL:HG13	2.19	0.41
22:LN:402:TRP:NE1	22:LN:416:LEU:HD13	2.35	0.41
25:LQ:589:ILE:HG21	25:LQ:621:VAL:HG11	2.01	0.41
37:ND:114:GLU:HA	37:ND:117:LEU:HD12	2.02	0.41
39:NF:132:VAL:O	39:NF:132:VAL:HG12	2.21	0.41
50:SD:123:ILE:O	50:SD:141:TYR:N	2.49	0.41
62:SS:268:SER:O	62:SS:268:SER:OG	2.32	0.41
63:ST:589:GLU:N	63:ST:589:GLU:OE1	2.53	0.41
5:L4:106:LYS:NZ	36:NC:233:HIS:O	2.54	0.41
7:L6:75:LEU:HD12	7:L6:97:VAL:HG21	2.03	0.41
14:LF:38:ASP:OD1	14:LF:39:GLU:N	2.51	0.41
35:NB:495:TYR:HD1	58:SN:23:GLN:NE2	2.07	0.41
41:NH:469:ASP:O	41:NH:473:LYS:N	2.50	0.41
48:SA:44:PHE:CE2	48:SA:48:ILE:HD11	2.56	0.41
48:SA:244:ASP:OD1	48:SA:244:ASP:N	2.53	0.41
54:SI:859:ILE:HD12	54:SI:1011:VAL:HG22	2.03	0.41
62:SS:372:GLU:OE1	62:SS:376:ARG:NH2	2.54	0.41
2:L1:956:C:OP1	2:L1:1072:C:O2'	2.36	0.41
16:LH:357:ILE:HD12	16:LH:371:PHE:CD1	2.55	0.41
21:LM:378:TYR:O	21:LM:382:LEU:HD23	2.19	0.41
21:LM:1671:GLY:O	21:LM:1675:SER:N	2.51	0.41
24:LP:175:ASN:O	24:LP:178:VAL:HG22	2.20	0.41
41:NH:1146:THR:HG21	41:NH:1180:ASN:ND2	2.34	0.41
48:SA:178:ILE:HD11	48:SA:313:ALA:CB	2.50	0.41
54:SI:157:ASN:O	54:SI:161:HIS:ND1	2.54	0.41
59:SP:1636:LEU:HA	59:SP:1639:ILE:HD12	2.02	0.41
29:LU:92:ILE:CD1	29:LU:136:MET:HE3	2.47	0.41
30:LV:397:LEU:HD21	30:LV:404:PHE:CG	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NH:128:LEU:O	41:NH:132:TYR:CD2	2.73	0.41
41:NH:404:GLY:N	41:NH:455:SER:OG	2.53	0.41
41:NH:655:LEU:O	44:NM:244:VAL:HG12	2.20	0.41
49:SB:199:VAL:HG13	49:SB:199:VAL:O	2.21	0.41
53:SH:19:LEU:HD22	54:SI:608:LEU:CD1	2.50	0.41
54:SI:131:ILE:HD11	54:SI:809:PRO:HG3	2.01	0.41
59:SP:561:LEU:O	59:SP:565:LEU:HD23	2.21	0.41
59:SP:1610:MET:HE1	59:SP:1654:VAL:HG22	2.03	0.41
9:L8:171:SER:OG	9:L8:172:ARG:N	2.53	0.41
16:LH:682:ASN:ND2	16:LH:689:ILE:HD11	2.36	0.41
16:LH:724:ILE:HG21	16:LH:762:TYR:HD1	1.84	0.41
18:LJ:11:SER:H	18:LJ:416:THR:HG22	1.85	0.41
20:LL:296:ILE:HG23	20:LL:296:ILE:O	2.21	0.41
22:LN:486:ILE:HD12	22:LN:500:LEU:HD11	2.03	0.41
25:LQ:178:ILE:HD11	25:LQ:231:LEU:HD11	2.02	0.41
25:LQ:206:GLU:OE1	25:LQ:206:GLU:N	2.49	0.41
25:LQ:941:THR:N	34:NA:464:SER:O	2.48	0.41
26:LR:689:ASP:OD1	26:LR:742:ARG:NH2	2.49	0.41
28:LT:724:SER:HB3	28:LT:880:LEU:HD13	2.02	0.41
30:LV:241:LEU:HD11	45:NN:485:TRP:CZ2	2.56	0.41
39:NF:31:GLU:O	39:NF:34:ILE:N	2.53	0.41
59:SP:323:PHE:HB2	59:SP:364:LEU:HD13	2.02	0.41
59:SP:1159:ARG:NE	59:SP:1204:SER:OG	2.53	0.41
59:SP:1527:LEU:HD21	59:SP:1590:LEU:HD21	2.02	0.41
63:ST:383:THR:OG1	63:ST:385:ASP:OD1	2.30	0.41
2:L1:559:C:H5'	54:SI:867:THR:HG21	2.03	0.41
8:L7:49:ILE:HD11	8:L7:172:VAL:HG22	2.03	0.41
8:L7:51:VAL:HG22	8:L7:52:ALA:N	2.35	0.41
41:NH:441:GLN:CG	41:NH:458:ILE:HD11	2.51	0.41
41:NH:976:ILE:HG22	41:NH:1042:ALA:HB3	2.02	0.41
48:SA:210:VAL:O	48:SA:210:VAL:HG23	2.21	0.41
57:SM:24:GLN:OE1	57:SM:24:GLN:N	2.52	0.41
3:L2:45:U:O2'	56:SL:23:GLN:OE1	2.24	0.41
12:LD:111:VAL:HA	12:LD:139:VAL:HB	2.03	0.41
26:LR:23:ALA:O	26:LR:294:LEU:HD11	2.20	0.41
26:LR:231:CYS:O	26:LR:232:LYS:NZ	2.46	0.41
30:LV:181:GLU:N	30:LV:181:GLU:OE2	2.54	0.41
30:LV:401:MET:HE3	59:SP:910:SER:O	2.21	0.41
31:LW:333:SER:HB3	31:LW:381:LEU:HD11	2.03	0.41
32:LX:297:ILE:HD13	32:LX:325:ILE:HD11	2.03	0.41
32:LY:579:ILE:HD13	45:NN:532:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LY:613:LEU:C	32:LY:613:LEU:HD23	2.46	0.41
48:SA:229:LEU:HD21	48:SA:255:ALA:CB	2.51	0.41
57:SM:192:ASP:OD1	57:SM:227:ARG:NH1	2.48	0.41
59:SP:340:ILE:HD12	59:SP:343:ILE:HD11	2.02	0.41
59:SP:972:LEU:HD11	59:SP:997:MET:HE1	2.02	0.41
60:SQ:173:ILE:H	60:SQ:173:ILE:HD12	1.86	0.41
63:ST:528:PHE:HB3	63:ST:532:ILE:HD12	2.02	0.41
64:SU:137:GLU:HB2	64:SU:140:ALA:HB2	2.02	0.41
66:SW:117:TYR:N	66:SW:118:PRO:CD	2.84	0.41
2:L1:513:U:H2'	2:L1:514:G:C8	2.56	0.41
8:L7:130:VAL:O	8:L7:133:THR:OG1	2.29	0.41
12:LD:84:ILE:HD11	12:LD:139:VAL:HG21	2.03	0.41
14:LF:40:LEU:O	14:LF:44:LEU:HD23	2.20	0.41
20:LL:253:LEU:CD2	20:LL:301:LEU:HD21	2.51	0.41
25:LQ:149:ASP:O	25:LQ:153:GLU:N	2.53	0.41
26:LR:591:ILE:HD11	26:LR:625:THR:CG2	2.51	0.41
32:LY:301:VAL:HG11	32:LY:359:ILE:HD13	2.03	0.41
41:NH:441:GLN:HG2	41:NH:458:ILE:HD11	2.03	0.41
41:NH:480:MET:SD	41:NH:484:SER:OG	2.77	0.41
41:NH:833:TYR:OH	41:NH:877:GLU:OE2	2.38	0.41
45:NN:532:ILE:HG23	45:NN:533:PHE:CD2	2.56	0.41
54:SI:348:ASP:OD1	54:SI:349:ASP:N	2.54	0.41
59:SP:1887:LEU:HD23	59:SP:1887:LEU:O	2.20	0.41
67:SY:149:GLU:O	67:SY:153:ASN:N	2.54	0.41
2:L1:924:A:H2'	2:L1:925:G:C8	2.56	0.40
16:LH:73:LEU:HD11	16:LH:77:ILE:HD11	2.03	0.40
16:LH:603:ASN:OD1	16:LH:604:PHE:N	2.55	0.40
16:LH:634:ASP:OD1	16:LH:635:PHE:N	2.54	0.40
17:LI:545:ARG:HA	17:LI:551:PHE:CZ	2.56	0.40
22:LN:681:ILE:HG22	22:LN:683:ASP:N	2.34	0.40
23:LO:351:LEU:HD12	23:LO:351:LEU:C	2.46	0.40
23:LO:424:THR:HG21	25:LQ:942:VAL:HB	2.04	0.40
28:LT:331:GLY:O	28:LT:332:SER:OG	2.28	0.40
32:LX:556:MET:SD	32:LX:564:LEU:HD11	2.61	0.40
32:LX:857:ASP:OD2	32:LY:784:ARG:HG2	2.21	0.40
32:LY:838:ASP:OD1	32:LY:841:ARG:NH1	2.55	0.40
36:NC:315:ALA:O	36:NC:319:VAL:N	2.52	0.40
41:NH:1227:GLY:HA3	41:NH:1231:VAL:HG13	2.03	0.40
52:SG:70:TYR:CZ	52:SG:74:LEU:HD11	2.56	0.40
59:SP:1202:LEU:HD13	59:SP:1224:LEU:HD22	2.02	0.40
9:L8:113:PHE:CE1	9:L8:121:LEU:HD12	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LD:71:LEU:HD12	12:LD:88:ARG:CZ	2.52	0.40
21:LM:230:LYS:O	21:LM:234:LEU:HD13	2.20	0.40
28:LT:484:ILE:HG21	28:LT:517:MET:HE1	2.02	0.40
32:LX:765:VAL:HG23	32:LX:774:LEU:HD22	2.01	0.40
32:LY:785:PHE:CZ	32:LY:789:LEU:HD21	2.57	0.40
41:NH:124:VAL:O	41:NH:128:LEU:HD23	2.20	0.40
43:NK:125:VAL:O	43:NK:184:ARG:NH2	2.54	0.40
58:SN:194:ASP:OD2	58:SN:195:ASN:N	2.49	0.40
59:SP:538:LEU:HD22	59:SP:574:LEU:CD2	2.50	0.40
59:SP:819:ILE:HD11	59:SP:822:SER:HB3	2.02	0.40
1:L0:63:G:N7	16:LH:223:LYS:NZ	2.64	0.40
1:L0:443:G:OP1	60:SQ:207:LYS:NZ	2.37	0.40
10:L9:31:ALA:O	10:L9:35:GLY:N	2.54	0.40
18:LJ:450:ILE:HG12	18:LJ:491:VAL:HG12	2.04	0.40
21:LM:63:GLU:OE1	21:LM:108:LYS:NZ	2.38	0.40
32:LX:64:LEU:HD22	32:LX:153:LYS:HE2	2.02	0.40
48:SA:163:VAL:O	48:SA:163:VAL:HG12	2.20	0.40
48:SA:281:LEU:HD11	49:SB:265:PHE:CE1	2.56	0.40
49:SB:409:THR:HG23	49:SB:409:THR:O	2.21	0.40
50:SD:230:TYR:OH	50:SD:256:ASN:OD1	2.39	0.40
59:SP:1643:LEU:HD11	59:SP:1693:THR:HG21	2.02	0.40
59:SP:1888:THR:C	59:SP:1924:LEU:HD21	2.46	0.40
61:SR:109:ARG:NE	61:SR:116:ASP:OD1	2.55	0.40
1:L0:388:C:OP1	33:LZ:22:LYS:NZ	2.35	0.40
3:L2:100:U:O3'	50:SD:138:LYS:NZ	2.54	0.40
4:L3:4:VAL:HG12	18:LJ:277:LEU:HD11	2.03	0.40
16:LH:372:LEU:HD21	16:LH:374:LEU:HD21	2.03	0.40
26:LR:730:ILE:O	26:LR:730:ILE:HG22	2.21	0.40
31:LW:102:LYS:HB3	31:LW:389:LEU:HD11	2.02	0.40
49:SB:47:PHE:CZ	49:SB:128:LEU:HD11	2.57	0.40
54:SI:221:LEU:O	54:SI:221:LEU:HD23	2.22	0.40
55:SJ:41:MET:HE3	55:SJ:241:PHE:CD2	2.56	0.40
59:SP:1275:PHE:CG	59:SP:1280:LEU:HD13	2.56	0.40
59:SP:1419:SER:O	59:SP:1422:SER:OG	2.31	0.40
59:SP:1511:ILE:HG21	59:SP:1547:LEU:HD12	2.04	0.40
20:LL:248:THR:OG1	20:LL:250:ASP:OD1	2.28	0.40
21:LM:181:LYS:HD2	49:SB:409:THR:HG21	2.02	0.40
21:LM:705:SER:O	21:LM:709:ASN:N	2.45	0.40
25:LQ:634:SER:OG	25:LQ:635:LYS:N	2.54	0.40
26:LR:328:GLN:N	26:LR:328:GLN:OE1	2.54	0.40
26:LR:394:LEU:HD13	26:LR:405:THR:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LS:409:ILE:HD13	27:LS:423:LEU:HA	2.04	0.40
29:LU:270:ASN:ND2	29:LU:273:GLU:OE1	2.54	0.40
29:LU:448:ARG:NH2	29:LU:450:ASP:O	2.55	0.40
32:LY:734:HIS:ND1	32:LY:762:MET:HE1	2.36	0.40
32:LY:895:ILE:HD11	32:LY:909:THR:HG22	2.03	0.40
36:NC:254:ASP:OD2	36:NC:254:ASP:C	2.65	0.40
55:SJ:246:GLU:O	55:SJ:250:ASN:N	2.54	0.40
58:SN:96:LEU:HD21	58:SN:180:LEU:HD12	2.04	0.40
59:SP:1151:ILE:HG23	59:SP:1201:LEU:HD13	2.03	0.40
66:SW:114:THR:HG23	66:SW:115:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L3	91/146 (62%)	90 (99%)	1 (1%)	0	100	100
5	L4	232/261 (89%)	230 (99%)	2 (1%)	0	100	100
6	L5	202/225 (90%)	197 (98%)	5 (2%)	0	100	100
7	L6	202/236 (86%)	202 (100%)	0	0	100	100
8	L7	165/190 (87%)	164 (99%)	1 (1%)	0	100	100
9	L8	167/200 (84%)	164 (98%)	3 (2%)	0	100	100
10	L9	169/197 (86%)	168 (99%)	1 (1%)	0	100	100
11	LC	123/143 (86%)	122 (99%)	1 (1%)	0	100	100
12	LD	135/156 (86%)	133 (98%)	2 (2%)	0	100	100
13	LE	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
14	LF	93/135 (69%)	91 (98%)	2 (2%)	0	100	100
15	LG	60/67 (90%)	60 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LH	790/896 (88%)	772 (98%)	18 (2%)	0	100	100
17	LI	582/713 (82%)	578 (99%)	4 (1%)	0	100	100
18	LJ	489/513 (95%)	476 (97%)	13 (3%)	0	100	100
19	LK	130/575 (23%)	130 (100%)	0	0	100	100
20	LL	496/643 (77%)	488 (98%)	8 (2%)	0	100	100
21	LM	1597/1769 (90%)	1566 (98%)	31 (2%)	0	100	100
