



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:31 AM UTC

PDB ID : 9PKG / pdb_00009pkg
EMDB ID : EMD-71696
Title : In situ human P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-07-14
Resolution : 3.26 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

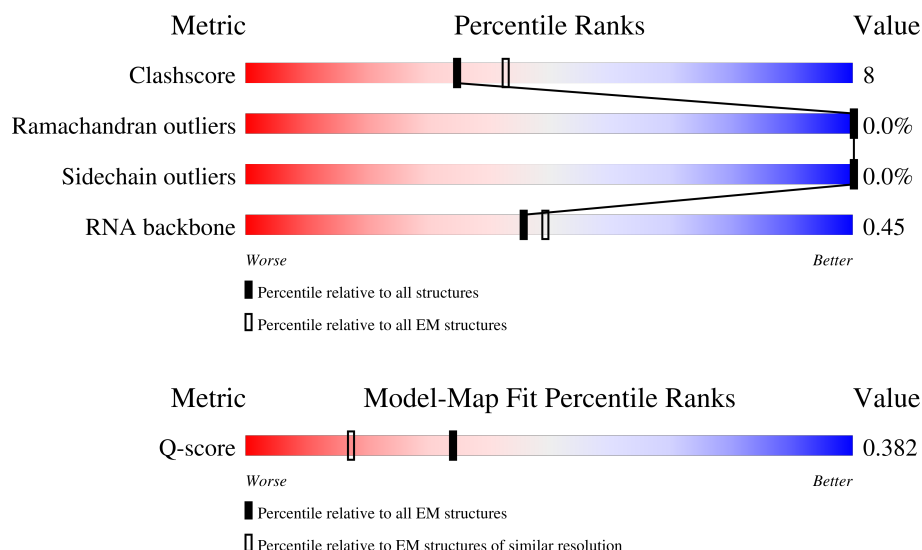
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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.






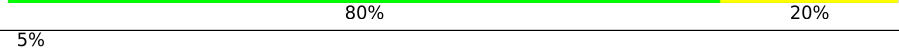
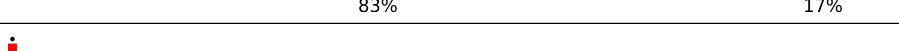







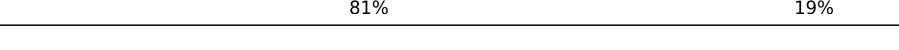

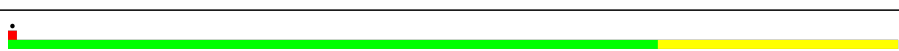



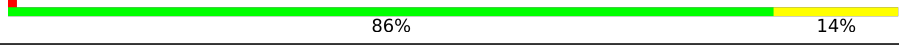






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	CI	31	
2	Pt	74	
3	L5	3655	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	124	
28	LX	120	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	157	
50	SD	227	
51	SF	189	
52	SK	98	
53	SM	122	

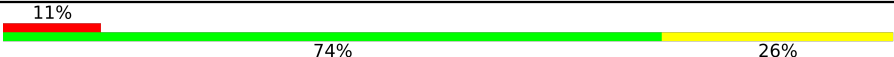



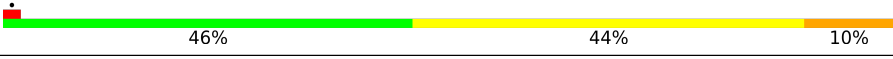
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	189	
71	SI	206	
72	SJ	185	
73	SL	153	
74	SN	150	
75	SO	140	
76	SV	83	
77	SW	129	
78	SX	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	SY	131	
80	Sa	102	
81	Sb	83	
82	Se	58	
83	S2	1740	

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 218355 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 protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CI	31	Total	C	N	O	S	0	0
			247	153	55	38	1		

- Molecule 2 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Pt	3	C	U	conflict	GB X64278
Pt	?	-	U	deletion	GB X64278
Pt	?	-	G	deletion	GB X64278
Pt	19	G	U	conflict	GB X64278
Pt	50	U	-	insertion	GB X64278
Pt	74	C	-	insertion	GB X64278

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3655	Total	C	N	O	P	0	0
			78421	34958	14341	25468	3654		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 11 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 14 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 25 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 30 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 40 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 47 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lt	134	Total	C	N	O	S	0	0
			998	626	180	189	3		

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 51 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 52 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 53 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 54 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 55 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 56 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 57 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 58 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 59 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 60 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 61 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 62 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 64 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 65 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 66 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 68 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 69 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 70 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 71 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 72 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 73 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 74 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 75 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 76 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 77 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 78 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 79 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 80 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 81 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

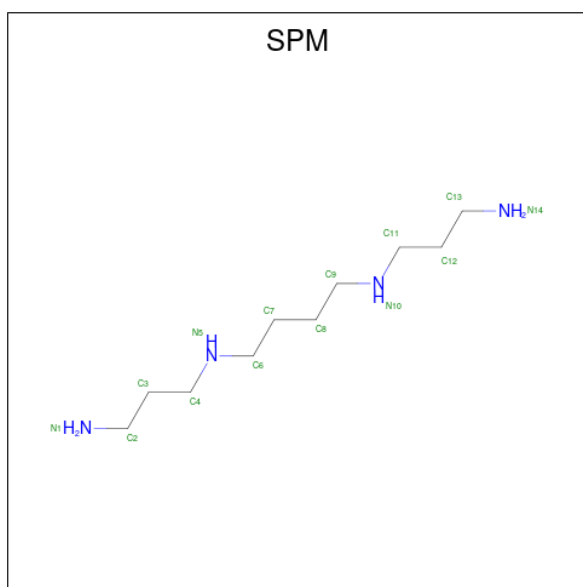
- Molecule 83 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	S2	1740	Total	C	N	O	P	0	0
			36953	16508	6600	12106	1739		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

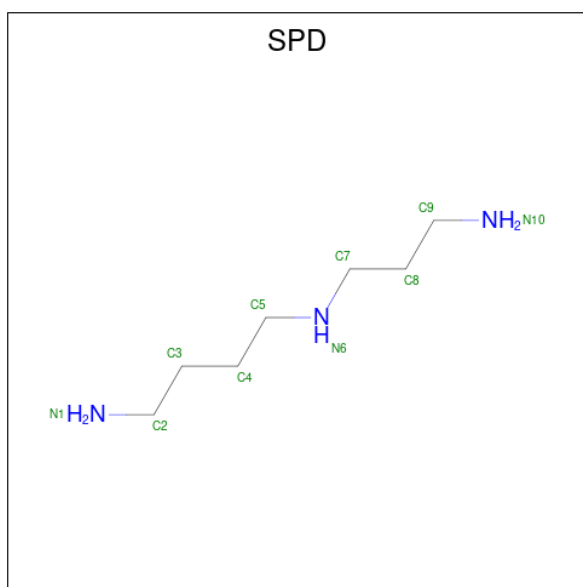
Mol	Chain	Residues	Atoms		AltConf
84	L5	181	Total	Mg	0
			181	181	
84	L7	2	Total	Mg	0
			2	2	
84	L8	4	Total	Mg	0
			4	4	
84	LA	1	Total	Mg	0
			1	1	
84	LV	1	Total	Mg	0
			1	1	
84	Le	1	Total	Mg	0
			1	1	
84	Lj	1	Total	Mg	0
			1	1	
84	Sa	1	Total	Mg	0
			1	1	
84	S2	27	Total	Mg	0
			27	27	

- Molecule 85 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			14	10	4	
85	L5	1	Total	C	N	0
			14	10	4	
85	L5	1	Total	C	N	0
			14	10	4	
85	L5	1	Total	C	N	0
			14	10	4	
85	L5	1	Total	C	N	0
			14	10	4	
85	L5	1	Total	C	N	0
			14	10	4	

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L8	1	Total	C	N	0
			10	7	3	
86	LN	1	Total	C	N	0
			10	7	3	

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
87	Lg	1	Total	Zn	0
			1	1	

Continued on next page...

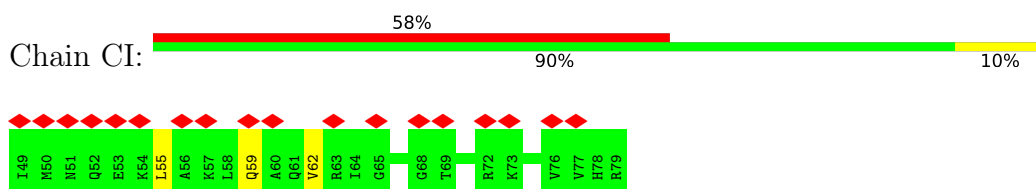
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	Lj	1	Total 1	Zn 1	0
87	Lm	1	Total 1	Zn 1	0
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0
87	Sa	1	Total 1	Zn 1	0

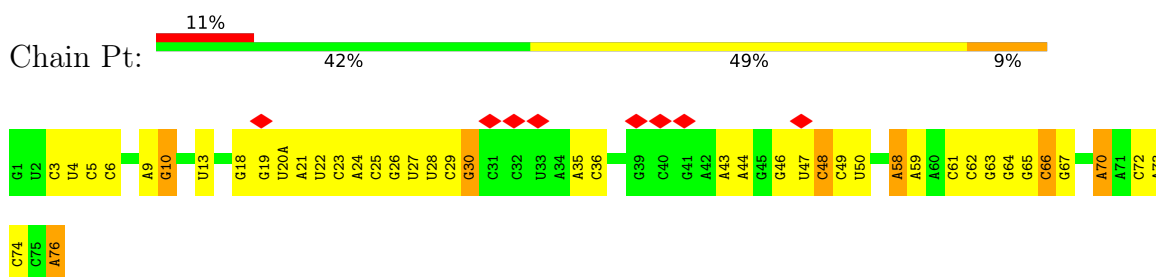
3 Residue-property plots [i](#)

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

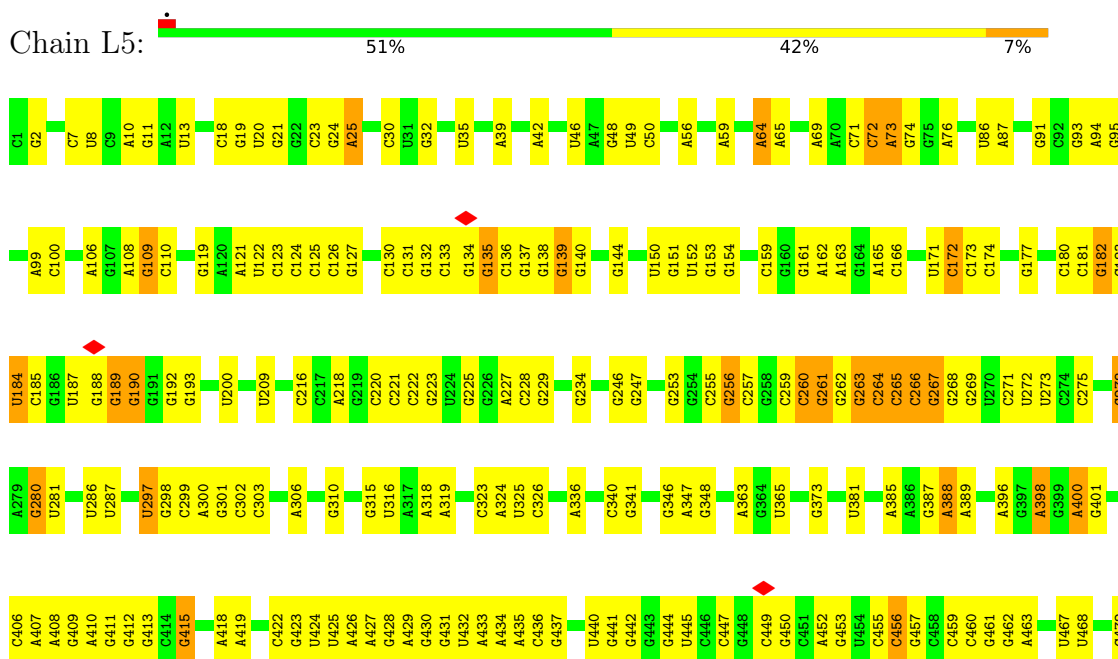
- Molecule 1: Transcription factor BTF3



- Molecule 2: P site tRNA



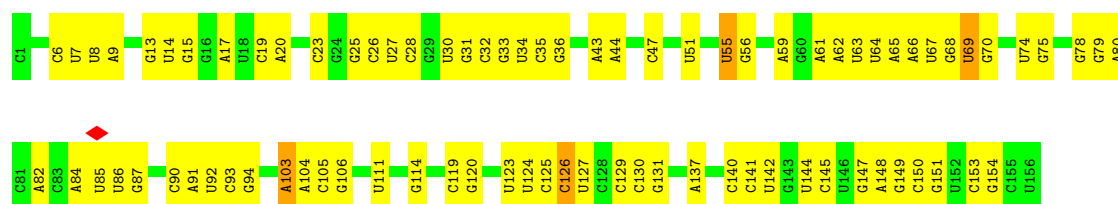
- Molecule 3: 28S rRNA



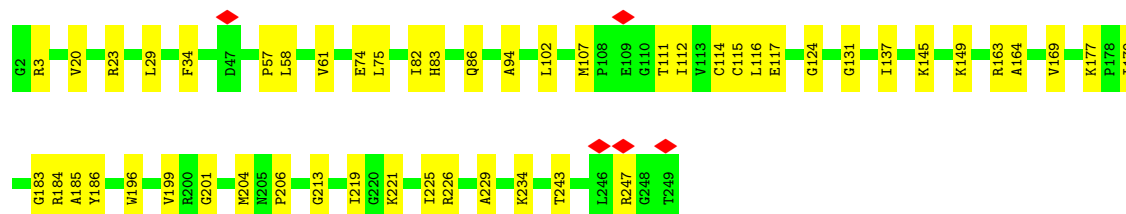
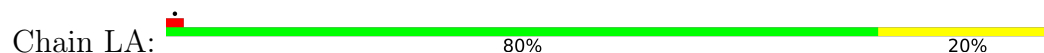
G181	G182	A183	G184	G185	A186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632</
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	---------

C4079	C4080	C4088	G4092	G4093	G4094	G4095	G4096	G4097	G4098	G4099	C4100	C4101	C4102	C4103	G4104	G4108	G4109	C4110	C4111	C4112	C4113	C4114	C4115	C4116	G4121	G4122	C4126	A4127	A4128	G4129	C4130	G4131	C4138	G4139	C4140	G4141	C4142	C4143	C4144	C4145	G4146	C4147	C4148	C4149	G4150	C4153	G4154	C4155	C4158	C4159																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U3914	U3915	U3916	U3917	U3918	U3919	U3920	U3921	U3922	A3923	A3924	U3925	C3926	U3927	A3928	C3929	U3930	C3931	U3932	C3933	C3934	C3935	A3936	C3937	C3938	C3939	A3942	A3943	A3944	A3945	A3946	A3947	C3948	A3949	U3950	C3951	A3952	C3953	A3954	A4056	C4057	U4058	C4059	U4060	C4061	C4062	U4063	C4064	U4065	U4066	U4067	U4068	U4069	U4070	U4071	C4072	G4076																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C3837	U3838	U3839	C3840	C3841	C3842	C3843	U3844	A3845	C3846	C3847	U3848	A3849	C3850	U3851	U3852	U3853	C3854	C3855	A3856	A3860	A3861	A3862	A3867	C3868	C3869	C3870	A3871	A3872	C3873	C3874	A3877	C3878	C3879	C3880	C3881	C3882	U3883	U3884	U3892	C3896	C3897	C3898	A3901	A3906	C3907	C3908	C3909	C3910	C3911	U3912	C3913																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C3735	A3736	A3737	C3738	C3739	C3740	C3741	G3744	U3745	A3746	A3747	A3748	C3749	G3753	G3754	A3760	U3764	G3765	U3770	A3774	A3775	C3776	U3777	C3782	A3785	U3786	C3791	C3792	C3808	C3809	C3810	C3811	C3812	C3813	A3817	U3818	C3819	U3822	C3823	A3824	A3825	A3830	U3831	U3832	C3833	C3834																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
C3652	A3653	G3661	C3662	A3663	C3664	C3665	C3670	C3673	C3674	C3683	C3684	C3685	U3690	C3691	A3692	U3695	U3697	C3698	C3699	C3700	C3701	C3706	U3707	C3708	U3709	G3710	A3711	A3712	U3713	C3714	U3715	C3716	A3717	A3718	A3719	C3720	U3721	C3722	A3723	A3724	C3725	A3726	A3727	A3728	U3729	U3730	C3731	A3732	A3733	U3734																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C3582	C3583	C3584	C3585	C3586	C3587	C3588	C3589	C3590	C3591	C3594	U3595	C3596	C3597	C3598	A3599	C3600	C3601	C3602	C3603	A3604	C3605	U3606	A3607	A3608	A3611	C3619	C3626	A3635	C3636	C3637	C3638	U3639	U3640	U3641	U3644	U3645	A3646	A3647	A3648																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C3274	C3275	C3276	C3277	C3278	C3279	C3280	C3281	C3282	C3283	C3284	C3285	C3286	C3287	C3288	C3289	C3290	C3291	C3292	C3293	C3294	C3295	C3296	C3297	C3298	C3299	C3300	C3301	C3302	C3303	C3304	C3305	C3306	C3307	C3308	C3309	C3310	C3311	C3312	C3313	C3314	C3315	C3316	C3317	C3318	C3319	C3320	C3321	C3322	C3323	C3324	C3325	C3326	C3327	C3328	C3329	C3330	C3331	C3332	C3333	C3334	C3335	C3336	C3337	C3338	C3339	C3340	C3341	C3342	C3343	C3344	C3345	C3346	C3347	C3348	C3349	C3350	C3351	C3352	C3353	C3354	C3355	C3356	C3357	C3358	C3359	C3360	C3361	C3362	C3363	C3364	C3365	C3366	C3367	C3368	C3369	C3370	C3371	C3372	C3373	C3374	C3375	C3376	C3377	C3378	C3379	C3380	C3381	C3382	C3383	C3384	C3385	C3386	C3387	C3388	C3389	C3390	C3391	C3392	C3393	C3394	C3395	C3396	C3397	C3398	C3399	C3400	C3401	C3402	C3403	C3404	C3405	C3406	C3407	C3408	C3409	C3410	C3411	C3412	C3413	C3414	C3415	C3416	C3417	C3418	C3419	C3420	C3421	C3422	C3423	C3424	C3425	C3426	C3427	C3428	C3429	C3430	C3431	C3432	C3433	C3434	C3435	C3436	C3437	C3438	C3439	C3440	C3441	C3442	C3443	C3444	C3445	C3446	C3447	C3448	C3449	C3450	C3451	C3452	C3453	C3454	C3455	C3456	C3457	C3458	C3459	C3460	C3461	C3462	C3463	C3464	C3465	C3466	C3467	C3468	C3469	C3470	C3471	C3472	C3473	C3474	C3475	C3476	C3477	C3478	C3479	C3480	C3481	C3482	C3483	C3484	C3485	C3486	C3487	C3488	C3489	C3490	C3491	C3492	C3493	C3494	C3495	C3496	C3497	C3498	C3499	C3500	C3501	C3502	C3503	C3504	C3505	C3506	C3507	C3508	C3509	C3510	C3511	C3512	C3513	C3514	C3515	C3516	C3517	C3518	C3519	C3520	C3521	C3522	C3523	C3524	C3525	C3526	C3527	C3528	C3529	C3530	C3531	C3532	C3533	C3534	C3535	C3536	C3537	C3538	C3539	C3540	C3541	C3542	C3543	C3544	C3545	C3546	C3547	C3548	C3549	C3550	C3551	C3552	C3553	C3554	C3555	C3556	C3557	C3558	C3559	C3560	C3561	C3562	C3563	C3564	C3565	C3566	C3567	C3568	C3569	C3570	C3571	C3572	C3573	C3574	C3575	C3576	C3577	C3578	C3579	C3580	C3581	C3582	C3583	C3584	C3585	C3586	C3587	C3588	C3589	C3590	C3591	C3592	C3593	C3594	C3595	C3596	C3597	C3598	C3599	C3600	C3601	C3602	C3603	C3604	C3605	C3606	C3607	C3608	C3609	C3610	C3611	C3612	C3613	C3614	C3615	C3616	C3617	C3618	C3619	C3620	C3621	C3622	C3623	C3624	C3625	C3626	C3627	C3628	C3629	C3630	C3631	C3632	C3633	C3634	C3635	C3636	C3637	C3638	C3639	C3640	C3641	C3642	C3643	C3644	C3645	C3646	C3647	C3648	C3649	C3650	C3651	C3652	C3653	C3654	C3655	C3656	C3657	C3658	C3659	C3660	C3661	C3662	C3663	C3664	C3665	C3666	C3667	C3668	C3669	C3670	C3671	C3672	C3673	C3674	C3675	C3676	C3677	C3678	C3679	C3680	C3681	C3682	C3683	C3684	C3685	C3686	C3687	C3688	C3689	C3690	C3691	C3692	C3693	C3694	C3695	C3696	C3697	C3698	C3699	C3700	C3701	C3702	C3703	C3704	C3705	C3706	C3707	C3708	C3709	C3710	C3711	C3712	C3713	C3714	C3715	C3716	C3717	C3718	C3719	C3720	C3721	C3722	C3723	C3724	C3725	C3726	C3727	C3728	C3729	C3730	C3731	C3732	C3733	C3734	C3735	C3736	C3737	C3738	C3739	C3740	C3741	C3742	C3743	C3744	C3745	C3746	C3747	C3748	C3749	C3750	C3751	C3752	C3753	C3754	C3755	C3756	C3757	C3758	C3759	C3760	C3761	C3762	C3763	C3764	C3765	C3766	C3767	C3768	C3769	C3770	C3771	C3772	C3773	C3774	C3775	C3776	C3777	C3778	C3779	C3780	C3781	C3782	C3783	C3784	C3785	C3786	C3787	C3788	C3789	C3790	C3791	C3792	C3793	C3794	C3795	C3796	C3797	C3798	C3799	C3800	C3801	C3802	C3803	C3804	C3805	C3806	C3807	C3808	C3809	C3810	C3811	C3812	C3813	C3814	C3815	C3816	C3817	C3818	C3819	C3820	C3821	C3822	C3823	C3824	C3825	C3826	C3827	C3828	C3829	C3830	C3831	C3832	C3833	C3834	C3835	C3836	C3837	C3838	C3839	C3840	C3841	C3842	C3843	C3844	C3845	C3846	C3847	C3848	C3849	C3850	C3851	C3852	C3853	C3854	C3855	C3856	C3857	C3858	C3859	C3860	C3861	C3862	C3863	C3864	C3865	C3866	C3867	C3868	C3869	C3870	C3871	C3872	C3873	C3874	C3875	C3876	C3877	C3878	C3879	C3880	C3881	C3882	C3883	C3884	C3885	C3886	C3887	C3888	C3889	C3890	C3891	C3892	C3893	C3894	C3895	C3896	C3897	C3898	C3899	C3900	C3901	C3902	C3903	C3904	C3905	C3906	C3907	C3908	C3909	C3910	C3911	C3912	C3913	C3914	C3915	C3916	C3917	C3918	C3919	C3920	C3921	C3922	C3923	C3924	C3925	C3926	C3927	C3928	C3929	C3930	C3931	C3932	C3933	C3934	C3935	C3936	C3937	C3938	C3939	C3940	C3941	C3942	C3943	C3944	C3945	C3946	C3947	C3948	C3949	C3950	C3951	C3952	C3953	C3954	C3955	C3956	C3957	C3958	C3959	C3960	C3961	C3962	C3963	C3964	C3965	C3966	C3967	C3968	C3969	C3970	C3971	C3972	C3973	C3974	C3975	C3976	C3977	C3978	C3979	C3980	C3981	C3982	C3983	C3984	C3985	C3986	C3987	C3988	C3989	C3990	C3991	C3992	C3993	C3994	C3995	C3996	C3997	C3998	C3999	C4000	C4001	C4002	C4003	C4004	C4005	C4006	C4007	C4008	C4009	C4010	C4011	C4012	C4013	C4014	C4015	C4016	C4017	C4018	C4019	C4020	C4021	C4022	C4023	C4024	C4025	C4026	C4027	C4028	C4029	C4030	C4031	C4032	C4033	C4034	C4035	C4036	C4037	C4038	C4039	C4040	C4041	C4042	C4043	C4044	C4045	C4046	C4047	C4048	C4049	C4050	C4051	C4052	C4053	C4054	C4055	C4056	C4057	C4058	C4059	C4060	C4061	C4062	C4063	C4064	C4065	C4066	C4067	C4068	C4069	C4070	C4071	C4072	C4073	C4074	C4075	C4076	C4077	C4078	C4079	C4080	C4081	C4082	C4083	C4084	C4085	C4086	C4087	C4088	C4089	C4090	C4091	C4092	C4093	C4094	C4095	C4096	C4097	C4098	C4099	C4100	C4101	C4102	C4103	C4104	C4105	C4106	C4107	C4108	C4109	C4110	C4111	C4112	C4113	C4114	C4115	C4116	C4117	C4118	C4119	C4120	C4121	C4122	C4123	C4124	C4125	C4126	C4127	C4128	C4129	C4130	C4131	C4132	C4133	C4134	C4135	C4136	C4137	C4138	C4139	C4140	C4141	C4142	C4143	C4144	C4145	C4146	C4147	C4148	C4149	C4150	C4151	C4152	C4153	C4154	C4155	C4156	C4157	C4158	C4159	C4160	C4161	C4162	C4163	C4164	C4165	C4166	C4167	C4168	C4169	C4170	C4171	C4172	C4173	C4174	C4175	C4176	C4177	C4178	C4179	C4180	C4181	C4182	C4183	C4184	C4185	C4186	C4187	C4188	C4189	C4190	C4191	C4192	C4193	C4194	C4195	C4196	C4197	C4198	C4199	C4200	C4201	C4202	C4203	C4204	C4205	C4206	C4207	C4208	C4209	C4210	C4211	C4212	C4213	C4214	C4215	C4216	C4217	C4218	C4219	C4220	C4221	C4222	C4223	C4224	C4225	C4226	C4227	C4228	C4229	C4230	C4231	C4232	C4233	C4234	C4235	C4236	C4237	C4238	C4239	C4240	C4241	C4242	C4243	C4244	C4245	C4246	C4247	C4248	C4249	C4250	C4251	C4252	C4253	C4254	C4255	C4256	C4257	C4258	C4259	C4260	C4261	C4262	C4263	C4264	C4265	C4266	C4267	C4268	C4269	C4270	C4271	C4272	C4273	C4274	C4275	C4276	C4277	C4278	C4279	C4280	C4281	C4282	C4283	C4284	C4285	C4286	C4287	C4288	C4289	C4290	C4291	C4292	C4293	C4294	C4295	C4296	C4297	C4298	C4299	C4300	C4301	C4302	C4303	C4304	C4305	C4306	C4307	C4308	C4309	C4310	C4311	C4312	C4313	C4314	C4315	C4316	C4317	C4318	C4

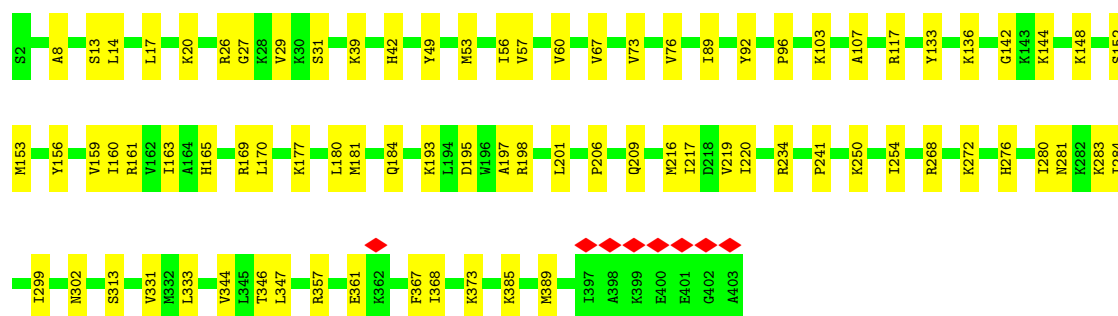
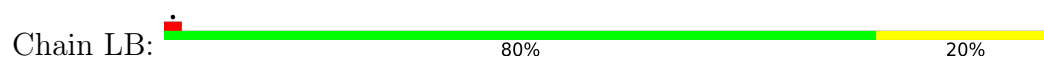




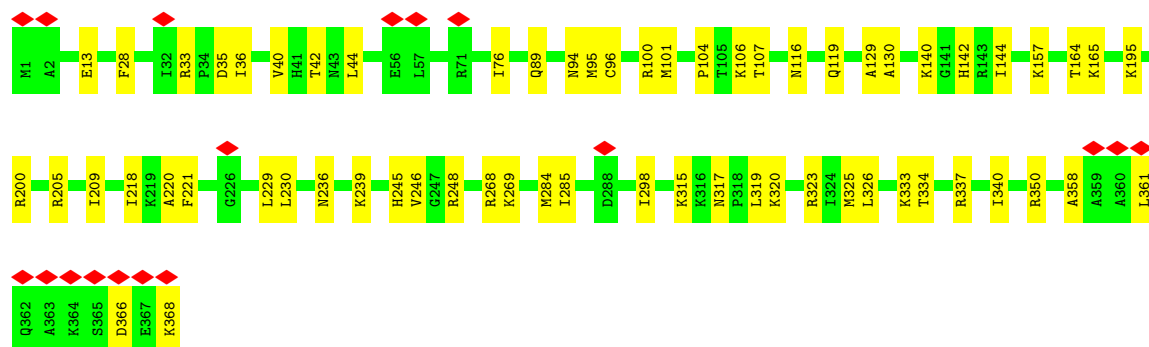
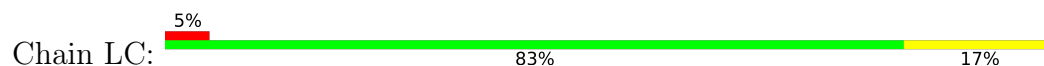
• Molecule 6: 60S ribosomal protein L8



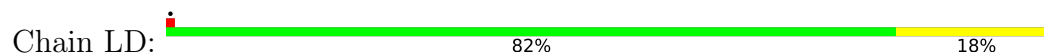
• Molecule 7: Large ribosomal subunit protein uL3



• Molecule 8: 60S ribosomal protein L4

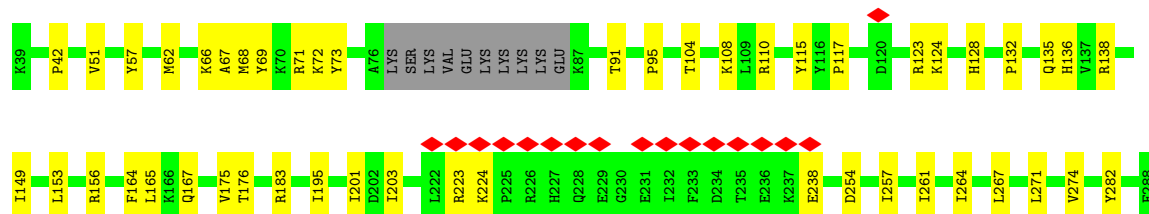
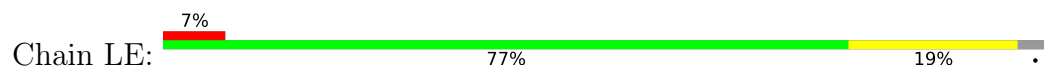


• Molecule 9: Large ribosomal subunit protein uL18

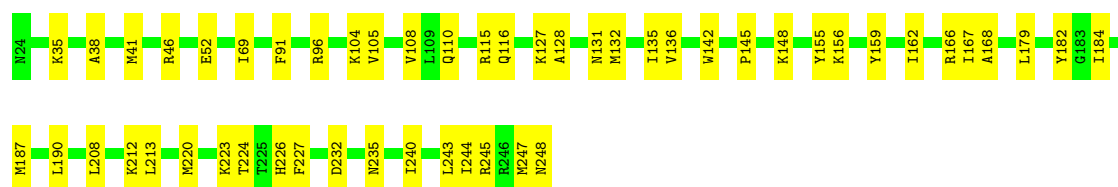
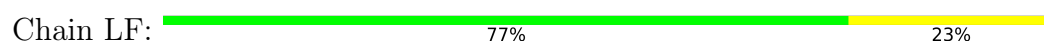




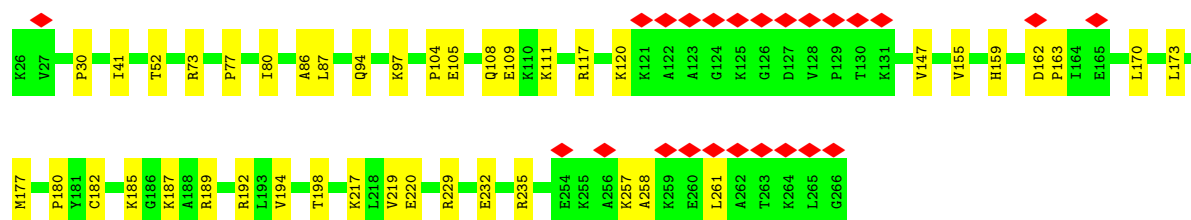
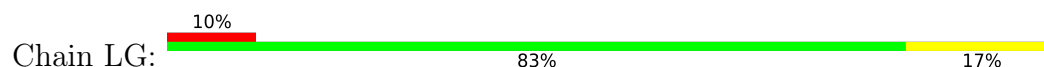
- Molecule 10: Large ribosomal subunit protein eL6



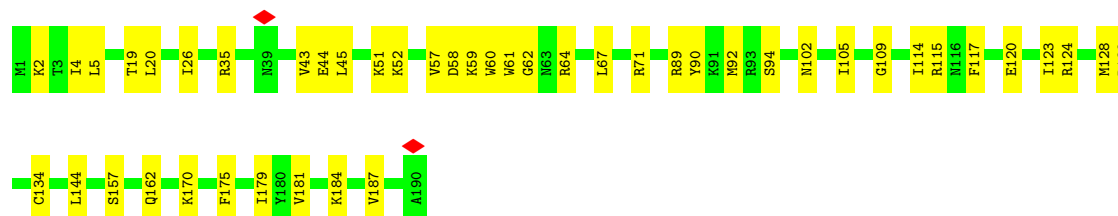
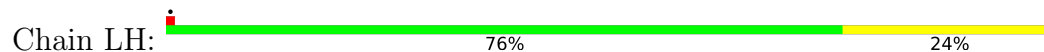
- Molecule 11: 60S ribosomal protein L7



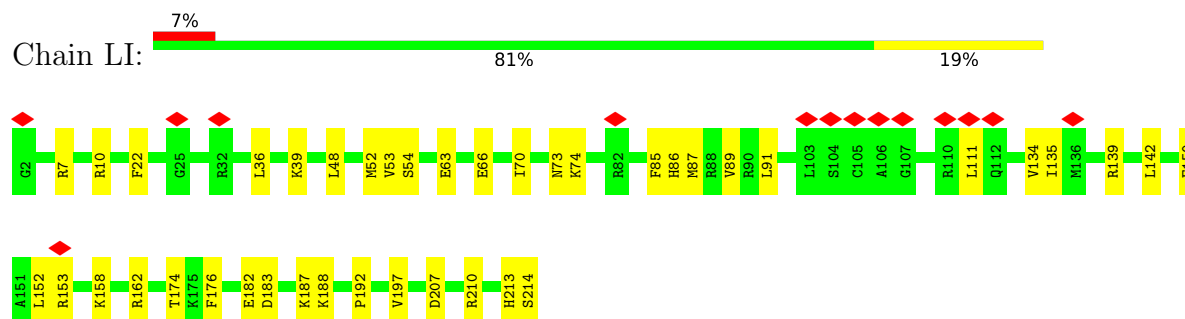
- Molecule 12: 60S ribosomal protein L7a



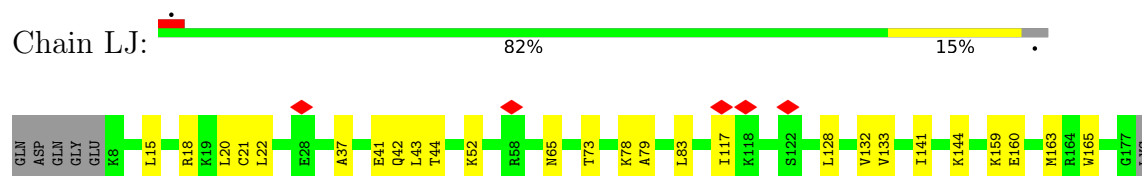
- Molecule 13: 60S ribosomal protein L9



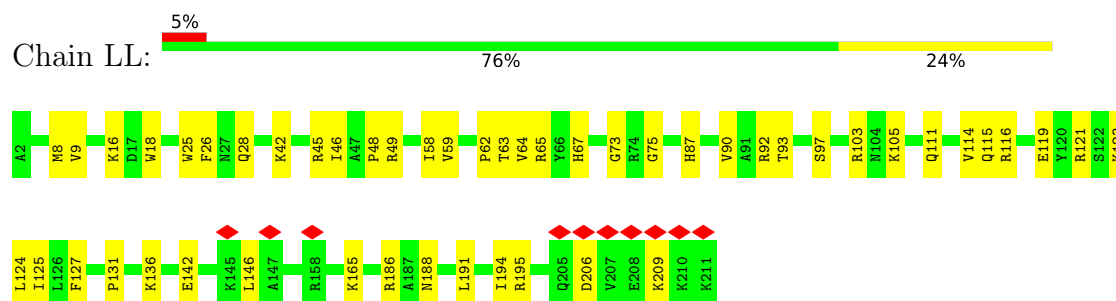
- Molecule 14: Ribosomal protein uL16-like



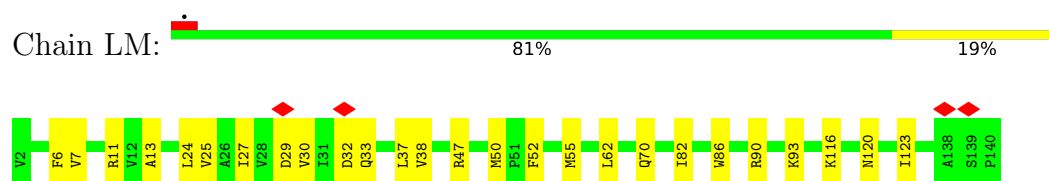
- Molecule 15: 60S ribosomal protein L11



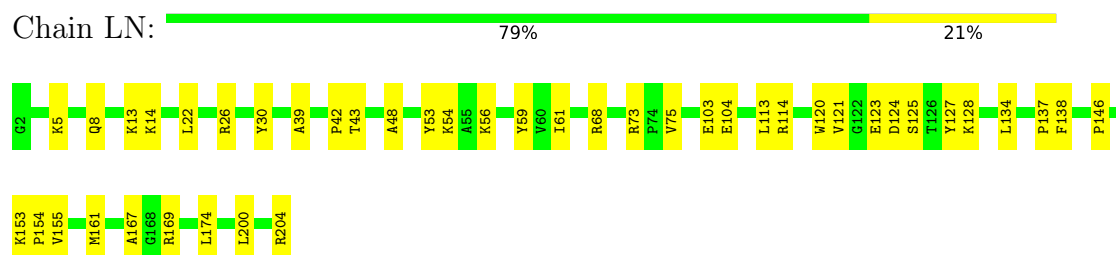
- Molecule 16: Large ribosomal subunit protein eL13



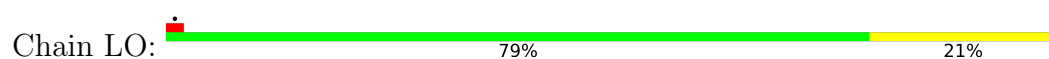
- Molecule 17: 60S ribosomal protein L14

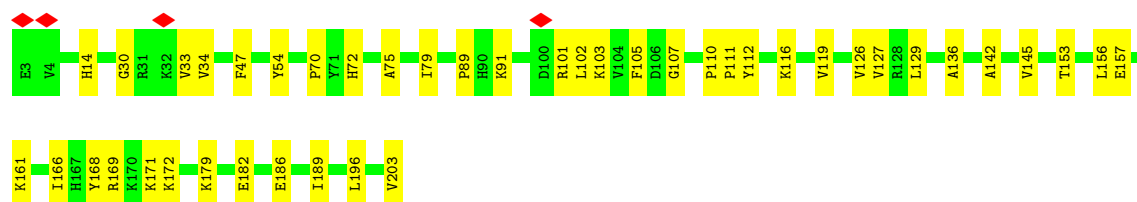


- Molecule 18: 60S ribosomal protein L15

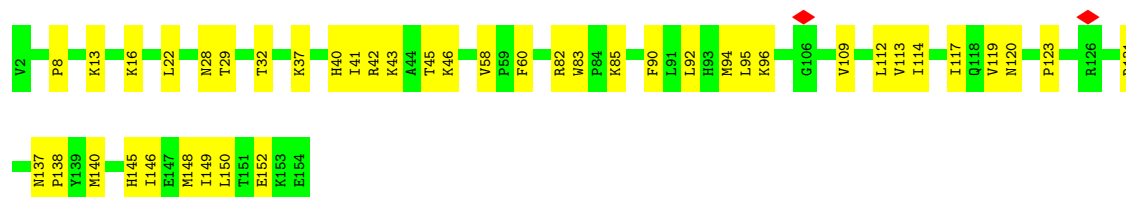
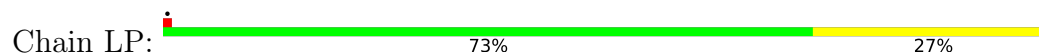


- Molecule 19: 60S ribosomal protein L13a

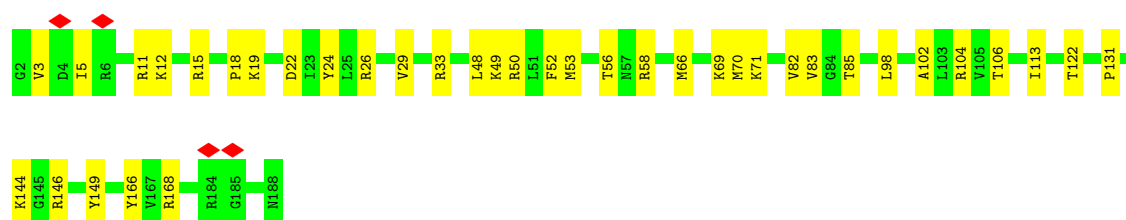
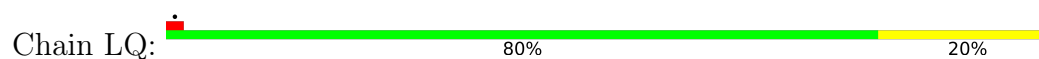




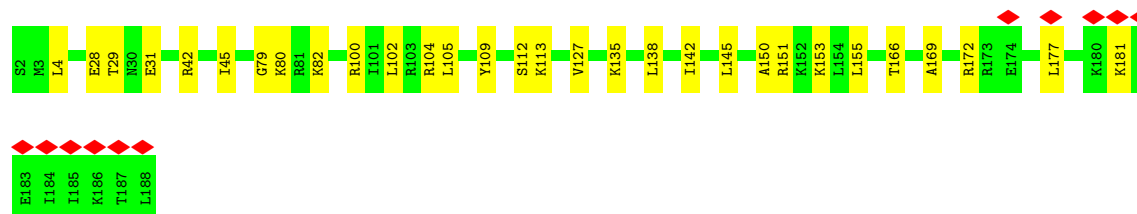
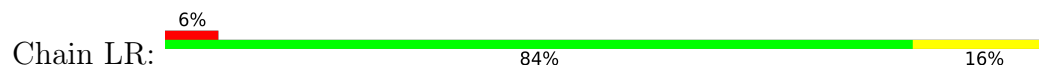
- Molecule 20: 60S ribosomal protein L17



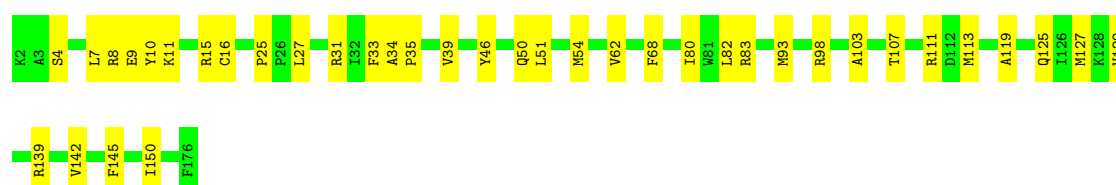
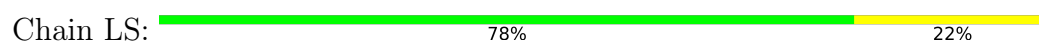
- Molecule 21: 60S ribosomal protein L18




- Molecule 22: 60S ribosomal protein L19




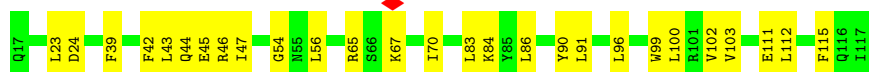
- Molecule 23: 60S ribosomal protein L18a




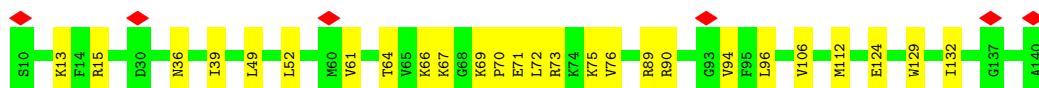
• Molecule 24: 60S ribosomal protein L21

Chain LT:  86% 14%


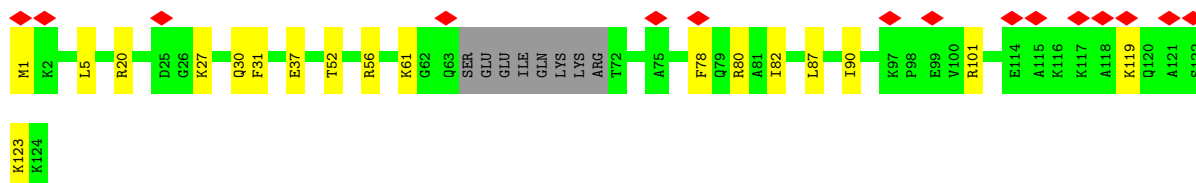
• Molecule 25: Heparin-binding protein HBp15

Chain LU:  73% 27%


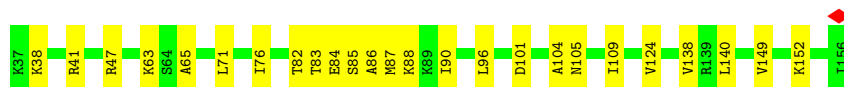
• Molecule 26: 60S ribosomal protein L23

Chain LV:  5% 80% 20%


• Molecule 27: Ribosomal protein L24

Chain LW:  12% 79% 15% 6%


• Molecule 28: 60S ribosomal protein L23a

Chain LX:  79% 21%

• Molecule 29: 60S ribosomal protein L26


Chain LY:  80% 20%

• Molecule 30: 60S ribosomal protein L27

Chain LZ:  79% 20%




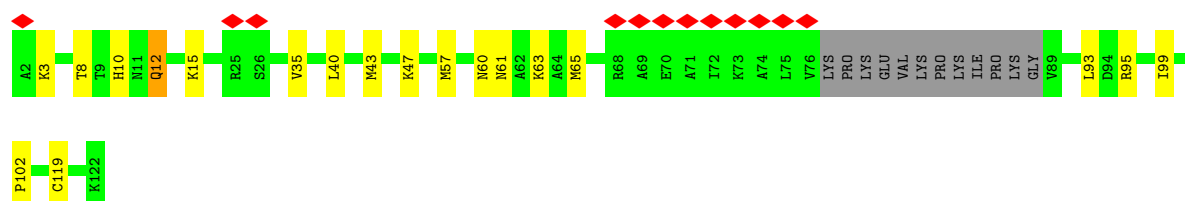
- Molecule 31: 60S ribosomal protein L27a

Chain La:  82% 18%




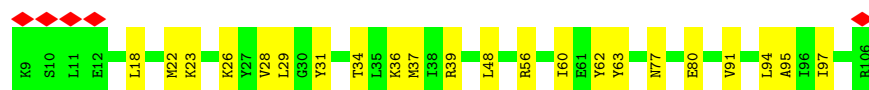
- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:  10% 74% 15% 10%



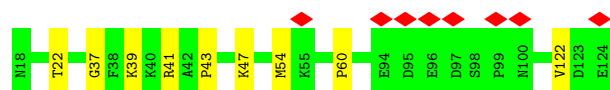
- Molecule 33: 60S ribosomal protein L30

Chain Lc:  5% 78% 22%



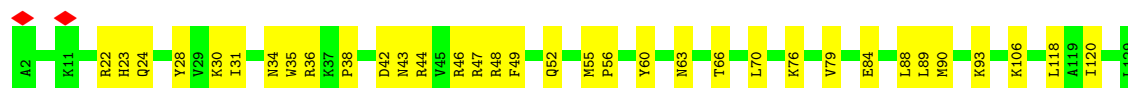
- Molecule 34: 60S ribosomal protein L31

Chain Ld:  7% 92% 8%




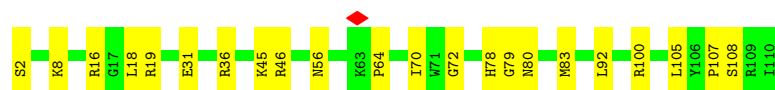
- Molecule 35: 60S ribosomal protein L32

Chain Le:  73% 27%

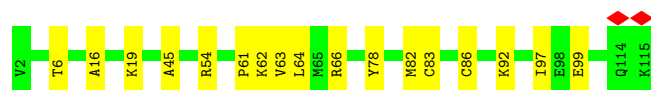
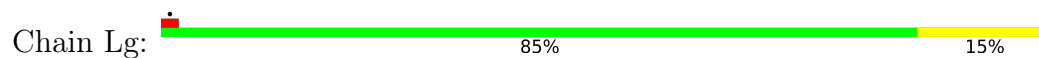


- Molecule 36: 60S ribosomal protein L35a

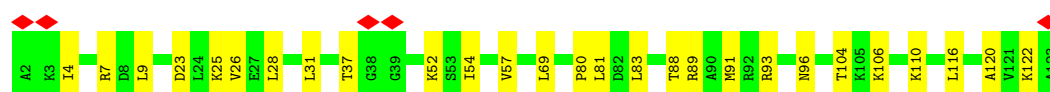
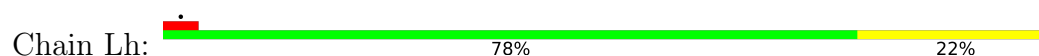
Chain Lf:  80% 20%



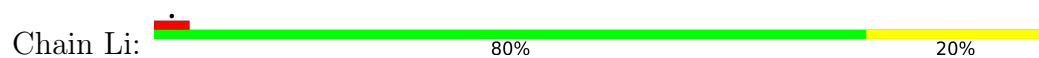
- Molecule 37: 60S ribosomal protein L34



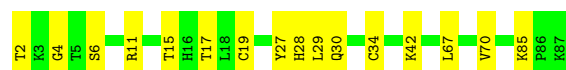
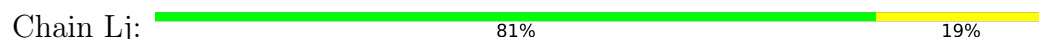
- Molecule 38: 60S ribosomal protein L35



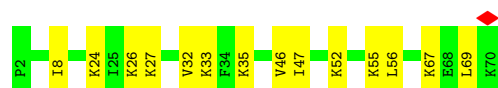
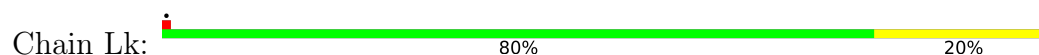
- Molecule 39: 60S ribosomal protein L36



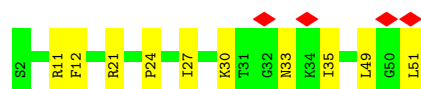
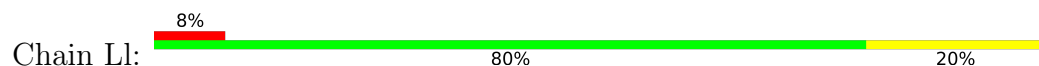
- Molecule 40: 60S ribosomal protein L37



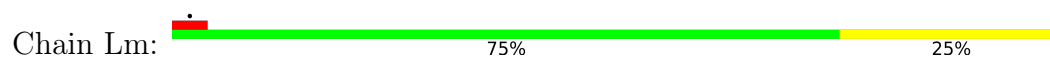
- Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein L39



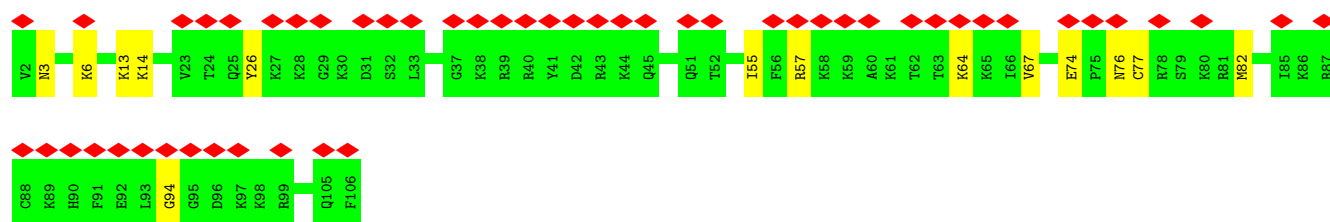
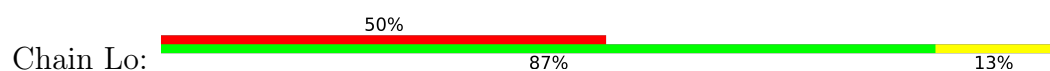
- Molecule 43: Large ribosomal subunit protein eL40



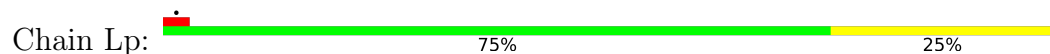
- Molecule 44: 60S ribosomal protein L41



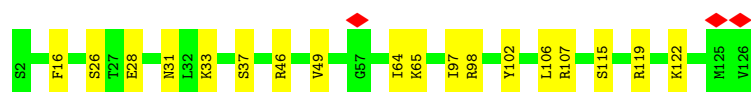
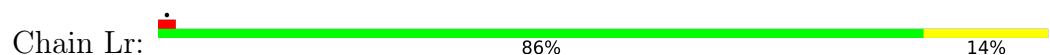
- Molecule 45: 60S ribosomal protein L36a



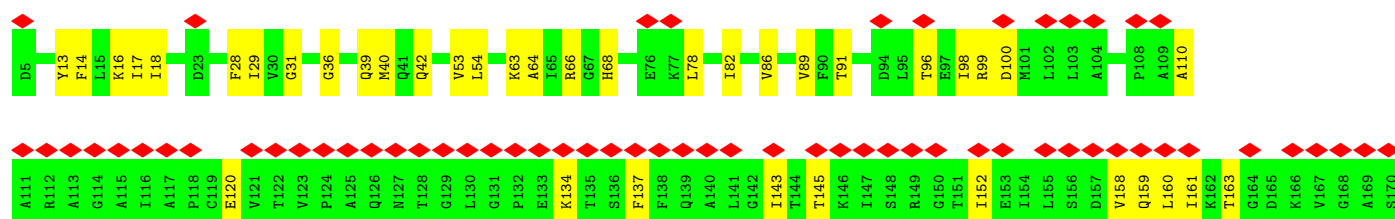
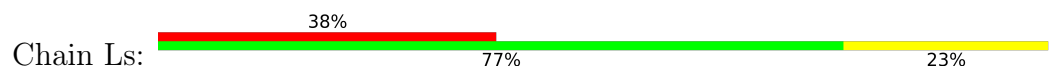
- Molecule 46: 60S ribosomal protein L37a

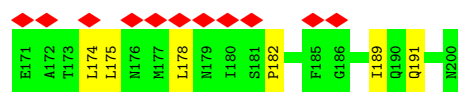


- Molecule 47: 60S ribosomal protein L28



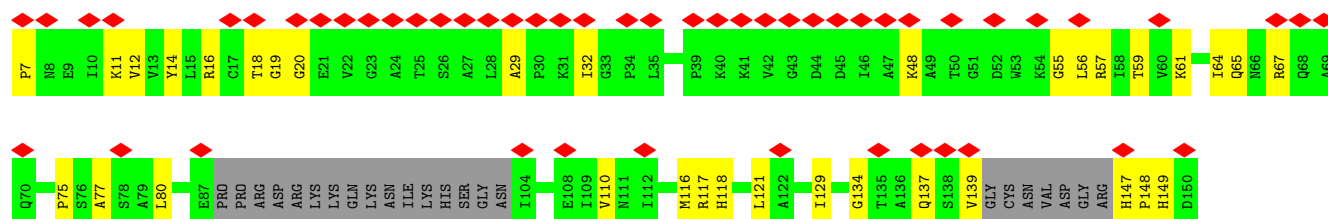
- Molecule 48: 60S acidic ribosomal protein P0





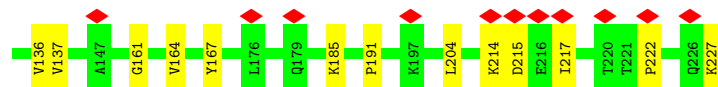
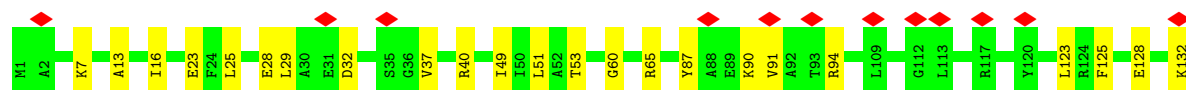
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt: 39% 63% 22% 15%



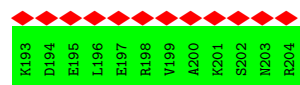
- Molecule 50: Small ribosomal subunit protein uS3

Chain SD: 10% 84% 16%



- Molecule 51: 40S ribosomal protein S5

Chain SF: 43% 83% 17%

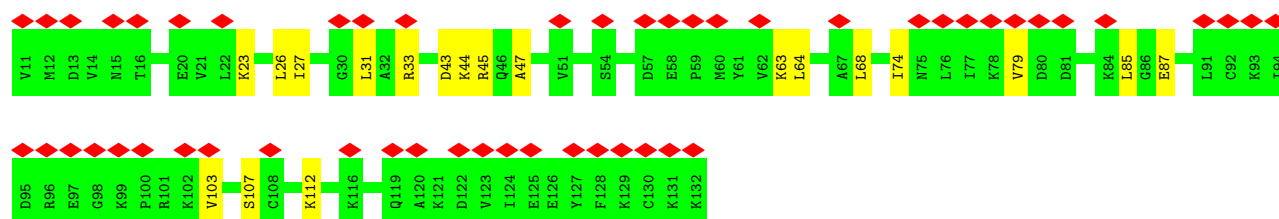
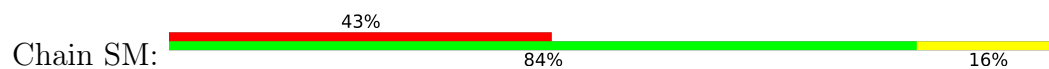


- Molecule 52: 40S ribosomal protein S10

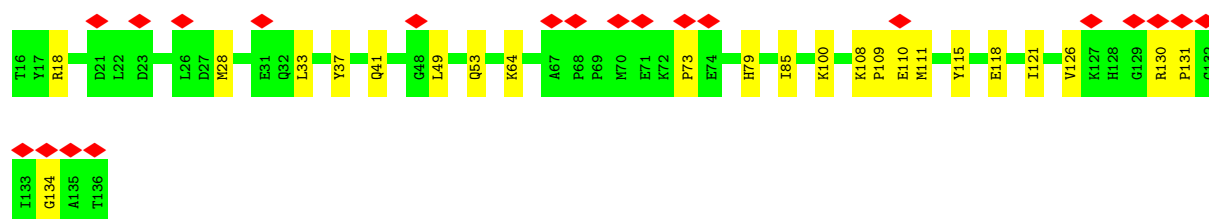
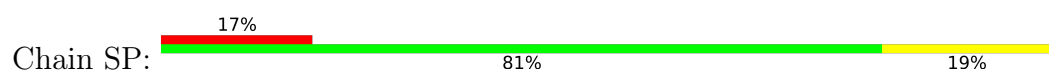
Chain SK: 15% 64% 36%



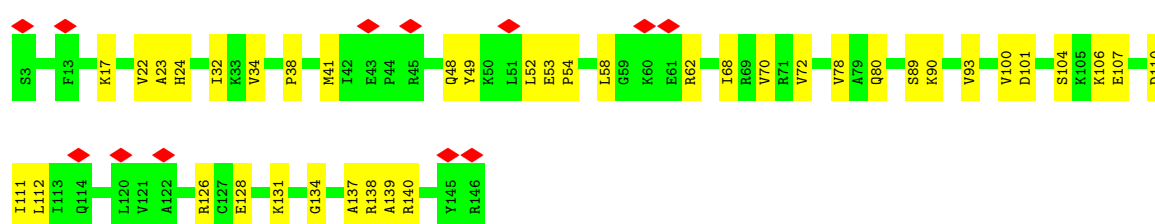
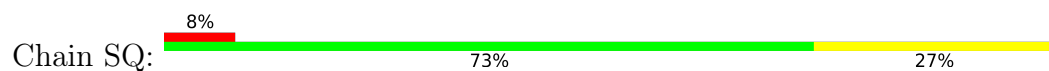
- Molecule 53: Small ribosomal subunit protein eS12



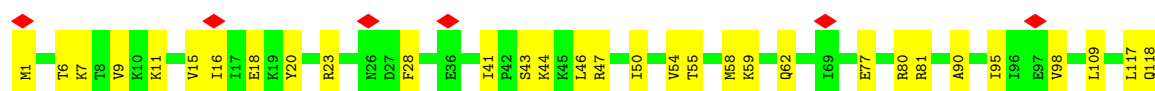
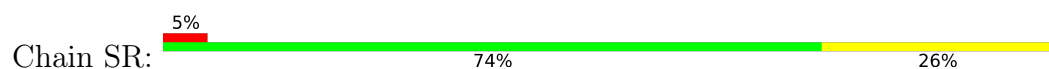
- Molecule 54: Small ribosomal subunit protein uS19

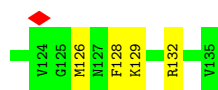


- Molecule 55: Small ribosomal subunit protein uS9

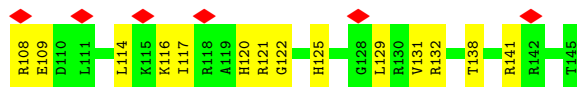
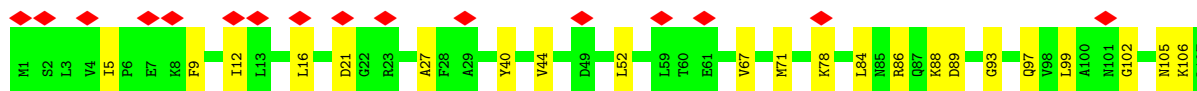
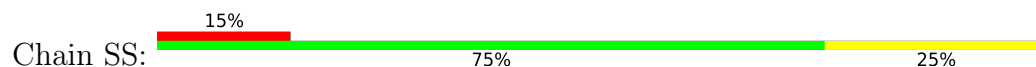


- Molecule 56: Small ribosomal subunit protein eS17

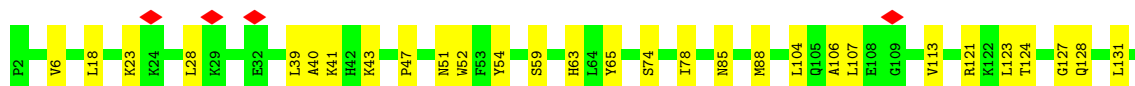
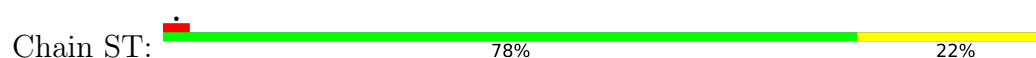




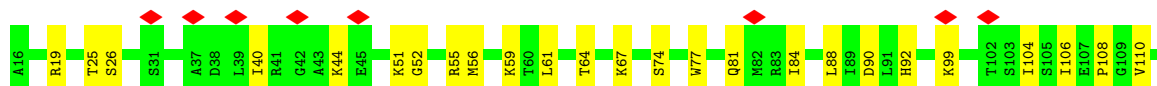
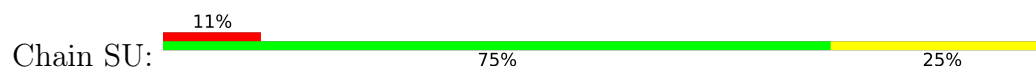
- Molecule 57: 40S ribosomal protein S18



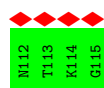
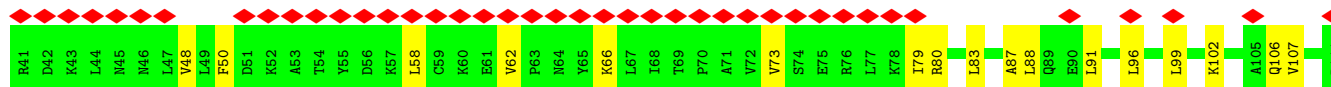
- Molecule 58: 40S ribosomal protein S19



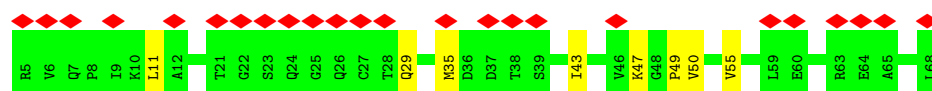
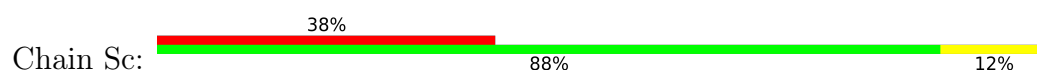
- Molecule 59: 40S ribosomal protein S20



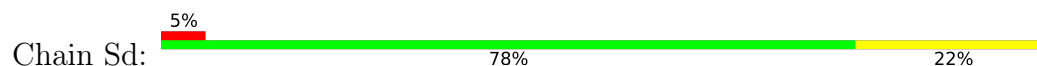
- Molecule 60: Small ribosomal subunit protein eS25



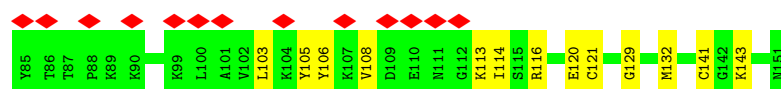
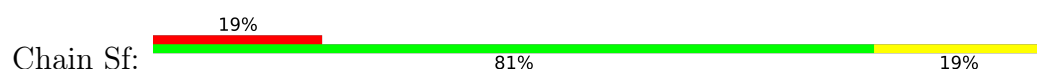
- Molecule 61: 40S ribosomal protein S28



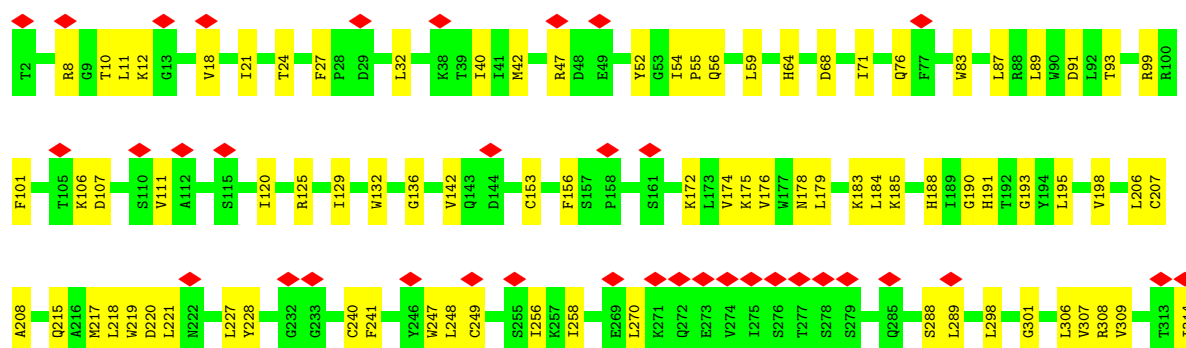
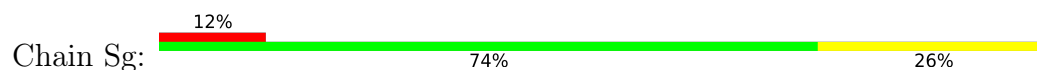
- Molecule 62: 40S ribosomal protein S29



