



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:56 AM UTC

PDB ID : 8RXX / pdb_00008rxx
EMDB ID : EMD-19582
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME
WITH A/P/E-site tRNA AND mRNA : LM32Cs3H1 sKO STRAIN
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2024-02-08
Resolution : 2.97 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:

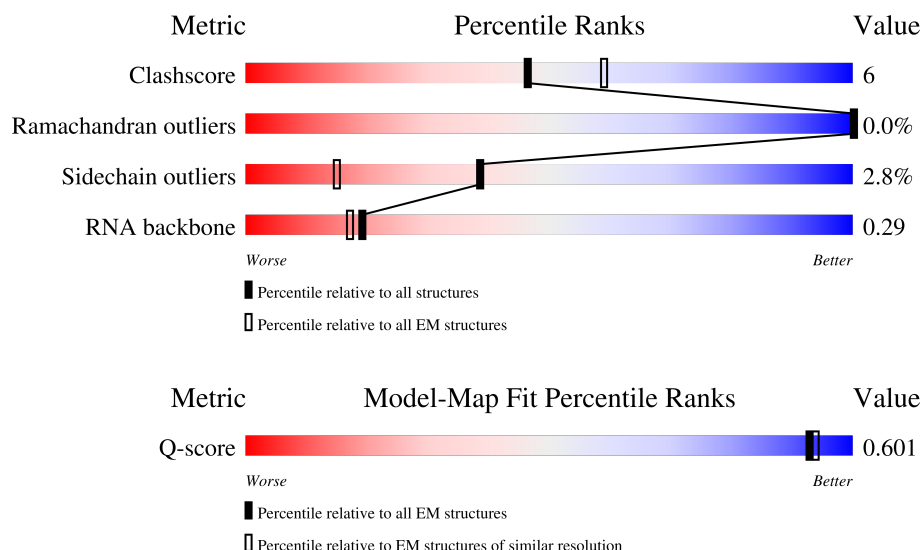
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	L1	1782	
2	L2	1526	
3	L3	216	

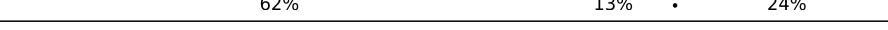
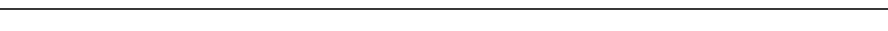
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Mol	Chain	Length	Quality of chain
4	L4	184	
5	L5	135	
6	L6	73	
7	L7	171	
8	L8	123	
9	LA	260	
10	LB	419	
11	LC	373	
12	LD	188	
13	LE	190	
14	LF	195	
15	LG	264	
16	LH	222	
17	LI	220	
18	LJ	139	
19	LK	175	
20	LL	145	
21	LM	204	
22	LN	213	
23	LO	305	
24	LP	198	
25	LQ	254	
26	LR	179	
27	LS	159	
28	LT	166	

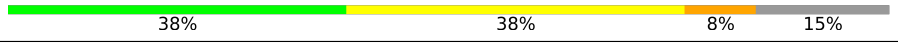
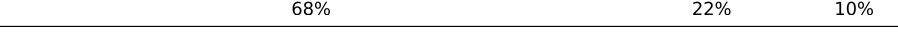
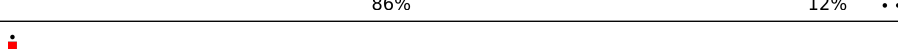
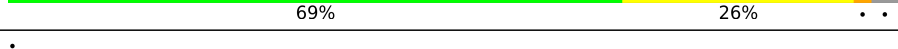
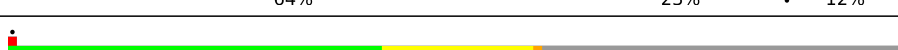
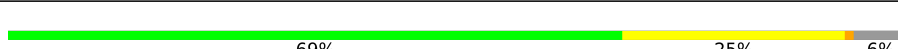
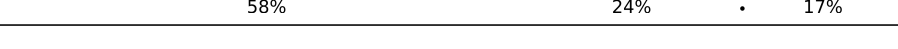
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Mol	Chain	Length	Quality of chain
29	LU	129	 81% 12% 5%
30	LV	145	 71% 11% 18%
31	LW	143	 62% 23% 15%
32	LX	124	 57% 11% 31%
33	LY	134	 81% 19%
34	LZ	147	 77% 20% ..
35	La	127	 77% 20% ..
36	Lb	70	 83% 14% .
37	Lc	252	 77% 13% 9%
38	Ld	104	 72% 20% . 7%
39	Le	188	 84% 14% ..
40	Lf	133	 77% 18% . .
41	Lg	144	 83% 17% .
42	Lh	168	 62% 13% . 24%
43	Li	105	 85% 12% .
44	Lj	83	 71% 27% .
45	Lk	83	 84% 10% 6%
46	Ll	51	 82% 16% .
47	Lm	128	 31% 9% 60%
48	Ln	34	 65% 29% . .
49	Lo	92	 76% 18% . .
50	Lp	106	 75% 17% 8%
51	S1	2204	 41% 33% 9% 17%
52	S2	76	 8% . 5% . 84%
53	S3	77	 40% 35% 17% 8%

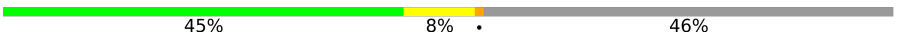
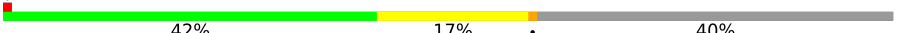
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Mol	Chain	Length	Quality of chain
54	S4	76	
55	S5	13	
56	SA	264	
57	SB	246	
58	SC	219	
59	SD	190	
60	SE	273	
61	SF	265	
62	SG	249	
63	SH	190	
64	SI	200	
65	SJ	130	
66	SK	220	
67	SL	149	
68	SM	116	
69	SN	168	
70	SO	144	
71	SP	143	
72	SQ	141	
73	SR	153	
74	SS	57	
75	ST	151	
76	SU	173	
77	SV	143	
78	SW	152	

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Mol	Chain	Length	Quality of chain
79	SX	161	
80	SY	164	
81	SZ	137	
82	Sa	120	
83	Sb	112	
84	Sc	86	
85	Sd	87	
86	Se	66	
87	Sf	152	
88	Sg	312	
89	Sh	235	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 213449 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1657	Total	C	N	O	P	1	0
			35568	15899	6506	11505	1658		

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	1149	Total	C	N	O	P	1	0
			24609	11017	4437	8005	1150		

- Molecule 3 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	183	Total	C	N	O	P	0	0
			3877	1735	669	1290	183		

- Molecule 4 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L4	184	Total	C	N	O	P	0	0
			3937	1756	712	1285	184		

- Molecule 5 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	122	Total	C	N	O	P	0	0
			2600	1160	466	852	122		

- Molecule 6 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 7 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	166	Total	C	N	O	P	0	0
			3532	1583	626	1158	165		

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	255	Total	C	N	O	S	0	0
			1931	1201	394	326	10		

- Molecule 10 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LB	401	Total	C	N	O	S	0	0
			3169	1997	629	530	13		

- Molecule 11 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	366	Total	C	N	O	S	0	0
			2815	1759	561	480	15		

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	175	Total	C	N	O	S	0	0
			1340	849	258	225	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	186	Total	C	N	O	S	0	0
			1472	934	273	259	6		

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	149	Total	C	N	O	S	0	0
			1151	731	216	202	2		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	241	Total	C	N	O	S	1	0
			1905	1200	380	318	7		

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	221	Total	C	N	O	S	0	0
			1764	1122	353	282	7		

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	208	Total	C	N	O	S	0	0
			1635	1022	331	274	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	135	Total	C	N	O	S	0	0
			1008	636	190	176	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	169	Total	C	N	O	S	0	0
			1327	829	261	229	8		

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	203	Total	C	N	O	S	0	0
			1711	1079	362	262	8		

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	199	Total	C	N	O	S	0	0
			1615	1018	321	262	14		

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	290	Total	C	N	O	S	0	0
			2212	1405	416	385	6		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	197	Total	C	N	O	S	0	0
			1535	965	306	258	6		

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	201	Total	C	N	O	S	0	0
			1679	1034	367	272	6		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	178	Total	C	N	O	S	0	0
			1455	925	279	246	5		

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LS	158	Total	C	N	O	S	0	0
			1247	793	243	207	4		

- Molecule 28 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	152	Total	C	N	O	S	0	0
			1218	761	241	205	11		

- Molecule 29 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	122	Total	C	N	O	S	0	0
			957	623	176	155	3		

- Molecule 30 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	119	Total	C	N	O	S	0	0
			945	599	180	164	2		

- Molecule 31 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	121	Total	C	N	O	S	0	0
			956	598	200	154	4		

- Molecule 32 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	85	Total	C	N	O	S	0	0
			714	461	140	109	4		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LY	133	Total	C	N	O	S	0	0
			1067	684	215	165	3		

- Molecule 34 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LZ	145	Total	C	N	O	S	0	0
			1113	682	237	189	5		

- Molecule 35 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	La	125	Total	C	N	O	S	0	0
			1043	650	217	172	4		

- Molecule 36 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lb	68	Total	C	N	O	S	0	0
			546	335	125	86			

- Molecule 37 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lc	229	Total	C	N	O	S	0	0
			1862	1185	358	308	11		

- Molecule 38 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ld	97	Total	C	N	O	S	0	0
			744	464	136	139	5		

- Molecule 39 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Le	186	Total	C	N	O	S	0	0
			1469	922	296	247	4		

- Molecule 40 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lf	128	Total	C	N	O	S	0	0
			1046	658	210	174	4		

- Molecule 41 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lg	143	Total	C	N	O	S	0	0
			1149	714	240	190	5		

- Molecule 42 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lh	127	Total	C	N	O	S	0	0
			1029	633	224	166	6		

- Molecule 43 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Li	102	Total	C	N	O	S	0	0
			807	508	163	133	3		

- Molecule 44 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lj	81	Total	C	N	O	S	0	0
			672	409	154	103	6		

- Molecule 45 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lk	78	Total	C	N	O	S	0	0
			581	365	115	98	3		

- Molecule 46 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ll	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lm	51	Total	C	N	O	S	0	0
			402	254	80	63	5		

- Molecule 48 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ln	33	Total	C	N	O	S	0	0
			290	178	73	37	2		

- Molecule 49 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lo	89	Total	C	N	O	S	0	0
			693	431	143	113	6		

- Molecule 50 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lp	97	Total	C	N	O	S	0	0
			780	494	158	123	5		

- Molecule 51 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S1	1836	Total	C	N	O	P	1	0
			39285	17572	7085	12791	1837		

- Molecule 52 is a RNA chain called A-site_tRNA_chain_S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S2	12	Total	C	N	O	P	0	0
			263	121	47	82	12		

- Molecule 53 is a RNA chain called P-site_tRNA_chain_S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	71	Total	C	N	O	P	0	0
			1513	676	277	490	70		

- Molecule 54 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S4	66	Total	C	N	O	P	0	0
			1406	628	253	460	65		

- Molecule 55 is a RNA chain called mRNA_chain_S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S5	11	Total	C	N	O	P	0	0
			229	103	38	77	11		

- Molecule 56 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SA	238	Total	C	N	O	S	0	0
			1909	1194	366	338	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SB	211	Total	C	N	O	S	0	0
			1649	1047	301	290	11		

- Molecule 58 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SC	212	Total	C	N	O	S	0	0
			1627	1030	297	287	13		

- Molecule 59 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SD	183	Total	C	N	O	S	0	0
			1504	947	305	244	8		

- Molecule 60 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SE	260	Total	C	N	O	S	0	0
			2054	1301	393	351	9		

- Molecule 61 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SF	218	Total	C	N	O	S	0	0
			1662	1063	297	293	9		

- Molecule 62 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SG	245	Total	C	N	O	S	0	0
			1948	1213	401	331	3		

- Molecule 63 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SH	182	Total	C	N	O	S	0	0
			1430	889	275	259	7		

- Molecule 64 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SI	200	Total	C	N	O	S	0	0
			1639	1044	316	271	8		

- Molecule 65 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

- Molecule 66 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SK	198	Total	C	N	O	S	0	0
			1600	998	330	270	2		

- Molecule 67 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SL	144	Total	C	N	O	S	0	0
			1140	731	210	196	3		

- Molecule 68 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SM	102	Total	C	N	O	S	0	0
			796	498	145	151	2		

- Molecule 69 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SN	99	Total	C	N	O	S	0	0
			808	518	141	142	7		

- Molecule 70 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SO	136	Total	C	N	O	S	0	0
			1010	624	197	182	7		

- Molecule 71 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SP	141	Total	C	N	O	S	0	0
			1096	691	216	186	3		

- Molecule 72 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SQ	98	Total	C	N	O	S	0	0
			655	400	119	131	5		

- Molecule 73 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SR	127	Total	C	N	O	S	0	0
			1011	641	195	171	4		

- Molecule 74 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SS	56	Total	C	N	O	S	0	0
			451	279	94	73	5		

- Molecule 75 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	ST	142	Total	C	N	O	S	0	0
			1159	731	230	190	8		

- Molecule 76 is a protein called Ribosomal protein S17 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SU	153	Total	C	N	O	S	0	0
			1251	792	248	206	5		

- Molecule 77 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SV	122	Total	C	N	O	S	0	0
			936	588	180	164	4		

- Molecule 78 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SW	115	Total	C	N	O	S	0	0
			925	590	176	155	4		

- Molecule 79 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SX	152	Total	C	N	O	S	0	0
			1206	766	237	199	4		

- Molecule 80 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SY	88	Total	C	N	O	S	0	0
			659	407	121	127	4		

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SZ	130	Total	C	N	O	S	0	0
			1051	675	204	169	3		

- Molecule 82 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sa	72	Total	C	N	O	S	0	0
			567	361	100	103	3		

- Molecule 83 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sb	104	Total	C	N	O	S	0	0
			827	513	177	130	7		

- Molecule 84 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sc	85	Total	C	N	O	S	0	0
			674	416	131	119	8		

- Molecule 85 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sd	66	Total	C	N	O	S	0	0
			479	293	96	86	4		

- Molecule 86 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Se	58	Total	C	N	O	S	0	0
			465	293	97	74	1		

- Molecule 87 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms				AltConf	Trace
87	Sf	46	Total	C	N	O	0	0
			300	187	63	50		

- Molecule 88 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Sg	301	Total	C	N	O	S	0	0
			2341	1468	418	442	13		

- Molecule 89 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Sh	103	Total	C	N	O	S	0	0
			826	520	158	145	3		

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	L1	34	Total 34	K 34	0
90	L2	22	Total 22	K 22	0
90	L3	3	Total 3	K 3	0
90	L4	6	Total 6	K 6	0
90	L5	1	Total 1	K 1	0
90	L7	2	Total 2	K 2	0
90	LA	1	Total 1	K 1	0
90	LM	1	Total 1	K 1	0
90	S1	19	Total 19	K 19	0

- Molecule 91 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
91	L1	16	Total 16	Na 16	0
91	L2	14	Total 14	Na 14	0
91	L8	1	Total 1	Na 1	0
91	LA	1	Total 1	Na 1	0
91	Lh	1	Total 1	Na 1	0
91	S1	7	Total 7	Na 7	0
91	SK	1	Total 1	Na 1	0

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	L1	73	Total 73	Mg 73	0
92	L2	42	Total 42	Mg 42	0

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Mol	Chain	Residues	Atoms		AltConf
92	L3	3	Total 3	Mg 3	0
92	L4	2	Total 2	Mg 2	0
92	L5	2	Total 2	Mg 2	0
92	L6	1	Total 1	Mg 1	0
92	L7	3	Total 3	Mg 3	0
92	L8	2	Total 2	Mg 2	0
92	LB	1	Total 1	Mg 1	0
92	LJ	1	Total 1	Mg 1	0
92	LT	1	Total 1	Mg 1	0
92	Lf	1	Total 1	Mg 1	0
92	Lj	1	Total 1	Mg 1	0
92	S1	31	Total 31	Mg 31	0
92	S5	1	Total 1	Mg 1	0
92	SK	1	Total 1	Mg 1	0

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
93	Lm	1	Total 1	Zn 1	0
93	SS	1	Total 1	Zn 1	0
93	Sb	1	Total 1	Zn 1	0

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	L1	337	Total 337	O 337	0
94	L2	235	Total 235	O 235	0
94	L3	21	Total 21	O 21	0
94	L4	39	Total 39	O 39	0
94	L5	30	Total 30	O 30	0
94	L6	6	Total 6	O 6	0
94	L7	38	Total 38	O 38	0
94	L8	2	Total 2	O 2	0
94	LA	14	Total 14	O 14	0
94	LB	20	Total 20	O 20	0
94	LC	18	Total 18	O 18	0
94	LF	3	Total 3	O 3	0
94	LG	2	Total 2	O 2	0
94	LH	6	Total 6	O 6	0
94	LI	5	Total 5	O 5	0
94	LJ	6	Total 6	O 6	0
94	LK	1	Total 1	O 1	0
94	LL	8	Total 8	O 8	0
94	LM	12	Total 12	O 12	0
94	LP	6	Total 6	O 6	0
94	LQ	8	Total 8	O 8	0
94	LR	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
94	LT	11	Total 11	O 11	0
94	LV	4	Total 4	O 4	0
94	LW	2	Total 2	O 2	0
94	LX	3	Total 3	O 3	0
94	LZ	1	Total 1	O 1	0
94	La	3	Total 3	O 3	0
94	Lb	1	Total 1	O 1	0
94	Lc	5	Total 5	O 5	0
94	Ld	1	Total 1	O 1	0
94	Le	3	Total 3	O 3	0
94	Lf	8	Total 8	O 8	0
94	Lg	7	Total 7	O 7	0
94	Lh	7	Total 7	O 7	0
94	Lj	11	Total 11	O 11	0
94	Lk	1	Total 1	O 1	0
94	Ll	4	Total 4	O 4	0
94	Lm	1	Total 1	O 1	0
94	Ln	1	Total 1	O 1	0
94	Lo	6	Total 6	O 6	0
94	Lp	1	Total 1	O 1	0
94	S1	78	Total 78	O 78	0