22	LN	649/776 (84%)	639 (98%)	10 (2%)	0	100	100
23	LO	829/923 (90%)	820 (99%)	9 (1%)	0	100	100
24	LP	376/440 (86%)	374 (100%)	2 (0%)	0	100	100
25	LQ	831/943 (88%)	814 (98%)	17 (2%)	0	100	100
26	LR	785/817 (96%)	769 (98%)	16 (2%)	0	100	100
27	LS	469/594 (79%)	462 (98%)	7 (2%)	0	100	100
28	LT	865/939 (92%)	851 (98%)	14 (2%)	0	100	100
29	LU	456/489 (93%)	449 (98%)	7 (2%)	0	100	100
30	LV	401/707 (57%)	392 (98%)	9 (2%)	0	100	100
31	LW	531/554 (96%)	520 (98%)	11 (2%)	0	100	100
32	LX	838/1056 (79%)	824 (98%)	14 (2%)	0	100	100
32	LY	834/1056 (79%)	825 (99%)	9 (1%)	0	100	100
33	LZ	179/183 (98%)	179 (100%)	0	0	100	100
34	NA	274/593 (46%)	269 (98%)	5 (2%)	0	100	100
35	NB	255/610 (42%)	254 (100%)	1 (0%)	0	100	100
36	NC	244/357 (68%)	240 (98%)	4 (2%)	0	100	100
37	ND	70/214 (33%)	70 (100%)	0	0	100	100
38	NE	207/346 (60%)	204 (99%)	3 (1%)	0	100	100
39	NF	139/151 (92%)	139 (100%)	0	0	100	100
40	NG	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
41	NH	1063/1237 (86%)	1050 (99%)	13 (1%)	0	100	100
42	NI	232/297 (78%)	226 (97%)	6 (3%)	0	100	100
43	NK	253/316 (80%)	250 (99%)	3 (1%)	0	100	100
44	NM	224/255 (88%)	223 (100%)	1 (0%)	0	100	100
45	NN	257/534 (48%)	257 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	NQ	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
47	OA	11/1729 (1%)	11 (100%)	0	0	100	100
48	SA	384/504 (76%)	380 (99%)	4 (1%)	0	100	100
49	SB	434/511 (85%)	427 (98%)	7 (2%)	0	100	100
50	SC	237/327 (72%)	234 (99%)	3 (1%)	0	100	100
50	SD	228/327 (70%)	223 (98%)	5 (2%)	0	100	100
51	SE	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
51	SF	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
52	SG	442/573 (77%)	433 (98%)	9 (2%)	0	100	100
53	SH	358/367 (98%)	354 (99%)	4 (1%)	0	100	100
54	SI	803/1183 (68%)	789 (98%)	14 (2%)	0	100	100
55	SJ	207/252 (82%)	205 (99%)	2 (1%)	0	100	100
55	SK	225/252 (89%)	224 (100%)	1 (0%)	0	100	100
56	SL	169/189 (89%)	165 (98%)	4 (2%)	0	100	100
57	SM	278/290 (96%)	276 (99%)	2 (1%)	0	100	100
58	SN	251/274 (92%)	251 (100%)	0	0	100	100
59	SP	2136/2493 (86%)	2111 (99%)	25 (1%)	0	100	100
60	SQ	129/217 (59%)	123 (95%)	6 (5%)	0	100	100
61	SR	102/145 (70%)	101 (99%)	1 (1%)	0	100	100
62	SS	243/899 (27%)	239 (98%)	4 (2%)	0	100	100
63	ST	572/810 (71%)	567 (99%)	5 (1%)	0	100	100
64	SU	528/552 (96%)	524 (99%)	4 (1%)	0	100	100
65	SV	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
66	SW	193/274 (70%)	189 (98%)	4 (2%)	0	100	100
67	SY	227/250 (91%)	227 (100%)	0	0	100	100
68	SZ	255/483 (53%)	252 (99%)	3 (1%)	0	100	100
All	All	26096/35160 (74%)	25725 (99%)	371 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	88/129 (68%)	88 (100%)	0	100	100
5	L4	202/222 (91%)	202 (100%)	0	100	100
6	L5	179/191 (94%)	179 (100%)	0	100	100
7	L6	175/201 (87%)	175 (100%)	0	100	100
8	L7	149/170 (88%)	149 (100%)	0	100	100
9	L8	138/161 (86%)	138 (100%)	0	100	100
10	L9	147/166 (89%)	147 (100%)	0	100	100
11	LC	105/119 (88%)	105 (100%)	0	100	100
12	LD	124/137 (90%)	124 (100%)	0	100	100
13	LE	110/111 (99%)	110 (100%)	0	100	100
14	LF	79/113 (70%)	79 (100%)	0	100	100
15	LG	55/60 (92%)	55 (100%)	0	100	100
16	LH	745/826 (90%)	744 (100%)	1 (0%)	88	89
17	LI	244/657 (37%)	244 (100%)	0	100	100
18	LJ	437/454 (96%)	437 (100%)	0	100	100
19	LK	124/533 (23%)	124 (100%)	0	100	100
20	LL	452/574 (79%)	452 (100%)	0	100	100
21	LM	421/1633 (26%)	421 (100%)	0	100	100
22	LN	603/713 (85%)	603 (100%)	0	100	100
23	LO	729/811 (90%)	729 (100%)	0	100	100
24	LP	360/414 (87%)	360 (100%)	0	100	100
25	LQ	746/832 (90%)	746 (100%)	0	100	100
26	LR	698/719 (97%)	698 (100%)	0	100	100
27	LS	423/528 (80%)	423 (100%)	0	100	100
28	LT	763/819 (93%)	763 (100%)	0	100	100
29	LU	415/443 (94%)	415 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	LV	366/636 (58%)	366 (100%)	0	100	100
31	LW	465/480 (97%)	465 (100%)	0	100	100
32	LX	760/934 (81%)	760 (100%)	0	100	100
32	LY	592/934 (63%)	592 (100%)	0	100	100
33	LZ	170/172 (99%)	170 (100%)	0	100	100
34	NA	194/535 (36%)	194 (100%)	0	100	100
35	NB	149/538 (28%)	149 (100%)	0	100	100
36	NC	121/315 (38%)	121 (100%)	0	100	100
37	ND	70/196 (36%)	70 (100%)	0	100	100
38	NE	166/304 (55%)	166 (100%)	0	100	100
39	NF	121/128 (94%)	121 (100%)	0	100	100
40	NG	90/105 (86%)	90 (100%)	0	100	100
41	NH	982/1125 (87%)	982 (100%)	0	100	100
42	NI	220/274 (80%)	220 (100%)	0	100	100
43	NK	233/289 (81%)	233 (100%)	0	100	100
44	NM	205/224 (92%)	205 (100%)	0	100	100
45	NN	44/482 (9%)	44 (100%)	0	100	100
46	NQ	68/71 (96%)	68 (100%)	0	100	100
47	OA	10/1544 (1%)	10 (100%)	0	100	100
48	SA	331/435 (76%)	331 (100%)	0	100	100
49	SB	360/433 (83%)	360 (100%)	0	100	100
50	SC	200/240 (83%)	200 (100%)	0	100	100
50	SD	197/240 (82%)	197 (100%)	0	100	100
51	SE	100/104 (96%)	100 (100%)	0	100	100
51	SF	100/104 (96%)	100 (100%)	0	100	100
52	SG	392/502 (78%)	392 (100%)	0	100	100
53	SH	307/312 (98%)	307 (100%)	0	100	100
54	SI	722/1039 (70%)	722 (100%)	0	100	100
55	SJ	192/222 (86%)	192 (100%)	0	100	100
55	SK	205/222 (92%)	205 (100%)	0	100	100
56	SL	155/169 (92%)	155 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	SM	251/258 (97%)	251 (100%)	0	100	100
58	SN	236/256 (92%)	236 (100%)	0	100	100
59	SP	2002/2307 (87%)	2002 (100%)	0	100	100
60	SQ	124/200 (62%)	124 (100%)	0	100	100
61	SR	86/120 (72%)	86 (100%)	0	100	100
62	SS	234/808 (29%)	234 (100%)	0	100	100
63	ST	443/732 (60%)	443 (100%)	0	100	100
64	SU	490/506 (97%)	490 (100%)	0	100	100
65	SV	42/192 (22%)	42 (100%)	0	100	100
66	SW	172/238 (72%)	172 (100%)	0	100	100
67	SY	218/234 (93%)	218 (100%)	0	100	100
68	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	21310/31319 (68%)	21309 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LH	868	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
5	L4	17	HIS
5	L4	67	GLN
5	L4	142	HIS
9	L8	116	HIS
10	L9	112	GLN
11	LC	74	HIS
13	LE	56	HIS
13	LE	98	GLN
13	LE	120	HIS
14	LF	29	HIS
16	LH	115	HIS
16	LH	364	ASN
16	LH	593	ASN
16	LH	868	ASN
17	LI	504	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	LI	529	HIS
17	LI	588	GLN
17	LI	597	GLN
17	LI	677	ASN
18	LJ	210	ASN
18	LJ	391	ASN
18	LJ	403	ASN
19	LK	450	ASN
20	LL	49	ASN
20	LL	240	GLN
20	LL	459	ASN
21	LM	10	GLN
21	LM	84	ASN
22	LN	216	GLN
22	LN	318	ASN
22	LN	385	ASN
22	LN	467	ASN
22	LN	766	GLN
23	LO	188	ASN
23	LO	254	HIS
23	LO	483	GLN
23	LO	552	ASN
23	LO	734	GLN
23	LO	752	ASN
23	LO	791	HIS
23	LO	825	GLN
24	LP	41	HIS
24	LP	90	GLN
24	LP	417	ASN
25	LQ	50	ASN
25	LQ	383	HIS
25	LQ	553	ASN
25	LQ	596	ASN
25	LQ	608	HIS
25	LQ	677	HIS
25	LQ	847	HIS
25	LQ	871	GLN
25	LQ	881	ASN
25	LQ	916	HIS
25	LQ	932	ASN
26	LR	642	GLN
27	LS	224	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	LS	245	HIS
27	LS	307	GLN
27	LS	309	GLN
27	LS	388	HIS
27	LS	412	GLN
27	LS	522	GLN
27	LS	528	GLN
27	LS	593	HIS
28	LT	86	HIS
28	LT	120	HIS
28	LT	736	HIS
29	LU	230	ASN
29	LU	353	GLN
29	LU	466	HIS
30	LV	80	GLN
30	LV	96	HIS
30	LV	185	HIS
31	LW	185	HIS
31	LW	278	ASN
31	LW	394	HIS
31	LW	506	GLN
31	LW	535	GLN
32	LX	215	ASN
32	LX	551	ASN
32	LX	721	HIS
32	LX	853	HIS
32	LX	891	GLN
32	LY	258	ASN
32	LY	545	HIS
32	LY	718	HIS
33	LZ	7	HIS
33	LZ	27	HIS
33	LZ	45	HIS
33	LZ	141	ASN
35	NB	499	GLN
35	NB	513	HIS
36	NC	233	HIS
36	NC	293	ASN
38	NE	237	HIS
41	NH	173	ASN
41	NH	606	ASN
41	NH	665	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	NH	687	GLN
41	NH	901	ASN
41	NH	923	HIS
41	NH	1076	GLN
42	NI	35	HIS
44	NM	74	GLN
44	NM	92	GLN
44	NM	199	ASN
46	NQ	19	HIS
48	SA	125	GLN
48	SA	235	HIS
48	SA	297	HIS
50	SC	93	HIS
50	SC	216	ASN
50	SC	264	GLN
50	SC	303	GLN
51	SE	18	GLN
52	SG	322	HIS
53	SH	176	GLN
54	SI	55	HIS
54	SI	173	HIS
54	SI	222	ASN
54	SI	289	HIS
54	SI	776	GLN
54	SI	803	ASN
54	SI	878	HIS
54	SI	986	HIS
54	SI	1049	ASN
55	SJ	165	ASN
55	SJ	250	ASN
55	SK	125	ASN
55	SK	250	ASN
56	SL	64	GLN
56	SL	77	GLN
57	SM	27	GLN
57	SM	53	GLN
57	SM	156	HIS
57	SM	236	HIS
58	SN	5	ASN
58	SN	132	HIS
58	SN	217	GLN
58	SN	248	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	SP	183	HIS
59	SP	388	ASN
59	SP	588	ASN
59	SP	776	ASN
59	SP	840	ASN
59	SP	1093	HIS
59	SP	1101	GLN
59	SP	1160	ASN
59	SP	1317	HIS
59	SP	1427	ASN
59	SP	1455	ASN
59	SP	1460	HIS
59	SP	1546	GLN
59	SP	1707	HIS
59	SP	1786	GLN
59	SP	1816	HIS
59	SP	2031	HIS
59	SP	2067	ASN
59	SP	2135	ASN
59	SP	2226	HIS
62	SS	316	ASN
63	ST	554	GLN
63	ST	713	HIS
66	SW	232	HIS
66	SW	239	HIS
67	SY	9	GLN
67	SY	45	GLN
67	SY	206	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	519/700 (74%)	88 (16%)	0
2	L1	1124/1808 (62%)	168 (14%)	1 (0%)
3	L2	170/333 (51%)	22 (12%)	0
All	All	1813/2841 (63%)	278 (15%)	1 (0%)