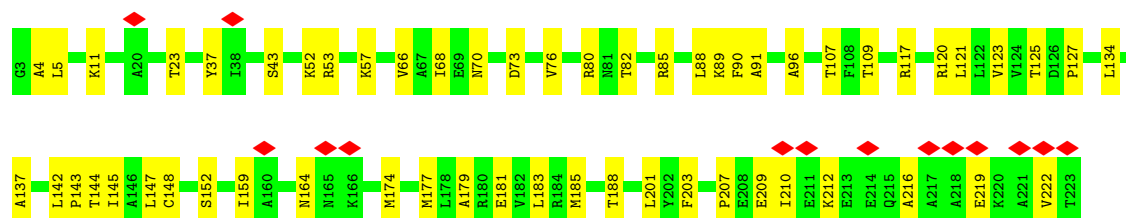
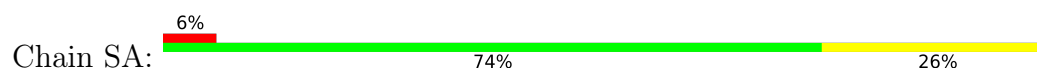
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



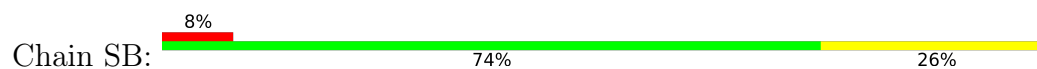
- Molecule 64: Receptor of activated protein C kinase 1

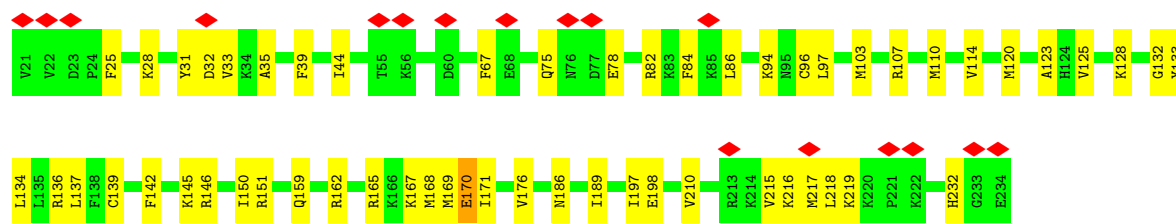


- Molecule 65: 40S ribosomal protein SA



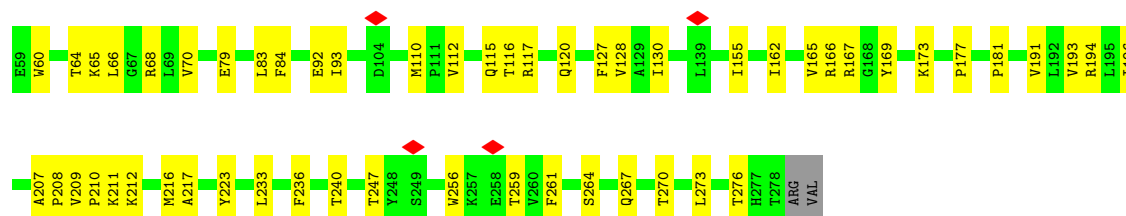
- Molecule 66: 40S ribosomal protein S3a





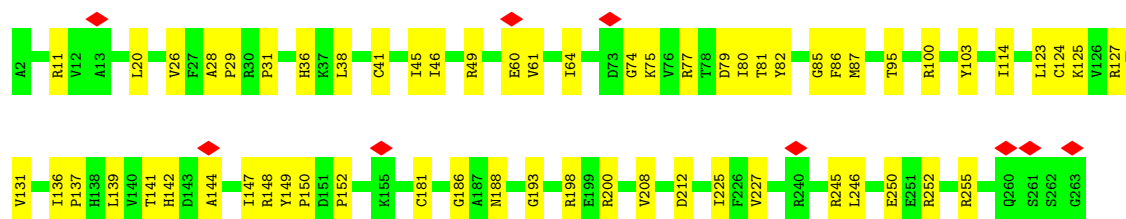
- Molecule 67: 40S ribosomal protein S2

Chain SC: 75% 24%



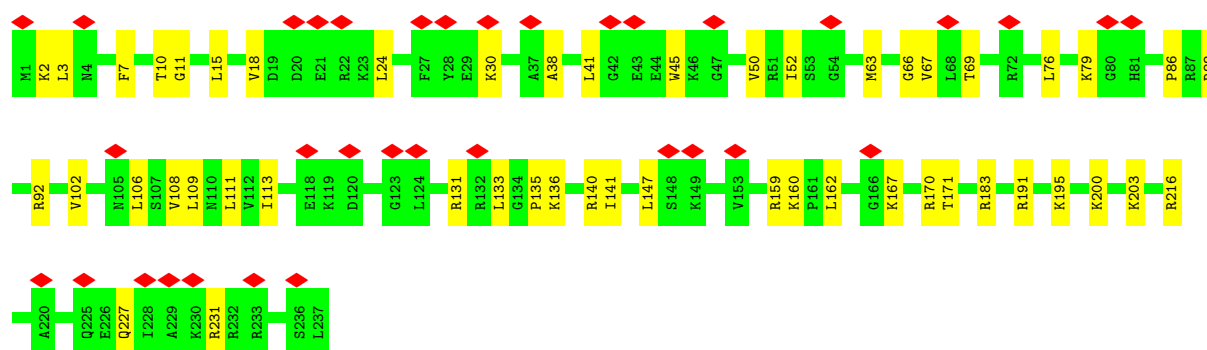
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

Chain SE: 77% 23%



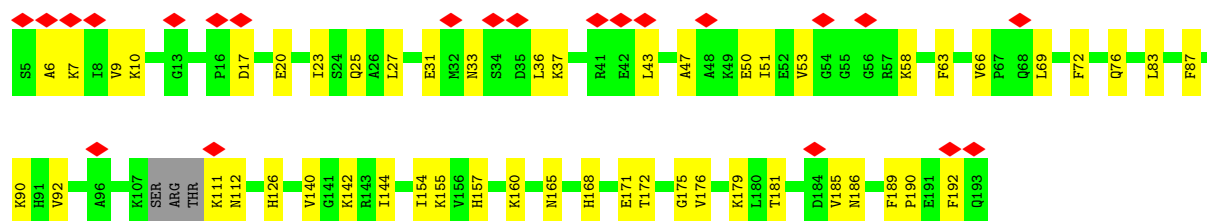
- Molecule 69: 40S ribosomal protein S6

Chain SG: 14% 79% 21%

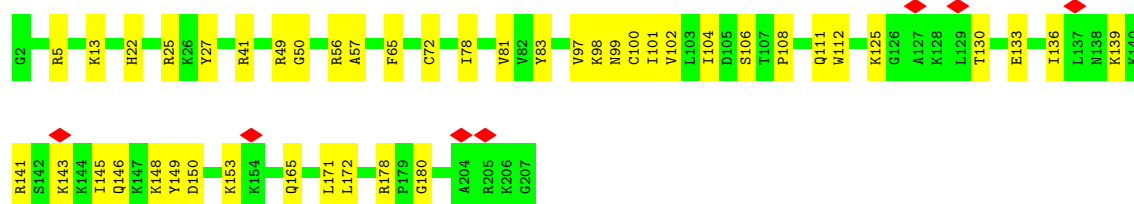
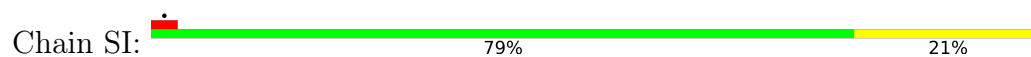


- Molecule 70: Small ribosomal subunit protein eS7

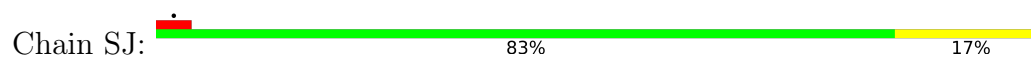
Chain SH: 12% 71% 27%



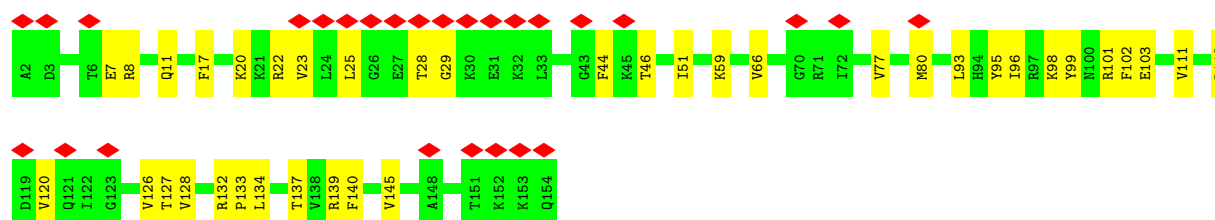
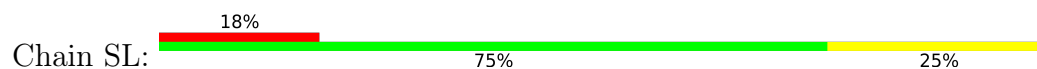
- Molecule 71: 40S ribosomal protein S8



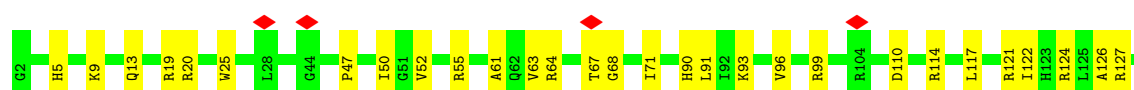
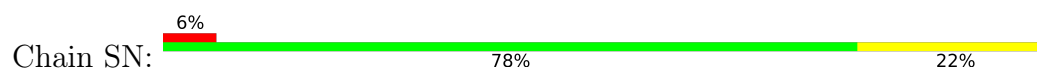
- Molecule 72: 40S ribosomal protein S9

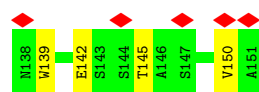


- Molecule 73: 40S ribosomal protein S11

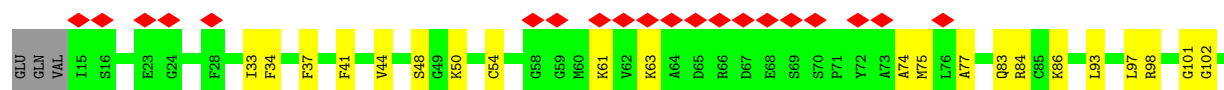
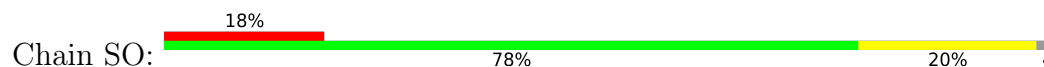


- Molecule 74: 40S ribosomal protein S13





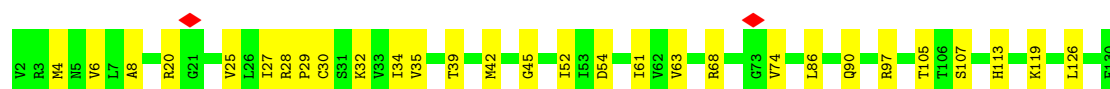
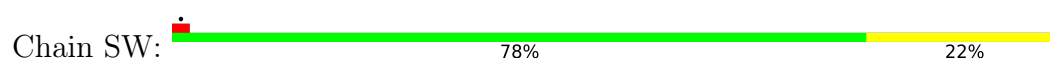
- Molecule 75: Small ribosomal subunit protein uS11



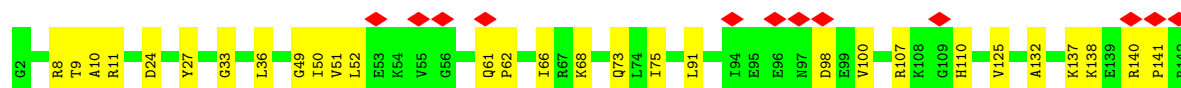
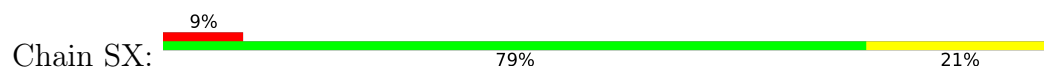
- Molecule 76: Small ribosomal subunit protein eS21



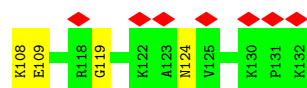
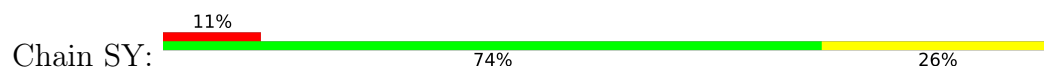
- Molecule 77: 40S ribosomal protein S15a



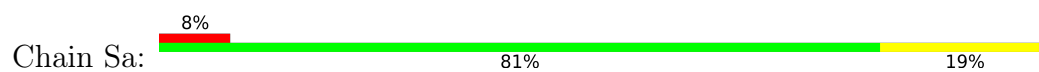
- Molecule 78: 40S ribosomal protein S23



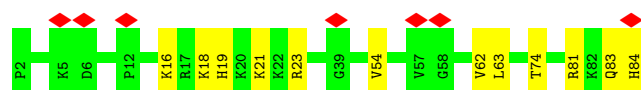
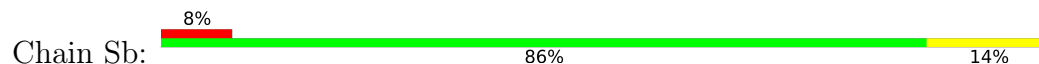
- Molecule 79: 40S ribosomal protein S24



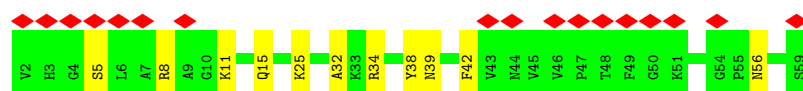
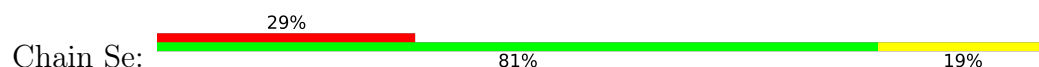
- Molecule 80: 40S ribosomal protein S26



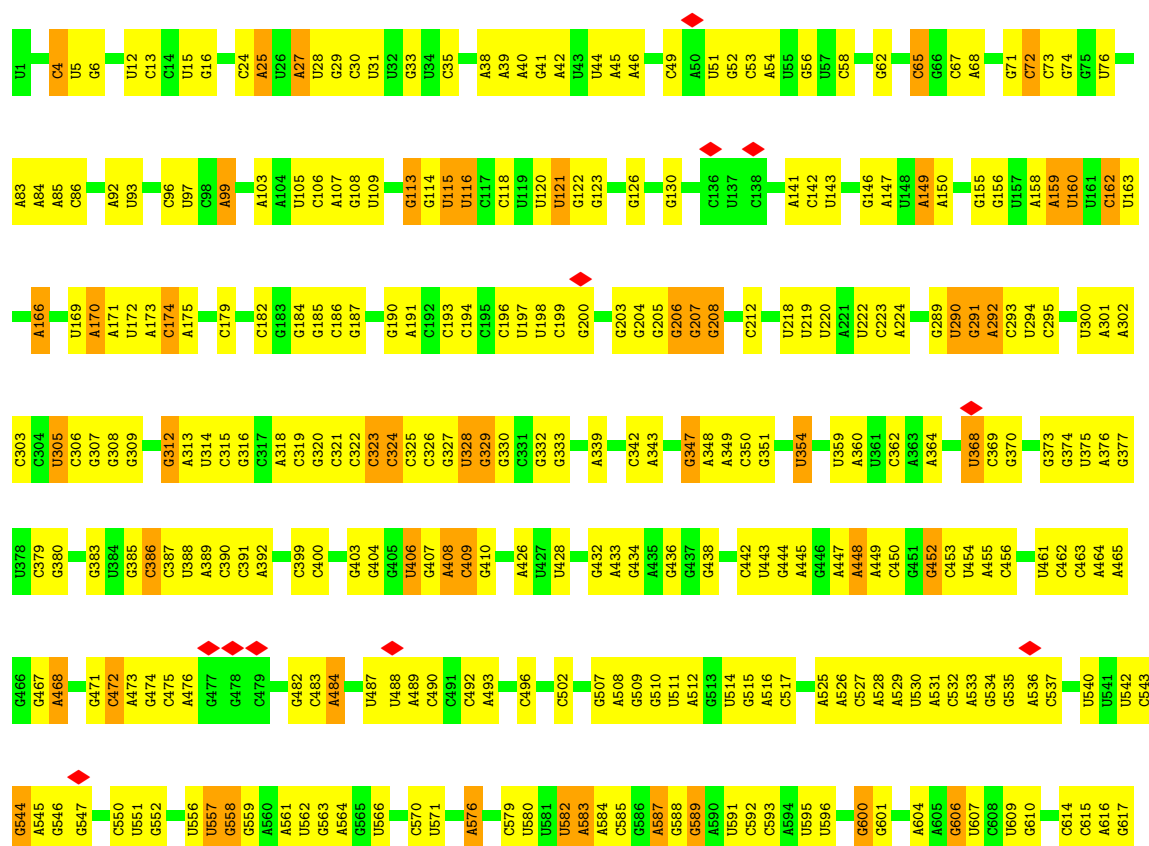
- Molecule 81: Small ribosomal subunit protein eS27

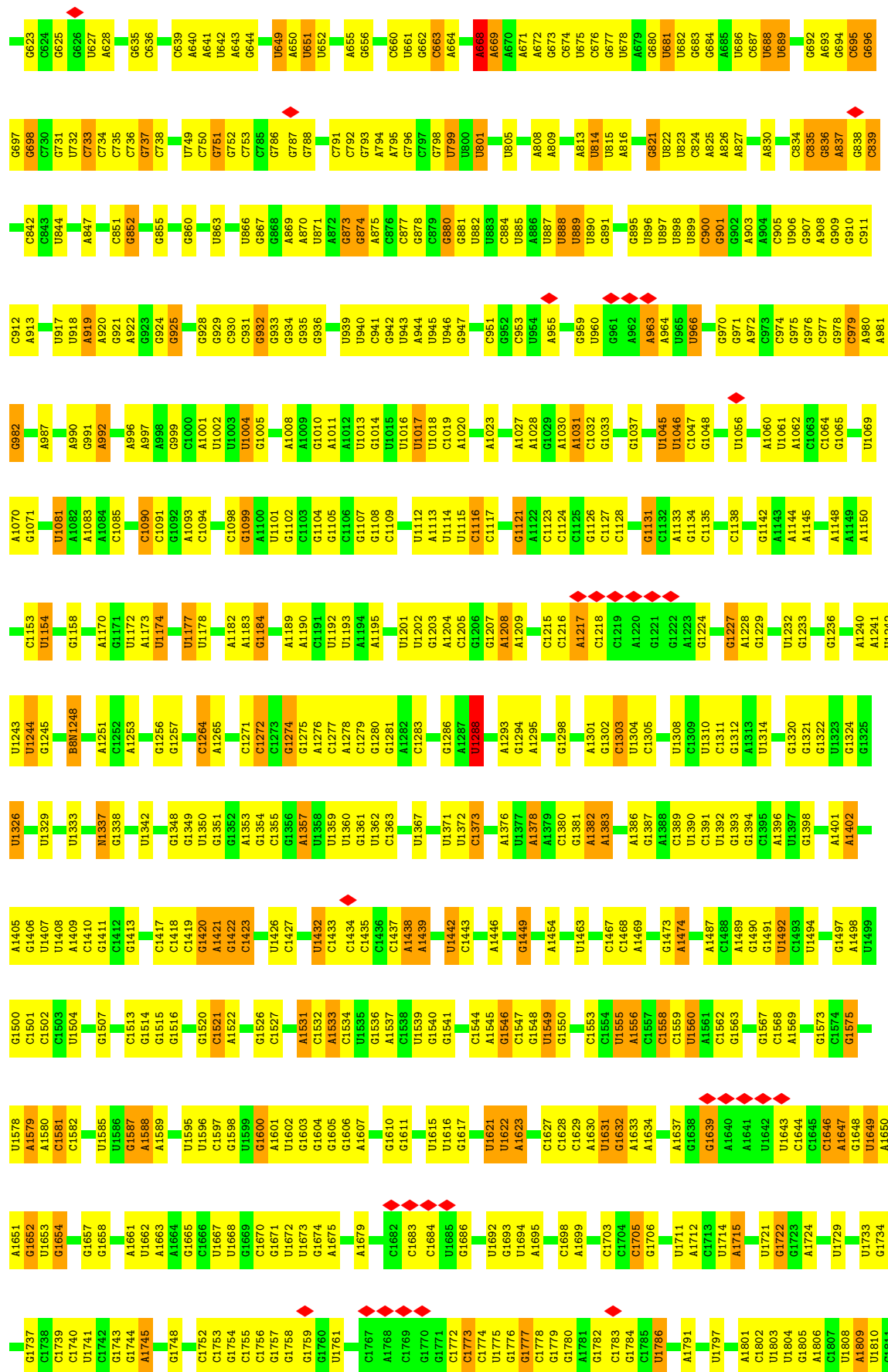


- Molecule 82: Small ribosomal subunit protein eS30



- Molecule 83: 18S rRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0108	Depositor
Map size (\AA)	512.64, 512.64, 512.64	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.89000005, 0.89000005, 0.89000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 1MA, UR3, SPM, OMG, SPD, 5MC, MA6, MG, OMU, G7M, UY1, 4AC, ZN, PSU, 6MZ, A2M, B8N

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	CI	0.13	0/247	0.34	0/323
2	Pt	0.14	0/1761	0.27	0/2741
3	L5	0.23	0/85072	0.31	0/132721
4	L7	0.21	0/2861	0.26	0/4459
5	L8	0.22	0/3631	0.30	0/5657
6	LA	0.24	0/1936	0.43	0/2596
7	LB	0.22	0/3306	0.42	0/4424
8	LC	0.23	0/2981	0.40	0/4002
9	LD	0.20	0/2428	0.40	0/3252
10	LE	0.20	0/1973	0.41	0/2645
11	LF	0.27	0/1905	0.44	0/2539
12	LG	0.21	0/1960	0.46	0/2637
13	LH	0.22	0/1537	0.45	0/2066
14	LI	0.22	0/1751	0.45	0/2340
15	LJ	0.18	0/1385	0.42	0/1852
16	LL	0.20	0/1732	0.37	0/2315
17	LM	0.22	0/1161	0.43	0/1554
18	LN	0.25	0/1746	0.41	0/2338
19	LO	0.24	0/1682	0.40	0/2250
20	LP	0.23	0/1268	0.46	0/1701
21	LQ	0.24	0/1537	0.42	0/2052
22	LR	0.21	0/1582	0.46	0/2091
23	LS	0.25	0/1493	0.43	0/2003
24	LT	0.20	0/1326	0.36	0/1770
25	LU	0.22	0/839	0.51	0/1126
26	LV	0.21	0/993	0.42	0/1332
27	LW	0.19	0/959	0.41	0/1270
28	LX	0.23	0/1002	0.39	0/1345
29	LY	0.24	0/1132	0.46	0/1504
30	LZ	0.21	0/1130	0.43	0/1507
31	La	0.21	0/1191	0.39	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.20	0/889	0.43	0/1175
33	Lc	0.21	0/774	0.45	0/1038
34	Ld	0.23	0/903	0.40	0/1216
35	Le	0.24	0/1071	0.47	0/1429
36	Lf	0.23	0/895	0.40	0/1198
37	Lg	0.20	0/916	0.39	0/1220
38	Lh	0.20	0/1023	0.48	0/1351
39	Li	0.20	0/843	0.44	0/1115
40	Lj	0.24	0/720	0.45	0/952
41	Lk	0.19	0/575	0.42	0/761
42	Ll	0.20	0/454	0.38	0/599
43	Lm	0.22	0/435	0.44	0/575
44	Ln	0.20	0/231	0.39	0/294
45	Lo	0.17	0/876	0.37	0/1156
46	Lp	0.24	0/718	0.48	0/953
47	Lr	0.24	0/1017	0.41	0/1364
48	Ls	0.16	0/1519	0.41	0/2052
49	Lt	0.18	0/1009	0.53	0/1363
50	SD	0.14	0/1793	0.36	0/2414
51	SF	0.16	0/1516	0.41	0/2037
52	SK	0.16	0/851	0.40	0/1147
53	SM	0.16	0/950	0.43	0/1275
54	SP	0.16	0/1003	0.45	0/1342
55	SQ	0.16	0/1160	0.43	0/1553
56	SR	0.16	0/1105	0.43	0/1484
57	SS	0.17	0/1216	0.48	0/1628
58	ST	0.16	0/1131	0.39	0/1515
59	SU	0.16	0/831	0.42	0/1115
60	SZ	0.18	0/604	0.47	0/810
61	Sc	0.15	0/508	0.41	0/680
62	Sd	0.16	0/470	0.41	0/623
63	Sf	0.18	0/560	0.51	0/745
64	Sg	0.15	0/2493	0.39	0/3394
65	SA	0.18	0/1778	0.41	0/2416
66	SB	0.17	0/1765	0.42	0/2362
67	SC	0.17	0/1744	0.42	0/2357
68	SE	0.16	0/2118	0.38	0/2849
69	SG	0.15	0/1946	0.40	0/2590
70	SH	0.18	0/1519	0.45	0/2033
71	SI	0.17	0/1715	0.44	0/2287
72	SJ	0.15	0/1550	0.38	0/2069
73	SL	0.17	0/1268	0.40	0/1696
74	SN	0.18	0/1232	0.36	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SO	0.18	0/1037	0.41	0/1391
76	SV	0.18	0/643	0.41	0/860
77	SW	0.17	0/1051	0.39	0/1406
78	SX	0.19	0/1116	0.46	0/1490
79	SY	0.16	0/1083	0.41	0/1438
80	Sa	0.16	0/836	0.36	0/1121
81	Sb	0.16	0/665	0.40	0/891
82	Se	0.15	0/465	0.44	0/612
83	S2	0.20	3/39756 (0.0%)	0.30	0/61939
All	All	0.21	3/229853 (0.0%)	0.36	0/337039