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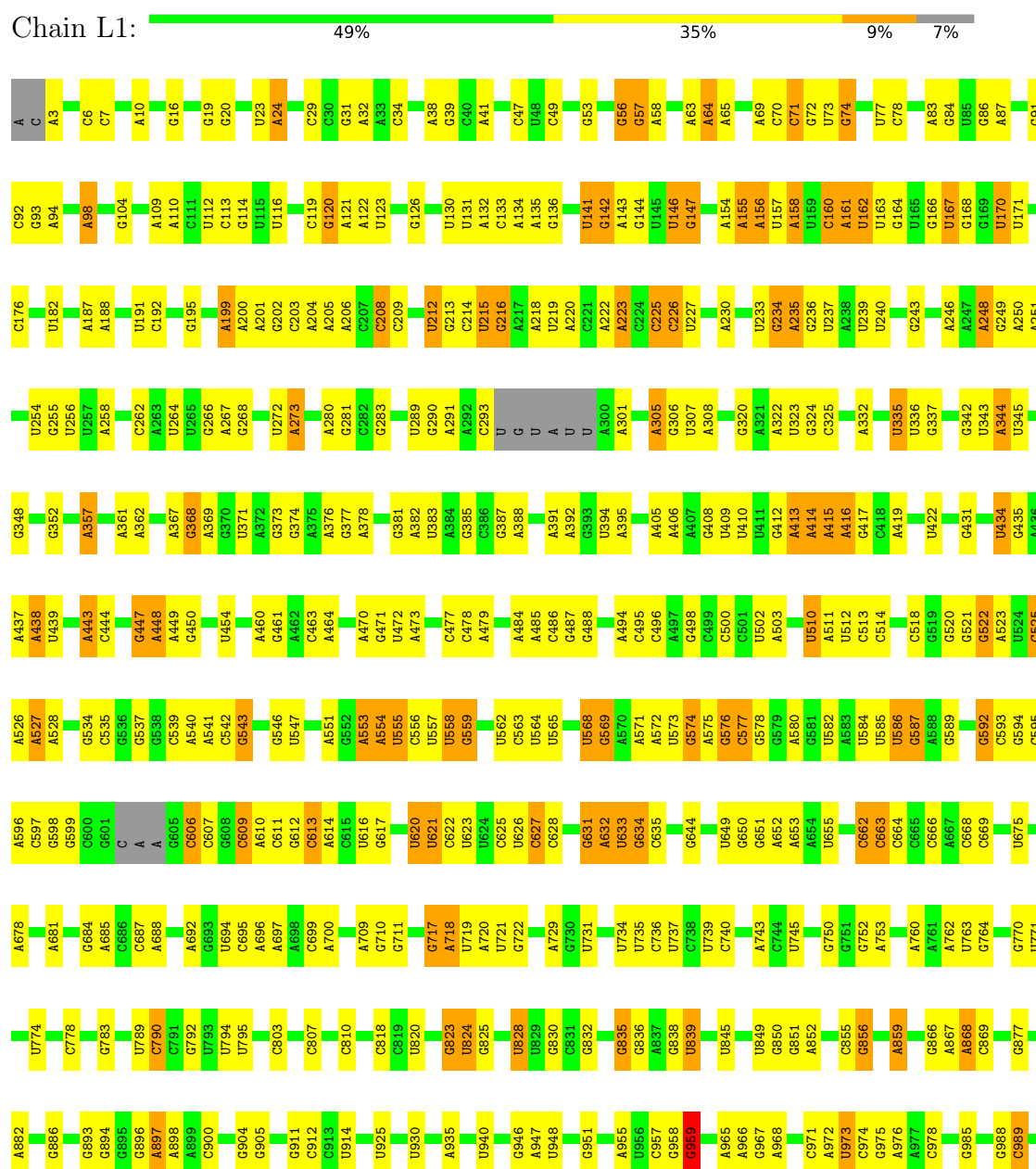
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Mol	Chain	Residues	Atoms		AltConf
94	S3	1	Total 1	O 1	0
94	S4	1	Total 1	O 1	0
94	S5	3	Total 3	O 3	0
94	SK	2	Total 2	O 2	0
94	SO	1	Total 1	O 1	0
94	SP	1	Total 1	O 1	0
94	ST	3	Total 3	O 3	0
94	Sb	1	Total 1	O 1	0

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: LSUa_rRNA_chain_1

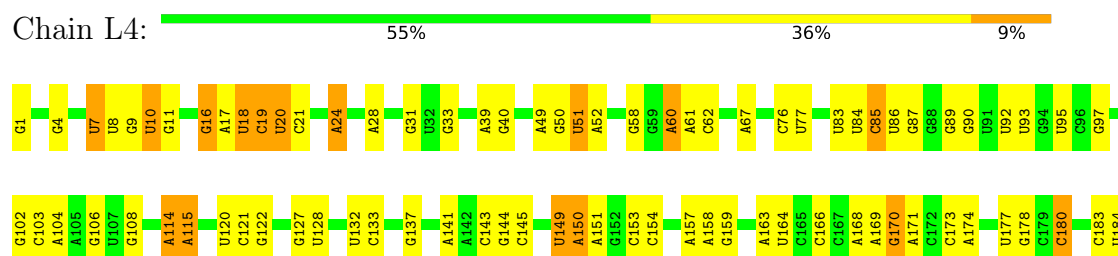


A1510	G1430	C1337	G1261	G1182	A1105	G1011	G	G	U	C812	A	G664	U665	C481	A391	G
G1511	G1433	G1342	G1262	C1183	A1106	U1012	G	G	G	U818	C	A665	A570	C489	C392	U
G1512	G1434	U1264	C1263	A1185	U1107	G	C	C	C	U819	A	U667	G571	A489	G403	C
U1514	A1435	U1265	U1264	A1189	C1109	A1017	U	U	U	G820	G742	G668	G495	G492	A404	A
G1526	A1436	U1266	U1266	U1193	U1110	G1018	G	G	C	A823	C743	G675	C579	G496	U405	C
	A1437	U1350	G1270	U1194	C1020	C1020	A	C	G	G824	G744	G683	U580	G497	G406	G
	U1438		G1271	U	A1021	U	C	U	U	U	G745	G684	G581	U408	C407	C
	U1439		A1276	A1199	U947	U947	U	C	A	A	A746	G685	U592	U409	U409	U
	G1440		G1277	A1200	G948	G948	U	U	A	A	A747	G686	U500			G
	C1441		C1278	A1118	U1024	U1024	U	U	U	A	G748	G687	A501	G414	G414	U
	G1442		G1279	A1119	G1025	G1025	U	U	U	A	A749	G688	A502	U415	U415	C
	A1443		U1280	C1120	A1030	A1030	C	C	A	U	U750	G689	C503	G416	G416	U
	G1444		U1281	C1121	U	U	C	U	U	U	G752	U692	U593	G417	G417	U
	A1445		U1282	A1123	A954	A954	G	G	A	U	U755	U693	U597	U418	U418	G
	A1446		C1282	A1205	C955	C955	G	U	U	G	U756	U694	G507	G419	G419	U
	A1447		U1283	A1206	C956	C956	C	C	C	C	G757	U695	A508	U420	U420	G
	A1448		G1207	G1125	C957	C957	C	C	C	C	A758	U696	C509	A421	A421	C
	A1449		A1208	G1041	A958	A958	G	U	U	G	U759	A696	U510	U422	U422	C
	G1450		A1209	G1046	U963	U963	U	U	U	G	U760	G698	C511	A423	A423	G
	U1453		C1287	A1130	G964	G964	C	C	C	U	U768	U	U514	G426	G426	C
	A1454		G1288	A1131	C965	C965	C	C	C	A	A769	U	U515	C427	C427	C
	U1455		A1289	A1132	U1053	U1053	C	C	C	A	U770	A	A516			C
	C1456		A1290	G1133	A1055	A1055	C	C	C	C	A772	A	A517	G431	G431	C
	C1457		G1291	U1136	U1058	U1058	C	C	C	C	A777	U	A518	U432	U432	C
	U1458		U1292	C1137	U1060	U1060	C	C	C	U847	U778	A	A525	G433	G433	A
	G1459		C1293	C1138	U1061	U1061	C	C	C	C848	U779	G	A526	U434	U434	C
	U1460		G1294	U1139	U1062	U1062	C	C	C	C849	U780	A	A527	U435	U435	C
	C1461		C1295	U1140	A1064	A1064	C	C	C	C850	U781	G	A528	U436	U436	C
	A1462		U1296	G1141	U1069	U1069	C	C	C	A	U782	G	C524	U437	U437	C
	A1463		U1297	G1142	A1070	A1070	U	U	U	U	U783	A	A529	U438	U438	C
	A1464		U1298	C1153	G1075	G1075	U	U	U	C	U784	A	C530	U439	U439	C
	U1465		U1299	C1154	U1077	U1077	C	C	C	U	U785	A	C531	A443	A443	C
	G1466		U1300	U1144	U1079	U1079	U	U	U	A	A786	C	U532	G447	G447	C
	U1468		U1303	C1147	A1083	A1083	C	C	C	A	U793	A	A541	A	A	C
	U1472		C1304	G1148	A1084	A1084	G	G	G	U	C797	G	A542	U	U	C
	G1474		C1305	G1152	G1076	G1076	U	U	U	U	G798	C	U543	G456	G456	C
	G1479		U1308	U1153	U1077	U1077	C	C	C	U	G799	C	U544	A	A	C
	U		G1309	C1154	U1078	U1078	C	C	C	U	U800	A	C550	A459	A459	C
	U		A1407	C1155	U1079	U1079	U	U	U	A	G801	C	C551	A460	A460	C
	U		A1408	U1156	U1083	U1083	C	C	C	U	U802	A	C552	U463	U463	C
	G1410		U1313	U1157	A1088	A1088	C	C	C	U	U803	A	C553			C
	G1411		C1314	A1158	G1088	G1088	U	U	U	U	U804	U	C554	G469	G469	C
	U1412		U1318	A1162	C1093	C1093	U	U	U	U	U805	A	C555	A470	A470	C
	G1413		U1324	U1170	U1096	U1096	U	U	U	U	G806	A	C556	U471	U471	C
	U1416		A1325	G1171	U1096	U1096	U	U	U	U	U807	A	C557	U472	U472	C
			A1326	C1172	U1100	U1100	U	U	U	U	U808	U	C558	A386	A386	C
	G1494		C1327	U1176	G1004	G1004	C	C	C	U	U809	A	C559	U387	U387	C
	A1495		U1328	A1175	A1105	A1105	C	C	C	U	U810	A	C560	A388	A388	C
	G1496		C1329	G1177	C1102	C1102	U	U	U	U	U811	U	C561	A389	A389	C
	C1497		U1329	G1178	U1006	U1006	C	C	C	U			C562	U478	U478	C
	G1498		C1330	C1179	G1006	G1006	C	C	C	U			C563	G450	G450	C
			U1332	G1179	U1007	U1007	U	U	U	U			C564			C
	G1506		G1333	A1100	A1005	A1005	C	C	C	U			C565			C
	U1507		C1334	A1101	C1102	C1102	U	U	U	U			C566			C
	A1508		U1427	A1179	U1007	U1007	C	C	C	U			C567			C
			U1428	A1180	G1104	G1104	C	C	C	U			C568			C
	G1509		G1336	G1181			C	C	C	U			C569			C

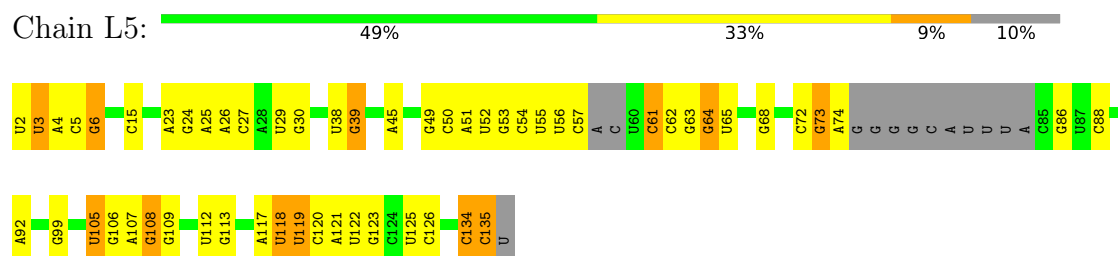
- Molecule 3: SR1_chain_3



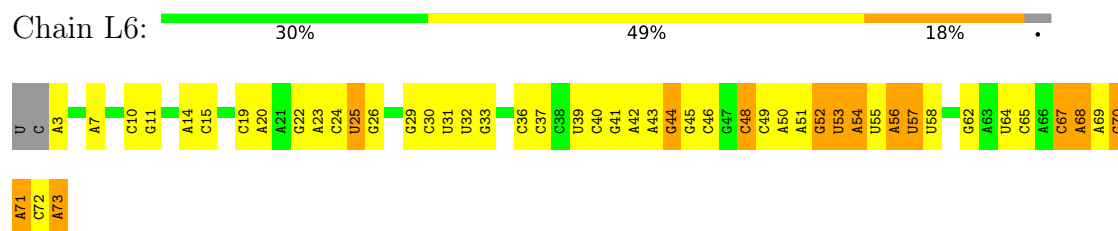
- Molecule 4: SR2_chain_4



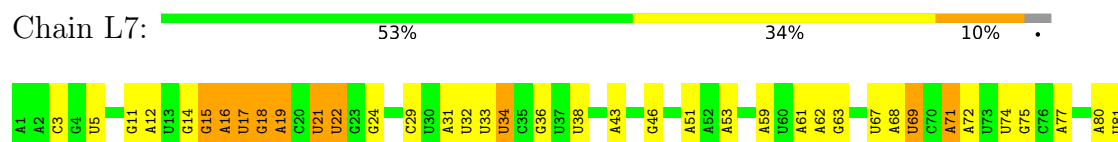
- Molecule 5: SR4_chain_5

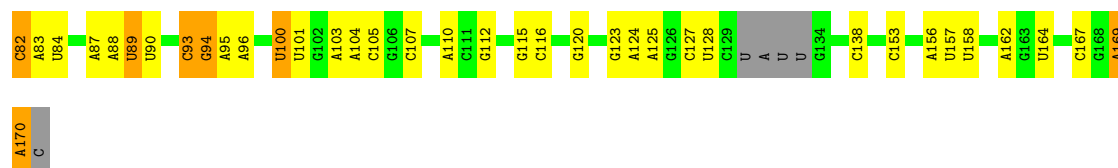


- Molecule 6: SR6_chain_6



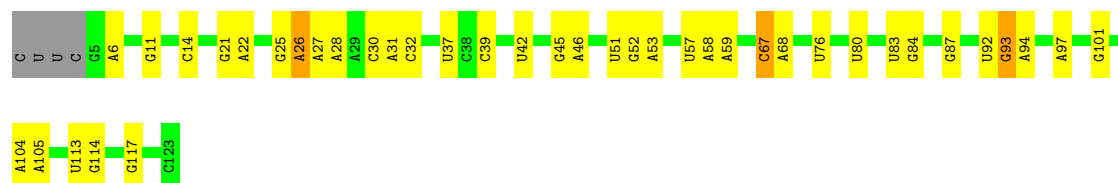
- Molecule 7: 5.8S_rRNA_chain_7





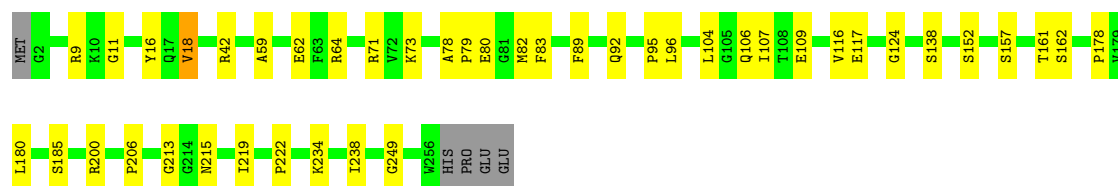
• Molecule 8: 5S_rRNA_chain_8

Chain L8: 64% 30% . .



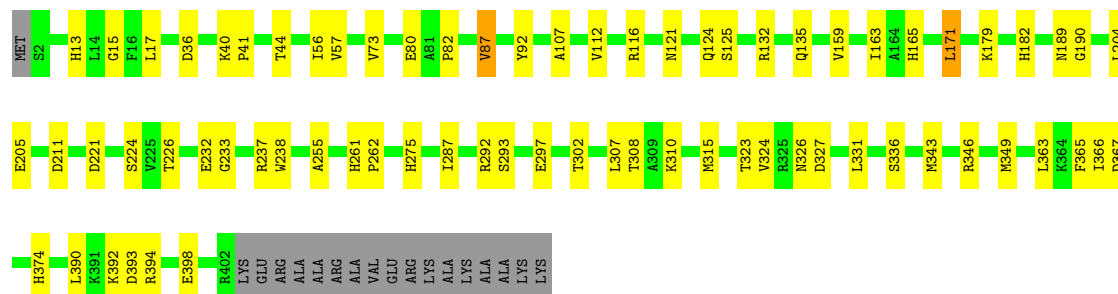
• Molecule 9: Putative 60S ribosomal protein L2

Chain LA: 82% 16% .



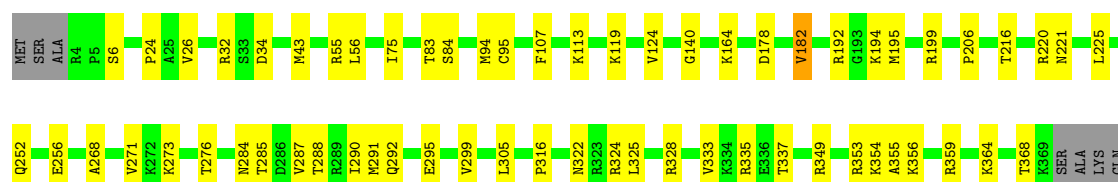
• Molecule 10: Putative ribosomal protein L3

Chain LB: 79% 17% .



• Molecule 11: Putative ribosomal protein L1a

Chain LC: 82% 16% .



Chain LD:

Chain LE:

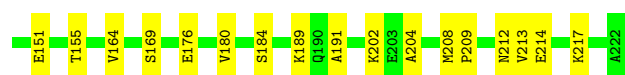
[illegible]

Chain LG:

78% 13% 9%

78% 13% 9%

Chain LH: 77% 21%



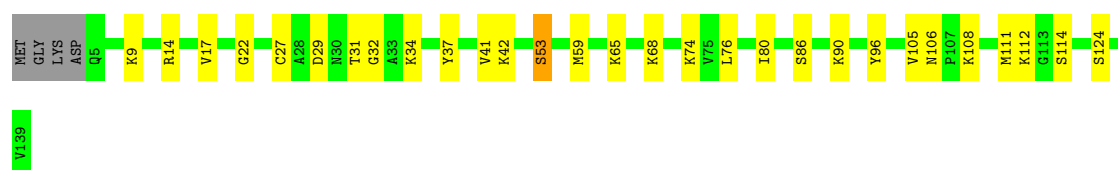
- Molecule 17: Putative 60S ribosomal protein L13

Chain LI: 87% 7% 5%



- Molecule 18: Putative 60S ribosomal protein L23

Chain LJ: 76% 20% ..



- Molecule 19: Putative 40S ribosomal protein L14

Chain LK: 81% 16% .



- Molecule 20: Putative 60S ribosomal protein L27A/L29

Chain LL: 77% 21% ..



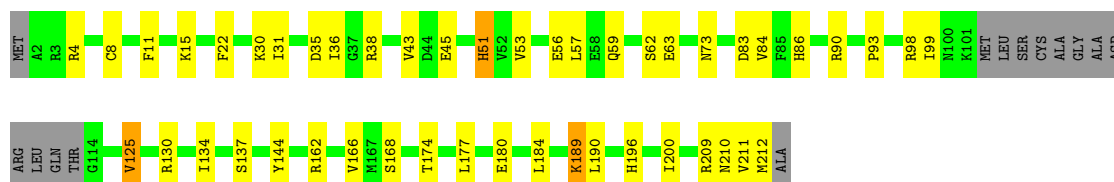
- Molecule 21: Ribosomal protein L15

Chain LM: 81% 18%



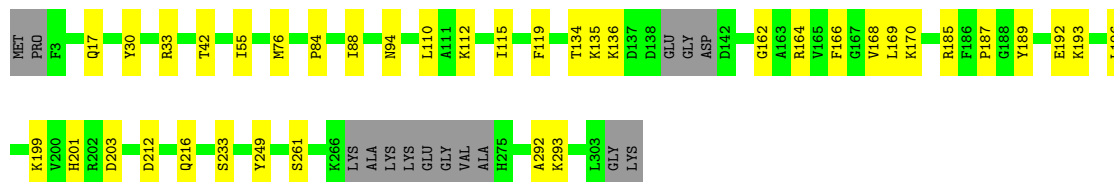
- Molecule 22: Putative 60S ribosomal protein L10

Chain LN: 71% 21% . 7%



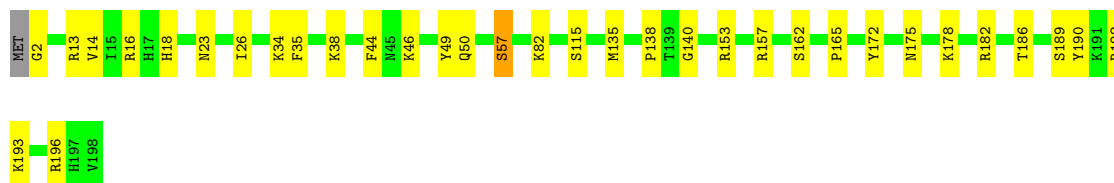
- Molecule 23: Putative 60S ribosomal protein L5

Chain LO: 83% 12% 5%



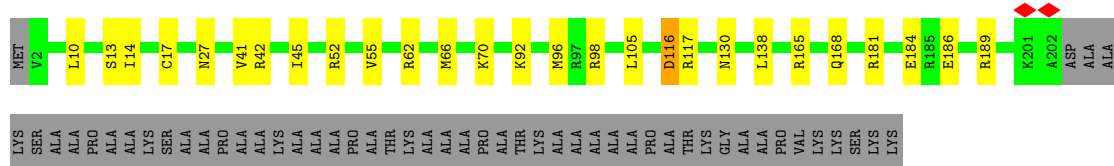
- Molecule 24: 60S ribosomal protein L18

Chain LP: 82% 17% ..