All (278) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	62	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L0	63	G
1	L0	64	U
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	89	C
1	L0	91	U
1	L0	103	G
1	L0	109	C
1	L0	110	G
1	L0	111	C
1	L0	122	U
1	L0	123	C
1	L0	125	G
1	L0	127	U
1	L0	128	C
1	L0	129	U
1	L0	130	G
1	L0	142	U
1	L0	144	C
1	L0	151	U
1	L0	171	G
1	L0	176	U
1	L0	177	U
1	L0	190	U
1	L0	200	A
1	L0	219	U
1	L0	227	U
1	L0	235	A
1	L0	240	C
1	L0	256	U
1	L0	259	G
1	L0	260	A
1	L0	267	U
1	L0	279	A
1	L0	280	A
1	L0	281	G
1	L0	304	U
1	L0	305	A
1	L0	310	U
1	L0	311	C
1	L0	316	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L0	325	U
1	L0	326	C
1	L0	346	G
1	L0	353	A
1	L0	354	G
1	L0	360	C
1	L0	365	G
1	L0	369	G
1	L0	370	U
1	L0	371	G
1	L0	372	A
1	L0	373	U
1	L0	381	G
1	L0	382	U
1	L0	383	G
1	L0	386	A
1	L0	395	C
1	L0	407	A
1	L0	427	A
1	L0	430	C
1	L0	431	A
1	L0	432	C
1	L0	461	A
1	L0	462	G
1	L0	464	G
1	L0	468	A
1	L0	481	U
1	L0	482	A
1	L0	487	A
1	L0	488	U
1	L0	489	G
1	L0	491	U
1	L0	492	G
1	L0	493	A
1	L0	517	A
1	L0	519	A
1	L0	525	U
1	L0	526	U
1	L0	533	G
1	L0	536	A
1	L0	539	A
1	L0	541	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L0	542	U
1	L0	546	G
1	L0	552	G
2	L1	-6	A
2	L1	5	U
2	L1	18	C
2	L1	23	G
2	L1	25	C
2	L1	34	G
2	L1	35	U
2	L1	36	C
2	L1	51	A
2	L1	52	U
2	L1	73	U
2	L1	74	U
2	L1	75	U
2	L1	76	A
2	L1	77	U
2	L1	93	A
2	L1	99	C
2	L1	101	U
2	L1	102	U
2	L1	105	A
2	L1	114	C
2	L1	116	U
2	L1	127	G
2	L1	128	U
2	L1	140	A
2	L1	145	A
2	L1	160	C
2	L1	168	A
2	L1	187	G
2	L1	188	A
2	L1	190	C
2	L1	192	U
2	L1	193	U
2	L1	195	G
2	L1	196	G
2	L1	202	A
2	L1	204	G
2	L1	249	U
2	L1	250	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	260	U
2	L1	261	U
2	L1	265	A
2	L1	275	C
2	L1	276	C
2	L1	277	U
2	L1	278	U
2	L1	279	G
2	L1	280	U
2	L1	299	A
2	L1	316	A
2	L1	319	U
2	L1	320	U
2	L1	321	C
2	L1	322	G
2	L1	334	G
2	L1	337	G
2	L1	359	A
2	L1	361	C
2	L1	400	A
2	L1	402	C
2	L1	423	G
2	L1	439	U
2	L1	444	C
2	L1	445	A
2	L1	454	U
2	L1	456	A
2	L1	473	A
2	L1	477	A
2	L1	495	C
2	L1	496	G
2	L1	501	U
2	L1	505	A
2	L1	506	A
2	L1	538	A
2	L1	539	G
2	L1	542	A
2	L1	545	A
2	L1	552	G
2	L1	564	G
2	L1	565	C
2	L1	575	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	579	A
2	L1	583	C
2	L1	594	A
2	L1	635	A
2	L1	863	A
2	L1	893	U
2	L1	898	A
2	L1	899	G
2	L1	906	A
2	L1	933	A
2	L1	935	U
2	L1	951	A
2	L1	960	U
2	L1	965	U
2	L1	970	A
2	L1	1027	A
2	L1	1030	A
2	L1	1033	C
2	L1	1036	A
2	L1	1040	G
2	L1	1076	A
2	L1	1079	U
2	L1	1084	A
2	L1	1085	G
2	L1	1114	G
2	L1	1122	G
2	L1	1127	G
2	L1	1128	C
2	L1	1132	A
2	L1	1134	C
2	L1	1158	C
2	L1	1159	C
2	L1	1167	G
2	L1	1175	U
2	L1	1191	U
2	L1	1192	C
2	L1	1193	A
2	L1	1207	C
2	L1	1208	A
2	L1	1218	G
2	L1	1220	C
2	L1	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	1228	G
2	L1	1232	U
2	L1	1256	A
2	L1	1267	G
2	L1	1268	G
2	L1	1269	U
2	L1	1270	G
2	L1	1436	A
2	L1	1437	U
2	L1	1438	G
2	L1	1440	C
2	L1	1472	C
2	L1	1474	G
2	L1	1485	C
2	L1	1492	A
2	L1	1493	A
2	L1	1506	G
2	L1	1577	A
2	L1	1590	G
2	L1	1595	U
2	L1	1596	C
2	L1	1601	G
2	L1	1602	C
2	L1	1611	A
2	L1	1618	C
2	L1	1619	C
2	L1	1633	A
2	L1	1657	U
2	L1	1658	G
2	L1	1664	C
2	L1	1680	G
2	L1	1683	C
2	L1	1701	A
2	L1	1702	A
2	L1	1703	C
2	L1	1715	G
2	L1	1716	C
2	L1	1721	A
2	L1	1745	G
2	L1	1747	G
2	L1	1768	G
2	L1	1778	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L1	1780	G
2	L1	1781	A
2	L1	1782	A
3	L2	4	G
3	L2	14	A
3	L2	24	U
3	L2	25	U
3	L2	27	U
3	L2	28	A
3	L2	30	A
3	L2	34	A
3	L2	35	U
3	L2	38	U
3	L2	39	C
3	L2	48	A
3	L2	56	A
3	L2	61	G
3	L2	62	C
3	L2	77	U
3	L2	90	C
3	L2	91	C
3	L2	109	G
3	L2	324	U
3	L2	325	C
3	L2	329	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L1	320	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SEP	LS	128	27	8,9,10	1.60	1 (12%)	7,12,14	1.33	1 (14%)
52	SEP	SG	50	52	8,9,10	1.60	1 (12%)	7,12,14	1.33	1 (14%)
23	SEP	LO	651	23	8,9,10	1.60	1 (12%)	7,12,14	1.29	1 (14%)