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1288	OMU	O3'-P	5.16	1.61	1.56
83	S2	1639	G7M	O3'-P	5.09	1.61	1.56
83	S2	1326	OMU	O3'-P	5.01	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	3	0
2	Pt	1576	0	803	29	0
3	L5	78421	0	39705	971	0
4	L7	2561	0	1295	25	0
5	L8	3315	0	1685	49	0
6	LA	1898	0	1993	41	0
7	LB	3238	0	3376	56	0
8	LC	2927	0	3104	50	0
9	LD	2382	0	2410	36	0
10	LE	1935	0	2096	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	LF	1870	0	1996	32	0
12	LG	1927	0	2074	28	0
13	LH	1518	0	1601	28	0
14	LI	1711	0	1749	28	0
15	LJ	1362	0	1399	14	0
16	LL	1701	0	1818	36	0
17	LM	1138	0	1204	20	0
18	LN	1701	0	1749	31	0
19	LO	1650	0	1794	29	0
20	LP	1242	0	1269	28	0
21	LQ	1513	0	1628	32	0
22	LR	1566	0	1729	21	0
23	LS	1453	0	1490	28	0
24	LT	1298	0	1366	17	0
25	LU	825	0	850	17	0
26	LV	979	0	1039	19	0
27	LW	945	0	1003	15	0
28	LX	985	0	1066	21	0
29	LY	1115	0	1205	20	0
30	LZ	1107	0	1182	19	0
31	La	1162	0	1213	19	0
32	Lb	876	0	948	15	0
33	Lc	764	0	804	13	0
34	Ld	888	0	930	5	0
35	Le	1053	0	1147	24	0
36	Lf	876	0	912	15	0
37	Lg	906	0	998	13	0
38	Lh	1015	0	1148	21	0
39	Li	832	0	917	16	0
40	Lj	705	0	737	13	0
41	Lk	569	0	637	9	0
42	Ll	444	0	483	7	0
43	Lm	429	0	465	12	0
44	Ln	230	0	276	7	0
45	Lo	862	0	929	9	0
46	Lp	708	0	756	20	0
47	Lr	1002	0	1068	16	0
48	Ls	1496	0	1540	27	0
49	Lt	998	0	1032	26	0
50	SD	1765	0	1865	25	0
51	SF	1495	0	1549	25	0
52	SK	827	0	854	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	SM	940	0	965	13	0
54	SP	985	0	1031	18	0
55	SQ	1142	0	1213	27	0
56	SR	1090	0	1149	23	0
57	SS	1198	0	1261	25	0
58	ST	1112	0	1146	21	0
59	SU	821	0	883	19	0
60	SZ	598	0	656	15	0
61	Sc	506	0	536	6	0
62	Sd	459	0	452	11	0
63	Sf	548	0	551	9	0
64	Sg	2436	0	2393	53	0
65	SA	1741	0	1746	38	0
66	SB	1738	0	1809	44	0
67	SC	1707	0	1791	40	0
68	SE	2076	0	2177	40	0
69	SG	1923	0	2089	36	0
70	SH	1497	0	1590	33	0
71	SI	1686	0	1772	35	0
72	SJ	1525	0	1640	22	0
73	SL	1247	0	1323	28	0
74	SN	1208	0	1294	21	0
75	SO	1024	0	1050	21	0
76	SV	636	0	637	21	0
77	SW	1034	0	1080	22	0
78	SX	1098	0	1167	20	0
79	SY	1065	0	1142	26	0
80	Sa	821	0	870	12	0
81	Sb	651	0	672	10	0
82	Se	459	0	503	10	0
83	S2	36953	0	18679	568	0
84	L5	181	0	0	0	0
84	L7	2	0	0	0	0
84	L8	4	0	0	0	0
84	LA	1	0	0	0	0
84	LV	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lj	1	0	0	0	0
84	S2	27	0	0	0	0
84	Sa	1	0	0	0	0
85	L5	98	0	182	7	0
86	L5	80	0	152	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L8	10	0	19	0	0
86	LN	10	0	19	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Sa	1	0	0	0	0
All	All	218355	0	162808	3048	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3048) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2845:A:H61	3:L5:3843:C:N4	1.53	1.04
3:L5:2845:A:N6	3:L5:3843:C:H42	1.56	1.03
3:L5:1095:A:H2	3:L5:1200:G:H1	1.14	0.96
83:S2:1324:G:H1	83:S2:1504:U:H3	1.14	0.95
3:L5:1100:U:H3	3:L5:1194:G:H1	0.95	0.95
3:L5:184:U:H3	3:L5:253:G:H1	1.05	0.95
3:L5:3946:G:H1	3:L5:4067:U:H3	1.18	0.92
3:L5:2557:G:H1	3:L5:2570:U:H3	0.99	0.91
3:L5:4887:C:H42	3:L5:4932:U:H3	1.16	0.90
83:S2:1351:G:H1	83:S2:1360:U:H3	1.13	0.90
83:S2:1652:G:H1	83:S2:1672:U:H3	0.90	0.90
3:L5:3944:G:H1	3:L5:4069:U:H3	1.21	0.86
9:LD:34:LYS:HG2	24:LT:27:LEU:HD21	1.58	0.85
18:LN:13:LYS:HZ1	39:Li:45:ARG:HE	1.25	0.85
3:L5:1095:A:C2	3:L5:1200:G:N1	2.43	0.85
3:L5:3929:G:H1	3:L5:4181:U:H3	1.23	0.85
3:L5:512:U:H3	3:L5:647:G:H1	0.85	0.83
68:SE:252:ARG:HA	68:SE:255:ARG:HE	1.41	0.83
8:LC:326:LEU:HD21	8:LC:333:LYS:HB2	1.62	0.82
17:LM:7:VAL:HG23	17:LM:27:ILE:HD13	1.61	0.81
67:SC:117:ARG:HH11	83:S2:1204:A:H5''	1.43	0.81
83:S2:1533:A:H62	83:S2:1602:U:H3	1.26	0.81
2:Pt:50:U:H3	2:Pt:64:G:H1	0.82	0.81
3:L5:184:U:O2	3:L5:253:G:N2	2.14	0.80
69:SG:183:ARG:HH12	83:S2:316:G:H5''	1.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:677:G:H21	83:S2:1028:A:H62	1.29	0.80
3:L5:4093:G:N2	3:L5:4114:C:O2	2.13	0.80
68:SE:198:ARG:HH11	68:SE:200:ARG:HD2	1.46	0.80
3:L5:3754:G:H1	3:L5:3770:U:H3	1.31	0.78
50:SD:51:LEU:HD12	50:SD:91:VAL:HG12	1.65	0.78
8:LC:116:ASN:HD22	8:LC:119:GLN:HE22	1.28	0.78
83:S2:600:G:H2'	83:S2:601:OMG:H8	1.49	0.77
43:Lm:103:LEU:HD21	43:Lm:110:CYS:HA	1.67	0.77
70:SH:6:ALA:H	70:SH:25:GLN:HE21	1.33	0.77
43:Lm:111:ARG:HG3	43:Lm:112:LYS:HG3	1.67	0.77
4:L7:2:U:H3	4:L7:117:G:H1	1.30	0.76
21:LQ:50:ARG:HB3	21:LQ:83:VAL:HG11	1.66	0.76
83:S2:1729:U:H3	83:S2:1805:G:H1	1.32	0.76
83:S2:928:G:H2'	83:S2:929:G:C8	2.21	0.75
3:L5:1952:G:H4'	23:LS:93:MET:HG3	1.68	0.75
3:L5:5002:U:H3	3:L5:5045:G:H1	1.34	0.75
83:S2:924:G:H1	83:S2:1018:U:H3	1.32	0.75
56:SR:41:ILE:HG21	56:SR:47:ARG:HB2	1.68	0.74
3:L5:2609:G:H1	3:L5:2730:U:H3	1.35	0.74
83:S2:1657:G:H1	83:S2:1667:U:H3	1.34	0.74
83:S2:1607:A:H62	83:S2:1632:G:N2	1.85	0.74
22:LR:155:LEU:HD11	73:SL:118:ARG:HH21	1.52	0.73
3:L5:310:G:H5''	39:Li:85:ARG:HH12	1.53	0.73
3:L5:513:U:H1'	3:L5:516:C:H41	1.52	0.73
10:LE:117:PRO:HB2	35:Le:93:LYS:HZ3	1.53	0.73
3:L5:4139:G:H21	3:L5:4140:C:H41	1.37	0.72
3:L5:4162:C:H5	12:LG:73:ARG:HH12	1.37	0.72
13:LH:114:ILE:HB	13:LH:124:ARG:HB2	1.71	0.72
55:SQ:23:ALA:HB1	55:SQ:68:ILE:HD11	1.71	0.72
66:SB:123:ALA:HB1	66:SB:169:MET:HE3	1.72	0.72
23:LS:34:ALA:HB1	23:LS:39:VAL:HG23	1.71	0.72
3:L5:1095:A:H2	3:L5:1200:G:N1	1.83	0.72
3:L5:665:C:H4'	3:L5:666:G:H5'	1.70	0.72
3:L5:4407:G:H1	3:L5:4435:U:H3	1.37	0.72
3:L5:4887:C:N4	3:L5:4932:U:H3	1.86	0.72
7:LB:57:VAL:HB	7:LB:367:PHE:HB3	1.72	0.72
3:L5:5024:C:H41	3:L5:5028:G:H21	1.38	0.71
64:Sg:247:TRP:HB3	64:Sg:258:ILE:HD11	1.72	0.71
69:SG:11:GLY:HA2	83:S2:166:A2M:HM'1	1.73	0.71
73:SL:20:LYS:HE3	73:SL:22:ARG:HH12	1.56	0.71
3:L5:3946:G:N2	3:L5:4067:U:O2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.73	0.70
3:L5:121:A:H62	3:L5:152:U:H3	1.37	0.70
83:S2:928:G:H1	83:S2:1013:U:H3	1.35	0.70
3:L5:1996:C:H42	3:L5:2000:G:N2	1.89	0.70
17:LM:116:LYS:HD3	19:LO:196:LEU:HD21	1.72	0.70
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.57	0.70
55:SQ:131:LYS:HB2	55:SQ:140:ARG:HH22	1.57	0.70
3:L5:2845:A:H61	3:L5:3843:C:H42	0.77	0.70
83:S2:1653:U:H3	83:S2:1671:G:H1	1.39	0.70
59:SU:52:GLY:HA3	83:S2:1401:A:H4'	1.74	0.70
21:LQ:98:LEU:HB2	21:LQ:113:ILE:HD11	1.72	0.70
83:S2:49:C:H2'	83:S2:472:C:H41	1.55	0.70
3:L5:1996:C:H42	3:L5:2000:G:H22	1.38	0.69
37:Lg:78:TYR:HB3	37:Lg:82:MET:HB3	1.72	0.69
3:L5:1095:A:N1	3:L5:1200:G:O6	2.25	0.69
83:S2:1841:C:H2'	83:S2:1842:4AC:H6	1.73	0.69
3:L5:2353:U:H5''	8:LC:89:GLN:HG2	1.73	0.69
76:SV:2:GLN:H	76:SV:8:PHE:HA	1.55	0.69
83:S2:1417:C:H42	83:S2:1422:G:H22	1.40	0.69
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.57	0.69
62:Sd:22:ARG:HG2	62:Sd:38:MET:HB3	1.74	0.69
71:SI:81:VAL:HG12	71:SI:102:VAL:HG12	1.74	0.69
3:L5:4926:C:H5''	3:L5:4927:G:H21	1.57	0.69
10:LE:136:HIS:HB2	10:LE:138:ARG:HH12	1.58	0.69
35:Le:90:MET:HG3	47:Lr:33:LYS:HA	1.74	0.69
83:S2:1112:U:O2	83:S2:1121:G:O6	2.11	0.69
3:L5:1348:U:H2'	3:L5:1349:G:H8	1.58	0.68
3:L5:1094:G:O6	3:L5:1201:U:O2	2.11	0.68
79:SY:43:LYS:HG2	79:SY:47:MET:HE1	1.74	0.68
85:L5:5291:SPM:H112	19:LO:91:LYS:HD3	1.75	0.68
31:La:102:ASP:HA	31:La:125:LYS:HB2	1.75	0.68
41:Lk:24:LYS:HZ3	41:Lk:67:LYS:HD2	1.57	0.68
3:L5:1435:G:N2	3:L5:1449:C:O2	2.19	0.68
3:L5:1351:G:H1'	8:LC:119:GLN:HE21	1.59	0.68
3:L5:2554:U:O2	3:L5:2764:A:N7	2.27	0.68
67:SC:191:VAL:HG11	67:SC:236:PHE:HA	1.75	0.68
70:SH:83:LEU:HB3	70:SH:92:VAL:HG21	1.76	0.68
83:S2:1829:G:H1'	83:S2:1850:MA6:H2	1.76	0.68
3:L5:1969:G:H4'	48:Ls:36:GLY:HA2	1.75	0.67
29:LY:10:ASP:HB3	29:LY:13:LYS:HB2	1.75	0.67
41:Lk:52:LYS:HA	41:Lk:55:LYS:HG2	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2608:G:H5'	22:LR:100:ARG:HH22	1.58	0.67
55:SQ:139:ALA:HB2	83:S2:1650:A:H5''	1.76	0.67
78:SX:9:THR:HG22	83:S2:681:PSU:H4'	1.76	0.67
71:SI:22:HIS:HB3	83:S2:433:A:H5''	1.77	0.67
3:L5:3930:U:H3	3:L5:4180:G:H1	1.40	0.67
3:L5:4126:C:H5''	3:L5:4127:A:H5''	1.75	0.67
7:LB:57:VAL:HG22	7:LB:73:VAL:HG22	1.77	0.66
50:SD:90:LYS:HG3	50:SD:94:ARG:HH21	1.59	0.66
64:Sg:206:LEU:HD12	64:Sg:218:LEU:HD12	1.77	0.66
15:LJ:141:ILE:HA	15:LJ:144:LYS:HE3	1.77	0.66
68:SE:31:PRO:HA	68:SE:81:THR:HB	1.75	0.66
83:S2:1748:G:H1	83:S2:1786:U:H3	0.75	0.66
70:SH:154:ILE:HB	70:SH:185:VAL:HG22	1.75	0.66
83:S2:885:U:O2	83:S2:901:G:O6	2.14	0.66
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.78	0.66
78:SX:107:ARG:HG3	78:SX:110:HIS:HB3	1.74	0.66
20:LP:8:PRO:HD3	20:LP:149:ILE:HD13	1.76	0.66
50:SD:137:VAL:HB	50:SD:185:LYS:HB2	1.78	0.66
77:SW:107:SER:HB2	83:S2:860:G:H21	1.59	0.66
83:S2:1533:A:N6	83:S2:1602:U:H3	1.93	0.66
3:L5:4093:G:H1	3:L5:4114:C:H2'	1.61	0.66
83:S2:149:A:H3'	83:S2:150:A:H8	1.60	0.66
83:S2:1417:C:N3	83:S2:1422:G:N1	2.44	0.66
3:L5:1442:C:H42	3:L5:2105:A:H1'	1.59	0.66
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.61	0.66
13:LH:102:ASN:HB3	13:LH:115:ARG:HB2	1.76	0.66
39:Li:55:ARG:HA	39:Li:58:MET:HE2	1.78	0.66
74:SN:13:GLN:HE22	83:S2:921:G:H5'	1.61	0.66
4:L7:63:C:H5'	4:L7:64:G:H5''	1.78	0.65
12:LG:173:LEU:HG	12:LG:177:MET:HE2	1.77	0.65
13:LH:128:MET:HE3	13:LH:134:CYS:HB2	1.78	0.65
29:LY:55:VAL:HG12	29:LY:106:ILE:HG22	1.78	0.65
3:L5:2017:A:HO2'	3:L5:2018:C:H6	1.44	0.65
51:SF:142:SER:HB3	61:Sc:50:VAL:HG22	1.78	0.65
3:L5:1696:C:H2'	3:L5:1697:G:C4	2.31	0.65
9:LD:197:LYS:HG3	9:LD:202:GLN:HB2	1.77	0.65
83:S2:655:A:H4'	83:S2:656:G:H3'	1.79	0.65
3:L5:511:C:H5''	16:LL:165:LYS:HZ2	1.61	0.65
71:SI:98:LYS:HD3	83:S2:377:G:H5'	1.79	0.65
67:SC:212:LYS:O	67:SC:216:MET:HB2	1.96	0.65
51:SF:127:ARG:HG2	51:SF:136:ARG:HE	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LP:138:PRO:HB3	20:LP:140:MET:HE3	1.77	0.65
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.61	0.65
57:SS:86:ARG:HE	57:SS:106:LYS:HD3	1.61	0.65
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.62	0.65
83:S2:1228:A:H2'	83:S2:1229:G:H8	1.62	0.65
7:LB:136:LYS:HB2	7:LB:142:GLY:HA3	1.79	0.65
64:Sg:176:VAL:HG23	64:Sg:185:LYS:HB2	1.79	0.65
3:L5:518:G:H1	3:L5:643:C:H2'	1.62	0.64
29:LY:74:TYR:HE2	29:LY:77:LYS:HG3	1.60	0.64
30:LZ:9:LYS:HB3	30:LZ:25:ILE:HD12	1.79	0.64
56:SR:20:TYR:HB3	56:SR:23:ARG:HB3	1.79	0.64
57:SS:105:ASN:HA	57:SS:108:ARG:HD3	1.78	0.64
55:SQ:38:PRO:HD2	55:SQ:41:MET:HE2	1.79	0.64
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.32	0.64
7:LB:8:ALA:HB2	26:LV:49:LEU:HD12	1.77	0.64
61:Sc:29:GLN:HG2	61:Sc:43:ILE:HD11	1.79	0.64
63:Sf:108:VAL:HB	63:Sf:113:LYS:H	1.61	0.64
64:Sg:76:GLN:HE22	64:Sg:91:ASP:HB2	1.61	0.64
55:SQ:78:VAL:HG12	83:S2:1673:U:H5''	1.80	0.64
73:SL:103:GLU:HG3	78:SX:11:ARG:HB2	1.80	0.64
81:Sb:16:LYS:HA	81:Sb:23:ARG:HH21	1.63	0.64
83:S2:28:U:H2'	83:S2:29:G:H8	1.61	0.64
27:LW:87:LEU:HD23	27:LW:90:ILE:HD11	1.79	0.64
63:Sf:108:VAL:HG12	63:Sf:114:ILE:HA	1.78	0.64
57:SS:138:THR:HA	57:SS:141:ARG:HH21	1.63	0.64
83:S2:106:C:H2'	83:S2:107:A:H8	1.62	0.64
5:L8:67:U:H2'	5:L8:68:G:H8	1.62	0.64
67:SC:79:GLU:HG2	76:SV:12:TYR:HB3	1.80	0.64
83:S2:1030:A:H2'	83:S2:1031:A2M:H8	1.81	0.64
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.63	0.63
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.63	0.63
3:L5:1973:G:H4'	49:Lt:117:ARG:HH22	1.62	0.63
6:LA:20:VAL:HA	6:LA:23:ARG:HD3	1.80	0.63
13:LH:20:LEU:HD13	13:LH:45:LEU:HB3	1.80	0.63
35:Le:63:ASN:HB3	35:Le:66:THR:HG22	1.80	0.63
36:Lf:70:ILE:HD11	36:Lf:92:LEU:HD23	1.79	0.63
81:Sb:54:VAL:HG13	81:Sb:63:LEU:HB2	1.79	0.63
55:SQ:140:ARG:HB2	83:S2:1644:C:H4'	1.81	0.63
62:Sd:14:PHE:HB2	83:S2:1661:A:H8	1.64	0.63
66:SB:146:ARG:HD3	83:S2:1123:C:H1'	1.80	0.63
3:L5:989:U:H3	3:L5:1064:G:H1	1.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2400:G:H21	37:Lg:6:THR:HG22	1.63	0.63
3:L5:4220:6MZ:O1P	3:L5:4220:6MZ:H8	1.98	0.63
67:SC:210:PRO:HB3	67:SC:240:THR:HG21	1.81	0.63
68:SE:45:ILE:HG13	68:SE:61:VAL:HG11	1.80	0.63
69:SG:2:LYS:HB2	69:SG:108:VAL:HG12	1.81	0.63
72:SJ:164:PRO:HB3	72:SJ:170:PRO:HA	1.81	0.63
83:S2:1010:G:H2'	83:S2:1011:A:C8	2.34	0.63
83:S2:1550:G:H3'	83:S2:1579:A:H61	1.62	0.63
39:Li:74:LYS:HE2	39:Li:80:HIS:HA	1.81	0.63
83:S2:527:C:H2'	83:S2:528:A:C8	2.34	0.63
3:L5:512:U:O4	3:L5:647:G:O6	2.17	0.63
3:L5:4897:G:H2'	3:L5:4898:G:H8	1.64	0.63
58:ST:128:GLN:HA	58:ST:131:LEU:HB2	1.80	0.63
65:SA:23:THR:HA	65:SA:164:ASN:HD22	1.64	0.63
2:Pt:3:C:H42	2:Pt:70:A:H61	1.46	0.62
3:L5:229:G:H5''	29:LY:11:ARG:HG3	1.81	0.62
3:L5:989:U:O2	3:L5:1064:G:N2	2.28	0.62
3:L5:2486:G:O6	3:L5:2493:G:O6	2.16	0.62
12:LG:87:LEU:HD21	12:LG:182:CYS:HB2	1.80	0.62
70:SH:142:LYS:HB3	77:SW:54:ASP:HB3	1.80	0.62
83:S2:677:G:N2	83:S2:1028:A:H62	1.96	0.62
83:S2:1547:C:H3'	83:S2:1548:G:H8	1.64	0.62
19:LO:34:VAL:HG22	19:LO:103:LYS:HB3	1.80	0.62
52:SK:10:ALA:HB1	52:SK:35:LEU:HD21	1.79	0.62
83:S2:5:U:H2'	83:S2:6:G:H8	1.65	0.62
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.81	0.62
3:L5:2701:U:H3	3:L5:2715:G:H1	1.47	0.62
11:LF:162:ILE:HB	11:LF:167:ILE:HD13	1.79	0.62
12:LG:105:GLU:HG3	12:LG:109:GLU:HG3	1.80	0.62
44:Ln:1:MET:HE2	44:Ln:6:ARG:HG2	1.80	0.62
66:SB:31:TYR:HA	66:SB:94:LYS:HD2	1.80	0.62
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.63	0.62
14:LI:63:GLU:HA	14:LI:66:GLU:OE1	1.99	0.62
83:S2:556:U:H3'	83:S2:557:U:H4'	1.82	0.62
3:L5:300:A:H2'	3:L5:301:G:H8	1.64	0.62
35:Le:38:PRO:HB2	35:Le:46:ARG:HB2	1.80	0.62
48:Ls:96:THR:HA	48:Ls:99:ARG:HG2	1.82	0.62
83:S2:1607:A:H62	83:S2:1632:G:H21	1.46	0.62
67:SC:193:VAL:HG11	67:SC:240:THR:HG22	1.82	0.62
73:SL:66:VAL:HA	73:SL:132:ARG:HH22	1.65	0.62
12:LG:104:PRO:HG2	12:LG:194:VAL:HG23	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SK:5:LYS:HD3	52:SK:8:ARG:HH21	1.64	0.62
79:SY:90:ARG:HA	79:SY:93:ARG:HD2	1.81	0.62
83:S2:1513:C:H2'	83:S2:1514:G:H8	1.64	0.62
3:L5:1207:C:H2'	3:L5:1208:G:H8	1.65	0.62
7:LB:284:ILE:HD13	7:LB:331:VAL:HG13	1.81	0.62
56:SR:98:VAL:HB	56:SR:117:LEU:HD12	1.81	0.62
57:SS:121:ARG:HG3	57:SS:131:VAL:HB	1.82	0.62
3:L5:4246:G:H2'	3:L5:4247:G:H8	1.64	0.61
14:LI:174:THR:HG23	14:LI:176:PHE:H	1.65	0.61
64:Sg:106:LYS:HG2	64:Sg:107:ASP:H	1.65	0.61
68:SE:79:ASP:HB3	68:SE:82:TYR:HB2	1.81	0.61
6:LA:107:MET:HB2	6:LA:111:THR:HG21	1.82	0.61
6:LA:112:ILE:HD11	46:Lp:79:VAL:HG22	1.81	0.61
11:LF:110:GLN:HA	11:LF:115:ARG:HH12	1.64	0.61
17:LM:29:ASP:H	17:LM:37:LEU:HB3	1.65	0.61
83:S2:1653:U:O2	83:S2:1671:G:N2	2.28	0.61
3:L5:73:A:H5''	16:LL:105:LYS:HD3	1.82	0.61
6:LA:179:ILE:HG21	6:LA:185:ALA:HB2	1.81	0.61
49:Lt:7:PRO:HB2	49:Lt:11:LYS:HD3	1.83	0.61
68:SE:125:LYS:HB3	68:SE:142:HIS:HB3	1.83	0.61
78:SX:50:ILE:HG22	78:SX:73:GLN:HB3	1.83	0.61
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.65	0.61
12:LG:117:ARG:HA	12:LG:120:LYS:HG2	1.82	0.61
50:SD:215:ASP:HB2	50:SD:217:ILE:HG12	1.83	0.61
3:L5:422:C:H2'	3:L5:423:G:H8	1.66	0.61
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.82	0.61
23:LS:4:SER:HB3	23:LS:111:ARG:HH22	1.66	0.61
49:Lt:134:GLY:HA3	49:Lt:152:ILE:HD11	1.83	0.61
83:S2:1417:C:O2	83:S2:1422:G:O6	2.19	0.61
38:Lh:106:LYS:HB3	38:Lh:110:LYS:HZ3	1.66	0.61
3:L5:2484:A:H62	3:L5:2494:U:H3	1.49	0.61
9:LD:288:LEU:HD23	9:LD:291:GLN:HE22	1.65	0.61
22:LR:169:ALA:HA	22:LR:172:ARG:HE	1.66	0.61
38:Lh:88:THR:HB	38:Lh:91:MET:HB2	1.83	0.61
83:S2:1534:C:H41	83:S2:1600:G:H1	1.49	0.61
3:L5:2647:A:H3'	3:L5:2648:G:H8	1.66	0.60
70:SH:140:VAL:HG12	74:SN:19:ARG:HD3	1.83	0.60
78:SX:100:VAL:HG12	78:SX:125:VAL:HG22	1.83	0.60
83:S2:587:A:H5'	83:S2:592:C:H41	1.66	0.60
83:S2:1337:4AC:H2'	83:S2:1338:G:H8	1.67	0.60
49:Lt:117:ARG:HG2	49:Lt:118:HIS:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1259:G:H2'	3:L5:1260:G:H8	1.66	0.60
22:LR:105:LEU:HD23	22:LR:138:LEU:HD23	1.82	0.60
79:SY:61:ARG:HH12	83:S2:580:U:H1'	1.66	0.60
83:S2:981:A:H2'	83:S2:982:G:C8	2.37	0.60
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.83	0.60
20:LP:37:LYS:HD3	20:LP:117:ILE:HG22	1.82	0.60
35:Le:44:ARG:HG3	35:Le:52:GLN:HE22	1.66	0.60
49:Lt:55:GLY:H	49:Lt:59:THR:HG21	1.67	0.60
64:Sg:76:GLN:HE21	64:Sg:93:THR:HG23	1.65	0.60
83:S2:368:U:H3'	83:S2:369:C:H2'	1.84	0.60
83:S2:525:A:H2'	83:S2:526:A:H8	1.64	0.60
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.67	0.60
68:SE:100:ARG:HB2	68:SE:114:ILE:HD13	1.84	0.60
16:LL:48:PRO:HB2	38:Lh:120:ALA:HB2	1.84	0.60
16:LL:59:VAL:HG21	16:LL:73:GLY:HA3	1.83	0.60
29:LY:111:LEU:HB3	29:LY:116:LYS:HE3	1.83	0.60
3:L5:1095:A:N1	3:L5:1200:G:C6	2.70	0.60
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.65	0.60
85:L5:5291:SPM:H132	19:LO:91:LYS:HG2	1.83	0.60
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.83	0.60
83:S2:27:A2M:H2'	83:S2:28:U:C6	2.37	0.60
83:S2:609:U:H2'	83:S2:610:G:H8	1.65	0.60
83:S2:1729:U:O2	83:S2:1805:G:N2	2.29	0.60
3:L5:138:G:H2'	3:L5:139:G:H8	1.67	0.60
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.65	0.60
74:SN:96:VAL:HG22	74:SN:99:ARG:HH22	1.66	0.60
3:L5:1346:C:H2'	3:L5:1347:G:H8	1.67	0.59
25:LU:23:LEU:HB2	25:LU:70:ILE:HG22	1.84	0.59
29:LY:34:LEU:HD11	29:LY:47:MET:HG2	1.84	0.59
83:S2:359:U:H3	83:S2:403:G:H1	1.48	0.59
83:S2:668:A2M:H2'	83:S2:669:A:N7	2.16	0.59
3:L5:262:G:H2'	3:L5:263:G:H8	1.65	0.59
3:L5:2884:G:H2'	3:L5:2885:A:H8	1.67	0.59
19:LO:157:GLU:O	19:LO:161:LYS:HG2	2.02	0.59
25:LU:43:LEU:HD12	25:LU:47:ILE:HD11	1.84	0.59
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.37	0.59
49:Lt:16:ARG:HH21	49:Lt:61:LYS:HE2	1.67	0.59
83:S2:1351:G:N2	83:S2:1360:U:O2	2.34	0.59
83:S2:1417:C:H42	83:S2:1422:G:N2	2.01	0.59
3:L5:735:G:H5''	17:LM:70:GLN:HG3	1.84	0.59
3:L5:2279:A:H4'	35:Le:48:ARG:HH22	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:135:PRO:HG2	69:SG:141:ILE:HG13	1.84	0.59
3:L5:3944:G:O6	3:L5:4069:U:O4	2.21	0.59
3:L5:4294:C:H4'	45:Lo:13:LYS:HD3	1.84	0.59
33:Lc:36:LYS:HZ3	33:Lc:37:MET:HE3	1.67	0.59
77:SW:30:CYS:HA	77:SW:34:ILE:HD11	1.84	0.59
28:LX:76:ILE:HD11	28:LX:104:ALA:HB2	1.83	0.59
31:La:2:PRO:HB2	31:La:5:LEU:HD13	1.83	0.59
31:La:4:ARG:HG3	31:La:5:LEU:HD12	1.84	0.59
83:S2:808:A:H2	83:S2:855:G:H22	1.51	0.59
6:LA:58:LEU:HD12	6:LA:75:LEU:HG	1.84	0.59
20:LP:41:ILE:HD13	20:LP:112:LEU:HB2	1.84	0.59
45:Lo:55:ILE:HG21	45:Lo:57:ARG:HH21	1.67	0.59
51:SF:134:VAL:HG12	51:SF:135:ARG:HG2	1.85	0.59
83:S2:155:G:H2'	83:S2:156:G:H8	1.67	0.59
83:S2:1101:U:H2'	83:S2:1102:G:C8	2.38	0.59
3:L5:1563:A:H2'	3:L5:1564:A:C8	2.37	0.59
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.85	0.59
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.37	0.59
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.84	0.59
21:LQ:26:ARG:HA	21:LQ:29:VAL:HG22	1.84	0.59
59:SU:51:LYS:HB2	59:SU:90:ASP:HB2	1.85	0.59
78:SX:66:ILE:HG21	82:Se:5:SER:HB2	1.84	0.59
67:SC:209:VAL:HG21	67:SC:233:LEU:HD13	1.85	0.59
75:SO:34:PHE:HB3	75:SO:41:PHE:HB2	1.85	0.59
83:S2:1348:G:H2'	83:S2:1349:G:H8	1.68	0.59
65:SA:85:ARG:HH21	65:SA:201:LEU:HD12	1.68	0.59
83:S2:888:U:H4'	83:S2:889:U:H5'	1.85	0.59
83:S2:1228:A:H2'	83:S2:1229:G:C8	2.38	0.59
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.68	0.58
3:L5:2903:G:H1'	3:L5:2904:U:H5	1.67	0.58
9:LD:61:ILE:HG12	9:LD:63:GLN:HE22	1.68	0.58
66:SB:35:ALA:HB2	66:SB:44:ILE:HD11	1.85	0.58
75:SO:98:ARG:HG3	75:SO:133:THR:HA	1.85	0.58
3:L5:490:C:H2'	3:L5:491:G:C8	2.38	0.58
72:SJ:109:ARG:HE	72:SJ:146:SER:HA	1.68	0.58
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.85	0.58
34:Ld:22:THR:HG23	34:Ld:122:VAL:HG23	1.85	0.58
2:Pt:29:C:H2'	2:Pt:30:G:H8	1.67	0.58
3:L5:459:C:H5'	10:LE:110:ARG:HA	1.85	0.58
67:SC:65:LYS:HD2	67:SC:273:LEU:HD22	1.85	0.58
77:SW:8:ALA:HA	77:SW:74:VAL:HG11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1277:C:H2'	83:S2:1278:A:H8	1.69	0.58
11:LF:190:LEU:HD21	11:LF:208:LEU:HD21	1.86	0.58
15:LJ:18:ARG:HB2	15:LJ:133:VAL:HG13	1.86	0.58
51:SF:144:LEU:HD22	61:Sc:49:PRO:HG2	1.85	0.58
64:Sg:288:SER:HB3	64:Sg:301:GLY:H	1.67	0.58
68:SE:144:ALA:HB3	83:S2:121:OMU:HM23	1.84	0.58
69:SG:170:ARG:HA	83:S2:72:C:H42	1.68	0.58
71:SI:97:VAL:HG22	71:SI:98:LYS:H	1.68	0.58
83:S2:5:U:H2'	83:S2:6:G:C8	2.39	0.58
24:LT:40:VAL:HG11	24:LT:96:ILE:HD12	1.86	0.58
69:SG:38:ALA:HB1	69:SG:41:LEU:HD12	1.85	0.58
79:SY:105:LYS:HZ1	79:SY:108:LYS:HE3	1.68	0.58
80:Sa:59:PHE:HB2	80:Sa:62:TYR:HB2	1.85	0.58
3:L5:150:U:H3	12:LG:163:PRO:HD2	1.68	0.58
43:Lm:94:MET:HB3	43:Lm:121:LEU:HD12	1.85	0.58
70:SH:72:PHE:O	70:SH:76:GLN:HB2	2.02	0.58
74:SN:142:GLU:HB2	74:SN:145:THR:HG22	1.85	0.58
7:LB:60:VAL:HG11	7:LB:67:VAL:HG13	1.86	0.58
47:Lr:98:ARG:HD2	47:Lr:107:ARG:HD3	1.86	0.58
74:SN:91:LEU:HB3	74:SN:122:ILE:HG12	1.85	0.58
7:LB:217:ILE:HD12	7:LB:347:LEU:HD12	1.84	0.58
7:LB:333:LEU:HD11	7:LB:347:LEU:HD11	1.85	0.58
12:LG:159:HIS:HD2	12:LG:185:LYS:HA	1.69	0.58
65:SA:183:LEU:HD12	65:SA:188:THR:HG21	1.85	0.58
3:L5:4302:U:H4'	24:LT:5:LYS:HD2	1.86	0.58
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.38	0.58
14:LI:53:VAL:HG22	14:LI:134:VAL:HG12	1.84	0.58
54:SP:115:TYR:HB2	54:SP:118:GLU:HG3	1.86	0.58
83:S2:1536:G:H2'	83:S2:1537:A:H8	1.68	0.58
18:LN:39:ALA:HB3	18:LN:61:ILE:HG22	1.85	0.57
23:LS:7:LEU:HD23	23:LS:107:THR:HG22	1.85	0.57
23:LS:15:ARG:HD2	23:LS:25:PRO:HG2	1.85	0.57
64:Sg:40:ILE:HB	64:Sg:59:LEU:HB2	1.85	0.57
65:SA:127:PRO:HG2	65:SA:152:SER:HB3	1.86	0.57
69:SG:162:LEU:HG	69:SG:167:LYS:HE3	1.86	0.57
71:SI:133:GLU:HA	71:SI:136:ILE:HG12	1.86	0.57
71:SI:165:GLN:HG2	71:SI:171:LEU:HD23	1.86	0.57
83:S2:1337:4AC:H2'	83:S2:1338:G:C8	2.39	0.57
3:L5:1759:G:H1	3:L5:1773:U:H3	1.52	0.57
3:L5:1982:G:H21	3:L5:2010:A:H5'	1.69	0.57
3:L5:3661:G:H4'	3:L5:3662:A:H5'	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SS:27:ALA:HB2	57:SS:52:LEU:HD12	1.87	0.57
65:SA:177:MET:HE3	65:SA:181:GLU:HG2	1.87	0.57
48:Ls:63:LYS:HG3	48:Ls:66:ARG:HH22	1.69	0.57
59:SU:104:ILE:HB	59:SU:106:ILE:HG12	1.86	0.57
80:Sa:41:ILE:HD12	80:Sa:68:TYR:HD2	1.69	0.57
83:S2:929:G:H2'	83:S2:930:C:O4'	2.04	0.57
3:L5:4910:G:H21	7:LB:96:PRO:HG3	1.68	0.57
23:LS:83:ARG:HG3	23:LS:125:GLN:HB3	1.87	0.57
67:SC:169:TYR:CE1	67:SC:173:LYS:HE3	2.39	0.57
80:Sa:11:ALA:HB3	80:Sa:33:ASP:HB2	1.86	0.57
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.40	0.57
48:Ls:91:THR:HG21	48:Ls:98:ILE:HG13	1.87	0.57
71:SI:57:ALA:H	71:SI:180:GLY:HA2	1.68	0.57
83:S2:388:U:H2'	83:S2:389:A:H8	1.69	0.57
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.70	0.57
55:SQ:34:VAL:HG22	55:SQ:70:VAL:HB	1.86	0.57
83:S2:640:A:H2'	83:S2:641:A:C8	2.39	0.57
83:S2:1417:C:N4	83:S2:1422:G:H22	2.02	0.57
3:L5:2375:A:H2'	3:L5:2376:A:H8	1.69	0.57
3:L5:4246:G:H2'	3:L5:4247:G:C8	2.39	0.57
10:LE:264:ILE:HD11	10:LE:267:LEU:HD12	1.84	0.57
42:LI:27:ILE:HD12	42:LI:30:LYS:HZ3	1.69	0.57
66:SB:128:LYS:HE2	66:SB:132:GLY:HA2	1.86	0.57
3:L5:1695:U:H3	3:L5:1696:C:H41	1.53	0.57
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.40	0.57
18:LN:120:TRP:HE1	18:LN:123:GLU:HB2	1.68	0.57
35:Le:47:ARG:HE	35:Le:49:PHE:HE2	1.51	0.57
60:SZ:99:LEU:HD21	60:SZ:102:LYS:HB2	1.87	0.57
70:SH:31:GLU:HA	70:SH:37:LYS:HG3	1.87	0.57
83:S2:159:A2M:H2'	83:S2:160:U:H6	1.70	0.57
3:L5:318:A:H2'	3:L5:319:A:C8	2.40	0.57
3:L5:1972:G:C6	3:L5:1973:G:O6	2.58	0.57
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.70	0.57
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.40	0.57
29:LY:4:ASN:HB3	29:LY:7:VAL:HG22	1.87	0.57
50:SD:60:GLY:HA3	50:SD:65:ARG:H	1.69	0.57
56:SR:16:ILE:HD11	56:SR:54:VAL:HG21	1.87	0.57
3:L5:976:G:H4'	8:LC:326:LEU:HD13	1.86	0.57
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	1.87	0.57
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.87	0.57
60:SZ:73:VAL:HG21	60:SZ:88:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SN:52:VAL:HG22	74:SN:55:ARG:HH12	1.69	0.57
75:SO:74:ALA:HB1	75:SO:115:ALA:HB2	1.87	0.57
3:L5:2543:A:H2	3:L5:2773:G:H22	1.52	0.56
52:SK:1:MET:HE3	52:SK:47:LYS:HB3	1.87	0.56
53:SM:44:LYS:O	53:SM:45:ARG:HD3	2.05	0.56
66:SB:168:MET:HA	66:SB:171:ILE:HG12	1.87	0.56
68:SE:61:VAL:HG22	68:SE:80:ILE:HD11	1.87	0.56
83:S2:388:U:H2'	83:S2:389:A:C8	2.40	0.56
3:L5:1779:U:H2'	3:L5:1780:A:C8	2.40	0.56
18:LN:5:LYS:HG3	39:Li:40:VAL:HG11	1.86	0.56
35:Le:70:LEU:HD21	35:Le:76:LYS:HE2	1.87	0.56
83:S2:1101:U:H2'	83:S2:1102:G:H8	1.70	0.56
83:S2:1562:C:H2'	83:S2:1563:G:C8	2.40	0.56
3:L5:908:G:H2'	3:L5:909:A:H8	1.71	0.56
3:L5:3754:G:O6	3:L5:3770:U:O4	2.22	0.56
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.40	0.56
8:LC:334:THR:HG22	8:LC:337:ARG:HH21	1.71	0.56
12:LG:147:VAL:HG22	12:LG:177:MET:HE3	1.86	0.56
14:LI:207:ASP:HA	14:LI:210:ARG:HG2	1.86	0.56
16:LL:63:THR:HG23	16:LL:65:ARG:H	1.70	0.56
41:Lk:47:ILE:HD11	41:Lk:52:LYS:HE3	1.87	0.56
56:SR:28:PHE:HA	56:SR:55:THR:HG21	1.87	0.56
64:Sg:24:THR:HG23	64:Sg:27:PHE:H	1.70	0.56
70:SH:9:VAL:HG11	70:SH:27:LEU:HD22	1.86	0.56
71:SI:25:ARG:HA	83:S2:448:A:H5''	1.87	0.56
83:S2:533:A:H61	83:S2:550:C:H42	1.53	0.56
83:S2:750:C:H42	83:S2:793:G:H1'	1.69	0.56
3:L5:3718:A2M:H2'	3:L5:3719:A:O4'	2.05	0.56
3:L5:4108:G:H2'	3:L5:4109:G:H8	1.70	0.56
3:L5:4347:G:H2'	3:L5:4348:A:C8	2.41	0.56
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.70	0.56
5:L8:90:C:H1'	29:LY:24:HIS:HB3	1.88	0.56
10:LE:138:ARG:HB3	10:LE:167:GLN:HE22	1.70	0.56
21:LQ:18:PRO:HG3	21:LQ:29:VAL:HG11	1.88	0.56
21:LQ:70:MET:HG2	21:LQ:98:LEU:HD11	1.86	0.56
49:Lt:57:ARG:NH1	49:Lt:59:THR:H	2.04	0.56
65:SA:143:PRO:HB3	76:SV:32:ILE:HG21	1.88	0.56
3:L5:926:G:H2'	3:L5:927:G:H8	1.70	0.56
3:L5:1350:C:H2'	3:L5:1351:G:H8	1.71	0.56
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.70	0.56
64:Sg:175:LYS:HB3	64:Sg:184:LEU:HD11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:261:G:H2'	3:L5:262:G:C8	2.40	0.56
3:L5:501:C:H41	3:L5:650:C:H41	1.54	0.56
13:LH:19:THR:HB	13:LH:26:ILE:HB	1.87	0.56
15:LJ:159:LYS:HG2	15:LJ:163:MET:HE1	1.87	0.56
23:LS:8:ARG:HB2	23:LS:10:TYR:HE1	1.70	0.56
57:SS:71:MET:HB3	57:SS:99:LEU:HG	1.88	0.56
83:S2:1748:G:N2	83:S2:1786:U:O2	2.28	0.56
3:L5:2075:G:H2'	3:L5:2076:G:H8	1.71	0.56
10:LE:164:PHE:HA	10:LE:175:VAL:HG12	1.88	0.56
70:SH:51:ILE:HD11	70:SH:176:VAL:HG12	1.87	0.56
80:Sa:44:ILE:HG22	80:Sa:67:LEU:HB2	1.87	0.56
83:S2:159:A2M:H2	83:S2:467:G:H21	1.71	0.56
83:S2:1422:G:H4'	83:S2:1423:C:H3'	1.88	0.56
3:L5:462:G:H2'	3:L5:463:A:H8	1.71	0.56
3:L5:4163:U:H5'	3:L5:4164:C:H5''	1.88	0.56
3:L5:4896:G:H2'	3:L5:4897:G:C8	2.41	0.56
9:LD:86:TYR:HE2	9:LD:247:ILE:HG13	1.70	0.56
21:LQ:85:THR:HG22	21:LQ:104:ARG:HB2	1.87	0.56
69:SG:66:GLY:HA2	83:S2:1745:A:H1'	1.88	0.56
70:SH:126:HIS:CE1	70:SH:181:THR:HG23	2.41	0.56
83:S2:207:G:H3'	83:S2:208:G:H8	1.70	0.56
83:S2:557:U:H2'	83:S2:558:G:C8	2.41	0.56
83:S2:1560:U:O2	83:S2:1575:G:O6	2.23	0.56
3:L5:4430:G:H1'	14:LI:158:LYS:HE3	1.88	0.56
51:SF:34:SER:HA	61:Sc:55:VAL:HG23	1.88	0.56
52:SK:32:HIS:HD2	52:SK:45:VAL:HG21	1.70	0.56
58:ST:124:THR:HG23	58:ST:127:GLY:H	1.70	0.56
71:SI:143:LYS:HD3	71:SI:146:GLN:HE21	1.71	0.56
78:SX:52:LEU:HD11	78:SX:73:GLN:HB2	1.88	0.56
83:S2:1845:A:H2'	83:S2:1846:G:C8	2.41	0.56
2:Pt:62:C:H2'	2:Pt:63:G:H8	1.70	0.56
3:L5:1079:C:H2'	3:L5:1080:C:H6	1.71	0.56
8:LC:142:HIS:HE1	8:LC:248:ARG:HD2	1.71	0.56
17:LM:30:VAL:HG11	23:LS:150:ILE:HD13	1.88	0.56
30:LZ:54:THR:H	30:LZ:57:MET:HE3	1.71	0.56
55:SQ:32:ILE:HA	55:SQ:68:ILE:HG22	1.88	0.56
76:SV:42:VAL:HG23	76:SV:43:THR:HG23	1.87	0.56
13:LH:162:GLN:HE21	13:LH:181:VAL:HG23	1.71	0.55
66:SB:146:ARG:HH11	83:S2:1123:C:H1'	1.70	0.55
72:SJ:46:VAL:HG11	72:SJ:106:LEU:HD21	1.87	0.55
83:S2:525:A:H2'	83:S2:526:A:C8	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1562:C:H2'	83:S2:1563:G:H8	1.70	0.55
3:L5:267:G:H2'	3:L5:268:G:H8	1.70	0.55
3:L5:2261:G:H8	47:Lr:98:ARG:HH12	1.55	0.55
16:LL:8:MET:HG2	21:LQ:166:TYR:HB3	1.88	0.55
20:LP:148:MET:HE3	20:LP:150:LEU:HD21	1.88	0.55
31:La:75:LEU:HD11	31:La:133:ALA:HA	1.88	0.55
31:La:95:THR:HG23	31:La:97:ALA:H	1.71	0.55
53:SM:85:LEU:HD23	53:SM:107:SER:HA	1.88	0.55
61:Sc:11:LEU:HB3	61:Sc:35:MET:HG3	1.88	0.55
83:S2:406:PSU:H2'	83:S2:408:A:H8	1.71	0.55
83:S2:1748:G:O6	83:S2:1786:U:O4	2.23	0.55
3:L5:1350:C:H2'	3:L5:1351:G:C8	2.41	0.55
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.42	0.55
25:LU:45:GLU:HA	25:LU:54:GLY:HA2	1.88	0.55
50:SD:53:THR:HA	50:SD:94:ARG:CZ	2.36	0.55
3:L5:137:G:H2'	3:L5:138:G:H8	1.71	0.55
27:LW:82:ILE:HD12	69:SG:131:ARG:HG3	1.88	0.55
54:SP:134:GLY:H	83:S2:1236:G:H4'	1.71	0.55
64:Sg:64:HIS:HB3	64:Sg:83:TRP:HB2	1.89	0.55
68:SE:188:ASN:HA	68:SE:245:ARG:HH12	1.70	0.55
71:SI:97:VAL:HG12	71:SI:100:CYS:HB3	1.88	0.55
83:S2:39:A:H3'	83:S2:40:A:H8	1.70	0.55
83:S2:223:C:H2'	83:S2:224:A:C8	2.42	0.55
83:S2:795:A:H2'	83:S2:796:G:C8	2.40	0.55
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.21	0.55
3:L5:1700:G:H5'	3:L5:1702:C:OP2	2.07	0.55
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.42	0.55
3:L5:1976:G:H22	49:Lt:139:VAL:HG11	1.70	0.55
3:L5:4421:C:H42	3:L5:4475:G:H22	1.54	0.55
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.72	0.55
8:LC:315:LYS:HD2	11:LF:168:ALA:HB1	1.88	0.55
19:LO:166:ILE:HD11	19:LO:169:ARG:HH21	1.71	0.55
25:LU:65:ARG:HG2	25:LU:67:LYS:H	1.72	0.55
63:Sf:132:MET:HE2	63:Sf:141:CYS:HB2	1.89	0.55
79:SY:36:PRO:HG3	83:S2:570:C:H4'	1.88	0.55
82:Se:8:ARG:HG2	82:Se:11:LYS:HD3	1.87	0.55
5:L8:86:U:H3'	38:Lh:7:ARG:HH12	1.71	0.55
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.89	0.55
49:Lt:19:GLY:HA2	49:Lt:48:LYS:HZ3	1.70	0.55
53:SM:87:GLU:HG3	53:SM:103:VAL:HG11	1.87	0.55
67:SC:207:ALA:HB2	83:S2:4:C:H4'	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SH:53:VAL:HG12	70:SH:175:GLY:HA3	1.89	0.55
83:S2:27:A2M:H2'	83:S2:28:U:H6	1.71	0.55
83:S2:1410:C:H2'	83:S2:1411:G:H8	1.71	0.55
3:L5:161:G:H2'	3:L5:162:A:H8	1.72	0.55
3:L5:1100:U:O4	3:L5:1194:G:O6	2.23	0.55
3:L5:1189:G:H2'	3:L5:1190:C:C6	2.42	0.55
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.89	0.55
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.41	0.55
20:LP:28:ASN:HD22	20:LP:60:PHE:HZ	1.53	0.55
30:LZ:28:ASN:C	30:LZ:28:ASN:HD22	2.14	0.55
30:LZ:81:MET:HE3	37:Lg:92:LYS:HD3	1.89	0.55
66:SB:39:PHE:HA	66:SB:75:GLN:HE22	1.71	0.55
72:SJ:63:LEU:HD21	72:SJ:69:ARG:HH21	1.70	0.55
83:S2:583:A:H3'	83:S2:584:A:H8	1.72	0.55
83:S2:907:G:H2'	83:S2:908:A:C8	2.42	0.55
3:L5:2111:G:H21	3:L5:2252:G:H5'	1.72	0.55
3:L5:4319:C:H2'	3:L5:4320:G:H8	1.71	0.55
6:LA:83:HIS:HB3	46:Lp:64:VAL:HG22	1.89	0.55
49:Lt:20:GLY:HA2	49:Lt:56:LEU:HD12	1.88	0.55
83:S2:528:A:H2'	83:S2:529:A:C8	2.42	0.55
83:S2:639:C:H2'	83:S2:640:A:C8	2.42	0.55
3:L5:137:G:H2'	3:L5:138:G:C8	2.42	0.55
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.89	0.55
3:L5:4743:G:H2'	3:L5:4744:A:H8	1.72	0.55
16:LL:206:ASP:HA	16:LL:209:LYS:HD3	1.89	0.55
30:LZ:4:PHE:HE1	33:Lc:39:ARG:HA	1.72	0.55
53:SM:26:LEU:HD12	53:SM:31:LEU:HD11	1.89	0.55
83:S2:159:A2M:O5'	83:S2:159:A2M:H8	2.07	0.55
3:L5:1558:A:H2'	3:L5:1559:G:H8	1.73	0.55
3:L5:4402:C:H42	3:L5:4441:A:H61	1.55	0.55
26:LV:64:THR:HG22	26:LV:76:VAL:HA	1.88	0.55
50:SD:227:LYS:HG2	64:Sg:184:LEU:HD23	1.89	0.55
52:SK:90:VAL:HG11	52:SK:95:ARG:HE	1.71	0.55
77:SW:90:GLN:HG2	77:SW:97:ARG:HH21	1.72	0.55
83:S2:329:G:H2'	83:S2:330:G:H8	1.72	0.55
3:L5:181:C:H2'	3:L5:182:G:C8	2.42	0.54
8:LC:195:LYS:HA	8:LC:200:ARG:HA	1.89	0.54
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	1.89	0.54
47:Lr:119:ARG:HD3	47:Lr:122:LYS:HZ1	1.72	0.54
67:SC:64:THR:HG22	67:SC:66:LEU:H	1.72	0.54
83:S2:751:G:H1'	83:S2:793:G:H21	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LV:69:LYS:HB3	26:LV:72:LEU:HD13	1.88	0.54
32:Lb:60:ASN:HA	32:Lb:63:LYS:HZ2	1.72	0.54
33:Lc:26:LYS:HB2	33:Lc:97:ILE:HB	1.88	0.54
44:Ln:21:ARG:HH12	83:S2:1174:PSU:H5'	1.72	0.54
49:Lt:110:VAL:HG11	49:Lt:137:GLN:HE22	1.72	0.54
49:Lt:117:ARG:HG2	49:Lt:118:HIS:N	2.23	0.54
55:SQ:72:VAL:HG11	55:SQ:80:GLN:HG3	1.89	0.54
68:SE:45:ILE:HB	68:SE:80:ILE:HG13	1.90	0.54
3:L5:2554:U:C2	3:L5:2764:A:N7	2.76	0.54
3:L5:4489:G:H4'	86:L5:5288:SPD:H91	1.90	0.54
9:LD:182:GLY:HA2	9:LD:194:VAL:HG23	1.89	0.54
22:LR:142:ILE:HA	22:LR:145:LEU:HG	1.87	0.54
48:Ls:175:LEU:HD21	48:Ls:182:PRO:HB3	1.89	0.54
83:S2:146:G:H1	83:S2:173:A:H61	1.56	0.54
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.36	0.54
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.42	0.54
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.43	0.54
17:LM:62:LEU:HD21	17:LM:82:ILE:HD11	1.88	0.54
22:LR:105:LEU:HD22	22:LR:135:LYS:HG3	1.88	0.54
26:LV:71:GLU:HG2	26:LV:72:LEU:HD12	1.90	0.54
31:La:75:LEU:HG	31:La:113:GLY:HA2	1.90	0.54
42:Ll:21:ARG:HH22	42:Ll:24:PRO:HG3	1.72	0.54
51:SF:30:ILE:HG23	51:SF:117:ILE:HD11	1.89	0.54
77:SW:6:VAL:HG13	77:SW:29:PRO:HB2	1.89	0.54
83:S2:1845:A:H2'	83:S2:1846:G:H8	1.73	0.54
3:L5:268:G:H2'	3:L5:269:G:H8	1.72	0.54
3:L5:481:G:H2'	3:L5:482:G:C8	2.42	0.54
3:L5:1647:U:H5''	86:L5:5289:SPD:H71	1.90	0.54
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.90	0.54
8:LC:358:ALA:HA	8:LC:361:LEU:HD12	1.89	0.54
10:LE:149:ILE:HD12	10:LE:271:LEU:HD21	1.88	0.54
23:LS:46:TYR:O	23:LS:50:GLN:HG2	2.08	0.54
23:LS:127:MET:HE1	24:LT:155:PRO:HA	1.88	0.54
35:Le:89:LEU:HD13	35:Le:118:LEU:HD22	1.89	0.54
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.42	0.54
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.42	0.54
7:LB:283:LYS:HE2	7:LB:361:GLU:HB2	1.90	0.54
46:Lp:9:GLY:HA3	46:Lp:27:LYS:HZ3	1.72	0.54
68:SE:87:MET:HG2	68:SE:100:ARG:HD2	1.90	0.54
6:LA:177:LYS:HD3	6:LA:184:ARG:HH22	1.73	0.54
29:LY:2:LYS:HD2	29:LY:7:VAL:HG23	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:149:A:N7	83:S2:169:U:O2	2.41	0.54
83:S2:588:G:H4'	83:S2:589:G:H5'	1.90	0.54
83:S2:649:PSU:H2'	83:S2:650:A:C8	2.43	0.54
3:L5:667:A:H5''	3:L5:668:C:H5''	1.88	0.54
3:L5:1350:C:H4'	8:LC:36:ILE:HD11	1.90	0.54
8:LC:230:LEU:HD21	8:LC:236:ASN:H	1.72	0.54
76:SV:14:PRO:HG2	76:SV:23:ILE:HD11	1.88	0.54
83:S2:851:C:H5''	83:S2:852:G:H5'	1.89	0.54
3:L5:162:A:H2'	3:L5:163:A:H8	1.73	0.54
5:L8:106:G:H4'	5:L8:137:A:H5'	1.90	0.54
32:Lb:95:ARG:O	32:Lb:99:ILE:HG12	2.07	0.54
74:SN:63:VAL:HG21	74:SN:71:ILE:HG13	1.89	0.54
83:S2:1037:G:H4'	83:S2:1845:A:H4'	1.88	0.54
3:L5:659:G:H2'	3:L5:660:A:H8	1.73	0.54
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.39	0.54
7:LB:217:ILE:HD11	7:LB:333:LEU:HD21	1.89	0.54
45:Lo:26:TYR:HB3	45:Lo:67:VAL:HB	1.90	0.54
74:SN:5:HIS:HB3	74:SN:117:LEU:HD13	1.89	0.54
3:L5:162:A:H2'	3:L5:163:A:C8	2.43	0.53
3:L5:3611:A:H2	3:L5:5016:A:H8	1.56	0.53
28:LX:82:THR:HG21	38:Lh:37:THR:HG22	1.90	0.53
48:Ls:143:ILE:HD12	48:Ls:158:VAL:HG11	1.89	0.53
66:SB:198:GLU:HB3	66:SB:210:VAL:HG21	1.90	0.53
71:SI:165:GLN:HE22	71:SI:172:LEU:HG	1.73	0.53
3:L5:462:G:H2'	3:L5:463:A:C8	2.42	0.53
13:LH:105:ILE:HD11	13:LH:109:GLY:HA2	1.89	0.53
46:Lp:29:ILE:HD11	46:Lp:69:TRP:CD1	2.43	0.53
68:SE:131:VAL:HA	68:SE:137:PRO:HA	1.91	0.53
83:S2:935:G:H2'	83:S2:936:G:H8	1.74	0.53
3:L5:481:G:H2'	3:L5:482:G:H8	1.73	0.53
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.44	0.53
3:L5:2683:C:H2'	3:L5:2684:C:H6	1.73	0.53
42:Ll:33:ASN:HB3	42:Ll:35:ILE:HG22	1.89	0.53
48:Ls:174:LEU:O	48:Ls:178:LEU:HB2	2.08	0.53
64:Sg:178:ASN:HB2	64:Sg:185:LYS:HD3	1.90	0.53
66:SB:170:GLU:HG2	66:SB:171:ILE:HG23	1.90	0.53
81:Sb:62:VAL:HG23	81:Sb:74:THR:HG21	1.90	0.53
83:S2:433:A:H2'	83:S2:434:G:C8	2.43	0.53
3:L5:958:G:C4	10:LE:124:LYS:HD2	2.43	0.53
3:L5:1982:G:H2'	3:L5:1983:A:O4'	2.09	0.53
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.74	0.53
4:L7:58:A:H2'	4:L7:59:G:C8	2.43	0.53
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	1.90	0.53
55:SQ:104:SER:HA	55:SQ:107:GLU:HG3	1.91	0.53
64:Sg:47:ARG:HG3	64:Sg:52:TYR:HE1	1.72	0.53
70:SH:160:LYS:HD3	70:SH:189:PHE:HB3	1.90	0.53
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.72	0.53
4:L7:117:G:H5'	9:LD:256:LYS:HD2	1.90	0.53
6:LA:247:ARG:HB3	83:S2:1069:U:H4'	1.90	0.53
23:LS:51:LEU:HD21	24:LT:153:PRO:HA	1.91	0.53
27:LW:56:ARG:HE	27:LW:61:LYS:HB2	1.74	0.53
34:Ld:54:MET:HE1	34:Ld:60:PRO:HA	1.90	0.53
48:Ls:29:ILE:HD11	48:Ls:191:GLN:HG2	1.90	0.53
56:SR:7:LYS:HG3	83:S2:1373:C:H5''	1.90	0.53
64:Sg:68:ASP:HB3	64:Sg:111:VAL:HG22	1.91	0.53
65:SA:145:ILE:HA	65:SA:159:ILE:HB	1.89	0.53
71:SI:78:ILE:HG13	71:SI:104:ILE:HG22	1.89	0.53
77:SW:4:MET:HB2	83:S2:683:OMG:H4'	1.88	0.53
3:L5:323:C:H2'	3:L5:324:A:H8	1.72	0.53
3:L5:1906:U:H2'	3:L5:1907:A:H8	1.73	0.53
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.42	0.53
5:L8:19:C:H2'	5:L8:20:A:H8	1.73	0.53
26:LV:106:VAL:HG12	26:LV:112:MET:HG2	1.91	0.53
52:SK:85:LEU:HD21	52:SK:89:ILE:HB	1.91	0.53
58:ST:28:LEU:HD12	58:ST:106:ALA:HB1	1.90	0.53
58:ST:40:ALA:HB3	58:ST:43:LYS:HG2	1.89	0.53
60:SZ:48:VAL:HG23	60:SZ:80:ARG:HD2	1.90	0.53
66:SB:136:ARG:HB3	66:SB:216:LYS:HG3	1.90	0.53
70:SH:10:LYS:HE3	70:SH:17:ASP:HB3	1.91	0.53
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.74	0.53
3:L5:5018:C:H2'	3:L5:5019:A:H8	1.74	0.53
64:Sg:89:LEU:HB3	64:Sg:99:ARG:HB3	1.91	0.53
3:L5:18:C:H4'	18:LN:138:PHE:CD2	2.44	0.53
3:L5:1172:C:HO2'	3:L5:1173:G:H8	1.57	0.53
3:L5:1907:A:H4'	11:LF:223:LYS:HD2	1.90	0.53
3:L5:2067:C:H5''	36:Lf:78:HIS:CE1	2.43	0.53
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.44	0.53
8:LC:268:ARG:HH12	8:LC:269:LYS:HE2	1.73	0.53
80:Sa:5:ARG:HH21	83:S2:1864:U:H3'	1.73	0.53
3:L5:974:C:H41	3:L5:1281:G:H21	1.57	0.53
3:L5:1996:C:N4	3:L5:2000:G:H22	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2375:A:H2'	3:L5:2376:A:C8	2.44	0.53
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.90	0.53
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.44	0.53
26:LV:13:LYS:HZ3	26:LV:124:GLU:HB3	1.74	0.53
43:Lm:99:CYS:HB2	43:Lm:114:LYS:HE3	1.90	0.53
43:Lm:106:ARG:HD3	43:Lm:106:ARG:H	1.74	0.53
67:SC:130:ILE:HG23	67:SC:162:ILE:HD11	1.91	0.53
67:SC:267:GLN:HA	67:SC:270:THR:HB	1.91	0.53
69:SG:41:LEU:HB3	69:SG:45:TRP:HE3	1.74	0.53
69:SG:191:ARG:HH22	83:S2:312:G:H2'	1.73	0.53
77:SW:4:MET:HE1	83:S2:1158:G:H21	1.72	0.53
83:S2:1801:A:H2'	83:S2:1802:C:C6	2.44	0.53
3:L5:1346:C:H2'	3:L5:1347:G:C8	2.43	0.52
3:L5:3721:U:H2'	3:L5:3722:G:H8	1.72	0.52
3:L5:3856:A:H4'	20:LP:85:LYS:HG2	1.91	0.52
26:LV:129:TRP:HB2	26:LV:132:ILE:HG12	1.91	0.52
68:SE:208:VAL:HG11	68:SE:225:ILE:HG13	1.90	0.52
72:SJ:108:ARG:HH22	72:SJ:154:GLN:HB3	1.73	0.52
83:S2:106:C:H2'	83:S2:107:A:C8	2.43	0.52
83:S2:1536:G:H2'	83:S2:1537:A:C8	2.43	0.52
83:S2:1568:C:H2'	83:S2:1569:A:C8	2.45	0.52
3:L5:1811:G:H21	32:Lb:57:MET:HE1	1.74	0.52
3:L5:4965:U:H4'	3:L5:4966:A:H5'	1.90	0.52
13:LH:115:ARG:HD3	13:LH:123:ILE:HD12	1.91	0.52
28:LX:71:LEU:HG	28:LX:76:ILE:HD13	1.91	0.52
30:LZ:57:MET:HB2	30:LZ:61:LYS:HD3	1.91	0.52
56:SR:6:THR:HA	83:S2:1373:C:H5'	1.90	0.52
64:Sg:12:LYS:HD3	64:Sg:306:LEU:HD12	1.90	0.52
83:S2:1579:A:H4'	83:S2:1581:C:H5	1.73	0.52
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.44	0.52
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.44	0.52
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.45	0.52
5:L8:67:U:H2'	5:L8:68:G:C8	2.43	0.52
18:LN:73:ARG:HG2	18:LN:75:VAL:HG23	1.91	0.52
30:LZ:91:LEU:HD12	30:LZ:96:VAL:HG21	1.91	0.52
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.44	0.52
5:L8:19:C:H2'	5:L8:20:A:C8	2.45	0.52
23:LS:80:ILE:HG22	23:LS:129:VAL:HA	1.92	0.52
47:Lr:97:ILE:HD13	47:Lr:107:ARG:HA	1.91	0.52
67:SC:165:VAL:HG21	67:SC:217:ALA:HB1	1.91	0.52
71:SI:106:SER:HB3	71:SI:171:LEU:HG	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:300:U:H2'	83:S2:301:A:C8	2.44	0.52
83:S2:1203:G:H2'	83:S2:1204:A:C8	2.44	0.52
3:L5:7:C:H2'	3:L5:8:U:C6	2.45	0.52
3:L5:1955:G:H2'	3:L5:1956:A:H8	1.75	0.52
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.45	0.52
3:L5:4421:C:H42	3:L5:4475:G:N2	2.08	0.52
26:LV:70:PRO:HG3	83:S2:1724:A:H5'	1.92	0.52
27:LW:56:ARG:HH21	27:LW:61:LYS:HB3	1.75	0.52
32:Lb:12:GLN:HA	32:Lb:12:GLN:HE21	1.75	0.52
52:SK:31:LYS:NZ	52:SK:40:VAL:H	2.08	0.52
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.45	0.52
5:L8:66:A:H2'	5:L8:67:U:C6	2.44	0.52
13:LH:4:ILE:HG13	13:LH:61:TRP:CH2	2.45	0.52
49:Lt:12:VAL:HG11	49:Lt:65:GLN:H	1.75	0.52
60:SZ:79:ILE:HB	60:SZ:83:LEU:HD23	1.91	0.52
66:SB:133:TYR:HB3	66:SB:217:MET:HE1	1.91	0.52
68:SE:127:ARG:HD2	68:SE:142:HIS:HA	1.90	0.52
71:SI:83:TYR:HB3	71:SI:101:ILE:HD11	1.91	0.52
71:SI:141:ARG:HD3	71:SI:145:ILE:HG21	1.92	0.52
83:S2:116:OMU:O5'	83:S2:116:OMU:H6	2.09	0.52
83:S2:342:C:H2'	83:S2:343:A:H8	1.74	0.52
83:S2:825:A:H2'	83:S2:826:A:C8	2.45	0.52
83:S2:980:A:H2'	83:S2:981:A:C8	2.45	0.52
83:S2:1804:U:H2'	83:S2:1805:G:C8	2.44	0.52
3:L5:3607:U:H2'	3:L5:3608:A:H8	1.73	0.52
3:L5:4098:A:H2'	3:L5:4099:G:H4'	1.92	0.52
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.45	0.52
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.74	0.52
8:LC:319:LEU:H	8:LC:325:MET:HE3	1.75	0.52
23:LS:11:LYS:HA	23:LS:31:ARG:HH21	1.75	0.52
64:Sg:11:LEU:HB2	64:Sg:307:VAL:HG13	1.92	0.52
83:S2:1513:C:H2'	83:S2:1514:G:C8	2.44	0.52
2:Pt:29:C:H2'	2:Pt:30:G:C8	2.45	0.52
3:L5:189:G:H2'	3:L5:190:G:H8	1.75	0.52
3:L5:300:A:H2'	3:L5:301:G:C8	2.44	0.52
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.45	0.52
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.75	0.52
4:L7:6:C:H4'	9:LD:52:ILE:HD13	1.92	0.52
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.50	0.52
75:SO:54:CYS:HB2	75:SO:84:ARG:HG2	1.92	0.52
83:S2:793:G:H2'	83:S2:794:A:H8	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1351:G:O6	83:S2:1360:U:O4	2.28	0.52
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.45	0.52
3:L5:1558:A:H2'	3:L5:1559:G:C8	2.45	0.52
3:L5:1675:C:H3'	3:L5:1677:PSU:HN1	1.73	0.52
3:L5:2007:G:H2'	3:L5:2008:U:C6	2.45	0.52
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.45	0.52
3:L5:3946:G:O6	3:L5:4067:U:O4	2.27	0.52
3:L5:4208:U:H2'	3:L5:4209:G:H8	1.74	0.52
3:L5:4530:UR3:H2'	3:L5:4531:U:H2'	1.90	0.52
5:L8:153:C:H2'	5:L8:154:G:H8	1.74	0.52
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.44	0.52
66:SB:33:VAL:HG12	66:SB:96:CYS:HB2	1.91	0.52
72:SJ:114:VAL:HG11	72:SJ:135:ILE:HG21	1.91	0.52
83:S2:1581:C:H5'	83:S2:1582:C:H5	1.74	0.52
3:L5:1683:PSU:H2'	3:L5:1684:A:H8	1.75	0.52
3:L5:1943:A:H5''	14:LI:162:ARG:HH12	1.75	0.52
3:L5:2018:C:H2'	3:L5:2019:C:C6	2.45	0.52
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.45	0.52
3:L5:2049:G:H2'	3:L5:2050:G:C8	2.45	0.52
3:L5:2859:G:H21	3:L5:3837:C:H1'	1.75	0.52
16:LL:191:LEU:HD22	16:LL:194:ILE:HD11	1.92	0.52
38:Lh:106:LYS:HB3	38:Lh:110:LYS:NZ	2.24	0.52
40:Lj:27:TYR:HA	40:Lj:34:CYS:HA	1.92	0.52
67:SC:83:LEU:HG	76:SV:15:ARG:NH1	2.25	0.52
69:SG:133:LEU:HD12	83:S2:65:C:C4	2.45	0.52
83:S2:874:G:H2'	83:S2:875:A:H8	1.75	0.52
83:S2:996:A:H2'	83:S2:997:A:C8	2.45	0.52
83:S2:1277:C:H2'	83:S2:1278:A:C8	2.45	0.52
83:S2:1432:U:H2'	83:S2:1438:A:C8	2.45	0.52
83:S2:1558:C:H2'	83:S2:1559:C:C6	2.44	0.52
2:Pt:50:U:O4	2:Pt:64:G:O6	2.28	0.51
3:L5:46:U:H5''	16:LL:16:LYS:HG3	1.92	0.51
3:L5:426:A:H2'	3:L5:427:A:H8	1.74	0.51
3:L5:980:U:H5'	10:LE:42:PRO:HA	1.92	0.51
4:L7:2:U:O4	4:L7:117:G:O6	2.28	0.51
39:Li:65:LYS:HG2	39:Li:68:ARG:HB3	1.92	0.51
54:SP:108:LYS:HD2	54:SP:109:PRO:HD2	1.91	0.51
60:SZ:106:GLN:HA	60:SZ:106:GLN:HE21	1.76	0.51
83:S2:1013:U:H2'	83:S2:1014:G:H8	1.75	0.51
3:L5:418:A:H4'	3:L5:2311:C:H5'	1.93	0.51
3:L5:460:C:H2'	3:L5:461:G:H8	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.75	0.51
18:LN:169:ARG:HG3	18:LN:174:LEU:HD12	1.90	0.51
39:Li:6:PRO:HB3	39:Li:16:LYS:HD3	1.91	0.51
41:Lk:8:ILE:HD11	41:Lk:56:LEU:HD13	1.90	0.51
41:Lk:24:LYS:HB2	41:Lk:35:LYS:HB2	1.91	0.51
43:Lm:103:LEU:HD22	43:Lm:121:LEU:HD11	1.90	0.51
52:SK:58:VAL:HG21	52:SK:69:TRP:HB3	1.92	0.51
64:Sg:156:PHE:HE1	64:Sg:179:LEU:HD11	1.74	0.51
76:SV:11:LEU:HG	76:SV:12:TYR:HD1	1.75	0.51
82:Se:32:ALA:HB2	83:S2:525:A:H5'	1.92	0.51
83:S2:1804:U:H2'	83:S2:1805:G:H8	1.75	0.51
3:L5:264:C:H2'	3:L5:265:C:C4	2.46	0.51
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	1.91	0.51
13:LH:5:LEU:HA	13:LH:60:TRP:CD1	2.45	0.51
23:LS:82:LEU:HD11	23:LS:113:MET:HE3	1.92	0.51
54:SP:121:ILE:HD13	57:SS:120:HIS:HD2	1.75	0.51
69:SG:67:VAL:HG12	69:SG:69:THR:HG22	1.91	0.51
79:SY:57:VAL:HB	79:SY:60:PHE:HE2	1.74	0.51
83:S2:121:OMU:HM22	83:S2:122:G:H5'	1.92	0.51
3:L5:921:C:H2'	3:L5:922:C:C6	2.46	0.51
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.44	0.51
3:L5:2557:G:O6	3:L5:2570:U:O4	2.29	0.51
7:LB:14:LEU:HD12	7:LB:17:LEU:HD11	1.92	0.51
14:LI:39:LYS:HA	14:LI:86:HIS:HD2	1.75	0.51
21:LQ:53:MET:HB2	21:LQ:58:ARG:HG3	1.91	0.51
35:Le:38:PRO:HD2	35:Le:55:MET:HE3	1.93	0.51
51:SF:49:LEU:HD12	55:SQ:49:TYR:HB2	1.92	0.51
64:Sg:107:ASP:HB2	64:Sg:125:ARG:HG3	1.91	0.51
72:SJ:33:GLY:HA3	82:Se:38:TYR:CG	2.45	0.51
3:L5:161:G:H2'	3:L5:162:A:C8	2.46	0.51
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.45	0.51
20:LP:120:ASN:HB2	20:LP:145:HIS:HB2	1.92	0.51
35:Le:22:ARG:HD2	35:Le:36:ARG:HB2	1.91	0.51
83:S2:929:G:N2	83:S2:1104:G:H4'	2.25	0.51
3:L5:93:G:H2'	3:L5:94:A:C8	2.45	0.51
3:L5:109:G:H5'	16:LL:92:ARG:HE	1.75	0.51
3:L5:4192:A:H2'	3:L5:4193:C:C6	2.46	0.51
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.45	0.51
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.93	0.51
14:LI:39:LYS:HA	14:LI:86:HIS:CD2	2.46	0.51
35:Le:70:LEU:HD21	35:Le:76:LYS:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SM:47:ALA:HB3	53:SM:74:ILE:HD13	1.93	0.51
57:SS:125:HIS:CD2	57:SS:131:VAL:HG11	2.46	0.51
70:SH:66:VAL:HA	70:SH:69:LEU:HD23	1.91	0.51
83:S2:1671:G:H2'	83:S2:1672:U:H6	1.74	0.51
3:L5:429:A:H2'	3:L5:430:G:C8	2.45	0.51
3:L5:959:G:C8	10:LE:123:ARG:HG2	2.46	0.51
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.46	0.51
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.45	0.51
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.92	0.51
7:LB:152:SER:O	7:LB:156:TYR:HB2	2.11	0.51
12:LG:52:THR:HG22	28:LX:41:ARG:HG3	1.92	0.51
14:LI:85:PHE:HE2	14:LI:87:MET:HE2	1.75	0.51
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.93	0.51
28:LX:87:MET:HA	28:LX:90:ILE:HG22	1.93	0.51
31:La:85:GLN:HA	31:La:88:VAL:HG12	1.91	0.51
44:Ln:15:ARG:HG2	44:Ln:18:ARG:HH22	1.74	0.51
69:SG:52:ILE:HA	69:SG:111:LEU:HD23	1.93	0.51
69:SG:76:LEU:HD21	69:SG:92:ARG:HE	1.74	0.51
83:S2:116:OMU:HN3	83:S2:347:G:H1	1.57	0.51
83:S2:1808:U:H2'	83:S2:1809:A:H8	1.76	0.51
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.46	0.51
3:L5:2250:C:H2'	3:L5:2251:G:C8	2.45	0.51
3:L5:3937:C:H1'	18:LN:125:SER:HB3	1.91	0.51
3:L5:4615:C:H5''	7:LB:357:ARG:HD2	1.92	0.51
10:LE:282:TYR:HE2	36:Lf:31:GLU:HG2	1.75	0.51
13:LH:92:MET:HB3	13:LH:144:LEU:HB2	1.91	0.51
15:LJ:21:CYS:HA	15:LJ:73:THR:HG22	1.92	0.51
16:LL:46:ILE:HB	16:LL:49:ARG:HB2	1.92	0.51
51:SF:72:LEU:HB3	51:SF:151:ILE:HD11	1.92	0.51
83:S2:432:G:H2'	83:S2:433:A:C8	2.46	0.51
83:S2:1652:G:O6	83:S2:1672:U:O4	2.28	0.51
83:S2:1722:G:O6	83:S2:1812:U:O2	2.27	0.51
83:S2:1737:G:H1	83:S2:1797:U:H3	1.59	0.51
3:L5:1323:A2M:H2'	3:L5:1324:A:O4'	2.11	0.51
3:L5:4370:OMG:H4'	45:Lo:64:LYS:HD3	1.93	0.51
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.45	0.51
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.46	0.51
3:L5:4770:U:H2'	3:L5:4771:C:C6	2.46	0.51
21:LQ:22:ASP:O	21:LQ:26:ARG:HG3	2.11	0.51
29:LY:82:ILE:HB	29:LY:85:VAL:HG12	1.92	0.51
51:SF:91:ARG:HA	51:SF:94:LYS:HE3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SM:26:LEU:HA	53:SM:31:LEU:HD21	1.92	0.51
58:ST:78:ILE:HD11	83:S2:1587:G:C5	2.45	0.51
70:SH:165:ASN:HA	70:SH:168:HIS:HE1	1.76	0.51
83:S2:925:G:H1	83:S2:1017:U:H3	1.58	0.51
83:S2:1010:G:H2'	83:S2:1011:A:H8	1.75	0.51
83:S2:1652:G:N2	83:S2:1672:U:O2	2.31	0.51
83:S2:1773:C:H2'	83:S2:1774:C:H5''	1.93	0.51
3:L5:10:A:H2'	3:L5:11:G:C8	2.46	0.51
3:L5:262:G:H2'	3:L5:263:G:C8	2.45	0.51
3:L5:700:G:N1	3:L5:701:G:C6	2.79	0.51
3:L5:1253:G:H2'	3:L5:1256:G:H5'	1.93	0.51
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.11	0.51
5:L8:92:U:H2'	5:L8:93:C:O4'	2.10	0.51
33:Lc:77:ASN:OD1	33:Lc:80:GLU:HG2	2.11	0.51
50:SD:23:GLU:HG2	52:SK:64:TRP:HE1	1.75	0.51
52:SK:50:GLN:HE22	83:S2:1276:A:H1'	1.76	0.51
64:Sg:120:ILE:HB	64:Sg:132:TRP:HB2	1.92	0.51
83:S2:15:U:H2'	83:S2:16:G:O4'	2.11	0.51
83:S2:186:C:H2'	83:S2:187:G:H8	1.76	0.51
83:S2:1144:A:H2'	83:S2:1145:A:C8	2.46	0.51
83:S2:1386:A:H3'	83:S2:1387:G:H8	1.75	0.51
2:Pt:18:G:H21	2:Pt:58:A:H5'	1.76	0.50
3:L5:268:G:H2'	3:L5:269:G:C8	2.46	0.50
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.93	0.50
3:L5:1972:G:C6	3:L5:1973:G:C6	2.99	0.50
6:LA:186:TYR:HB2	6:LA:196:TRP:CZ3	2.46	0.50
7:LB:29:VAL:HG12	7:LB:31:SER:H	1.76	0.50
7:LB:89:ILE:HG12	7:LB:197:ALA:HB1	1.94	0.50
8:LC:366:ASP:HB3	8:LC:368:LYS:HE2	1.92	0.50
18:LN:124:ASP:HB3	18:LN:127:TYR:H	1.76	0.50
25:LU:84:LYS:HE2	25:LU:102:VAL:HG23	1.92	0.50
75:SO:33:ILE:HG23	75:SO:97:LEU:HD23	1.93	0.50
83:S2:28:U:H2'	83:S2:29:G:C8	2.45	0.50
83:S2:159:A2M:H2'	83:S2:160:U:C6	2.45	0.50
83:S2:374:G:H2'	83:S2:375:U:C6	2.46	0.50
83:S2:1348:G:H2'	83:S2:1349:G:C8	2.46	0.50
3:L5:256:G:H2'	3:L5:257:C:C6	2.46	0.50
3:L5:299:C:H2'	3:L5:300:A:C8	2.46	0.50
3:L5:299:C:H2'	3:L5:300:A:H8	1.77	0.50
3:L5:2017:A:O2'	3:L5:2018:C:H6	1.92	0.50
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:123:U:H2'	5:L8:126:C:H42	1.76	0.50
27:LW:119:LYS:O	27:LW:123:LYS:HB2	2.10	0.50
75:SO:149:ARG:HH22	83:S2:960:U:H5''	1.75	0.50
83:S2:1244:PSU:H2'	83:S2:1245:G:H8	1.77	0.50
3:L5:318:A:H2'	3:L5:319:A:H8	1.74	0.50
3:L5:697:G:H2'	3:L5:698:G:H8	1.77	0.50
3:L5:1959:U:H4'	3:L5:1960:A:H5''	1.93	0.50
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.47	0.50
16:LL:8:MET:HE1	21:LQ:168:ARG:HB3	1.93	0.50
27:LW:123:LYS:HD2	83:S2:320:G:H5''	1.93	0.50
39:Li:44:ILE:HA	39:Li:47:VAL:HG12	1.92	0.50
42:Ll:12:PHE:HE2	42:Ll:51:LEU:HD22	1.76	0.50
47:Lr:26:SER:HB3	47:Lr:31:ASN:ND2	2.26	0.50
58:ST:104:LEU:HD23	58:ST:107:LEU:HD12	1.94	0.50
65:SA:4:ALA:HA	76:SV:80:SER:HB3	1.92	0.50
20:LP:114:ILE:HD11	20:LP:117:ILE:HB	1.92	0.50
23:LS:113:MET:HG3	23:LS:119:ALA:HB3	1.93	0.50
58:ST:85:ASN:HB3	58:ST:88:MET:HB2	1.94	0.50
64:Sg:174:VAL:HG23	64:Sg:188:HIS:HB2	1.93	0.50
64:Sg:218:LEU:HB2	64:Sg:228:TYR:HB2	1.93	0.50
68:SE:26:VAL:HG22	72:SJ:4:ALA:HB2	1.93	0.50
73:SL:46:THR:HG21	73:SL:51:ILE:HD11	1.94	0.50
77:SW:27:ILE:HG13	77:SW:61:ILE:HB	1.93	0.50
3:L5:1876:U:H2'	3:L5:1877:G:C8	2.47	0.50
3:L5:4503:A:H2'	3:L5:4504:C:C6	2.46	0.50
32:Lb:12:GLN:HE22	32:Lb:15:LYS:HE2	1.77	0.50
56:SR:44:LYS:HG3	56:SR:47:ARG:HH21	1.77	0.50
59:SU:19:ARG:HH11	59:SU:92:HIS:HB3	1.76	0.50
2:Pt:76:A:H2'	3:L5:4397:A:H1'	1.94	0.50
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.46	0.50
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.46	0.50
3:L5:2413:U:H2'	3:L5:2414:G:C8	2.47	0.50
3:L5:2764:A:H2'	3:L5:2765:A:H8	1.75	0.50
3:L5:2770:C:H2'	3:L5:2771:G:H8	1.77	0.50
3:L5:3945:A:H2'	3:L5:3946:G:C8	2.46	0.50
3:L5:4403:PSU:HN3	3:L5:4440:G:H1	1.58	0.50
4:L7:58:A:H2'	4:L7:59:G:H8	1.76	0.50
6:LA:225:ILE:HG21	6:LA:234:LYS:HA	1.93	0.50
8:LC:221:PHE:HB3	8:LC:229:LEU:HD11	1.92	0.50
12:LG:30:PRO:HG2	30:LZ:124:THR:HA	1.94	0.50
13:LH:89:ARG:HB2	13:LH:187:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LO:54:TYR:HD2	19:LO:145:VAL:HG21	1.77	0.50
25:LU:83:LEU:HD23	25:LU:86:LEU:HD21	1.92	0.50
33:Lc:34:THR:HG23	33:Lc:95:ALA:HB2	1.93	0.50
47:Lr:49:VAL:HG23	47:Lr:64:ILE:HG22	1.92	0.50
64:Sg:32:LEU:HA	64:Sg:42:MET:HA	1.93	0.50
83:S2:327:G:H5'	83:S2:328:U:C2	2.47	0.50
83:S2:609:U:H2'	83:S2:610:G:C8	2.44	0.50
83:S2:1545:A:H2'	83:S2:1546:G:C8	2.46	0.50
3:L5:223:G:H4'	3:L5:225:G:N7	2.27	0.50
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.47	0.50
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.47	0.50
4:L7:15:C:H2'	4:L7:16:A:H8	1.77	0.50
19:LO:105:PHE:HE2	19:LO:112:TYR:HE2	1.60	0.50
20:LP:92:LEU:O	20:LP:96:LYS:HG2	2.12	0.50
31:La:36:GLY:HA3	31:La:40:HIS:CE1	2.47	0.50
65:SA:142:LEU:HD12	65:SA:143:PRO:HD2	1.93	0.50
68:SE:139:LEU:HB3	68:SE:147:ILE:HG22	1.94	0.50
3:L5:87:A:H4'	31:La:63:LEU:HD12	1.94	0.50
3:L5:418:A:C2	5:L8:17:A:H1'	2.47	0.50
3:L5:425:U:H2'	3:L5:426:A:H8	1.75	0.50
3:L5:1578:U:H2'	3:L5:1579:C:H6	1.77	0.50
3:L5:2517:A:H5'	37:Lg:62:LYS:HD2	1.94	0.50
4:L7:110:G:H2'	4:L7:111:C:C6	2.47	0.50
13:LH:43:VAL:HG12	13:LH:59:LYS:HB2	1.94	0.50
35:Le:28:TYR:HB3	35:Le:30:LYS:HG2	1.93	0.50
64:Sg:208:ALA:HB2	64:Sg:218:LEU:HD13	1.94	0.50
69:SG:159:ARG:HH21	69:SG:171:THR:HG23	1.76	0.50
80:Sa:10:ARG:HD2	80:Sa:34:LYS:HD2	1.94	0.50
3:L5:1441:C:H2'	3:L5:1442:C:C5	2.47	0.50
3:L5:1999:A:H62	48:Ls:40:MET:HE2	1.76	0.50
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.46	0.50
3:L5:3721:U:H2'	3:L5:3722:G:C8	2.46	0.50
3:L5:4071:U:H2'	3:L5:4072:C:H6	1.77	0.50
6:LA:229:ALA:HB3	6:LA:234:LYS:HB3	1.94	0.50
44:Ln:14:LYS:HD3	44:Ln:18:ARG:HH11	1.76	0.50
50:SD:29:LEU:HG	50:SD:32:ASP:HB2	1.94	0.50
50:SD:222:PRO:HB3	64:Sg:190:GLY:HA3	1.94	0.50
59:SU:81:GLN:HB2	62:Sd:55:LEU:HD23	1.94	0.50
60:SZ:91:LEU:HD22	60:SZ:96:LEU:HD21	1.92	0.50
69:SG:191:ARG:HH12	83:S2:312:G:H2'	1.77	0.50
83:S2:1515:G:H2'	83:S2:1516:G:H8	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Pt:50:U:O2	2:Pt:64:G:N2	2.27	0.49
3:L5:267:G:H2'	3:L5:268:G:C8	2.47	0.49
3:L5:278:G:H5''	18:LN:8:GLN:HE22	1.77	0.49
3:L5:474:C:H2'	3:L5:475:G:C8	2.47	0.49
3:L5:1399:G:H2'	3:L5:1400:G:H8	1.76	0.49
3:L5:1732:C:H2'	3:L5:1733:G:C8	2.47	0.49
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.47	0.49
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.77	0.49
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	1.94	0.49
32:Lb:8:THR:HB	32:Lb:10:HIS:H	1.77	0.49
59:SU:26:SER:HB3	59:SU:110:VAL:HG23	1.94	0.49
80:Sa:70:LYS:HD3	83:S2:987:A:H4'	1.93	0.49
83:S2:118:C:H1'	83:S2:445:A:C5	2.46	0.49
83:S2:403:G:H2'	83:S2:404:G:H8	1.77	0.49
3:L5:246:G:H2'	3:L5:247:G:H8	1.75	0.49
3:L5:1373:A:H5''	8:LC:44:LEU:HD12	1.94	0.49
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.77	0.49
3:L5:1636:U:H5''	3:L5:1637:A:H5'	1.94	0.49
49:Lt:121:LEU:HD22	49:Lt:129:ILE:HA	1.94	0.49
49:Lt:147:HIS:CE1	49:Lt:149:HIS:HB3	2.47	0.49
64:Sg:87:LEU:HB2	64:Sg:101:PHE:HB2	1.92	0.49
65:SA:57:LYS:HZ1	65:SA:159:ILE:C	2.20	0.49
65:SA:207:PRO:HA	65:SA:210:ILE:HB	1.93	0.49
73:SL:96:ILE:HD11	78:SX:10:ALA:HB1	1.93	0.49
73:SL:133:PRO:HG2	83:S2:383:G:H21	1.76	0.49
83:S2:1288:OMU:HN3	83:S2:1311:C:H42	1.57	0.49
83:S2:1802:C:H2'	83:S2:1803:U:C6	2.47	0.49
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.76	0.49
3:L5:4685:U:H2'	3:L5:4686:G:H8	1.78	0.49
3:L5:4897:G:H2'	3:L5:4898:G:C8	2.47	0.49
52:SK:27:VAL:HB	52:SK:43:LEU:HD12	1.94	0.49
54:SP:64:LYS:HD2	54:SP:73:PRO:HG2	1.94	0.49
64:Sg:129:ILE:HB	64:Sg:142:VAL:HB	1.93	0.49
66:SB:134:LEU:HD22	66:SB:219:LYS:HZ2	1.77	0.49
70:SH:87:PHE:HB3	70:SH:90:LYS:HD2	1.94	0.49
73:SL:7:GLU:HB3	73:SL:11:GLN:HE22	1.77	0.49
82:Se:39:ASN:HD21	83:S2:551:U:H4'	1.77	0.49
83:S2:909:G:H2'	83:S2:910:G:C8	2.48	0.49
3:L5:1613:A:H5''	6:LA:183:GLY:HA3	1.94	0.49
3:L5:2413:U:H2'	3:L5:2414:G:H8	1.77	0.49
3:L5:2631:U:H5''	3:L5:2632:PSU:H5''	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4939:C:P	10:LE:156:ARG:HH22	2.35	0.49
3:L5:5054:C:H4'	3:L5:5055:G:H8	1.77	0.49
7:LB:96:PRO:HB3	19:LO:153:THR:HG22	1.93	0.49
16:LL:127:PHE:HZ	16:LL:131:PRO:HB3	1.78	0.49
19:LO:75:ALA:O	19:LO:79:ILE:HG12	2.11	0.49
83:S2:52:G:H2'	83:S2:53:C:C6	2.47	0.49
83:S2:115:U:H2'	83:S2:116:OMU:C6	2.42	0.49
3:L5:444:G:H2'	3:L5:445:U:H6	1.77	0.49
3:L5:1960:A:H5'	48:Ls:63:LYS:HG2	1.95	0.49
3:L5:2305:U:C2	35:Le:106:LYS:HD3	2.47	0.49
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.77	0.49
3:L5:4208:U:H2'	3:L5:4209:G:C8	2.48	0.49
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.48	0.49
15:LJ:160:GLU:HA	15:LJ:163:MET:HE2	1.94	0.49
46:Lp:51:ALA:H	46:Lp:54:ILE:HB	1.78	0.49
83:S2:291:G:H2'	83:S2:292:A:C8	2.48	0.49
83:S2:1777:G:H2'	83:S2:1778:C:H6	1.76	0.49
3:L5:429:A:H2'	3:L5:430:G:H8	1.76	0.49
3:L5:1081:C:O2'	3:L5:1082:C:H5'	2.12	0.49
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.77	0.49
3:L5:2474:G:C5	28:LX:47:ARG:HG2	2.47	0.49
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	1.93	0.49
6:LA:177:LYS:HB2	46:Lp:29:ILE:HD13	1.95	0.49
65:SA:181:GLU:O	65:SA:185:MET:HG2	2.11	0.49
3:L5:426:A:H2'	3:L5:427:A:C8	2.48	0.49
3:L5:2751:G:H2'	3:L5:2752:G:H8	1.76	0.49
3:L5:4567:G:H5'	7:LB:20:LYS:HB3	1.95	0.49
7:LB:206:PRO:HG2	7:LB:209:GLN:HG3	1.94	0.49
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.95	0.49
14:LI:192:PRO:HA	14:LI:197:VAL:HG12	1.94	0.49
18:LN:68:ARG:HG2	18:LN:128:LYS:HG3	1.95	0.49
30:LZ:81:MET:HE1	33:Lc:63:TYR:HE1	1.78	0.49
35:Le:23:HIS:HD2	35:Le:24:GLN:HG2	1.78	0.49
59:SU:74:SER:H	83:S2:1338:G:H4'	1.77	0.49
64:Sg:18:VAL:HB	64:Sg:301:GLY:HA3	1.95	0.49
67:SC:112:VAL:HG11	83:S2:1357:A:H5'	1.94	0.49
75:SO:50:LYS:HZ1	83:S2:951:C:H1'	1.78	0.49
77:SW:39:THR:HG23	77:SW:42:MET:HE2	1.94	0.49
83:S2:375:U:H2'	83:S2:376:A:C8	2.46	0.49
3:L5:710:G:H2'	3:L5:711:A:C8	2.48	0.49
3:L5:932:A:H61	23:LS:68:PHE:HZ	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1186:U:H3'	3:L5:1187:G:H21	1.77	0.49
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.48	0.49
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.47	0.49
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.94	0.49
3:L5:5005:G:H22	3:L5:5041:G:H1'	1.78	0.49
10:LE:66:LYS:HB3	10:LE:68:MET:HE3	1.95	0.49
12:LG:159:HIS:CD2	12:LG:185:LYS:HA	2.47	0.49
34:Ld:43:PRO:O	34:Ld:47:LYS:HG2	2.12	0.49
54:SP:108:LYS:HB3	54:SP:111:MET:HE3	1.94	0.49
63:Sf:116:ARG:HD2	63:Sf:120:GLU:HG2	1.94	0.49
83:S2:155:G:H2'	83:S2:156:G:C8	2.48	0.49
83:S2:1278:A:H2'	83:S2:1279:C:C6	2.48	0.49
3:L5:422:C:H2'	3:L5:423:G:C8	2.48	0.49
3:L5:444:G:H2'	3:L5:445:U:C6	2.48	0.49
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.47	0.49
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.47	0.49
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.47	0.49
3:L5:4147:G:H2'	3:L5:4148:C:H6	1.76	0.49
5:L8:141:C:H2'	5:L8:142:U:C6	2.47	0.49
8:LC:209:ILE:HG12	8:LC:221:PHE:HE2	1.78	0.49
12:LG:187:LYS:HB2	12:LG:198:THR:HG23	1.95	0.49
23:LS:9:GLU:HB3	23:LS:33:PHE:CE2	2.48	0.49
23:LS:83:ARG:HG2	23:LS:127:MET:HE3	1.95	0.49
30:LZ:51:ARG:HB2	30:LZ:65:ARG:HB3	1.94	0.49
75:SO:75:MET:SD	75:SO:118:ALA:HB2	2.52	0.49
83:S2:509:OMG:H2'	83:S2:510:G:H8	1.77	0.49
3:L5:1273:G:C6	10:LE:73:TYR:HB2	2.48	0.49
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.48	0.49
51:SF:78:MET:HE3	51:SF:159:ARG:NH1	2.28	0.49
67:SC:166:ARG:HG2	67:SC:181:PRO:HG3	1.95	0.49
72:SJ:65:GLU:O	72:SJ:66:LYS:HG2	2.13	0.49
79:SY:34:THR:HG23	79:SY:69:THR:HG21	1.94	0.49
83:S2:323:C:H5'	83:S2:324:C:OP1	2.12	0.49
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.48	0.48
3:L5:1377:G:H4'	3:L5:1378:C:H3'	1.94	0.48
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.48	0.48
3:L5:4775:C:H5	3:L5:4859:C:H42	1.61	0.48
10:LE:57:TYR:HB2	10:LE:62:MET:HE2	1.94	0.48
10:LE:165:LEU:HD11	10:LE:176:THR:HG22	1.95	0.48
12:LG:155:VAL:HG11	12:LG:170:LEU:HD21	1.95	0.48
12:LG:180:PRO:HG3	12:LG:219:VAL:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:162:GLN:NE2	13:LH:181:VAL:H	2.10	0.48
26:LV:94:VAL:HG11	27:LW:20:ARG:HH21	1.78	0.48
60:SZ:99:LEU:HD11	60:SZ:102:LYS:HB2	1.95	0.48
70:SH:7:LYS:HD3	70:SH:10:LYS:HB3	1.94	0.48
83:S2:461:U:H2'	83:S2:462:OMC:C6	2.48	0.48
83:S2:1805:G:H2'	83:S2:1806:A:C8	2.48	0.48
3:L5:10:A:H2'	3:L5:11:G:H8	1.78	0.48
3:L5:419:A:H61	5:L8:15:G:H1'	1.78	0.48
3:L5:1730:U:H2'	3:L5:1731:C:C6	2.49	0.48
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.78	0.48
25:LU:100:LEU:HD12	25:LU:112:LEU:HB3	1.95	0.48
30:LZ:100:VAL:HG23	30:LZ:106:LEU:HB3	1.95	0.48
51:SF:19:LEU:HD22	51:SF:109:LEU:HD21	1.96	0.48
57:SS:84:LEU:HG	57:SS:97:GLN:HB2	1.95	0.48
73:SL:17:PHE:CG	83:S2:222:U:H5''	2.47	0.48
83:S2:1304:U:H2'	83:S2:1305:C:C6	2.48	0.48
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.49	0.48
3:L5:4277:G:H5''	24:LT:17:ARG:HG2	1.96	0.48
3:L5:4389:C:H2'	3:L5:4390:A:H8	1.79	0.48
6:LA:20:VAL:HG12	6:LA:23:ARG:HH11	1.78	0.48
7:LB:195:ASP:HA	7:LB:198:ARG:HG2	1.95	0.48
16:LL:125:ILE:HD11	38:Lh:122:LYS:HG3	1.95	0.48
20:LP:16:LYS:HG2	20:LP:149:ILE:HG12	1.95	0.48
24:LT:48:VAL:HG11	24:LT:94:GLU:HG3	1.95	0.48
49:Lt:77:ALA:HB3	49:Lt:80:LEU:HB2	1.93	0.48
50:SD:123:LEU:HD13	50:SD:136:VAL:HG22	1.95	0.48
62:Sd:14:PHE:HB2	83:S2:1661:A:C8	2.46	0.48
65:SA:80:ARG:HD3	65:SA:82:THR:HG23	1.94	0.48
83:S2:1393:G:H2'	83:S2:1394:G:C8	2.47	0.48
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.12	0.48
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.48	0.48
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.79	0.48
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.48	0.48
3:L5:4601:U:H2'	3:L5:4602:A:C8	2.46	0.48
48:Ls:53:VAL:HG23	48:Ls:89:VAL:HB	1.94	0.48
55:SQ:138:ARG:HD3	83:S2:1646:C:H5''	1.94	0.48
57:SS:12:ILE:HG22	57:SS:21:ASP:HA	1.95	0.48
64:Sg:10:THR:HG22	64:Sg:308:ARG:HG2	1.95	0.48
73:SL:132:ARG:HE	83:S2:114:G:H5'	1.78	0.48
83:S2:349:A:H2'	83:S2:350:C:C6	2.48	0.48
83:S2:399:C:H5	83:S2:680:G:H5''	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1628:C:H2'	83:S2:1629:C:C6	2.49	0.48
3:L5:325:U:H2'	3:L5:326:C:C6	2.49	0.48
3:L5:1348:U:H2'	3:L5:1349:G:C8	2.43	0.48
3:L5:4951:G:H2'	3:L5:4952:G:H8	1.79	0.48
11:LF:166:ARG:HH12	11:LF:212:LYS:NZ	2.11	0.48
17:LM:7:VAL:HG21	17:LM:52:PHE:HE1	1.78	0.48
36:Lf:45:LYS:HD2	36:Lf:105:LEU:HA	1.95	0.48
59:SU:61:LEU:HD13	59:SU:84:ILE:HD13	1.95	0.48
65:SA:90:PHE:HD1	65:SA:179:ALA:HB2	1.79	0.48
83:S2:677:G:H21	83:S2:1028:A:N6	2.04	0.48
83:S2:1407:U:H2'	83:S2:1408:U:C6	2.49	0.48
3:L5:702:U:H2'	3:L5:703:G:O4'	2.13	0.48
3:L5:1876:U:H2'	3:L5:1877:G:H8	1.79	0.48
3:L5:3867:A2M:H2'	3:L5:3868:G:C8	2.48	0.48
3:L5:4253:A:H5'	3:L5:4254:G:C8	2.49	0.48
3:L5:4466:C:H2'	3:L5:4467:A:H8	1.77	0.48
5:L8:75:OMG:H8	5:L8:75:OMG:OP1	1.96	0.48
14:LI:36:LEU:HD22	14:LI:73:ASN:HD21	1.79	0.48
15:LJ:37:ALA:O	15:LJ:41:GLU:HG2	2.14	0.48
26:LV:36:ASN:HD21	26:LV:66:LYS:HB2	1.79	0.48
27:LW:78:PHE:HE2	27:LW:80:ARG:HB2	1.78	0.48
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	1.95	0.48
46:Lp:10:ILE:H	46:Lp:27:LYS:HZ3	1.60	0.48
58:ST:18:LEU:HD13	58:ST:134:ILE:HD13	1.95	0.48
64:Sg:8:ARG:HB3	64:Sg:309:VAL:HG13	1.95	0.48
74:SN:90:HIS:HA	74:SN:93:LYS:HG2	1.96	0.48
83:S2:71:G:H2'	83:S2:72:C:H4'	1.94	0.48
83:S2:484:A2M:H8	83:S2:484:A2M:O5'	2.13	0.48
83:S2:786:G:H2'	83:S2:787:G:C8	2.49	0.48
3:L5:72:C:H5	16:LL:67:HIS:HD1	1.62	0.48
3:L5:713:C:H2'	3:L5:714:G:H8	1.79	0.48
3:L5:972:C:H2'	3:L5:973:G:H8	1.78	0.48
7:LB:92:TYR:HB2	7:LB:159:VAL:HG13	1.96	0.48
26:LV:39:ILE:HG12	26:LV:61:VAL:HG11	1.95	0.48
40:Lj:67:LEU:HA	40:Lj:70:VAL:HG12	1.94	0.48
46:Lp:26:VAL:HA	46:Lp:29:ILE:HG22	1.95	0.48
55:SQ:128:GLU:HG2	55:SQ:137:ALA:HB1	1.96	0.48
58:ST:23:LYS:HE3	58:ST:51:ASN:HB3	1.95	0.48
58:ST:63:HIS:CE1	58:ST:78:ILE:HG21	2.49	0.48
79:SY:89:HIS:CE1	79:SY:90:ARG:HG3	2.49	0.48
83:S2:1280:G:H2'	83:S2:1281:G:H8	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:153:G:H2'	3:L5:154:G:H8	1.79	0.48
3:L5:1086:C:H2'	3:L5:1087:A:H8	1.79	0.48
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.49	0.48
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.48	0.48
7:LB:26:ARG:HE	7:LB:181:MET:HE3	1.79	0.48
8:LC:268:ARG:NH1	8:LC:269:LYS:HE2	2.28	0.48
14:LI:70:ILE:O	14:LI:74:LYS:HG2	2.12	0.48
19:LO:33:VAL:HG13	19:LO:102:LEU:HD13	1.95	0.48
48:Ls:160:LEU:HD23	48:Ls:161:ILE:HB	1.96	0.48
50:SD:28:GLU:HA	52:SK:61:GLN:HG3	1.95	0.48
75:SO:102:GLY:H	75:SO:134:PRO:HB2	1.79	0.48
75:SO:149:ARG:HH12	83:S2:960:U:H5''	1.79	0.48
77:SW:86:LEU:HD11	77:SW:113:HIS:HB2	1.95	0.48
83:S2:374:G:H2'	83:S2:375:U:H6	1.79	0.48
3:L5:1315:C:H2'	3:L5:1316:OMG:H8	1.79	0.48
3:L5:1888:A:N7	3:L5:2049:G:H5'	2.29	0.48
3:L5:2018:C:H2'	3:L5:2019:C:H6	1.78	0.48
3:L5:2638:G:H22	3:L5:2719:C:P	2.36	0.48
3:L5:3842:C:H1'	26:LV:52:LEU:HD12	1.95	0.48
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.49	0.48
4:L7:15:C:H2'	4:L7:16:A:C8	2.49	0.48
12:LG:94:GLN:HG3	12:LG:97:LYS:NZ	2.28	0.48
18:LN:114:ARG:HH11	18:LN:137:PRO:HG3	1.79	0.48
20:LP:95:LEU:HD23	20:LP:148:MET:HE1	1.96	0.48
22:LR:151:ARG:HH21	22:LR:155:LEU:HD12	1.79	0.48
32:Lb:61:ASN:O	32:Lb:65:MET:HG2	2.14	0.48
54:SP:130:ARG:HD3	54:SP:131:PRO:HD2	1.96	0.48
57:SS:129:LEU:HD13	83:S2:1521:C:H5'	1.95	0.48
68:SE:148:ARG:NH1	83:S2:123:G:H4'	2.28	0.48
69:SG:7:PHE:HD2	69:SG:10:THR:HG22	1.78	0.48
82:Se:38:TYR:O	82:Se:42:PHE:HB2	2.14	0.48
83:S2:35:C:H5''	83:S2:579:C:H5''	1.96	0.48
83:S2:835:C:H4'	83:S2:836:G:C8	2.48	0.48
83:S2:1643:U:H2'	83:S2:1644:C:C6	2.49	0.48
2:Pt:10:G:N2	2:Pt:26:G:H1'	2.29	0.48
3:L5:2045:G:O2'	3:L5:2046:G:H5''	2.14	0.48
3:L5:2696:A:H62	41:Lk:35:LYS:NZ	2.12	0.48
3:L5:3924:C:H2'	3:L5:3925:OMU:H6	1.96	0.48
3:L5:4319:C:H2'	3:L5:4320:G:C8	2.49	0.48
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.49	0.48
12:LG:232:GLU:HB2	12:LG:235:ARG:HE	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LI:48:LEU:HB2	14:LI:142:LEU:HA	1.96	0.48
43:Lm:110:CYS:HB3	43:Lm:115:CYS:SG	2.53	0.48
51:SF:17:ILE:HG13	51:SF:46:ALA:HB3	1.95	0.48
56:SR:109:LEU:HD13	65:SA:52:LYS:HE2	1.96	0.48
3:L5:1725:U:H2'	3:L5:1726:U:C6	2.49	0.47
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.49	0.47
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.49	0.47
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.49	0.47
4:L7:23:A:H2'	4:L7:24:C:C6	2.49	0.47
10:LE:261:ILE:HG23	10:LE:267:LEU:HD22	1.95	0.47
13:LH:51:LYS:HG3	13:LH:52:LYS:H	1.79	0.47
18:LN:42:PRO:HG3	18:LN:53:TYR:CE2	2.48	0.47
52:SK:64:TRP:CZ3	62:Sd:23:VAL:HG22	2.49	0.47
56:SR:95:ILE:HB	56:SR:118:GLN:HE22	1.79	0.47
57:SS:44:VAL:HG21	57:SS:71:MET:HE1	1.95	0.47
62:Sd:3:HIS:CE1	62:Sd:5:GLN:HB2	2.49	0.47
66:SB:103:MET:HB3	66:SB:215:VAL:HG12	1.96	0.47
66:SB:137:LEU:HD11	66:SB:176:VAL:HG21	1.96	0.47
71:SI:27:TYR:HB3	71:SI:49:ARG:HH22	1.78	0.47
73:SL:101:ARG:HB2	78:SX:10:ALA:HB2	1.95	0.47
83:S2:696:G:H8	83:S2:733:C:H41	1.62	0.47
83:S2:1359:U:H2'	83:S2:1360:U:H6	1.78	0.47
83:S2:1417:C:O2	83:S2:1422:G:C6	2.67	0.47
3:L5:138:G:H2'	3:L5:139:G:C8	2.47	0.47
3:L5:690:C:H2'	3:L5:691:C:C6	2.49	0.47
3:L5:1091:C:H2'	3:L5:1092:G:C8	2.49	0.47
8:LC:28:PHE:HA	8:LC:129:ALA:HA	1.96	0.47
15:LJ:22:LEU:HD11	15:LJ:128:LEU:HB2	1.96	0.47
19:LO:186:GLU:HA	19:LO:189:ILE:HB	1.96	0.47
57:SS:89:ASP:HB3	57:SS:93:GLY:H	1.79	0.47
69:SG:227:GLN:HB3	69:SG:231:ARG:HH21	1.78	0.47
75:SO:44:VAL:HG23	75:SO:93:LEU:HD11	1.96	0.47
83:S2:375:U:H2'	83:S2:376:A:H8	1.79	0.47
83:S2:1396:A:N7	83:S2:1449:G:O6	2.46	0.47
83:S2:1547:C:H1'	83:S2:1670:C:H4'	1.97	0.47
83:S2:1610:G:H2'	83:S2:1611:G:H8	1.79	0.47
83:S2:1651:A:H2'	83:S2:1652:G:H8	1.78	0.47
3:L5:425:U:H2'	3:L5:426:A:C8	2.49	0.47
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.79	0.47
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.49	0.47
3:L5:1788:A:H2'	14:LI:22:PHE:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.50	0.47
3:L5:2401:A2M:HM'3	3:L5:2401:A2M:H1'	1.74	0.47
71:SI:72:CYS:HG	71:SI:112:TRP:CG	2.32	0.47
73:SL:93:LEU:HD11	78:SX:8:ARG:HE	1.79	0.47
78:SX:137:LYS:HE2	83:S2:30:C:O3'	2.15	0.47
83:S2:51:U:H2'	83:S2:52:G:H8	1.79	0.47
83:S2:1098:C:H2'	83:S2:1099:G:C8	2.48	0.47
83:S2:1204:A:H2'	83:S2:1205:C:C6	2.49	0.47
83:S2:1276:A:C5	83:S2:1322:G:H1'	2.49	0.47
83:S2:1329:U:O2	83:S2:1500:G:O6	2.31	0.47
83:S2:1588:A:H2'	83:S2:1589:A:C8	2.49	0.47
3:L5:265:C:H1'	3:L5:266:C:H5''	1.94	0.47
3:L5:1878:G:H2'	3:L5:1879:C:C6	2.49	0.47
5:L8:148:A:H2'	5:L8:149:G:C8	2.50	0.47
27:LW:78:PHE:CE2	27:LW:80:ARG:HB2	2.49	0.47
71:SI:49:ARG:HD3	71:SI:50:GLY:N	2.29	0.47
73:SL:111:VAL:HG12	73:SL:140:PHE:HB2	1.95	0.47
77:SW:28:ARG:NH2	83:S2:921:G:H3'	2.30	0.47
3:L5:2374:A:H2'	3:L5:2375:A:H8	1.80	0.47
3:L5:4066:U:H2'	3:L5:4067:U:H6	1.79	0.47
5:L8:55:PSU:H2'	5:L8:56:G:H8	1.79	0.47
5:L8:78:G:H2'	5:L8:79:G:C8	2.49	0.47
8:LC:298:ILE:HD13	21:LQ:131:PRO:HG3	1.97	0.47
16:LL:9:VAL:HG13	21:LQ:168:ARG:HH12	1.80	0.47
22:LR:112:SER:O	22:LR:113:LYS:HG3	2.15	0.47
28:LX:96:LEU:HB2	28:LX:138:VAL:HG13	1.96	0.47
31:La:103:VAL:HG22	31:La:125:LYS:O	2.15	0.47
38:Lh:4:ILE:HD12	38:Lh:9:LEU:HD11	1.95	0.47
54:SP:49:LEU:HD13	54:SP:53:GLN:HG3	1.95	0.47
59:SU:40:ILE:HG22	59:SU:44:LYS:NZ	2.30	0.47
59:SU:56:MET:HE3	59:SU:88:LEU:HB2	1.96	0.47
60:SZ:106:GLN:HA	60:SZ:106:GLN:NE2	2.29	0.47
67:SC:64:THR:HG22	67:SC:66:LEU:N	2.28	0.47
70:SH:47:ALA:HB3	70:SH:63:PHE:HD2	1.79	0.47
72:SJ:86:VAL:HG11	72:SJ:105:PHE:HD1	1.78	0.47
78:SX:49:GLY:HA2	78:SX:75:ILE:HG23	1.96	0.47
79:SY:21:LYS:HE2	79:SY:75:ILE:HD11	1.97	0.47
83:S2:941:C:H2'	83:S2:942:G:H8	1.79	0.47
2:Pt:27:U:H2'	2:Pt:28:U:C6	2.50	0.47
3:L5:2079:G:H2'	3:L5:2080:U:H6	1.80	0.47
8:LC:33:ARG:HG3	8:LC:35:ASP:OD1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:223:ARG:HH22	10:LE:238:GLU:HG3	1.80	0.47
26:LV:90:ARG:HH22	26:LV:96:LEU:HD13	1.79	0.47
27:LW:52:THR:O	27:LW:56:ARG:HG2	2.14	0.47
32:Lb:43:MET:HE3	32:Lb:47:LYS:HG3	1.96	0.47
53:SM:68:LEU:HD11	63:Sf:106:TYR:HE2	1.79	0.47
55:SQ:58:LEU:HB3	55:SQ:62:ARG:HD2	1.97	0.47
59:SU:55:ARG:HD2	83:S2:1446:A:N3	2.29	0.47
75:SO:101:GLY:HA3	75:SO:134:PRO:HD2	1.96	0.47
83:S2:146:G:H2'	83:S2:147:A:H8	1.80	0.47
83:S2:467:G:H2'	83:S2:468:A2M:H8	1.97	0.47
83:S2:1383:A2M:HM'3	83:S2:1383:A2M:H1'	1.69	0.47
83:S2:1829:G:H1'	83:S2:1850:MA6:C2	2.43	0.47
1:CI:62:VAL:HG21	25:LU:115:PHE:CD2	2.49	0.47
3:L5:1079:C:H2'	3:L5:1080:C:C6	2.50	0.47
3:L5:1471:U:H2'	3:L5:1472:C:C6	2.49	0.47
3:L5:1511:U:H2'	3:L5:1512:G:C8	2.49	0.47
3:L5:1631:A:C8	6:LA:199:VAL:HG11	2.50	0.47
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.50	0.47
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.78	0.47
3:L5:4758:U:H5''	19:LO:116:LYS:HG2	1.95	0.47
3:L5:4775:C:H41	3:L5:4859:C:N4	2.13	0.47
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.80	0.47
7:LB:103:LYS:HB3	7:LB:153:MET:HE2	1.96	0.47
14:LI:7:ARG:HA	14:LI:10:ARG:HG3	1.97	0.47
35:Le:22:ARG:NH2	35:Le:31:ILE:HG23	2.30	0.47
46:Lp:77:VAL:HG13	46:Lp:80:LYS:HZ3	1.79	0.47
51:SF:141:VAL:HG12	61:Sc:47:LYS:HG2	1.96	0.47
58:ST:23:LYS:HG2	58:ST:54:TYR:HD2	1.79	0.47
65:SA:76:VAL:HG12	65:SA:123:VAL:HB	1.96	0.47
65:SA:209:GLU:HA	65:SA:212:LYS:HG2	1.97	0.47
66:SB:67:PHE:CE1	75:SO:48:SER:HB3	2.50	0.47
66:SB:150:ILE:HG12	83:S2:1124:C:H5''	1.97	0.47
67:SC:259:THR:HG23	76:SV:16:LYS:HZ3	1.80	0.47
67:SC:261:PHE:HD2	76:SV:52:THR:HG23	1.80	0.47
72:SJ:28:GLU:O	72:SJ:32:ILE:HG12	2.15	0.47
73:SL:28:THR:HA	73:SL:29:GLY:HA2	1.61	0.47
77:SW:28:ARG:HB3	77:SW:29:PRO:HD3	1.96	0.47
83:S2:24:C:O2'	83:S2:25:A:H8	1.98	0.47
83:S2:329:G:H2'	83:S2:330:G:C8	2.50	0.47
83:S2:511:U:H2'	83:S2:512:A:C8	2.49	0.47
83:S2:929:G:H21	83:S2:1104:G:H4'	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1405:A:H2'	83:S2:1406:G:O4'	2.15	0.47
83:S2:1775:U:H2'	83:S2:1776:G:C2	2.50	0.47
3:L5:687:U:N3	10:LE:95:PRO:HG2	2.30	0.47
3:L5:714:G:H2'	3:L5:715:G:H8	1.79	0.47
3:L5:1179:U:H3'	3:L5:1180:C:H5''	1.97	0.47
3:L5:1339:U:H2'	3:L5:1340:OMC:H6	1.80	0.47
3:L5:1471:U:H2'	3:L5:1472:C:H6	1.79	0.47
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.49	0.47
3:L5:2824:OMC:H1'	3:L5:2824:OMC:HM23	1.61	0.47
3:L5:4066:U:H2'	3:L5:4067:U:C6	2.50	0.47
3:L5:4627:U:H4'	7:LB:373:LYS:HE2	1.95	0.47
9:LD:287:PHE:HZ	14:LI:214:SER:HB3	1.79	0.47
10:LE:274:VAL:HG21	36:Lf:2:SER:HB2	1.97	0.47
12:LG:189:ARG:HG2	12:LG:192:ARG:HH22	1.80	0.47
16:LL:87:HIS:HB3	16:LL:90:VAL:HG22	1.97	0.47
35:Le:38:PRO:HB3	35:Le:43:ASN:ND2	2.29	0.47
48:Ls:16:LYS:HZ3	48:Ls:54:LEU:HD11	1.79	0.47
65:SA:66:VAL:HG11	65:SA:185:MET:HG3	1.96	0.47
66:SB:33:VAL:HG23	66:SB:44:ILE:HB	1.97	0.47
67:SC:166:ARG:H	67:SC:247:THR:HG21	1.79	0.47
67:SC:167:ARG:HB3	67:SC:177:PRO:HB2	1.97	0.47
71:SI:139:LYS:HE3	71:SI:149:TYR:CZ	2.50	0.47
83:S2:96:C:H2'	83:S2:97:U:C6	2.49	0.47
83:S2:141:A:H4'	83:S2:142:C:H3'	1.97	0.47
3:L5:35:U:H4'	3:L5:1525:A:C2	2.50	0.47
3:L5:1900:C:H4'	35:Le:60:TYR:CE1	2.50	0.47
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.50	0.47
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.96	0.47
3:L5:5010:PSU:H2'	3:L5:5011:A:C8	2.50	0.47
13:LH:64:ARG:HA	13:LH:67:LEU:HB2	1.97	0.47
23:LS:8:ARG:HB2	23:LS:10:TYR:CE1	2.49	0.47
55:SQ:48:GLN:HG2	55:SQ:52:LEU:HD13	1.97	0.47
79:SY:9:THR:H	83:S2:837:A:N6	2.13	0.47
83:S2:941:C:H2'	83:S2:942:G:C8	2.50	0.47
83:S2:1420:G:H21	83:S2:1421:A:H1'	1.80	0.47
83:S2:1468:C:H2'	83:S2:1469:A:H8	1.80	0.47
83:S2:1491:G:H2'	83:S2:1492:U:C6	2.49	0.47
3:L5:434:A:H3'	3:L5:435:A:H8	1.80	0.47
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.15	0.47
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.50	0.47
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4079:C:H2'	3:L5:4080:C:H6	1.80	0.47
3:L5:4237:C:H2'	3:L5:4238:G:H8	1.80	0.47
3:L5:4421:C:N4	3:L5:4475:G:H22	2.12	0.47
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.15	0.47
39:Li:76:ARG:HD3	39:Li:76:ARG:HA	1.72	0.47
46:Lp:41:PHE:CD2	46:Lp:62:LYS:HG2	2.49	0.47
58:ST:39:LEU:HD21	58:ST:52:TRP:CZ3	2.49	0.47
58:ST:47:PRO:HA	83:S2:1539:U:H4'	1.96	0.47
63:Sf:103:LEU:HB2	63:Sf:105:TYR:CE2	2.49	0.47
68:SE:36:HIS:CG	68:SE:85:GLY:HA3	2.49	0.47
68:SE:77:ARG:NH1	83:S2:121:OMU:H5'	2.30	0.47
69:SG:3:LEU:HD13	69:SG:109:LEU:HB3	1.97	0.47
83:S2:1116:C:H2'	83:S2:1117:C:C6	2.50	0.47
3:L5:436:C:H2'	3:L5:437:G:H8	1.80	0.46
3:L5:1511:U:H2'	3:L5:1512:G:H8	1.79	0.46
3:L5:4523:A2M:H2'	3:L5:4559:A:N7	2.30	0.46
5:L8:6:C:H2'	5:L8:7:U:C6	2.50	0.46
10:LE:72:LYS:HD3	32:Lb:119:CYS:HB3	1.97	0.46
29:LY:37:GLU:HA	29:LY:40:GLN:CD	2.40	0.46
33:Lc:48:LEU:HD11	33:Lc:60:ILE:HG21	1.96	0.46
48:Ls:120:GLU:HB2	48:Ls:163:THR:HG22	1.96	0.46
49:Lt:57:ARG:HD3	49:Lt:80:LEU:HG	1.96	0.46
56:SR:132:ARG:HE	66:SB:151:ARG:HA	1.79	0.46
66:SB:114:VAL:HG11	83:S2:987:A:H2'	1.96	0.46
68:SE:136:ILE:HD12	68:SE:149:TYR:HE1	1.79	0.46
82:Se:56:ASN:HB3	83:S2:606:G:H5''	1.96	0.46
83:S2:795:A:H2'	83:S2:796:G:H8	1.78	0.46
83:S2:1093:A:H2'	83:S2:1094:C:H6	1.79	0.46
83:S2:1610:G:H2'	83:S2:1611:G:C8	2.50	0.46
3:L5:509:A:C4	31:La:82:VAL:HG12	2.50	0.46
3:L5:3785:A2M:HM'1	3:L5:4537:C:H1'	1.98	0.46
3:L5:3883:U:H2'	3:L5:3884:PSU:C6	2.49	0.46
3:L5:4723:A:H2'	3:L5:4724:A:H8	1.80	0.46
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.49	0.46
4:L7:4:U:H2'	4:L7:5:A:C8	2.49	0.46
5:L8:119:C:H2'	5:L8:120:G:C8	2.50	0.46
8:LC:140:LYS:HD3	8:LC:245:HIS:HB2	1.97	0.46
9:LD:209:ARG:HA	9:LD:212:MET:HE3	1.97	0.46
20:LP:40:HIS:CG	20:LP:42:ARG:HH11	2.33	0.46
51:SF:102:LEU:O	60:SZ:66:LYS:HD3	2.16	0.46
55:SQ:17:LYS:H	55:SQ:126:ARG:NH2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SR:126:MET:HB3	65:SA:43:SER:HB2	1.97	0.46
68:SE:193:GLY:HA2	68:SE:212:ASP:HA	1.97	0.46
71:SI:65:PHE:HE1	71:SI:78:ILE:HD11	1.80	0.46
83:S2:1382:A:H2'	83:S2:1383:A2M:H8	1.97	0.46
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.50	0.46
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.51	0.46
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.50	0.46
3:L5:4906:C:H2'	3:L5:4907:G:H8	1.80	0.46
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.50	0.46
9:LD:204:VAL:O	9:LD:208:MET:HG2	2.15	0.46
11:LF:52:GLU:HG3	32:Lb:93:LEU:HD13	1.96	0.46
17:LM:6:PHE:H	17:LM:11:ARG:NH2	2.14	0.46
18:LN:13:LYS:NZ	39:Li:45:ARG:HA	2.29	0.46
46:Lp:9:GLY:HA3	46:Lp:27:LYS:NZ	2.30	0.46
65:SA:125:THR:HA	65:SA:147:LEU:HD12	1.98	0.46
66:SB:35:ALA:HB1	66:SB:39:PHE:HD2	1.80	0.46
83:S2:455:A:H2'	83:S2:456:C:H6	1.80	0.46
83:S2:931:C:H2'	83:S2:932:G:C8	2.51	0.46
83:S2:991:G:N1	83:S2:1134:G:H4'	2.30	0.46
3:L5:1195:G:H2'	3:L5:1196:G:H8	1.81	0.46
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.51	0.46
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.65	0.46
3:L5:4079:C:H2'	3:L5:4080:C:C6	2.51	0.46
3:L5:4236:G:H2'	3:L5:4237:C:C6	2.50	0.46
3:L5:4590:A2M:HM'3	3:L5:4590:A2M:H1'	1.51	0.46
36:Lf:46:ARG:HD3	36:Lf:72:GLY:O	2.15	0.46
48:Ls:134:LYS:HD2	48:Ls:137:PHE:HE2	1.80	0.46
51:SF:127:ARG:HG2	51:SF:136:ARG:HB2	1.97	0.46
67:SC:264:SER:H	67:SC:267:GLN:HE21	1.64	0.46
73:SL:66:VAL:HA	73:SL:132:ARG:HH12	1.80	0.46
83:S2:409:C:H2'	83:S2:410:G:H8	1.81	0.46
83:S2:880:G:H3'	83:S2:881:G:H8	1.78	0.46
83:S2:900:C:H5'	83:S2:901:G:N7	2.30	0.46
3:L5:1411:C:H2'	3:L5:1412:G:C8	2.51	0.46
3:L5:1884:C:H4'	3:L5:2070:U:C4	2.49	0.46
3:L5:2610:G:H2'	3:L5:2611:A:H8	1.79	0.46
3:L5:4232:U:H1'	3:L5:4233:A:C2	2.51	0.46
3:L5:4448:G:H5''	3:L5:4449:A:H5'	1.97	0.46
9:LD:7:VAL:HG13	9:LD:8:LYS:HG3	1.97	0.46
9:LD:166:ALA:HB1	9:LD:171:LEU:HD12	1.98	0.46
10:LE:223:ARG:HA	10:LE:224:LYS:HA	1.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LG:108:GLN:O	12:LG:111:LYS:HG2	2.16	0.46
16:LL:188:ASN:HA	16:LL:195:ARG:HH21	1.80	0.46
31:La:148:ALA:HB3	39:Li:6:PRO:HB2	1.97	0.46
33:Lc:18:LEU:HG	33:Lc:22:MET:HE1	1.97	0.46
35:Le:22:ARG:HD3	35:Le:34:ASN:O	2.15	0.46
45:Lo:74:GLU:HG3	45:Lo:76:ASN:H	1.80	0.46
58:ST:74:SER:O	58:ST:78:ILE:HD12	2.15	0.46
65:SA:148:CYS:HB3	65:SA:152:SER:HB2	1.96	0.46
72:SJ:121:LYS:HD3	83:S2:527:C:H4'	1.97	0.46
83:S2:348:A:H2'	83:S2:349:A:C8	2.50	0.46
3:L5:20:U:H3'	3:L5:21:G:C8	2.50	0.46
3:L5:23:C:H2'	3:L5:24:G:O4'	2.16	0.46
3:L5:189:G:H2'	3:L5:190:G:C8	2.51	0.46
3:L5:676:C:H2'	3:L5:677:G:C8	2.50	0.46
3:L5:689:U:H2'	3:L5:690:C:C6	2.51	0.46
3:L5:4523:A2M:H1'	3:L5:4558:U:C4	2.51	0.46
9:LD:49:TYR:HB3	9:LD:64:ILE:HD11	1.97	0.46
14:LI:162:ARG:NE	14:LI:162:ARG:HA	2.30	0.46
65:SA:5:LEU:HD11	76:SV:41:LYS:HD3	1.98	0.46
65:SA:107:THR:HG22	65:SA:117:ARG:HG2	1.98	0.46
66:SB:134:LEU:HG	66:SB:218:LEU:HD12	1.97	0.46
83:S2:1396:A:C5	83:S2:1449:G:O6	2.68	0.46
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.50	0.46
3:L5:1654:G:C6	3:L5:3914:U:H5''	2.51	0.46
3:L5:4952:G:H2'	3:L5:4953:G:C8	2.51	0.46
8:LC:142:HIS:CE1	8:LC:248:ARG:HD2	2.51	0.46
23:LS:98:ARG:HG3	23:LS:142:VAL:HG23	1.97	0.46
33:Lc:62:TYR:HE2	37:Lg:99:GLU:HG3	1.80	0.46
64:Sg:215:GLN:HE22	64:Sg:217:MET:HG2	1.81	0.46
69:SG:50:VAL:HG23	69:SG:113:ILE:HG13	1.98	0.46
83:S2:314:U:H2'	83:S2:315:C:C6	2.50	0.46
83:S2:1337:4AC:O5'	83:S2:1337:4AC:H6	2.15	0.46
3:L5:221:C:H2'	3:L5:222:C:C6	2.50	0.46
3:L5:676:C:H2'	3:L5:677:G:H8	1.80	0.46
3:L5:1449:C:H2'	3:L5:1450:C:C6	2.51	0.46
3:L5:1700:G:H2'	3:L5:1704:C:H42	1.81	0.46
9:LD:279:ARG:HG2	9:LD:283:LYS:HE2	1.98	0.46
38:Lh:23:ASP:O	38:Lh:26:VAL:HG22	2.16	0.46
54:SP:28:MET:HG3	54:SP:33:LEU:HB2	1.96	0.46
64:Sg:21:ILE:HD11	64:Sg:307:VAL:HG21	1.98	0.46
68:SE:87:MET:HE1	68:SE:123:LEU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:293:C:O2'	83:S2:294:U:H3'	2.16	0.46
83:S2:354:OMU:HM23	83:S2:354:OMU:H1'	1.79	0.46
83:S2:543:C:H3'	83:S2:544:G:H8	1.79	0.46
3:L5:32:G:H21	3:L5:50:C:H5	1.64	0.46
3:L5:126:C:H2'	3:L5:127:G:H8	1.81	0.46
3:L5:474:C:H2'	3:L5:475:G:H8	1.81	0.46
3:L5:1199:G:H2'	3:L5:1200:G:C8	2.51	0.46
3:L5:1779:U:H2'	3:L5:1780:A:H8	1.80	0.46
3:L5:1845:U:H2'	3:L5:1846:G:H8	1.81	0.46
3:L5:2369:U:H1'	34:Ld:39:LYS:NZ	2.30	0.46
3:L5:4173:G:H2'	3:L5:4174:U:C6	2.51	0.46
3:L5:5018:C:H2'	3:L5:5019:A:C8	2.50	0.46
7:LB:250:LYS:HE2	7:LB:250:LYS:HB2	1.81	0.46
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.96	0.46
29:LY:103:LYS:HA	29:LY:103:LYS:HD3	1.81	0.46
31:La:89:ASN:HA	31:La:92:LYS:HG2	1.98	0.46
64:Sg:24:THR:HA	64:Sg:71:ILE:HD13	1.98	0.46
66:SB:169:MET:HE2	66:SB:169:MET:HA	1.98	0.46
77:SW:25:VAL:HG12	77:SW:63:VAL:HB	1.97	0.46
83:S2:693:A:H2'	83:S2:694:G:N7	2.31	0.46
83:S2:890:U:H3	83:S2:895:G:H22	1.62	0.46
2:Pt:22:U:H2'	2:Pt:23:C:C6	2.51	0.46
2:Pt:65:G:H2'	2:Pt:66:C:C6	2.51	0.46
3:L5:86:U:H2'	3:L5:87:A:C8	2.51	0.46
3:L5:710:G:H2'	3:L5:711:A:H8	1.81	0.46
3:L5:1598:C:H2'	3:L5:1599:A:H8	1.80	0.46
3:L5:2081:C:H2'	3:L5:2082:G:H8	1.81	0.46
3:L5:4549:G:H2'	3:L5:4550:G:H8	1.81	0.46
10:LE:132:PRO:HG2	10:LE:135:GLN:OE1	2.16	0.46
11:LF:159:TYR:HD1	11:LF:168:ALA:HA	1.80	0.46
19:LO:171:LYS:HA	19:LO:171:LYS:HD3	1.63	0.46
29:LY:85:VAL:HG22	29:LY:97:VAL:HB	1.98	0.46
37:Lg:61:PRO:HA	37:Lg:64:LEU:HD23	1.98	0.46
40:Lj:42:LYS:HA	40:Lj:42:LYS:HD3	1.78	0.46
49:Lt:16:ARG:HD3	49:Lt:18:THR:HG22	1.97	0.46
53:SM:23:LYS:O	53:SM:27:ILE:HG12	2.16	0.46
54:SP:108:LYS:HG3	54:SP:110:GLU:H	1.80	0.46
55:SQ:17:LYS:H	55:SQ:126:ARG:CZ	2.29	0.46
69:SG:88:ARG:HH12	83:S2:452:G:H4'	1.80	0.46
70:SH:33:ASN:ND2	70:SH:36:LEU:HB3	2.30	0.46
78:SX:68:LYS:HG2	78:SX:91:LEU:HD13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SY:9:THR:HA	79:SY:25:ILE:HG22	1.98	0.46
83:S2:205:G:H2'	83:S2:206:G:H8	1.81	0.46
83:S2:1324:G:O6	83:S2:1504:U:O4	2.34	0.46
3:L5:227:A:H4'	29:LY:1:MET:HE2	1.98	0.45
3:L5:490:C:H2'	3:L5:491:G:H8	1.79	0.45
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.52	0.45
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.51	0.45
3:L5:2340:C:H4'	8:LC:42:THR:HG23	1.98	0.45
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.97	0.45
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.16	0.45
3:L5:3844:PSU:H2'	3:L5:3845:A:H8	1.81	0.45
4:L7:112:U:H2'	4:L7:113:G:H8	1.81	0.45
5:L8:153:C:H2'	5:L8:154:G:C8	2.52	0.45
11:LF:220:MET:HB3	11:LF:232:ASP:OD2	2.16	0.45
51:SF:60:ARG:HE	83:S2:1679:A:P	2.40	0.45
83:S2:534:G:H2'	83:S2:535:G:H8	1.81	0.45
83:S2:1183:A:H2'	83:S2:1184:G:H8	1.81	0.45
3:L5:667:A:H5'	47:Lr:46:ARG:NH2	2.31	0.45
3:L5:713:C:H2'	3:L5:714:G:C8	2.51	0.45
3:L5:956:A:H1'	3:L5:2076:G:H5''	1.98	0.45
3:L5:1394:G:H4'	16:LL:186:ARG:HH22	1.80	0.45
3:L5:1505:C:H2'	3:L5:1506:G:C8	2.52	0.45
3:L5:2476:G:H2'	3:L5:2477:A:C8	2.51	0.45
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.51	0.45
10:LE:201:ILE:HG13	10:LE:203:ILE:HG23	1.97	0.45
17:LM:120:ASN:HA	17:LM:123:ILE:HG22	1.99	0.45
32:Lb:43:MET:HG3	32:Lb:47:LYS:NZ	2.31	0.45
37:Lg:54:ARG:HD3	37:Lg:54:ARG:H	1.80	0.45
40:Lj:19:CYS:SG	40:Lj:34:CYS:HB2	2.55	0.45
55:SQ:100:VAL:HG22	55:SQ:101:ASP:H	1.80	0.45
79:SY:39:GLU:HA	79:SY:42:GLU:CD	2.41	0.45
83:S2:113:G:H22	83:S2:292:A:H2'	1.81	0.45
83:S2:348:A:H2'	83:S2:349:A:H8	1.80	0.45
83:S2:1777:G:H2'	83:S2:1778:C:C6	2.51	0.45
2:Pt:5:C:H2'	2:Pt:6:C:C6	2.51	0.45
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.51	0.45
3:L5:4346:U:H2'	3:L5:4347:G:C8	2.51	0.45
3:L5:4761:G:H2'	3:L5:4762:A:H8	1.81	0.45
7:LB:144:LYS:HZ3	7:LB:148:LYS:HE2	1.81	0.45
16:LL:111:GLN:HA	16:LL:114:VAL:HG22	1.98	0.45
17:LM:13:ALA:HB1	17:LM:55:MET:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LN:43:THR:HG21	18:LN:121:VAL:HG21	1.97	0.45
28:LX:83:THR:HG23	28:LX:86:ALA:H	1.82	0.45
59:SU:64:THR:HG22	59:SU:77:TRP:HE3	1.81	0.45
70:SH:111:LYS:HE3	83:S2:796:G:H21	1.81	0.45
83:S2:656:G:N2	83:S2:663:C:H5''	2.31	0.45
83:S2:1090:C:H2'	83:S2:1091:C:C6	2.52	0.45
3:L5:1692:C:H5''	21:LQ:53:MET:HE1	1.98	0.45
3:L5:1971:C:H2'	3:L5:1972:G:C8	2.52	0.45
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.16	0.45
3:L5:2846:G:H2'	3:L5:2847:G:H8	1.82	0.45
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.79	0.45
3:L5:4159:C:H2'	3:L5:4160:C:C6	2.52	0.45
3:L5:4237:C:H2'	3:L5:4238:G:C8	2.51	0.45
11:LF:179:LEU:HB3	11:LF:184:ILE:HB	1.98	0.45
15:LJ:42:GLN:HG3	15:LJ:117:ILE:HD12	1.98	0.45
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.52	0.45
44:Ln:14:LYS:HA	44:Ln:17:ARG:HG2	1.98	0.45
56:SR:90:ALA:HB3	65:SA:203:PHE:HE2	1.82	0.45
58:ST:121:ARG:HH21	83:S2:1563:G:H5''	1.81	0.45
60:SZ:58:LEU:HD12	60:SZ:62:VAL:HG21	1.97	0.45
64:Sg:191:HIS:CG	64:Sg:195:LEU:HD21	2.52	0.45
82:Se:11:LYS:O	82:Se:15:GLN:HG3	2.16	0.45
83:S2:544:G:H2'	83:S2:545:A:C8	2.51	0.45
2:Pt:23:C:H2'	2:Pt:24:A:C8	2.51	0.45
3:L5:495:C:H2'	3:L5:496:G:C8	2.52	0.45
3:L5:962:C:H2'	3:L5:1702:C:H41	1.82	0.45
3:L5:1258:G:H2'	3:L5:1259:G:C8	2.52	0.45
3:L5:1725:U:O2	11:LF:132:MET:HE1	2.16	0.45
3:L5:1943:A:H5''	14:LI:162:ARG:NH1	2.32	0.45
3:L5:2888:G:H5''	22:LR:80:LYS:NZ	2.31	0.45
3:L5:4467:A:H61	3:L5:4490:C:H42	1.62	0.45
3:L5:4623:OMG:HM23	3:L5:4623:OMG:H1'	1.66	0.45
3:L5:4704:C:H4'	13:LH:129:ARG:HH22	1.80	0.45
85:L5:5263:SPM:H111	85:L5:5263:SPM:H82	1.68	0.45
10:LE:68:MET:HE2	10:LE:71:ARG:HD3	1.98	0.45
23:LS:139:ARG:HB2	23:LS:142:VAL:HG12	1.97	0.45
33:Lc:23:LYS:HE3	33:Lc:23:LYS:HB3	1.83	0.45
35:Le:42:ASP:HA	35:Le:47:ARG:HH12	1.81	0.45
64:Sg:256:ILE:HB	64:Sg:270:LEU:HB2	1.98	0.45
68:SE:60:GLU:O	68:SE:64:ILE:HG13	2.15	0.45
68:SE:95:THR:HG22	79:SY:16:ARG:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SY:108:LYS:HZ2	83:S2:54:A:H5'	1.81	0.45
83:S2:1351:G:N1	83:S2:1360:U:N3	2.43	0.45
2:Pt:3:C:H42	2:Pt:70:A:N6	2.12	0.45
2:Pt:35:A:H2'	2:Pt:36:C:H6	1.82	0.45
3:L5:49:U:H2'	3:L5:50:C:H6	1.82	0.45
3:L5:319:A:H1'	3:L5:3726:A:N3	2.32	0.45
3:L5:1479:G:H2'	3:L5:1480:C:C6	2.52	0.45
3:L5:3916:G:H2'	3:L5:3917:A:H8	1.82	0.45
3:L5:4122:G:C5	37:Lg:97:ILE:HG21	2.52	0.45
3:L5:4127:A:O2'	3:L5:4128:A:H8	1.99	0.45
3:L5:4608:G:H3'	3:L5:4609:G:H8	1.81	0.45
18:LN:54:LYS:HB3	18:LN:59:TYR:CE2	2.51	0.45
21:LQ:49:LYS:HD2	21:LQ:49:LYS:HA	1.74	0.45
23:LS:35:PRO:HD2	23:LS:39:VAL:HG21	1.98	0.45
27:LW:101:ARG:HH12	69:SG:147:LEU:HD22	1.82	0.45
28:LX:85:SER:HA	28:LX:88:LYS:HE3	1.99	0.45
30:LZ:10:VAL:HG23	30:LZ:86:SER:HA	1.98	0.45
44:Ln:12:ARG:HG2	44:Ln:15:ARG:HH22	1.81	0.45
50:SD:132:LYS:HG2	50:SD:191:PRO:HB3	1.98	0.45
64:Sg:153:CYS:HB3	64:Sg:198:VAL:HG12	1.98	0.45
64:Sg:207:CYS:HB3	64:Sg:221:LEU:HD21	1.98	0.45
71:SI:99:ASN:HB2	83:S2:377:G:O5'	2.17	0.45
73:SL:44:PHE:HZ	73:SL:127:THR:HG21	1.82	0.45
83:S2:386:C:H2'	83:S2:387:C:C6	2.52	0.45
83:S2:884:C:H2'	83:S2:885:U:O4'	2.17	0.45
83:S2:1217:A:H2'	83:S2:1218:C:C6	2.52	0.45
83:S2:1801:A:H2'	83:S2:1802:C:H6	1.82	0.45
3:L5:734:G:H22	3:L5:929:A:H2	1.64	0.45
3:L5:1450:C:H2'	3:L5:1451:G:O4'	2.17	0.45
3:L5:1818:G:O2'	3:L5:1819:G:H5''	2.17	0.45
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.17	0.45
3:L5:2072:C:H5''	11:LF:116:GLN:HE21	1.81	0.45
3:L5:2898:G:H5''	22:LR:104:ARG:HH22	1.82	0.45
3:L5:4954:G:H2'	3:L5:4955:A:H8	1.81	0.45
6:LA:57:PRO:HB3	46:Lp:54:ILE:HD11	1.98	0.45
7:LB:133:TYR:O	7:LB:136:LYS:HG3	2.17	0.45
8:LC:285:ILE:HG12	21:LQ:122:THR:HG21	1.98	0.45
11:LF:156:LYS:HD3	11:LF:248:ASN:HB2	1.98	0.45
13:LH:5:LEU:HG	13:LH:60:TRP:HE1	1.81	0.45
14:LI:89:VAL:HG22	14:LI:91:LEU:H	1.82	0.45
16:LL:58:ILE:HG13	16:LL:116:ARG:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	1.98	0.45
52:SK:31:LYS:HZ3	52:SK:39:ASN:N	2.14	0.45
59:SU:67:LYS:HB3	83:S2:1337:4AC:H5''	1.99	0.45
68:SE:64:ILE:HG12	79:SY:18:LEU:HD11	1.99	0.45
71:SI:130:THR:HA	71:SI:133:GLU:HG3	1.99	0.45
83:S2:113:G:N2	83:S2:292:A:H2'	2.32	0.45
83:S2:551:U:H2'	83:S2:552:G:C8	2.51	0.45
83:S2:1033:G:N2	83:S2:1081:PSU:HN1	2.15	0.45
83:S2:1671:G:H2'	83:S2:1672:U:C6	2.51	0.45
3:L5:965:G:H21	3:L5:2092:G:H1'	1.81	0.45
3:L5:1960:A:H5'	48:Ls:63:LYS:HE2	1.98	0.45
3:L5:2081:C:H5''	21:LQ:11:ARG:HD3	1.98	0.45
3:L5:3588:C:H2'	3:L5:3589:G:O4'	2.17	0.45
3:L5:3927:U:H2'	3:L5:3928:A:H8	1.82	0.45
85:L5:5263:SPM:HN11	85:L5:5263:SPM:H42	1.61	0.45
5:L8:74:U:P	29:LY:76:LYS:HD2	2.57	0.45
9:LD:52:ILE:O	9:LD:62:CYS:HA	2.17	0.45
12:LG:229:ARG:HB2	12:LG:232:GLU:OE2	2.16	0.45
14:LI:52:MET:HB2	14:LI:152:LEU:HD22	1.98	0.45
21:LQ:3:VAL:HG13	21:LQ:5:ILE:HG12	1.99	0.45
21:LQ:15:ARG:HB3	21:LQ:52:PHE:HB3	1.98	0.45
51:SF:78:MET:HE3	51:SF:159:ARG:HH12	1.82	0.45
53:SM:43:ASP:OD1	63:Sf:129:GLY:HA2	2.17	0.45
55:SQ:24:HIS:O	55:SQ:68:ILE:HA	2.17	0.45
71:SI:145:ILE:O	71:SI:148:LYS:HG2	2.17	0.45
71:SI:145:ILE:HG22	71:SI:149:TYR:CE2	2.52	0.45
74:SN:61:ALA:HB1	83:S2:1016:U:H6	1.82	0.45
83:S2:1240:A:H2'	83:S2:1241:A:C8	2.52	0.45
83:S2:1839:U:H2'	83:S2:1840:U:C6	2.52	0.45
2:Pt:62:C:H2'	2:Pt:63:G:C8	2.50	0.45
3:L5:1368:A:H2'	3:L5:1369:C:O4'	2.17	0.45
3:L5:4311:A:H2'	3:L5:4312:PSU:C6	2.52	0.45
11:LF:155:TYR:HE1	11:LF:187:MET:HB3	1.82	0.45
39:Li:23:LYS:HG2	39:Li:24:PRO:HD2	1.98	0.45
57:SS:114:LEU:HD23	57:SS:117:ILE:HD11	1.97	0.45
58:ST:59:SER:HB3	83:S2:1541:G:H5''	1.99	0.45
60:SZ:102:LYS:HA	60:SZ:107:VAL:HG23	1.98	0.45
65:SA:89:LYS:HD2	65:SA:201:LEU:HG	1.97	0.45
68:SE:38:LEU:HA	68:SE:41:CYS:SG	2.56	0.45
71:SI:141:ARG:HB3	71:SI:145:ILE:HB	1.99	0.45
79:SY:37:LYS:HG3	83:S2:571:U:H5''	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:174:OMC:HM23	83:S2:174:OMC:H1'	1.81	0.45
83:S2:963:A:H61	83:S2:1065:G:H1'	1.82	0.45
83:S2:1093:A:H2'	83:S2:1094:C:C6	2.52	0.45
83:S2:1531:A:H2'	83:S2:1532:C:C6	2.52	0.45
83:S2:1539:U:H2'	83:S2:1540:G:C8	2.52	0.45
3:L5:123:C:H2'	3:L5:124:C:H6	1.82	0.45
3:L5:683:C:H2'	3:L5:684:G:O4'	2.17	0.45
3:L5:739:G:HO2'	3:L5:740:G:H8	1.65	0.45
3:L5:1097:C:H2'	3:L5:1098:G:H8	1.80	0.45
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.51	0.45
3:L5:2544:G:H22	5:L8:124:U:H5'	1.82	0.45
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.17	0.45
3:L5:3718:A2M:HM'3	3:L5:3718:A2M:H1'	1.81	0.45
3:L5:4571:A2M:H2'	3:L5:4572:U:C6	2.52	0.45
4:L7:82:G:H2'	4:L7:83:A:C8	2.52	0.45
9:LD:41:LYS:HG3	24:LT:93:ILE:HG21	1.99	0.45
18:LN:103:GLU:OE2	18:LN:167:ALA:HB3	2.16	0.45
21:LQ:69:LYS:HD3	21:LQ:69:LYS:HA	1.77	0.45
22:LR:28:GLU:OE1	22:LR:31:GLU:HB2	2.17	0.45
35:Le:88:LEU:HB2	35:Le:120:ILE:HD13	1.99	0.45
52:SK:80:ARG:NH2	52:SK:90:VAL:HG12	2.32	0.45
52:SK:90:VAL:HG21	52:SK:95:ARG:HB2	1.98	0.45
67:SC:194:ARG:HH11	83:S2:1154:U:H1'	1.80	0.45
69:SG:18:VAL:HG21	69:SG:24:LEU:HD21	1.99	0.45
79:SY:33:ALA:HB2	83:S2:582:U:H1'	1.99	0.45
83:S2:218:U:H2'	83:S2:219:U:C6	2.52	0.45
83:S2:935:G:H2'	83:S2:936:G:C8	2.51	0.45
83:S2:1192:U:H2'	83:S2:1193:U:C6	2.52	0.45
2:Pt:24:A:H2'	2:Pt:25:C:C6	2.52	0.44
3:L5:679:C:H2'	3:L5:680:G:C8	2.52	0.44
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.31	0.44
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.52	0.44
3:L5:3700:C:H2'	3:L5:3746:A:H61	1.82	0.44
3:L5:4227:OMU:HM21	3:L5:4336:A:H1'	1.98	0.44
3:L5:4622:A:H4'	7:LB:13:SER:HB2	1.99	0.44
7:LB:163:ILE:HG22	7:LB:180:LEU:HD22	1.99	0.44
9:LD:288:LEU:HD23	9:LD:291:GLN:NE2	2.30	0.44
18:LN:26:ARG:HD2	18:LN:30:TYR:OH	2.16	0.44
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.17	0.44
48:Ls:31:GLY:HA2	48:Ls:86:VAL:HG12	1.98	0.44
56:SR:1:MET:HA	83:S2:1467:C:H5''	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:ST:39:LEU:HA	58:ST:39:LEU:HD23	1.66	0.44
63:Sf:121:CYS:HA	63:Sf:132:MET:HE3	1.99	0.44
67:SC:208:PRO:HA	67:SC:211:LYS:HE3	1.98	0.44
69:SG:160:LYS:HE2	83:S2:65:C:O2	2.17	0.44
72:SJ:3:VAL:HB	72:SJ:5:ARG:HG2	1.99	0.44
72:SJ:39:ASN:HB2	83:S2:642:U:P	2.57	0.44
3:L5:1266:G:H5'	32:Lb:99:ILE:HD11	2.00	0.44
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.17	0.44
3:L5:2486:G:N7	3:L5:2493:G:N1	2.57	0.44
3:L5:3860:A:H2	20:LP:131:ARG:HH22	1.64	0.44
3:L5:4236:G:H2'	3:L5:4237:C:H6	1.82	0.44
3:L5:4906:C:H2'	3:L5:4907:G:C8	2.52	0.44
5:L8:90:C:H2'	5:L8:91:A:C8	2.51	0.44
9:LD:60:ILE:HB	9:LD:80:ALA:HB2	1.99	0.44
10:LE:91:THR:HA	10:LE:108:LYS:HA	1.99	0.44
11:LF:38:ALA:HA	11:LF:41:MET:HE2	1.98	0.44
11:LF:104:LYS:O	11:LF:108:VAL:HG22	2.16	0.44
17:LM:24:LEU:HD11	17:LM:86:TRP:CG	2.52	0.44
36:Lf:36:ARG:HB2	36:Lf:80:ASN:HA	2.00	0.44
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.70	0.44
40:Lj:2:THR:HG22	40:Lj:4:GLY:H	1.82	0.44
67:SC:128:VAL:HG11	67:SC:155:ILE:HG13	2.00	0.44
73:SL:128:VAL:HG22	73:SL:140:PHE:HB3	2.00	0.44
82:Se:25:LYS:HD2	82:Se:25:LYS:HA	1.83	0.44
83:S2:12:U:H2'	83:S2:13:C:C6	2.52	0.44
83:S2:1127:C:H2'	83:S2:1128:C:C6	2.52	0.44
83:S2:1653:U:H2'	83:S2:1654:G:C8	2.52	0.44
83:S2:1739:C:H2'	83:S2:1740:C:C6	2.52	0.44
83:S2:1808:U:H2'	83:S2:1809:A:C8	2.52	0.44
83:S2:1856:C:H2'	83:S2:1857:G:C8	2.52	0.44
3:L5:947:C:H5''	10:LE:51:VAL:HG11	1.99	0.44
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.52	0.44
3:L5:2017:A:H2'	3:L5:2017:A:OP2	2.17	0.44
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.50	0.44
3:L5:2780:C:H2'	3:L5:2781:G:H8	1.81	0.44
3:L5:4143:G:N3	3:L5:4145:C:H1'	2.32	0.44
7:LB:220:ILE:HB	7:LB:346:THR:OG1	2.17	0.44
12:LG:258:ALA:HA	12:LG:261:LEU:HB2	1.98	0.44
46:Lp:38:THR:HA	46:Lp:45:THR:HA	1.99	0.44
51:SF:101:HIS:HB2	51:SF:108:PRO:HG3	1.99	0.44
55:SQ:22:VAL:HG21	83:S2:1443:C:H1'	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Sg:289:LEU:HD11	64:Sg:298:LEU:HD21	2.00	0.44
67:SC:177:PRO:HD3	76:SV:9:VAL:HG11	1.99	0.44
77:SW:105:THR:HB	77:SW:126:LEU:HD11	1.99	0.44
83:S2:1019:C:H2'	83:S2:1020:A:O4'	2.17	0.44
83:S2:1533:A:N6	83:S2:1602:U:N3	2.55	0.44
83:S2:1692:U:H2'	83:S2:1693:G:C8	2.52	0.44
3:L5:228:C:H2'	3:L5:229:G:H8	1.82	0.44
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.48	0.44
3:L5:419:A:N6	5:L8:15:G:H1'	2.32	0.44
3:L5:674:G:H2'	3:L5:675:C:C6	2.52	0.44
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.53	0.44
3:L5:1700:G:H5''	3:L5:1704:C:N4	2.32	0.44
3:L5:3748:A:H2'	3:L5:3749:C:C6	2.53	0.44
3:L5:3846:C:H2'	3:L5:3847:C:H6	1.83	0.44
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.83	0.44
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.52	0.44
5:L8:14:U:H5''	20:LP:123:PRO:HD3	2.00	0.44
7:LB:299:ILE:HB	7:LB:313:SER:HB3	1.98	0.44
11:LF:96:ARG:HH12	11:LF:224:THR:HG23	1.83	0.44
13:LH:2:LYS:HZ1	13:LH:62:GLY:HA2	1.83	0.44
13:LH:94:SER:HB3	13:LH:179:ILE:HD13	2.00	0.44
17:LM:37:LEU:HD21	17:LM:47:ARG:HD3	1.99	0.44
21:LQ:19:LYS:HE2	21:LQ:19:LYS:HB2	1.82	0.44
21:LQ:50:ARG:O	21:LQ:53:MET:HG2	2.18	0.44
27:LW:27:LYS:HA	27:LW:27:LYS:HD3	1.82	0.44
28:LX:124:VAL:HG12	28:LX:138:VAL:HA	1.98	0.44
36:Lf:45:LYS:NZ	36:Lf:108:SER:HA	2.33	0.44
37:Lg:45:ALA:HB3	37:Lg:82:MET:HE2	1.99	0.44
49:Lt:12:VAL:HG11	49:Lt:64:ILE:HA	1.99	0.44
55:SQ:134:GLY:HA3	55:SQ:140:ARG:HA	1.98	0.44
62:Sd:13:LYS:HG3	83:S2:1556:A:C8	2.52	0.44
67:SC:60:TRP:CD1	67:SC:92:GLU:HG3	2.51	0.44
70:SH:157:HIS:CD2	70:SH:190:PRO:HG3	2.53	0.44
73:SL:59:LYS:HD3	73:SL:134:LEU:HB3	1.99	0.44
76:SV:60:ARG:HB3	76:SV:65:SER:HB3	1.98	0.44
80:Sa:30:VAL:HG21	80:Sa:74:CYS:HB3	2.00	0.44
83:S2:675:U:H2'	83:S2:676:C:H6	1.81	0.44
83:S2:974:C:H2'	83:S2:975:G:H8	1.82	0.44
83:S2:976:G:H2'	83:S2:977:C:H6	1.83	0.44
83:S2:1070:A:H2'	83:S2:1071:G:O4'	2.16	0.44
83:S2:1426:U:H2'	83:S2:1427:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1616:U:H2'	83:S2:1617:G:C8	2.52	0.44
3:L5:679:C:H2'	3:L5:680:G:H8	1.82	0.44
3:L5:1176:C:H2'	3:L5:1177:U:C6	2.53	0.44
3:L5:1259:G:H2'	3:L5:1260:G:C8	2.48	0.44
3:L5:2059:C:H2'	3:L5:2060:G:H8	1.82	0.44
3:L5:3869:OMC:N4	85:L5:5291:SPM:H72	2.33	0.44
3:L5:4154:G:H2'	3:L5:4155:C:C6	2.53	0.44
3:L5:4194:U:H5''	32:Lb:3:LYS:HG2	2.00	0.44
5:L8:32:C:H3'	5:L8:33:G:H8	1.81	0.44
16:LL:111:GLN:O	16:LL:115:GLN:HG2	2.18	0.44
20:LP:29:THR:HG23	20:LP:119:VAL:HG11	1.98	0.44
48:Ls:145:THR:HG21	48:Ls:152:ILE:HG23	1.99	0.44
59:SU:19:ARG:HB2	59:SU:117:ALA:HB2	1.99	0.44
70:SH:50:GLU:OE2	70:SH:58:LYS:HB3	2.18	0.44
83:S2:1064:C:H2'	83:S2:1065:G:H8	1.83	0.44
83:S2:1567:G:H2'	83:S2:1568:C:C6	2.52	0.44
83:S2:1627:C:H2'	83:S2:1628:C:C6	2.51	0.44
83:S2:1805:G:H2'	83:S2:1806:A:H8	1.81	0.44
3:L5:25:A:C8	3:L5:341:G:C8	3.05	0.44
3:L5:223:G:N7	8:LC:165:LYS:HE3	2.33	0.44
3:L5:946:C:HO2'	8:LC:340:ILE:HG22	1.83	0.44
3:L5:1326:A2M:HM'3	3:L5:1326:A2M:H1'	1.51	0.44
3:L5:1405:C:H2'	3:L5:1406:G:H8	1.83	0.44
3:L5:1449:C:H2'	3:L5:1450:C:H6	1.83	0.44
3:L5:1534:A2M:N3	40:Lj:11:ARG:HB2	2.33	0.44
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.52	0.44
3:L5:2081:C:H2'	3:L5:2082:G:C8	2.52	0.44
3:L5:2374:A:H2'	3:L5:2375:A:C8	2.52	0.44
5:L8:66:A:H2'	5:L8:67:U:H6	1.83	0.44
7:LB:17:LEU:HA	7:LB:17:LEU:HD23	1.80	0.44
7:LB:234:ARG:HG3	7:LB:272:LYS:HB3	2.00	0.44
9:LD:211:LEU:HB3	9:LD:219:TYR:HB2	2.00	0.44
10:LE:67:ALA:HA	10:LE:69:TYR:CE2	2.53	0.44
13:LH:45:LEU:HD13	13:LH:57:VAL:HG12	2.00	0.44
16:LL:119:GLU:O	16:LL:123:LYS:HG3	2.18	0.44
29:LY:118:ILE:HD12	29:LY:118:ILE:HA	1.89	0.44
33:Lc:28:VAL:O	33:Lc:94:LEU:HD12	2.18	0.44
53:SM:31:LEU:HB3	53:SM:33:ARG:HG3	1.98	0.44
62:Sd:20:SER:HB3	62:Sd:27:ARG:CZ	2.47	0.44
64:Sg:172:LYS:HG2	64:Sg:193:GLY:O	2.17	0.44
72:SJ:40:LYS:HG2	82:Se:34:ARG:HH12	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SJ:169:ARG:HD2	72:SJ:169:ARG:HA	1.91	0.44
83:S2:534:G:H2'	83:S2:535:G:C8	2.52	0.44
83:S2:1650:A:H2'	83:S2:1651:A:O4'	2.18	0.44
83:S2:1714:U:H2'	83:S2:1715:A:C8	2.52	0.44
3:L5:1687:U:H2'	3:L5:1688:G:C8	2.53	0.44
3:L5:2891:U:H2'	3:L5:2892:C:O4'	2.18	0.44
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.83	0.44
3:L5:4169:G:H4'	3:L5:4171:C:C2	2.53	0.44
6:LA:234:LYS:H	6:LA:234:LYS:HG2	1.66	0.44
9:LD:263:LYS:HD3	9:LD:263:LYS:HA	1.74	0.44
11:LF:131:ASN:O	11:LF:135:ILE:HG12	2.17	0.44
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.81	0.44
52:SK:5:LYS:HZ1	83:S2:1312:G:H4'	1.83	0.44
66:SB:25:PHE:HA	66:SB:28:LYS:HG3	1.99	0.44
70:SH:58:LYS:HD2	70:SH:58:LYS:HA	1.75	0.44
74:SN:9:LYS:HE3	83:S2:1131:G:P	2.58	0.44
75:SO:33:ILE:HD12	75:SO:41:PHE:O	2.17	0.44
83:S2:509:OMG:H2'	83:S2:510:G:C8	2.53	0.44
83:S2:656:G:H5'	83:S2:662:G:N2	2.32	0.44
83:S2:693:A:H2'	83:S2:694:G:C8	2.53	0.44
83:S2:881:G:N2	83:S2:906:U:H1'	2.33	0.44
3:L5:64:A:H1'	3:L5:76:A:H1'	1.98	0.44
3:L5:106:A:H1'	3:L5:336:A:N3	2.32	0.44
3:L5:259:C:H2'	3:L5:260:C:C6	2.53	0.44
3:L5:1315:C:H2'	3:L5:1316:OMG:C8	2.53	0.44
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.18	0.44
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.77	0.44
3:L5:3744:OMG:HM23	3:L5:3744:OMG:H1'	1.79	0.44
3:L5:4279:A:H5'	3:L5:4281:A:H1'	2.00	0.44
3:L5:4759:C:H2'	3:L5:4760:G:C8	2.53	0.44
4:L7:48:G:H2'	4:L7:49:A:C8	2.53	0.44
5:L8:47:C:H1'	5:L8:61:A:H2'	2.00	0.44
11:LF:213:LEU:HD23	11:LF:247:MET:HG3	1.99	0.44
15:LJ:43:LEU:HA	15:LJ:117:ILE:HD11	2.00	0.44
17:LM:82:ILE:H	17:LM:82:ILE:HD12	1.82	0.44
25:LU:44:GLN:HB2	25:LU:56:LEU:HD21	2.00	0.44
31:La:8:THR:HG23	31:La:17:HIS:CE1	2.52	0.44
51:SF:79:HIS:HB2	51:SF:159:ARG:HD3	2.00	0.44
57:SS:67:VAL:O	57:SS:71:MET:HG2	2.18	0.44
66:SB:120:MET:HE2	66:SB:142:PHE:HE2	1.82	0.44
71:SI:49:ARG:HD3	71:SI:50:GLY:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:12:U:H2'	83:S2:13:C:H6	1.82	0.44
83:S2:468:A2M:HM'3	83:S2:468:A2M:H1'	1.68	0.44
83:S2:1177:PSU:H2'	83:S2:1178:U:C6	2.52	0.44
83:S2:1595:U:H2'	83:S2:1596:U:C6	2.53	0.44
1:CI:55:LEU:HD13	25:LU:99:TRP:CE3	2.53	0.44
3:L5:272:U:H2'	3:L5:273:U:C6	2.53	0.44
3:L5:737:C:C4	3:L5:739:G:H5''	2.53	0.44
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.52	0.44
3:L5:2804:OMC:H2'	3:L5:2805:C:H6	1.83	0.44
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.53	0.44
3:L5:4383:U:H2'	3:L5:4384:U:C6	2.53	0.44
3:L5:4748:U:H2'	3:L5:4749:C:C6	2.53	0.44
3:L5:4927:G:H5''	3:L5:4928:C:C5	2.53	0.44
3:L5:5027:C:O2'	3:L5:5028:G:H5''	2.18	0.44
85:L5:5291:SPM:H82	85:L5:5291:SPM:H111	1.81	0.44
4:L7:9:C:OP1	24:LT:26:PRO:HB2	2.18	0.44
6:LA:131:GLY:H	6:LA:169:VAL:HG13	1.82	0.44
7:LB:367:PHE:HB2	27:LW:1:MET:HG2	2.00	0.44
9:LD:64:ILE:HG21	9:LD:109:LEU:HD12	1.99	0.44
11:LF:142:TRP:CZ2	11:LF:235:ASN:HB2	2.53	0.44
43:Lm:94:MET:HG2	43:Lm:105:PRO:HA	2.00	0.44
50:SD:40:ARG:HA	59:SU:108:PRO:HB3	2.00	0.44
83:S2:116:OMU:HM23	83:S2:116:OMU:H1'	1.74	0.44
83:S2:813:A:H2'	83:S2:814:PSU:O4'	2.18	0.44
83:S2:1438:A:H2'	83:S2:1439:A:C8	2.52	0.44
3:L5:441:G:H2'	3:L5:442:G:H8	1.82	0.43
3:L5:1399:G:H2'	3:L5:1400:G:C8	2.53	0.43
3:L5:1505:C:H2'	3:L5:1506:G:H8	1.82	0.43
3:L5:1777:C:H2'	3:L5:1778:C:C6	2.53	0.43
3:L5:2249:C:H2'	3:L5:2250:C:C5	2.53	0.43
3:L5:2804:OMC:H2'	3:L5:2805:C:C6	2.53	0.43
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.18	0.43
3:L5:3707:U:H2'	3:L5:3708:C:H6	1.83	0.43
3:L5:4364:G:H2'	3:L5:4365:C:C6	2.52	0.43
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.53	0.43
3:L5:4676:G:H4'	7:LB:280:ILE:HD11	2.00	0.43
6:LA:83:HIS:CE1	6:LA:86:GLN:HB2	2.52	0.43
8:LC:101:MET:SD	8:LC:104:PRO:HA	2.57	0.43
16:LL:25:TRP:HE3	16:LL:28:GLN:HG3	1.83	0.43
19:LO:30:GLY:HA2	19:LO:101:ARG:NE	2.32	0.43
21:LQ:82:VAL:O	21:LQ:102:ALA:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LU:39:PHE:HD1	25:LU:90:TYR:CD2	2.36	0.43
50:SD:214:LYS:HG3	50:SD:215:ASP:H	1.82	0.43
52:SK:91:PRO:HB2	52:SK:94:LEU:HD23	1.99	0.43
73:SL:126:VAL:HG12	73:SL:145:VAL:HG12	2.00	0.43
76:SV:36:VAL:O	76:SV:50:PHE:HB2	2.18	0.43
83:S2:1104:G:H2'	83:S2:1105:G:C8	2.52	0.43
83:S2:1548:G:H2'	83:S2:1549:U:C6	2.52	0.43
83:S2:1683:C:H2'	83:S2:1684:C:H6	1.83	0.43
83:S2:1743:G:H21	83:S2:1791:A:H62	1.65	0.43
2:Pt:35:A:H2'	2:Pt:36:C:C6	2.53	0.43
3:L5:381:U:H4'	3:L5:415:G:H5'	1.99	0.43
3:L5:1508:A:H2'	3:L5:1509:C:C6	2.54	0.43
3:L5:1524:A2M:HM'1	3:L5:3916:G:H21	1.82	0.43
3:L5:1613:A:H5''	6:LA:183:GLY:CA	2.48	0.43
3:L5:1812:C:H2'	3:L5:1813:U:C6	2.53	0.43
3:L5:4392:OMG:N3	3:L5:4447:5MC:HM52	2.32	0.43
10:LE:95:PRO:HA	10:LE:104:THR:HG22	2.00	0.43
14:LI:36:LEU:HD22	14:LI:73:ASN:ND2	2.33	0.43
45:Lo:82:MET:HE3	45:Lo:82:MET:HB3	1.91	0.43
48:Ls:99:ARG:HG3	48:Ls:100:ASP:N	2.32	0.43
51:SF:76:MET:HG2	51:SF:155:CYS:SG	2.58	0.43
56:SR:43:SER:HB3	56:SR:46:LEU:HD12	2.01	0.43
58:ST:6:VAL:HG12	58:ST:135:ALA:HB2	1.99	0.43
71:SI:108:PRO:O	71:SI:111:GLN:HG3	2.18	0.43
74:SN:124:ARG:HG2	74:SN:127:ARG:HH22	1.83	0.43
78:SX:51:VAL:HB	78:SX:98:ASP:H	1.82	0.43
83:S2:321:C:H2'	83:S2:322:C:C6	2.53	0.43
83:S2:1515:G:H2'	83:S2:1516:G:C8	2.53	0.43
83:S2:1693:G:H2'	83:S2:1694:U:C6	2.53	0.43
2:Pt:27:U:H2'	2:Pt:28:U:H6	1.83	0.43
3:L5:125:C:H2'	3:L5:126:C:H6	1.82	0.43
3:L5:400:A2M:H2'	3:L5:401:G:O4'	2.18	0.43
3:L5:1274:A:O2'	3:L5:1275:G:H8	2.01	0.43
3:L5:2080:U:H2'	3:L5:2081:C:C6	2.52	0.43
3:L5:2273:G:H2'	3:L5:2274:C:C6	2.53	0.43
3:L5:2674:A:N6	46:Lp:42:CYS:HA	2.34	0.43
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.19	0.43
3:L5:4627:U:H2'	3:L5:4628:PSU:H6	1.82	0.43
3:L5:5002:U:H2'	3:L5:5003:U:H6	1.82	0.43
3:L5:5010:PSU:H2'	3:L5:5011:A:H8	1.83	0.43
5:L8:140:C:H2'	5:L8:141:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:94:ALA:HB3	6:LA:102:LEU:HB3	2.00	0.43
19:LO:142:ALA:HA	19:LO:145:VAL:HG12	2.01	0.43
24:LT:107:LYS:HE3	24:LT:107:LYS:HB3	1.85	0.43
27:LW:5:LEU:HB3	27:LW:30:GLN:HG3	2.00	0.43
34:Ld:37:GLY:O	34:Ld:41:ARG:HG3	2.17	0.43
54:SP:37:TYR:HB3	54:SP:41:GLN:HB2	2.00	0.43
54:SP:126:VAL:HG11	83:S2:1520:G:N2	2.34	0.43
59:SU:59:LYS:HD2	59:SU:59:LYS:HA	1.68	0.43
66:SB:145:LYS:HB2	66:SB:145:LYS:HE3	1.75	0.43
74:SN:25:TRP:HE1	81:Sb:83:GLN:HG2	1.83	0.43
74:SN:47:PRO:HA	74:SN:50:ILE:HD12	2.00	0.43
83:S2:159:A2M:O2'	83:S2:160:U:H5'	2.18	0.43
83:S2:391:C:H2'	83:S2:392:A:H8	1.83	0.43
83:S2:649:PSU:H2'	83:S2:650:A:H8	1.82	0.43
83:S2:1779:G:H2'	83:S2:1780:G:C8	2.53	0.43
3:L5:221:C:H2'	3:L5:222:C:H6	1.83	0.43
3:L5:742:G:H2'	3:L5:743:G:C8	2.54	0.43
3:L5:1199:G:H2'	3:L5:1200:G:H8	1.83	0.43
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.53	0.43
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.54	0.43
3:L5:3619:G:H4'	22:LR:79:GLY:O	2.19	0.43
3:L5:4407:G:O6	3:L5:4435:U:O4	2.37	0.43
3:L5:4552:PSU:H2'	3:L5:4553:A:C8	2.53	0.43
6:LA:219:ILE:HG22	6:LA:221:LYS:H	1.84	0.43
9:LD:164:LYS:HA	9:LD:167:VAL:HG22	1.99	0.43
11:LF:46:ARG:NH2	32:Lb:102:PRO:HG3	2.33	0.43
15:LJ:20:LEU:HD23	15:LJ:79:ALA:HB1	2.01	0.43
21:LQ:144:LYS:HA	21:LQ:149:TYR:CD2	2.54	0.43
38:Lh:31:LEU:HD23	38:Lh:31:LEU:HA	1.79	0.43
54:SP:79:HIS:CD2	83:S2:1298:G:C8	3.07	0.43
60:SZ:99:LEU:HD21	60:SZ:102:LYS:HD2	2.01	0.43
63:Sf:143:LYS:HD3	83:S2:1310:U:O3'	2.18	0.43
76:SV:17:CYS:HB2	76:SV:56:CYS:HB3	2.00	0.43
79:SY:23:MET:HE2	79:SY:48:TYR:HE2	1.83	0.43
83:S2:162:C:H2'	83:S2:163:U:O4'	2.19	0.43
83:S2:461:U:H2'	83:S2:462:OMC:H6	1.84	0.43
2:Pt:43:A:H2'	2:Pt:44:A:H8	1.84	0.43
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.83	0.43
3:L5:2259:G:H22	10:LE:110:ARG:HH21	1.66	0.43
3:L5:2308:A:H4'	3:L5:2334:C:H4'	1.99	0.43
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4637:OMG:H1'	3:L5:4637:OMG:HM23	1.66	0.43
3:L5:4970:C:C2	3:L5:4971:A:C8	3.07	0.43
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	2.01	0.43
20:LP:32:THR:HA	20:LP:58:VAL:HG21	2.00	0.43
21:LQ:66:MET:HE1	21:LQ:98:LEU:HG	2.00	0.43
25:LU:24:ASP:HB2	25:LU:111:GLU:HB3	2.01	0.43
46:Lp:37:TYR:HB2	46:Lp:47:MET:HB2	1.99	0.43
47:Lr:49:VAL:HG12	47:Lr:106:LEU:HD13	2.00	0.43
65:SA:121:LEU:HD11	65:SA:145:ILE:HG13	2.01	0.43
66:SB:159:GLN:O	66:SB:162:ARG:HG2	2.18	0.43
66:SB:186:ASN:HA	66:SB:189:ILE:HD12	2.00	0.43
74:SN:110:ASP:O	74:SN:114:ARG:HG2	2.18	0.43
75:SO:50:LYS:HA	83:S2:976:G:H1'	2.01	0.43
83:S2:601:OMG:H1'	83:S2:601:OMG:HM23	1.68	0.43
83:S2:1201:U:H2'	83:S2:1202:U:C6	2.53	0.43
83:S2:1739:C:H2'	83:S2:1740:C:H6	1.83	0.43
3:L5:297:U:H2'	3:L5:298:G:C8	2.54	0.43
3:L5:2019:C:H2'	3:L5:2020:U:H6	1.83	0.43
3:L5:2034:G:H2'	3:L5:2035:C:C6	2.54	0.43
3:L5:2461:G:H2'	3:L5:2462:C:C6	2.53	0.43
3:L5:2744:A:H2'	3:L5:2745:A:H8	1.81	0.43
3:L5:3830:A2M:H1'	3:L5:3830:A2M:HM'3	1.57	0.43
3:L5:3933:G:H2'	3:L5:3934:G:H8	1.83	0.43
3:L5:4887:C:N3	3:L5:4932:U:O2	2.52	0.43
11:LF:148:LYS:HD2	11:LF:245:ARG:HH21	1.83	0.43
22:LR:42:ARG:HA	22:LR:45:ILE:HG22	2.01	0.43
50:SD:53:THR:HA	50:SD:94:ARG:NH1	2.33	0.43
65:SA:147:LEU:HD13	65:SA:174:MET:SD	2.58	0.43
70:SH:51:ILE:HG21	70:SH:179:LYS:HG2	1.99	0.43
74:SN:64:ARG:NH1	74:SN:68:GLY:HA2	2.33	0.43
74:SN:93:LYS:HA	74:SN:150:VAL:HG21	2.01	0.43
76:SV:11:LEU:HD23	76:SV:11:LEU:H	1.83	0.43
83:S2:406:PSU:H2'	83:S2:408:A:C8	2.52	0.43
83:S2:1134:G:H2'	83:S2:1135:C:C6	2.54	0.43
83:S2:1828:C:H2'	83:S2:1829:G:C8	2.53	0.43
3:L5:967:C:H2'	10:LE:110:ARG:HH22	1.83	0.43
3:L5:2492:C:H2'	3:L5:2493:G:H8	1.84	0.43
3:L5:3600:G:H2'	3:L5:3601:C:C6	2.54	0.43
3:L5:3867:A2M:H1'	3:L5:3867:A2M:HM'3	1.48	0.43
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.54	0.43
3:L5:4910:G:H22	19:LO:107:GLY:HA3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4923:C:O2	3:L5:4924:C:O2	2.36	0.43
5:L8:26:C:H2'	5:L8:27:U:C6	2.54	0.43
6:LA:34:PHE:CE2	12:LG:41:ILE:HD11	2.54	0.43
6:LA:131:GLY:N	6:LA:169:VAL:HG13	2.33	0.43
8:LC:94:ASN:HA	8:LC:100:ARG:O	2.19	0.43
20:LP:22:LEU:HD12	20:LP:90:PHE:CD2	2.54	0.43
24:LT:112:ASN:HB3	24:LT:128:LEU:HD23	2.00	0.43
48:Ls:14:PHE:CD1	48:Ls:64:ALA:HB2	2.54	0.43
48:Ls:110:ALA:HA	48:Ls:182:PRO:HG2	2.00	0.43
66:SB:97:LEU:HD23	66:SB:232:HIS:CG	2.54	0.43
67:SC:84:PHE:CE1	67:SC:264:SER:HA	2.53	0.43
68:SE:181:CYS:HA	68:SE:227:VAL:HA	1.99	0.43
69:SG:133:LEU:HD23	69:SG:133:LEU:H	1.82	0.43
70:SH:155:LYS:HD2	70:SH:186:ASN:HB2	2.00	0.43
71:SI:13:LYS:HB2	73:SL:137:THR:HG21	2.01	0.43
77:SW:20:ARG:HA	77:SW:20:ARG:HD2	1.84	0.43
83:S2:432:G:H2'	83:S2:433:A:H8	1.84	0.43
83:S2:489:A:H2'	83:S2:490:C:C6	2.53	0.43
83:S2:909:G:H2'	83:S2:910:G:H8	1.84	0.43
83:S2:1392:U:H2'	83:S2:1393:G:C8	2.54	0.43
83:S2:1615:U:H2'	83:S2:1616:U:C6	2.54	0.43
2:Pt:48:C:H2'	2:Pt:59:A:O4'	2.18	0.43
3:L5:7:C:H2'	3:L5:8:U:H6	1.83	0.43
3:L5:280:G:H5''	18:LN:14:LYS:HE2	2.00	0.43
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.19	0.43
3:L5:691:C:H2'	3:L5:692:A:C8	2.54	0.43
3:L5:1494:U:H2'	3:L5:1495:G:C8	2.53	0.43
3:L5:2561:C:H2'	3:L5:2562:G:O4'	2.19	0.43
3:L5:3845:A:H2'	3:L5:3846:C:C6	2.54	0.43
3:L5:4071:U:H2'	3:L5:4072:C:C6	2.53	0.43
3:L5:4113:U:H4'	3:L5:4115:G:C6	2.54	0.43
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.82	0.43
3:L5:4919:G:H2'	3:L5:4920:C:H6	1.84	0.43
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.17	0.43
5:L8:130:C:H2'	5:L8:131:G:C8	2.54	0.43
7:LB:27:GLY:HA2	7:LB:276:HIS:CD2	2.54	0.43
9:LD:36:LEU:CD2	9:LD:50:ARG:HD2	2.49	0.43
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.54	0.43
17:LM:32:ASP:O	17:LM:33:GLN:HG3	2.19	0.43
18:LN:153:LYS:HD2	18:LN:154:PRO:HD2	2.00	0.43
18:LN:153:LYS:HG3	18:LN:155:VAL:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LT:18:PRO:HD2	24:LT:21:LYS:HB2	2.01	0.43
28:LX:65:ALA:HB2	38:Lh:69:LEU:HD11	2.00	0.43
28:LX:88:LYS:HE3	28:LX:88:LYS:HB2	1.84	0.43
37:Lg:16:ALA:HA	37:Lg:19:LYS:HE2	2.01	0.43
50:SD:161:GLY:O	50:SD:164:VAL:HG12	2.18	0.43
51:SF:90:VAL:HA	51:SF:93:VAL:HG12	2.01	0.43
56:SR:81:ARG:HH21	65:SA:88:LEU:HD22	1.83	0.43
65:SA:91:ALA:HA	65:SA:96:ALA:HB3	2.01	0.43
66:SB:123:ALA:HB3	66:SB:139:CYS:SG	2.58	0.43
71:SI:145:ILE:HG23	71:SI:148:LYS:HE2	1.99	0.43
79:SY:29:HIS:HB2	79:SY:32:LYS:HB2	2.00	0.43
79:SY:119:GLY:HA2	83:S2:85:A:H5'	2.00	0.43
83:S2:99:A2M:H62	83:S2:433:A:H1'	1.84	0.43
83:S2:186:C:H2'	83:S2:187:G:C8	2.54	0.43
83:S2:462:OMC:HM23	83:S2:462:OMC:H1'	1.76	0.43
83:S2:595:U:H2'	83:S2:596:U:C6	2.54	0.43
83:S2:661:U:H3'	83:S2:662:G:H2'	2.00	0.43
83:S2:1182:A:C5	83:S2:1183:A:H1'	2.53	0.43
3:L5:727:C:H4'	11:LF:69:ILE:HG12	2.00	0.43
3:L5:1077:C:H4'	3:L5:1215:C:C4	2.54	0.43
3:L5:1541:C:H2'	3:L5:1542:U:C6	2.54	0.43
3:L5:1915:C:H5'	36:Lf:16:ARG:NH1	2.33	0.43
3:L5:2685:C:H2'	3:L5:2686:G:O4'	2.19	0.43
3:L5:4323:A:C6	9:LD:153:THR:HG21	2.53	0.43
3:L5:5036:C:H2'	3:L5:5037:U:H6	1.84	0.43
10:LE:183:ARG:HA	10:LE:183:ARG:HD2	1.79	0.43
15:LJ:15:LEU:HD12	15:LJ:165:TRP:HB2	2.01	0.43
16:LL:93:THR:HA	38:Lh:116:LEU:HD13	2.01	0.43
20:LP:60:PHE:CE2	20:LP:82:ARG:HB2	2.54	0.43
22:LR:4:LEU:HD11	22:LR:29:THR:HG23	1.99	0.43
38:Lh:25:LYS:O	38:Lh:28:LEU:HG	2.19	0.43
57:SS:106:LYS:HA	57:SS:109:GLU:HG2	2.01	0.43
66:SB:97:LEU:HB3	66:SB:232:HIS:NE2	2.33	0.43
66:SB:171:ILE:HG13	66:SB:197:ILE:HG12	1.99	0.43
67:SC:70:VAL:HG21	67:SC:93:ILE:HG23	2.01	0.43
68:SE:186:GLY:HA3	83:S2:809:A:OP1	2.19	0.43
72:SJ:5:ARG:HB3	83:S2:38:A:H5''	2.00	0.43
75:SO:83:GLN:HA	75:SO:86:LYS:HG2	2.00	0.43
77:SW:90:GLN:HG2	77:SW:97:ARG:NH2	2.33	0.43
83:S2:83:A:H2'	83:S2:84:A:O4'	2.19	0.43
83:S2:1144:A:H5'	83:S2:1355:C:H41	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1189:A:H2'	83:S2:1190:A:C8	2.54	0.43
83:S2:1705:C:H2'	83:S2:1706:G:C8	2.54	0.43
2:Pt:4:U:H2'	2:Pt:5:C:H6	1.84	0.43
3:L5:717:U:H2'	3:L5:718:C:C6	2.53	0.43
3:L5:1281:G:H5'	8:LC:323:ARG:HB2	2.00	0.43
3:L5:1884:C:H2'	3:L5:1885:G:H8	1.84	0.43
3:L5:2351:OMC:HM23	3:L5:2351:OMC:H1'	1.70	0.43
3:L5:2870:A:H2'	3:L5:2871:A:H8	1.83	0.43
3:L5:3748:A:H5''	6:LA:243:THR:OG1	2.19	0.43
3:L5:4215:C:C2	3:L5:4216:G:C8	3.07	0.43
3:L5:4424:A:H5'	43:Lm:125:LYS:HE3	2.00	0.43
3:L5:4466:C:H2'	3:L5:4467:A:C8	2.53	0.43
3:L5:4593:C:H2'	3:L5:4594:U:H6	1.83	0.43
3:L5:4637:OMG:H2'	3:L5:4638:U:C6	2.54	0.43
5:L8:119:C:H2'	5:L8:120:G:H8	1.83	0.43
5:L8:141:C:H2'	5:L8:142:U:H6	1.81	0.43
9:LD:208:MET:CB	9:LD:233:PRO:HG3	2.49	0.43
22:LR:82:LYS:HA	22:LR:82:LYS:HD2	1.92	0.43
29:LY:34:LEU:HG	29:LY:106:ILE:HD11	2.00	0.43
35:Le:79:VAL:HG23	35:Le:84:GLU:HB2	2.01	0.43
64:Sg:217:MET:HE2	64:Sg:219:TRP:CH2	2.54	0.43
65:SA:134:LEU:HD21	65:SA:144:THR:HG21	1.99	0.43
65:SA:137:ALA:HB1	65:SA:142:LEU:HB3	2.01	0.43
67:SC:196:ILE:HB	67:SC:223:TYR:HB2	2.01	0.43
73:SL:23:VAL:HG23	73:SL:25:LEU:HG	2.01	0.43
75:SO:63:LYS:HD3	75:SO:63:LYS:HA	1.81	0.43
83:S2:96:C:H2'	83:S2:97:U:H6	1.83	0.43
83:S2:120:U:H2'	83:S2:121:OMU:H6	2.01	0.43
83:S2:193:C:H2'	83:S2:194:C:C6	2.54	0.43
83:S2:289:G:H2'	83:S2:290:U:C6	2.54	0.43
83:S2:475:C:H1'	83:S2:507:G:H1'	1.99	0.43
3:L5:461:G:H2'	3:L5:462:G:H8	1.84	0.42
3:L5:1304:C:H2'	3:L5:1305:C:C6	2.54	0.42
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.54	0.42
3:L5:2676:A:H8	3:L5:2676:A:OP2	2.02	0.42
3:L5:4195:G:C8	3:L5:4442:PSU:H5'	2.53	0.42
3:L5:4219:A:H2'	3:L5:4220:6MZ:C8	2.49	0.42
3:L5:4600:G:H4'	3:L5:4601:U:O5'	2.19	0.42
3:L5:4919:G:H2'	3:L5:4920:C:C6	2.54	0.42
4:L7:33:U:H2'	4:L7:34:C:C6	2.53	0.42
5:L8:69:PSU:H2'	5:L8:70:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:116:LEU:HD13	6:LA:164:ALA:HB2	2.01	0.42
7:LB:181:MET:HE1	7:LB:346:THR:HG21	2.01	0.42
8:LC:13:GLU:CD	8:LC:157:LYS:HE3	2.44	0.42
28:LX:76:ILE:HD12	28:LX:101:ASP:HB3	1.99	0.42
39:Li:51:ALA:HB3	39:Li:54:GLU:OE1	2.19	0.42
48:Ls:39:GLN:O	48:Ls:42:GLN:HG3	2.19	0.42
58:ST:65:TYR:HE1	58:ST:128:GLN:HB2	1.84	0.42
72:SJ:111:GLN:HE21	72:SJ:123:ILE:HG13	1.84	0.42
74:SN:5:HIS:CE1	74:SN:121:ARG:HG3	2.54	0.42
83:S2:99:A2M:H1'	83:S2:99:A2M:HM'3	1.55	0.42
83:S2:483:C:H2'	83:S2:484:A2M:C8	2.49	0.42
83:S2:1114:U:O2'	83:S2:1115:U:H2'	2.19	0.42
83:S2:1391:OMC:H1'	83:S2:1391:OMC:HM23	1.78	0.42
83:S2:1533:A:N6	83:S2:1602:U:C2	2.86	0.42
3:L5:424:U:H2'	3:L5:425:U:C6	2.54	0.42
3:L5:711:A:H2'	3:L5:712:C:C6	2.53	0.42
3:L5:2066:C:O2'	36:Lf:79:GLY:HA2	2.19	0.42
3:L5:2898:G:H2'	3:L5:2899:C:H6	1.84	0.42
3:L5:3825:A2M:HM'3	3:L5:3825:A2M:H1'	1.66	0.42
3:L5:4673:PSU:H5'	26:LV:89:ARG:NH2	2.34	0.42
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.55	0.42
5:L8:64:U:C2	5:L8:65:A:C8	3.08	0.42
6:LA:114:CYS:SG	6:LA:169:VAL:HB	2.58	0.42
6:LA:145:LYS:HA	6:LA:145:LYS:HD3	1.74	0.42
15:LJ:52:LYS:HB3	15:LJ:65:ASN:HA	2.01	0.42
18:LN:56:LYS:HD3	18:LN:56:LYS:HA	1.87	0.42
47:Lr:16:PHE:CD2	47:Lr:28:GLU:HB3	2.53	0.42
52:SK:51:SER:HA	83:S2:1276:A:O2'	2.19	0.42
56:SR:9:VAL:HG23	56:SR:50:ILE:HG12	2.01	0.42
66:SB:123:ALA:HB2	66:SB:165:ARG:HG2	2.00	0.42
69:SG:200:LYS:HA	69:SG:203:LYS:HG2	2.01	0.42
76:SV:74:LYS:NZ	76:SV:83:PHE:HB3	2.34	0.42
81:Sb:18:LYS:NZ	81:Sb:23:ARG:HA	2.34	0.42
83:S2:185:G:H2'	83:S2:186:C:H6	1.85	0.42
83:S2:453:C:H2'	83:S2:454:U:C6	2.54	0.42
83:S2:530:U:H2'	83:S2:531:A:H8	1.83	0.42
83:S2:651:PSU:H2'	83:S2:652:U:C6	2.54	0.42
83:S2:919:A:H8	83:S2:919:A:OP2	2.02	0.42
83:S2:1775:U:H2'	83:S2:1776:G:N3	2.34	0.42
3:L5:1290:G:H2'	3:L5:1291:G:C8	2.54	0.42
3:L5:3833:C:H2'	3:L5:3834:C:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.53	0.42
3:L5:4092:G:N2	3:L5:4158:C:C2	2.87	0.42
4:L7:4:U:H2'	4:L7:5:A:H8	1.83	0.42
5:L8:7:U:H2'	5:L8:8:U:C6	2.54	0.42
5:L8:8:U:H2'	5:L8:9:A:C8	2.54	0.42
6:LA:58:LEU:HD13	6:LA:58:LEU:HA	1.89	0.42
11:LF:179:LEU:HD13	11:LF:182:TYR:HD2	1.84	0.42
16:LL:121:ARG:NH2	16:LL:124:LEU:HD11	2.34	0.42
17:LM:24:LEU:HD21	17:LM:86:TRP:CE2	2.53	0.42
19:LO:47:PHE:HA	19:LO:136:ALA:HB2	2.01	0.42
21:LQ:33:ARG:HA	21:LQ:48:LEU:HD22	2.01	0.42
52:SK:85:LEU:HD12	52:SK:86:PRO:HD2	2.01	0.42
66:SB:167:LYS:HB2	66:SB:167:LYS:HE2	1.86	0.42
70:SH:112:ASN:ND2	83:S2:875:A:H5''	2.34	0.42
71:SI:41:ARG:CZ	83:S2:305:U:H4'	2.49	0.42
73:SL:59:LYS:HD3	73:SL:134:LEU:HD13	2.02	0.42
74:SN:20:ARG:NH2	83:S2:918:U:H4'	2.35	0.42
76:SV:30:ALA:HA	76:SV:60:ARG:HH21	1.84	0.42
77:SW:32:LYS:HA	77:SW:35:VAL:HG22	2.00	0.42
78:SX:24:ASP:OD1	78:SX:27:TYR:HB3	2.20	0.42
81:Sb:81:ARG:HA	81:Sb:81:ARG:HD2	1.79	0.42
83:S2:30:C:H2'	83:S2:31:U:C6	2.54	0.42
83:S2:184:G:H2'	83:S2:185:G:H8	1.84	0.42
83:S2:314:U:H2'	83:S2:315:C:H6	1.85	0.42
83:S2:945:U:H2'	83:S2:946:U:C6	2.55	0.42
83:S2:991:G:C6	83:S2:1134:G:H4'	2.53	0.42
83:S2:1004:PSU:H2'	83:S2:1005:G:C8	2.54	0.42
83:S2:1107:G:H2'	83:S2:1108:G:H8	1.83	0.42
3:L5:347:A:H2'	3:L5:348:G:C8	2.54	0.42
3:L5:700:G:C6	3:L5:701:G:C6	3.07	0.42
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.20	0.42
3:L5:2020:U:H2'	3:L5:2021:G:C8	2.50	0.42
3:L5:2539:C:H2'	3:L5:2540:C:H6	1.81	0.42
3:L5:2875:C:H5'	3:L5:2876:OMG:C5	2.54	0.42
3:L5:3928:A:H3'	3:L5:3929:G:H8	1.84	0.42
3:L5:4454:G:H2'	3:L5:4455:G:H8	1.84	0.42
3:L5:4524:G:H2'	3:L5:4525:C:H6	1.84	0.42
3:L5:4928:C:H2'	3:L5:4929:C:C6	2.54	0.42
3:L5:4968:A:H2'	3:L5:4969:C:C6	2.55	0.42
4:L7:18:C:H2'	4:L7:19:C:C6	2.54	0.42
7:LB:49:TYR:CE2	7:LB:344:VAL:HG22	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LI:150:GLU:O	14:LI:153:ARG:HG3	2.20	0.42
15:LJ:83:LEU:HD11	15:LJ:132:VAL:HG21	2.01	0.42
19:LO:70:PRO:HB2	19:LO:72:HIS:CE1	2.53	0.42
20:LP:43:LYS:HA	20:LP:46:LYS:HG2	2.01	0.42
26:LV:90:ARG:HH22	26:LV:96:LEU:HD22	1.83	0.42
31:La:100:ILE:HG13	31:La:123:ILE:HB	2.01	0.42
37:Lg:63:VAL:HG13	37:Lg:66:ARG:CZ	2.49	0.42
49:Lt:29:ALA:HA	49:Lt:32:ILE:HD13	2.02	0.42
53:SM:112:LYS:HE2	53:SM:112:LYS:HB2	1.90	0.42
64:Sg:10:THR:HB	64:Sg:306:LEU:HD21	2.00	0.42
64:Sg:289:LEU:HD12	64:Sg:289:LEU:HA	1.91	0.42
66:SB:75:GLN:HB2	66:SB:78:GLU:CD	2.44	0.42
70:SH:192:PHE:HE1	81:Sb:84:HIS:HB3	1.84	0.42
71:SI:56:ARG:HH12	83:S2:379:C:H5''	1.85	0.42
83:S2:92:A:N6	83:S2:444:G:H1'	2.34	0.42
83:S2:616:A:H62	83:S2:625:G:N2	2.18	0.42
83:S2:1173:A:H2'	83:S2:1174:PSU:H6	1.84	0.42
83:S2:1303:C:H2'	83:S2:1304:U:C6	2.55	0.42
83:S2:1320:G:H2'	83:S2:1321:G:O4'	2.19	0.42
83:S2:1555:U:H5'	83:S2:1556:A:C5	2.54	0.42
83:S2:1621:U:O2'	83:S2:1622:U:H2'	2.20	0.42
83:S2:1649:U:H2'	83:S2:1650:A:H8	1.84	0.42
83:S2:1651:A:H2'	83:S2:1652:G:C8	2.54	0.42
3:L5:742:G:H2'	3:L5:743:G:H8	1.84	0.42
3:L5:1354:A:OP2	21:LQ:106:THR:HG21	2.18	0.42
3:L5:1534:A2M:H8	40:Lj:15:THR:HG23	2.01	0.42
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.55	0.42
3:L5:3871:A:H2'	3:L5:3872:A:C8	2.54	0.42
3:L5:3927:U:H2'	3:L5:3928:A:C8	2.55	0.42
3:L5:3936:A:H2'	3:L5:3937:C:C6	2.54	0.42
3:L5:4153:C:H5''	28:LX:38:LYS:HD2	2.01	0.42
3:L5:4518:A:OP2	3:L5:4518:A:H8	2.01	0.42
3:L5:4592:C:H2'	3:L5:4593:C:C6	2.53	0.42
5:L8:27:U:H2'	5:L8:28:C:C6	2.54	0.42
5:L8:55:PSU:H2'	5:L8:56:G:C8	2.54	0.42
8:LC:130:ALA:HB3	8:LC:246:VAL:HG21	2.00	0.42
14:LI:188:LYS:NZ	14:LI:213:HIS:H	2.17	0.42
19:LO:14:HIS:CE1	19:LO:119:VAL:HG13	2.55	0.42
40:Lj:28:HIS:HE1	40:Lj:30:GLN:HB3	1.84	0.42
55:SQ:90:LYS:HA	55:SQ:93:VAL:HG22	2.02	0.42
56:SR:54:VAL:O	56:SR:58:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SZ:50:PHE:HE2	60:SZ:87:ALA:HB2	1.83	0.42
64:Sg:54:ILE:HD12	64:Sg:55:PRO:HD2	2.02	0.42
68:SE:137:PRO:HG2	68:SE:150:PRO:HD2	2.02	0.42
69:SG:63:MET:HE1	69:SG:106:LEU:HD21	2.02	0.42
73:SL:8:ARG:HH21	83:S2:390:C:H4'	1.85	0.42
83:S2:1070:A:H3'	83:S2:1071:G:H8	1.85	0.42
83:S2:1501:C:H2'	83:S2:1502:C:H6	1.83	0.42
83:S2:1643:U:H2'	83:S2:1644:C:H6	1.83	0.42
2:Pt:72:C:H3'	2:Pt:73:A:H8	1.84	0.42
3:L5:35:U:H4'	3:L5:1525:A:H2	1.85	0.42
3:L5:74:G:H1'	16:LL:62:PRO:HG3	2.01	0.42
3:L5:2875:C:H3'	46:Lp:7:LYS:HG2	2.01	0.42
3:L5:3760:A:C5	83:S2:1826:G:H4'	2.55	0.42
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.55	0.42
3:L5:4147:G:H2'	3:L5:4148:C:C6	2.53	0.42
3:L5:4407:G:H1'	3:L5:4438:U:C2	2.54	0.42
3:L5:4568:A:P	7:LB:20:LYS:HB2	2.59	0.42
4:L7:111:C:H2'	4:L7:112:U:O4'	2.19	0.42
5:L8:144:U:H2'	5:L8:145:C:C6	2.55	0.42
6:LA:29:LEU:HG	6:LA:124:GLY:H	1.84	0.42
6:LA:179:ILE:HA	6:LA:184:ARG:HH21	1.83	0.42
7:LB:169:ARG:HG3	7:LB:170:LEU:HD22	2.01	0.42
7:LB:216:MET:HG3	7:LB:281:ASN:HA	2.01	0.42
16:LL:18:TRP:CD1	16:LL:18:TRP:H	2.36	0.42
18:LN:48:ALA:C	18:LN:53:TYR:HB3	2.44	0.42
20:LP:114:ILE:HA	20:LP:150:LEU:HD13	2.01	0.42
22:LR:150:ALA:O	22:LR:153:LYS:HG2	2.19	0.42
28:LX:90:ILE:HD13	28:LX:96:LEU:HA	2.02	0.42
42:Ll:11:ARG:HD2	42:Ll:12:PHE:N	2.34	0.42
47:Lr:119:ARG:HD3	47:Lr:119:ARG:HA	1.78	0.42
50:SD:125:PHE:HA	50:SD:128:GLU:HG2	2.00	0.42
51:SF:164:ARG:HH21	83:S2:1533:A:H3'	1.84	0.42
52:SK:31:LYS:HE3	52:SK:36:ALA:HA	2.01	0.42
57:SS:78:LYS:HD3	57:SS:78:LYS:HA	1.75	0.42
65:SA:11:LYS:HD2	65:SA:11:LYS:HA	1.83	0.42
67:SC:233:LEU:HD23	67:SC:233:LEU:HA	1.78	0.42
68:SE:46:ILE:HG22	68:SE:49:ARG:HH21	1.84	0.42
76:SV:74:LYS:HZ3	76:SV:83:PHE:HB3	1.85	0.42
83:S2:1090:C:H2'	83:S2:1091:C:H6	1.84	0.42
3:L5:180:C:H2'	3:L5:181:C:H6	1.85	0.42
3:L5:677:G:H2'	3:L5:678:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.85	0.42
3:L5:1191:C:H2'	3:L5:1192:C:H6	1.83	0.42
3:L5:1867:A:H2'	3:L5:1868:A:C8	2.55	0.42
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.20	0.42
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.85	0.42
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.85	0.42
3:L5:3855:C:H2'	3:L5:3856:A:H8	1.84	0.42
3:L5:4093:G:H3'	3:L5:4094:G:H8	1.84	0.42
3:L5:4456:OMC:HM21	7:LB:241:PRO:HD3	2.01	0.42
3:L5:5029:C:O2'	3:L5:5030:U:H6	2.02	0.42
20:LP:40:HIS:HA	20:LP:113:VAL:HG12	2.02	0.42
20:LP:42:ARG:HA	20:LP:45:THR:HG22	2.01	0.42
36:Lf:18:LEU:HD23	36:Lf:19:ARG:NH1	2.35	0.42
36:Lf:56:ASN:HD21	36:Lf:64:PRO:HB2	1.85	0.42
45:Lo:6:LYS:HG3	45:Lo:94:GLY:HA3	2.01	0.42
46:Lp:75:SER:O	46:Lp:79:VAL:HG23	2.19	0.42
54:SP:100:LYS:HB2	83:S2:1240:A:C5	2.54	0.42
64:Sg:183:LYS:HD2	64:Sg:183:LYS:HA	1.89	0.42
76:SV:64:GLU:OE2	76:SV:67:ASP:HB3	2.19	0.42
83:S2:386:C:H2'	83:S2:387:C:H6	1.84	0.42
3:L5:286:U:H2'	3:L5:287:U:C6	2.55	0.42
3:L5:909:A:H2'	3:L5:910:G:H8	1.85	0.42
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.55	0.42
3:L5:1717:C:H2'	3:L5:1718:C:C4	2.55	0.42
3:L5:2006:U:H2'	3:L5:2007:G:O4'	2.19	0.42
3:L5:4232:U:H5''	45:Lo:3:ASN:O	2.20	0.42
3:L5:4697:U:H4'	43:Lm:104:HIS:ND1	2.33	0.42
8:LC:104:PRO:HB2	8:LC:106:LYS:NZ	2.35	0.42
16:LL:42:LYS:HG3	16:LL:45:ARG:HH22	1.84	0.42
20:LP:131:ARG:HG3	20:LP:137:ASN:OD1	2.19	0.42
46:Lp:83:ILE:HD13	46:Lp:83:ILE:HA	1.93	0.42
48:Ls:13:TYR:O	48:Ls:17:ILE:HG12	2.20	0.42
49:Lt:11:LYS:HA	49:Lt:11:LYS:HD2	1.84	0.42
59:SU:61:LEU:HG	62:Sd:34:TYR:CZ	2.54	0.42
65:SA:37:TYR:HA	65:SA:53:ARG:HD3	2.02	0.42
67:SC:208:PRO:O	67:SC:211:LYS:HG2	2.20	0.42
70:SH:157:HIS:HB3	70:SH:190:PRO:HG3	2.02	0.42
73:SL:95:TYR:HB2	73:SL:102:PHE:CE1	2.54	0.42
79:SY:105:LYS:O	79:SY:109:GLU:HG2	2.20	0.42
80:Sa:10:ARG:HH12	83:S2:1859:A:P	2.42	0.42
83:S2:688:U:H1'	83:S2:689:U:OP2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:885:U:O2	83:S2:901:G:C6	2.73	0.42
83:S2:1409:A:H2'	83:S2:1410:C:C6	2.54	0.42
3:L5:152:U:H5''	18:LN:54:LYS:HG2	2.01	0.42
3:L5:171:U:H5''	3:L5:172:C:C5	2.55	0.42
3:L5:440:U:H2'	3:L5:441:G:C8	2.55	0.42
3:L5:1677:PSU:H4'	3:L5:1680:G:C2	2.53	0.42
3:L5:1811:G:H2'	3:L5:1812:C:H6	1.84	0.42
3:L5:1848:C:H2'	3:L5:1849:U:O4'	2.20	0.42
3:L5:2082:G:H5''	21:LQ:12:LYS:HD3	2.02	0.42
3:L5:2499:C:H2'	3:L5:2500:U:H6	1.85	0.42
3:L5:4139:G:N2	3:L5:4140:C:H41	2.12	0.42
3:L5:4727:A:H2'	3:L5:4728:U:O4'	2.19	0.42
11:LF:91:PHE:HB2	11:LF:145:PRO:HG3	2.01	0.42
12:LG:77:PRO:HD2	12:LG:80:ILE:HD13	2.02	0.42
17:LM:38:VAL:HG21	17:LM:50:MET:HE2	2.01	0.42
22:LR:42:ARG:O	22:LR:45:ILE:HG22	2.19	0.42
28:LX:105:ASN:O	28:LX:109:ILE:HD12	2.20	0.42
54:SP:85:ILE:HD13	54:SP:111:MET:HG3	2.01	0.42
56:SR:15:VAL:O	56:SR:18:GLU:HG2	2.20	0.42
68:SE:86:PHE:HE1	68:SE:103:TYR:H	1.68	0.42
68:SE:136:ILE:HD12	68:SE:149:TYR:CE1	2.55	0.42
70:SH:171:GLU:HG2	70:SH:172:THR:N	2.34	0.42
71:SI:98:LYS:HD2	71:SI:178:ARG:HG2	2.01	0.42
77:SW:119:LYS:HA	77:SW:119:LYS:HD3	1.82	0.42
83:S2:1362:U:H5''	83:S2:1363:C:H5	1.83	0.42
83:S2:1657:G:H2'	83:S2:1658:G:H8	1.85	0.42
3:L5:678:C:H2'	3:L5:679:C:C6	2.55	0.42
3:L5:1340:OMC:HN41	3:L5:1516:G:H1	1.66	0.42
3:L5:4561:C:H2'	3:L5:4562:C:C6	2.55	0.42
3:L5:4697:U:H4'	43:Lm:104:HIS:CE1	2.55	0.42
3:L5:4896:G:H2'	3:L5:4897:G:H8	1.83	0.42
8:LC:40:VAL:O	8:LC:44:LEU:HB2	2.20	0.42
8:LC:284:MET:HB3	21:LQ:24:TYR:HD2	1.85	0.42
11:LF:226:HIS:HD2	11:LF:227:PHE:N	2.17	0.42
18:LN:104:GLU:OE1	18:LN:161:MET:HG2	2.19	0.42
21:LQ:18:PRO:HD3	21:LQ:52:PHE:CE1	2.54	0.42
47:Lr:26:SER:HB3	47:Lr:31:ASN:HD22	1.84	0.42
50:SD:13:ALA:HA	50:SD:16:ILE:HG22	2.02	0.42
52:SK:32:HIS:CD2	52:SK:45:VAL:HG21	2.52	0.42
60:SZ:106:GLN:HE21	60:SZ:106:GLN:CA	2.32	0.42
66:SB:82:ARG:HD3	66:SB:103:MET:HE2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SC:116:THR:HA	83:S2:1203:G:H4'	2.01	0.42
72:SJ:150:ARG:HG3	83:S2:821:G:C6	2.54	0.42
75:SO:136:PRO:HB3	83:S2:944:A:H1'	2.00	0.42
83:S2:1208:A:H2'	83:S2:1209:A:H8	1.84	0.42
83:S2:1264:C:H4'	83:S2:1265:A:O4'	2.20	0.42
3:L5:192:G:H2'	3:L5:193:G:H8	1.85	0.41
3:L5:1997:U:O2'	3:L5:1998:A:H8	2.02	0.41
3:L5:2638:G:N1	3:L5:2718:U:H2'	2.35	0.41
3:L5:4102:C:H1'	3:L5:4108:G:H1	1.85	0.41
3:L5:4694:G:H4'	13:LH:71:ARG:HH12	1.85	0.41
4:L7:57:C:H2'	4:L7:58:A:C8	2.55	0.41
8:LC:205:ARG:HD3	8:LC:205:ARG:HA	1.88	0.41
12:LG:162:ASP:HB3	12:LG:163:PRO:HD3	2.01	0.41
23:LS:107:THR:O	23:LS:111:ARG:HG2	2.19	0.41
29:LY:74:TYR:CE2	29:LY:77:LYS:HG3	2.48	0.41
31:La:125:LYS:HD3	31:La:125:LYS:HA	1.89	0.41
32:Lb:35:VAL:HB	32:Lb:40:LEU:HD21	2.01	0.41
47:Lr:65:LYS:HE3	47:Lr:65:LYS:HB2	1.82	0.41
49:Lt:61:LYS:HA	49:Lt:75:PRO:HD2	2.03	0.41
53:SM:79:VAL:HG11	53:SM:85:LEU:HD22	2.01	0.41
56:SR:128:PHE:CD2	56:SR:129:LYS:HG3	2.55	0.41
57:SS:102:GLY:O	57:SS:106:LYS:HG2	2.20	0.41
65:SA:219:GLU:HA	65:SA:222:VAL:HG12	2.02	0.41
66:SB:32:ASP:HB2	66:SB:94:LYS:NZ	2.35	0.41
67:SC:110:MET:HE1	67:SC:127:PHE:CZ	2.55	0.41
73:SL:77:VAL:HG11	73:SL:80:MET:HE2	2.01	0.41
74:SN:63:VAL:O	74:SN:67:THR:HG22	2.20	0.41
83:S2:674:C:H2'	83:S2:675:U:C6	2.55	0.41
83:S2:959:G:H1'	83:S2:964:A:N6	2.35	0.41
83:S2:1047:C:H2'	83:S2:1048:G:O4'	2.20	0.41
2:Pt:27:U:C2	2:Pt:28:U:C5	3.09	0.41
3:L5:1181:C:O2'	3:L5:1183:C:H5''	2.20	0.41
3:L5:1534:A2M:C8	40:Lj:15:THR:HG23	2.50	0.41
3:L5:1820:C:H2'	3:L5:1822:U:H5'	2.02	0.41
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.84	0.41
3:L5:4910:G:C4	19:LO:156:LEU:HD13	2.55	0.41
4:L7:113:G:H2'	4:L7:114:U:C6	2.55	0.41
5:L8:43:A:H2'	5:L8:44:A:H8	1.84	0.41
6:LA:20:VAL:HG12	6:LA:23:ARG:NH1	2.35	0.41
8:LC:218:ILE:HG12	8:LC:229:LEU:HD22	2.02	0.41
13:LH:44:GLU:HG3	13:LH:58:ASP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:117:PHE:O	13:LH:120:GLU:HG3	2.20	0.41
14:LI:183:ASP:O	14:LI:187:LYS:HG2	2.20	0.41
17:LM:33:GLN:HB3	23:LS:145:PHE:HZ	1.85	0.41
36:Lf:8:LYS:HB3	36:Lf:100:ARG:CZ	2.50	0.41
40:Lj:17:THR:HB	40:Lj:29:LEU:HD21	2.01	0.41
41:Lk:27:LYS:HD2	41:Lk:32:VAL:HG22	2.01	0.41
42:Ll:49:LEU:HD23	42:Ll:49:LEU:HA	1.91	0.41
49:Lt:147:HIS:HA	49:Lt:148:PRO:HD3	1.88	0.41
52:SK:41:PRO:HG2	52:SK:44:HIS:HB2	2.03	0.41
56:SR:77:GLU:HG2	56:SR:80:ARG:HH21	1.84	0.41
57:SS:102:GLY:HA2	57:SS:105:ASN:ND2	2.35	0.41
60:SZ:80:ARG:HH11	83:S2:1598:G:H5''	1.85	0.41
64:Sg:191:HIS:CE1	64:Sg:217:MET:HB2	2.55	0.41
70:SH:23:ILE:HD12	70:SH:23:ILE:HA	1.97	0.41
73:SL:133:PRO:HB3	73:SL:139:ARG:NH1	2.35	0.41
75:SO:37:PHE:CE1	75:SO:110:PRO:HD3	2.55	0.41
83:S2:403:G:H2'	83:S2:404:G:C8	2.54	0.41
83:S2:943:U:H2'	83:S2:944:A:H8	1.85	0.41
83:S2:1740:C:H2'	83:S2:1741:U:C6	2.54	0.41
3:L5:135:G:C6	38:Lh:96:ASN:HA	2.55	0.41
3:L5:325:U:H3'	39:Li:28:ARG:HH21	1.85	0.41
3:L5:1281:G:C6	10:LE:128:HIS:HB2	2.55	0.41
3:L5:1514:U:H2'	3:L5:1515:A:H8	1.85	0.41
3:L5:3706:C:H5''	6:LA:226:ARG:N	2.35	0.41
3:L5:3823:G:H2'	3:L5:3824:A:H8	1.85	0.41
3:L5:3920:PSU:H2'	3:L5:3921:U:C6	2.56	0.41
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.56	0.41
3:L5:4164:C:H2'	3:L5:4165:C:C6	2.55	0.41
3:L5:4210:U:H3	3:L5:4222:G:H1	1.68	0.41
3:L5:4460:U:H2'	3:L5:4461:C:H6	1.84	0.41
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.54	0.41
3:L5:4592:C:H2'	3:L5:4593:C:H6	1.86	0.41
3:L5:4872:G:C2	19:LO:203:VAL:HG23	2.55	0.41
3:L5:4923:C:C2	3:L5:4924:C:N3	2.89	0.41
4:L7:7:G:H5''	9:LD:22:ARG:HD3	2.01	0.41
4:L7:119:U:C2	9:LD:261:VAL:HG11	2.55	0.41
14:LI:182:GLU:HG2	14:LI:183:ASP:N	2.35	0.41
20:LP:109:VAL:HA	20:LP:112:LEU:HD13	2.00	0.41
24:LT:122:LYS:NZ	24:LT:124:THR:HB	2.36	0.41
30:LZ:26:VAL:HG22	30:LZ:91:LEU:HD11	2.01	0.41
43:Lm:99:CYS:HB3	43:Lm:115:CYS:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:ST:113:VAL:HG22	58:ST:123:LEU:HD23	2.02	0.41
65:SA:109:THR:HG21	83:S2:1378:A:H61	1.84	0.41
68:SE:11:ARG:NH1	68:SE:20:LEU:HB3	2.35	0.41
68:SE:28:ALA:O	83:S2:496:C:H4'	2.19	0.41
69:SG:30:LYS:O	69:SG:102:VAL:HG12	2.20	0.41
70:SH:43:LEU:HB3	70:SH:72:PHE:CE1	2.54	0.41
78:SX:140:ARG:HE	78:SX:141:PRO:HD2	1.84	0.41
83:S2:943:U:H2'	83:S2:944:A:C8	2.55	0.41
83:S2:1647:A:N1	83:S2:1675:A:H5''	2.36	0.41
3:L5:1198:G:H2'	3:L5:1199:G:H8	1.84	0.41
3:L5:2327:G:H2'	3:L5:2328:G:H8	1.85	0.41
3:L5:2474:G:C6	28:LX:47:ARG:HG2	2.55	0.41
3:L5:2749:C:H4'	37:Lg:64:LEU:HB3	2.02	0.41
3:L5:3601:C:H2'	3:L5:3602:C:C6	2.55	0.41
3:L5:4130:C:H2'	3:L5:4131:G:C8	2.55	0.41
3:L5:4130:C:H2'	3:L5:4131:G:H8	1.85	0.41
3:L5:4683:U:H2'	3:L5:4684:A:C8	2.56	0.41
6:LA:117:GLU:HG2	6:LA:163:ARG:O	2.19	0.41
9:LD:89:LYS:HD2	9:LD:90:VAL:HB	2.01	0.41
9:LD:179:ARG:HD3	9:LD:179:ARG:HA	1.81	0.41
10:LE:223:ARG:HB3	10:LE:224:LYS:HB2	2.03	0.41
22:LR:105:LEU:HD11	22:LR:109:TYR:CZ	2.55	0.41
23:LS:103:ALA:O	23:LS:107:THR:HG23	2.21	0.41
25:LU:42:PHE:CZ	25:LU:46:ARG:HG3	2.55	0.41
36:Lf:45:LYS:HA	36:Lf:107:PRO:HD2	2.02	0.41
50:SD:49:ILE:HG22	50:SD:87:TYR:HB3	2.02	0.41
62:Sd:55:LEU:HD12	83:S2:1391:OMC:H4'	2.02	0.41
66:SB:32:ASP:HB2	66:SB:94:LYS:HZ2	1.85	0.41
66:SB:107:ARG:HA	66:SB:110:MET:HG2	2.03	0.41
69:SG:136:LYS:HB3	83:S2:170:A:O5'	2.20	0.41
71:SI:5:ARG:NH1	83:S2:380:G:H1'	2.36	0.41
80:Sa:15:ARG:HH22	83:S2:992:A:H3'	1.85	0.41
81:Sb:19:HIS:NE2	81:Sb:21:LYS:HE2	2.35	0.41
83:S2:51:U:H2'	83:S2:52:G:C8	2.55	0.41
83:S2:159:A2M:HM'3	83:S2:159:A2M:H1'	1.48	0.41
83:S2:681:PSU:H2'	83:S2:682:U:C6	2.55	0.41
83:S2:1189:A:H2'	83:S2:1190:A:H8	1.85	0.41
83:S2:1244:PSU:H2'	83:S2:1245:G:C8	2.54	0.41
83:S2:1329:U:C2	83:S2:1500:G:O6	2.74	0.41
83:S2:1380:C:H2'	83:S2:1381:G:C8	2.56	0.41
83:S2:1852:C:H2'	83:S2:1853:C:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Pt:43:A:H2'	2:Pt:44:A:C8	2.55	0.41
3:L5:228:C:H2'	3:L5:229:G:C8	2.55	0.41
3:L5:678:C:H2'	3:L5:679:C:H6	1.86	0.41
3:L5:727:C:H2'	3:L5:728:U:C6	2.55	0.41
3:L5:1270:A:H8	3:L5:2106:G:H21	1.67	0.41
3:L5:1578:U:H2'	3:L5:1579:C:C6	2.55	0.41
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.55	0.41
3:L5:1997:U:H2'	3:L5:1998:A:H3'	2.01	0.41
3:L5:2519:U:H1'	3:L5:2520:C:C6	2.55	0.41
3:L5:2624:G:H2'	3:L5:2625:U:H6	1.83	0.41
3:L5:2774:C:H2'	3:L5:2775:C:C6	2.56	0.41
3:L5:4629:U:C2	3:L5:4630:G:C8	3.08	0.41
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.55	0.41
4:L7:94:C:H2'	4:L7:95:C:H6	1.85	0.41
5:L8:30:U:H2'	5:L8:31:G:C8	2.56	0.41
6:LA:201:GLY:HA2	6:LA:204:MET:HG3	2.02	0.41
7:LB:385:LYS:O	7:LB:389:MET:HG2	2.21	0.41
11:LF:243:LEU:HG	11:LF:247:MET:HE3	2.02	0.41
25:LU:103:VAL:O	25:LU:111:GLU:HG3	2.21	0.41
30:LZ:32:GLY:HA2	30:LZ:36:ARG:O	2.20	0.41
46:Lp:48:LYS:HE3	46:Lp:48:LYS:HB3	1.87	0.41
47:Lr:64:ILE:HB	47:Lr:102:TYR:CZ	2.55	0.41
49:Lt:12:VAL:HA	49:Lt:14:TYR:CE2	2.55	0.41
51:SF:151:ILE:HD12	51:SF:151:ILE:HA	1.95	0.41
65:SA:70:ASN:HB3	65:SA:73:ASP:HB2	2.03	0.41
68:SE:124:CYS:HB3	68:SE:141:THR:HB	2.02	0.41
71:SI:125:LYS:HA	71:SI:125:LYS:HD3	1.93	0.41
75:SO:61:LYS:HG3	75:SO:77:ALA:HB2	2.02	0.41
83:S2:85:A:H2'	83:S2:86:C:H6	1.86	0.41
83:S2:146:G:H2'	83:S2:147:A:C8	2.55	0.41
83:S2:514:U:H2'	83:S2:515:G:O4'	2.21	0.41
83:S2:695:C:H2'	83:S2:735:C:N4	2.35	0.41
83:S2:1595:U:H2'	83:S2:1596:U:H6	1.86	0.41
3:L5:126:C:H2'	3:L5:127:G:C8	2.56	0.41
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.84	0.41
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.36	0.41
3:L5:2497:C:H2'	3:L5:2498:C:H6	1.86	0.41
3:L5:2532:C:H2'	3:L5:2533:C:C6	2.56	0.41
3:L5:2610:G:H2'	3:L5:2611:A:C8	2.55	0.41
3:L5:2682:G:H2'	3:L5:2683:C:C6	2.55	0.41
3:L5:4571:A2M:H8	3:L5:4571:A2M:O5'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4575:G:H2'	3:L5:4576:PSU:H6	1.85	0.41
3:L5:4708:A:N3	3:L5:4709:U:H5'	2.35	0.41
5:L8:103:A:H5'	5:L8:104:A:H8	1.86	0.41
5:L8:123:U:H2'	5:L8:126:C:N4	2.36	0.41
8:LC:106:LYS:HD3	8:LC:106:LYS:HA	1.80	0.41
10:LE:254:ASP:HA	10:LE:257:ILE:HB	2.03	0.41
12:LG:257:LYS:HZ3	12:LG:261:LEU:HD11	1.86	0.41
17:LM:90:ARG:HA	17:LM:93:LYS:HG2	2.01	0.41
29:LY:34:LEU:HD23	29:LY:38:LEU:HB3	2.03	0.41
33:Lc:31:TYR:CD1	33:Lc:56:ARG:HD2	2.56	0.41
56:SR:7:LYS:HB3	56:SR:11:LYS:HE2	2.02	0.41
58:ST:41:LYS:HD2	83:S2:1627:C:H5''	2.02	0.41
62:Sd:10:HIS:HB3	83:S2:1513:C:OP1	2.20	0.41
64:Sg:314:ILE:HD12	64:Sg:314:ILE:HA	1.93	0.41
65:SA:216:ALA:O	65:SA:219:GLU:HG2	2.21	0.41
66:SB:84:PHE:HB3	66:SB:86:LEU:HD23	2.03	0.41
72:SJ:86:VAL:HG21	72:SJ:105:PHE:HE1	1.84	0.41
78:SX:33:GLY:HA2	78:SX:36:LEU:HD13	2.03	0.41
80:Sa:45:VAL:HG11	80:Sa:53:ILE:HD11	2.02	0.41
83:S2:107:A:H2'	83:S2:108:G:C8	2.54	0.41
83:S2:508:A:H5'	83:S2:509:OMG:OP2	2.21	0.41
83:S2:1173:A:H2'	83:S2:1174:PSU:C6	2.56	0.41
83:S2:1597:C:H4'	83:S2:1603:G:O6	2.21	0.41
83:S2:1630:A:H2'	83:S2:1630:A:N3	2.34	0.41
83:S2:1854:U:H2'	83:S2:1855:G:H8	1.86	0.41
3:L5:302:C:H2'	3:L5:303:C:C6	2.56	0.41
3:L5:388:A:H5'	3:L5:389:A:H5'	2.02	0.41
3:L5:724:C:OP1	8:LC:350:ARG:HD3	2.20	0.41
3:L5:1458:C:C2	3:L5:1459:A:C8	3.09	0.41
3:L5:1754:U:H2'	3:L5:1755:C:C5	2.55	0.41
3:L5:2283:G:H2'	3:L5:2284:G:C8	2.55	0.41
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.56	0.41
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.62	0.41
3:L5:2431:A:H2'	3:L5:2432:U:C6	2.56	0.41
3:L5:3641:U:H5	3:L5:3646:A:N7	2.19	0.41
3:L5:3664:G:H2'	3:L5:3665:G:C8	2.50	0.41
3:L5:3785:A2M:H2	3:L5:4551:U:O2	2.20	0.41
3:L5:4719:G:O2'	3:L5:4720:C:H5''	2.20	0.41
3:L5:4761:G:H2'	3:L5:4762:A:C8	2.55	0.41
7:LB:302:ASN:HB2	7:LB:313:SER:HA	2.03	0.41
9:LD:150:LEU:HD23	9:LD:150:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:90:TYR:CZ	13:LH:184:LYS:HG2	2.56	0.41
13:LH:170:LYS:HD2	13:LH:175:PHE:CE1	2.56	0.41
18:LN:22:LEU:HD12	18:LN:26:ARG:NH1	2.36	0.41
31:La:72:THR:OG1	31:La:112:LEU:HG	2.20	0.41
38:Lh:54:ILE:HA	38:Lh:57:VAL:HG12	2.01	0.41
40:Lj:2:THR:HB	40:Lj:6:SER:HB2	2.02	0.41
68:SE:246:LEU:HD13	68:SE:250:GLU:HG2	2.03	0.41
83:S2:698:G:H5'	83:S2:733:C:N3	2.35	0.41
83:S2:734:C:H42	83:S2:737:G:H22	1.68	0.41
83:S2:835:C:H2'	83:S2:837:A:C6	2.54	0.41
83:S2:1104:G:H2'	83:S2:1105:G:H8	1.84	0.41
83:S2:1402:A:H3'	83:S2:1405:A:N6	2.36	0.41
3:L5:69:A:H2	3:L5:71:C:H42	1.68	0.41
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.56	0.41
3:L5:440:U:H2'	3:L5:441:G:H8	1.86	0.41
3:L5:1247:U:H2'	3:L5:1248:C:C6	2.56	0.41
3:L5:1444:G:H22	3:L5:2104:G:N2	2.19	0.41
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.85	0.41
3:L5:2611:A:H2'	3:L5:2612:G:H8	1.86	0.41
3:L5:2722:G:H2'	3:L5:2723:U:O4'	2.20	0.41
3:L5:3718:A2M:H2	3:L5:3934:G:C1'	2.51	0.41
5:L8:75:OMG:C8	42:Ll:30:LYS:HG2	2.55	0.41
8:LC:76:ILE:HG12	8:LC:96:CYS:SG	2.61	0.41
8:LC:116:ASN:HB2	8:LC:119:GLN:OE1	2.20	0.41
8:LC:236:ASN:HB3	8:LC:239:LYS:HG2	2.03	0.41
10:LE:153:LEU:HD11	10:LE:195:ILE:HG13	2.03	0.41
12:LG:86:ALA:HB3	12:LG:185:LYS:HE2	2.03	0.41
17:LM:25:VAL:HB	17:LM:38:VAL:HG13	2.03	0.41
19:LO:179:LYS:O	19:LO:182:GLU:HG3	2.21	0.41
21:LQ:18:PRO:HD3	21:LQ:52:PHE:CD1	2.56	0.41
22:LR:166:THR:HG21	83:S2:873:G:H5'	2.02	0.41
46:Lp:62:LYS:HE3	46:Lp:62:LYS:HB2	1.87	0.41
56:SR:59:LYS:O	56:SR:62:GLN:HG3	2.21	0.41
64:Sg:241:PHE:CE2	64:Sg:248:LEU:HD12	2.56	0.41
68:SE:74:GLY:O	68:SE:75:LYS:HD2	2.20	0.41
69:SG:191:ARG:O	69:SG:195:LYS:HG3	2.20	0.41
83:S2:218:U:H2'	83:S2:219:U:H6	1.86	0.41
83:S2:462:OMC:H2'	83:S2:463:C:C6	2.56	0.41
83:S2:635:G:H2'	83:S2:636:C:C6	2.55	0.41
83:S2:639:C:H2'	83:S2:640:A:H8	1.82	0.41
83:S2:815:U:C2	83:S2:816:A:C8	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:59:GLN:HB2	25:LU:99:TRP:HE1	1.86	0.41
3:L5:94:A:C5	3:L5:95:G:H1'	2.55	0.41
3:L5:135:G:H5''	3:L5:136:C:O4'	2.21	0.41
3:L5:428:G:H2'	3:L5:429:A:C8	2.56	0.41
3:L5:441:G:H2'	3:L5:442:G:C8	2.56	0.41
3:L5:697:G:H2'	3:L5:698:G:C8	2.56	0.41
3:L5:946:C:H2'	3:L5:947:C:C6	2.56	0.41
3:L5:1628:C:H42	6:LA:3:ARG:HD3	1.84	0.41
3:L5:1728:U:H2'	3:L5:1729:A:H8	1.85	0.41
3:L5:1768:C:H2'	3:L5:1770:A:N7	2.36	0.41
3:L5:1863:U:H2'	3:L5:1864:G:H8	1.84	0.41
3:L5:1908:A:H2'	3:L5:1909:G:O4'	2.20	0.41
3:L5:2019:C:H2'	3:L5:2020:U:C6	2.55	0.41
3:L5:2249:C:H2'	3:L5:2250:C:H5	1.85	0.41
3:L5:2275:G:H2'	3:L5:2276:A:C8	2.56	0.41
3:L5:2386:U:H2'	3:L5:2387:G:H8	1.86	0.41
3:L5:2730:U:H2'	3:L5:2731:C:H6	1.86	0.41
3:L5:3723:A:H2'	3:L5:3724:A:H8	1.86	0.41
3:L5:4277:G:H2'	3:L5:4278:C:C6	2.55	0.41
3:L5:4301:U:H4'	24:LT:54:HIS:CD2	2.55	0.41
3:L5:4303:C:H1'	3:L5:4306:OMU:H5	2.03	0.41
3:L5:4323:A:C2	9:LD:146:LEU:HD23	2.56	0.41
3:L5:4336:A:H5''	3:L5:4337:C:H5'	2.02	0.41
3:L5:4524:G:H2'	3:L5:4525:C:C6	2.56	0.41
3:L5:4628:PSU:C4	3:L5:4629:U:C5	3.09	0.41
3:L5:4775:C:H41	3:L5:4859:C:H42	1.67	0.41
3:L5:4923:C:N3	3:L5:4924:C:N3	2.69	0.41
3:L5:4974:C:H1'	3:L5:4985:U:O2	2.21	0.41
85:L5:5291:SPM:H31	85:L5:5291:SPM:H62	1.91	0.41
5:L8:36:G:C5	38:Lh:89:ARG:HD3	2.55	0.41
5:L8:129:C:H2'	5:L8:130:C:C6	2.56	0.41
7:LB:56:ILE:HD12	7:LB:368:ILE:HG12	2.01	0.41
7:LB:160:ILE:HD11	7:LB:193:LYS:HB3	2.03	0.41
7:LB:165:HIS:HB3	7:LB:180:LEU:HD23	2.03	0.41
8:LC:317:ASN:HB3	8:LC:320:LYS:HB2	2.02	0.41
12:LG:159:HIS:CD2	12:LG:185:LYS:HD3	2.56	0.41
15:LJ:44:THR:HA	15:LJ:78:LYS:HE2	2.02	0.41
18:LN:13:LYS:HZ1	39:Li:45:ARG:HA	1.84	0.41
20:LP:13:LYS:HB3	20:LP:152:GLU:HB3	2.03	0.41
22:LR:102:LEU:HB3	22:LR:127:VAL:HG21	2.03	0.41
23:LS:7:LEU:H	23:LS:107:THR:CG2	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LS:27:LEU:HD22	23:LS:62:VAL:HG11	2.03	0.41
25:LU:65:ARG:HG2	25:LU:67:LYS:N	2.36	0.41
28:LX:63:LYS:NZ	38:Lh:81:LEU:HD11	2.36	0.41
28:LX:149:VAL:HA	28:LX:152:LYS:HG3	2.03	0.41
30:LZ:103:ASP:HB3	30:LZ:106:LEU:HB2	2.03	0.41
40:Lj:85:LYS:HE3	40:Lj:85:LYS:HB3	1.76	0.41
44:Ln:14:LYS:HD3	44:Ln:18:ARG:NH1	2.34	0.41
50:SD:7:LYS:HD3	59:SU:25:THR:HG21	2.02	0.41
50:SD:25:LEU:HD22	50:SD:37:VAL:HB	2.02	0.41
51:SF:76:MET:HE3	51:SF:76:MET:HB3	1.93	0.41
52:SK:25:LYS:HB2	52:SK:67:PHE:HE1	1.86	0.41
57:SS:40:TYR:OH	57:SS:97:GLN:HG2	2.20	0.41
57:SS:132:ARG:HD3	83:S2:1623:A:C5	2.56	0.41
59:SU:99:LYS:HZ3	59:SU:99:LYS:HG2	1.72	0.41
64:Sg:52:TYR:CE2	64:Sg:309:VAL:HG21	2.55	0.41
64:Sg:240:CYS:SG	64:Sg:249:CYS:HB3	2.61	0.41
66:SB:114:VAL:HG22	66:SB:120:MET:HE1	2.01	0.41
67:SC:60:TRP:CG	67:SC:92:GLU:HG3	2.55	0.41
67:SC:68:ARG:CZ	67:SC:276:THR:HB	2.51	0.41
67:SC:115:GLN:HA	67:SC:120:GLN:HG3	2.03	0.41
69:SG:140:ARG:HD2	83:S2:170:A:OP1	2.21	0.41
70:SH:144:ILE:HB	77:SW:52:ILE:HB	2.02	0.41
72:SJ:60:LEU:HD11	72:SJ:73:GLU:HB3	2.01	0.41
74:SN:126:ALA:HB1	74:SN:139:TRP:HZ3	1.86	0.41
78:SX:132:ALA:HB1	78:SX:138:LYS:HG2	2.03	0.41
79:SY:68:LYS:HB3	79:SY:68:LYS:HE2	1.81	0.41
80:Sa:26:CYS:SG	80:Sa:28:ARG:HG3	2.61	0.41
83:S2:379:C:H2'	83:S2:380:G:C8	2.55	0.41
83:S2:561:A:H2'	83:S2:562:U:C6	2.55	0.41
83:S2:570:C:H2'	83:S2:571:U:O4'	2.20	0.41
83:S2:615:C:H2'	83:S2:616:A:O4'	2.21	0.41
83:S2:910:G:H2'	83:S2:911:C:O4'	2.21	0.41
83:S2:930:C:H42	83:S2:1011:A:H62	1.69	0.41
83:S2:1353:A:H2'	83:S2:1354:G:C8	2.56	0.41
83:S2:1501:C:H2'	83:S2:1502:C:C6	2.56	0.41
83:S2:1733:U:H2'	83:S2:1734:G:O4'	2.21	0.41
83:S2:1802:C:H2'	83:S2:1803:U:H6	1.85	0.41
3:L5:20:U:H3'	3:L5:21:G:H8	1.85	0.41
3:L5:271:C:H2'	3:L5:272:U:H6	1.86	0.41
3:L5:714:G:H2'	3:L5:715:G:C8	2.56	0.41
3:L5:1323:A2M:HM'3	3:L5:1323:A2M:H1'	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1524:A2M:H8	3:L5:3915:U:O2	2.20	0.41
3:L5:2858:A:H2'	3:L5:2859:G:H8	1.83	0.41
3:L5:4458:C:H2'	3:L5:4459:U:H6	1.86	0.41
3:L5:4523:A2M:H1'	3:L5:4523:A2M:HM'3	1.74	0.41
3:L5:4674:C:H2'	3:L5:4675:U:C6	2.56	0.41
6:LA:61:VAL:HB	6:LA:74:GLU:OE2	2.21	0.41
7:LB:49:TYR:HE2	7:LB:344:VAL:HG22	1.86	0.41
7:LB:219:VAL:HG22	7:LB:347:LEU:HD13	2.02	0.41
11:LF:240:ILE:O	11:LF:244:ILE:HD12	2.21	0.41
18:LN:200:LEU:HD22	18:LN:204:ARG:NH1	2.36	0.41
19:LO:189:ILE:HD13	19:LO:189:ILE:HA	1.96	0.41
22:LR:177:LEU:O	22:LR:181:LYS:HG2	2.21	0.41
26:LV:72:LEU:HA	26:LV:75:LYS:HZ2	1.86	0.41
30:LZ:67:LYS:HA	30:LZ:119:GLU:OE2	2.21	0.41
33:Lc:29:LEU:HD12	33:Lc:91:VAL:HG21	2.02	0.41
48:Ls:28:PHE:HB3	48:Ls:189:ILE:HD11	2.03	0.41
50:SD:167:TYR:CE2	50:SD:204:LEU:HD23	2.56	0.41
54:SP:108:LYS:O	54:SP:111:MET:HG2	2.21	0.41
55:SQ:78:VAL:HG11	83:S2:1674:G:P	2.61	0.41
57:SS:114:LEU:HB3	57:SS:122:GLY:HA3	2.03	0.41
67:SC:256:TRP:CE2	77:SW:68:ARG:HD3	2.55	0.41
68:SE:29:PRO:HA	83:S2:496:C:H5'	2.02	0.41
69:SG:41:LEU:HB3	69:SG:45:TRP:CE3	2.56	0.41
70:SH:20:GLU:O	70:SH:23:ILE:HG22	2.21	0.41
81:Sb:19:HIS:CD2	81:Sb:21:LYS:H	2.39	0.41
83:S2:39:A:H3'	83:S2:40:A:C8	2.54	0.41
83:S2:455:A:H2'	83:S2:456:C:C6	2.55	0.41
83:S2:1227:G:H5''	83:S2:1639:G7M:O6	2.21	0.41
83:S2:1349:G:H2'	83:S2:1350:U:C6	2.55	0.41
83:S2:1406:G:H2'	83:S2:1407:U:C6	2.55	0.41
3:L5:86:U:H2'	3:L5:87:A:H8	1.84	0.40
3:L5:173:C:H2'	3:L5:174:C:C6	2.56	0.40
3:L5:473:C:H2'	3:L5:474:C:C6	2.56	0.40
3:L5:659:G:H2'	3:L5:660:A:C8	2.55	0.40
3:L5:1490:G:H2'	3:L5:1491:A:C8	2.57	0.40
3:L5:1603:C:H2'	3:L5:1604:G:H8	1.86	0.40
3:L5:1972:G:C6	3:L5:1995:G:N1	2.89	0.40
3:L5:2390:G:H22	3:L5:2825:A:H2	1.68	0.40
3:L5:2528:G:H4'	3:L5:2783:A:H4'	2.03	0.40
3:L5:2888:G:H2'	3:L5:2889:G:H8	1.86	0.40
3:L5:4471:PSU:H2'	3:L5:4472:G:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4577:U:H2'	3:L5:4578:G:C8	2.56	0.40
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	2.02	0.40
7:LB:39:LYS:HG2	7:LB:42:HIS:CE1	2.56	0.40
13:LH:26:ILE:HG13	13:LH:35:ARG:NE	2.36	0.40
14:LI:48:LEU:O	14:LI:139:ARG:HA	2.20	0.40
16:LL:142:GLU:O	16:LL:146:LEU:HB3	2.21	0.40
20:LP:94:MET:HE3	20:LP:146:ILE:HG22	2.03	0.40
21:LQ:56:THR:HB	21:LQ:146:ARG:NH1	2.37	0.40
30:LZ:23:ALA:HB1	30:LZ:43:VAL:HG22	2.03	0.40
36:Lf:78:HIS:HB3	36:Lf:83:MET:HB2	2.03	0.40
37:Lg:83:CYS:SG	37:Lg:86:CYS:HB2	2.61	0.40
48:Ls:78:LEU:O	48:Ls:82:ILE:HG12	2.21	0.40
52:SK:55:ARG:HG3	83:S2:1277:C:H4'	2.03	0.40
55:SQ:89:SER:HB2	55:SQ:112:LEU:HD11	2.03	0.40
55:SQ:106:LYS:NZ	55:SQ:110:ASP:HB3	2.36	0.40
64:Sg:101:PHE:CE2	64:Sg:136:GLY:HA2	2.55	0.40
77:SW:45:GLY:O	77:SW:68:ARG:HD2	2.21	0.40
78:SX:33:GLY:HA2	78:SX:36:LEU:HB2	2.03	0.40
78:SX:61:GLN:HG3	78:SX:62:PRO:HD3	2.02	0.40
83:S2:92:A:C8	83:S2:447:A:C4	3.09	0.40
83:S2:342:C:H2'	83:S2:343:A:C8	2.54	0.40
83:S2:389:A:H2'	83:S2:390:C:C6	2.56	0.40
83:S2:979:C:H2'	83:S2:980:A:C8	2.57	0.40
83:S2:1389:C:H2'	83:S2:1390:U:C6	2.56	0.40
3:L5:19:G:H2'	3:L5:20:U:C6	2.57	0.40
3:L5:423:G:H2'	3:L5:424:U:C6	2.57	0.40
3:L5:455:C:O2'	3:L5:456:C:H5'	2.21	0.40
3:L5:674:G:H2'	3:L5:675:C:H6	1.87	0.40
3:L5:746:A:H2'	3:L5:747:A:C8	2.56	0.40
3:L5:1481:C:H41	39:Li:4:ARG:HG3	1.86	0.40
3:L5:1490:G:H2'	3:L5:1491:A:H8	1.87	0.40
3:L5:1807:C:H2'	3:L5:1808:C:C6	2.57	0.40
3:L5:2476:G:H2'	3:L5:2477:A:H8	1.86	0.40
3:L5:3652:A:H2'	3:L5:3653:A:C5	2.57	0.40
3:L5:4139:G:H21	3:L5:4140:C:N4	2.12	0.40
8:LC:164:THR:HG22	8:LC:220:ALA:O	2.21	0.40
10:LE:115:TYR:HD1	47:Lr:115:SER:HB3	1.84	0.40
13:LH:128:MET:SD	13:LH:157:SER:HB3	2.62	0.40
16:LL:75:GLY:HA2	16:LL:97:SER:OG	2.22	0.40
18:LN:22:LEU:HD12	18:LN:26:ARG:HH12	1.86	0.40
19:LO:110:PRO:N	19:LO:111:PRO:HD2	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LX:84:GLU:O	28:LX:87:MET:HG3	2.21	0.40
40:Lj:28:HIS:CE1	40:Lj:30:GLN:HB3	2.55	0.40
41:Lk:33:LYS:HG2	41:Lk:46:VAL:HG22	2.03	0.40
45:Lo:14:LYS:HB3	45:Lo:77:CYS:SG	2.61	0.40
49:Lt:116:MET:H	49:Lt:116:MET:HG3	1.77	0.40
57:SS:5:ILE:HD11	57:SS:9:PHE:CG	2.57	0.40
65:SA:68:ILE:HG23	65:SA:120:ARG:NH1	2.36	0.40
69:SG:79:LYS:HG2	69:SG:86:PRO:HB3	2.02	0.40
79:SY:42:GLU:HA	79:SY:52:PRO:HB3	2.03	0.40
81:Sb:16:LYS:HA	81:Sb:16:LYS:HD3	1.78	0.40
83:S2:939:U:H2'	83:S2:940:U:C6	2.56	0.40
83:S2:1233:G:C6	83:S2:1526:G:C6	3.09	0.40
83:S2:1407:U:H2'	83:S2:1408:U:H6	1.85	0.40
83:S2:1473:G:H5'	83:S2:1474:A:OP2	2.22	0.40
3:L5:73:A:N6	16:LL:103:ARG:HH22	2.20	0.40
3:L5:286:U:H3	3:L5:301:G:H1	1.68	0.40
3:L5:978:G:H2'	3:L5:979:C:C6	2.55	0.40
3:L5:1298:C:H2'	3:L5:1299:G:H8	1.86	0.40
3:L5:1509:C:H5''	31:La:2:PRO:HG3	2.03	0.40
3:L5:1572:U:H2'	3:L5:1573:G:C8	2.57	0.40
3:L5:2521:G:H2'	3:L5:2522:G:H8	1.86	0.40
3:L5:3831:U:H2'	3:L5:3832:U:H6	1.87	0.40
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.56	0.40
3:L5:4888:U:H2'	3:L5:4889:G:C8	2.56	0.40
3:L5:5026:U:H4'	3:L5:5027:C:O4'	2.22	0.40
5:L8:13:G:C5	5:L8:14:U:C4	3.09	0.40
8:LC:144:ILE:HG13	8:LC:144:ILE:O	2.22	0.40
18:LN:113:LEU:HB3	18:LN:134:LEU:HD23	2.03	0.40
25:LU:91:LEU:HD13	25:LU:96:LEU:HB2	2.04	0.40
28:LX:96:LEU:HD12	28:LX:140:LEU:HD11	2.03	0.40
48:Ls:18:ILE:HD13	48:Ls:68:HIS:HB3	2.04	0.40
50:SD:167:TYR:HE2	50:SD:204:LEU:HD23	1.86	0.40
54:SP:18:ARG:NE	57:SS:88:LYS:HG2	2.36	0.40
55:SQ:53:GLU:HB3	55:SQ:54:PRO:HD3	2.02	0.40
66:SB:125:VAL:HB	66:SB:169:MET:SD	2.61	0.40
67:SC:208:PRO:O	67:SC:212:LYS:HG2	2.21	0.40
68:SE:152:PRO:HG2	69:SG:216:ARG:HG3	2.03	0.40
76:SV:27:LYS:HD3	76:SV:29:HIS:CE1	2.55	0.40
83:S2:442:C:H2'	83:S2:443:U:C6	2.56	0.40
83:S2:808:A:H2'	83:S2:809:A:C8	2.57	0.40
83:S2:974:C:H2'	83:S2:975:G:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1031:A2M:H2'	83:S2:1032:C:O4'	2.21	0.40
83:S2:1631:U:H2'	83:S2:1632:G:C4	2.57	0.40
2:Pt:3:C:N4	2:Pt:70:A:H61	2.16	0.40
2:Pt:10:G:C2	2:Pt:26:G:H1'	2.56	0.40
3:L5:124:C:H2'	3:L5:125:C:H6	1.86	0.40
3:L5:716:C:OP1	8:LC:317:ASN:HB2	2.20	0.40
3:L5:1086:C:H2'	3:L5:1087:A:C8	2.56	0.40
3:L5:3764:U:H3'	3:L5:3765:G:H8	1.86	0.40
3:L5:4420:U:H5''	3:L5:4421:C:H5	1.86	0.40
3:L5:5036:C:H2'	3:L5:5037:U:C6	2.57	0.40
6:LA:82:ILE:HD13	6:LA:82:ILE:HA	1.93	0.40
7:LB:53:MET:HB2	7:LB:76:VAL:O	2.21	0.40
12:LG:217:LYS:O	12:LG:220:GLU:HG2	2.22	0.40
16:LL:136:LYS:HE2	16:LL:136:LYS:HB2	1.85	0.40
23:LS:16:CYS:HA	23:LS:54:MET:HE1	2.02	0.40
24:LT:119:ALA:HA	24:LT:122:LYS:HG3	2.03	0.40
26:LV:67:LYS:HD2	26:LV:73:ARG:NH2	2.36	0.40
26:LV:106:VAL:HA	26:LV:112:MET:HA	2.03	0.40
30:LZ:10:VAL:HG11	30:LZ:129:TRP:HZ3	1.87	0.40
31:La:146:LEU:HD23	31:La:146:LEU:HA	1.87	0.40
50:SD:91:VAL:HG22	50:SD:94:ARG:NH1	2.37	0.40
55:SQ:110:ASP:OD1	55:SQ:111:ILE:HD12	2.21	0.40
64:Sg:42:MET:SD	64:Sg:56:GLN:HB3	2.61	0.40
64:Sg:220:ASP:HB2	64:Sg:227:LEU:HD12	2.02	0.40
69:SG:2:LYS:HD3	69:SG:15:LEU:HD21	2.04	0.40
73:SL:80:MET:HE1	73:SL:120:VAL:HG13	2.03	0.40
79:SY:124:ASN:ND2	83:S2:84:A:H5''	2.36	0.40
83:S2:946:U:H2'	83:S2:947:G:C8	2.55	0.40
83:S2:1272:OMC:HM21	83:S2:1274:G:C6	2.57	0.40
83:S2:1360:U:H3'	83:S2:1361:G:C8	2.56	0.40
83:S2:1432:U:H2'	83:S2:1438:A:H8	1.84	0.40
83:S2:1711:U:H2'	83:S2:1712:A:C8	2.56	0.40
3:L5:99:A:H2'	3:L5:100:C:O2	2.21	0.40
3:L5:130:C:H2'	3:L5:131:C:C6	2.57	0.40
3:L5:222:C:H2'	3:L5:223:G:O4'	2.22	0.40
3:L5:271:C:H2'	3:L5:272:U:C6	2.56	0.40
3:L5:502:C:H3'	3:L5:503:C:H3'	2.03	0.40
3:L5:946:C:O2'	8:LC:340:ILE:HG22	2.20	0.40
3:L5:1419:G:H5''	21:LQ:71:LYS:NZ	2.37	0.40
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.57	0.40
3:L5:2267:U:P	47:Lr:37:SER:HB2	2.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2535:G:H2'	3:L5:2536:A:C8	2.57	0.40
3:L5:2846:G:H2'	3:L5:2847:G:C8	2.57	0.40
3:L5:2877:G:H2'	3:L5:2878:G:O4'	2.22	0.40
3:L5:3896:C:H1'	7:LB:268:ARG:NH2	2.36	0.40
3:L5:4093:G:H3'	3:L5:4094:G:C8	2.57	0.40
8:LC:107:THR:HG22	16:LL:26:PHE:HE2	1.87	0.40
9:LD:103:LEU:HG	9:LD:247:ILE:HG21	2.03	0.40
9:LD:171:LEU:HB3	9:LD:173:ILE:HD11	2.03	0.40
11:LF:35:LYS:HE3	11:LF:35:LYS:HB3	1.97	0.40
11:LF:128:ALA:O	11:LF:132:MET:HG2	2.21	0.40
14:LI:111:LEU:HD12	14:LI:111:LEU:HA	1.95	0.40
17:LM:25:VAL:HG21	17:LM:50:MET:HE1	2.04	0.40
19:LO:129:LEU:HD23	19:LO:129:LEU:HA	1.87	0.40
27:LW:31:PHE:CD2	27:LW:37:GLU:HG3	2.57	0.40
29:LY:58:VAL:HG23	29:LY:59:ARG:HG2	2.03	0.40
35:Le:76:LYS:HA	35:Le:76:LYS:HD3	1.95	0.40
48:Ls:16:LYS:NZ	48:Ls:54:LEU:HD11	2.36	0.40
51:SF:123:GLU:HA	51:SF:140:ASP:HA	2.04	0.40
52:SK:59:LYS:HD3	52:SK:72:THR:HG22	2.03	0.40
53:SM:63:LYS:HD3	53:SM:64:LEU:HD22	2.03	0.40
54:SP:108:LYS:HG2	57:SS:116:LYS:NZ	2.37	0.40
66:SB:167:LYS:O	66:SB:171:ILE:HG12	2.22	0.40
71:SI:150:ASP:HA	71:SI:153:LYS:CG	2.51	0.40
72:SJ:37:LEU:HD23	72:SJ:109:ARG:NH1	2.36	0.40
73:SL:98:LYS:HD3	73:SL:99:TYR:CE2	2.57	0.40
75:SO:50:LYS:NZ	83:S2:951:C:H1'	2.37	0.40
79:SY:8:ARG:HA	83:S2:837:A:H62	1.86	0.40
79:SY:10:ARG:HA	83:S2:839:C:H41	1.86	0.40
83:S2:1410:C:H2'	83:S2:1411:G:C8	2.54	0.40
83:S2:1558:C:H2'	83:S2:1559:C:H6	1.85	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	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
7	LB	400/402 (100%)	380 (95%)	20 (5%)	0	100	100
8	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
9	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
10	LE	236/250 (94%)	220 (93%)	16 (7%)	0	100	100
11	LF	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
12	LG	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
13	LH	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
14	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
15	LJ	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
16	LL	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	LM	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
19	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
20	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
21	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
26	LV	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
27	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
32	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
33	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
34	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Le	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
36	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
37	Lg	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
38	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
41	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
42	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
46	Lp	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
47	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/157 (82%)	109 (85%)	19 (15%)	0	100	100
50	SD	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
51	SF	187/189 (99%)	177 (95%)	10 (5%)	0	100	100
52	SK	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
53	SM	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
54	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
55	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
56	SR	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
57	SS	143/145 (99%)	137 (96%)	5 (4%)	1 (1%)	18	48
58	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
59	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
60	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
61	Sc	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
62	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
63	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
64	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
65	SA	219/221 (99%)	204 (93%)	15 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	SB	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
67	SC	218/222 (98%)	203 (93%)	15 (7%)	0	100	100
68	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
69	SG	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
70	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
71	SI	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
72	SJ	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
73	SL	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
74	SN	148/150 (99%)	147 (99%)	1 (1%)	0	100	100
75	SO	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
76	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
77	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
78	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
79	SY	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
80	Sa	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
81	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
82	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
All	All	11672/11907 (98%)	11108 (95%)	563 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	SS	16	LEU