- Molecule 25: Putative 60S ribosomal protein L19

Chain LQ: 69% 10% 21%



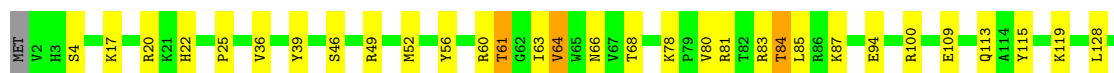
- Molecule 26: 60S ribosomal protein L18a

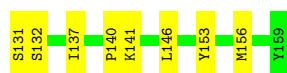
Chain LR: 83% 16% ..



- Molecule 27: Putative 60S ribosomal protein L21

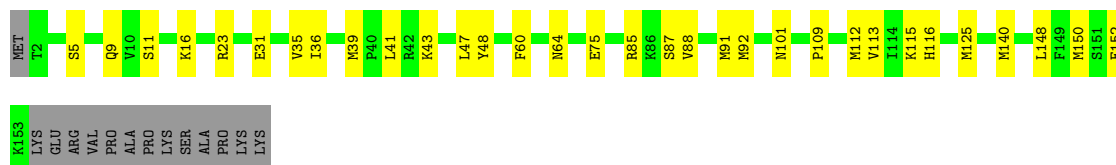
Chain LS: 75% 23% ..





- Molecule 28: Putative 60S ribosomal protein L17

Chain LT: 72% 19% 8%



- Molecule 29: Putative 60S ribosomal protein L22

Chain LU: 81% 12% 5%



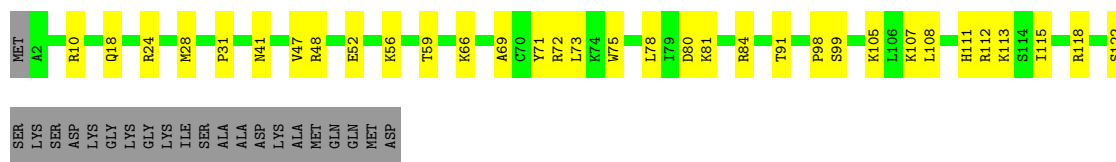
- Molecule 30: Putative 60S ribosomal protein L23a

Chain LV: 71% 11% 18%



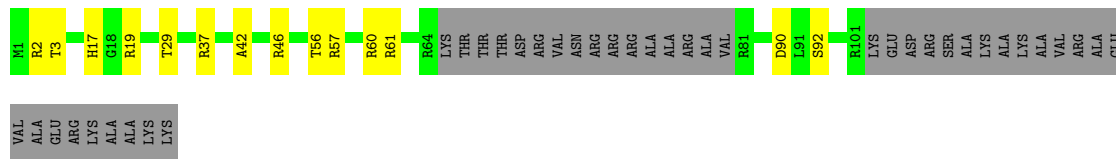
- Molecule 31: Putative 60S ribosomal protein L26

Chain LW: 62% 23% 15%



- Molecule 32: Putative ribosomal protein L24

Chain LX: 57% 11% 31%



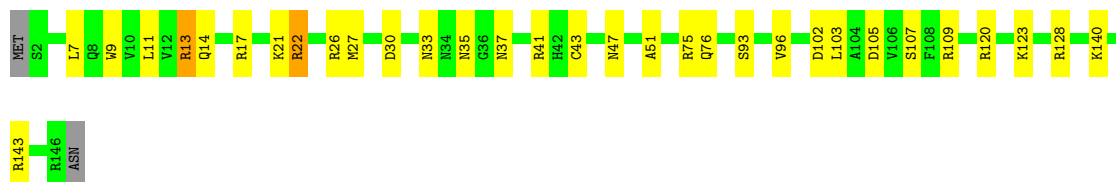
- Molecule 33: 60S ribosomal protein L27

Chain LY: 81% 19%



- Molecule 34: Putative 60S ribosomal protein L28

Chain LZ: 77% 20% ..



- Molecule 35: Putative 60S ribosomal protein L35

Chain La: 77% 20% ..



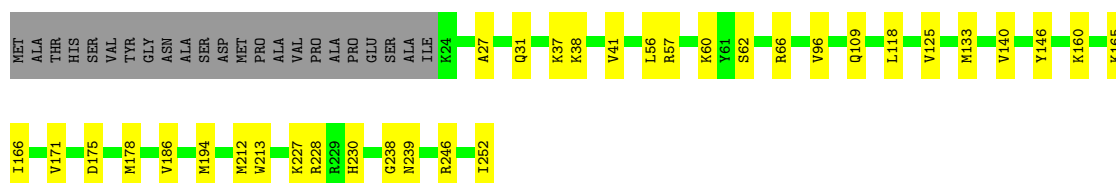
- Molecule 36: 60S ribosomal protein L29

Chain Lb: 83% 14% .



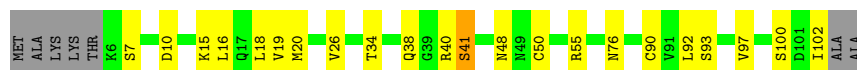
- Molecule 37: Putative 60S ribosomal protein L7

Chain Lc: 77% 13% 9%



- Molecule 38: 60S ribosomal protein L30

Chain Ld: 72% 20% 7%

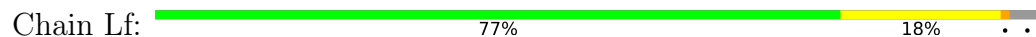


- Molecule 39: Putative 60S ribosomal subunit protein L31

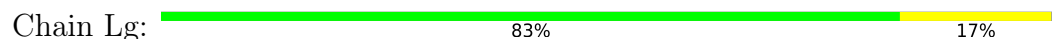
Chain Le: 84% 14% ..



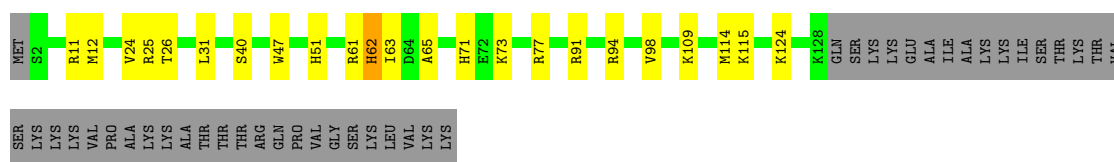
- Molecule 40: 60S ribosomal protein L32



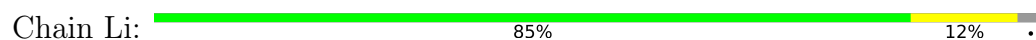
- Molecule 41: Putative ribosomal protein l35a



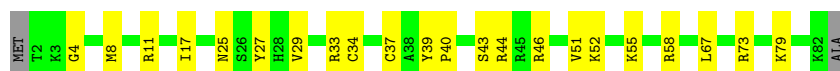
- Molecule 42: Putative 60S ribosomal protein L34



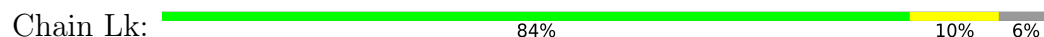
- Molecule 43: Putative 60S Ribosomal protein L36



- Molecule 44: Ribosomal protein L37



- Molecule 45: Putative ribosomal protein L38



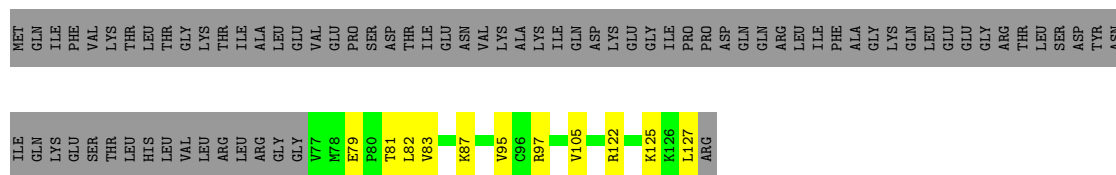
- Molecule 46: Putative 60S ribosomal protein L39

Chain Ll:  82% 16%



- Molecule 47: Ubiquitin-60S ribosomal protein L40

Chain Lm:  31% 9% 60%



- Molecule 48: 60S ribosomal protein L41

Chain Ln:  65% 29%



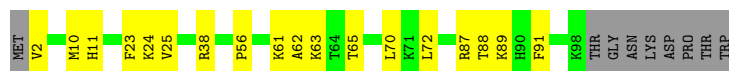
- Molecule 49: 60S ribosomal protein L37a

Chain Lo:  76% 18%

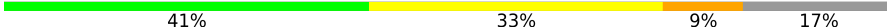


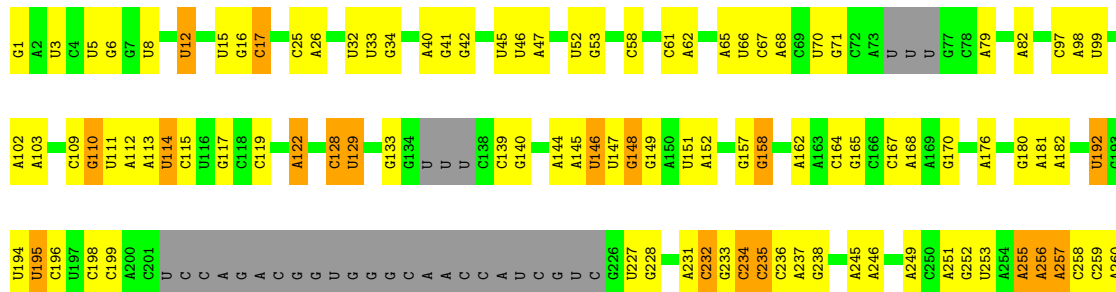
- Molecule 50: Putative 60S ribosomal protein L44

Chain Lp:  75% 17% 8%



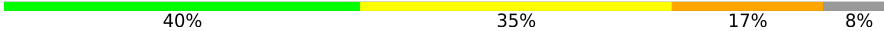
- Molecule 51: SSU_rRNA_chain_S1

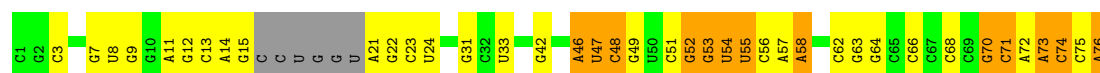
Chain S1:  41% 33% 9% 17%



WORLDWIDE
PDB
PROTEIN DATA BANK

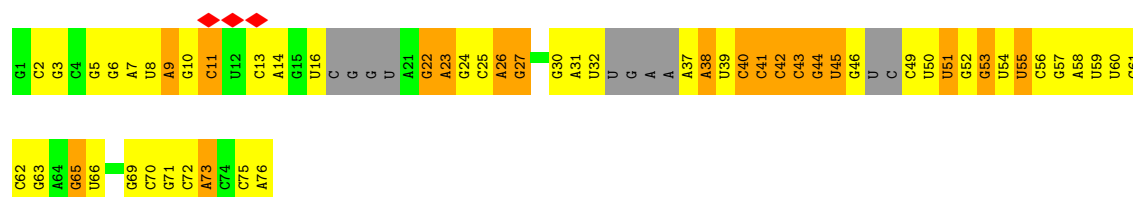
- Molecule 52: A-site tRNA chain S2

Chain S3: 

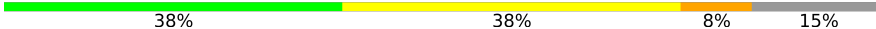


• Molecule 54: E-site_tRNA_chain_S4

Chain S4: 



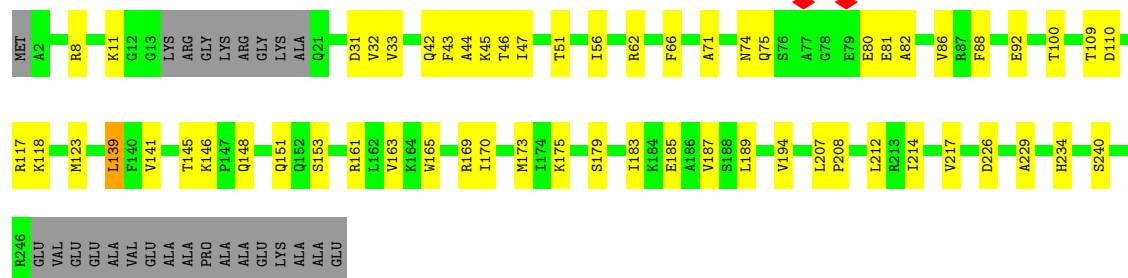
• Molecule 55: mRNA_chain_S5

Chain S5: 



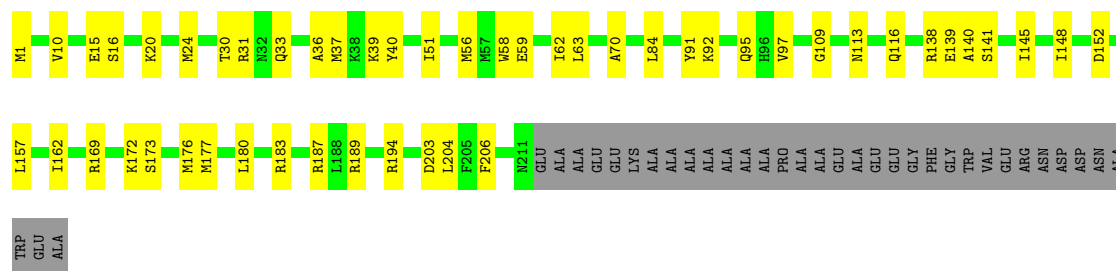
• Molecule 56: 40S ribosomal protein S3a

Chain SA: 



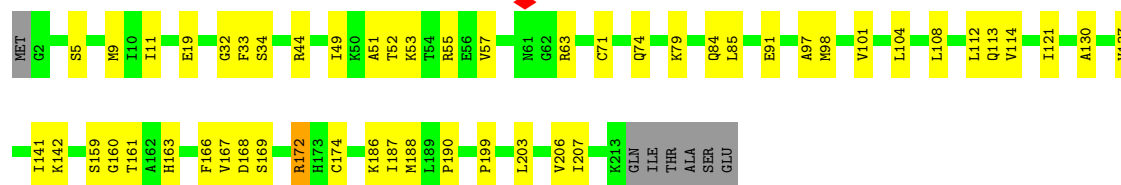
• Molecule 57: 40S ribosomal protein SA

Chain SB: 



• Molecule 58: Putative 40S ribosomal protein S3

Chain SC:  73% 23% .



- Molecule 59: Putative 40S ribosomal protein S9

Chain SD:  76% 19% . .



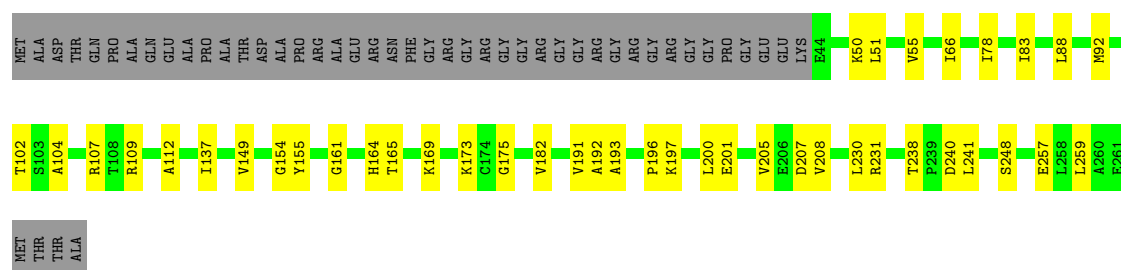
- Molecule 60: 40S ribosomal protein S4

Chain SE:  81% 14% 5%



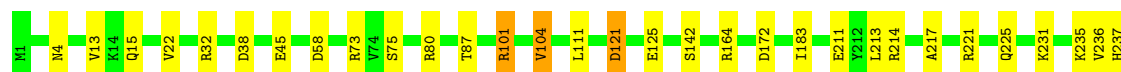
- Molecule 61: 40S ribosomal protein S2

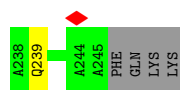
Chain SF:  66% 16% 18%



- Molecule 62: 40S ribosomal protein S6

Chain SG:  86% 12% . .





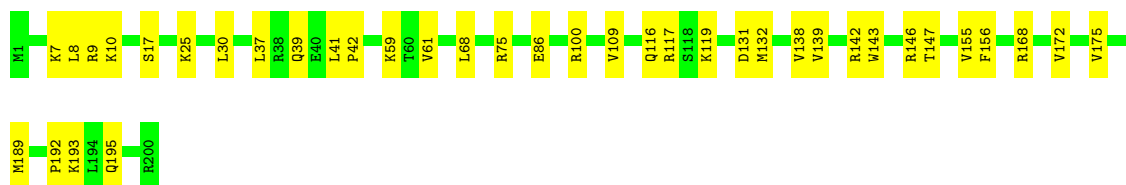
- Molecule 63: 40S ribosomal protein S5

Chain SH: 80% 15% . .



- Molecule 64: 40S ribosomal protein S7

Chain SI: 81% 19%



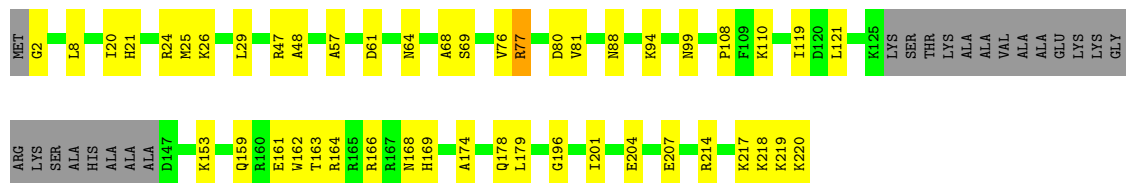
- Molecule 65: Putative 40S ribosomal protein S15A

Chain SJ: 82% 17% .



- Molecule 66: 40S ribosomal protein S8

Chain SK: 69% 21% 10%



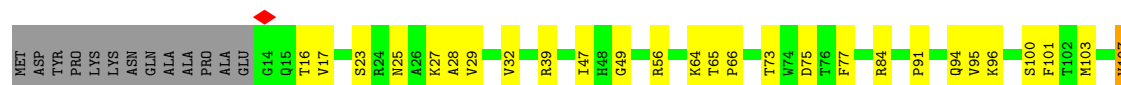
- Molecule 67: Putative 40S ribosomal protein S16

Chain SL: 69% 26% . .