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
27	SEP	LS	128	27	-	0/6/8/10	-
52	SEP	SG	50	52	-	0/6/8/10	-
23	SEP	LO	651	23	-	1/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	SG	50	SEP	P-O1P	3.53	1.61	1.50
23	LO	651	SEP	P-O1P	3.49	1.61	1.50
27	LS	128	SEP	P-O1P	3.48	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	LS	128	SEP	OG-CB-CA	2.94	111.01	108.14
52	SG	50	SEP	OG-CB-CA	2.88	110.95	108.14
23	LO	651	SEP	OG-CB-CA	2.76	110.83	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	LO	651	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 27 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	ATP	NH	1300	69	32,33,33	0.28	0	48,52,52	0.68	0
72	GTP	SI	2001	69	33,34,34	1.82	4 (12%)	50,54,54	1.49	7 (14%)

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
70	ATP	NH	1300	69	-	1/22/38/38	0/3/3/3
72	GTP	SI	2001	69	-	0/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	SI	2001	GTP	C5-N7	6.72	1.52	1.39
72	SI	2001	GTP	C8-N9	-4.19	1.28	1.37
72	SI	2001	GTP	C4-N9	-3.78	1.28	1.38
72	SI	2001	GTP	C4-N3	2.31	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	SI	2001	GTP	C8-N9-C4	7.14	119.40	106.03
72	SI	2001	GTP	N9-C4-N3	2.71	131.36	125.95
72	SI	2001	GTP	C6-C5-N7	2.55	134.93	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	SI	2001	GTP	C1'-N9-C8	-2.32	120.15	126.73
72	SI	2001	GTP	C8-N7-C5	-2.06	100.58	104.26
72	SI	2001	GTP	C5-C4-N9	-2.06	101.97	105.66
72	SI	2001	GTP	C1'-N9-C4	-2.05	120.44	126.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