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	
1	CI	25/25 (100%)	25 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	180/180 (100%)	180 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	116 (99%)	1 (1%)	70	76
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	87 (99%)	1 (1%)	65	75
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	161 (99%)	1 (1%)	78	81
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SD	190/190 (100%)	190 (100%)	0	100	100
51	SF	159/159 (100%)	159 (100%)	0	100	100
52	SK	89/89 (100%)	89 (100%)	0	100	100
53	SM	102/104 (98%)	102 (100%)	0	100	100
54	SP	107/107 (100%)	107 (100%)	0	100	100
55	SQ	119/119 (100%)	119 (100%)	0	100	100
56	SR	122/122 (100%)	122 (100%)	0	100	100
57	SS	126/126 (100%)	126 (100%)	0	100	100
58	ST	113/113 (100%)	113 (100%)	0	100	100
59	SU	94/94 (100%)	94 (100%)	0	100	100
60	SZ	66/66 (100%)	66 (100%)	0	100	100
61	Sc	57/57 (100%)	57 (100%)	0	100	100
62	Sd	48/48 (100%)	48 (100%)	0	100	100
63	Sf	60/60 (100%)	60 (100%)	0	100	100
64	Sg	272/272 (100%)	272 (100%)	0	100	100
65	SA	183/183 (100%)	183 (100%)	0	100	100
66	SB	195/195 (100%)	194 (100%)	1 (0%)	81	82
67	SC	186/188 (99%)	186 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	SE	224/224 (100%)	224 (100%)	0	100	100
69	SG	207/207 (100%)	207 (100%)	0	100	100
70	SH	166/169 (98%)	166 (100%)	0	100	100
71	SI	178/178 (100%)	178 (100%)	0	100	100
72	SJ	161/161 (100%)	161 (100%)	0	100	100
73	SL	137/137 (100%)	137 (100%)	0	100	100
74	SN	130/130 (100%)	130 (100%)	0	100	100
75	SO	107/110 (97%)	107 (100%)	0	100	100
76	SV	67/67 (100%)	67 (100%)	0	100	100
77	SW	112/112 (100%)	112 (100%)	0	100	100
78	SX	113/113 (100%)	113 (100%)	0	100	100
79	SY	113/113 (100%)	113 (100%)	0	100	100
80	Sa	89/89 (100%)	89 (100%)	0	100	100
81	Sb	75/75 (100%)	75 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
All	All	10147/10221 (99%)	10143 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	LZ	28	ASN
32	Lb	12	GLN
48	Ls	159	GLN
66	SB	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
6	LA	22	HIS
6	LA	83	HIS
6	LA	86	GLN
6	LA	194	ASN
6	LA	215	ASN
7	LB	184	GLN
7	LB	213	GLN
8	LC	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	LC	43	ASN
8	LC	119	GLN
8	LC	276	ASN
8	LC	362	GLN
9	LD	17	GLN
9	LD	225	GLN
9	LD	282	GLN
9	LD	291	GLN
10	LE	167	GLN
11	LF	116	GLN
11	LF	226	HIS
12	LG	81	ASN
12	LG	112	GLN
12	LG	159	HIS
12	LG	208	ASN
13	LH	162	GLN
14	LI	73	ASN
16	LL	205	GLN
18	LN	91	GLN
18	LN	149	GLN
19	LO	167	HIS
20	LP	54	GLN
20	LP	75	GLN
20	LP	93	HIS
20	LP	97	ASN
20	LP	116	HIS
21	LQ	44	ASN
21	LQ	162	HIS
25	LU	94	ASN
26	LV	27	ASN
27	LW	59	HIS
29	LY	14	ASN
29	LY	56	GLN
29	LY	61	HIS
30	LZ	28	ASN
31	La	17	HIS
31	La	34	ASN
31	La	62	HIS
32	Lb	6	ASN
32	Lb	10	HIS
32	Lb	12	GLN
32	Lb	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	Ld	28	ASN
35	Le	24	GLN
35	Le	34	ASN
36	Lf	21	GLN
36	Lf	55	ASN
37	Lg	28	ASN
37	Lg	114	GLN
40	Lj	13	ASN
42	Ll	33	ASN
45	Lo	45	GLN
47	Lr	21	ASN
47	Lr	95	HIS
47	Lr	121	GLN
48	Ls	159	GLN
48	Ls	191	GLN
49	Lt	65	GLN
49	Lt	70	GLN
49	Lt	137	GLN
49	Lt	149	HIS
50	SD	159	HIS
52	SK	32	HIS
52	SK	44	HIS
52	SK	50	GLN
56	SR	56	HIS
57	SS	87	GLN
57	SS	120	HIS
57	SS	125	HIS
59	SU	18	HIS
60	SZ	112	ASN
62	Sd	37	ASN
64	Sg	76	GLN
64	Sg	119	GLN
64	Sg	196	ASN
64	Sg	215	GLN
65	SA	9	GLN
65	SA	29	ASN
65	SA	84	GLN
66	SB	76	ASN
66	SB	95	ASN
66	SB	149	GLN
67	SC	120	GLN
67	SC	267	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
68	SE	50	ASN
68	SE	67	GLN
69	SG	56	ASN
69	SG	186	GLN
71	SI	64	ASN
71	SI	146	GLN
71	SI	165	GLN
73	SL	13	GLN
73	SL	108	ASN
74	SN	13	GLN
74	SN	36	GLN
74	SN	105	ASN
75	SO	79	GLN
77	SW	44	HIS
77	SW	56	HIS
77	SW	90	GLN
79	SY	85	ASN
80	Sa	25	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	18 (25%)	0
3	L5	3644/3655 (99%)	808 (22%)	13 (0%)
4	L7	119/120 (99%)	15 (12%)	0
5	L8	155/156 (99%)	24 (15%)	0
83	S2	1714/1740 (98%)	422 (24%)	3 (0%)
All	All	5704/5745 (99%)	1287 (22%)	16 (0%)