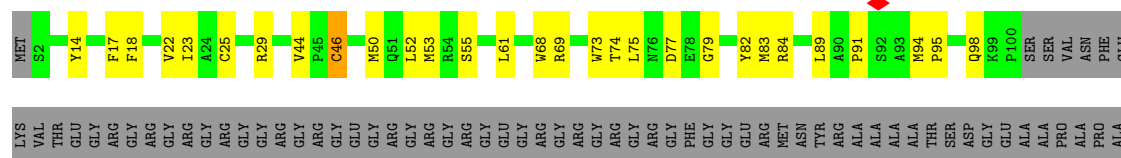




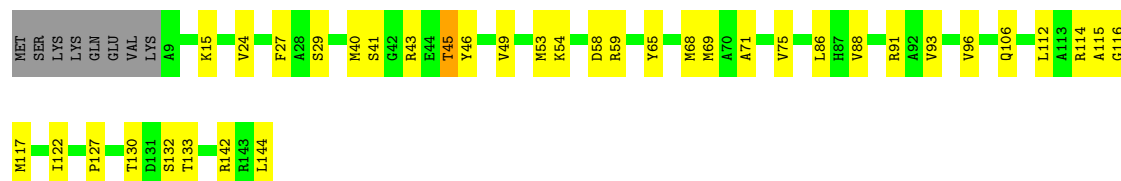
- Molecule 68: Putative ribosomal protein S20



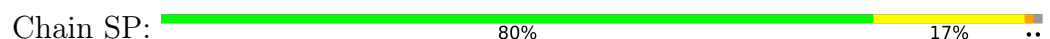
- Molecule 69: Putative 40S ribosomal protein S10



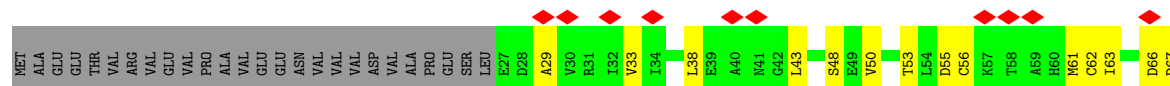
- Molecule 70: 40S ribosomal protein S14

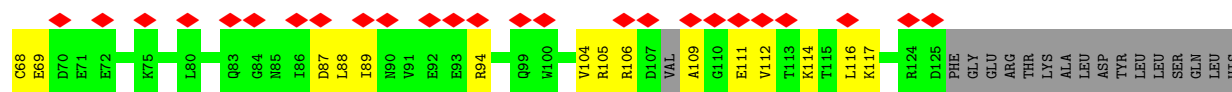


- Molecule 71: Putative 40S ribosomal protein S23



- Molecule 72: 40S ribosomal protein S12

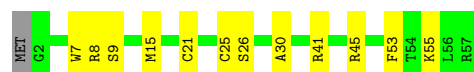
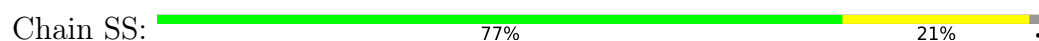




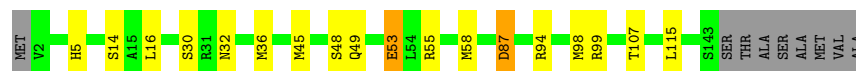
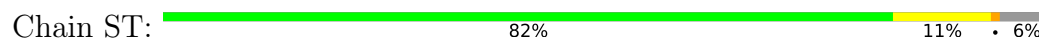
- Molecule 73: Putative 40S ribosomal protein S18



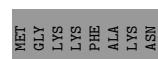
- Molecule 74: Putative ribosomal protein S29



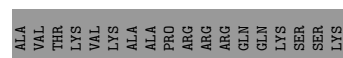
- Molecule 75: Putative 40S ribosomal protein S13



- Molecule 76: Ribosomal protein S17 family protein

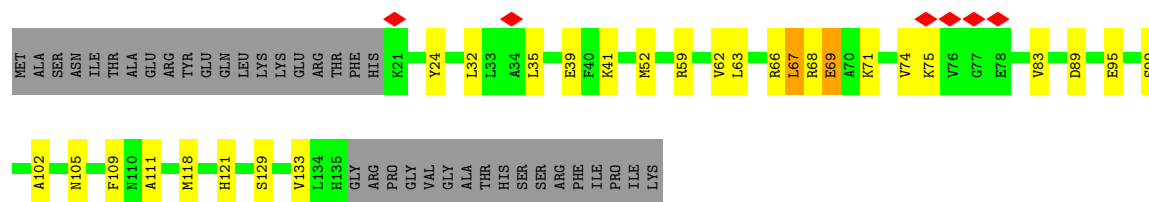


- Molecule 77: Putative 40S ribosomal protein S17



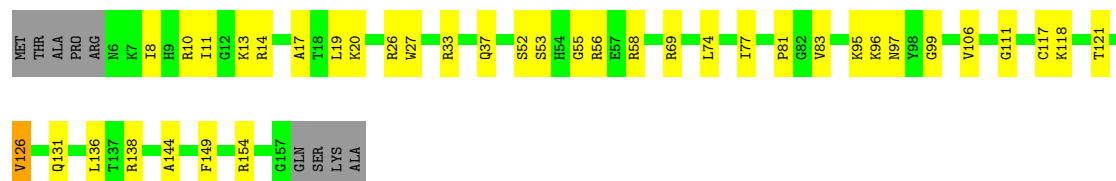
- Molecule 78: Putative 40S ribosomal protein S15

Chain SW: 

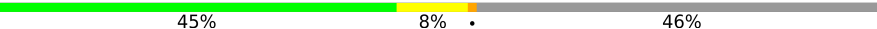


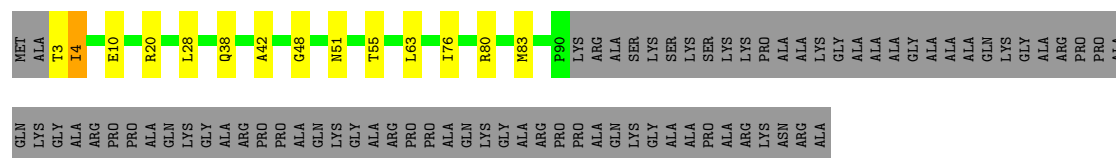
- Molecule 79: 40S ribosomal protein S19-like protein

Chain SX: 



- Molecule 80: Putative 40S ribosomal protein S21

Chain SY: 

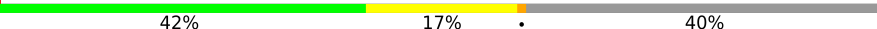


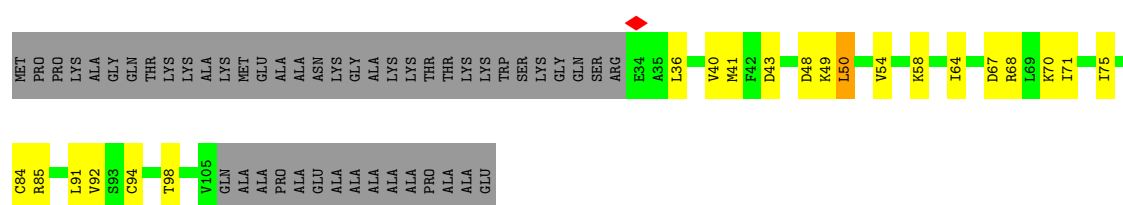
- Molecule 81: 40S ribosomal protein S24

Chain SZ: 



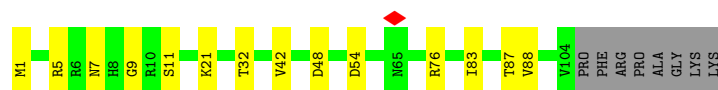
- Molecule 82: 40S ribosomal protein S25

Chain Sa: 

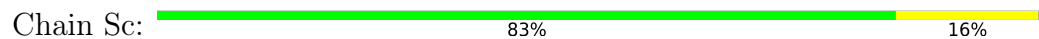


- Molecule 83: 40S ribosomal protein S26

Chain Sb: 



- Molecule 84: Putative 40S ribosomal protein S27-1



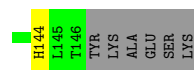
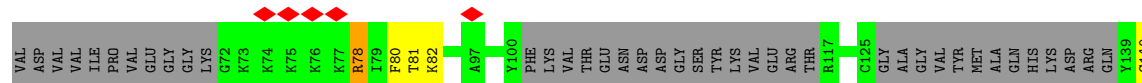
- Molecule 85: Putative 40S ribosomal protein S33



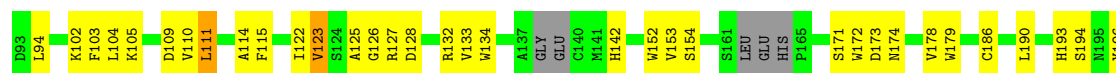
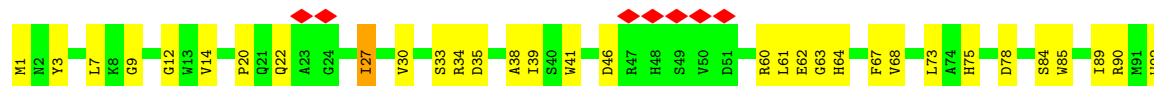
- Molecule 86: 40S ribosomal protein S30

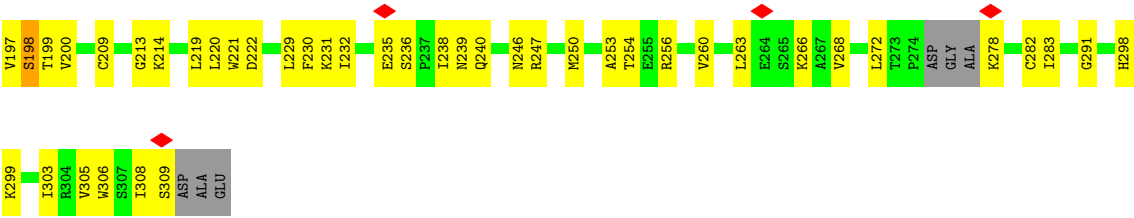


- Molecule 87: Ubiquitin-60S ribosomal protein L40

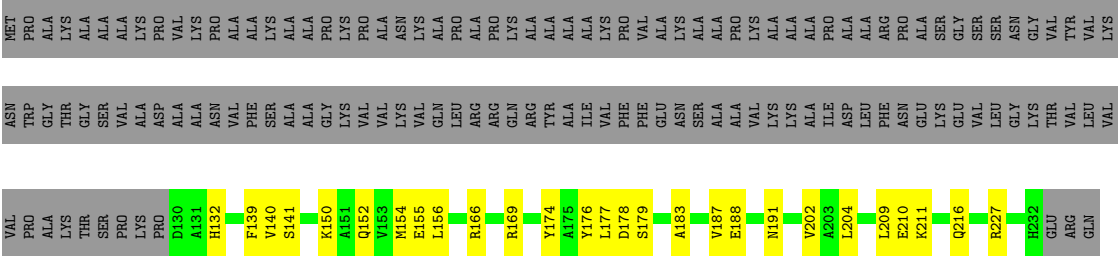
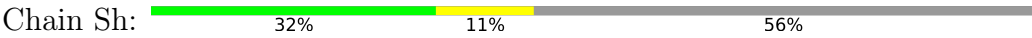


- Molecule 88: Guanine nucleotide-binding protein subunit beta-like protein





• Molecule 89: Putative RNA binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.273	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 5MC, NA, OMU, A2M, MIA, B8N, ZN, MG, OMC, PSU, MA6, 1MA, 7MG, K

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	L1	0.65	0/38810	0.89	4/60514 (0.0%)
2	L2	0.66	2/25898 (0.0%)	0.89	4/40361 (0.0%)
3	L3	0.65	0/4302	0.88	0/6687
4	L4	0.64	0/4376	0.88	0/6822
5	L5	0.65	0/2903	0.89	0/4518
6	L6	0.65	0/1683	0.89	0/2618
7	L7	0.64	0/3802	0.90	1/5917 (0.0%)
8	L8	0.66	0/2829	0.86	0/4405
9	LA	0.18	0/1972	0.36	0/2646
10	LB	0.17	0/3236	0.35	0/4354
11	LC	0.18	0/2865	0.32	0/3854
12	LD	0.28	0/1363	0.41	0/1825
13	LE	0.23	0/1492	0.41	0/2011
14	LF	0.15	0/1173	0.31	0/1586
15	LG	0.14	0/1932	0.30	0/2599
16	LH	0.14	0/1800	0.30	0/2418
17	LI	0.29	0/1668	0.44	0/2236
18	LJ	0.15	0/1025	0.34	0/1383
19	LK	0.20	0/1346	0.34	0/1805
20	LL	0.24	0/1151	0.39	0/1538
21	LM	0.17	0/1751	0.36	1/2338 (0.0%)
22	LN	0.11	0/1647	0.32	1/2203 (0.0%)
23	LO	0.24	0/2252	0.36	0/3024
24	LP	0.15	0/1560	0.32	0/2088
25	LQ	0.18	0/1698	0.30	0/2246
26	LR	0.20	0/1489	0.33	0/2008
27	LS	0.16	0/1276	0.30	0/1720
28	LT	0.17	0/1242	0.36	0/1666
29	LU	0.12	0/973	0.31	0/1299
30	LV	0.17	0/960	0.30	0/1293
31	LW	0.23	0/970	0.40	0/1296
32	LX	0.14	0/735	0.28	0/989

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LY	0.12	0/1088	0.24	0/1455
34	LZ	0.26	0/1129	0.38	0/1512
35	La	0.18	0/1054	0.34	0/1399
36	Lb	0.15	0/557	0.34	0/743
37	Lc	0.16	0/1896	0.31	0/2540
38	Ld	0.18	0/754	0.37	0/1019
39	Le	0.14	0/1488	0.29	0/1979
40	Lf	0.14	0/1066	0.28	0/1424
41	Lg	0.30	0/1172	0.49	1/1573 (0.1%)
42	Lh	0.36	0/1045	0.50	0/1390
43	Li	0.14	0/822	0.29	0/1099
44	Lj	0.17	0/686	0.35	0/915
45	Lk	0.13	0/590	0.26	0/798
46	Ll	0.14	0/463	0.26	0/617
47	Lm	0.11	0/408	0.29	0/545
48	Ln	0.16	0/294	0.38	0/383
49	Lo	0.33	0/705	0.57	0/940
50	Lp	0.14	0/793	0.30	0/1048
51	S1	0.67	0/42900	0.88	2/66828 (0.0%)
52	S2	0.71	0/260	0.90	0/400
53	S3	0.70	0/1690	0.86	0/2631
54	S4	0.70	0/1568	0.89	0/2436
55	S5	0.67	0/254	0.87	0/392
56	SA	0.12	0/1933	0.33	0/2596
57	SB	0.13	0/1683	0.31	0/2279
58	SC	0.33	0/1650	0.43	0/2209
59	SD	0.17	0/1532	0.33	0/2054
60	SE	0.12	0/2092	0.29	0/2819
61	SF	0.13	0/1698	0.31	0/2301
62	SG	0.13	0/1972	0.29	0/2635
63	SH	0.10	0/1452	0.26	0/1948
64	SI	0.13	0/1669	0.28	0/2244
65	SJ	0.13	0/1038	0.31	0/1391
66	SK	0.13	0/1623	0.29	0/2169
67	SL	0.36	0/1161	0.51	0/1559
68	SM	0.12	0/806	0.33	0/1093
69	SN	3.36	1/831 (0.1%)	1.23	2/1127 (0.2%)
70	SO	0.13	0/1025	0.35	0/1379
71	SP	0.12	0/1116	0.29	0/1496
72	SQ	0.14	0/655	0.42	0/890
73	SR	0.24	0/1029	0.42	0/1384
74	SS	0.10	0/457	0.32	0/606
75	ST	0.15	0/1182	0.32	0/1584

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SU	0.18	0/1280	0.29	0/1720
77	SV	0.11	0/945	0.29	0/1265
78	SW	0.12	0/945	0.30	0/1271
79	SX	0.11	0/1237	0.29	0/1661
80	SY	0.11	0/669	0.27	0/908
81	SZ	0.11	0/1071	0.29	0/1425
82	Sa	0.13	0/572	0.29	0/769
83	Sb	0.13	0/844	0.32	0/1129
84	Sc	0.12	0/688	0.30	0/921
85	Sd	0.10	0/481	0.27	0/647
86	Se	0.17	0/473	0.34	0/627
87	Sf	1.07	0/303	1.11	0/408
88	Sg	0.12	0/2398	0.36	0/3256
89	Sh	0.13	0/843	0.35	0/1134
All	All	0.56	3/224214 (0.0%)	0.73	16/329237 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	LE	0	1
17	LI	0	1
25	LQ	0	1
34	LZ	0	2
49	Lo	0	1
58	SC	0	1
73	SR	0	1
87	Sf	0	1
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	SN	91	PRO	N-CD	95.92	2.82	1.47
2	L2	502[A]	A2M	O3'-P	5.09	1.61	1.56
2	L2	502[B]	A2M	O3'-P	5.09	1.61	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	SN	91	PRO	N-CD-CG	-33.16	53.46	103.20
69	SN	91	PRO	CA-N-CD	-14.92	91.11	112.00
2	L2	1293	C	O3'-P-O5'	5.97	112.95	104.00
7	L7	93	C	C4'-C3'-C2'	-5.86	96.74	102.60
1	L1	170	U	C2'-C3'-O3'	5.58	117.87	109.50
1	L1	208	C	C4'-C3'-C2'	-5.39	97.21	102.60
22	LN	211	VAL	N-CA-C	-5.34	108.29	113.53
51	S1	328	C	C2'-C3'-O3'	5.33	121.69	113.70
21	LM	148	ILE	N-CA-C	-5.28	108.13	113.20
41	Lg	99	THR	N-CA-C	-5.25	106.85	113.20
2	L2	502[A]	A2M	OP2-P-O3'	5.24	116.72	105.20
2	L2	502[B]	A2M	OP2-P-O3'	5.24	116.72	105.20
1	L1	1742	G	C2'-C3'-O3'	5.23	121.55	113.70
51	S1	958	G	O3'-P-O5'	-5.20	96.20	104.00
1	L1	1412	G	O3'-P-O5'	-5.18	96.22	104.00
2	L2	1136	U	C2'-C3'-O3'	5.15	121.42	113.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	LE	155	ARG	Sidechain
17	LI	157	ARG	Sidechain
25	LQ	117	ARG	Sidechain
34	LZ	13	ARG	Sidechain
34	LZ	22	ARG	Sidechain
49	Lo	4	ARG	Sidechain
58	SC	172	ARG	Sidechain
73	SR	32	ARG	Sidechain
87	Sf	78	ARG	Sidechain