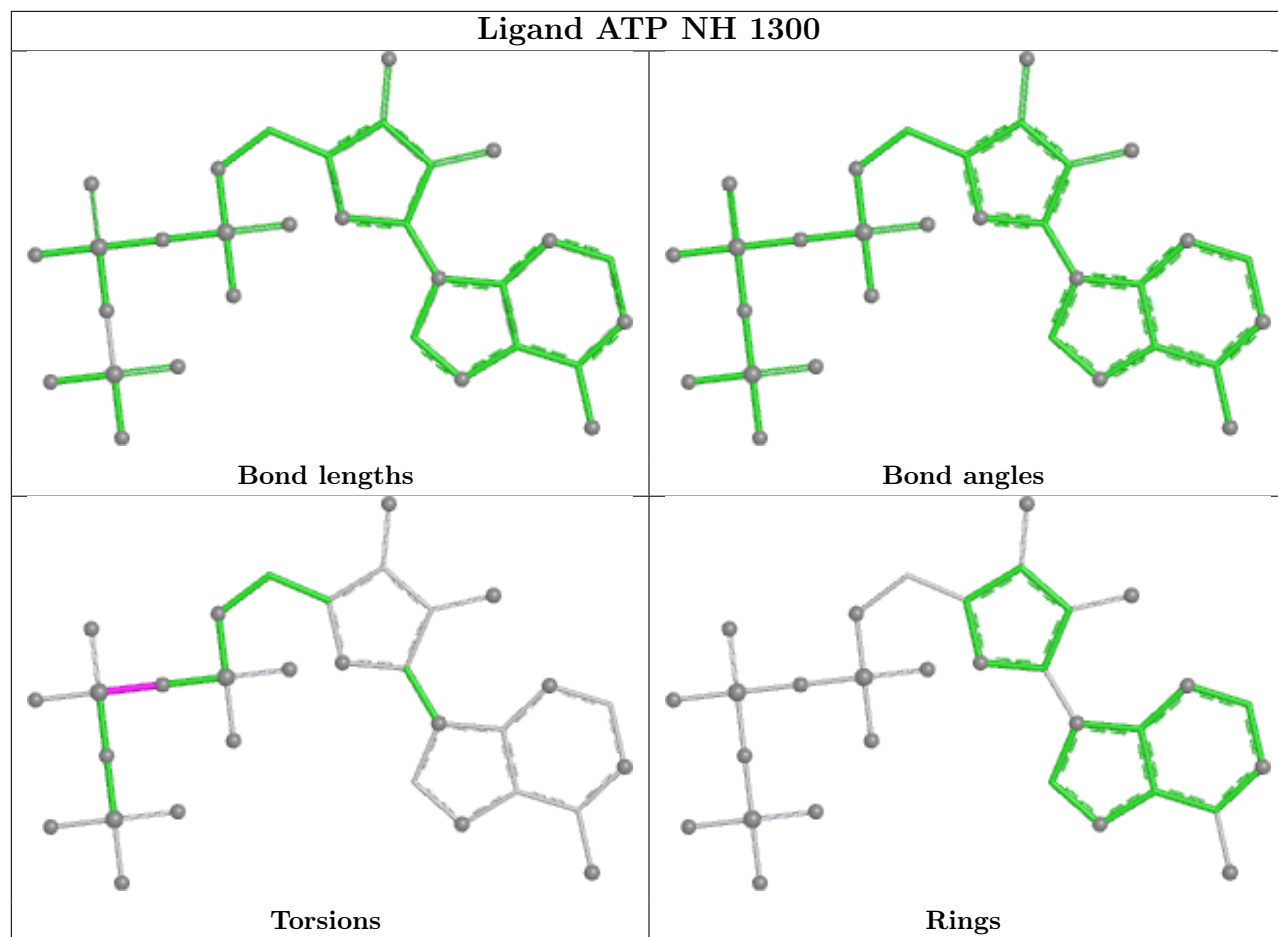
Mol	Chain	Res	Type	Atoms
70	NH	1300	ATP	PA-O3A-PB-O3B

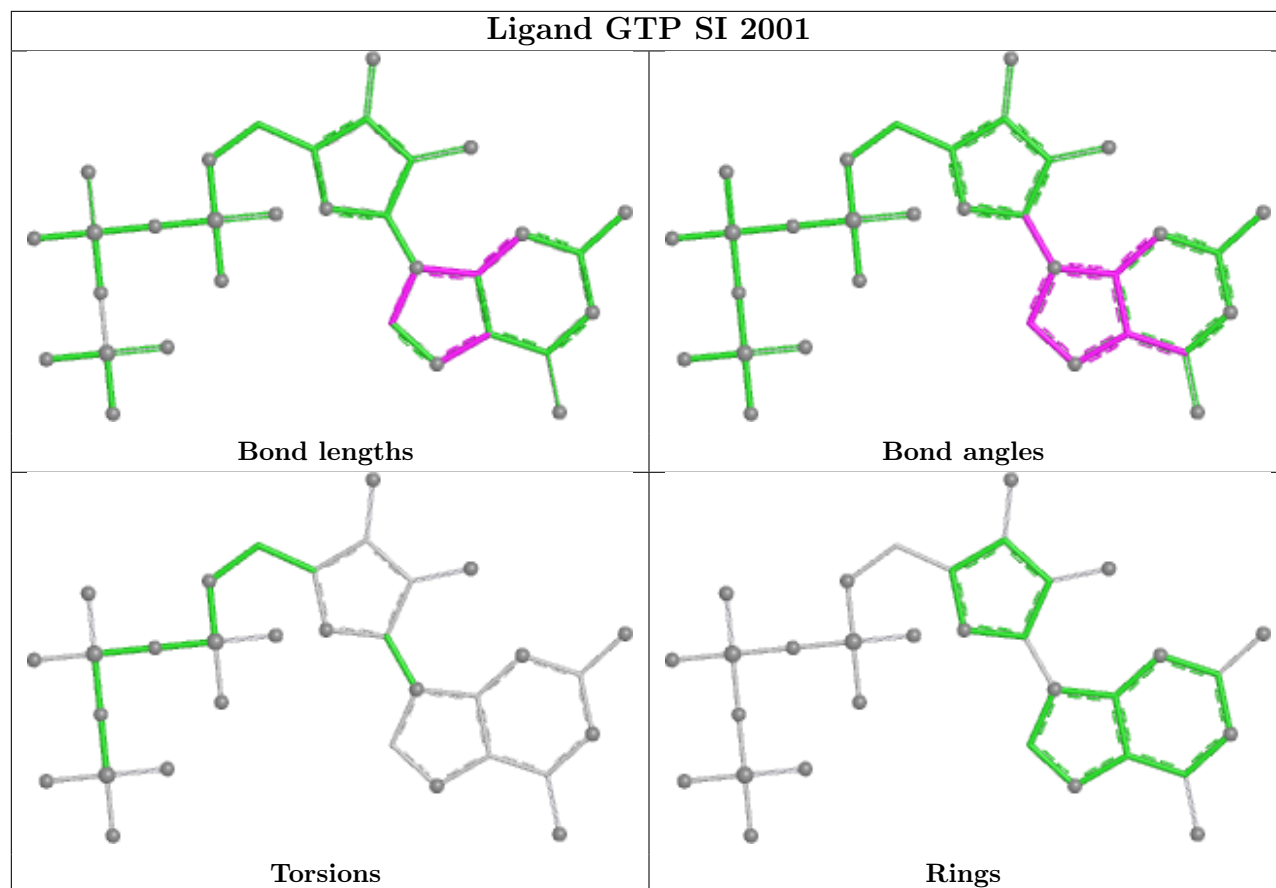
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	NH	1300	ATP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

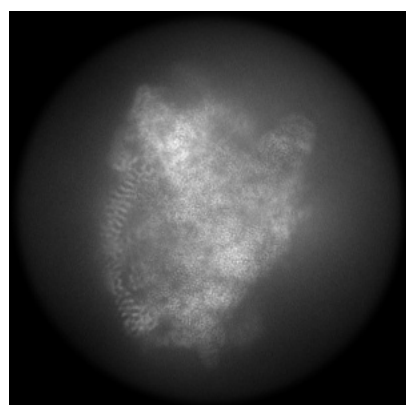
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49075. These allow visual inspection of the internal detail of the map and identification of artifacts.