All (1287) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	10	G
2	Pt	13	U
2	Pt	19	G
2	Pt	20(A)	U
2	Pt	21	A
2	Pt	30	G
2	Pt	46	G
2	Pt	47	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Pt	48	C
2	Pt	49	C
2	Pt	58	A
2	Pt	61	C
2	Pt	66	C
2	Pt	67	G
2	Pt	70	A
2	Pt	74	C
2	Pt	76	A
3	L5	2	G
3	L5	13	U
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	72	C
3	L5	73	A
3	L5	91	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	122	U
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	139	G
3	L5	140	G
3	L5	144	G
3	L5	151	G
3	L5	159	C
3	L5	165	A
3	L5	166	C
3	L5	172	C
3	L5	177	G
3	L5	182	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	183	C
3	L5	184	U
3	L5	185	C
3	L5	187	U
3	L5	188	G
3	L5	189	G
3	L5	190	G
3	L5	200	U
3	L5	209	U
3	L5	216	C
3	L5	218	A
3	L5	220	C
3	L5	234	G
3	L5	255	C
3	L5	256	G
3	L5	260	C
3	L5	261	G
3	L5	263	G
3	L5	264	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	275	C
3	L5	278	G
3	L5	280	G
3	L5	281	U
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	346	G
3	L5	363	A
3	L5	365	U
3	L5	373	G
3	L5	385	A
3	L5	387	G
3	L5	388	A
3	L5	396	A
3	L5	407	A
3	L5	408	A
3	L5	409	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	415	G
3	L5	431	G
3	L5	432	U
3	L5	447	C
3	L5	449	C
3	L5	450	G
3	L5	452	A
3	L5	453	G
3	L5	456	C
3	L5	457	G
3	L5	467	U
3	L5	468	U
3	L5	472	C
3	L5	479	G
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	493	G
3	L5	494	U
3	L5	497	G
3	L5	498	C
3	L5	499	G
3	L5	502	C
3	L5	503	C
3	L5	504	G
3	L5	505	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	518	G
3	L5	519	C
3	L5	643	C
3	L5	646	G
3	L5	654	C
3	L5	655	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	656	C
3	L5	659	G
3	L5	666	G
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	672	C
3	L5	673	C
3	L5	674	G
3	L5	685	C
3	L5	686	A
3	L5	687	U
3	L5	696	C
3	L5	704	C
3	L5	729	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	742	G
3	L5	746	A
3	L5	750	U
3	L5	758	G
3	L5	759	G
3	L5	904	C
3	L5	905	C
3	L5	910	G
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	923	C
3	L5	924	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	941	C
3	L5	943	A
3	L5	944	A
3	L5	945	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	956	A
3	L5	957	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	969	C
3	L5	970	G
3	L5	982	U
3	L5	985	C
3	L5	989	U
3	L5	1070	G
3	L5	1072	C
3	L5	1075	G
3	L5	1076	C
3	L5	1082	C
3	L5	1083	U
3	L5	1088	C
3	L5	1168	G
3	L5	1170	G
3	L5	1171	G
3	L5	1172	C
3	L5	1173	G
3	L5	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C
3	L5	1187	G
3	L5	1202	C
3	L5	1203	G
3	L5	1206	C
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1216	C
3	L5	1218	G
3	L5	1219	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	1221	G
3	L5	1222	A
3	L5	1241	C
3	L5	1243	C
3	L5	1245	C
3	L5	1246	G
3	L5	1247	U
3	L5	1254	A
3	L5	1257	A
3	L5	1258	G
3	L5	1262	G
3	L5	1266	G
3	L5	1267	C
3	L5	1269	G
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1275	G
3	L5	1277	G
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1314	C
3	L5	1326	A2M
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1367	C
3	L5	1379	C
3	L5	1387	A
3	L5	1394	G
3	L5	1398	A
3	L5	1403	G
3	L5	1404	G
3	L5	1407	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	1409	C
3	L5	1410	U
3	L5	1411	C
3	L5	1417	C
3	L5	1420	A
3	L5	1437	C
3	L5	1438	U
3	L5	1439	C
3	L5	1442	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1457	G
3	L5	1465	G
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1504	G
3	L5	1516	G
3	L5	1517	G
3	L5	1523	A
3	L5	1534	A2M
3	L5	1537	A
3	L5	1547	A
3	L5	1549	G
3	L5	1563	A
3	L5	1564	A
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1612	G
3	L5	1613	A
3	L5	1621	A
3	L5	1624	G
3	L5	1625	OMG
3	L5	1626	G
3	L5	1631	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1641	G
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1678	C
3	L5	1691	G
3	L5	1696	C
3	L5	1698	C
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1702	C
3	L5	1703	C
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C
3	L5	1719	A
3	L5	1731	C
3	L5	1742	A
3	L5	1745	G
3	L5	1753	G
3	L5	1757	U
3	L5	1758	G
3	L5	1760	G
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1767	A
3	L5	1768	C
3	L5	1770	A
3	L5	1772	C
3	L5	1775	A
3	L5	1787	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	1803	G
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1811	G
3	L5	1815	G
3	L5	1821	G
3	L5	1822	U
3	L5	1833	G
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1869	G
3	L5	1897	A
3	L5	1899	G
3	L5	1915	C
3	L5	1917	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1936	C
3	L5	1946	G
3	L5	1948	G
3	L5	1951	G
3	L5	1957	U
3	L5	1961	G
3	L5	1962	A
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
3	L5	1991	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	1993	C
3	L5	1997	U
3	L5	1998	A
3	L5	1999	A
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2004	U
3	L5	2005	G
3	L5	2011	C
3	L5	2017	A
3	L5	2018	C
3	L5	2021	G
3	L5	2024	G
3	L5	2026	A
3	L5	2034	G
3	L5	2046	G
3	L5	2048	U
3	L5	2052	G
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2072	C
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2094	G
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2099	G
3	L5	2101	C
3	L5	2102	G
3	L5	2107	C
3	L5	2112	G
3	L5	2250	C
3	L5	2252	G
3	L5	2256	C
3	L5	2258	C
3	L5	2269	C
3	L5	2270	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2316	G
3	L5	2331	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2382	A
3	L5	2383	C
3	L5	2395	A
3	L5	2397	G
3	L5	2398	U
3	L5	2410	C
3	L5	2416	G
3	L5	2417	A
3	L5	2425	U
3	L5	2450	G
3	L5	2453	A
3	L5	2463	G
3	L5	2464	C
3	L5	2465	C
3	L5	2469	C
3	L5	2471	G
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2479	G
3	L5	2483	G
3	L5	2484	A
3	L5	2485	U
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2494	U
3	L5	2504	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2537	A
3	L5	2544	G
3	L5	2546	G
3	L5	2547	G
3	L5	2553	A
3	L5	2554	U
3	L5	2555	G
3	L5	2556	G
3	L5	2558	C
3	L5	2560	C
3	L5	2565	A
3	L5	2567	G
3	L5	2573	A
3	L5	2583	C
3	L5	2586	G
3	L5	2587	A
3	L5	2589	C
3	L5	2602	G
3	L5	2606	G
3	L5	2618	G
3	L5	2627	C
3	L5	2638	G
3	L5	2653	C
3	L5	2658	G
3	L5	2662	G
3	L5	2669	C
3	L5	2673	G
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2702	C
3	L5	2703	G
3	L5	2706	G
3	L5	2707	U
3	L5	2708	U
3	L5	2709	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	2710	C
3	L5	2711	G
3	L5	2719	C
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2727	C
3	L5	2736	G
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2746	A
3	L5	2761	U
3	L5	2763	U
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2799	G
3	L5	2806	A
3	L5	2814	C
3	L5	2826	U
3	L5	2827	G
3	L5	2828	U
3	L5	2829	U
3	L5	2833	A
3	L5	2835	A
3	L5	2855	G
3	L5	2867	C
3	L5	2876	OMG
3	L5	2877	G
3	L5	2900	U
3	L5	2901	G
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2907	G
3	L5	2908	U
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G
3	L5	3604	A
3	L5	3605	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3683	C
3	L5	3684	G
3	L5	3692	A
3	L5	3701	OMC
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3727	A
3	L5	3748	A
3	L5	3753	G
3	L5	3760	A
3	L5	3770	U
3	L5	3774	A
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3778	U
3	L5	3785	A2M
3	L5	3786	U
3	L5	3791	C
3	L5	3792	OMG
3	L5	3810	C
3	L5	3811	G
3	L5	3812	C
3	L5	3813	A
3	L5	3817	A
3	L5	3819	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3892	U
3	L5	3897	G
3	L5	3898	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3938	G
3	L5	3939	G
3	L5	3942	A
3	L5	3947	A
3	L5	3949	A
3	L5	3950	U
3	L5	3951	G
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4065	G
3	L5	4068	U
3	L5	4076	G
3	L5	4093	G
3	L5	4095	G
3	L5	4097	G
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	4115	G
3	L5	4116	C
3	L5	4121	G
3	L5	4122	G
3	L5	4127	A
3	L5	4138	C
3	L5	4139	G
3	L5	4140	C
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4146	G
3	L5	4149	C
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4168	G
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4220	6MZ
3	L5	4222	G
3	L5	4225	G
3	L5	4228	OMG
3	L5	4229	U
3	L5	4233	A
3	L5	4241	C
3	L5	4243	C
3	L5	4251	A
3	L5	4254	G
3	L5	4258	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4290	U
3	L5	4291	G
3	L5	4295	U
3	L5	4297	G
3	L5	4304	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	4305	G
3	L5	4314	C
3	L5	4319	C
3	L5	4326	G
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4349	C
3	L5	4350	C
3	L5	4354	U
3	L5	4364	G
3	L5	4373	G
3	L5	4377	G
3	L5	4378	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4410	G
3	L5	4421	C
3	L5	4422	A
3	L5	4430	G
3	L5	4432	C
3	L5	4441	A
3	L5	4444	C
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4488	A
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4522	G
3	L5	4524	G
3	L5	4525	C
3	L5	4528	G
3	L5	4545	G
3	L5	4548	A
3	L5	4549	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	4557	U
3	L5	4560	C
3	L5	4567	G
3	L5	4570	G
3	L5	4575	G
3	L5	4589	A
3	L5	4590	A2M
3	L5	4599	A
3	L5	4601	U
3	L5	4608	G
3	L5	4617	G
3	L5	4635	A
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4687	A
3	L5	4693	C
3	L5	4694	G
3	L5	4695	C
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4733	C
3	L5	4734	A
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4775	C
3	L5	4859	C
3	L5	4860	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	4862	G
3	L5	4863	G
3	L5	4865	C
3	L5	4867	G
3	L5	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4881	U
3	L5	4882	U
3	L5	4883	C
3	L5	4887	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4897	G
3	L5	4899	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4925	U
3	L5	4926	C
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4941	G
3	L5	4943	A
3	L5	4947	U
3	L5	4949	G
3	L5	4952	G
3	L5	4955	A
3	L5	4960	G
3	L5	4976	U
3	L5	4985	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	4995	U
3	L5	5013	C
3	L5	5014	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5026	U
3	L5	5027	C
3	L5	5028	G
3	L5	5030	U
3	L5	5034	A
3	L5	5040	U
3	L5	5041	G
3	L5	5047	C
3	L5	5048	A
3	L5	5050	C
3	L5	5054	C
3	L5	5055	G
3	L5	5060	A
3	L5	5061	A
3	L5	5069	U
4	L7	22	A
4	L7	33	U
4	L7	37	G
4	L7	38	U
4	L7	50	A
4	L7	53	U
4	L7	54	A
4	L7	63	C
4	L7	64	G
4	L7	74	A
4	L7	97	G
4	L7	100	A
4	L7	102	U
4	L7	110	G
4	L7	120	U
5	L8	23	C
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	51	U
5	L8	59	A
5	L8	62	A
5	L8	63	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L8	80	A
5	L8	82	A
5	L8	84	A
5	L8	85	U
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	111	U
5	L8	114	G
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	147	G
5	L8	150	C
5	L8	151	G
83	S2	4	C
83	S2	25	A
83	S2	33	G
83	S2	41	G
83	S2	42	A
83	S2	44	U
83	S2	45	A
83	S2	46	A
83	S2	56	G
83	S2	58	C
83	S2	62	G
83	S2	65	C
83	S2	67	C
83	S2	68	A
83	S2	72	C
83	S2	73	C
83	S2	74	G
83	S2	76	U
83	S2	103	A
83	S2	113	G
83	S2	115	U
83	S2	126	G
83	S2	130	G
83	S2	143	U
83	S2	149	A
83	S2	158	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	160	U
83	S2	162	C
83	S2	170	A
83	S2	171	A
83	S2	175	A
83	S2	179	C
83	S2	182	C
83	S2	190	G
83	S2	191	A
83	S2	196	C
83	S2	197	U
83	S2	198	U
83	S2	199	C
83	S2	200	G
83	S2	203	G
83	S2	204	G
83	S2	206	G
83	S2	207	G
83	S2	208	G
83	S2	212	C
83	S2	220	U
83	S2	290	U
83	S2	291	G
83	S2	292	A
83	S2	295	C
83	S2	302	A
83	S2	303	C
83	S2	305	U
83	S2	306	C
83	S2	307	G
83	S2	308	G
83	S2	309	G
83	S2	312	G
83	S2	313	A
83	S2	318	A
83	S2	319	C
83	S2	323	C
83	S2	324	C
83	S2	325	C
83	S2	326	C
83	S2	328	U
83	S2	329	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	332	G
83	S2	333	G
83	S2	339	A
83	S2	347	G
83	S2	351	G
83	S2	360	A
83	S2	362	C
83	S2	364	A
83	S2	368	U
83	S2	370	G
83	S2	373	G
83	S2	385	G
83	S2	386	C
83	S2	400	C
83	S2	407	G
83	S2	408	A
83	S2	409	C
83	S2	426	A
83	S2	436	OMG
83	S2	438	G
83	S2	448	A
83	S2	449	A
83	S2	450	C
83	S2	452	G
83	S2	464	A
83	S2	465	A
83	S2	471	G
83	S2	472	C
83	S2	473	A
83	S2	474	G
83	S2	476	A
83	S2	482	G
83	S2	487	U
83	S2	488	U
83	S2	492	C
83	S2	493	A
83	S2	502	C
83	S2	516	A
83	S2	517	OMC
83	S2	532	C
83	S2	536	A
83	S2	537	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	540	U
83	S2	542	U
83	S2	544	G
83	S2	546	G
83	S2	547	G
83	S2	557	U
83	S2	558	G
83	S2	559	G
83	S2	563	G
83	S2	564	A
83	S2	566	U
83	S2	576	A2M
83	S2	582	U
83	S2	583	A
83	S2	585	C
83	S2	587	A
83	S2	589	G
83	S2	591	U
83	S2	593	C
83	S2	600	G
83	S2	604	A
83	S2	606	G
83	S2	607	U
83	S2	614	C
83	S2	617	G
83	S2	623	G
83	S2	628	A
83	S2	643	A
83	S2	644	OMG
83	S2	660	C
83	S2	663	C
83	S2	664	A
83	S2	668	A2M
83	S2	669	A
83	S2	671	A
83	S2	672	A
83	S2	673	G
83	S2	678	U
83	S2	684	G
83	S2	687	C
83	S2	688	U
83	S2	689	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	692	G
83	S2	695	C
83	S2	696	G
83	S2	697	G
83	S2	698	G
83	S2	731	G
83	S2	732	U
83	S2	733	C
83	S2	736	C
83	S2	737	G
83	S2	738	C
83	S2	749	U
83	S2	751	G
83	S2	752	G
83	S2	753	C
83	S2	788	G
83	S2	791	C
83	S2	792	C
83	S2	798	G
83	S2	799	OMU
83	S2	801	PSU
83	S2	805	U
83	S2	821	G
83	S2	822	U
83	S2	823	U
83	S2	824	C
83	S2	827	A
83	S2	830	A
83	S2	834	C
83	S2	835	C
83	S2	836	G
83	S2	837	A
83	S2	838	G
83	S2	839	C
83	S2	842	C
83	S2	844	U
83	S2	847	A
83	S2	852	G
83	S2	867	OMG
83	S2	869	A
83	S2	870	A
83	S2	871	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	873	G
83	S2	874	G
83	S2	877	C
83	S2	878	G
83	S2	880	G
83	S2	882	U
83	S2	887	U
83	S2	888	U
83	S2	889	U
83	S2	891	G
83	S2	896	U
83	S2	897	U
83	S2	898	U
83	S2	899	U
83	S2	900	C
83	S2	901	G
83	S2	903	A
83	S2	905	C
83	S2	912	C
83	S2	913	A
83	S2	917	U
83	S2	919	A
83	S2	920	A
83	S2	922	A
83	S2	925	G
83	S2	932	G
83	S2	933	G
83	S2	934	G
83	S2	953	C
83	S2	955	A
83	S2	963	A
83	S2	966	PSU
83	S2	970	G
83	S2	971	G
83	S2	972	A
83	S2	978	G
83	S2	979	C
83	S2	982	G
83	S2	990	A
83	S2	992	A
83	S2	999	G
83	S2	1001	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	1002	U
83	S2	1008	A
83	S2	1017	U
83	S2	1023	A
83	S2	1027	A
83	S2	1045	PSU
83	S2	1046	PSU
83	S2	1060	A
83	S2	1061	U
83	S2	1062	A
83	S2	1083	A
83	S2	1085	C
83	S2	1090	C
83	S2	1099	G
83	S2	1109	C
83	S2	1113	A
83	S2	1116	C
83	S2	1121	G
83	S2	1126	G
83	S2	1131	G
83	S2	1133	A
83	S2	1138	C
83	S2	1142	G
83	S2	1148	A
83	S2	1150	A
83	S2	1153	C
83	S2	1154	U
83	S2	1170	A
83	S2	1172	U
83	S2	1184	G
83	S2	1195	A
83	S2	1207	G
83	S2	1208	A
83	S2	1215	C
83	S2	1216	C
83	S2	1217	A
83	S2	1224	G
83	S2	1227	G
83	S2	1242	U
83	S2	1243	U
83	S2	1248	B8N
83	S2	1251	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	1253	A
83	S2	1256	G
83	S2	1257	G
83	S2	1264	C
83	S2	1271	C
83	S2	1272	OMC
83	S2	1274	G
83	S2	1275	G
83	S2	1283	C
83	S2	1286	G
83	S2	1288	OMU
83	S2	1293	A
83	S2	1294	G
83	S2	1295	A
83	S2	1301	A
83	S2	1302	G
83	S2	1303	C
83	S2	1308	U
83	S2	1314	U
83	S2	1326	OMU
83	S2	1333	U
83	S2	1342	U
83	S2	1357	A
83	S2	1371	U
83	S2	1372	U
83	S2	1373	C
83	S2	1376	A
83	S2	1378	A
83	S2	1382	A
83	S2	1398	G
83	S2	1402	A
83	S2	1413	G
83	S2	1418	C
83	S2	1419	C
83	S2	1420	G
83	S2	1421	A
83	S2	1422	G
83	S2	1423	C
83	S2	1432	U
83	S2	1433	C
83	S2	1434	C
83	S2	1435	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	1437	C
83	S2	1438	A
83	S2	1439	A
83	S2	1442	OMU
83	S2	1449	G
83	S2	1454	A
83	S2	1463	U
83	S2	1474	A
83	S2	1487	A
83	S2	1489	A
83	S2	1490	OMG
83	S2	1492	U
83	S2	1494	U
83	S2	1497	G
83	S2	1498	A
83	S2	1507	G
83	S2	1521	C
83	S2	1522	A
83	S2	1527	C
83	S2	1531	A
83	S2	1533	A
83	S2	1544	C
83	S2	1546	G
83	S2	1549	U
83	S2	1553	C
83	S2	1555	U
83	S2	1556	A
83	S2	1558	C
83	S2	1560	U
83	S2	1573	G
83	S2	1575	G
83	S2	1578	U
83	S2	1579	A
83	S2	1580	A
83	S2	1581	C
83	S2	1585	U
83	S2	1587	G
83	S2	1588	A
83	S2	1600	G
83	S2	1601	A
83	S2	1604	G
83	S2	1605	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	1606	G
83	S2	1621	U
83	S2	1622	U
83	S2	1623	A
83	S2	1631	U
83	S2	1632	G
83	S2	1633	A
83	S2	1634	A
83	S2	1637	A
83	S2	1646	C
83	S2	1647	A
83	S2	1648	G
83	S2	1649	U
83	S2	1652	G
83	S2	1654	G
83	S2	1662	U
83	S2	1663	A
83	S2	1665	G
83	S2	1668	U
83	S2	1686	G
83	S2	1695	A
83	S2	1698	C
83	S2	1699	A
83	S2	1705	C
83	S2	1715	A
83	S2	1721	U
83	S2	1722	G
83	S2	1744	G
83	S2	1745	A
83	S2	1752	C
83	S2	1753	C
83	S2	1754	G
83	S2	1755	C
83	S2	1756	C
83	S2	1757	G
83	S2	1758	G
83	S2	1759	G
83	S2	1761	U
83	S2	1772	C
83	S2	1773	C
83	S2	1777	G
83	S2	1782	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	S2	1783	C
83	S2	1784	G
83	S2	1786	U
83	S2	1809	A
83	S2	1810	U
83	S2	1821	U
83	S2	1825	A
83	S2	1826	G
83	S2	1831	A
83	S2	1835	A
83	S2	1838	U
83	S2	1849	G
83	S2	1851	MA6
83	S2	1852	C
83	S2	1861	G
83	S2	1862	G
83	S2	1863	A
83	S2	1865	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	406	C
3	L5	493	G
3	L5	914	U
3	L5	1082	C
3	L5	1633	G
3	L5	1977	C
3	L5	2416	G
3	L5	2675	G
3	L5	2760	G
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
83	S2	291	G
83	S2	563	G
83	S2	688	U