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	L1	35568	0	17933	261	0
2	L2	24609	0	12476	180	0
3	L3	3877	0	1966	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L4	3937	0	1989	31	0
5	L5	2600	0	1319	28	0
6	L6	1506	0	768	16	0
7	L7	3532	0	1790	31	0
8	L8	2531	0	1283	11	0
9	LA	1931	0	1987	31	0
10	LB	3169	0	3272	48	0
11	LC	2815	0	2919	46	0
12	LD	1340	0	1343	26	0
13	LE	1472	0	1551	32	0
14	LF	1151	0	1216	18	0
15	LG	1905	0	2035	30	0
16	LH	1764	0	1870	26	0
17	LI	1635	0	1696	13	0
18	LJ	1008	0	1051	19	0
19	LK	1327	0	1390	22	0
20	LL	1124	0	1151	22	0
21	LM	1711	0	1791	28	0
22	LN	1615	0	1678	26	0
23	LO	2212	0	2223	27	0
24	LP	1535	0	1637	24	0
25	LQ	1679	0	1799	15	0
26	LR	1455	0	1492	22	0
27	LS	1247	0	1278	24	0
28	LT	1218	0	1254	24	0
29	LU	957	0	985	10	0
30	LV	945	0	1001	10	0
31	LW	956	0	1029	24	0
32	LX	714	0	727	8	0
33	LY	1067	0	1140	15	0
34	LZ	1113	0	1154	24	0
35	La	1043	0	1142	19	0
36	Lb	546	0	575	6	0
37	Lc	1862	0	1959	20	0
38	Ld	744	0	770	11	0
39	Le	1469	0	1599	19	0
40	Lf	1046	0	1106	17	0
41	Lg	1149	0	1203	17	0
42	Lh	1029	0	1084	21	0
43	Li	807	0	865	10	0
44	Lj	672	0	688	15	0
45	Lk	581	0	579	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Ll	450	0	483	7	0
47	Lm	402	0	424	6	0
48	Ln	290	0	331	11	0
49	Lo	693	0	716	19	0
50	Lp	780	0	839	14	0
51	S1	39285	0	19847	390	0
52	S2	263	0	141	3	0
53	S3	1513	0	774	22	0
54	S4	1406	0	718	29	0
55	S5	229	0	119	2	0
56	SA	1909	0	1999	36	0
57	SB	1649	0	1663	33	0
58	SC	1627	0	1684	36	0
59	SD	1504	0	1578	25	0
60	SE	2054	0	2148	26	0
61	SF	1662	0	1708	25	0
62	SG	1948	0	2075	21	0
63	SH	1430	0	1456	21	0
64	SI	1639	0	1730	27	0
65	SJ	1021	0	1050	14	0
66	SK	1600	0	1687	31	0
67	SL	1140	0	1197	31	0
68	SM	796	0	838	21	0
69	SN	808	0	786	33	0
70	SO	1010	0	1025	25	0
71	SP	1096	0	1135	13	0
72	SQ	655	0	589	19	0
73	SR	1011	0	1046	34	0
74	SS	451	0	457	13	0
75	ST	1159	0	1231	11	0
76	SU	1251	0	1288	16	0
77	SV	936	0	976	28	0
78	SW	925	0	953	18	0
79	SX	1206	0	1231	31	0
80	SY	659	0	654	10	0
81	SZ	1051	0	1130	15	0
82	Sa	567	0	612	12	0
83	Sb	827	0	864	10	0
84	Sc	674	0	676	10	0
85	Sd	479	0	488	8	0
86	Se	465	0	521	9	0
87	Sf	300	0	238	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	Sg	2341	0	2263	72	0
89	Sh	826	0	829	18	0
90	L1	34	0	0	0	0
90	L2	22	0	0	0	0
90	L3	3	0	0	0	0
90	L4	6	0	0	0	0
90	L5	1	0	0	0	0
90	L7	2	0	0	0	0
90	LA	1	0	0	0	0
90	LM	1	0	0	0	0
90	S1	19	0	0	0	0
91	L1	16	0	0	0	0
91	L2	14	0	0	0	0
91	L8	1	0	0	0	0
91	LA	1	0	0	0	0
91	Lh	1	0	0	0	0
91	S1	7	0	0	0	0
91	SK	1	0	0	0	0
92	L1	73	0	0	0	0
92	L2	42	0	0	0	0
92	L3	3	0	0	0	0
92	L4	2	0	0	0	0
92	L5	2	0	0	0	0
92	L6	1	0	0	0	0
92	L7	3	0	0	0	0
92	L8	2	0	0	0	0
92	LB	1	0	0	0	0
92	LJ	1	0	0	0	0
92	LT	1	0	0	0	0
92	Lf	1	0	0	0	0
92	Lj	1	0	0	0	0
92	S1	31	0	0	0	0
92	S5	1	0	0	0	0
92	SK	1	0	0	0	0
93	Lm	1	0	0	0	0
93	SS	1	0	0	0	0
93	Sb	1	0	0	0	0
94	L1	337	0	0	0	0
94	L2	235	0	0	0	0
94	L3	21	0	0	0	0
94	L4	39	0	0	0	0
94	L5	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	L6	6	0	0	0	0
94	L7	38	0	0	0	0
94	L8	2	0	0	0	0
94	LA	14	0	0	0	0
94	LB	20	0	0	0	0
94	LC	18	0	0	0	0
94	LF	3	0	0	0	0
94	LG	2	0	0	0	0
94	LH	6	0	0	0	0
94	LI	5	0	0	0	0
94	LJ	6	0	0	0	0
94	LK	1	0	0	0	0
94	LL	8	0	0	0	0
94	LM	12	0	0	0	0
94	LP	6	0	0	0	0
94	LQ	8	0	0	0	0
94	LR	1	0	0	0	0
94	LT	11	0	0	0	0
94	LV	4	0	0	0	0
94	LW	2	0	0	1	0
94	LX	3	0	0	0	0
94	LZ	1	0	0	0	0
94	La	3	0	0	0	0
94	Lb	1	0	0	0	0
94	Lc	5	0	0	0	0
94	Ld	1	0	0	0	0
94	Le	3	0	0	0	0
94	Lf	8	0	0	1	0
94	Lg	7	0	0	0	0
94	Lh	7	0	0	0	0
94	Lj	11	0	0	0	0
94	Lk	1	0	0	0	0
94	Ll	4	0	0	0	0
94	Lm	1	0	0	0	0
94	Ln	1	0	0	0	0
94	Lo	6	0	0	0	0
94	Lp	1	0	0	0	0
94	S1	78	0	0	0	0
94	S3	1	0	0	0	0
94	S4	1	0	0	0	0
94	S5	3	0	0	0	0
94	SK	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	SO	1	0	0	0	0
94	SP	1	0	0	0	0
94	ST	3	0	0	0	0
94	Sb	1	0	0	0	0
All	All	213449	0	155960	2201	0