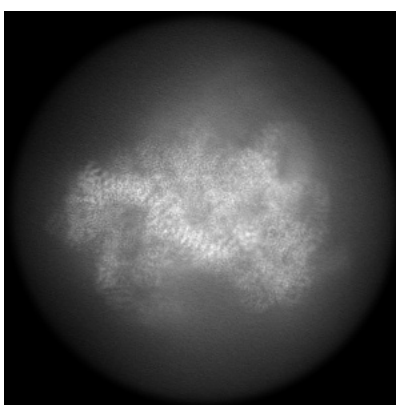
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

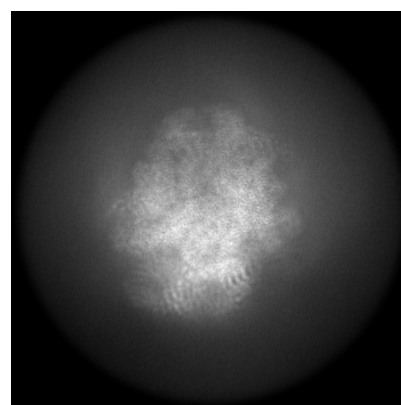
6.1.1 Primary map



X



Y

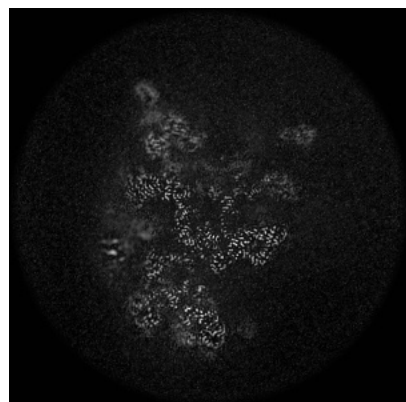


Z

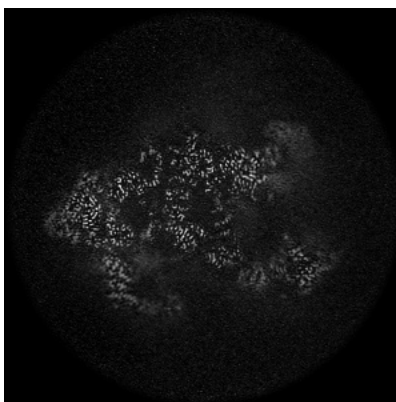
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

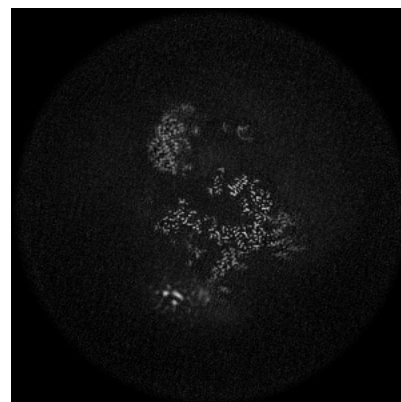
6.2.1 Primary map



X Index: 252



Y Index: 252

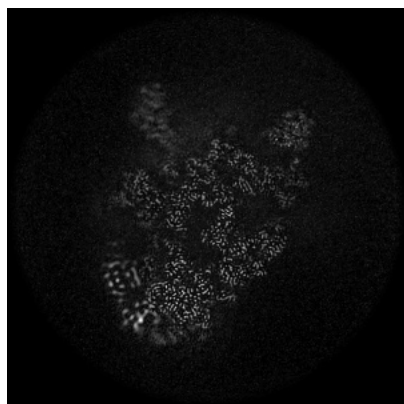


Z Index: 252

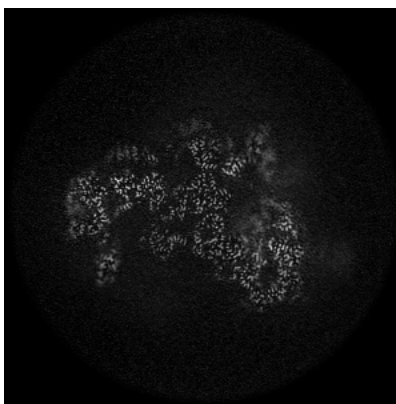
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

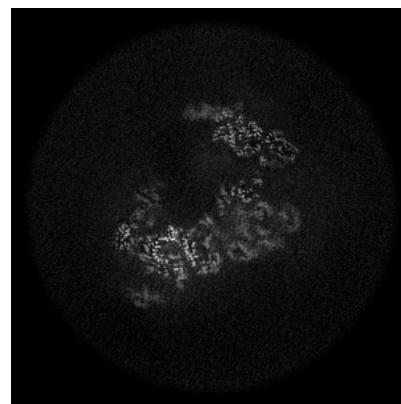
6.3.1 Primary map



X Index: 274



Y Index: 221

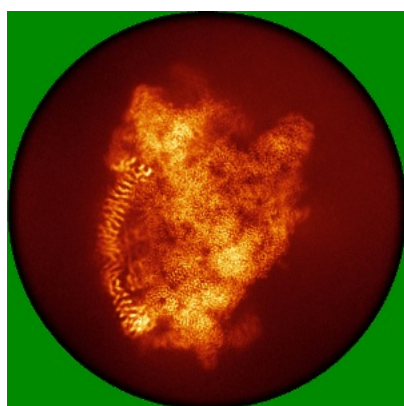


Z Index: 334

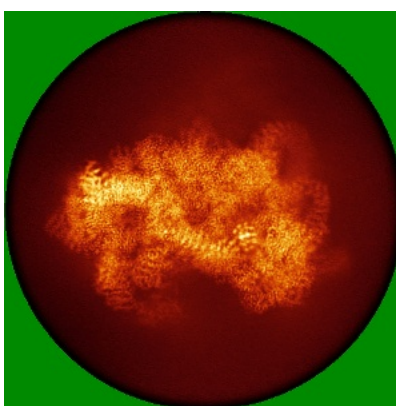
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

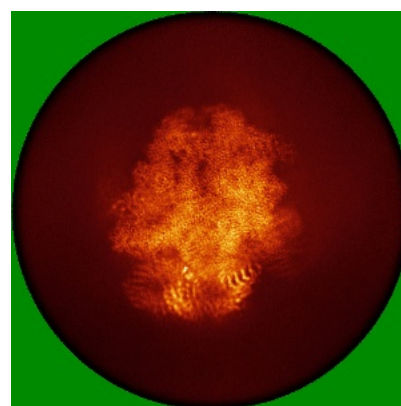
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