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

178 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$
3	PSU	L5	1782	3	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
83	OMC	S2	462	83	19,22,23	0.52	0	25,31,34	0.65	0
5	PSU	L8	55	5	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
3	A2M	L5	2815	3	22,25,26	1.18	1 (4%)	30,36,39	1.50	8 (26%)
83	OMU	S2	627	83	19,22,23	3.39	7 (36%)	25,31,34	1.81	4 (16%)
3	OMG	L5	4392	3	23,26,27	0.53	0	32,38,41	0.47	0
83	OMU	S2	428	83	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
83	PSU	S2	686	83	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
3	6MZ	L5	4220	3	22,25,26	4.00	11 (50%)	29,36,39	2.41	12 (41%)
3	A2M	L5	400	3	22,25,26	1.24	1 (4%)	30,36,39	1.58	9 (30%)
83	G7M	S2	1639	83,2	23,26,27	2.69	8 (34%)	34,39,42	2.57	11 (32%)
3	PSU	L5	1781	3	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
3	A2M	L5	1323	3	22,25,26	1.25	3 (13%)	30,36,39	1.56	9 (30%)
3	OMG	L5	2424	3	23,26,27	0.51	0	32,38,41	0.46	0
3	PSU	L5	1860	3	18,21,22	1.05	1 (5%)	21,30,33	1.75	4 (19%)
83	PSU	S2	801	83	18,21,22	1.16	1 (5%)	21,30,33	1.71	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
3	OMG	L5	4637	3	23,26,27	0.52	0	32,38,41	0.49	0
3	A2M	L5	2787	3	22,25,26	1.17	1 (4%)	30,36,39	1.54	8 (26%)
83	OMG	S2	1328	83	23,26,27	0.46	0	32,38,41	0.48	0
3	OMC	L5	3701	3	19,22,23	0.60	0	25,31,34	1.03	2 (8%)
3	PSU	L5	3639	3	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
3	A2M	L5	4571	3	22,25,26	1.28	2 (9%)	30,36,39	1.61	7 (23%)
3	OMC	L5	2824	3	19,22,23	0.57	0	25,31,34	0.66	0
3	PSU	L5	4312	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	105	83	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L5	4636	3	18,21,22	1.10	2 (11%)	21,30,33	2.10	6 (28%)
3	PSU	L5	1582	3	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
83	MA6	S2	1851	83	23,26,27	1.28	2 (8%)	33,38,41	3.42	13 (39%)
83	PSU	S2	863	83	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1744	84,3	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	2363	84,3	22,25,26	1.19	1 (4%)	30,36,39	1.50	8 (26%)
83	A2M	S2	576	83	22,25,26	1.20	2 (9%)	30,36,39	1.53	6 (20%)
3	PSU	L5	3822	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	6 (28%)
83	B8N	S2	1248	83	25,29,30	3.28	6 (24%)	28,42,45	2.06	9 (32%)
3	OMG	L5	4494	3	23,26,27	0.52	0	32,38,41	0.52	0
3	PSU	L5	1677	3	18,21,22	1.05	2 (11%)	21,30,33	1.89	4 (19%)
3	OMG	L5	1522	3	23,26,27	0.54	0	32,38,41	0.66	0
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
3	A2M	L5	4523	84,3	22,25,26	1.31	3 (13%)	30,36,39	1.48	7 (23%)
83	PSU	S2	1046	83	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	1871	84,3	22,25,26	1.21	1 (4%)	30,36,39	1.68	6 (20%)
3	OMG	L5	1625	3	23,26,27	0.51	0	32,38,41	0.50	0
83	PSU	S2	406	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
3	A2M	L5	1534	84,3	22,25,26	1.16	1 (4%)	30,36,39	1.51	7 (23%)
3	A2M	L5	3867	3	22,25,26	1.26	2 (9%)	30,36,39	1.54	9 (30%)
83	MA6	S2	1850	83	23,26,27	1.30	3 (13%)	33,38,41	3.22	11 (33%)
3	OMG	L5	4228	3	23,26,27	0.56	0	32,38,41	0.65	0
3	PSU	L5	2839	3	18,21,22	1.11	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.09	2 (11%)	21,30,33	1.92	4 (19%)
3	OMU	L5	2837	3	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
3	OMG	L5	4618	3	23,26,27	0.54	0	32,38,41	0.52	0
83	OMU	S2	172	83	19,22,23	3.40	7 (36%)	25,31,34	1.82	5 (20%)
83	A2M	S2	99	84,83	22,25,26	1.25	1 (4%)	30,36,39	1.58	8 (26%)
3	PSU	L5	4521	84,3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
3	A2M	L5	4590	3	22,25,26	1.20	1 (4%)	30,36,39	1.52	6 (20%)
3	PSU	L5	4576	3	18,21,22	1.06	1 (5%)	21,30,33	1.87	5 (23%)
3	OMU	L5	4306	3	19,22,23	3.19	7 (36%)	25,31,34	1.72	4 (16%)
83	OMG	S2	867	83	23,26,27	0.48	0	32,38,41	0.52	0
83	OMC	S2	1703	83	19,22,23	0.52	0	25,31,34	0.72	1 (4%)
5	OMG	L8	75	5	23,26,27	0.52	0	32,38,41	0.45	0
3	PSU	L5	4628	3	18,21,22	1.01	1 (5%)	21,30,33	1.78	4 (19%)
83	OMU	S2	1326	83	19,22,23	3.40	7 (36%)	25,31,34	1.87	5 (20%)
3	PSU	L5	5010	3	18,21,22	1.06	1 (5%)	21,30,33	1.89	4 (19%)
83	A2M	S2	668	84,83	22,25,26	1.33	2 (9%)	30,36,39	1.65	7 (23%)
3	OMC	L5	3808	84,3	19,22,23	0.60	0	25,31,34	0.94	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1792	3	18,21,22	1.03	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
83	OMU	S2	1288	83	19,22,23	3.41	7 (36%)	25,31,34	1.76	4 (16%)
3	PSU	L5	4689	3	18,21,22	1.04	2 (11%)	21,30,33	1.80	4 (19%)
83	PSU	S2	1232	83	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.07	1 (5%)	21,30,33	1.78	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.07	1 (5%)	21,30,33	1.95	5 (23%)
83	OMC	S2	174	83	19,22,23	0.53	0	25,31,34	0.73	1 (4%)
3	OMC	L5	3869	3	19,22,23	0.57	0	25,31,34	0.62	0
83	OMC	S2	1272	83	19,22,23	0.49	0	25,31,34	0.73	0
83	PSU	S2	1056	83	18,21,22	1.08	1 (5%)	21,30,33	1.80	4 (19%)
83	PSU	S2	1004	83	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
83	PSU	S2	966	84,83	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
83	OMU	S2	354	83	19,22,23	3.33	7 (36%)	25,31,34	1.72	4 (16%)
83	PSU	S2	1177	83	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
83	OMG	S2	683	83	23,26,27	0.47	0	32,38,41	0.51	0
3	OMU	L5	4498	3	19,22,23	3.31	7 (36%)	25,31,34	1.86	5 (20%)
3	PSU	L5	1862	3	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
3	OMG	L5	4499	3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMC	L5	1340	3	19,22,23	0.61	0	25,31,34	0.72	0
3	A2M	L5	3825	3	22,25,26	1.21	1 (4%)	30,36,39	1.51	8 (26%)
83	A2M	S2	468	83	22,25,26	1.22	1 (4%)	30,36,39	1.56	6 (20%)
3	PSU	L5	4299	3	18,21,22	1.13	1 (5%)	21,30,33	1.96	4 (19%)
3	PSU	L5	2632	3	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
83	PSU	S2	1244	83	18,21,22	1.14	1 (5%)	21,30,33	1.97	5 (23%)
83	OMU	S2	121	83	19,22,23	3.33	7 (36%)	25,31,34	1.73	4 (16%)
83	PSU	S2	814	83	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	3853	84,3	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
3	5MC	L5	4447	3	19,22,23	0.73	0	26,32,35	0.68	0
83	A2M	S2	27	83	22,25,26	1.23	1 (4%)	30,36,39	1.49	5 (16%)
83	A2M	S2	166	83	22,25,26	1.31	1 (4%)	30,36,39	1.59	8 (26%)
3	UR3	L5	4530	3	19,22,23	2.69	7 (36%)	26,32,35	1.59	3 (11%)
83	4AC	S2	1842	83	21,24,25	0.41	0	28,34,37	0.51	0
3	PSU	L5	4673	3	18,21,22	1.13	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMG	S2	601	83	23,26,27	0.51	0	32,38,41	0.60	0
3	OMC	L5	4536	3	19,22,23	0.56	0	25,31,34	0.62	0
3	OMG	L5	3792	3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMU	L5	4227	3	19,22,23	3.30	7 (36%)	25,31,34	1.79	5 (20%)
3	OMG	L5	1316	3	23,26,27	0.54	0	32,38,41	0.57	0
3	A2M	L5	3785	84,3	22,25,26	1.14	1 (4%)	30,36,39	1.54	9 (30%)
3	OMU	L5	3925	3	19,22,23	3.28	7 (36%)	25,31,34	1.75	4 (16%)
3	OMG	L5	2364	84,3	23,26,27	0.54	0	32,38,41	0.45	0
3	1MA	L5	1322	84,3	21,25,26	0.56	0	30,37,40	0.74	1 (3%)
3	PSU	L5	4972	3	18,21,22	1.04	1 (5%)	21,30,33	1.85	4 (19%)
83	PSU	S2	866	83	18,21,22	1.15	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	2876	3	23,26,27	0.50	0	32,38,41	0.53	0
3	PSU	L5	4442	3	18,21,22	1.12	3 (16%)	21,30,33	2.10	6 (28%)
3	PSU	L5	4500	3	18,21,22	1.12	1 (5%)	21,30,33	2.08	6 (28%)
3	PSU	L5	4973	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
83	6MZ	S2	1832	84,83	26,26,26	2.86	5 (19%)	36,39,39	2.07	10 (27%)
83	A2M	S2	1031	83	22,25,26	1.24	1 (4%)	30,36,39	1.52	7 (23%)
3	OMG	L5	3744	3	23,26,27	0.49	0	32,38,41	0.49	0
3	PSU	L5	4403	3	18,21,22	1.06	1 (5%)	21,30,33	1.94	6 (28%)
3	OMC	L5	2365	84,3	19,22,23	0.55	0	25,31,34	0.64	0
3	OMC	L5	2804	3	19,22,23	0.57	0	25,31,34	0.64	0
3	PSU	L5	3844	3	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
83	PSU	S2	681	83	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
5	PSU	L8	69	5	18,21,22	1.10	1 (5%)	21,30,33	1.88	5 (23%)
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.78	2 (7%)
3	5MC	L5	3782	84,3	19,22,23	0.61	0	26,32,35	0.81	1 (3%)
83	PSU	S2	1174	83	18,21,22	1.02	1 (5%)	21,30,33	1.86	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.23	1 (4%)	30,36,39	1.54	6 (20%)
83	PSU	S2	1367	83	18,21,22	1.12	1 (5%)	21,30,33	1.98	6 (28%)
83	OMU	S2	116	83	19,22,23	3.35	7 (36%)	25,31,34	1.71	5 (20%)
3	A2M	L5	398	3	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
83	A2M	S2	484	83	22,25,26	1.23	1 (4%)	30,36,39	1.49	7 (23%)
3	OMG	L5	3627	3	23,26,27	0.49	0	32,38,41	0.61	0
3	PSU	L5	3695	3	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
3	OMG	L5	4623	3	23,26,27	0.50	0	32,38,41	0.52	0
83	OMU	S2	1442	83	19,22,23	3.41	7 (36%)	25,31,34	1.78	5 (20%)
83	PSU	S2	93	83	18,21,22	1.15	1 (5%)	21,30,33	1.78	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	PSU	S2	651	83	18,21,22	1.17	1 (5%)	21,30,33	1.88	4 (19%)
3	OMU	L5	4620	3	19,22,23	3.26	7 (36%)	25,31,34	1.74	4 (16%)
83	PSU	S2	1045	83	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
83	OMC	S2	1391	83	19,22,23	0.51	0	25,31,34	0.68	0
83	PSU	S2	109	83	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	3920	84,3	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
3	OMG	L5	4196	2,3	23,26,27	0.51	0	32,38,41	0.48	0
83	PSU	S2	1081	83	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
83	OMG	S2	644	83	23,26,27	0.45	0	32,38,41	0.52	0
3	OMC	L5	2861	3	19,22,23	0.58	0	25,31,34	0.94	2 (8%)
3	OMC	L5	3887	3	19,22,23	0.56	0	25,31,34	0.65	0
83	A2M	S2	1383	83	22,25,26	1.25	1 (4%)	30,36,39	1.69	5 (16%)
83	A2M	S2	159	83	22,25,26	1.21	1 (4%)	30,36,39	1.52	7 (23%)
83	OMU	S2	799	83	19,22,23	3.36	7 (36%)	25,31,34	1.79	4 (16%)
3	OMG	L5	3899	3	23,26,27	0.55	0	32,38,41	0.50	0
83	OMG	S2	436	83	23,26,27	0.51	0	32,38,41	0.49	0
3	UY1	L5	3818	3	19,22,23	4.91	10 (52%)	21,31,34	2.07	5 (23%)
83	OMC	S2	517	83	19,22,23	0.54	0	25,31,34	0.72	0
3	A2M	L5	3718	3	22,25,26	1.15	1 (4%)	30,36,39	1.49	5 (16%)
3	OMC	L5	2422	84,3	19,22,23	0.58	0	25,31,34	0.77	1 (4%)
83	OMG	S2	1490	83	23,26,27	0.52	0	32,38,41	0.46	0
3	A2M	L5	1524	3	22,25,26	1.25	2 (9%)	30,36,39	1.51	6 (20%)
3	PSU	L5	5001	3	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.05	2 (11%)	21,30,33	1.96	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.19	1 (4%)	30,36,39	1.48	8 (26%)
3	OMG	L5	4370	3	23,26,27	0.48	0	32,38,41	0.57	0
3	OMC	L5	2351	84,3	19,22,23	0.58	0	25,31,34	0.80	1 (4%)
3	PSU	L5	4431	3	18,21,22	1.10	1 (5%)	21,30,33	1.95	4 (19%)
83	OMG	S2	509	83	23,26,27	0.47	0	32,38,41	0.52	0
83	PSU	S2	649	83	18,21,22	1.20	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	4457	3	18,21,22	1.08	1 (5%)	21,30,33	2.02	6 (28%)
3	A2M	L5	2401	3	22,25,26	1.21	1 (4%)	30,36,39	1.58	8 (26%)
3	PSU	L5	3637	3	18,21,22	1.06	1 (5%)	21,30,33	2.02	5 (23%)
3	PSU	L5	4353	3	18,21,22	1.10	1 (5%)	21,30,33	1.96	4 (19%)
3	PSU	L5	3851	3	18,21,22	1.06	1 (5%)	21,30,33	1.96	6 (28%)
3	OMC	L5	4456	3	19,22,23	0.61	0	25,31,34	0.80	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1683	3	18,21,22	1.15	1 (5%)	21,30,33	1.87	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.57	0	25,31,34	0.48	0

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
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	462	83	-	1/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	627	83	-	5/9/27/28	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	428	83	-	6/9/27/28	0/2/2/2
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
83	G7M	S2	1639	83,2	-	0/7/25/26	0/3/3/3
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
83	OMG	S2	1328	83	-	1/9/27/28	0/3/3/3
3	OMC	L5	3701	3	-	5/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
83	MA6	S2	1851	83	-	1/11/29/30	0/3/3/3
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	84,3	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2363	84,3	-	0/9/27/28	0/3/3/3
83	A2M	S2	576	83	-	3/9/27/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
83	B8N	S2	1248	83	-	8/16/34/35	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	84,3	-	0/9/27/28	0/3/3/3
83	PSU	S2	1046	83	-	2/7/25/26	0/2/2/2
3	A2M	L5	1871	84,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	3/9/27/28	0/3/3/3
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	84,3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3
83	MA6	S2	1850	83	-	0/11/29/30	0/3/3/3
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	172	83	-	0/9/27/28	0/2/2/2
83	A2M	S2	99	84,83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4521	84,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	2/9/27/28	0/2/2/2
83	OMG	S2	867	83	-	2/9/27/28	0/3/3/3
83	OMC	S2	1703	83	-	0/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1326	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	668	84,83	-	2/9/27/28	0/3/3/3
3	OMC	L5	3808	84,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1792	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	2/9/27/28	0/2/2/2
83	OMC	S2	1272	83	-	2/9/27/28	0/2/2/2
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	966	84,83	-	0/7/25/26	0/2/2/2
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
83	OMG	S2	683	83	-	0/9/27/28	0/3/3/3
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3825	3	-	1/9/27/28	0/3/3/3
83	A2M	S2	468	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1244	83	-	1/7/25/26	0/2/2/2
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	84,3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
83	A2M	S2	27	83	-	1/9/27/28	0/3/3/3
83	A2M	S2	166	83	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	1/7/25/26	0/2/2/2
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	601	83	-	1/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3785	84,3	-	2/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	2364	84,3	-	2/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1MA	L5	1322	84,3	-	2/7/25/26	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
83	6MZ	S2	1832	84,83	-	6/12/28/28	0/3/3/3
83	A2M	S2	1031	83	-	1/9/27/28	0/3/3/3
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	84,3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2
3	5MC	L5	3782	84,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	3/9/27/28	0/3/3/3
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
83	OMU	S2	116	83	-	1/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
83	A2M	S2	484	83	-	0/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	651	83	-	1/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2
83	OMC	S2	1391	83	-	1/9/27/28	0/2/2/2
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	84,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	2,3	-	1/9/27/28	0/3/3/3
83	PSU	S2	1081	83	-	1/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	644	83	-	3/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
83	A2M	S2	1383	83	-	3/9/27/28	0/3/3/3
83	A2M	S2	159	83	-	1/9/27/28	0/3/3/3
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
83	OMG	S2	436	83	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2422	84,3	-	3/9/27/28	0/2/2/2
83	OMG	S2	1490	83	-	1/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2351	84,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	509	83	-	0/9/27/28	0/3/3/3
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1832	6MZ	C6-N6	12.90	1.48	1.34
3	L5	3818	UY1	C6-C5	12.81	1.49	1.35
3	L5	4220	6MZ	C6-N6	12.32	1.48	1.34
3	L5	3818	UY1	C2-N1	11.77	1.52	1.36
83	S2	1288	OMU	C2-N1	8.58	1.51	1.38
83	S2	1442	OMU	C2-N1	8.45	1.51	1.38
83	S2	172	OMU	C2-N1	8.42	1.51	1.38
83	S2	799	OMU	C2-N1	8.42	1.51	1.38
3	L5	4220	6MZ	C3'-C2'	-8.42	1.30	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	627	OMU	C2-N1	8.37	1.51	1.38
83	S2	1326	OMU	C2-N1	8.34	1.51	1.38
83	S2	428	OMU	C2-N1	8.16	1.51	1.38
83	S2	121	OMU	C2-N1	8.15	1.51	1.38
83	S2	354	OMU	C2-N1	8.11	1.51	1.38
83	S2	116	OMU	C2-N1	8.10	1.51	1.38
3	L5	4498	OMU	C2-N1	8.06	1.51	1.38
3	L5	2837	OMU	C2-N1	8.01	1.51	1.38
3	L5	3925	OMU	C2-N1	8.00	1.51	1.38
3	L5	4620	OMU	C2-N1	7.97	1.50	1.38
3	L5	4227	OMU	C2-N1	7.90	1.50	1.38
3	L5	3818	UY1	C2-N3	7.87	1.50	1.37
83	S2	1248	B8N	C6-N1	7.85	1.55	1.36
3	L5	4306	OMU	C2-N1	7.83	1.50	1.38
83	S2	1248	B8N	C4-N3	-7.77	1.26	1.40
83	S2	1248	B8N	C4-C5	7.17	1.63	1.47
83	S2	116	OMU	C2-N3	7.06	1.50	1.38
83	S2	1326	OMU	C2-N3	7.03	1.50	1.38
83	S2	1442	OMU	C2-N3	6.98	1.50	1.38
83	S2	172	OMU	C2-N3	6.96	1.50	1.38
83	S2	428	OMU	C2-N3	6.94	1.50	1.38
83	S2	627	OMU	C2-N3	6.93	1.50	1.38
83	S2	1288	OMU	C2-N3	6.89	1.50	1.38
83	S2	354	OMU	C2-N3	6.80	1.49	1.38
83	S2	799	OMU	C2-N3	6.78	1.49	1.38
3	L5	4227	OMU	C2-N3	6.77	1.49	1.38
3	L5	2837	OMU	C2-N3	6.76	1.49	1.38
83	S2	1639	G7M	C4-N3	6.76	1.49	1.34
3	L5	4498	OMU	C2-N3	6.74	1.49	1.38
3	L5	3925	OMU	C2-N3	6.73	1.49	1.38
3	L5	4620	OMU	C2-N3	6.70	1.49	1.38
83	S2	121	OMU	C2-N3	6.70	1.49	1.38
3	L5	4306	OMU	C2-N3	6.47	1.49	1.38
3	L5	4530	UR3	C6-C5	6.22	1.49	1.35
3	L5	4530	UR3	C2-N1	6.16	1.47	1.38
83	S2	172	OMU	C6-C5	5.96	1.48	1.35
83	S2	1288	OMU	C6-C5	5.94	1.48	1.35
83	S2	1248	B8N	C2-N1	5.91	1.56	1.39
83	S2	428	OMU	C6-C5	5.90	1.48	1.35
83	S2	121	OMU	C6-C5	5.89	1.48	1.35
3	L5	4227	OMU	C6-C5	5.87	1.48	1.35
83	S2	354	OMU	C6-C5	5.86	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	627	OMU	C6-C5	5.85	1.48	1.35
83	S2	1326	OMU	C6-C5	5.84	1.48	1.35
83	S2	1442	OMU	C6-C5	5.80	1.48	1.35
83	S2	116	OMU	C6-C5	5.79	1.48	1.35
3	L5	4498	OMU	C6-C5	5.76	1.48	1.35
83	S2	799	OMU	C6-C5	5.76	1.48	1.35
3	L5	2837	OMU	C6-C5	5.75	1.48	1.35
3	L5	4530	UR3	C2-N3	5.75	1.50	1.39
3	L5	3925	OMU	C6-C5	5.71	1.48	1.35
3	L5	4620	OMU	C6-C5	5.69	1.48	1.35
83	S2	1639	G7M	C2-N3	5.64	1.46	1.33
3	L5	4306	OMU	C6-C5	5.55	1.47	1.35
83	S2	799	OMU	O4-C4	-5.54	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.54	1.13	1.24
3	L5	2837	OMU	O4-C4	-5.53	1.13	1.24
3	L5	4306	OMU	O4-C4	-5.52	1.13	1.24
3	L5	4620	OMU	O4-C4	-5.51	1.13	1.24
83	S2	1442	OMU	O4-C4	-5.49	1.13	1.24
3	L5	4227	OMU	O4-C4	-5.47	1.13	1.24
83	S2	1326	OMU	O4-C4	-5.45	1.13	1.24
83	S2	354	OMU	O4-C4	-5.45	1.13	1.24
3	L5	3925	OMU	O4-C4	-5.45	1.13	1.24
83	S2	172	OMU	O4-C4	-5.40	1.14	1.24
83	S2	627	OMU	O4-C4	-5.40	1.14	1.24
83	S2	1248	B8N	C6-C5	5.39	1.42	1.35
83	S2	116	OMU	O4-C4	-5.38	1.14	1.24
83	S2	1288	OMU	O4-C4	-5.38	1.14	1.24
83	S2	428	OMU	O4-C4	-5.36	1.14	1.24
83	S2	121	OMU	O4-C4	-5.36	1.14	1.24
3	L5	3818	UY1	C6-N1	5.30	1.45	1.36
83	S2	1639	G7M	C2-N2	4.96	1.45	1.34
3	L5	4220	6MZ	O4'-C4'	4.71	1.55	1.45
3	L5	4220	6MZ	O4'-C1'	-4.70	1.31	1.42
83	S2	1639	G7M	C5-N7	-4.58	1.33	1.39
3	L5	3818	UY1	C4-N3	4.54	1.47	1.38
83	S2	428	OMU	C4-N3	4.51	1.46	1.38
83	S2	1442	OMU	C4-N3	4.50	1.46	1.38
83	S2	116	OMU	C4-N3	4.46	1.46	1.38
83	S2	1326	OMU	C4-N3	4.46	1.46	1.38
3	L5	4220	6MZ	C5'-C4'	-4.45	1.38	1.51
83	S2	627	OMU	C4-N3	4.44	1.46	1.38
83	S2	1288	OMU	C4-N3	4.36	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	172	OMU	C4-N3	4.35	1.46	1.38
3	L5	2837	OMU	C4-N3	4.31	1.46	1.38
3	L5	3925	OMU	C4-N3	4.28	1.46	1.38
83	S2	354	OMU	C4-N3	4.24	1.45	1.38
3	L5	4498	OMU	C4-N3	4.24	1.45	1.38
83	S2	121	OMU	C4-N3	4.21	1.45	1.38
83	S2	799	OMU	C4-N3	4.21	1.45	1.38
3	L5	4227	OMU	C4-N3	4.13	1.45	1.38
83	S2	649	PSU	C6-C5	4.05	1.39	1.35
3	L5	4620	OMU	C4-N3	3.98	1.45	1.38
83	S2	801	PSU	C6-C5	3.98	1.39	1.35
83	S2	1639	G7M	C5-C6	3.95	1.54	1.43
83	S2	93	PSU	C6-C5	3.94	1.39	1.35
83	S2	1248	B8N	C1'-C5	3.84	1.58	1.50
83	S2	651	PSU	C6-C5	3.84	1.39	1.35
3	L5	4306	OMU	C4-N3	3.83	1.45	1.38
83	S2	866	PSU	C6-C5	3.75	1.39	1.35
3	L5	1683	PSU	C6-C5	3.73	1.39	1.35
83	S2	1244	PSU	C6-C5	3.71	1.39	1.35
3	L5	3844	PSU	C6-C5	3.71	1.39	1.35
83	S2	863	PSU	C6-C5	3.69	1.39	1.35
3	L5	3818	UY1	O4-C4	-3.64	1.16	1.23
5	L8	55	PSU	C6-C5	3.64	1.39	1.35
83	S2	406	PSU	C6-C5	3.61	1.39	1.35
83	S2	1004	PSU	C6-C5	3.61	1.39	1.35
3	L5	1782	PSU	C6-C5	3.60	1.39	1.35
83	S2	1056	PSU	C6-C5	3.60	1.39	1.35
83	S2	1045	PSU	C6-C5	3.59	1.39	1.35
83	S2	1367	PSU	C6-C5	3.58	1.39	1.35
3	L5	4299	PSU	C6-C5	3.58	1.39	1.35
83	S2	1232	PSU	C6-C5	3.57	1.39	1.35
3	L5	4673	PSU	C6-C5	3.56	1.39	1.35
83	S2	814	PSU	C6-C5	3.55	1.39	1.35
3	L5	3830	A2M	O5'-C5'	-3.52	1.33	1.44
83	S2	668	A2M	O5'-C5'	-3.52	1.33	1.44
3	L5	4353	PSU	C6-C5	3.52	1.39	1.35
3	L5	4361	PSU	C6-C5	3.51	1.39	1.35
3	L5	1744	PSU	C6-C5	3.51	1.39	1.35
3	L5	2839	PSU	C6-C5	3.51	1.39	1.35
83	S2	99	A2M	O5'-C5'	-3.49	1.34	1.44
83	S2	966	PSU	C6-C5	3.49	1.39	1.35
83	S2	1177	PSU	C6-C5	3.49	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4471	PSU	C6-C5	3.49	1.39	1.35
83	S2	681	PSU	C6-C5	3.48	1.39	1.35
5	L8	69	PSU	C6-C5	3.47	1.39	1.35
83	S2	109	PSU	C6-C5	3.47	1.39	1.35
3	L5	3825	A2M	O5'-C5'	-3.47	1.34	1.44
3	L5	4312	PSU	C6-C5	3.47	1.39	1.35
3	L5	4431	PSU	C6-C5	3.46	1.39	1.35
83	S2	105	PSU	C6-C5	3.45	1.39	1.35
3	L5	1871	A2M	O5'-C5'	-3.45	1.34	1.44
83	S2	1046	PSU	C6-C5	3.44	1.39	1.35
3	L5	2815	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	4532	PSU	C6-C5	3.43	1.39	1.35
83	S2	686	PSU	C6-C5	3.43	1.39	1.35
3	L5	4552	PSU	C6-C5	3.42	1.39	1.35
3	L5	2401	A2M	O5'-C5'	-3.42	1.34	1.44
3	L5	4296	PSU	C6-C5	3.42	1.39	1.35
3	L5	1323	A2M	O5'-C5'	-3.42	1.34	1.44
3	L5	1862	PSU	C6-C5	3.42	1.39	1.35
3	L5	1781	PSU	C6-C5	3.41	1.39	1.35
83	S2	166	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	5010	PSU	C6-C5	3.39	1.39	1.35
3	L5	400	A2M	O5'-C5'	-3.39	1.34	1.44
83	S2	1031	A2M	O5'-C5'	-3.39	1.34	1.44
3	L5	2787	A2M	O5'-C5'	-3.37	1.34	1.44
3	L5	1582	PSU	C6-C5	3.37	1.39	1.35
3	L5	3639	PSU	C6-C5	3.36	1.39	1.35
83	S2	484	A2M	O5'-C5'	-3.36	1.34	1.44
3	L5	3695	PSU	C6-C5	3.36	1.39	1.35
3	L5	4500	PSU	C6-C5	3.35	1.39	1.35
83	S2	1081	PSU	C6-C5	3.35	1.39	1.35
3	L5	5001	PSU	C6-C5	3.35	1.39	1.35
3	L5	4571	A2M	O5'-C5'	-3.34	1.34	1.44
3	L5	4973	PSU	C6-C5	3.34	1.39	1.35
3	L5	3920	PSU	C6-C5	3.34	1.39	1.35
3	L5	4521	PSU	C6-C5	3.34	1.39	1.35
3	L5	2363	A2M	O5'-C5'	-3.34	1.34	1.44
3	L5	1536	PSU	C6-C5	3.33	1.39	1.35
83	S2	1383	A2M	O5'-C5'	-3.33	1.34	1.44
3	L5	1524	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	2632	PSU	C6-C5	3.31	1.39	1.35
3	L5	4493	PSU	C6-C5	3.31	1.39	1.35
3	L5	4523	A2M	O5'-C5'	-3.31	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1860	PSU	C6-C5	3.31	1.39	1.35
3	L5	4590	A2M	O5'-C5'	-3.29	1.34	1.44
3	L5	4442	PSU	C6-C5	3.29	1.38	1.35
3	L5	3785	A2M	O5'-C5'	-3.29	1.34	1.44
3	L5	4972	PSU	C6-C5	3.28	1.38	1.35
3	L5	4220	6MZ	C5-N7	-3.27	1.33	1.39
3	L5	3867	A2M	O5'-C5'	-3.26	1.34	1.44
3	L5	1792	PSU	C6-C5	3.26	1.38	1.35
3	L5	4636	PSU	C6-C5	3.25	1.38	1.35
3	L5	398	A2M	O5'-C5'	-3.25	1.34	1.44
3	L5	4579	PSU	C6-C5	3.23	1.38	1.35
3	L5	4457	PSU	C6-C5	3.23	1.38	1.35
3	L5	3853	PSU	C6-C5	3.22	1.38	1.35
3	L5	1326	A2M	O5'-C5'	-3.21	1.34	1.44
3	L5	3637	PSU	C6-C5	3.21	1.38	1.35
3	L5	3818	UY1	O2-C2	-3.21	1.16	1.23
3	L5	3822	PSU	C6-C5	3.21	1.38	1.35
3	L5	3718	A2M	O5'-C5'	-3.20	1.34	1.44
3	L5	3818	UY1	C1'-C5	3.20	1.57	1.50
3	L5	4293	PSU	C6-C5	3.19	1.38	1.35
83	S2	1174	PSU	C6-C5	3.18	1.38	1.35
83	S2	468	A2M	O5'-C5'	-3.17	1.34	1.44
3	L5	4220	6MZ	C2'-C1'	3.16	1.63	1.53
3	L5	3851	PSU	C6-C5	3.15	1.38	1.35
3	L5	3884	PSU	C6-C5	3.14	1.38	1.35
3	L5	4220	6MZ	C5-C4	-3.11	1.33	1.39
3	L5	4403	PSU	C6-C5	3.11	1.38	1.35
83	S2	576	A2M	O5'-C5'	-3.10	1.35	1.44
83	S2	27	A2M	O5'-C5'	-3.09	1.35	1.44
3	L5	1534	A2M	O5'-C5'	-3.08	1.35	1.44
83	S2	1832	6MZ	C5-N7	-3.08	1.33	1.39
3	L5	4220	6MZ	C8-N9	-3.07	1.32	1.37
3	L5	1677	PSU	C6-C5	3.07	1.38	1.35
83	S2	1851	MA6	C6-N6	3.07	1.45	1.36
3	L5	4576	PSU	C6-C5	3.07	1.38	1.35
83	S2	1832	6MZ	C5-C4	-3.05	1.33	1.39
83	S2	159	A2M	O5'-C5'	-3.05	1.35	1.44
83	S2	1850	MA6	C6-N6	3.02	1.45	1.36
3	L5	4689	PSU	C6-C5	3.01	1.38	1.35
83	S2	1288	OMU	C5-C4	2.94	1.50	1.43
83	S2	172	OMU	C5-C4	2.92	1.50	1.43
3	L5	4628	PSU	C6-C5	2.87	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	627	OMU	C5-C4	2.86	1.49	1.43
83	S2	121	OMU	C5-C4	2.86	1.49	1.43
83	S2	1639	G7M	C2-N1	2.84	1.44	1.37
83	S2	1326	OMU	C5-C4	2.84	1.49	1.43
83	S2	428	OMU	C5-C4	2.84	1.49	1.43
83	S2	1832	6MZ	C8-N9	-2.83	1.32	1.37
83	S2	354	OMU	C5-C4	2.82	1.49	1.43
3	L5	4227	OMU	C5-C4	2.81	1.49	1.43
83	S2	799	OMU	C5-C4	2.80	1.49	1.43
3	L5	4220	6MZ	O3'-C3'	2.79	1.49	1.43
83	S2	121	OMU	C6-N1	2.76	1.44	1.38
83	S2	1442	OMU	C5-C4	2.74	1.49	1.43
3	L5	4498	OMU	C5-C4	2.72	1.49	1.43
83	S2	1442	OMU	C6-N1	2.71	1.44	1.38
83	S2	116	OMU	C5-C4	2.71	1.49	1.43
83	S2	1326	OMU	C6-N1	2.70	1.44	1.38
83	S2	1288	OMU	C6-N1	2.70	1.44	1.38
3	L5	2837	OMU	C5-C4	2.69	1.49	1.43
83	S2	799	OMU	C6-N1	2.68	1.44	1.38
83	S2	627	OMU	C6-N1	2.67	1.44	1.38
83	S2	172	OMU	C6-N1	2.67	1.44	1.38
83	S2	354	OMU	C6-N1	2.67	1.44	1.38
3	L5	2837	OMU	C6-N1	2.65	1.44	1.38
83	S2	428	OMU	C6-N1	2.64	1.44	1.38
3	L5	4498	OMU	C6-N1	2.62	1.44	1.38
3	L5	4227	OMU	C6-N1	2.60	1.44	1.38
3	L5	4530	UR3	O2-C2	-2.60	1.17	1.22
83	S2	668	A2M	O4'-C4'	-2.59	1.39	1.45
83	S2	116	OMU	C6-N1	2.57	1.44	1.38
3	L5	4620	OMU	C5-C4	2.56	1.49	1.43
3	L5	3925	OMU	C5-C4	2.55	1.49	1.43
3	L5	4620	OMU	C6-N1	2.53	1.44	1.38
3	L5	4530	UR3	C6-N1	2.53	1.44	1.38
83	S2	1639	G7M	O6-C6	-2.51	1.18	1.23
83	S2	1639	G7M	C6-N1	2.50	1.43	1.38
3	L5	4306	OMU	C6-N1	2.50	1.44	1.38
83	S2	1850	MA6	C5-C4	-2.50	1.34	1.39
83	S2	1851	MA6	C5-C4	-2.49	1.34	1.39
3	L5	3925	OMU	C6-N1	2.47	1.44	1.38
3	L5	4306	OMU	C5-C4	2.47	1.49	1.43
3	L5	1524	A2M	O4'-C4'	-2.36	1.39	1.45
3	L5	3867	A2M	O4'-C4'	-2.31	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4530	UR3	C3U-N3	2.27	1.51	1.47
3	L5	4523	A2M	O4'-C4'	-2.25	1.40	1.45
3	L5	4530	UR3	C5-C4	2.25	1.49	1.43
3	L5	4220	6MZ	C6-N1	-2.19	1.31	1.35
3	L5	4571	A2M	O4'-C4'	-2.19	1.40	1.45
3	L5	3818	UY1	O4'-C1'	-2.17	1.40	1.43
3	L5	4442	PSU	O4'-C1'	-2.12	1.40	1.43
3	L5	4523	A2M	O3'-C3'	-2.11	1.37	1.43
3	L5	4689	PSU	C4-C5	-2.09	1.38	1.44
83	S2	1832	6MZ	C6-N1	-2.09	1.31	1.35
3	L5	1323	A2M	O4'-C4'	-2.08	1.40	1.45
3	L5	1677	PSU	C4-C5	-2.08	1.38	1.44
3	L5	1536	PSU	C4-C5	-2.06	1.38	1.44
83	S2	1850	MA6	C4-N9	-2.06	1.33	1.37
3	L5	4636	PSU	C4-C5	-2.05	1.38	1.44
3	L5	2839	PSU	C4-C5	-2.05	1.38	1.44
3	L5	3884	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4442	PSU	C4-C5	-2.04	1.38	1.44
3	L5	3639	PSU	C4-C5	-2.03	1.38	1.44
3	L5	1323	A2M	O3'-C3'	-2.02	1.37	1.43
3	L5	4673	PSU	C4-C5	-2.02	1.38	1.44
3	L5	3818	UY1	C4-C5	2.02	1.49	1.44
83	S2	576	A2M	C5-C4	2.01	1.42	1.39
3	L5	4293	PSU	C4-C5	-2.00	1.38	1.44