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

All (2201) 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)
88:Sg:173:ASP:O	88:Sg:174:ASN:OD1	1.68	1.11
4:L4:164:U:H4'	10:LB:349:MET:HE1	1.14	1.06
58:SC:63:ARG:HD2	69:SN:98:GLN:HE22	1.26	1.00
81:SZ:13:ARG:NH2	81:SZ:31:GLU:OE1	1.97	0.96
73:SR:6:ILE:HD13	82:Sa:43:ASP:OD1	1.66	0.96
67:SL:105:GLU:HG3	88:Sg:60:ARG:HB2	1.49	0.94
1:L1:1238:C:H5''	1:L1:1239:U:H5'	1.50	0.94
88:Sg:3:TYR:HB2	88:Sg:306:TRP:CZ3	2.05	0.91
54:S4:43:C:H5'	54:S4:44:G:OP2	1.71	0.91
60:SE:85:ASP:OD1	60:SE:119:LYS:NZ	2.05	0.90
64:SI:100:ARG:NH2	64:SI:131:ASP:OD2	2.06	0.88
61:SF:197:LYS:O	61:SF:201:GLU:HG3	1.74	0.88
51:S1:1589:G:H1	51:S1:1600:C:H5	1.22	0.87
4:L4:164:U:H4'	10:LB:349:MET:CE	2.04	0.86
67:SL:100:GLN:NE2	88:Sg:62:GLU:HG3	1.92	0.84
2:L2:1261:G:H1	2:L2:1305:C:H5	1.25	0.84
51:S1:1714:C:H5''	79:SX:8:ILE:HG21	1.60	0.84
57:SB:39:LYS:O	84:Sc:3:PHE:CE1	2.30	0.83
77:SV:25:ASN:OD1	77:SV:26:PHE:N	2.10	0.83
4:L4:24:A:H5''	16:LH:7:LYS:HB2	1.60	0.83
69:SN:14:TYR:CD2	69:SN:83:MET:HE3	2.15	0.82
88:Sg:173:ASP:O	88:Sg:173:ASP:OD1	1.97	0.82
10:LB:224:SER:HB3	10:LB:343:MET:HG2	1.62	0.81
2:L2:1510:A:H61	10:LB:327:ASP:H	1.26	0.80
69:SN:14:TYR:CD2	69:SN:83:MET:CE	2.64	0.80
54:S4:9:A:H2'	54:S4:11:C:H41	1.45	0.80
87:Sf:78:ARG:HD2	87:Sf:80:PHE:CE1	2.17	0.79
51:S1:340:G:H5''	60:SE:137:VAL:HG11	1.64	0.79
69:SN:23:ILE:HG21	69:SN:53:MET:HE1	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:Sh:154:MET:HA	89:Sh:154:MET:HE3	1.65	0.78
4:L4:164:U:C4'	10:LB:349:MET:HE1	2.07	0.78
17:LI:145:GLU:O	17:LI:149:LYS:HG2	1.82	0.78
45:Lk:73:SER:H	45:Lk:76:LYS:HE2	1.49	0.78
11:LC:295:GLU:OE1	24:LP:135:MET:HE3	1.83	0.78
2:L2:954:A:C5	42:Lh:114:MET:HE1	2.19	0.77
2:L2:1506:G:N2	39:Le:40:ARG:HH12	1.83	0.77
13:LE:149:ASP:HB3	13:LE:152:GLN:HB2	1.67	0.77
51:S1:1708:A:H4'	79:SX:138:ARG:HH12	1.49	0.77
62:SG:4:ASN:HD22	62:SG:111:LEU:HD11	1.50	0.76
88:Sg:173:ASP:C	88:Sg:174:ASN:OD1	2.28	0.76
48:Ln:10:MET:HG3	51:S1:2062:G:H5'	1.67	0.76
51:S1:876:G:H1	51:S1:885:C:H5	1.34	0.75
88:Sg:283:ILE:HD11	88:Sg:299:LYS:HE3	1.68	0.75
25:LQ:98:ARG:NH2	25:LQ:130:ASN:OD1	2.20	0.75
51:S1:996:C:H5''	64:SI:59:LYS:HE3	1.69	0.75
73:SR:6:ILE:HG13	82:Sa:41:MET:HB2	1.67	0.75
51:S1:146:U:H5'	62:SG:183:ILE:HD11	1.68	0.74
1:L1:77:U:H5''	21:LM:186:PRO:HG3	1.70	0.73
1:L1:1683:C:H42	1:L1:1709:U:H3	1.33	0.73
51:S1:878:C:H2'	51:S1:879:A:H8	1.53	0.73
88:Sg:238:ILE:HA	88:Sg:254:THR:HG22	1.69	0.73
72:SQ:111:GLU:N	72:SQ:111:GLU:OE2	2.20	0.73
1:L1:594:G:H1	1:L1:613:C:H5	1.36	0.73
2:L2:1214:G:H1	2:L2:1222:C:H5	1.32	0.73
59:SD:77:ARG:O	59:SD:81:GLU:HG2	1.88	0.73
2:L2:1225:A:H1'	20:LL:58:MET:HE3	1.71	0.73
58:SC:63:ARG:HH11	69:SN:98:GLN:NE2	1.87	0.73
51:S1:264:C:H5	51:S1:273:G:H1	1.37	0.73
2:L2:1012:U:OP1	15:LG:49[B]:ARG:NH1	2.22	0.72
67:SL:100:GLN:HE22	88:Sg:62:GLU:HG3	1.54	0.72
48:Ln:2:GLY:HA2	51:S1:2167:C:H5''	1.71	0.72
75:ST:36:MET:HE1	75:ST:58:MET:HE2	1.71	0.72
2:L2:954:A:C5	42:Lh:114:MET:CE	2.73	0.72
56:SA:44:ALA:HB2	70:SO:40:MET:HE2	1.71	0.72
67:SL:27:VAL:HG22	67:SL:71:ILE:HG12	1.71	0.72
5:L5:63:G:H2'	5:L5:64:G:O4'	1.90	0.72
51:S1:255:A:H5''	51:S1:943:U:H1'	1.72	0.72
19:LK:43:ASP:HB3	19:LK:46:MET:HB2	1.69	0.72
51:S1:878:C:H5	51:S1:883:G:H1	1.38	0.72
61:SF:92:MET:HE1	61:SF:112:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SM:77:PHE:HB3	74:SS:53:PHE:HB3	1.71	0.71
1:L1:596:A:H61	1:L1:609:C:H5	1.38	0.71
21:LM:4:PHE:CE2	21:LM:50:MET:HE2	2.25	0.71
84:Sc:47:VAL:HG12	84:Sc:55:VAL:HG11	1.70	0.71
51:S1:1980:U:H4'	51:S1:2019:C:H4'	1.71	0.71
66:SK:161:GLU:OE2	66:SK:164:ARG:NH2	2.24	0.71
71:SP:11:ARG:NH2	76:SU:117:LYS:O	2.24	0.71
51:S1:273:G:H4'	89:Sh:227:ARG:HH21	1.56	0.71
72:SQ:29:ALA:O	72:SQ:33:VAL:HG12	1.91	0.71
2:L2:1100:A:H5''	12:LD:97:ASN:HD22	1.55	0.71
1:L1:447:G:H1'	7:L7:16:A:H61	1.54	0.70
7:L7:169:A:H3'	7:L7:170:A:H8	1.55	0.70
1:L1:1352:C:H2'	1:L1:1353:A:C8	2.25	0.70
49:Lo:50:LYS:O	49:Lo:51:ALA:CB	2.38	0.70
57:SB:63:LEU:HD22	80:SY:83:MET:HE2	1.74	0.70
71:SP:48:LYS:HD3	71:SP:99:GLU:OE2	1.90	0.70
1:L1:163:U:H2'	1:L1:164:G:C8	2.27	0.70
8:L8:53:A:H5''	23:LO:233:SER:HB2	1.73	0.70
13:LE:5:LYS:HD3	13:LE:7:LEU:HD11	1.74	0.70
25:LQ:184:GLU:OE2	64:SI:10:LYS:NZ	2.25	0.70
19:LK:136:PRO:HB3	19:LK:141:LYS:HB3	1.73	0.69
73:SR:6:ILE:H	73:SR:6:ILE:HD12	1.57	0.69
57:SB:152:ASP:OD2	57:SB:169:ARG:NH1	2.25	0.69
2:L2:502[A]:A2M:N6	51:S1:2160:G:OP2	2.26	0.69
49:Lo:52:VAL:HG23	49:Lo:68:ALA:HB1	1.73	0.69
51:S1:1207:U:H5'	75:ST:55:ARG:HD3	1.75	0.69
61:SF:238:THR:HG22	61:SF:240:ASP:H	1.58	0.68
28:LT:9:GLN:HE21	28:LT:9:GLN:HA	1.58	0.68
28:LT:48:TYR:HB3	28:LT:92:MET:HE3	1.75	0.68
51:S1:1684:U:H3	51:S1:1820:G:H22	1.40	0.68
22:LN:36:ILE:HD12	22:LN:73:ASN:HB2	1.75	0.68
39:Le:133:THR:O	39:Le:137:HIS:HB3	1.94	0.68
51:S1:1908:A:H5''	51:S1:1909:C:H5	1.58	0.68
54:S4:26:A:H3'	54:S4:27:G:C8	2.29	0.68
59:SD:107:ARG:HH22	59:SD:125:ARG:HH21	1.40	0.68
68:SM:91:PRO:HD2	68:SM:94:GLN:HE21	1.59	0.68
1:L1:255:G:O6	31:LW:59:THR:HG22	1.94	0.68
1:L1:790:C:H5	11:LC:305:LEU:H	1.39	0.68
1:L1:1363:A:H4'	1:L1:1364:A:H5''	1.76	0.68
21:LM:9:GLU:OE1	43:Li:44:LYS:NZ	2.27	0.68
54:S4:26:A:H3'	54:S4:27:G:H8	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L4:4:G:H1	4:L4:20:U:H3	1.41	0.68
51:S1:694:U:H3	51:S1:751:G:H1	1.42	0.67
56:SA:123:MET:HG2	56:SA:163:VAL:HG13	1.76	0.67
37:Lc:57:ARG:NH2	37:Lc:186:VAL:O	2.27	0.67
2:L2:954:A:C4	42:Lh:114:MET:HE3	2.29	0.67
10:LB:80:GLU:HG3	10:LB:324:VAL:HG13	1.76	0.67
1:L1:820:U:H6	1:L1:823:G:H1	1.42	0.67
73:SR:6:ILE:CD1	82:Sa:43:ASP:OD1	2.41	0.67
12:LD:43:CYS:HB3	12:LD:45:GLN:HG2	1.77	0.67
51:S1:693:C:H42	51:S1:752:C:H42	1.42	0.67
61:SF:92:MET:HE2	61:SF:137:ILE:HG12	1.77	0.67
2:L2:746:A:H2'	2:L2:747:A:C8	2.29	0.67
51:S1:1663:U:H4'	77:SV:4:ILE:HD11	1.76	0.67
72:SQ:38:LEU:HD13	72:SQ:43:LEU:HD12	1.76	0.67
24:LP:23:ASN:HB3	24:LP:26:ILE:HB	1.77	0.67
2:L2:1335:C:H5''	47:Lm:125:LYS:HG3	1.77	0.67
24:LP:57:SER:O	24:LP:153:ARG:NH2	2.27	0.66
10:LB:13:HIS:HD2	10:LB:15:GLY:H	1.42	0.66
50:Lp:25:VAL:HG22	50:Lp:72:LEU:HD23	1.77	0.66
34:LZ:120:ARG:NH1	40:Lf:114:MET:O	2.28	0.66
51:S1:2199:C:H1'	83:Sb:7:ASN:HD21	1.59	0.66
10:LB:13:HIS:CD2	10:LB:15:GLY:H	2.13	0.66
28:LT:9:GLN:HA	28:LT:9:GLN:NE2	2.11	0.66
61:SF:55:VAL:HG21	61:SF:78:ILE:HG23	1.77	0.66
63:SH:83:LEU:HD22	63:SH:94:PRO:HB2	1.77	0.66
24:LP:165:PRO:HB3	24:LP:193:LYS:HB2	1.77	0.66
88:Sg:199:THR:HG21	88:Sg:240:GLN:HA	1.78	0.66
23:LO:55:ILE:HG21	23:LO:164:ARG:HH21	1.60	0.66
18:LJ:17:VAL:HB	18:LJ:53:SER:HB3	1.78	0.66
58:SC:63:ARG:HH11	69:SN:98:GLN:HE22	1.44	0.66
70:SO:96:VAL:HG12	70:SO:132:SER:HB2	1.76	0.66
1:L1:700:A:C2	1:L1:845:OMU:H5	2.31	0.66
1:L1:112:U:H3	1:L1:357:A:H62	1.44	0.65
18:LJ:42:LYS:HG3	18:LJ:59:MET:HG2	1.78	0.65
58:SC:207:ILE:HD13	77:SV:50:ILE:HD11	1.76	0.65
75:ST:45:MET:HE1	75:ST:53:GLU:HG2	1.77	0.65
14:LF:194:ASN:O	19:LK:110:ARG:NH2	2.29	0.65
58:SC:71:CYS:SG	69:SN:22:VAL:HG11	2.36	0.65
61:SF:83:ILE:HG21	61:SF:88:LEU:HD13	1.79	0.65
79:SX:55:GLY:HA2	79:SX:96:LYS:HD2	1.78	0.65
46:Ll:7:LEU:O	46:Ll:11:LYS:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ln:3:THR:HG23	51:S1:2196:G:H5''	1.78	0.65
2:L2:1485:G:H1'	19:LK:164:MET:HA	1.78	0.65
10:LB:232:GLU:HG3	10:LB:275:HIS:HB3	1.77	0.65
25:LQ:116:ASP:OD1	25:LQ:116:ASP:N	2.30	0.65
24:LP:35:PHE:HA	24:LP:38:LYS:HE2	1.79	0.65
78:SW:63:LEU:O	78:SW:67:LEU:HD23	1.96	0.65
79:SX:8:ILE:HD11	79:SX:154:ARG:HD3	1.79	0.65
88:Sg:9:GLY:O	88:Sg:60:ARG:NH2	2.29	0.65
1:L1:586:U:H5''	11:LC:335:ARG:HD2	1.78	0.64
19:LK:8:CYS:HB3	26:LR:150:SER:HB3	1.79	0.64
20:LL:72:THR:HG22	20:LL:108:LYS:HB3	1.79	0.64
57:SB:172:LYS:NZ	77:SV:90:ASP:OD2	2.30	0.64
1:L1:1685:G:H22	1:L1:1707:U:H3	1.45	0.64
31:LW:28:MET:HB3	31:LW:98:PRO:HG2	1.80	0.64
33:LY:54:VAL:HG22	33:LY:57:MET:HE3	1.79	0.64
51:S1:1398:C:H42	56:SA:161:ARG:HG3	1.61	0.64
69:SN:61:LEU:HD13	69:SN:79:GLY:HA2	1.79	0.64
78:SW:71:LYS:NZ	78:SW:95:GLU:O	2.30	0.64
51:S1:784:C:H3'	51:S1:787:G:H1	1.63	0.64
2:L2:5:A:H1'	3:L3:18:A:H1'	1.80	0.64
60:SE:97:ARG:HB2	60:SE:111:LEU:HD11	1.78	0.64
49:Lo:50:LYS:O	49:Lo:51:ALA:HB2	1.97	0.64
71:SP:101:LEU:HB3	71:SP:124:LYS:HB2	1.78	0.64
5:L5:55:U:H3	5:L5:61:C:H41	1.44	0.64
62:SG:164:ARG:NH1	62:SG:172:ASP:OD2	2.28	0.64
2:L2:1514:U:H5'	39:Le:30:ARG:NH1	2.12	0.64
21:LM:4:PHE:CZ	21:LM:50:MET:HE2	2.33	0.64
22:LN:177:LEU:HB2	22:LN:180:GLU:HG3	1.80	0.64
85:Sd:61:ARG:NH2	85:Sd:77:GLU:O	2.31	0.64
1:L1:216:G:H5'	34:LZ:128:ARG:HG2	1.80	0.63
2:L2:743:C:H2'	2:L2:744:G:H8	1.62	0.63
31:LW:48:ARG:HE	31:LW:107:LYS:HG2	1.64	0.63
64:SI:132:MET:CE	64:SI:172:VAL:HG13	2.28	0.63
18:LJ:32:GLY:HA3	18:LJ:68:LYS:HD3	1.80	0.63
60:SE:121:MET:HE1	60:SE:159:TYR:CD2	2.33	0.63
85:Sd:59:ILE:HG13	85:Sd:81:GLU:HG2	1.80	0.63
34:LZ:22:ARG:HB3	40:Lf:76:PRO:HG2	1.81	0.63
69:SN:69:ARG:NH1	74:SS:21:CYS:SG	2.72	0.63
1:L1:1675:A:H3'	1:L1:1676:G:H8	1.63	0.63
9:LA:234:LYS:HG2	9:LA:238:ILE:HG12	1.79	0.63
51:S1:606:G:N3	86:Se:60:GLN:NE2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SA:88:PHE:HB3	56:SA:100:THR:HB	1.79	0.63
1:L1:1609:A:H5''	28:LT:125:MET:HE1	1.80	0.63
10:LB:125:SER:O	39:Le:23:ARG:NH2	2.32	0.63
2:L2:683:G:H1	2:L2:756:C:H5	1.46	0.63
81:SZ:89:LEU:O	81:SZ:93:GLU:HB2	1.99	0.63
84:Sc:47:VAL:CG1	84:Sc:55:VAL:HG11	2.29	0.63
10:LB:374:HIS:O	32:LX:37:ARG:NH2	2.31	0.62
51:S1:1513:C:H2'	51:S1:1514:A:H8	1.64	0.62
51:S1:1870:A:H4'	51:S1:1960:G:H4'	1.81	0.62
54:S4:9:A:H1'	54:S4:45:U:H2'	1.81	0.62
56:SA:175:LYS:O	56:SA:179:SER:OG	2.13	0.62
51:S1:825:C:H1'	51:S1:826:A:H5'	1.81	0.62
84:Sc:20:HIS:HB3	84:Sc:23:ARG:HB2	1.80	0.62
51:S1:1976:U:H3'	73:SR:122:ARG:NH2	2.14	0.62
71:SP:107:ARG:HB3	71:SP:110:HIS:HB3	1.80	0.62
79:SX:52:SER:OG	79:SX:69:ARG:NH2	2.31	0.62
34:LZ:103:LEU:O	34:LZ:107:SER:OG	2.17	0.62
2:L2:479:C:H5	2:L2:1030:A:H1'	1.65	0.62
51:S1:792:G:H3'	51:S1:793:G:H21	1.64	0.62
66:SK:68:ALA:HB2	66:SK:201:ILE:HD11	1.80	0.62
79:SX:131:GLN:HG2	79:SX:131:GLN:O	1.99	0.62
62:SG:235:LYS:O	62:SG:239:GLN:HG2	1.99	0.62
2:L2:1456:C:H5	2:L2:1468:G:H1	1.47	0.62
10:LB:57:VAL:HG22	10:LB:73:VAL:HG22	1.82	0.62
49:Lo:76:ASN:O	49:Lo:80:ARG:HG3	2.00	0.62
2:L2:502[A]:A2M:HM'3	51:S1:2065:G:H21	1.65	0.62
35:La:77:ARG:HA	35:La:80:ARG:HE	1.65	0.62
53:S3:57:A:H2'	53:S3:58:A:H5''	1.81	0.61
68:SM:64:LYS:O	74:SS:45:ARG:NH1	2.33	0.61
53:S3:55:U:H2'	53:S3:57:A:N7	2.15	0.61
58:SC:207:ILE:HD11	77:SV:46:LEU:HD13	1.82	0.61
60:SE:247:ILE:O	60:SE:251:GLU:HG2	2.00	0.61
18:LJ:105:VAL:HG12	18:LJ:111:MET:HA	1.82	0.61
51:S1:2121:C:H2'	51:S1:2122:G:C8	2.36	0.61
5:L5:73:G:H3'	5:L5:74:A:H8	1.65	0.61
12:LD:19:LEU:HD12	12:LD:131:VAL:HG22	1.83	0.61
51:S1:955:A:HO2'	51:S1:956:A:H8	1.48	0.61
56:SA:31:ASP:OD1	56:SA:45:LYS:NZ	2.33	0.61
51:S1:2005:U:H2'	51:S1:2006:A:H8	1.66	0.61
68:SM:17:VAL:HG11	68:SM:95:VAL:HG21	1.82	0.61
73:SR:39:ILE:HG21	79:SX:58:ARG:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LS:83:ARG:HE	27:LS:85:LEU:HD21	1.65	0.61
28:LT:112:MET:SD	28:LT:152:GLU:HG3	2.40	0.61
2:L2:1279:G:H5'	2:L2:1280:U:H5''	1.81	0.61
51:S1:2059:C:H5	51:S1:2166:A:H61	1.46	0.61
1:L1:1110:G:H21	27:LS:61:THR:HG21	1.64	0.61
1:L1:514:C:H5''	26:LR:70:LYS:HG3	1.83	0.61
12:LD:43:CYS:CB	12:LD:71:CYS:HG	2.14	0.61
1:L1:745:U:H5'	1:L1:830:G:H1'	1.83	0.61
51:S1:286:G:H1'	62:SG:217:ALA:HB1	1.82	0.61
2:L2:469:G:H2'	2:L2:470:A:C8	2.36	0.60
34:LZ:22:ARG:NH1	40:Lf:82:ASP:OD2	2.34	0.60
62:SG:211:GLU:OE2	62:SG:214:ARG:NH1	2.32	0.60
88:Sg:220:LEU:HD11	88:Sg:250:MET:HE1	1.83	0.60
42:Lh:65:ALA:O	42:Lh:73:LYS:NZ	2.33	0.60
53:S3:57:A:H2'	53:S3:58:A:C5'	2.31	0.60
80:SY:3:THR:OG1	80:SY:4:ILE:N	2.30	0.60
51:S1:695:G:H22	51:S1:750:U:H3	1.49	0.60
51:S1:918:A:H3'	51:S1:919:G:H8	1.66	0.60
58:SC:166:PHE:CD2	58:SC:199:PRO:HG2	2.37	0.60
69:SN:14:TYR:CD2	69:SN:83:MET:HE1	2.35	0.60
88:Sg:89:ILE:HB	88:Sg:103:PHE:CE1	2.36	0.60
11:LC:355:ALA:O	11:LC:359:ARG:HG3	2.02	0.60
28:LT:87:SER:O	28:LT:91:MET:HG2	2.00	0.60
71:SP:68:LYS:HB3	71:SP:91:LEU:HD13	1.82	0.60
51:S1:1398:C:H2'	56:SA:165:TRP:CE2	2.36	0.60
62:SG:221:ARG:O	62:SG:225:GLN:HG2	2.01	0.60
69:SN:18:PHE:HD2	69:SN:83:MET:HB3	1.67	0.60
69:SN:53:MET:HE3	69:SN:73:TRP:CE3	2.37	0.60
34:LZ:21:LYS:HG2	34:LZ:26:ARG:HG2	1.83	0.60
59:SD:177:LYS:HB3	59:SD:181:ARG:HH12	1.67	0.60
88:Sg:22:GLN:NE2	88:Sg:75:HIS:O	2.34	0.60
44:Lj:4:GLY:O	44:Lj:8:MET:HG2	2.02	0.60
1:L1:1687:G:H1	1:L1:1705:G:H22	1.48	0.60
12:LD:27:GLU:OE1	12:LD:31:ARG:NH1	2.35	0.60
78:SW:41:LYS:HG2	78:SW:52:MET:HE3	1.83	0.60
81:SZ:85:ASP:N	81:SZ:85:ASP:OD1	2.33	0.60
1:L1:1048:A:H3'	1:L1:1049:A:H8	1.67	0.59
51:S1:148:G:H2'	51:S1:149:G:C8	2.37	0.59
51:S1:1281:C:HO2'	65:SJ:2:THR:N	1.99	0.59
1:L1:160:C:O2'	1:L1:161:A:O5'	2.19	0.59
3:L3:16:G:H1	3:L3:20:C:H2'	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:2183:G:H3'	51:S1:2184:MA6:H8	1.84	0.59
67:SL:35:ILE:HG12	67:SL:71:ILE:HB	1.84	0.59
51:S1:547:U:H3'	51:S1:548:G:H8	1.67	0.59
51:S1:817:A:H2'	51:S1:819:G:H2'	1.82	0.59
72:SQ:61:MET:HG3	72:SQ:87:ASP:OD1	2.01	0.59
11:LC:364:LYS:O	11:LC:368:THR:HG23	2.03	0.59
34:LZ:51:ALA:HB3	34:LZ:96:VAL:HG13	1.84	0.59
51:S1:878:C:H2'	51:S1:879:A:C8	2.36	0.59
51:S1:879:A:H3'	51:S1:880:U:H6	1.68	0.59
61:SF:51:LEU:HD21	61:SF:66:ILE:HD13	1.84	0.59
69:SN:94:MET:HE3	69:SN:98:GLN:HG3	1.83	0.59
2:L2:969:A:H1'	9:LA:95:PRO:HB3	1.83	0.59
27:LS:25:PRO:HG2	27:LS:94:GLU:HG2	1.84	0.59