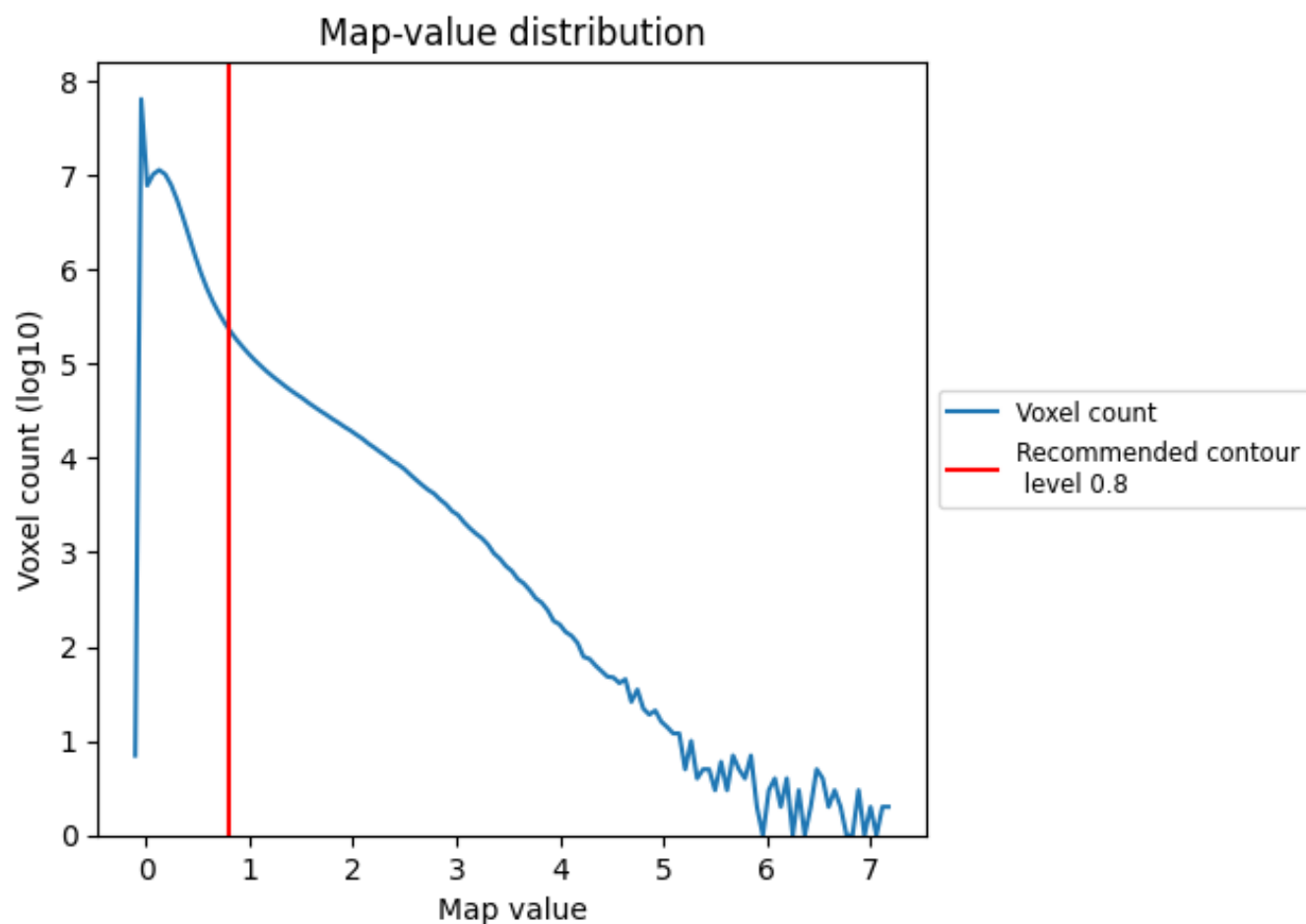
6.6 Mask visualisation

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

7 Map analysis [i](#)

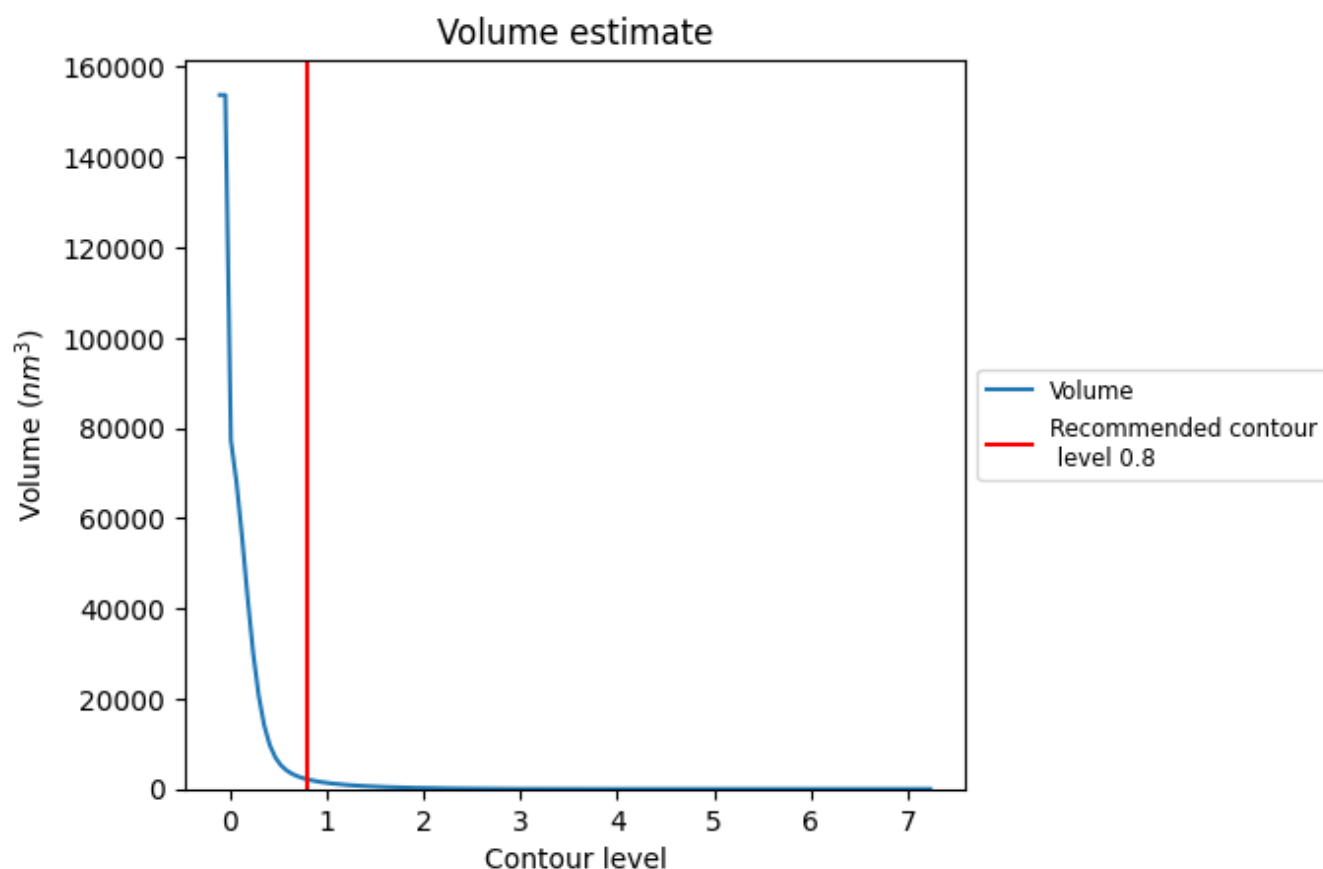
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

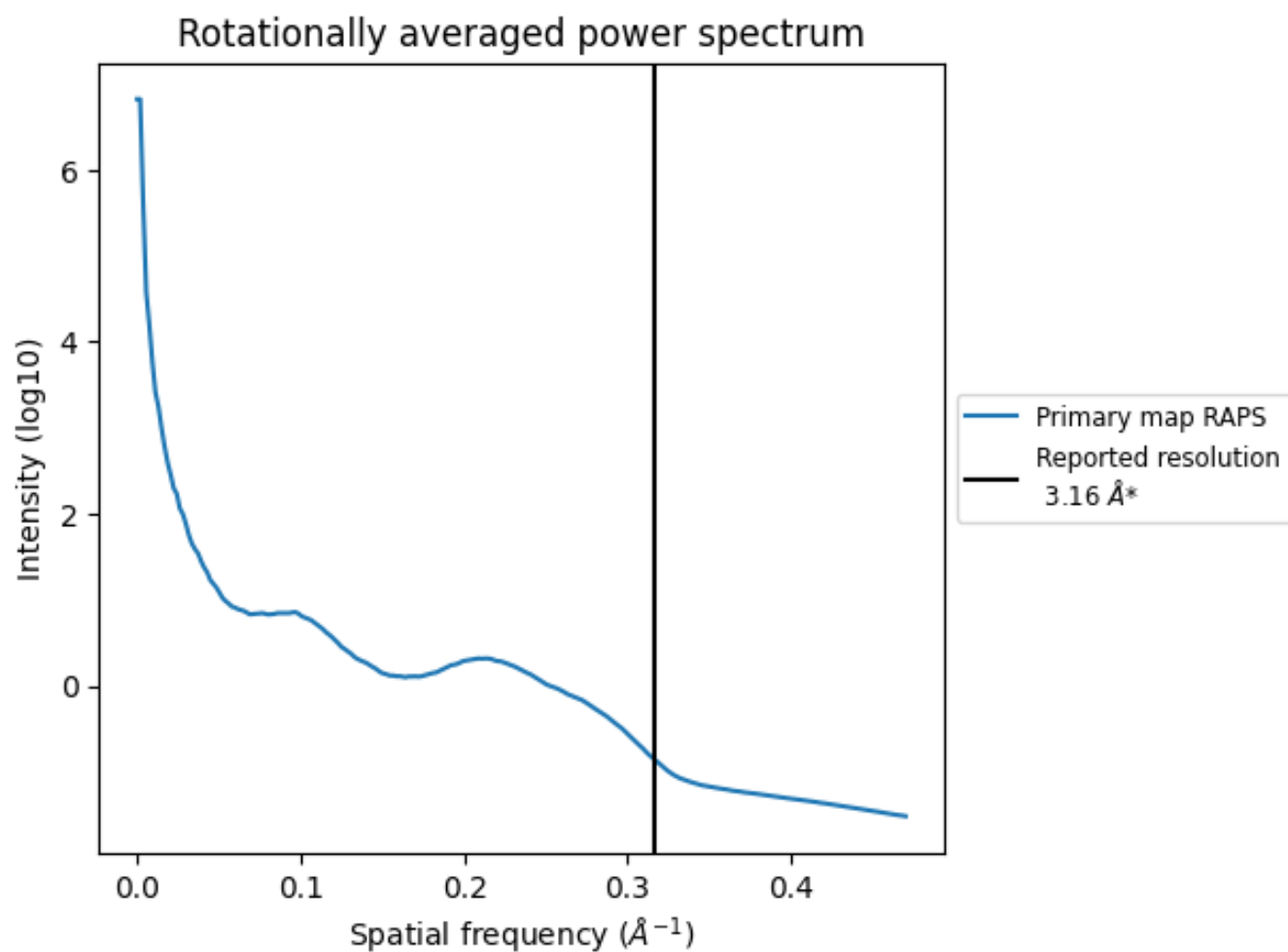
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2153 nm^3 ; this corresponds to an approximate mass of 1945 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 0.316 Å⁻¹