All (687) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-11.98	102.25	116.86
83	S2	1850	MA6	N1-C6-N6	-11.35	103.02	116.86
83	S2	1851	MA6	C5-C6-N6	7.70	137.53	125.33
83	S2	1850	MA6	C5-C6-N6	7.41	137.06	125.33
83	S2	1639	G7M	C1'-N9-C4	7.36	148.24	126.49
83	S2	1639	G7M	C1'-N9-C8	-7.35	101.93	126.74
3	L5	4498	OMU	C4-N3-C2	-5.77	119.45	126.61
83	S2	1326	OMU	C4-N3-C2	-5.71	119.52	126.61
83	S2	1832	6MZ	N1-C2-N3	-5.69	119.97	128.58
83	S2	172	OMU	C4-N3-C2	-5.66	119.58	126.61
83	S2	627	OMU	C4-N3-C2	-5.62	119.63	126.61
3	L5	2837	OMU	C4-N3-C2	-5.61	119.64	126.61
83	S2	1851	MA6	N1-C2-N3	-5.60	120.10	128.58
3	L5	4530	UR3	C4-N3-C2	-5.60	120.07	124.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N9-C8-N7	-5.59	106.01	113.94
3	L5	4227	OMU	C4-N3-C2	-5.57	119.70	126.61
83	S2	799	OMU	C4-N3-C2	-5.55	119.72	126.61
83	S2	428	OMU	C4-N3-C2	-5.51	119.78	126.61
83	S2	1850	MA6	N9-C8-N7	-5.46	106.18	113.94
83	S2	1288	OMU	C4-N3-C2	-5.43	119.86	126.61
83	S2	1248	B8N	C5-C4-N3	5.43	126.02	116.15
83	S2	1850	MA6	N1-C2-N3	-5.42	120.37	128.58
3	L5	4220	6MZ	N1-C2-N3	-5.38	120.43	128.58
83	S2	1442	OMU	C4-N3-C2	-5.37	119.95	126.61
83	S2	354	OMU	C4-N3-C2	-5.31	120.01	126.61
3	L5	4636	PSU	C4-N3-C2	-5.26	119.12	126.37
3	L5	4306	OMU	C4-N3-C2	-5.19	120.17	126.61
3	L5	3925	OMU	C4-N3-C2	-5.17	120.19	126.61
3	L5	3637	PSU	N1-C2-N3	5.17	120.62	115.17
3	L5	4442	PSU	N1-C2-N3	5.13	120.58	115.17
3	L5	4457	PSU	C4-N3-C2	-5.12	119.32	126.37
3	L5	4500	PSU	N1-C2-N3	5.11	120.56	115.17
83	S2	121	OMU	C4-N3-C2	-5.09	120.30	126.61
3	L5	4500	PSU	C4-N3-C2	-5.06	119.40	126.37
3	L5	4620	OMU	C4-N3-C2	-5.06	120.33	126.61
3	L5	4636	PSU	N1-C2-N3	5.06	120.50	115.17
83	S2	116	OMU	C4-N3-C2	-5.05	120.34	126.61
3	L5	3851	PSU	C4-N3-C2	-5.05	119.42	126.37
3	L5	4293	PSU	C4-N3-C2	-5.04	119.42	126.37
83	S2	686	PSU	C4-N3-C2	-5.04	119.43	126.37
3	L5	4431	PSU	C4-N3-C2	-5.01	119.47	126.37
3	L5	4457	PSU	N1-C2-N3	5.01	120.45	115.17
3	L5	1677	PSU	C4-N3-C2	-4.99	119.50	126.37
83	S2	1081	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	4442	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	4296	PSU	C4-N3-C2	-4.97	119.52	126.37
3	L5	4532	PSU	N1-C2-N3	4.97	120.41	115.17
3	L5	3637	PSU	C4-N3-C2	-4.96	119.54	126.37
3	L5	4296	PSU	N1-C2-N3	4.95	120.39	115.17
83	S2	1248	B8N	C4-N3-C2	-4.95	119.53	125.62
3	L5	1862	PSU	C4-N3-C2	-4.95	119.55	126.37
83	S2	1367	PSU	C4-N3-C2	-4.94	119.57	126.37
3	L5	4353	PSU	N1-C2-N3	4.94	120.38	115.17
83	S2	105	PSU	N1-C2-N3	4.93	120.37	115.17
83	S2	966	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	4299	PSU	N1-C2-N3	4.92	120.36	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1862	PSU	N1-C2-N3	4.90	120.34	115.17
3	L5	2632	PSU	N1-C2-N3	4.90	120.33	115.17
3	L5	4493	PSU	N1-C2-N3	4.89	120.32	115.17
83	S2	1851	MA6	C5-C4-N3	-4.89	119.99	126.72
3	L5	3853	PSU	C4-N3-C2	-4.88	119.65	126.37
3	L5	4521	PSU	N1-C2-N3	4.88	120.31	115.17
83	S2	1244	PSU	N1-C2-N3	4.88	120.31	115.17
83	S2	1367	PSU	N1-C2-N3	4.87	120.31	115.17
3	L5	4353	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	4521	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	4973	PSU	N1-C2-N3	4.87	120.31	115.17
83	S2	966	PSU	C4-N3-C2	-4.87	119.67	126.37
3	L5	2632	PSU	C4-N3-C2	-4.86	119.67	126.37
83	S2	686	PSU	N1-C2-N3	4.86	120.30	115.17
3	L5	1582	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	3818	UY1	C4-N3-C2	-4.86	119.68	126.37
3	L5	3884	PSU	N1-C2-N3	4.85	120.28	115.17
83	S2	863	PSU	N1-C2-N3	4.85	120.28	115.17
3	L5	4299	PSU	C4-N3-C2	-4.85	119.69	126.37
83	S2	814	PSU	C4-N3-C2	-4.84	119.70	126.37
83	S2	1832	6MZ	C5-C4-N3	-4.84	120.05	126.72
83	S2	1232	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	1792	PSU	N1-C2-N3	4.84	120.27	115.17
3	L5	3639	PSU	N1-C2-N3	4.83	120.27	115.17
3	L5	1536	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	4431	PSU	N1-C2-N3	4.83	120.26	115.17
83	S2	1244	PSU	C4-N3-C2	-4.83	119.72	126.37
83	S2	1232	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	4220	6MZ	C5-C4-N3	-4.82	120.07	126.72
3	L5	4972	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L5	1871	A2M	C3'-C2'-C1'	-4.82	93.58	102.81
3	L5	5010	PSU	N1-C2-N3	4.82	120.25	115.17
3	L5	4312	PSU	N1-C2-N3	4.81	120.25	115.17
83	S2	863	PSU	C4-N3-C2	-4.81	119.75	126.37
83	S2	1045	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L5	3851	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	4493	PSU	C4-N3-C2	-4.80	119.76	126.37
3	L5	3853	PSU	N1-C2-N3	4.79	120.22	115.17
83	S2	1832	6MZ	N9-C8-N7	-4.79	107.13	113.94
3	L5	4293	PSU	N1-C2-N3	4.79	120.22	115.17
3	L5	1536	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L5	4673	PSU	C4-N3-C2	-4.78	119.79	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	105	PSU	C4-N3-C2	-4.78	119.79	126.37
83	S2	651	PSU	C4-N3-C2	-4.78	119.79	126.37
3	L5	4673	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	4576	PSU	C4-N3-C2	-4.77	119.81	126.37
3	L5	1782	PSU	N1-C2-N3	4.76	120.19	115.17
83	S2	1046	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	4973	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	1781	PSU	N1-C2-N3	4.75	120.18	115.17
83	S2	109	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	4361	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	3822	PSU	N1-C2-N3	4.74	120.17	115.17
3	L5	2839	PSU	N1-C2-N3	4.74	120.16	115.17
5	L8	69	PSU	N1-C2-N3	4.73	120.16	115.17
83	S2	651	PSU	N1-C2-N3	4.73	120.16	115.17
3	L5	3822	PSU	C4-N3-C2	-4.72	119.86	126.37
83	S2	1081	PSU	N1-C2-N3	4.72	120.15	115.17
3	L5	4403	PSU	C4-N3-C2	-4.71	119.88	126.37
83	S2	109	PSU	N1-C2-N3	4.71	120.13	115.17
3	L5	1744	PSU	N1-C2-N3	4.71	120.13	115.17
5	L8	69	PSU	C4-N3-C2	-4.70	119.89	126.37
83	S2	1046	PSU	C4-N3-C2	-4.70	119.90	126.37
83	S2	1177	PSU	C4-N3-C2	-4.70	119.90	126.37
83	S2	406	PSU	N1-C2-N3	4.70	120.12	115.17
3	L5	3695	PSU	C4-N3-C2	-4.70	119.90	126.37
83	S2	1174	PSU	N1-C2-N3	4.70	120.12	115.17
3	L5	4532	PSU	C4-N3-C2	-4.69	119.91	126.37
3	L5	4403	PSU	N1-C2-N3	4.69	120.12	115.17
3	L5	3639	PSU	C4-N3-C2	-4.69	119.91	126.37
83	S2	681	PSU	N1-C2-N3	4.68	120.11	115.17
3	L5	4552	PSU	N1-C2-N3	4.68	120.10	115.17
83	S2	866	PSU	C4-N3-C2	-4.67	119.93	126.37
83	S2	814	PSU	N1-C2-N3	4.67	120.09	115.17
83	S2	1177	PSU	N1-C2-N3	4.66	120.09	115.17
3	L5	4579	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	4552	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	5001	PSU	C4-N3-C2	-4.65	119.96	126.37
5	L8	55	PSU	N1-C2-N3	4.65	120.07	115.17
83	S2	1174	PSU	C4-N3-C2	-4.64	119.98	126.37
3	L5	4361	PSU	N1-C2-N3	4.63	120.05	115.17
83	S2	1045	PSU	N1-C2-N3	4.63	120.05	115.17
83	S2	866	PSU	N1-C2-N3	4.62	120.04	115.17
3	L5	3884	PSU	C4-N3-C2	-4.62	120.01	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1582	PSU	N1-C2-N3	4.61	120.03	115.17
83	S2	649	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	1683	PSU	C4-N3-C2	-4.60	120.03	126.37
3	L5	1677	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	1683	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	1744	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	4972	PSU	N1-C2-N3	4.59	120.01	115.17
5	L8	55	PSU	C4-N3-C2	-4.59	120.05	126.37
83	S2	1004	PSU	N1-C2-N3	4.59	120.01	115.17
3	L5	1781	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	3695	PSU	N1-C2-N3	4.59	120.00	115.17
3	L5	1782	PSU	C4-N3-C2	-4.58	120.06	126.37
83	S2	681	PSU	C4-N3-C2	-4.58	120.06	126.37
3	L5	4471	PSU	N1-C2-N3	4.58	120.00	115.17
3	L5	5010	PSU	C4-N3-C2	-4.57	120.07	126.37
3	L5	3844	PSU	N1-C2-N3	4.57	119.99	115.17
3	L5	5001	PSU	N1-C2-N3	4.57	119.98	115.17
83	S2	406	PSU	C4-N3-C2	-4.56	120.09	126.37
3	L5	4312	PSU	C4-N3-C2	-4.55	120.10	126.37
3	L5	4576	PSU	N1-C2-N3	4.55	119.97	115.17
3	L5	1792	PSU	C4-N3-C2	-4.54	120.11	126.37
3	L5	3920	PSU	N1-C2-N3	4.53	119.95	115.17
83	S2	1056	PSU	N1-C2-N3	4.52	119.94	115.17
83	S2	1639	G7M	C2-N3-C4	4.51	120.07	112.30
83	S2	1056	PSU	C4-N3-C2	-4.51	120.16	126.37
83	S2	93	PSU	N1-C2-N3	4.50	119.91	115.17
3	L5	4628	PSU	C4-N3-C2	-4.49	120.19	126.37
3	L5	4579	PSU	C4-N3-C2	-4.49	120.19	126.37
3	L5	4689	PSU	N1-C2-N3	4.48	119.90	115.17
83	S2	1383	A2M	C3'-C2'-C1'	-4.48	94.23	102.81
83	S2	801	PSU	N1-C2-N3	4.46	119.87	115.17
3	L5	3818	UY1	N1-C2-N3	4.44	119.86	115.17
3	L5	2839	PSU	C4-N3-C2	-4.44	120.26	126.37
83	S2	1850	MA6	C4-N9-C8	4.42	110.38	105.74
3	L5	4471	PSU	C4-N3-C2	-4.41	120.30	126.37
83	S2	93	PSU	C4-N3-C2	-4.39	120.32	126.37
3	L5	4628	PSU	N1-C2-N3	4.38	119.79	115.17
3	L5	3844	PSU	C4-N3-C2	-4.38	120.34	126.37
3	L5	1860	PSU	N1-C2-N3	4.37	119.78	115.17
83	S2	649	PSU	C4-N3-C2	-4.36	120.36	126.37
3	L5	3920	PSU	C4-N3-C2	-4.35	120.38	126.37
3	L5	4220	6MZ	N9-C8-N7	-4.35	107.77	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1860	PSU	C4-N3-C2	-4.34	120.40	126.37
83	S2	1004	PSU	C4-N3-C2	-4.32	120.42	126.37
83	S2	1851	MA6	C4-N9-C8	4.22	110.17	105.74
83	S2	1850	MA6	C5-C4-N3	-4.11	121.06	126.72
3	L5	4689	PSU	C4-N3-C2	-4.11	120.71	126.37
83	S2	1639	G7M	C5-C4-N3	-4.10	120.41	128.15
3	L5	4498	OMU	N3-C2-N1	4.03	120.13	114.89
83	S2	1639	G7M	C5-C6-N1	4.01	120.14	111.84
83	S2	801	PSU	C4-N3-C2	-4.00	120.86	126.37
83	S2	172	OMU	N3-C2-N1	3.98	120.07	114.89
83	S2	121	OMU	N3-C2-N1	3.97	120.06	114.89
3	L5	398	A2M	C3'-C2'-C1'	-3.93	95.28	102.81
3	L5	4227	OMU	N3-C2-N1	3.92	120.00	114.89
3	L5	4220	6MZ	C9-N6-C6	-3.85	119.28	122.85
83	S2	1326	OMU	N3-C2-N1	3.83	119.88	114.89
3	L5	2837	OMU	N3-C2-N1	3.83	119.87	114.89
83	S2	428	OMU	N3-C2-N1	3.81	119.85	114.89
83	S2	799	OMU	C5-C4-N3	3.78	120.09	114.80
83	S2	468	A2M	C3'-C2'-C1'	-3.77	95.58	102.81
3	L5	4498	OMU	C5-C4-N3	3.76	120.07	114.80
3	L5	2837	OMU	C5-C4-N3	3.74	120.04	114.80
3	L5	4306	OMU	N3-C2-N1	3.73	119.75	114.89
3	L5	2787	A2M	O3'-C3'-C2'	3.72	121.61	111.19
3	L5	4620	OMU	N3-C2-N1	3.71	119.72	114.89
83	S2	1442	OMU	C5-C4-N3	3.71	120.00	114.80
3	L5	3925	OMU	N3-C2-N1	3.70	119.71	114.89
83	S2	1288	OMU	N3-C2-N1	3.70	119.71	114.89
83	S2	627	OMU	N3-C2-N1	3.69	119.69	114.89
83	S2	1851	MA6	C4-C5-C6	3.69	119.72	115.91
83	S2	354	OMU	N3-C2-N1	3.69	119.69	114.89
83	S2	1326	OMU	C5-C4-N3	3.68	119.95	114.80
83	S2	627	OMU	C5-C4-N3	3.68	119.95	114.80
3	L5	3830	A2M	C3'-C2'-C1'	-3.66	95.80	102.81
83	S2	1383	A2M	O3'-C3'-C2'	3.65	121.41	111.19
83	S2	799	OMU	N3-C2-N1	3.64	119.64	114.89
3	L5	4571	A2M	C3'-C2'-C1'	-3.64	95.83	102.81
83	S2	116	OMU	N3-C2-N1	3.64	119.63	114.89
83	S2	1248	B8N	C1'-C5-C4	3.64	123.13	117.61
83	S2	1851	MA6	N3-C4-N9	3.62	133.32	127.17
3	L5	3818	UY1	C6-C5-C4	3.56	120.58	118.17
3	L5	1871	A2M	O3'-C3'-C2'	3.55	121.13	111.19
83	S2	1288	OMU	C5-C4-N3	3.54	119.77	114.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4227	OMU	C5-C4-N3	3.54	119.76	114.80
3	L5	4530	UR3	C5-C4-N3	3.54	119.70	115.04
83	S2	354	OMU	C5-C4-N3	3.53	119.74	114.80
83	S2	1832	6MZ	C2-N3-C4	3.51	120.41	111.83
83	S2	172	OMU	C5-C4-N3	3.50	119.70	114.80
83	S2	428	OMU	C5-C4-N3	3.49	119.68	114.80
83	S2	1442	OMU	N3-C2-N1	3.48	119.42	114.89
83	S2	1248	B8N	N3-C2-N1	3.47	120.96	116.72
83	S2	668	A2M	C4-N9-C1'	-3.45	118.57	126.63
83	S2	1851	MA6	C5-N7-C8	3.44	108.85	103.45
3	L5	4571	A2M	O3'-C3'-C2'	3.43	120.79	111.19
83	S2	1850	MA6	C2-N1-C6	3.43	120.21	111.83
83	S2	576	A2M	C3'-C2'-C1'	-3.41	96.28	102.81
83	S2	576	A2M	O3'-C3'-C2'	3.40	120.71	111.19
3	L5	3925	OMU	C5-C4-N3	3.38	119.54	114.80
3	L5	2401	A2M	O3'-C3'-C2'	3.37	120.61	111.19
3	L5	4306	OMU	C5-C4-N3	3.37	119.51	114.80
3	L5	1524	A2M	O3'-C3'-C2'	3.36	120.59	111.19
83	S2	1851	MA6	C2-N3-C4	3.34	119.98	111.83
83	S2	1851	MA6	C2-N1-C6	3.34	119.98	111.83
3	L5	4620	OMU	C5-C4-N3	3.34	119.47	114.80
83	S2	1832	6MZ	C5-N7-C8	3.33	108.68	103.45
3	L5	4220	6MZ	C4-C5-C6	3.32	119.54	116.78
83	S2	1639	G7M	N9-C4-N3	3.32	132.60	125.95
3	L5	4220	6MZ	C2-N3-C4	3.31	119.91	111.83
3	L5	4220	6MZ	N3-C4-N9	3.31	132.79	127.17
3	L5	1534	A2M	C3'-C2'-C1'	-3.30	96.50	102.81
83	S2	1850	MA6	C4-C5-C6	3.28	119.30	115.91
83	S2	99	A2M	C3'-C2'-C1'	-3.28	96.53	102.81
83	S2	116	OMU	C5-C4-N3	3.28	119.39	114.80
83	S2	121	OMU	C5-C4-N3	3.27	119.38	114.80
3	L5	4689	PSU	C6-N1-C2	-3.26	119.66	122.69
83	S2	99	A2M	O3'-C3'-C2'	3.26	120.31	111.19
83	S2	1639	G7M	O6-C6-C5	-3.25	120.75	128.01
3	L5	398	A2M	O3'-C3'-C2'	3.23	120.23	111.19
3	L5	4973	PSU	O2-C2-N1	-3.23	119.46	122.79
83	S2	468	A2M	O3'-C3'-C2'	3.23	120.22	111.19
83	S2	166	A2M	O3'-C3'-C2'	3.22	120.19	111.19
3	L5	3639	PSU	O2-C2-N1	-3.21	119.48	122.79
3	L5	2839	PSU	O2-C2-N1	-3.19	119.50	122.79
83	S2	1031	A2M	C3'-C2'-C1'	-3.17	96.74	102.81
83	S2	1326	OMU	O4-C4-C5	-3.17	119.70	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	O3'-C3'-C2'	3.17	120.05	111.19
3	L5	1744	PSU	O2-C2-N1	-3.14	119.55	122.79
83	S2	1442	OMU	O4-C4-C5	-3.14	119.75	125.16
3	L5	3818	UY1	C6-N1-C2	-3.12	119.80	122.69
83	S2	668	A2M	C1'-N9-C8	3.12	134.02	127.09
3	L5	4500	PSU	C6-C5-C4	3.11	120.27	118.17
3	L5	4532	PSU	O2-C2-N1	-3.11	119.58	122.79
83	S2	863	PSU	O2-C2-N1	-3.10	119.59	122.79
3	L5	2839	PSU	C6-N1-C2	-3.10	119.82	122.69
83	S2	1383	A2M	C4-N9-C1'	-3.09	119.41	126.63
3	L5	5010	PSU	O2-C2-N1	-3.09	119.61	122.79
3	L5	2837	OMU	O4-C4-C5	-3.06	119.89	125.16
83	S2	159	A2M	O3'-C3'-C2'	3.05	119.71	111.19
3	L5	1683	PSU	O2-C2-N1	-3.05	119.65	122.79
3	L5	3925	OMU	O4-C4-C5	-3.03	119.93	125.16
83	S2	116	OMU	O4-C4-C5	-3.03	119.93	125.16
83	S2	1832	6MZ	N3-C4-N9	3.03	132.32	127.17
3	L5	3785	A2M	O3'-C3'-C2'	3.03	119.67	111.19
3	L5	4523	A2M	C3'-C2'-C1'	-3.03	97.01	102.81
83	S2	1850	MA6	C5-N7-C8	3.02	108.20	103.45
83	S2	428	OMU	O4-C4-C5	-3.02	119.95	125.16
3	L5	1677	PSU	O2-C2-N1	-3.02	119.68	122.79
83	S2	1850	MA6	N3-C4-N9	3.02	132.29	127.17
3	L5	4293	PSU	O2-C2-N1	-3.01	119.68	122.79
83	S2	1031	A2M	O3'-C3'-C2'	3.01	119.62	111.19
3	L5	2815	A2M	C2'-C1'-N9	3.01	118.71	113.75
83	S2	1832	6MZ	C4-C5-C6	3.01	119.28	116.78
3	L5	3830	A2M	O3'-C3'-C2'	3.00	119.57	111.19
83	S2	1850	MA6	C2-N3-C4	3.00	119.15	111.83
83	S2	627	OMU	O4-C4-C5	-2.99	120.00	125.16
3	L5	400	A2M	O3'-C3'-C2'	2.99	119.56	111.19
83	S2	649	PSU	C6-N1-C2	-2.99	119.92	122.69
83	S2	1639	G7M	C2-N1-C6	-2.98	119.71	125.11
3	L5	4442	PSU	O2-C2-N1	-2.97	119.72	122.79
3	L5	4590	A2M	C4-N9-C1'	-2.97	119.68	126.63
3	L5	1792	PSU	O2-C2-N1	-2.97	119.72	122.79
3	L5	4636	PSU	C6-C5-C4	2.97	120.18	118.17
3	L5	4498	OMU	O4-C4-C5	-2.97	120.04	125.16
3	L5	3867	A2M	C2'-C1'-N9	2.96	118.63	113.75
3	L5	3808	OMC	C1'-N1-C2	2.95	124.97	118.44
83	S2	1248	B8N	O4-C4-N3	-2.95	115.19	119.99
3	L5	2401	A2M	C3'-C2'-C1'	-2.95	97.16	102.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	27	A2M	C4-N9-C1'	-2.95	119.73	126.63
83	S2	799	OMU	O4-C4-C5	-2.95	120.08	125.16
3	L5	3884	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L5	4403	PSU	O2-C2-N1	-2.94	119.76	122.79
3	L5	1536	PSU	O2-C2-N1	-2.94	119.76	122.79
3	L5	3825	A2M	O3'-C3'-C2'	2.93	119.39	111.19
83	S2	1832	6MZ	C4-N9-C8	2.93	108.81	105.74
83	S2	1177	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	5010	PSU	C6-N1-C2	-2.92	119.98	122.69
3	L5	4312	PSU	C6-N1-C2	-2.92	119.98	122.69
3	L5	3718	A2M	C3'-C2'-C1'	-2.92	97.21	102.81
83	S2	966	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L5	4299	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L5	4312	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L5	1871	A2M	C4-N9-C1'	-2.92	119.81	126.63
83	S2	801	PSU	C6-N1-C2	-2.91	119.99	122.69
83	S2	109	PSU	O2-C2-N1	-2.90	119.79	122.79
83	S2	484	A2M	O3'-C3'-C2'	2.90	119.31	111.19
3	L5	3701	OMC	C1'-N1-C2	2.90	124.84	118.44
3	L5	4590	A2M	C3'-C2'-C1'	-2.90	97.26	102.81
3	L5	4552	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	3884	PSU	C6-N1-C2	-2.89	120.01	122.69
3	L5	2632	PSU	O2-C2-N1	-2.89	119.81	122.79
83	S2	99	A2M	C4-N9-C1'	-2.89	119.88	126.63
3	L5	4457	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L5	3639	PSU	C6-N1-C2	-2.88	120.02	122.69
3	L5	4220	6MZ	C4-N9-C8	2.88	108.76	105.74
83	S2	1045	PSU	O2-C2-N1	-2.87	119.82	122.79
83	S2	668	A2M	O3'-C3'-C2'	2.87	119.23	111.19
83	S2	1004	PSU	C6-N1-C2	-2.87	120.03	122.69
3	L5	1524	A2M	O4'-C1'-C2'	2.86	111.51	106.59
3	L5	3822	PSU	O2-C2-N1	-2.86	119.84	122.79
83	S2	1081	PSU	O2-C2-N1	-2.86	119.84	122.79
83	S2	93	PSU	O2-C2-N1	-2.85	119.84	122.79
3	L5	4628	PSU	O2-C2-N1	-2.85	119.84	122.79
3	L5	4620	OMU	O4-C4-C5	-2.85	120.25	125.16
83	S2	1288	OMU	O4-C4-C5	-2.85	120.25	125.16
5	L8	55	PSU	O2-C2-N1	-2.85	119.85	122.79
3	L5	4523	A2M	C4-N9-C1'	-2.84	119.99	126.63
3	L5	4590	A2M	C1'-N9-C8	2.84	133.40	127.09
83	S2	172	OMU	O4-C4-C5	-2.84	120.27	125.16
3	L5	2861	OMC	C1'-N1-C2	2.84	124.71	118.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1232	PSU	O2-C2-N1	-2.84	119.86	122.79
83	S2	1639	G7M	CN7-N7-C5	2.83	130.33	126.80
3	L5	3853	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L5	2401	A2M	C4-N9-C1'	-2.83	120.02	126.63
3	L5	4590	A2M	O3'-C3'-C2'	2.83	119.10	111.19
3	L5	1323	A2M	C4-N9-C1'	-2.83	120.02	126.63
3	L5	2815	A2M	O3'-C3'-C2'	2.82	119.09	111.19
3	L5	1326	A2M	O3'-C3'-C2'	2.82	119.07	111.19
3	L5	4628	PSU	C6-N1-C2	-2.81	120.08	122.69
83	S2	649	PSU	O2-C2-N1	-2.81	119.89	122.79
83	S2	1337	4AC	N4-C4-N3	2.81	118.42	113.87
3	L5	4972	PSU	O2-C2-N1	-2.80	119.90	122.79
3	L5	4532	PSU	C6-N1-C2	-2.80	120.09	122.69
3	L5	3637	PSU	C6-N1-C2	-2.80	120.10	122.69
83	S2	1174	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	4353	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	3637	PSU	O2-C2-N1	-2.79	119.92	122.79
83	S2	166	A2M	C4-N9-C1'	-2.79	120.12	126.63
3	L5	4576	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	4220	6MZ	C5-N7-C8	2.78	107.83	103.45
83	S2	159	A2M	C1'-N9-C8	2.78	133.26	127.09
83	S2	354	OMU	O4-C4-C5	-2.78	120.37	125.16
83	S2	159	A2M	C4-N9-C1'	-2.78	120.14	126.63
3	L5	4521	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	4636	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	3851	PSU	O2-C2-N1	-2.77	119.93	122.79
3	L5	3844	PSU	C6-N1-C2	-2.77	120.12	122.69
83	S2	1046	PSU	O2-C2-N1	-2.77	119.93	122.79
3	L5	3818	UY1	O2-C2-N1	-2.77	119.93	122.79
3	L5	4673	PSU	O2-C2-N1	-2.77	119.93	122.79
3	L5	4973	PSU	C6-N1-C2	-2.77	120.12	122.69
83	S2	406	PSU	O2-C2-N1	-2.76	119.94	122.79
3	L5	3830	A2M	C4-N9-C1'	-2.76	120.18	126.63
3	L5	1744	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	4579	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	398	A2M	C4-N9-C1'	-2.76	120.18	126.63
3	L5	4552	PSU	C6-N1-C2	-2.76	120.13	122.69
83	S2	1174	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	3695	PSU	O2-C2-N1	-2.76	119.95	122.79
83	S2	468	A2M	C4-N9-C1'	-2.75	120.19	126.63
83	S2	484	A2M	C1'-N9-C8	2.75	133.20	127.09
3	L5	1871	A2M	C1'-N9-C8	2.75	133.20	127.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4306	OMU	O4-C4-C5	-2.75	120.42	125.16
3	L5	400	A2M	C3'-C2'-C1'	-2.75	97.55	102.81
83	S2	166	A2M	C3'-C2'-C1'	-2.75	97.55	102.81
83	S2	1383	A2M	C1'-N9-C8	2.74	133.18	127.09
3	L5	1683	PSU	C6-N1-C2	-2.74	120.15	122.69
83	S2	1244	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L5	3785	A2M	C4-N9-C1'	-2.74	120.23	126.63
83	S2	484	A2M	C4-N9-C1'	-2.73	120.24	126.63
3	L5	400	A2M	C4-N9-C1'	-2.73	120.24	126.63
3	L5	4689	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L5	3825	A2M	C3'-C2'-C1'	-2.73	97.57	102.81
3	L5	4442	PSU	C6-N1-C2	-2.73	120.16	122.69
3	L5	1323	A2M	C3'-C2'-C1'	-2.73	97.58	102.81
83	S2	814	PSU	O2-C2-N1	-2.73	119.97	122.79
83	S2	27	A2M	O3'-C3'-C2'	2.73	118.82	111.19
3	L5	4442	PSU	C6-C5-C4	2.72	120.01	118.17
3	L5	1792	PSU	C6-N1-C2	-2.72	120.17	122.69
83	S2	1004	PSU	O2-C2-N1	-2.72	119.98	122.79
83	S2	866	PSU	O2-C2-N1	-2.72	119.98	122.79
83	S2	27	A2M	C1'-N9-C8	2.72	133.13	127.09
83	S2	27	A2M	O4'-C1'-C2'	2.71	111.26	106.59
3	L5	1536	PSU	C6-N1-C2	-2.71	120.17	122.69
3	L5	4500	PSU	O2-C2-N1	-2.71	119.99	122.79
3	L5	4493	PSU	O2-C2-N1	-2.70	120.00	122.79
83	S2	99	A2M	C1'-N9-C8	2.70	133.09	127.09
83	S2	1031	A2M	C4-N9-C1'	-2.69	120.33	126.63
83	S2	651	PSU	O2-C2-N1	-2.69	120.01	122.79
3	L5	1862	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L5	3718	A2M	C1'-N9-C8	2.68	133.05	127.09
3	L5	1782	PSU	C6-N1-C2	-2.68	120.21	122.69
3	L5	1781	PSU	O2-C2-N1	-2.67	120.03	122.79
83	S2	406	PSU	C6-N1-C2	-2.67	120.21	122.69
3	L5	4227	OMU	O4-C4-C5	-2.67	120.56	125.16
3	L5	1782	PSU	O2-C2-N1	-2.66	120.04	122.79
3	L5	1323	A2M	C1'-N9-C8	2.66	133.00	127.09
3	L5	2363	A2M	O3'-C3'-C2'	2.66	118.62	111.19
3	L5	4471	PSU	O2-C2-N1	-2.65	120.05	122.79
3	L5	398	A2M	C1'-N9-C8	2.65	132.98	127.09
3	L5	4471	PSU	C6-N1-C2	-2.65	120.23	122.69
83	S2	1367	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L5	4523	A2M	C1'-N9-C8	2.64	132.96	127.09
3	L5	1323	A2M	O3'-C3'-C2'	2.64	118.58	111.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	668	A2M	O4'-C1'-C2'	2.64	111.14	106.59
3	L5	3867	A2M	O3'-C3'-C2'	2.63	118.55	111.19
3	L5	4579	PSU	O2-C2-N1	-2.63	120.07	122.79
3	L5	4673	PSU	C6-N1-C2	-2.63	120.25	122.69
83	S2	468	A2M	C1'-N9-C8	2.63	132.93	127.09
3	L5	4353	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	3718	A2M	C4-N9-C1'	-2.62	120.49	126.63
3	L5	4431	PSU	O2-C2-N1	-2.62	120.08	122.79
3	L5	3920	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	2401	A2M	C1'-N9-C8	2.61	132.88	127.09
3	L5	4571	A2M	C4-N9-C1'	-2.61	120.53	126.63
3	L5	1860	PSU	C6-N1-C2	-2.61	120.27	122.69
83	S2	681	PSU	O2-C2-N1	-2.61	120.10	122.79
3	L5	1534	A2M	C1'-N9-C8	2.61	132.88	127.09
83	S2	93	PSU	C6-N1-C2	-2.60	120.28	122.69
83	S2	1056	PSU	O2-C2-N1	-2.60	120.11	122.79
83	S2	651	PSU	C6-N1-C2	-2.59	120.28	122.69
3	L5	1582	PSU	O2-C2-N1	-2.59	120.11	122.79
3	L5	3867	A2M	C4-N9-C1'	-2.59	120.57	126.63
3	L5	4299	PSU	C6-N1-C2	-2.58	120.30	122.69
3	L5	1534	A2M	O3'-C3'-C2'	2.58	118.41	111.19
3	L5	4296	PSU	O2-C2-N1	-2.58	120.13	122.79
83	S2	121	OMU	O4-C4-C5	-2.58	120.71	125.16
83	S2	576	A2M	C4-N9-C1'	-2.58	120.60	126.63
3	L5	4530	UR3	C6-N1-C2	-2.58	119.69	121.80
3	L5	2363	A2M	C4-N9-C1'	-2.57	120.61	126.63
3	L5	3844	PSU	O2-C2-N1	-2.57	120.14	122.79
3	L5	1781	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	3822	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	3867	A2M	O4'-C1'-C2'	2.57	111.01	106.59
83	S2	681	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	3825	A2M	C4-N9-C1'	-2.57	120.63	126.63
3	L5	3695	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	2787	A2M	O4'-C1'-C2'	2.56	111.00	106.59
3	L5	400	A2M	C1'-N9-C8	2.56	132.77	127.09
83	S2	109	PSU	C6-N1-C2	-2.56	120.32	122.69
5	L8	55	PSU	C6-N1-C2	-2.55	120.32	122.69
5	L8	69	PSU	C6-N1-C2	-2.55	120.33	122.69
3	L5	3830	A2M	C1'-N9-C8	2.55	132.75	127.09
83	S2	1046	PSU	C6-N1-C2	-2.54	120.33	122.69
5	L8	69	PSU	O2-C2-N1	-2.54	120.17	122.79
83	S2	686	PSU	O2-C2-N1	-2.54	120.17	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1244	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4361	PSU	O2-C2-N1	-2.53	120.18	122.79
3	L5	3785	A2M	C1'-N9-C8	2.52	132.70	127.09
83	S2	1639	G7M	CN7-N7-C8	-2.52	120.97	124.79
83	S2	1177	PSU	C6-N1-C2	-2.52	120.35	122.69
83	S2	863	PSU	C6-N1-C2	-2.52	120.36	122.69
3	L5	2787	A2M	C4-N9-C1'	-2.51	120.76	126.63
83	S2	1031	A2M	C1'-N9-C8	2.51	132.66	127.09
83	S2	866	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	1326	A2M	C4-N9-C1'	-2.50	120.80	126.63
83	S2	166	A2M	C1'-N9-C8	2.50	132.63	127.09
83	S2	1244	PSU	C6-C5-C4	2.50	119.86	118.17
83	S2	1367	PSU	C6-C5-C4	2.49	119.86	118.17
83	S2	1851	MA6	C1'-N9-C8	-2.49	121.57	127.09
3	L5	4500	PSU	C6-N1-C2	-2.49	120.38	122.69
83	S2	801	PSU	O2-C2-N1	-2.49	120.22	122.79
83	S2	105	PSU	O2-C2-N1	-2.49	120.22	122.79
3	L5	1534	A2M	C4-N9-C1'	-2.49	120.82	126.63
3	L5	5001	PSU	O2-C2-N1	-2.48	120.23	122.79
83	S2	1832	6MZ	C4-C5-N7	-2.48	107.74	110.58
3	L5	3825	A2M	C1'-N9-C8	2.47	132.58	127.09
3	L5	4493	PSU	C6-C5-C4	2.46	119.84	118.17
3	L5	4523	A2M	O3'-C3'-C2'	2.46	118.08	111.19
3	L5	4403	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L5	3920	PSU	O2-C2-N1	-2.45	120.26	122.79
83	S2	105	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L5	4571	A2M	C1'-N9-C8	2.45	132.53	127.09
3	L5	1860	PSU	O2-C2-N1	-2.45	120.27	122.79
3	L5	2632	PSU	C6-N1-C2	-2.44	120.42	122.69
3	L5	2363	A2M	C3'-C2'-C1'	-2.44	98.13	102.81
83	S2	966	PSU	C6-C5-C4	2.44	119.82	118.17
3	L5	4493	PSU	C6-N1-C2	-2.44	120.42	122.69
3	L5	2363	A2M	C1'-N9-C8	2.44	132.51	127.09
3	L5	4576	PSU	C6-N1-C2	-2.44	120.43	122.69
3	L5	4442	PSU	O4'-C1'-C2'	2.44	108.52	105.15
3	L5	4521	PSU	C6-N1-C2	-2.43	120.43	122.69
83	S2	576	A2M	C1'-N9-C8	2.43	132.49	127.09
83	S2	484	A2M	O4'-C4'-C3'	2.43	109.98	105.15
83	S2	668	A2M	C6-C5-C4	-2.43	113.86	117.18
83	S2	668	A2M	C4'-O4'-C1'	-2.43	104.11	109.47
83	S2	1639	G7M	N9-C8-N7	-2.43	106.59	112.48
83	S2	1232	PSU	C6-N1-C2	-2.42	120.44	122.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3867	A2M	C1'-N9-C8	2.42	132.47	127.09
83	S2	159	A2M	C2'-C1'-N9	2.42	117.73	113.75
3	L5	1326	A2M	C1'-N9-C8	2.42	132.46	127.09
83	S2	159	A2M	C3'-C2'-C1'	-2.41	98.20	102.81
3	L5	4296	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L5	2363	A2M	C2'-C1'-N9	2.39	117.69	113.75
3	L5	2815	A2M	C3'-C2'-C1'	-2.39	98.23	102.81
3	L5	1862	PSU	C6-N1-C2	-2.39	120.47	122.69
83	S2	1367	PSU	C6-N1-C2	-2.39	120.47	122.69
83	S2	966	PSU	C6-N1-C2	-2.39	120.47	122.69
83	S2	1056	PSU	C6-N1-C2	-2.39	120.48	122.69
3	L5	3867	A2M	C3'-C2'-C1'	-2.38	98.25	102.81
3	L5	4457	PSU	C6-N1-C2	-2.38	120.48	122.69
3	L5	4403	PSU	O4'-C1'-C2'	2.38	108.44	105.15
83	S2	814	PSU	C6-N1-C2	-2.38	120.48	122.69
3	L5	3701	OMC	C1'-N1-C6	-2.38	115.70	120.78
3	L5	4590	A2M	O4'-C1'-C2'	2.38	110.68	106.59
3	L5	1323	A2M	O4'-C1'-C2'	2.37	110.67	106.59
3	L5	1323	A2M	C2'-C1'-N9	2.37	117.66	113.75
3	L5	4403	PSU	C6-C5-C4	2.37	119.77	118.17
83	S2	484	A2M	O4'-C1'-C2'	2.36	110.66	106.59
3	L5	4220	6MZ	C5-C6-N1	2.36	120.69	118.15
3	L5	4456	OMC	C1'-N1-C2	2.36	123.66	118.44
3	L5	2787	A2M	C1'-N9-C8	2.35	132.31	127.09
3	L5	4590	A2M	C6-C5-C4	-2.34	113.98	117.18
3	L5	4361	PSU	C6-N1-C2	-2.34	120.52	122.69
83	S2	1045	PSU	C6-N1-C2	-2.34	120.52	122.69
83	S2	1248	B8N	C31-N3-C2	2.34	121.09	117.64
3	L5	3853	PSU	C6-N1-C2	-2.33	120.53	122.69
3	L5	2861	OMC	C1'-N1-C6	-2.33	115.81	120.78
3	L5	4523	A2M	O4'-C1'-C2'	2.32	110.58	106.59
3	L5	1862	PSU	C6-C5-C4	2.32	119.74	118.17
83	S2	1442	OMU	C1'-N1-C2	2.31	121.75	117.59
3	L5	4431	PSU	C6-N1-C2	-2.31	120.54	122.69
83	S2	686	PSU	C6-N1-C2	-2.31	120.55	122.69
3	L5	5001	PSU	C6-N1-C2	-2.30	120.55	122.69
3	L5	4227	OMU	O2-C2-N1	-2.30	119.80	122.80
83	S2	1383	A2M	C6-C5-C4	-2.29	114.06	117.18
3	L5	3822	PSU	O4'-C1'-C2'	2.28	108.31	105.15
3	L5	2401	A2M	O4'-C1'-C2'	2.27	110.49	106.59
3	L5	3785	A2M	O4'-C4'-C3'	2.26	109.65	105.15
3	L5	1326	A2M	O4'-C1'-C2'	2.26	110.48	106.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1326	A2M	C3'-C2'-C1'	-2.26	98.48	102.81
3	L5	4636	PSU	C6-N1-C2	-2.26	120.60	122.69
3	L5	3637	PSU	C6-C5-C4	2.25	119.69	118.17
3	L5	1524	A2M	C3'-C2'-C1'	-2.25	98.51	102.81
3	L5	2815	A2M	C4-N9-C1'	-2.24	121.39	126.63
83	S2	166	A2M	O4'-C1'-C2'	2.24	110.45	106.59
3	L5	2422	OMC	C1'-N1-C2	2.24	123.39	118.44
3	L5	2363	A2M	O4'-C1'-C2'	2.23	110.42	106.59
3	L5	4972	PSU	C6-N1-C2	-2.22	120.63	122.69
3	L5	3808	OMC	C1'-N1-C6	-2.22	116.04	120.78
3	L5	1871	A2M	C4'-O4'-C1'	-2.21	104.58	109.47
83	S2	99	A2M	C6-C5-C4	-2.21	114.16	117.18
3	L5	1524	A2M	C4-N9-C1'	-2.21	121.46	126.63
3	L5	1871	A2M	C6-C5-C4	-2.21	114.16	117.18
3	L5	3785	A2M	C2-N1-C6	-2.20	115.12	118.73
3	L5	1326	A2M	C2'-C1'-N9	2.19	117.36	113.75
83	S2	1248	B8N	O4-C4-C5	-2.19	118.79	122.58
3	L5	400	A2M	C2'-C1'-N9	2.19	117.36	113.75
3	L5	3825	A2M	O4'-C1'-C2'	2.19	110.36	106.59
3	L5	3782	5MC	C1'-N1-C6	-2.19	117.55	121.15
83	S2	166	A2M	C6-C5-C4	-2.19	114.19	117.18
83	S2	428	OMU	O2-C2-N1	-2.18	119.96	122.80
3	L5	1582	PSU	C6-N1-C2	-2.18	120.67	122.69
3	L5	1323	A2M	C6-C5-C4	-2.18	114.20	117.18
3	L5	400	A2M	O4'-C1'-C2'	2.18	110.34	106.59
83	S2	1326	OMU	O2-C2-N1	-2.17	119.97	122.80
3	L5	1677	PSU	C6-N1-C2	-2.17	120.68	122.69
3	L5	2787	A2M	C6-C5-C4	-2.17	114.21	117.18
3	L5	2401	A2M	C6-C5-C4	-2.17	114.22	117.18
3	L5	2351	OMC	C1'-N1-C2	2.17	123.23	118.44
3	L5	1524	A2M	C1'-N9-C8	2.17	131.91	127.09
83	S2	116	OMU	O2-C2-N1	-2.17	119.97	122.80
3	L5	4457	PSU	C6-C5-C4	2.16	119.63	118.17
3	L5	400	A2M	C6-C5-C4	-2.16	114.22	117.18
3	L5	3867	A2M	C2-N1-C6	-2.16	115.18	118.73
3	L5	3718	A2M	C2-N1-C6	-2.16	115.19	118.73
3	L5	1322	1MA	N1-C6-N6	2.15	125.11	119.71
3	L5	1534	A2M	C2'-C1'-N9	2.15	117.28	113.75
83	S2	686	PSU	C6-C5-C4	2.14	119.62	118.17
83	S2	1248	B8N	O4'-C1'-C2'	2.14	108.11	105.15
3	L5	2815	A2M	C1'-N9-C8	2.14	131.85	127.09
3	L5	2815	A2M	C2-N1-C6	-2.14	115.21	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	C3'-C2'-C1'	-2.14	98.71	102.81
3	L5	4498	OMU	O2-C2-N1	-2.14	120.01	122.80
83	S2	27	A2M	C6-C5-C4	-2.14	114.26	117.18
83	S2	1832	6MZ	C5-C6-N1	2.13	120.44	118.15
3	L5	4571	A2M	C6-C5-C4	-2.13	114.27	117.18
3	L5	4521	PSU	C6-C5-C4	2.13	119.61	118.17
3	L5	3867	A2M	C6-C5-C4	-2.13	114.27	117.18
83	S2	1031	A2M	O4'-C1'-C2'	2.13	110.25	106.59
3	L5	4523	A2M	C6-C5-C4	-2.12	114.29	117.18
5	L8	69	PSU	O4'-C1'-C2'	2.11	108.07	105.15
3	L5	3785	A2M	C5-C6-N1	2.11	122.87	117.51
3	L5	4220	6MZ	C3'-C2'-C1'	2.11	105.45	101.46
3	L5	3785	A2M	C3'-C2'-C1'	-2.10	98.78	102.81
3	L5	4636	PSU	O4'-C1'-C2'	2.10	108.06	105.15
83	S2	1031	A2M	C5-C6-N1	2.10	122.84	117.51
3	L5	400	A2M	C5-C6-N1	2.10	122.83	117.51
3	L5	4576	PSU	O4'-C1'-C2'	2.10	108.05	105.15
83	S2	576	A2M	C6-C5-C4	-2.10	114.32	117.18
3	L5	1326	A2M	C6-C5-C4	-2.09	114.32	117.18
3	L5	3830	A2M	C6-C5-C4	-2.09	114.32	117.18
83	S2	1337	4AC	C5-C4-N4	-2.09	119.42	122.94
3	L5	4293	PSU	C6-N1-C2	-2.09	120.76	122.69
3	L5	4296	PSU	C6-C5-C4	2.09	119.58	118.17
3	L5	3785	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	3851	PSU	C6-N1-C2	-2.08	120.76	122.69
83	S2	1031	A2M	C2-N1-C6	-2.08	115.31	118.73
83	S2	166	A2M	C5-C6-N1	2.08	122.79	117.51
83	S2	468	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	2787	A2M	O4'-C4'-C3'	2.08	109.28	105.15
3	L5	4571	A2M	C5-C6-N1	2.08	122.78	117.51
83	S2	484	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	3851	PSU	O4'-C1'-C2'	2.07	108.02	105.15
3	L5	2837	OMU	O2-C2-N1	-2.07	120.10	122.80
3	L5	3825	A2M	C2-N1-C6	-2.07	115.33	118.73
3	L5	1534	A2M	C2-N1-C6	-2.07	115.33	118.73
3	L5	3825	A2M	C6-C5-C4	-2.07	114.36	117.18
3	L5	2401	A2M	C5-C6-N1	2.06	122.75	117.51
3	L5	3830	A2M	C5-C6-N1	2.06	122.75	117.51
83	S2	99	A2M	C5-C6-N1	2.06	122.75	117.51
3	L5	4293	PSU	C6-C5-C4	2.06	119.56	118.17
83	S2	668	A2M	C2'-C1'-N9	2.06	117.14	113.75
83	S2	99	A2M	O4'-C1'-C2'	2.06	110.13	106.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	576	A2M	C5-C6-N1	2.06	122.73	117.51
3	L5	398	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	1524	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	2632	PSU	C6-C5-C4	2.05	119.56	118.17
3	L5	2363	A2M	C6-C5-C4	-2.05	114.38	117.18
3	L5	398	A2M	C6-C5-C4	-2.05	114.38	117.18
3	L5	2787	A2M	C5-C6-N1	2.05	122.71	117.51
3	L5	3825	A2M	C2'-C1'-N9	2.05	117.12	113.75
83	S2	406	PSU	C6-C5-C4	2.04	119.55	118.17
3	L5	3867	A2M	C5-C6-N1	2.04	122.69	117.51
3	L5	2401	A2M	C2-N1-C6	-2.04	115.38	118.73
83	S2	159	A2M	C2-N1-C6	-2.04	115.38	118.73
83	S2	484	A2M	C5-C6-N1	2.04	122.68	117.51
3	L5	3853	PSU	C6-C5-C4	2.04	119.55	118.17
83	S2	1248	B8N	O36-C34-O35	-2.04	119.46	124.08
3	L5	4523	A2M	C2-N1-C6	-2.04	115.39	118.73
3	L5	3822	PSU	C6-C5-C4	2.03	119.55	118.17
83	S2	1081	PSU	C6-C5-C4	2.03	119.54	118.17
3	L5	1534	A2M	C5-C6-N1	2.02	122.65	117.51
3	L5	3851	PSU	C6-C5-C4	2.02	119.54	118.17
3	L5	4457	PSU	O4'-C1'-C2'	2.02	107.95	105.15
83	S2	1851	MA6	C4-C5-N7	-2.02	108.27	110.58
3	L5	398	A2M	C5-C6-N1	2.02	122.65	117.51
3	L5	1323	A2M	C2-N1-C6	-2.02	115.41	118.73
83	S2	1367	PSU	O4'-C1'-C2'	2.02	107.94	105.15
3	L5	1323	A2M	C5-C6-N1	2.02	122.64	117.51
83	S2	99	A2M	C2-N1-C6	-2.02	115.41	118.73
3	L5	1326	A2M	C5-C6-N1	2.02	122.64	117.51
83	S2	174	OMC	C1'-N1-C2	2.02	122.90	118.44
3	L5	400	A2M	C2-N1-C6	-2.02	115.42	118.73
83	S2	172	OMU	O2-C2-N1	-2.01	120.17	122.80
3	L5	2363	A2M	C2-N1-C6	-2.01	115.42	118.73
3	L5	2815	A2M	O4'-C1'-C2'	2.01	110.05	106.59
3	L5	4220	6MZ	C4'-O4'-C1'	-2.01	105.02	109.47
83	S2	468	A2M	C5-C6-N1	2.01	122.62	117.51
3	L5	2815	A2M	C5-C6-N1	2.01	122.61	117.51
83	S2	159	A2M	O4'-C1'-C2'	2.01	110.05	106.59
3	L5	4571	A2M	C2-N1-C6	-2.01	115.43	118.73
3	L5	4500	PSU	O4'-C1'-C2'	2.00	107.92	105.15
3	L5	3785	A2M	C4'-O4'-C1'	-2.00	105.04	109.47
83	S2	1703	OMC	C1'-N1-C2	2.00	122.87	118.44
83	S2	166	A2M	C2-N1-C6	-2.00	115.44	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1045	PSU	C6-C5-C4	2.00	119.53	118.17

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1316	OMG	C1'-C2'-O2'-CM2
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2422	OMC	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	2824	OMC	C1'-C2'-O2'-CM2
3	L5	2876	OMG	O4'-C4'-C5'-O5'
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	3808	OMC	C1'-C2'-O2'-CM2
3	L5	3830	A2M	C1'-C2'-O2'-CM'
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4220	6MZ	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C1'-C2'-O2'-CM'
3	L5	4623	OMG	C1'-C2'-O2'-CM2
3	L5	4637	OMG	O4'-C4'-C5'-O5'
3	L5	4637	OMG	C1'-C2'-O2'-CM2
83	S2	27	A2M	C1'-C2'-O2'-CM'
83	S2	99	A2M	C1'-C2'-O2'-CM'
83	S2	116	OMU	C1'-C2'-O2'-CM2
83	S2	159	A2M	C1'-C2'-O2'-CM'
83	S2	462	OMC	C1'-C2'-O2'-CM2
83	S2	601	OMG	C1'-C2'-O2'-CM2
83	S2	644	OMG	O4'-C4'-C5'-O5'
83	S2	801	PSU	C3'-C4'-C5'-O5'
83	S2	1031	A2M	C1'-C2'-O2'-CM'
83	S2	1248	B8N	O4'-C4'-C5'-O5'
83	S2	1248	B8N	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
83	S2	1272	OMC	C3'-C4'-C5'-O5'
83	S2	1272	OMC	O4'-C4'-C5'-O5'
83	S2	1288	OMU	C3'-C4'-C5'-O5'
83	S2	1288	OMU	O4'-C4'-C5'-O5'
83	S2	1337	4AC	N3-C4-N4-C7
83	S2	1383	A2M	C1'-C2'-O2'-CM'
83	S2	1832	6MZ	C5-C6-N6-C9
83	S2	1832	6MZ	N1-C6-N6-C9
83	S2	1832	6MZ	C5'-O5'-P-O1P
83	S2	1832	6MZ	C5'-O5'-P-O3P
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	2876	OMG	C3'-C4'-C5'-O5'
3	L5	4306	OMU	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	O4'-C4'-C5'-O5'
83	S2	517	OMC	C3'-C4'-C5'-O5'
83	S2	576	A2M	O4'-C4'-C5'-O5'
83	S2	799	OMU	C3'-C4'-C5'-O5'
83	S2	799	OMU	O4'-C4'-C5'-O5'
83	S2	867	OMG	C3'-C4'-C5'-O5'
83	S2	1046	PSU	O4'-C4'-C5'-O5'
83	S2	1326	OMU	C3'-C4'-C5'-O5'
83	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	1536	PSU	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
83	S2	517	OMC	O4'-C4'-C5'-O5'
83	S2	576	A2M	C3'-C4'-C5'-O5'
83	S2	801	PSU	O4'-C4'-C5'-O5'
83	S2	1045	PSU	O4'-C4'-C5'-O5'
83	S2	1326	OMU	O4'-C4'-C5'-O5'
83	S2	1442	OMU	C3'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'
3	L5	4220	6MZ	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
83	S2	644	OMG	C3'-C4'-C5'-O5'
83	S2	668	A2M	C3'-C4'-C5'-O5'
83	S2	1248	B8N	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
83	S2	428	OMU	C2'-C1'-N1-C6
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	2632	PSU	C3'-C4'-C5'-O5'
83	S2	668	A2M	O4'-C4'-C5'-O5'
83	S2	867	OMG	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	1677	PSU	O4'-C4'-C5'-O5'
3	L5	2632	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
3	L5	3830	A2M	O4'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
3	L5	4306	OMU	O4'-C4'-C5'-O5'
3	L5	1677	PSU	C3'-C4'-C5'-O5'
3	L5	4571	A2M	O4'-C4'-C5'-O5'
83	S2	1045	PSU	C3'-C4'-C5'-O5'
83	S2	1046	PSU	C3'-C4'-C5'-O5'
83	S2	1383	A2M	O4'-C4'-C5'-O5'
3	L5	1323	A2M	C3'-C4'-C5'-O5'
3	L5	3830	A2M	C3'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
83	S2	627	OMU	C2'-C1'-N1-C6
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	1792	PSU	O4'-C4'-C5'-O5'
83	S2	1383	A2M	C3'-C4'-C5'-O5'
83	S2	1248	B8N	N34-C33-C34-O35
3	L5	4571	A2M	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	3825	A2M	C1'-C2'-O2'-CM'
3	L5	3841	OMC	C1'-C2'-O2'-CM2
83	S2	468	A2M	C1'-C2'-O2'-CM'
83	S2	1391	OMC	C1'-C2'-O2'-CM2
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
83	S2	1248	B8N	C31-C32-C33-N34
83	S2	428	OMU	O4'-C1'-N1-C6
83	S2	428	OMU	C2'-C1'-N1-C2
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	1582	PSU	C3'-C4'-C5'-O5'
83	S2	1244	PSU	O4'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
83	S2	1832	6MZ	C5'-O5'-P-O2P
3	L5	1534	A2M	C4'-C5'-O5'-P
83	S2	428	OMU	O4'-C4'-C5'-O5'
83	S2	428	OMU	O4'-C1'-N1-C2
83	S2	627	OMU	O4'-C1'-N1-C6
83	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	4636	PSU	O4'-C1'-C5-C4
83	S2	651	PSU	O4'-C1'-C5-C4
83	S2	1248	B8N	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	1625	OMG	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	3785	A2M	C3'-C2'-O2'-CM'
3	L5	4499	OMG	C3'-C2'-O2'-CM2
3	L5	3887	OMC	C4'-C5'-O5'-P
83	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	3869	OMC	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	1322	1MA	C2'-C1'-N9-C4
83	S2	576	A2M	C4'-C5'-O5'-P
83	S2	644	OMG	C4'-C5'-O5'-P
3	L5	3818	UY1	C3'-C4'-C5'-O5'
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	3744	OMG	C1'-C2'-O2'-CM2
83	S2	1328	OMG	C1'-C2'-O2'-CM2
83	S2	1081	PSU	C4'-C5'-O5'-P
83	S2	428	OMU	C3'-C4'-C5'-O5'
83	S2	1248	B8N	N34-C33-C34-O36
83	S2	1248	B8N	O4'-C1'-C5-C6
83	S2	627	OMU	C2'-C1'-N1-C2
3	L5	3869	OMC	C3'-C2'-O2'-CM2
83	S2	627	OMU	O4'-C1'-N1-C2
3	L5	4530	UR3	C3'-C4'-C5'-O5'
3	L5	1524	A2M	O4'-C1'-N9-C8
3	L5	1582	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	1792	PSU	C3'-C4'-C5'-O5'
83	S2	627	OMU	C4'-C5'-O5'-P
83	S2	1832	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

94 monomers are involved in 162 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	S2	462	OMC	4	0
5	L8	55	PSU	2	0
3	L5	4392	OMG	1	0
3	L5	4220	6MZ	2	0
3	L5	400	A2M	2	0
83	S2	1639	G7M	1	0
3	L5	1323	A2M	2	0
3	L5	4637	OMG	2	0
3	L5	4571	A2M	2	0
3	L5	2824	OMC	1	0
3	L5	4312	PSU	1	0
3	L5	2363	A2M	1	0
3	L5	1677	PSU	2	0
3	L5	4523	A2M	4	0
3	L5	1871	A2M	1	0
83	S2	406	PSU	2	0
3	L5	1534	A2M	3	0
3	L5	3867	A2M	3	0
83	S2	1850	MA6	2	0
3	L5	4618	OMG	1	0
83	S2	99	A2M	2	0
3	L5	4590	A2M	1	0
3	L5	4576	PSU	1	0
3	L5	4306	OMU	1	0
5	L8	75	OMG	2	0
3	L5	4628	PSU	2	0
3	L5	5010	PSU	2	0
83	S2	668	A2M	1	0
83	S2	1288	OMU	1	0
3	L5	4689	PSU	1	0
3	L5	4471	PSU	1	0
83	S2	174	OMC	1	0
3	L5	3869	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	S2	1272	OMC	1	0
83	S2	1004	PSU	1	0
83	S2	354	OMU	1	0
83	S2	1177	PSU	1	0
83	S2	683	OMG	1	0
3	L5	1340	OMC	3	0
3	L5	3825	A2M	1	0
83	S2	468	A2M	2	0
3	L5	2632	PSU	1	0
3	L5	4579	PSU	2	0
83	S2	1244	PSU	2	0
83	S2	121	OMU	4	0
83	S2	814	PSU	1	0
3	L5	4447	5MC	1	0
83	S2	27	A2M	2	0
83	S2	166	A2M	1	0
3	L5	4530	UR3	1	0
83	S2	1842	4AC	1	0
3	L5	4673	PSU	1	0
3	L5	3884	PSU	1	0
83	S2	601	OMG	2	0
3	L5	4227	OMU	1	0
3	L5	1316	OMG	2	0
3	L5	3785	A2M	2	0
3	L5	3925	OMU	2	0
3	L5	2876	OMG	2	0
3	L5	4442	PSU	1	0
83	S2	1031	A2M	2	0
3	L5	3744	OMG	1	0
3	L5	4403	PSU	1	0
3	L5	2804	OMC	2	0
3	L5	3844	PSU	1	0
83	S2	681	PSU	2	0
5	L8	69	PSU	1	0
83	S2	1337	4AC	4	0
83	S2	1174	PSU	3	0
3	L5	3830	A2M	1	0
83	S2	116	OMU	4	0
3	L5	398	A2M	2	0
83	S2	484	A2M	2	0
3	L5	4623	OMG	1	0
83	S2	651	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4620	OMU	1	0
83	S2	1391	OMC	2	0
3	L5	3920	PSU	1	0
83	S2	1081	PSU	1	0
3	L5	4552	PSU	1	0
83	S2	1383	A2M	2	0
83	S2	159	A2M	6	0
3	L5	3718	A2M	6	0
3	L5	2422	OMC	1	0
3	L5	1524	A2M	2	0
3	L5	1326	A2M	2	0
3	L5	4370	OMG	1	0
3	L5	2351	OMC	2	0
83	S2	509	OMG	3	0
83	S2	649	PSU	2	0
3	L5	2401	A2M	1	0
3	L5	4456	OMC	1	0
3	L5	1683	PSU	2	0
3	L5	3841	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 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	$\# Z > 2$
86	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	0.94	0
86	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.75	0
85	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	1.05	0
86	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	0.96	0
85	SPM	L5	5263	-	13,13,13	0.33	0	12,12,12	0.92	0
86	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.85	0
85	SPM	L5	5291	-	13,13,13	0.36	0	12,12,12	0.88	0
85	SPM	L5	5287	-	13,13,13	0.35	0	12,12,12	0.96	0
85	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.78	0
86	SPD	L5	5288	-	9,9,9	0.35	0	8,8,8	0.93	0
86	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.83	0
86	SPD	LN	301	-	9,9,9	0.34	0	8,8,8	0.84	0
85	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	0.94	0
86	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.85	0
86	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.85	0
86	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.82	0