14:LF:192:ARG:NH2	41:Lg:66:ASP:OD1	2.34	0.59
88:Sg:250:MET:HE2	88:Sg:263:LEU:HD21	1.84	0.59
88:Sg:263:LEU:O	88:Sg:266:LYS:NZ	2.29	0.59
12:LD:63:ARG:NH1	12:LD:64:ASN:OD1	2.36	0.59
62:SG:101:ARG:NH2	62:SG:104:VAL:O	2.36	0.59
9:LA:62:GLU:HG3	9:LA:73:LYS:HG3	1.85	0.59
16:LH:131:VAL:HG12	16:LH:132:ARG:HG3	1.84	0.59
62:SG:38:ASP:C	62:SG:38:ASP:OD2	2.45	0.59
79:SX:117:CYS:O	79:SX:121:THR:HG23	2.02	0.59
1:L1:1779:G:H1'	3:L3:18:A:H2'	1.85	0.58
2:L2:1004:G:H3'	2:L2:1005:A:H2'	1.85	0.58
48:Ln:4:VAL:HG21	51:S1:2175:C:H4'	1.83	0.58
58:SC:108:LEU:HD11	58:SC:114:VAL:HG12	1.83	0.58
4:L4:170:G:H4'	4:L4:171:A:H3'	1.84	0.58
14:LF:50:ARG:NH1	14:LF:180:SER:OG	2.36	0.58
75:ST:87:ASP:OD1	75:ST:87:ASP:N	2.32	0.58
1:L1:73:U:H5''	17:LI:63:VAL:HB	1.84	0.58
9:LA:80:GLU:CG	49:Lo:66:GLY:HA3	2.34	0.58
11:LC:299:VAL:HG21	24:LP:138:PRO:HB2	1.85	0.58
28:LT:60:PHE:O	28:LT:64:ASN:ND2	2.36	0.58
31:LW:52:GLU:HG3	31:LW:105:LYS:HB3	1.85	0.58
51:S1:436:C:H2'	51:S1:437:C:C6	2.38	0.58
53:S3:33:U:OP2	67:SL:149:ARG:NH1	2.34	0.58
63:SH:45:ARG:HB2	63:SH:48:TYR:HB2	1.85	0.58
1:L1:447:G:O2'	7:L7:15:G:N2	2.37	0.58
1:L1:1051:C:H5	1:L1:1097:A:H62	1.50	0.58
1:L1:1538:U:H2'	1:L1:1539:A2M:H8	1.85	0.58
10:LB:124:GLN:O	39:Le:3:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:S4:37:A:H3'	54:S4:38:A:C8	2.39	0.58
62:SG:58:ASP:HB3	62:SG:101:ARG:HG3	1.84	0.58
1:L1:1276:U:H5	1:L1:1353:A:N1	2.01	0.58
51:S1:879:A:H3'	51:S1:880:U:C6	2.38	0.58
51:S1:880:U:N3	81:SZ:13:ARG:HD2	2.19	0.58
22:LN:30:LYS:HG3	22:LN:63:GLU:HG3	1.86	0.58
65:SJ:86:TYR:O	65:SJ:90:MET:HG3	2.03	0.58
1:L1:576:G:H3'	1:L1:577:C:H5''	1.86	0.58
14:LF:100:PRO:HG2	14:LF:156:LYS:HE2	1.86	0.58
51:S1:259:C:H2'	51:S1:260:A:C8	2.39	0.58
34:LZ:75:ARG:HG3	34:LZ:76:GLN:HG3	1.86	0.58
51:S1:2037:U:H2'	51:S1:2038:C:C6	2.39	0.58
54:S4:7:A:H2'	54:S4:49:C:H1'	1.86	0.58
60:SE:29:ARG:HG3	60:SE:30:PRO:HD2	1.86	0.58
88:Sg:63:GLY:O	88:Sg:90:ARG:NH2	2.37	0.58
1:L1:554:A:H5''	1:L1:555:U:H5	1.68	0.57
7:L7:89:U:H2'	7:L7:90:U:C6	2.39	0.57
9:LA:64:ARG:NH2	15:LG:39:GLN:O	2.35	0.57
51:S1:701:G:H22	51:S1:745:G:H1	1.50	0.57
51:S1:1885:A:H5'	67:SL:20:THR:HG21	1.86	0.57
5:L5:38:U:H5''	10:LB:315:MET:HE2	1.85	0.57
9:LA:92:GLN:OE1	9:LA:106:GLN:NE2	2.37	0.57
18:LJ:86:SER:OG	32:LX:19:ARG:NH1	2.37	0.57
51:S1:1976:U:H3'	73:SR:122:ARG:HH21	1.69	0.57
76:SU:48:ARG:NH1	76:SU:68:TYR:O	2.37	0.57
12:LD:88:VAL:HG11	12:LD:108:ILE:HG13	1.85	0.57
51:S1:2026:U:H2'	51:S1:2027:G:C8	2.39	0.57
61:SF:50:LYS:HD2	61:SF:259:LEU:HD13	1.84	0.57
58:SC:55:ARG:HD2	58:SC:55:ARG:H	1.69	0.57
75:ST:45:MET:HE3	75:ST:49:GLN:HB3	1.86	0.57
1:L1:447:G:H1'	7:L7:16:A:N6	2.20	0.57
4:L4:149:U:H1'	4:L4:150:A:H2'	1.86	0.57
21:LM:121:VAL:HG11	21:LM:131:GLU:HG3	1.86	0.57
51:S1:256:A:H5'	51:S1:944:U:H1'	1.86	0.57
1:L1:593:C:H2'	1:L1:594:G:C8	2.40	0.57
5:L5:73:G:H3'	5:L5:74:A:C8	2.39	0.57
11:LC:252:GLN:O	11:LC:256:GLU:HG3	2.04	0.57
50:Lp:10:MET:HE1	50:Lp:72:LEU:HD13	1.86	0.57
50:Lp:63:LYS:HD2	50:Lp:87:ARG:NH1	2.20	0.57
51:S1:1911:U:H5	51:S1:1928:G:H1	1.52	0.57
1:L1:1371:OMU:H5'	1:L1:1372:G:H3'	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:382:A2M:H2	2:L2:389:A:N7	2.18	0.57
2:L2:760:U:H5'	15:LG:69:ARG:HG3	1.87	0.57
20:LL:134:ILE:HG21	20:LL:141:VAL:HG23	1.85	0.57
22:LN:38:ARG:NH1	22:LN:45:GLU:OE1	2.38	0.57
29:LU:13:TYR:HE1	29:LU:15:ARG:HD3	1.69	0.57
51:S1:895:A:H3'	51:S1:896:A:H8	1.69	0.57
2:L2:1485:G:C4	19:LK:164:MET:HG2	2.39	0.57
3:L3:171:U:H3'	3:L3:172:G:H21	1.69	0.57
63:SH:107:PRO:HG3	63:SH:179:LYS:HA	1.87	0.57
2:L2:1175:A:H2'	2:L2:1176:A:C8	2.40	0.57
13:LE:20:VAL:HG11	13:LE:45:LEU:HB2	1.85	0.57
27:LS:56:TYR:O	27:LS:60:ARG:NH1	2.38	0.57
39:Le:86:MET:HE2	39:Le:119:LEU:HD21	1.87	0.57
43:Li:93:MET:HA	43:Li:93:MET:HE2	1.85	0.57
64:SI:61:VAL:HG11	64:SI:175:VAL:HG21	1.86	0.57
68:SM:96:LYS:O	68:SM:100:SER:OG	2.20	0.57
1:L1:823:G:H2'	1:L1:823:G:N3	2.20	0.56
2:L2:1069:A:H2'	2:L2:1070:A:C8	2.40	0.56
51:S1:695:G:H1	51:S1:750:U:H3	1.52	0.56
61:SF:154:GLY:N	61:SF:165:THR:O	2.31	0.56
68:SM:23:SER:HB3	68:SM:29:VAL:HB	1.87	0.56
3:L3:151:A:H5'	45:Lk:26:LYS:HE2	1.87	0.56
31:LW:47:VAL:HG21	31:LW:98:PRO:HB3	1.86	0.56
38:Ld:41:SER:HG	38:Ld:93:SER:HG	1.49	0.56
51:S1:1523:A:H2'	51:S1:1524:G:C8	2.39	0.56
68:SM:39:ARG:HH12	68:SM:101:PHE:HB3	1.69	0.56
85:Sd:22:GLN:HG2	85:Sd:46:LEU:HD12	1.88	0.56
1:L1:882:A:N1	1:L1:914:U:H5	2.02	0.56
1:L1:998:A:H5''	40:Lf:56:LYS:HG2	1.87	0.56
3:L3:198:A:H5'	49:Lo:52:VAL:HB	1.87	0.56
13:LE:18:VAL:HG22	13:LE:27:VAL:HG22	1.87	0.56
33:LY:104:LYS:HG3	33:LY:107:ARG:HH21	1.69	0.56
51:S1:918:A:H3'	51:S1:919:G:C8	2.40	0.56
51:S1:2121:C:H2'	51:S1:2122:G:H8	1.69	0.56
61:SF:102:THR:HG22	61:SF:104:ALA:H	1.69	0.56
73:SR:25:ARG:HB2	73:SR:30:ALA:HB2	1.87	0.56
26:LR:48:ARG:HG3	26:LR:54:LYS:HD3	1.87	0.56
28:LT:41:LEU:HD13	28:LT:150:MET:HE1	1.88	0.56
51:S1:640:A:H2'	51:S1:641:A:C8	2.41	0.56
60:SE:138:THR:OG1	60:SE:140:ASP:OD1	2.21	0.56
66:SK:76:VAL:HG12	66:SK:108:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:93:PRO:HB2	22:LN:125:VAL:HG13	1.87	0.56
51:S1:2102:A:H61	51:S1:2121:C:H42	1.53	0.56
1:L1:699:C:H2'	1:L1:700:A:C8	2.41	0.56
28:LT:9:GLN:HE21	28:LT:9:GLN:CA	2.16	0.56
28:LT:35:VAL:HG13	28:LT:36:ILE:HG23	1.87	0.56
86:Se:42:ARG:O	86:Se:47:LYS:HD3	2.06	0.56
88:Sg:125:ALA:HB1	88:Sg:153:VAL:HB	1.87	0.56
1:L1:93:G:H2'	1:L1:94:A:C8	2.40	0.56
10:LB:226:THR:HG22	10:LB:336:SER:HB3	1.87	0.56
51:S1:180:G:H22	51:S1:316:A:H5'	1.70	0.56
64:SI:146:ARG:HA	65:SJ:49:GLU:OE1	2.06	0.56
67:SL:37:VAL:HB	67:SL:45:ILE:HD11	1.88	0.56
67:SL:99:PHE:HB3	67:SL:108:LYS:HB2	1.86	0.56
1:L1:381:G:N7	11:LC:192:ARG:HD3	2.21	0.56
15:LG:47:LEU:O	15:LG:51:MET:HG3	2.06	0.56
21:LM:73:ARG:NH1	21:LM:88:GLY:O	2.39	0.56
51:S1:1716:A:N1	79:SX:26:ARG:NH1	2.54	0.56
59:SD:112:VAL:HG13	59:SD:117:LEU:HB2	1.86	0.56
78:SW:102:ALA:HB1	78:SW:109:PHE:HB3	1.88	0.56
1:L1:3:A:C6	7:L7:169:A:H1'	2.40	0.56
22:LN:11:PHE:O	22:LN:59:GLN:NE2	2.27	0.56
32:LX:2:ARG:NH2	32:LX:3:THR:O	2.39	0.56
37:Lc:96:VAL:HG13	37:Lc:146:TYR:HB3	1.87	0.56
60:SE:49:LEU:HD11	60:SE:96:PHE:HZ	1.71	0.56
1:L1:1533:PSU:H2'	1:L1:1534:G:C8	2.41	0.56
2:L2:1506:G:H21	39:Le:40:ARG:HH12	1.52	0.56
10:LB:107:ALA:HB1	10:LB:205:GLU:HG3	1.88	0.56
13:LE:92:ARG:HD3	13:LE:142:GLU:HG3	1.87	0.56
51:S1:381:G:H3'	76:SU:148:LYS:HB3	1.87	0.56
2:L2:1136:U:H2'	2:L2:1137:G:C8	2.41	0.55
2:L2:1279:G:H3'	2:L2:1282:C:N4	2.21	0.55
44:Lj:55:LYS:HA	44:Lj:58:ARG:HD2	1.87	0.55
88:Sg:193:HIS:CE1	88:Sg:197:VAL:HG22	2.40	0.55
1:L1:1571:C:H5	28:LT:85:ARG:HH21	1.52	0.55
51:S1:1531:G:H21	51:S1:1861:A:H2	1.53	0.55
57:SB:30:THR:O	57:SB:31:ARG:HG2	2.06	0.55
67:SL:131:GLU:OE1	67:SL:140:ALA:HB1	2.06	0.55
73:SR:106:THR:HG23	73:SR:109:ARG:NH2	2.21	0.55
1:L1:1527:OMC:HM23	11:LC:94:MET:HG3	1.88	0.55
22:LN:35:ASP:OD1	22:LN:86:HIS:NE2	2.38	0.55
32:LX:90:ASP:OD2	32:LX:92:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S3:56:C:H3'	53:S3:57:A:H8	1.71	0.55
5:L5:2:U:H5	5:L5:134:C:H5'	1.71	0.55
51:S1:606:G:H1'	86:Se:60:GLN:HE21	1.71	0.55
51:S1:1659:U:H2'	51:S1:1660:G:H8	1.70	0.55
51:S1:1835:U:H4'	74:SS:25:CYS:HB2	1.88	0.55
88:Sg:114:ALA:HB3	88:Sg:123:VAL:HG23	1.89	0.55
1:L1:83:A:H61	1:L1:98:A:H3'	1.71	0.55
2:L2:1019:A:H4'	2:L2:1020:C:H5'	1.89	0.55
9:LA:206:PRO:HG3	9:LA:213:GLY:HA3	1.89	0.55
4:L4:114:A:H3'	4:L4:115:A:H8	1.71	0.55
51:S1:1618:U:H2'	51:S1:1619:G:C8	2.42	0.55
69:SN:69:ARG:HD2	74:SS:26:SER:HB3	1.89	0.55
51:S1:793:G:H3'	51:S1:794:U:H6	1.72	0.55
51:S1:889:A:C2	60:SE:16:MET:HG2	2.42	0.55
51:S1:948:G:H2'	51:S1:949:U:H5'	1.88	0.55
75:ST:94:ARG:HG2	75:ST:98:MET:HE3	1.89	0.55
12:LD:42:LEU:HD13	12:LD:116:ILE:HD11	1.88	0.55
51:S1:443:A:H5''	66:SK:25:MET:HA	1.89	0.55
72:SQ:61:MET:HE3	72:SQ:89:ILE:HD13	1.89	0.55
82:Sa:91:LEU:HD21	82:Sa:94:CYS:HB2	1.89	0.55
88:Sg:85:TRP:HA	88:Sg:109:ASP:HB2	1.89	0.55
1:L1:554:A:H5''	1:L1:555:U:C5	2.42	0.55
37:Lc:194:MET:HE1	37:Lc:212:MET:HE3	1.89	0.55
60:SE:56:ARG:O	60:SE:60:MET:HG3	2.07	0.55
1:L1:273:A:C6	44:Lj:79:LYS:HA	2.42	0.55
10:LB:57:VAL:HB	10:LB:365:PHE:HB3	1.89	0.55
51:S1:1577:U:H3'	51:S1:1578:G:H8	1.72	0.55
72:SQ:62:CYS:SG	72:SQ:63:ILE:N	2.80	0.55
1:L1:120:G:H1'	1:L1:122:A:H62	1.72	0.54
2:L2:1379:A:H5''	2:L2:1381:G:H4'	1.88	0.54
51:S1:1725:C:N3	79:SX:11:ILE:HG23	2.23	0.54
13:LE:109:ILE:HD11	13:LE:131:VAL:HG21	1.90	0.54
65:SJ:18:GLU:HG3	65:SJ:69:LEU:HD23	1.89	0.54
71:SP:41:PHE:HZ	71:SP:102:VAL:HG22	1.72	0.54
13:LE:95:TYR:HA	13:LE:176:ASP:HB3	1.89	0.54
51:S1:234:C:HO2'	51:S1:235:C:H6	1.55	0.54
51:S1:1909:C:H2'	51:S1:1910:C:C6	2.43	0.54
58:SC:19:GLU:HG2	69:SN:68:TRP:CE3	2.42	0.54
51:S1:1014:C:H2'	51:S1:1015:G:C8	2.42	0.54
2:L2:1318:PSU:H1'	10:LB:255:ALA:HB3	1.89	0.54
13:LE:75:HIS:O	13:LE:79:MET:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:459:A:H2'	2:L2:460:A:C8	2.43	0.54
12:LD:43:CYS:HG	12:LD:71:CYS:CB	2.21	0.54
12:LD:43:CYS:HG	12:LD:71:CYS:HB3	1.71	0.54
77:SV:38:VAL:HG23	77:SV:39:THR:HG23	1.89	0.54
2:L2:1407:A:N7	9:LA:215:ASN:ND2	2.56	0.54
51:S1:949:U:H2'	51:S1:950:U:C6	2.42	0.54
51:S1:1101:A:H2'	51:S1:1102:G:C4	2.43	0.54
1:L1:344:A:N1	2:L2:1221:U:H5	2.06	0.54
2:L2:1250:C:H2'	2:L2:1251:A:C8	2.42	0.54
2:L2:1506:G:H21	39:Le:40:ARG:NH1	2.06	0.54
9:LA:249:GLY:HA2	51:S1:1234:G:C6	2.43	0.54
13:LE:184:THR:OG1	13:LE:185:ASN:N	2.40	0.54
16:LH:176:GLU:O	16:LH:180:VAL:HG23	2.08	0.54
25:LQ:186:GLU:CD	25:LQ:189:ARG:HH12	2.16	0.54
51:S1:374:U:H2'	51:S1:375:G:C8	2.42	0.54
53:S3:71:C:H2'	53:S3:72:A:C8	2.43	0.54
54:S4:43:C:C5'	54:S4:44:G:OP2	2.50	0.54
57:SB:15:GLU:OE2	77:SV:118:ARG:N	2.40	0.54
1:L1:1098:A:H2'	1:L1:1099:A:C8	2.43	0.54
2:L2:1124:A:H2'	2:L2:1125:G:C8	2.42	0.54
7:L7:21:U:H6	11:LC:195:MET:HE2	1.73	0.54
47:Lm:97:ARG:HG2	47:Lm:122:ARG:HG2	1.90	0.54
58:SC:74:GLN:NE2	69:SN:22:VAL:O	2.41	0.54
86:Se:41:THR:HA	86:Se:45:LEU:HB2	1.90	0.54
88:Sg:111:LEU:HD21	88:Sg:127:ARG:HG2	1.90	0.54
1:L1:161:A:H2'	1:L1:162:U:C6	2.43	0.54
12:LD:108:ILE:HG12	12:LD:114:LEU:HD21	1.89	0.54
76:SU:36:PRO:HG3	76:SU:47:ILE:HD11	1.89	0.54
1:L1:443:A:N3	46:Ll:36:LYS:NZ	2.55	0.53
2:L2:655:OMG:HM21	2:L2:657:U:H5''	1.90	0.53
5:L5:62:C:H3'	5:L5:63:G:H21	1.73	0.53
10:LB:390:LEU:O	10:LB:394:ARG:HG3	2.07	0.53
23:LO:189:TYR:HA	23:LO:196:LEU:HA	1.89	0.53
51:S1:1142:G:H21	70:SO:45:THR:HG21	1.73	0.53
51:S1:2061:5MC:H2'	51:S1:2062:G:C8	2.42	0.53
61:SF:173:LYS:NZ	61:SF:175:GLY:O	2.39	0.53
88:Sg:133:VAL:HB	88:Sg:142:HIS:HB2	1.90	0.53
88:Sg:172:TRP:HA	88:Sg:196:TYR:HB2	1.90	0.53
7:L7:169:A:H3'	7:L7:170:A:C8	2.40	0.53
18:LJ:74:LYS:HE2	18:LJ:76:LEU:HD21	1.90	0.53
40:Lf:77:ILE:HD11	40:Lf:97:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lj:39:TYR:CD1	44:Lj:40:PRO:HA	2.43	0.53
51:S1:1945:A:H4'	67:SL:47:PRO:HG3	1.90	0.53
59:SD:101:PRO:O	59:SD:105:GLU:HG2	2.07	0.53
66:SK:26:LYS:HG2	66:SK:29:LEU:HD23	1.89	0.53
1:L1:56:G:H2'	1:L1:57:G:C8	2.43	0.53
11:LC:216:THR:O	11:LC:220:ARG:HG3	2.08	0.53
51:S1:324:U:H4'	51:S1:325:G:C4	2.43	0.53
64:SI:132:MET:HE3	64:SI:172:VAL:HG13	1.90	0.53
73:SR:122:ARG:HD3	73:SR:122:ARG:N	2.21	0.53
89:Sh:187:VAL:HG21	89:Sh:204:LEU:HD22	1.90	0.53
2:L2:743:C:H2'	2:L2:744:G:C8	2.44	0.53
2:L2:1100:A:H4'	12:LD:105:GLY:C	2.34	0.53
2:L2:1136:U:H2'	2:L2:1137:G:H8	1.74	0.53
28:LT:39:MET:HE1	28:LT:47:LEU:HD22	1.90	0.53
51:S1:321:G:H3'	51:S1:322:C:C6	2.43	0.53
51:S1:996:C:H2'	51:S1:997:C:C6	2.44	0.53
64:SI:143:TRP:HZ3	65:SJ:54:ASP:HB2	1.74	0.53
1:L1:1161:A:N6	24:LP:13:ARG:HD2	2.23	0.53
2:L2:525:A:N7	2:L2:532:U:H5	2.06	0.53
2:L2:957:C:H2'	2:L2:958:A:C8	2.43	0.53
2:L2:1102:C:H41	12:LD:24:CYS:HB3	1.74	0.53
11:LC:113:LYS:HG2	21:LM:203:LYS:HB3	1.90	0.53
14:LF:76:ILE:H	14:LF:154:GLN:HE22	1.57	0.53
51:S1:1972:G:H4'	74:SS:15:MET:HE1	1.90	0.53
58:SC:168:ASP:OD1	58:SC:187:ILE:HB	2.09	0.53
61:SF:169:LYS:HD2	65:SJ:95:PRO:HA	1.91	0.53
63:SH:58:LEU:HD23	63:SH:137:ILE:HG23	1.91	0.53
88:Sg:219:LEU:HD22	88:Sg:231:LYS:HG3	1.91	0.53
29:LU:97:PHE:O	29:LU:101:LYS:HG2	2.07	0.53
51:S1:1614:U:H2'	51:S1:1615:G:C8	2.43	0.53
51:S1:1992:G:H4'	51:S1:1993:A:C8	2.44	0.53
53:S3:72:A:H3'	53:S3:73:A:H8	1.74	0.53
56:SA:169:ARG:O	56:SA:173:MET:HG3	2.08	0.53
70:SO:106:GLN:OE1	83:Sb:48:ASP:OD1	2.26	0.53
79:SX:33:ARG:HG3	79:SX:33:ARG:HH11	1.74	0.53
79:SX:126:VAL:HG12	79:SX:136:LEU:HD23	1.90	0.53
56:SA:80:GLU:HG2	56:SA:81:GLU:OE1	2.09	0.53
68:SM:32:VAL:HG21	68:SM:107:VAL:HG21	1.90	0.53
1:L1:1098:A:N3	2:L2:1060:PSU:O2'	2.40	0.53
51:S1:1916:G:H5''	51:S1:1917:A:H2'	1.89	0.53
51:S1:1956:C:H1'	51:S1:1957:U:H5	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:S4:55:U:H2'	54:S4:57:G:N7	2.24	0.53
76:SU:73:CYS:O	76:SU:77:SER:OG	2.19	0.53
1:L1:1475:U:H5''	34:LZ:17:ARG:HE	1.74	0.53
45:Lk:57:GLU:HA	45:Lk:60:ILE:HD12	1.91	0.53
54:S4:40:C:H2'	54:S4:41:C:C6	2.43	0.53
79:SX:27:TRP:HH2	79:SX:74:LEU:HD23	1.74	0.53
2:L2:506:U:HO2'	2:L2:507:G:H8	1.57	0.53
13:LE:112:ARG:HG2	13:LE:120:VAL:HG22	1.91	0.53
22:LN:184:LEU:HB3	22:LN:190:LEU:HD13	1.90	0.53
51:S1:321:G:H3'	51:S1:322:C:H6	1.74	0.53
51:S1:994:U:H2'	51:S1:995:U:C6	2.44	0.53
57:SB:92:LYS:HE2	57:SB:204:LEU:HB3	1.91	0.53
2:L2:1510:A:N6	10:LB:327:ASP:H	2.03	0.52
5:L5:4:A:H62	5:L5:134:C:H5	1.57	0.52
13:LE:46:ARG:NH2	19:LK:6:TYR:OH	2.42	0.52
31:LW:24:ARG:HD3	31:LW:72:ARG:O	2.09	0.52
31:LW:41:ASN:HD22	31:LW:122:SER:HB3	1.75	0.52
58:SC:63:ARG:HD2	69:SN:98:GLN:NE2	2.10	0.52