8 Fourier-Shell correlation

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

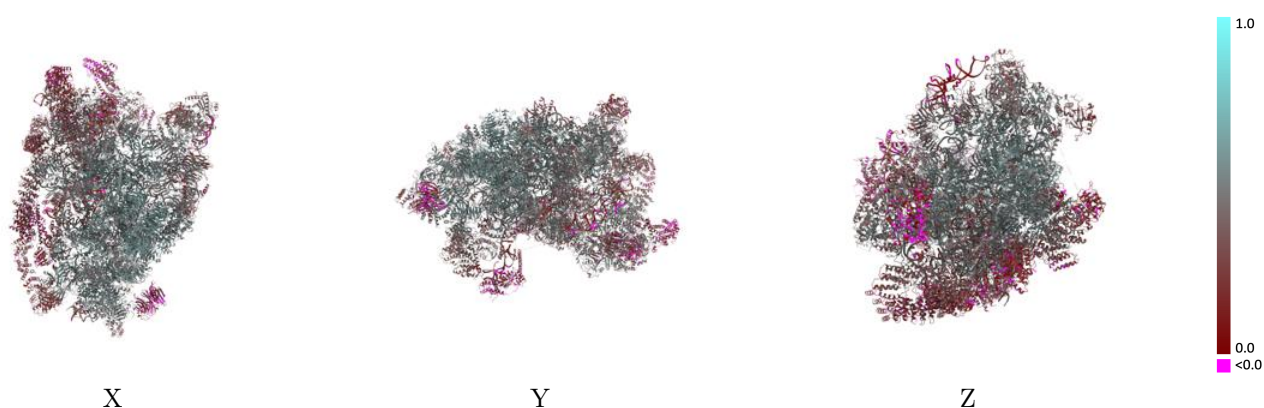
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49075 and PDB model 9N6V. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

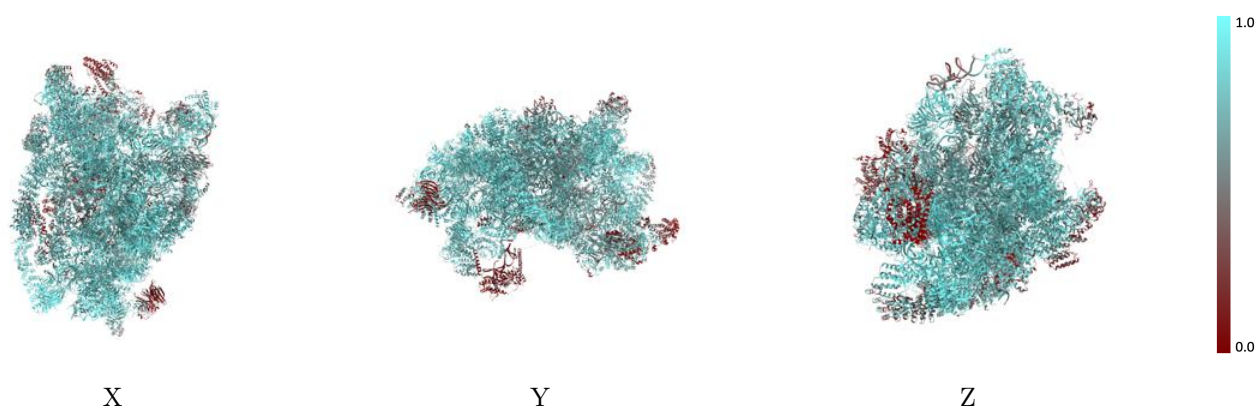
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



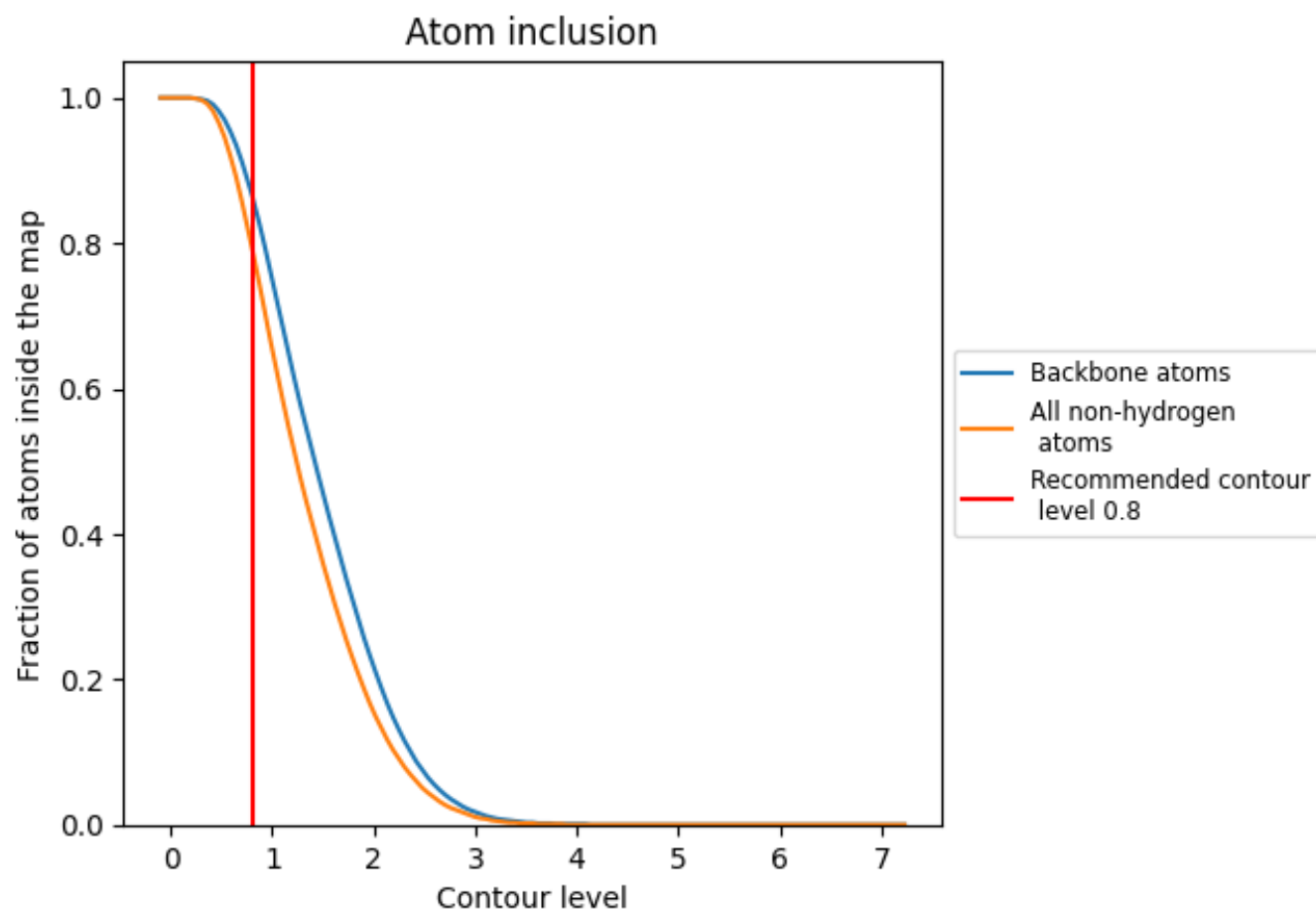
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7950	 0.4310
L0	 0.8730	 0.4680
L1	 0.8570	 0.4190
L2	 0.8840	 0.4710
L3	 0.2010	 0.2460
L4	 0.9290	 0.4230
L5	 0.8770	 0.5290
L6	 0.9210	 0.4180
L7	 0.8160	 0.3500
L8	 0.9540	 0.4660
L9	 0.8620	 0.5150
LC	 0.9050	 0.5530
LD	 0.9030	 0.3390
LE	 0.9260	 0.4990
LF	 0.8950	 0.3170
LG	 0.8600	 0.5360
LH	 0.9050	 0.5170
LI	 0.4710	 0.2690
LJ	 0.9220	 0.5240
LK	 0.7240	 0.3630
LL	 0.8800	 0.5120
LM	 0.8400	 0.3320
LN	 0.9210	 0.4880
LO	 0.8940	 0.5610
LP	 0.6280	 0.3960
LQ	 0.8400	 0.4230
LR	 0.6450	 0.4000
LS	 0.9090	 0.5490
LT	 0.8690	 0.5510
LU	 0.9330	 0.5420
LV	 0.8470	 0.4520
LW	 0.8630	 0.5520
LX	 0.7880	 0.4270
LY	 0.6240	 0.3560
LZ	 0.9050	 0.5860



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NA	 0.7010	 0.4370
NB	 0.6050	 0.3580
NC	 0.6170	 0.2880
ND	 0.7050	 0.3840
NE	 0.7110	 0.4590
NF	 0.8930	 0.5040
NG	 0.7680	 0.5050
NH	 0.8120	 0.4390
NI	 0.5620	 0.3560
NK	 0.7890	 0.4930
NM	 0.7650	 0.4960
NN	 0.3220	 0.1940
NQ	 0.8960	 0.5010
OA	 0.4420	 0.3790
SA	 0.7080	 0.4120
SB	 0.7230	 0.3920
SC	 0.8470	 0.5430
SD	 0.8000	 0.4720
SE	 0.9340	 0.5450
SF	 0.8270	 0.5060
SG	 0.8120	 0.4670
SH	 0.7620	 0.4920
SI	 0.8390	 0.5070
SJ	 0.7800	 0.3760
SK	 0.9120	 0.4260
SL	 0.8800	 0.5580
SM	 0.8280	 0.5340
SN	 0.7160	 0.4700
SP	 0.7100	 0.2520
SQ	 0.7050	 0.4820
SR	 0.8680	 0.5430
SS	 0.6460	 0.4130
ST	 0.6110	 0.3470
SU	 0.8110	 0.3860
SV	 0.7620	 0.3060
SW	 0.5840	 0.4280
SY	 0.8410	 0.5160
SZ	 0.1690	 0.1810