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
86	SPD	L5	5261	-	-	4/7/7/7	-
86	SPD	L5	5289	-	-	4/7/7/7	-
85	SPM	L5	5267	-	-	4/11/11/11	-
86	SPD	L5	5282	-	-	1/7/7/7	-
85	SPM	L5	5264	-	-	1/11/11/11	-
85	SPM	L5	5263	-	-	6/11/11/11	-
86	SPD	L5	5286	-	-	2/7/7/7	-
85	SPM	L5	5291	-	-	3/11/11/11	-
85	SPM	L5	5287	-	-	5/11/11/11	-
85	SPM	L5	5290	-	-	6/11/11/11	-
86	SPD	L5	5288	-	-	5/7/7/7	-
86	SPD	L5	5285	-	-	1/7/7/7	-
86	SPD	LN	301	-	-	2/7/7/7	-
85	SPM	L5	5259	-	-	3/11/11/11	-
86	SPD	L5	5284	-	-	1/7/7/7	-
86	SPD	L5	5283	-	-	1/7/7/7	-
86	SPD	L8	202	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L5	5290	SPM	N10-C11-C12-C13
85	L5	5267	SPM	C2-C3-C4-N5
86	L8	202	SPD	C3-C4-C5-N6
86	L5	5261	SPD	C3-C4-C5-N6
86	L5	5288	SPD	C3-C4-C5-N6
85	L5	5287	SPM	N10-C11-C12-C13
85	L5	5290	SPM	C2-C3-C4-N5
86	L5	5261	SPD	N6-C7-C8-C9
85	L5	5267	SPM	C7-C6-N5-C4
86	L5	5288	SPD	C8-C7-N6-C5
86	L5	5289	SPD	C4-C5-N6-C7
86	L5	5289	SPD	C8-C7-N6-C5
86	L5	5286	SPD	N6-C7-C8-C9
86	L5	5288	SPD	C4-C5-N6-C7
86	L5	5286	SPD	C8-C7-N6-C5
86	L5	5288	SPD	N6-C7-C8-C9
86	LN	301	SPD	C2-C3-C4-C5
85	L5	5290	SPM	C6-C7-C8-C9
85	L5	5263	SPM	C2-C3-C4-N5
85	L5	5259	SPM	C6-C7-C8-C9
86	L5	5282	SPD	C2-C3-C4-C5
85	L5	5263	SPM	C6-C7-C8-C9
86	L8	202	SPD	C2-C3-C4-C5
85	L5	5259	SPM	N5-C6-C7-C8
85	L5	5287	SPM	C6-C7-C8-C9
85	L5	5263	SPM	C11-C12-C13-N14
86	L5	5261	SPD	C7-C8-C9-N10
85	L5	5287	SPM	C3-C4-N5-C6
85	L5	5291	SPM	C7-C6-N5-C4
86	L5	5261	SPD	C4-C5-N6-C7
85	L5	5290	SPM	N5-C6-C7-C8
86	L5	5283	SPD	C3-C4-C5-N6
85	L5	5259	SPM	C2-C3-C4-N5
85	L5	5263	SPM	N1-C2-C3-C4
85	L5	5287	SPM	N1-C2-C3-C4
85	L5	5290	SPM	C8-C9-N10-C11
86	L5	5285	SPD	C7-C8-C9-N10
86	L5	5289	SPD	C7-C8-C9-N10
86	L5	5284	SPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

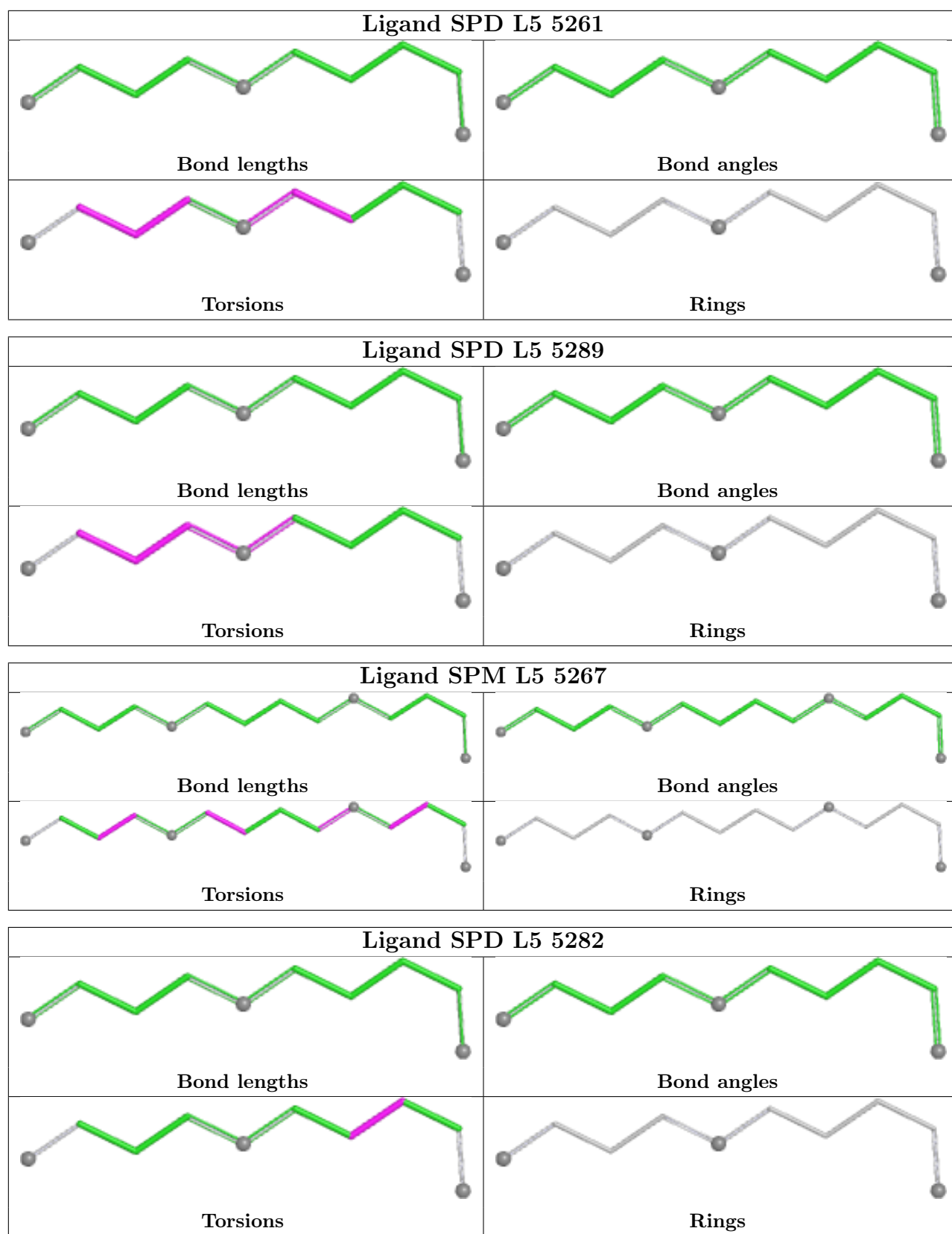
Mol	Chain	Res	Type	Atoms
85	L5	5287	SPM	C2-C3-C4-N5
85	L5	5291	SPM	N10-C11-C12-C13
86	L5	5289	SPD	N6-C7-C8-C9
85	L5	5263	SPM	C3-C4-N5-C6
86	LN	301	SPD	C8-C7-N6-C5
85	L5	5291	SPM	C2-C3-C4-N5
85	L5	5290	SPM	C3-C4-N5-C6
85	L5	5263	SPM	C8-C9-N10-C11
85	L5	5267	SPM	N10-C11-C12-C13
85	L5	5264	SPM	C11-C12-C13-N14
86	L5	5288	SPD	N1-C2-C3-C4
85	L5	5267	SPM	C7-C8-C9-N10

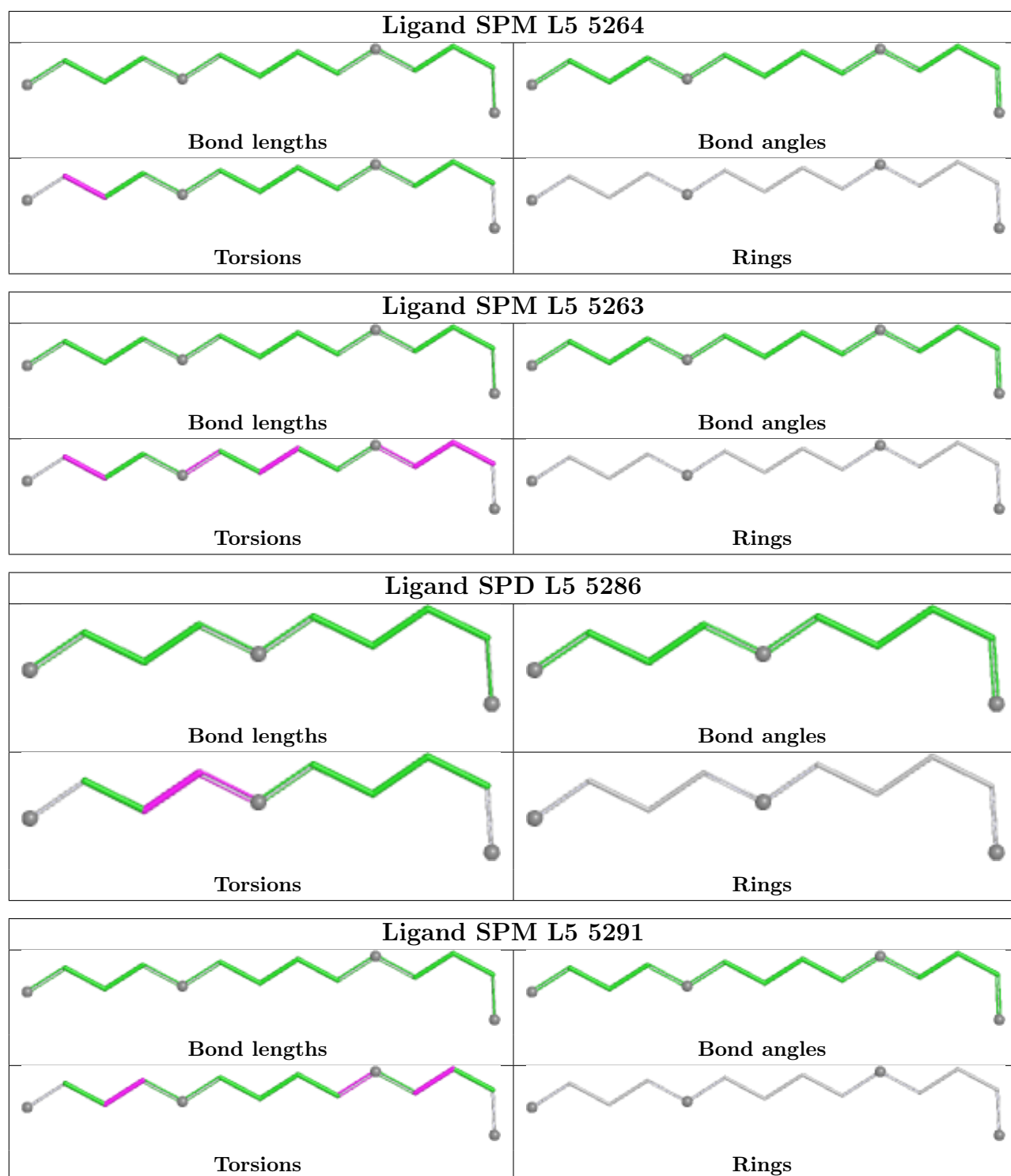
There are no ring outliers.

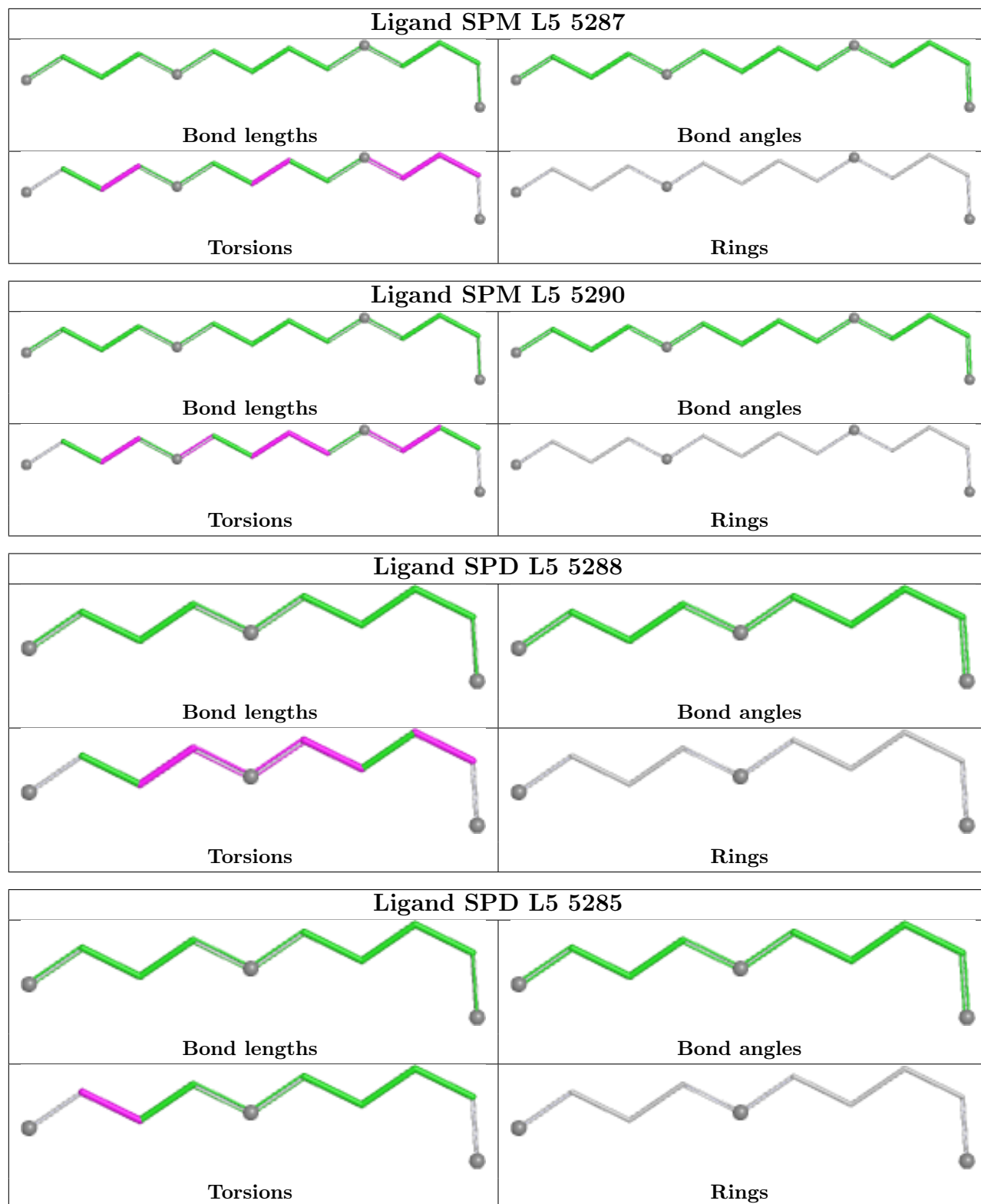
4 monomers are involved in 9 short contacts:

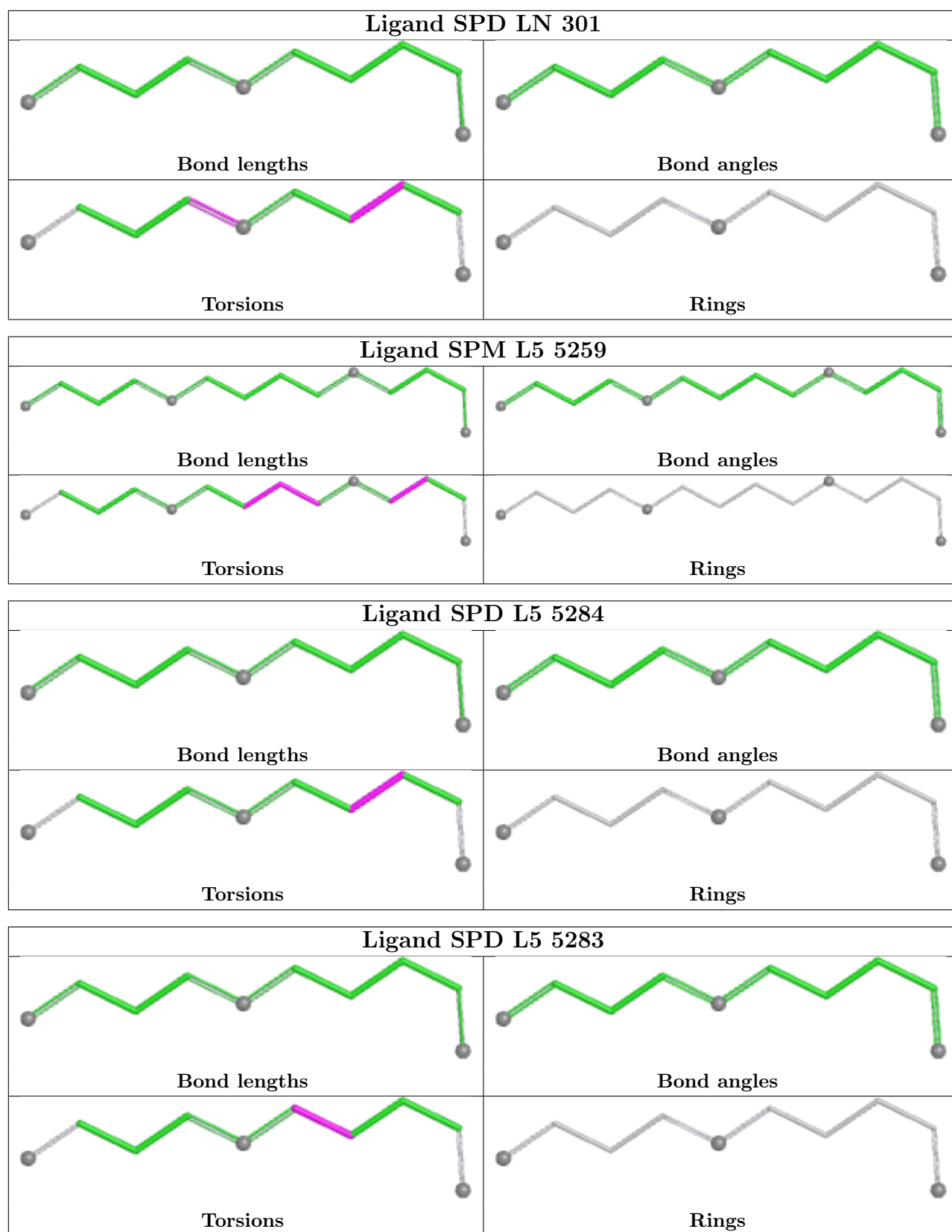
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5289	SPD	1	0
85	L5	5263	SPM	2	0
85	L5	5291	SPM	5	0
86	L5	5288	SPD	1	0

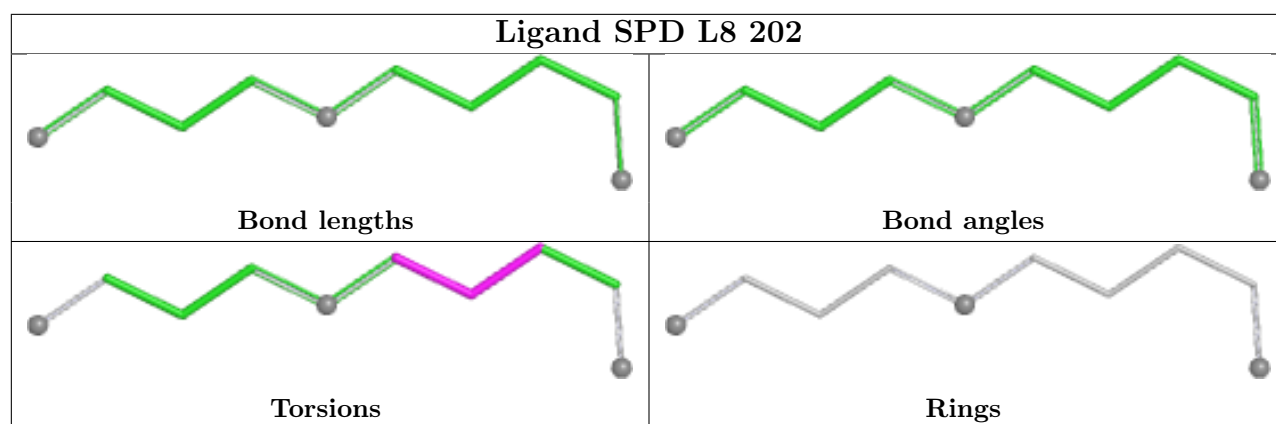
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L5	10
83	S2	5
2	Pt	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.90
1	L5	1706:A	O3'	1716:G	P	21.53
1	L5	2910:G	O3'	3584:C	P	21.03
1	L5	760:G	O3'	903:C	P	17.11
1	L5	2112:G	O3'	2249:C	P	15.56
1	L5	519:C	O3'	642:G	P	15.45
1	L5	4776:G	O3'	4858:C	P	14.45
1	L5	3954:A	O3'	4056:A	P	14.38
1	S2	698:G	O3'	730:C	P	14.05
1	S2	739:C	O3'	746:C	P	13.08
1	L5	990:C	O3'	1064:G	P	12.83
1	L5	1222:A	O3'	1234:G	P	10.44
1	Pt	15:G	O3'	18:G	P	9.76
1	S2	225:G	O3'	287:U	P	7.89
1	L5	1100:U	O3'	1167:C	P	7.20
1	S2	1831:A	O3'	1832:6MZ	P	4.49

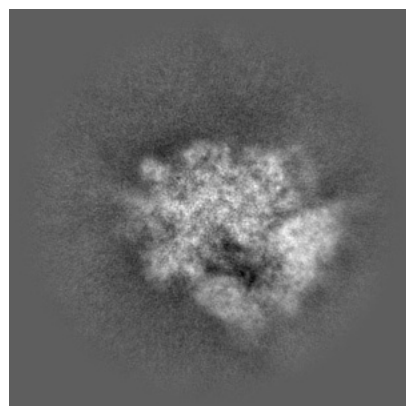
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71696. These allow visual inspection of the internal detail of the map and identification of artifacts.

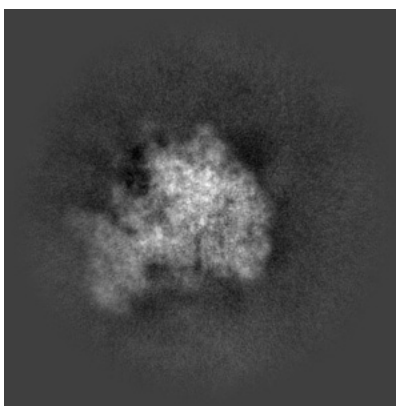
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

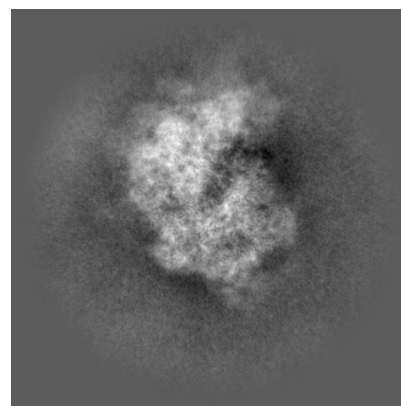
6.1.1 Primary map



X

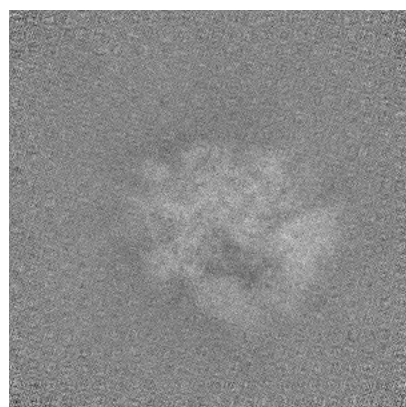


Y

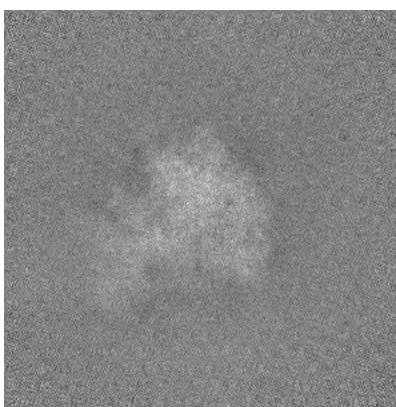


Z

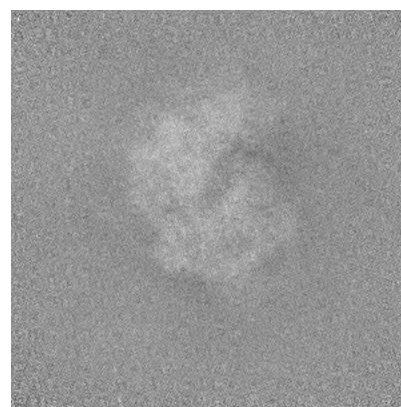
6.1.2 Raw map



X



Y

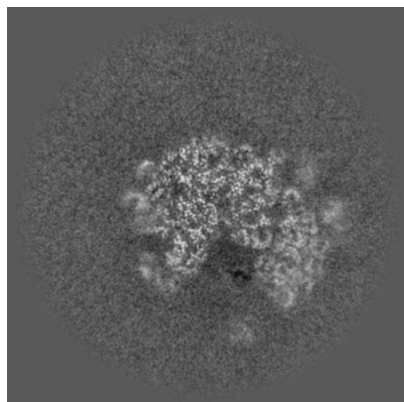


Z

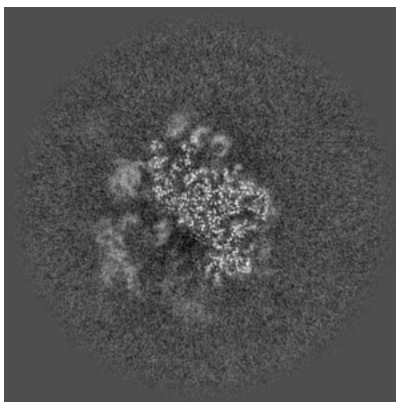
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

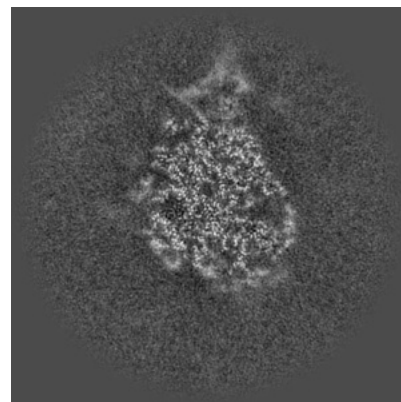
6.2.1 Primary map



X Index: 288

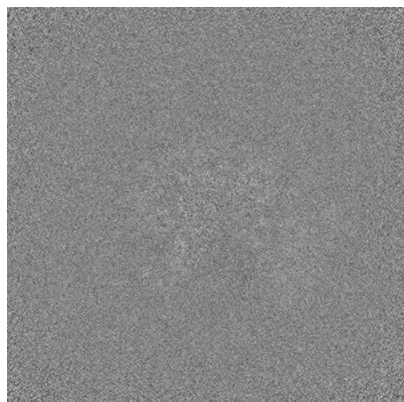


Y Index: 288

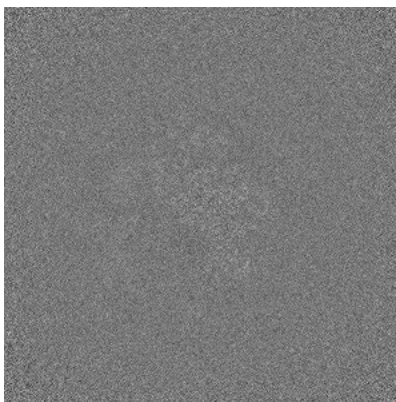


Z Index: 288

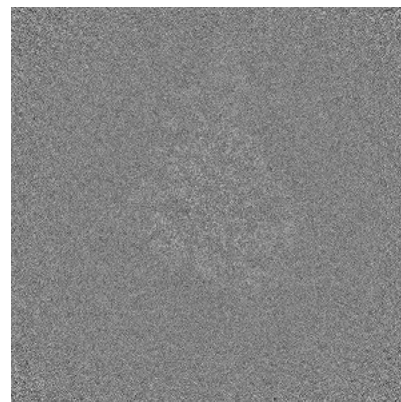
6.2.2 Raw map



X Index: 288



Y Index: 288

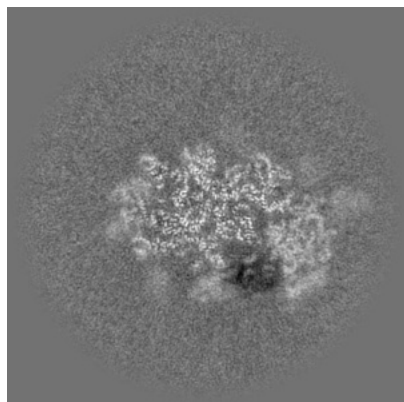


Z Index: 288

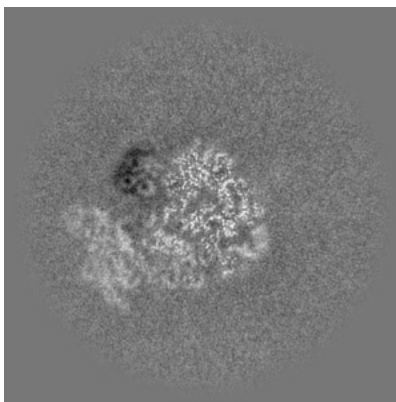
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

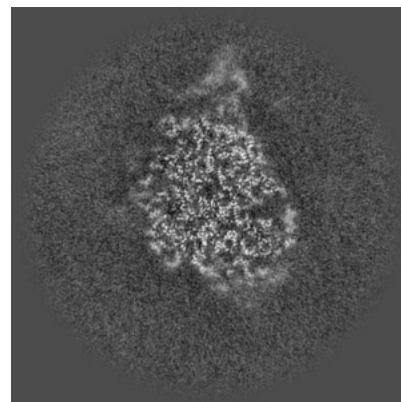
6.3.1 Primary map



X Index: 314

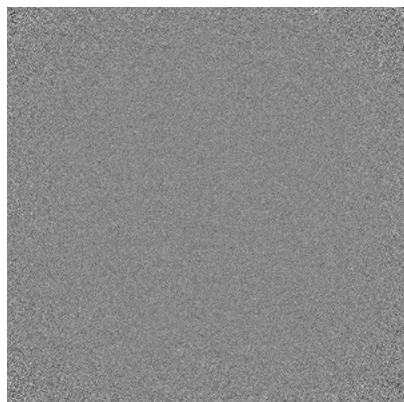


Y Index: 352

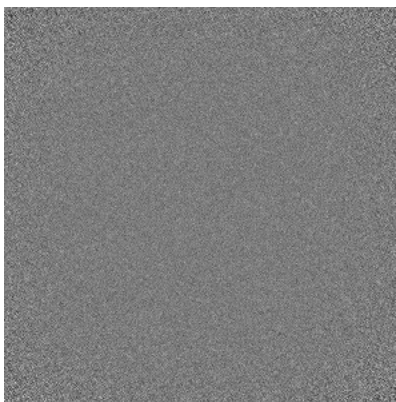


Z Index: 291

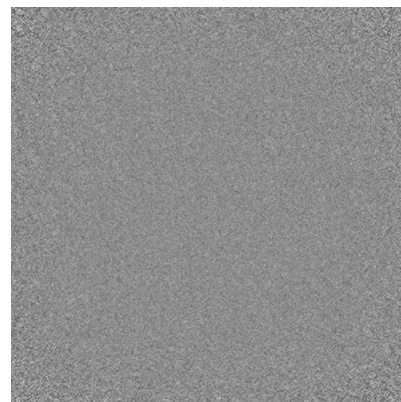
6.3.2 Raw map



X Index: 0



Y Index: 0

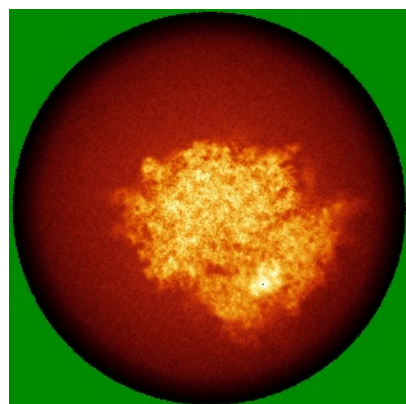


Z Index: 0

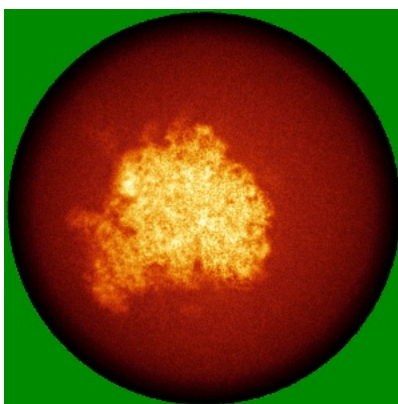
The images above show the largest variance slices of the map in three orthogonal directions.

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

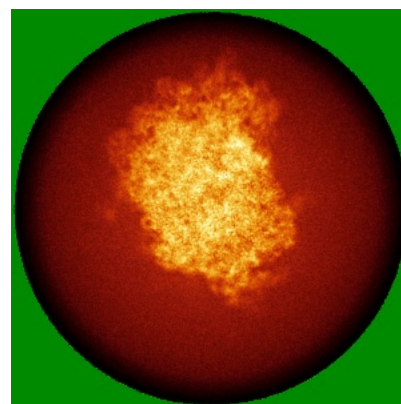
6.4.1 Primary map



X

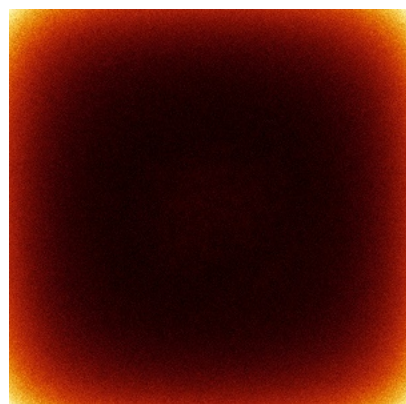


Y

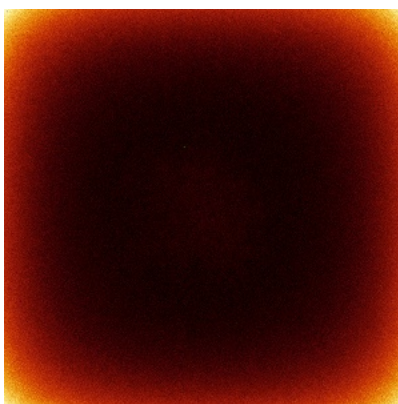


Z

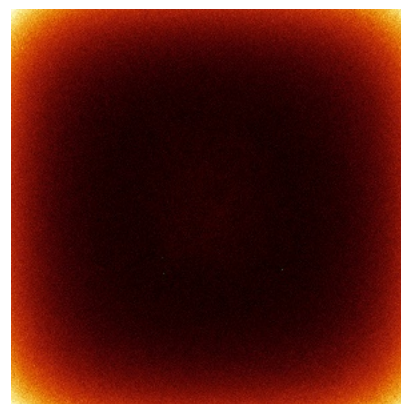
6.4.2 Raw map



X



Y

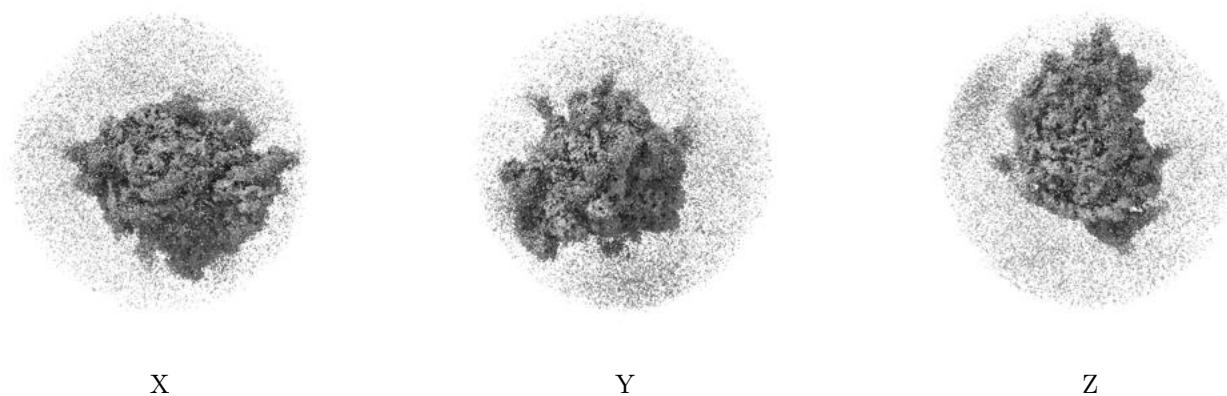


Z

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

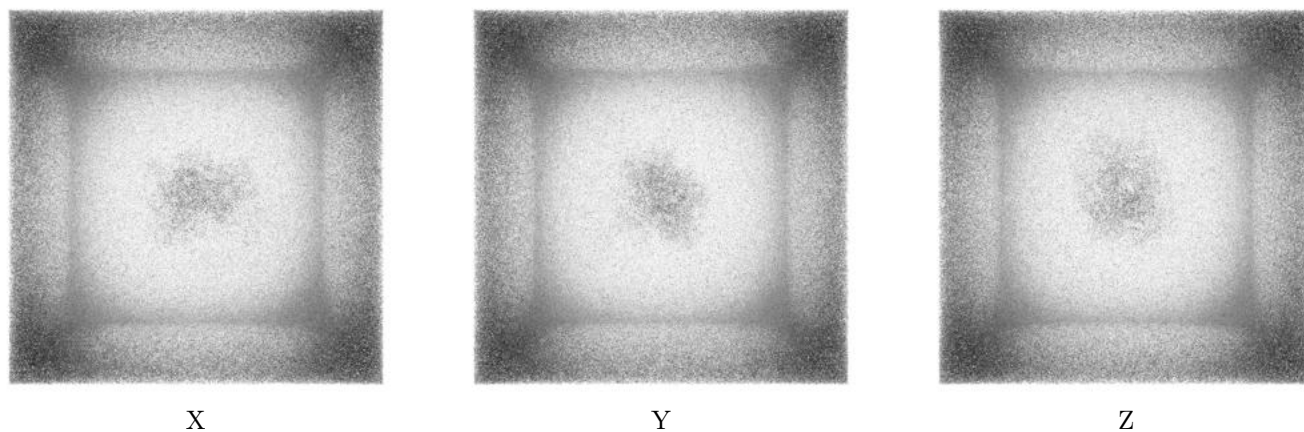
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0108. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

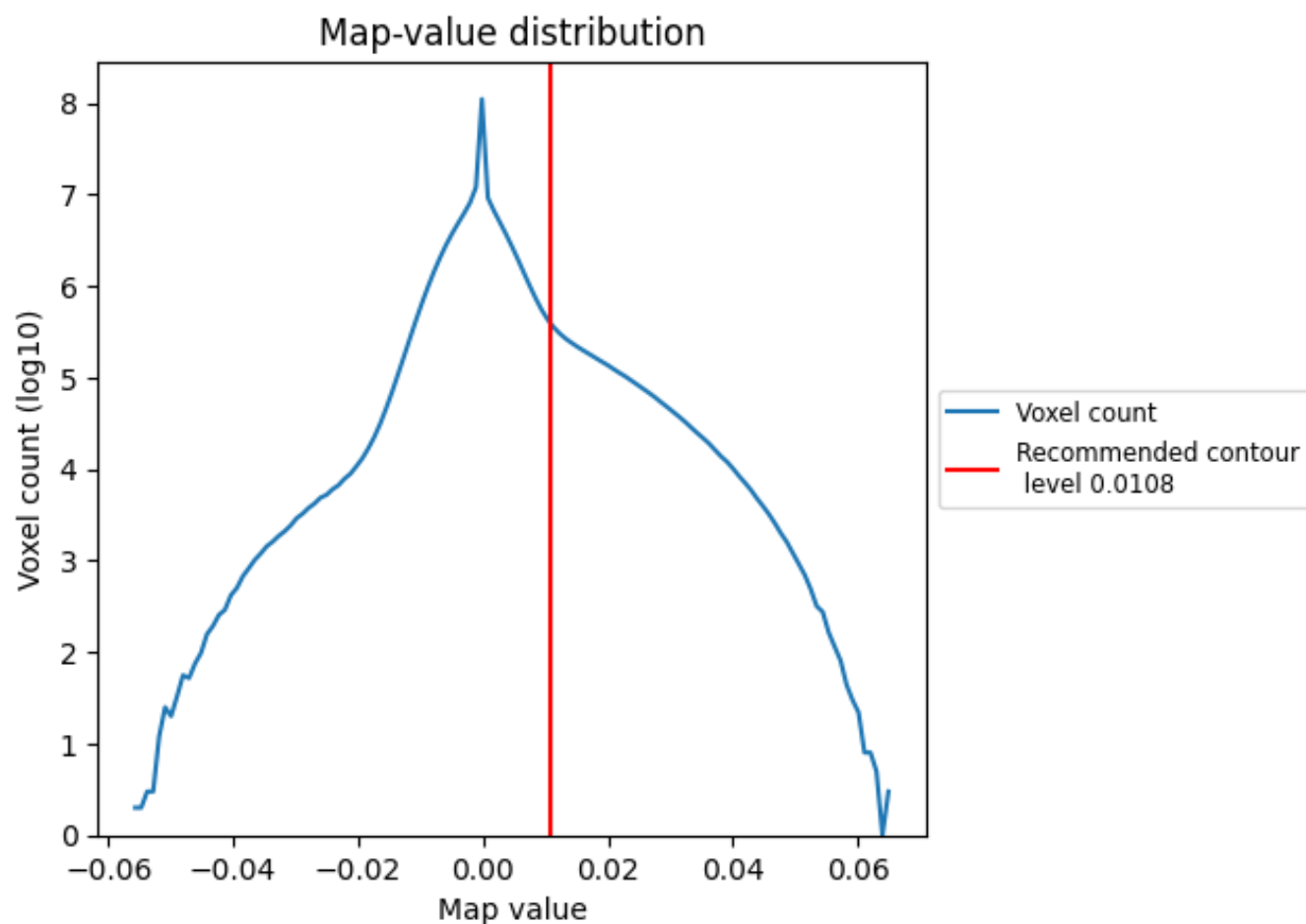
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

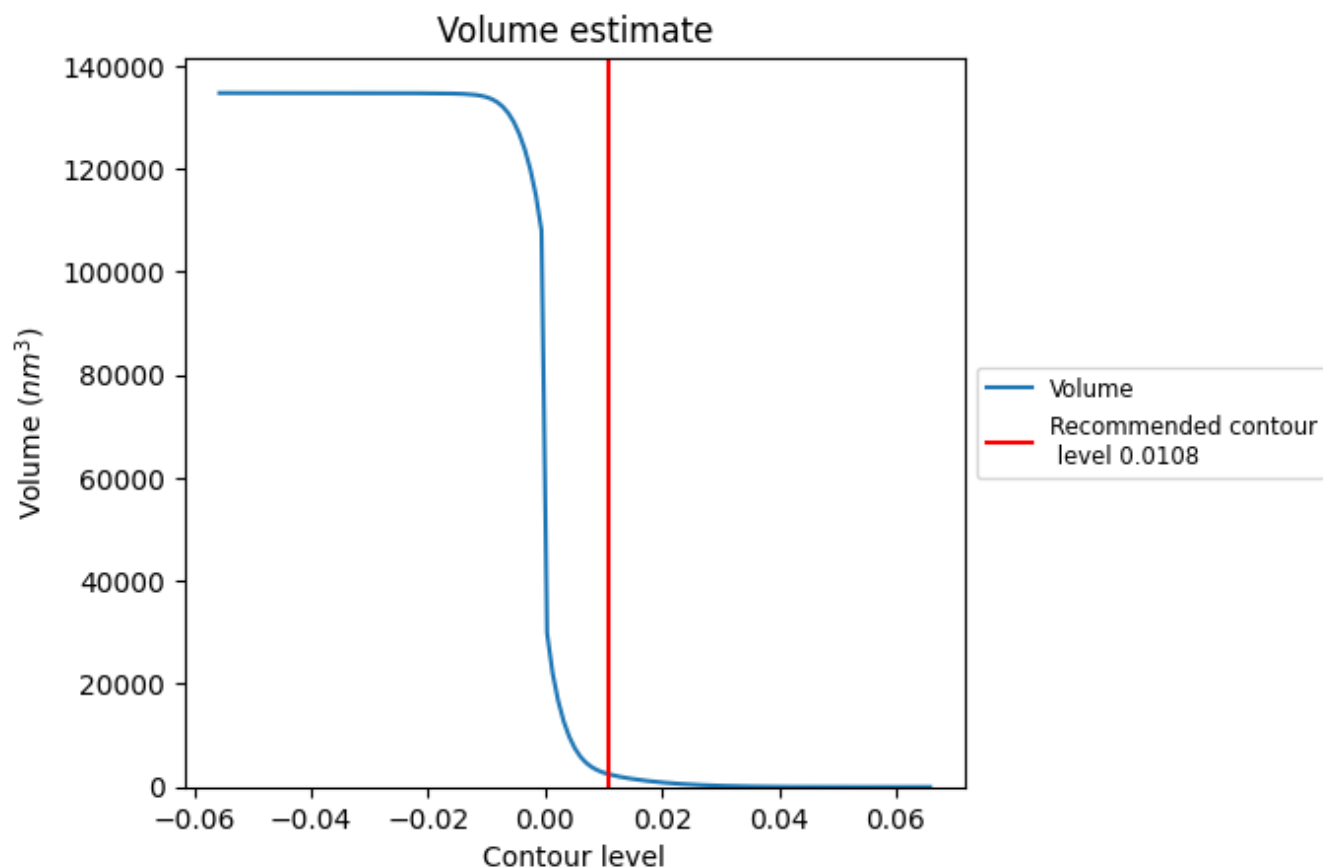
This section contains the results of statistical analysis of the map.

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.

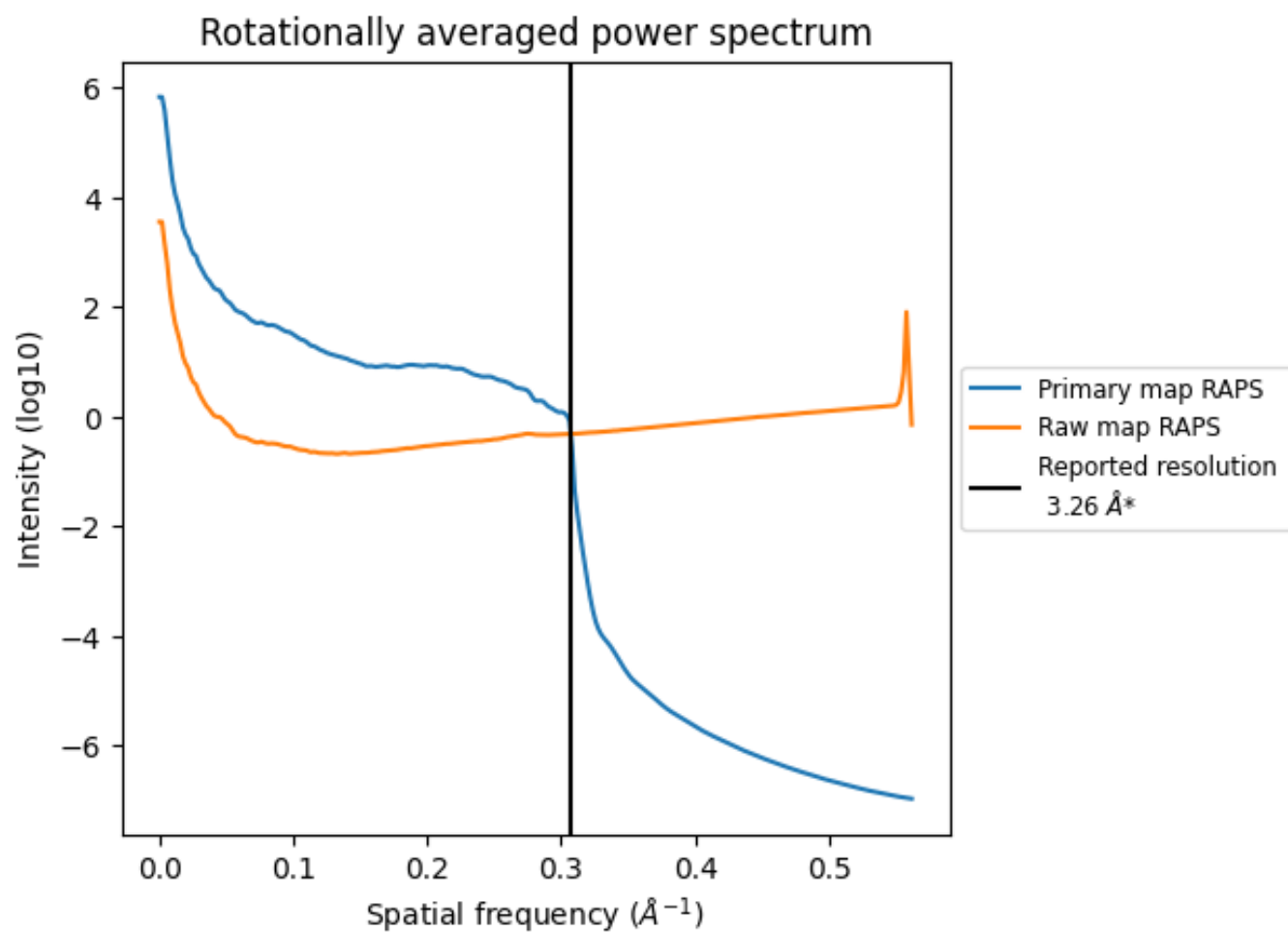
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2501 nm^3 ; this corresponds to an approximate mass of 2259 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

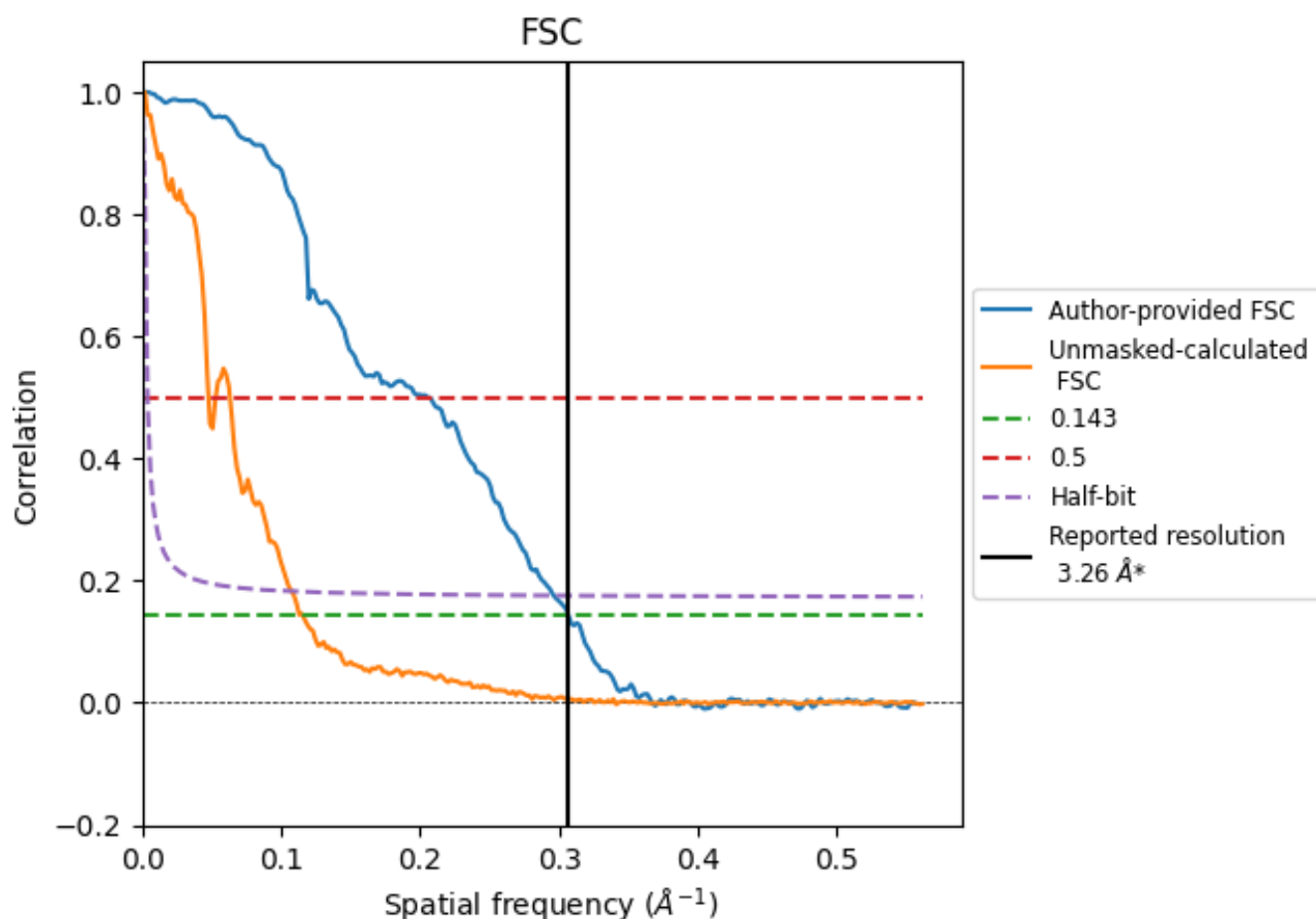


*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

8.2 Resolution estimates [i](#)

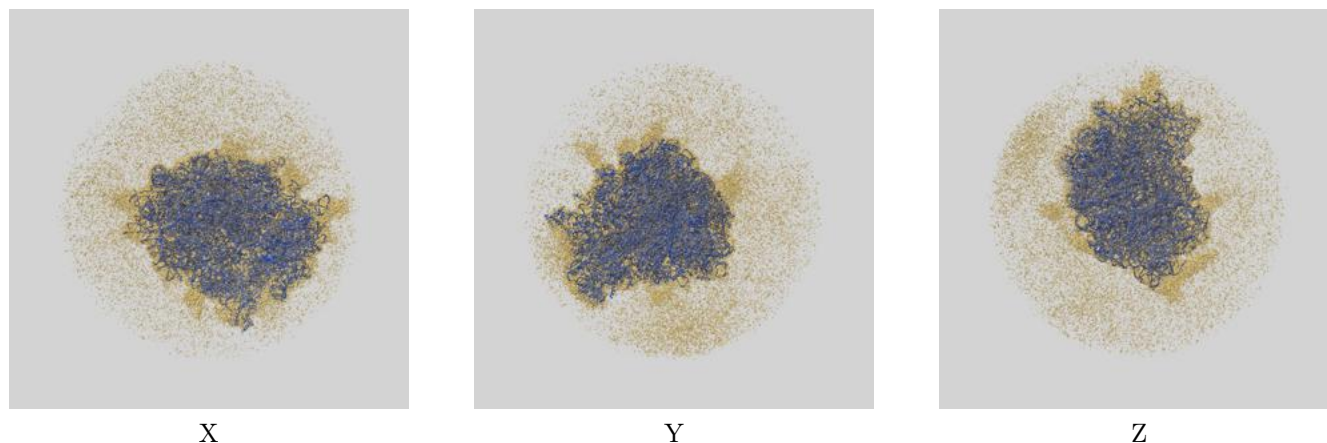
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	4.86	3.37
Unmasked-calculated*	8.65	20.92	9.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.65 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

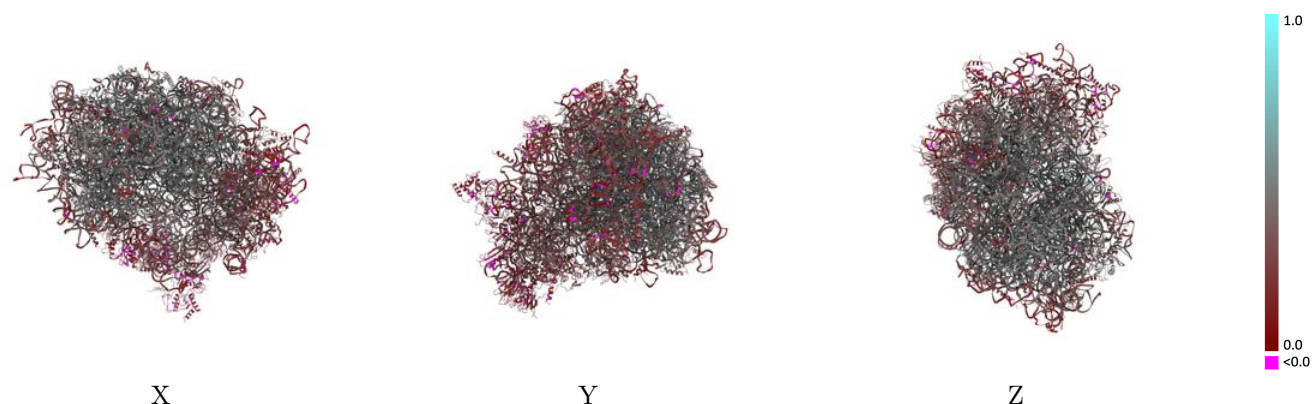
This section contains information regarding the fit between EMDB map EMD-71696 and PDB model 9PKG. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



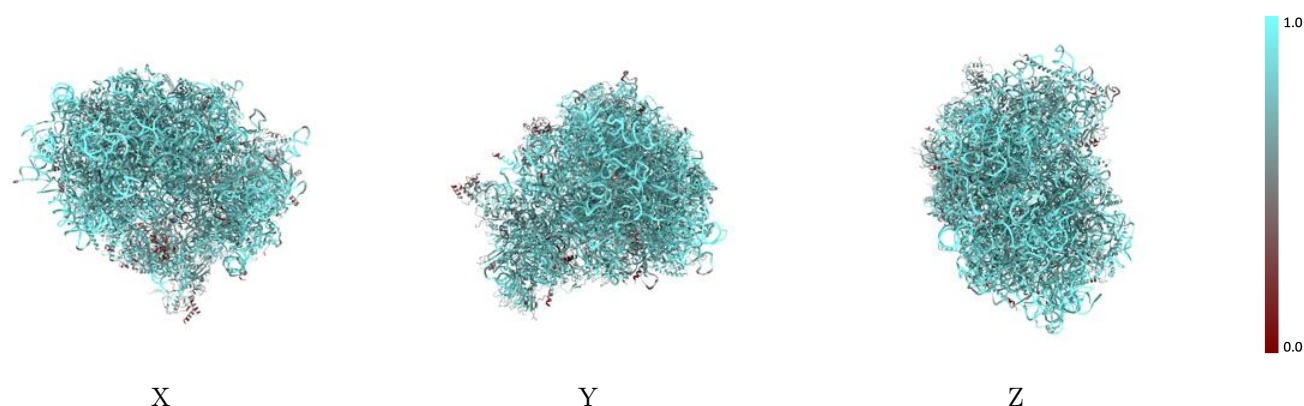
The images above show the 3D surface view of the map at the recommended contour level 0.0108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



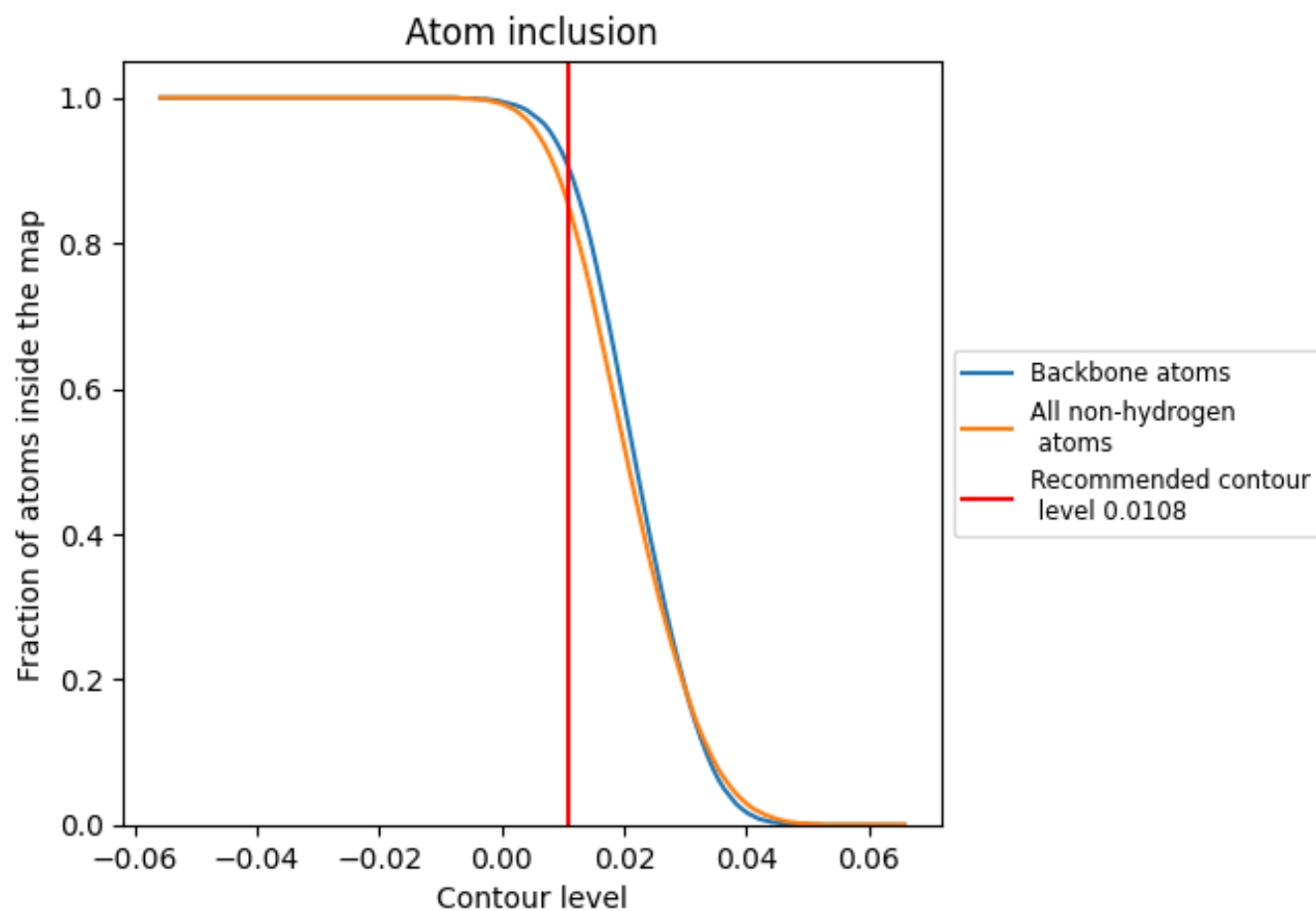
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0108).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.0108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3820
CI	 0.3980	 0.2800
L5	 0.9340	 0.4250
L7	 0.9830	 0.4510
L8	 0.9520	 0.4420
LA	 0.8220	 0.4920
LB	 0.8210	 0.4660
LC	 0.8000	 0.4690
LD	 0.8700	 0.4130
LE	 0.8130	 0.3970
LF	 0.8210	 0.4570
LG	 0.7810	 0.3970
LH	 0.8050	 0.4230
LI	 0.7630	 0.4390
LJ	 0.7990	 0.3680
LL	 0.7990	 0.4280
LM	 0.8440	 0.4350
LN	 0.8580	 0.4860
LO	 0.8070	 0.4590
LP	 0.8230	 0.4770
LQ	 0.8040	 0.4790
LR	 0.7800	 0.4130
LS	 0.8490	 0.4830
LT	 0.8200	 0.4610
LU	 0.8400	 0.3760
LV	 0.7400	 0.4680
LW	 0.7110	 0.3290
LX	 0.8120	 0.4430
LY	 0.8590	 0.4580
LZ	 0.8890	 0.4230
La	 0.8500	 0.4850
Lb	 0.7560	 0.3770
Lc	 0.8070	 0.4100
Ld	 0.7980	 0.4420
Le	 0.7900	 0.4840

















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lf	 0.8420	 0.4950
Lg	 0.8140	 0.4550
Lh	 0.7800	 0.4150
Li	 0.8120	 0.4280
Lj	 0.8530	 0.4980
Lk	 0.8370	 0.3910
Ll	 0.7900	 0.4610
Lm	 0.8030	 0.4520
Ln	 0.7610	 0.3940
Lo	 0.4350	 0.4700
Lp	 0.7590	 0.4520
Lr	 0.8270	 0.4750
Ls	 0.5290	 0.1800
Lt	 0.4650	 0.1460
Pt	 0.6740	 0.3020
S2	 0.9190	 0.3240
SA	 0.7860	 0.2890
SB	 0.7560	 0.3520
SC	 0.8120	 0.3350
SD	 0.6970	 0.2430
SE	 0.8160	 0.2970
SF	 0.4640	 0.2450
SG	 0.7180	 0.2330
SH	 0.6880	 0.2450
SI	 0.7590	 0.3290
SJ	 0.8050	 0.2920
SK	 0.7030	 0.1980
SL	 0.7040	 0.3570
SM	 0.4590	 0.1390
SN	 0.7520	 0.3590
SO	 0.6420	 0.3410
SP	 0.6900	 0.2250
SQ	 0.7530	 0.2390
SR	 0.7770	 0.2850
SS	 0.6890	 0.2470
ST	 0.8020	 0.2380
SU	 0.7240	 0.2150
SV	 0.7860	 0.2940
SW	 0.7940	 0.3550
SX	 0.7120	 0.3600
SY	 0.7650	 0.2320
SZ	 0.3460	 0.2230

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sa	 0.8130	 0.3820
Sb	 0.7840	 0.3230
Sc	 0.5060	 0.2340
Sd	 0.8160	 0.2390
Se	 0.6370	 0.2590
Sf	 0.6720	 0.1790
Sg	 0.7240	 0.1840