72:SQ:69:GLU:CD	72:SQ:94:ARG:HH12	2.16	0.52
73:SR:88:GLN:HA	73:SR:96:THR:HG23	1.89	0.52
1:L1:113:C:H5'	21:LM:147:ARG:HD3	1.91	0.52
5:L5:2:U:P	5:L5:135:C:H3'	2.50	0.52
37:Lc:146:TYR:CZ	37:Lc:239:ASN:HB2	2.44	0.52
78:SW:68:ARG:HG3	78:SW:69:GLU:OE2	2.08	0.52
1:L1:1672:U:H2'	1:L1:1673:G:C8	2.44	0.52
2:L2:1213:PSU:H2'	2:L2:1214:G:C8	2.43	0.52
51:S1:139:C:H2'	51:S1:140:G:C8	2.45	0.52
51:S1:377:A:H5'	66:SK:48:ALA:HB1	1.92	0.52
51:S1:979:U:H2'	51:S1:980:G:C8	2.44	0.52
67:SL:23:ALA:HB2	67:SL:75:VAL:HG13	1.90	0.52
73:SR:118:MET:HG3	78:SW:118:MET:HG2	1.91	0.52
2:L2:554:C:H2'	2:L2:555:A:C8	2.45	0.52
10:LB:56:ILE:HD13	10:LB:363:LEU:HD22	1.90	0.52
12:LD:43:CYS:SG	12:LD:71:CYS:HB3	2.49	0.52
42:Lh:94:ARG:O	42:Lh:98:VAL:HG23	2.09	0.52
51:S1:256:A:N7	51:S1:943:U:H5	2.08	0.52
59:SD:56:ARG:HG3	59:SD:96:LEU:HD21	1.90	0.52
81:SZ:14:THR:HG21	81:SZ:54:TYR:HE2	1.75	0.52
1:L1:700:A:N1	1:L1:845:OMU:H5	2.24	0.52
18:LJ:86:SER:HA	18:LJ:96:TYR:HB3	1.89	0.52
22:LN:53:VAL:HG22	22:LN:134:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:209:ARG:O	22:LN:210:ASN:ND2	2.42	0.52
34:LZ:30:ASP:HB3	34:LZ:33:ASN:HB2	1.92	0.52
51:S1:262:U:H2'	51:S1:263:G:C8	2.44	0.52
51:S1:308:C:H5'	51:S1:309:G:C4	2.43	0.52
76:SU:107:HIS:ND1	76:SU:118:ARG:NH1	2.58	0.52
88:Sg:190:LEU:HB3	88:Sg:221:TRP:CZ3	2.44	0.52
1:L1:593:C:H42	1:L1:614:A:H61	1.56	0.52
21:LM:123:MET:HB3	21:LM:128:LYS:HG3	1.91	0.52
40:Lf:98:SER:O	40:Lf:106:ARG:NH2	2.42	0.52
48:Ln:22:LEU:HD21	51:S1:2153:A:H5''	1.92	0.52
1:L1:266:G:H2'	1:L1:267:A:C8	2.44	0.52
20:LL:39:HIS:O	20:LL:40:HIS:ND1	2.43	0.52
40:Lf:80:VAL:HG13	40:Lf:112:LYS:HG2	1.92	0.52
51:S1:1108:A:H5''	75:ST:16:LEU:HD12	1.90	0.52
63:SH:110:ASP:HA	63:SH:186:ALA:HB2	1.90	0.52
1:L1:307:U:H2'	1:L1:308:A:C8	2.45	0.52
1:L1:1262:G:H5'	1:L1:1262:G:H8	1.75	0.52
2:L2:1102:C:N4	12:LD:24:CYS:HB3	2.25	0.52
2:L2:1369:C:H5''	18:LJ:42:LYS:HD3	1.90	0.52
9:LA:80:GLU:HG2	49:Lo:66:GLY:HA3	1.92	0.52
10:LB:297:GLU:HG3	10:LB:297:GLU:O	2.10	0.52
15:LG:104:LYS:O	15:LG:108:GLU:HG3	2.10	0.52
21:LM:9:GLU:HB2	43:Li:47:ILE:HG13	1.90	0.52
26:LR:97:ARG:HG2	26:LR:141:ILE:HG23	1.92	0.52
51:S1:1690:C:H2'	51:S1:1691:U:C6	2.45	0.52
69:SN:94:MET:CE	69:SN:98:GLN:HG3	2.40	0.52
1:L1:631:G:H1'	1:L1:632:A:H2'	1.91	0.52
2:L2:1024:U:H2'	2:L2:1025:G:C8	2.44	0.52
5:L5:112:U:H5	5:L5:121:A:N7	2.08	0.52
13:LE:48:ASP:OD2	13:LE:51:ASN:ND2	2.34	0.52
54:S4:38:A:H3'	54:S4:39:U:H6	1.75	0.52
69:SN:77:ASP:OD1	69:SN:77:ASP:N	2.40	0.52
72:SQ:104:VAL:HG21	72:SQ:111:GLU:HG3	1.92	0.52
88:Sg:236:SER:HB3	88:Sg:256:ARG:NH1	2.25	0.52
11:LC:316:PRO:HB3	11:LC:322:ASN:OD1	2.10	0.52
24:LP:153:ARG:O	24:LP:157:ARG:HG2	2.09	0.52
51:S1:582:U:H2'	51:S1:583:A:C8	2.45	0.52
39:Le:127:ILE:HG23	39:Le:131:LEU:HD23	1.93	0.51
51:S1:1702:A:N1	51:S1:1773:U:H5	2.08	0.51
60:SE:89:ILE:O	60:SE:93:GLY:N	2.43	0.51
70:SO:114:ARG:HD3	83:Sb:54:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:SU:148:LYS:HG3	76:SU:149:THR:HG23	1.90	0.51
2:L2:502[A]:A2M:H2'	51:S1:2160:G:H1'	1.92	0.51
51:S1:958:G:H3'	51:S1:959:U:C6	2.44	0.51
53:S3:21:A:H3'	53:S3:46:A:H62	1.75	0.51
70:SO:49:VAL:HG13	70:SO:53:MET:HE2	1.93	0.51
1:L1:141:U:H1'	1:L1:142:G:H5''	1.91	0.51
2:L2:819:U:H2'	2:L2:820:G:C8	2.45	0.51
4:L4:28:A:N1	4:L4:177:U:H5	2.08	0.51
17:LI:190:LEU:HB2	20:LL:143:LEU:HD11	1.93	0.51
25:LQ:14:ILE:HD13	25:LQ:42:ARG:HG3	1.91	0.51
38:Ld:10:ASP:OD1	38:Ld:10:ASP:N	2.36	0.51
1:L1:626:U:HO2'	1:L1:627:C:H6	1.58	0.51
1:L1:1086:G:H3'	1:L1:1087:A:H8	1.76	0.51
2:L2:665:A2M:H2'	2:L2:666:C:C6	2.45	0.51
3:L3:157:C:H2'	3:L3:158:U:C6	2.45	0.51
7:L7:43:A2M:N1	7:L7:100:U:H5	2.08	0.51
12:LD:162:MET:O	12:LD:166:GLU:HG3	2.10	0.51
13:LE:88:ARG:HD3	13:LE:90:LYS:HE2	1.91	0.51
29:LU:33:PRO:HB2	29:LU:39:PHE:HB2	1.91	0.51
85:Sd:41:GLN:OE1	85:Sd:62:ASN:ND2	2.34	0.51
1:L1:1216:U:H5'	24:LP:2:GLY:HA3	1.93	0.51
1:L1:1257[B]:U:H4'	1:L1:1258:A:O5'	2.11	0.51
16:LH:11:ARG:O	16:LH:15:LYS:HG2	2.11	0.51
51:S1:1635:U:H3'	51:S1:1636:U:H2'	1.93	0.51
60:SE:45:ILE:HD12	60:SE:49:LEU:HD12	1.92	0.51
69:SN:52:LEU:O	69:SN:55:SER:OG	2.22	0.51
77:SV:99:VAL:HB	77:SV:120:VAL:HG12	1.93	0.51
88:Sg:174:ASN:ND2	88:Sg:194:SER:O	2.25	0.51
2:L2:479:C:H3'	2:L2:480:G:H8	1.75	0.51
2:L2:1076:G:N3	2:L2:1185:A2M:H2	2.26	0.51
2:L2:1086:G:H4'	2:L2:1179:A:O2'	2.11	0.51
73:SR:116:LYS:HD2	73:SR:127:ALA:HB2	1.92	0.51
1:L1:1255:G:H2'	1:L1:1256:A:C8	2.45	0.51
57:SB:109:GLY:N	57:SB:139:GLU:OE2	2.34	0.51
79:SX:19:LEU:HD22	79:SX:144:ALA:HB1	1.93	0.51
88:Sg:68:VAL:HA	88:Sg:84:SER:HA	1.92	0.51
88:Sg:173:ASP:O	88:Sg:173:ASP:CG	2.53	0.51
1:L1:1666:G:H4'	1:L1:1667:G:C8	2.45	0.51
4:L4:24:A:N6	5:L5:2:U:H3	2.09	0.51
22:LN:174:THR:HG22	22:LN:196:HIS:HA	1.92	0.51
32:LX:42:ALA:O	32:LX:46:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1031:A:C8	1:L1:1162:G:H1'	2.46	0.51
4:L4:92:U:H2'	4:L4:93:U:C6	2.45	0.51
10:LB:292:ARG:HG3	10:LB:293:SER:H	1.76	0.51
51:S1:1107:G:H2'	51:S1:1108:A:C8	2.46	0.51
51:S1:1851:U:H4'	74:SS:8:ARG:HG2	1.93	0.51
88:Sg:30:VAL:HG21	88:Sg:73:LEU:HD21	1.92	0.51
88:Sg:198:SER:H	88:Sg:213:GLY:HA2	1.76	0.51
7:L7:18:G:H2'	7:L7:19:A:C8	2.45	0.51
21:LM:4:PHE:HE2	21:LM:50:MET:HE2	1.72	0.51
24:LP:196:ARG:HH11	24:LP:196:ARG:HG3	1.76	0.51
40:Lf:37:ARG:NH2	94:Lf:1401:HOH:O	2.43	0.51
51:S1:97:C:H2'	51:S1:421:A:H4'	1.93	0.51
51:S1:1403:A:N3	56:SA:148:GLN:NE2	2.59	0.51
51:S1:2195:G:O4'	83:Sb:1:MET:N	2.42	0.51
56:SA:151:GLN:HE21	56:SA:153:SER:HB2	1.75	0.51
72:SQ:68:CYS:O	72:SQ:69:GLU:HG2	2.10	0.51
2:L2:419:G:H5''	9:LA:18:VAL:HG23	1.93	0.50
16:LH:151:GLU:OE2	26:LR:155:GLN:NE2	2.44	0.50
22:LN:56:GLU:HG3	22:LN:162:ARG:H	1.76	0.50
30:LV:96:THR:HG22	30:LV:100:LYS:HE3	1.92	0.50
34:LZ:41:ARG:HH11	34:LZ:102:ASP:HB2	1.76	0.50
56:SA:117:ARG:CG	56:SA:117:ARG:HH11	2.24	0.50
57:SB:24:MET:HE2	77:SV:91:VAL:HB	1.93	0.50
59:SD:89:LYS:HB2	59:SD:94:TYR:CD1	2.46	0.50
65:SJ:42:GLN:NE2	65:SJ:48:GLY:O	2.34	0.50
88:Sg:193:HIS:HE1	88:Sg:197:VAL:HG22	1.76	0.50
1:L1:225:C:HO2'	1:L1:226:C:H6	1.58	0.50
1:L1:387:G:H2'	1:L1:388:A:C8	2.46	0.50
2:L2:1110:U:H2'	2:L2:1111:C:C6	2.47	0.50
21:LM:97:ASN:ND2	21:LM:171:HIS:HB3	2.26	0.50
51:S1:1820:G:H21	58:SC:161:THR:HG23	1.76	0.50
51:S1:1980:U:H3'	51:S1:1981:G:H21	1.77	0.50
61:SF:164:HIS:ND1	61:SF:207:ASP:OD2	2.44	0.50
64:SI:86:GLU:OE2	64:SI:168:ARG:NH1	2.44	0.50
81:SZ:62:VAL:HG22	81:SZ:82:ILE:HG12	1.93	0.50
7:L7:29:C:H5'	17:LI:35:ALA:HB1	1.94	0.50
10:LB:392:LYS:HG2	10:LB:393:ASP:N	2.26	0.50
15:LG:187:LEU:HB3	15:LG:196:ALA:HB3	1.93	0.50
17:LI:145:GLU:O	17:LI:149:LYS:CG	2.56	0.50
42:Lh:62:HIS:O	42:Lh:63:ILE:HG22	2.11	0.50
51:S1:139:C:H2'	51:S1:140:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:S4:41:C:H2'	54:S4:42:C:C6	2.46	0.50
58:SC:97:ALA:O	58:SC:101:VAL:HG23	2.11	0.50
70:SO:75:VAL:HG21	70:SO:115:ALA:HB3	1.93	0.50
81:SZ:12:ILE:HG21	81:SZ:50:LEU:HD13	1.94	0.50
1:L1:290:G:H2'	1:L1:291:A:C8	2.46	0.50
21:LM:168:GLY:HA2	21:LM:171:HIS:CD2	2.46	0.50
51:S1:1704:U:H2'	51:S1:1705:C:C6	2.46	0.50
65:SJ:18:GLU:OE1	65:SJ:18:GLU:HA	2.10	0.50
1:L1:1479:A:H5''	1:L1:1481:G:O4'	2.12	0.50
3:L3:99:U:H2'	3:L3:100:U:C6	2.46	0.50
6:L6:30:C:H3'	13:LE:50:LYS:HD3	1.93	0.50
14:LF:42:LEU:HD11	14:LF:85:ILE:HG13	1.94	0.50
18:LJ:106:ASN:HD21	18:LJ:108:LYS:HB2	1.76	0.50
20:LL:51:GLY:HA2	24:LP:182:ARG:N	2.27	0.50
51:S1:877:U:H3	51:S1:884:A:H62	1.60	0.50
51:S1:904:G:H1'	51:S1:905:A:N7	2.27	0.50
57:SB:84:LEU:HG	57:SB:84:LEU:O	2.12	0.50
59:SD:43:ARG:O	59:SD:47:THR:HG23	2.12	0.50
1:L1:1680:U:H3	1:L1:1712:G:H1	1.59	0.50
23:LO:110:LEU:HD13	23:LO:115:ILE:HG22	1.92	0.50
31:LW:80:ASP:OD1	31:LW:81:LYS:N	2.45	0.50
51:S1:810:G:H1'	51:S1:811:C:H5'	1.93	0.50
51:S1:1227:G:H4'	51:S1:2179:A:H4'	1.94	0.50
62:SG:125:GLU:H	62:SG:125:GLU:CD	2.20	0.50
73:SR:36:GLY:O	73:SR:98:HIS:NE2	2.41	0.50
73:SR:67:LYS:HD2	73:SR:71:ILE:HD11	1.93	0.50
1:L1:1394:U:O2	37:Lc:246:ARG:NH1	2.44	0.50
20:LL:114:HIS:O	20:LL:116:GLN:NE2	2.44	0.50
31:LW:112:ARG:HA	31:LW:115:ILE:HD12	1.94	0.50
51:S1:998:C:H2'	51:S1:999:A:C8	2.47	0.50
51:S1:1532:U:H4'	51:S1:1861:A:H61	1.77	0.50
59:SD:31:GLY:HA3	86:Se:40:TYR:CG	2.46	0.50
85:Sd:60:VAL:HG12	85:Sd:82:ALA:HB3	1.94	0.50
1:L1:345:U:H1'	2:L2:469:G:H21	1.77	0.50
2:L2:692:U:H2'	2:L2:693:C:C6	2.47	0.50
22:LN:31:ILE:HG22	22:LN:62:SER:HB2	1.94	0.50
51:S1:594:A:H61	51:S1:643:A:H5''	1.76	0.50
56:SA:74:ASN:C	56:SA:75:GLN:HG3	2.36	0.50
64:SI:138:VAL:HG13	64:SI:155:VAL:HG13	1.93	0.50
73:SR:64:GLU:HA	73:SR:67:LYS:HB3	1.93	0.50
77:SV:44:LYS:O	77:SV:48:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:364:G:H3'	2:L2:365:G:H8	1.77	0.50
7:L7:11:G:H1'	28:LT:5:SER:HB3	1.93	0.50
10:LB:82:PRO:HG3	10:LB:171:LEU:HB2	1.93	0.50
34:LZ:43:CYS:O	34:LZ:47:ASN:ND2	2.43	0.50
51:S1:1551:G:H5''	74:SS:30:ALA:HB2	1.94	0.50
51:S1:1963:C:H2'	51:S1:1964:C:C6	2.47	0.50
58:SC:34:SER:HA	58:SC:98:MET:HE3	1.94	0.50
64:SI:142:ARG:HG3	64:SI:156:PHE:HE2	1.76	0.50
88:Sg:89:ILE:HB	88:Sg:103:PHE:HE1	1.77	0.50
1:L1:498:G:H1	1:L1:562:U:H5	1.59	0.49
2:L2:590:U:H2'	2:L2:591:A2M:H8	1.92	0.49
2:L2:1289:A:H2'	2:L2:1289:A:N3	2.26	0.49
26:LR:75:ASN:ND2	26:LR:145:HIS:HE1	2.09	0.49
37:Lc:175:ASP:OD1	37:Lc:178:MET:HG3	2.12	0.49
41:Lg:61:VAL:HG13	41:Lg:66:ASP:HB3	1.94	0.49
51:S1:256:A:H2'	51:S1:257:A:H5''	1.94	0.49
51:S1:274:C:H1'	51:S1:275:A:N7	2.26	0.49
51:S1:357:U:O4	51:S1:1482:G:H1'	2.12	0.49
86:Se:7:SER:O	86:Se:7:SER:OG	2.21	0.49
88:Sg:246:ASN:OD1	88:Sg:291:GLY:HA3	2.12	0.49
1:L1:592:G:H2'	1:L1:593:C:C6	2.47	0.49
1:L1:855:C:H5'	11:LC:94:MET:HE1	1.93	0.49
2:L2:998:G:H2'	2:L2:999:U:C6	2.46	0.49
2:L2:1157:U:H5	2:L2:1237:A:N1	2.10	0.49
17:LI:145:GLU:HG3	17:LI:149:LYS:HE3	1.93	0.49
23:LO:199:LYS:NZ	23:LO:203:ASP:OD2	2.35	0.49
25:LQ:105:LEU:HD23	25:LQ:138:LEU:HD23	1.95	0.49
51:S1:667:U:H5''	51:S1:1277:A:C5	2.48	0.49
51:S1:1298:U:H1'	51:S1:1365:U:C4	2.46	0.49
73:SR:85:LEU:HD12	73:SR:96:THR:HG22	1.94	0.49
8:L8:83:U:H2'	8:L8:84:G:H8	1.76	0.49
10:LB:80:GLU:HG2	10:LB:326:ASN:HB2	1.95	0.49
13:LE:154:SER:O	13:LE:155:ARG:HB3	2.13	0.49
27:LS:115:TYR:OH	27:LS:119:LYS:NZ	2.38	0.49
49:Lo:51:ALA:O	49:Lo:52:VAL:C	2.55	0.49
57:SB:39:LYS:O	84:Sc:3:PHE:CD1	2.65	0.49
1:L1:1352:C:H2'	1:L1:1353:A:H8	1.72	0.49
2:L2:1120:C:H1'	2:L2:1133:G:H5''	1.95	0.49
4:L4:1:G:H1'	6:L6:3:A:H5'	1.93	0.49
6:L6:52:G:O6	41:Lg:28:ARG:NH2	2.46	0.49
6:L6:73:A:H5'	41:Lg:29:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:204:ALA:O	16:LH:208:MET:HG2	2.12	0.49
42:Lh:47:TRP:HA	42:Lh:51:HIS:HB2	1.94	0.49
43:Li:63:PHE:HB3	43:Li:72:ALA:HB2	1.94	0.49
51:S1:846:U:H2'	51:S1:847:A:H8	1.77	0.49
59:SD:16:ARG:O	59:SD:22:ARG:NH1	2.46	0.49
65:SJ:86:TYR:OH	65:SJ:121:THR:O	2.26	0.49
69:SN:17:PHE:CZ	69:SN:75:LEU:HG	2.47	0.49
1:L1:120:G:O6	15:LG:142:ARG:NH2	2.44	0.49
1:L1:959:OMG:HM22	1:L1:959:OMG:N3	2.27	0.49
2:L2:954:A:C4	42:Lh:114:MET:CE	2.96	0.49
11:LC:284:ASN:O	11:LC:285:THR:HG22	2.13	0.49
14:LF:50:ARG:O	14:LF:72:ASN:ND2	2.46	0.49
16:LH:111:LYS:O	16:LH:115:LYS:HG3	2.13	0.49
23:LO:110:LEU:HD22	23:LO:115:ILE:HG21	1.95	0.49
35:La:77:ARG:HA	35:La:80:ARG:NE	2.27	0.49
51:S1:546:U:C2	51:S1:547:U:H1'	2.47	0.49
51:S1:787:G:H8	51:S1:833:G:H1	1.60	0.49
51:S1:793:G:H3'	51:S1:794:U:C6	2.47	0.49
51:S1:939:G:H3'	51:S1:940:C:C6	2.47	0.49
51:S1:1397:A:H1'	56:SA:169:ARG:NH2	2.27	0.49
73:SR:30:ALA:O	73:SR:33:MET:HG3	2.13	0.49
79:SX:17:ALA:HB3	79:SX:149:PHE:HA	1.94	0.49
1:L1:368:G:OP2	11:LC:55:ARG:NH1	2.45	0.49
1:L1:1391:U:C5	19:LK:19:PRO:HB2	2.47	0.49
4:L4:174:A:C6	16:LH:4:PRO:HD3	2.47	0.49
9:LA:109:GLU:HG2	9:LA:138:SER:HA	1.94	0.49
11:LC:349:ARG:HD3	11:LC:353:ARG:NH2	2.27	0.49
15:LG:111:GLN:O	15:LG:115:GLU:HG2	2.12	0.49
51:S1:809:C:H4'	51:S1:810:G:H5'	1.95	0.49
57:SB:194:ARG:HH11	80:SY:48:GLY:HA3	1.78	0.49
80:SY:76:ILE:O	80:SY:80:ARG:HG2	2.12	0.49
1:L1:335:U:C5	43:Li:41:ARG:HD2	2.48	0.49
2:L2:623:A:H5''	2:L2:624:C:H5	1.76	0.49
27:LS:49:ARG:HA	27:LS:52:MET:HE2	1.94	0.49
30:LV:71:THR:HG21	35:La:38:THR:HG22	1.94	0.49
40:Lf:64:THR:HA	40:Lf:67:ILE:HD12	1.93	0.49
69:SN:46:CYS:O	69:SN:50:MET:HG3	2.13	0.49
70:SO:116:GLY:O	70:SO:117:MET:HG2	2.13	0.49
1:L1:1706:C:H2'	1:L1:1707:U:C6	2.48	0.49
2:L2:947:U:H2'	2:L2:948:G:C8	2.48	0.49
2:L2:1276:A:N6	2:L2:1288:G:H1'	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:147:A:H4'	45:Lk:4:GLU:HG3	1.94	0.49
10:LB:233:GLY:O	10:LB:237:ARG:HB2	2.12	0.49
35:La:8:LYS:O	35:La:12:GLU:HG3	2.11	0.49
51:S1:869:U:C2	59:SD:142:ILE:HG13	2.48	0.49
63:SH:38:THR:O	63:SH:38:THR:OG1	2.30	0.49
1:L1:187:A:H2'	1:L1:248:A:N1	2.28	0.49
1:L1:361:A:H2'	1:L1:362:A:C8	2.48	0.49
1:L1:405:A:H1'	11:LC:83:THR:CG2	2.42	0.49
2:L2:1102:C:H2'	2:L2:1103:A:C8	2.47	0.49
4:L4:122:G:OP1	18:LJ:14:ARG:NH2	2.45	0.49
10:LB:92:TYR:HB2	10:LB:159:VAL:HB	1.95	0.49
51:S1:70:U:H2'	51:S1:71:G:C8	2.47	0.49
51:S1:263:G:H5'	89:Sh:169:ARG:HB2	1.94	0.49
51:S1:880:U:H4'	51:S1:881:U:H5'	1.95	0.49
51:S1:2100:A:H3'	51:S1:2101:C:H5''	1.95	0.49
51:S1:2197:G:H1'	83:Sb:83:ILE:HD13	1.94	0.49
51:S1:2202:PSU:H2'	56:SA:118:LYS:HB2	1.95	0.49
56:SA:139:LEU:HD13	56:SA:217:VAL:HG22	1.95	0.49
66:SK:159:GLN:O	66:SK:163:THR:HG23	2.12	0.49
88:Sg:179:TRP:HA	88:Sg:186:CYS:HA	1.95	0.49
51:S1:1586:A:H5''	51:S1:1597:G:H2'	1.93	0.49
1:L1:448:A:C2	7:L7:16:A:H1'	2.48	0.48
4:L4:85:C:H4'	39:Le:97:LYS:HE3	1.95	0.48
7:L7:17:U:H2'	7:L7:18:G:C8	2.48	0.48
11:LC:43:MET:HE2	11:LC:119:LYS:HD2	1.95	0.48
15:LG:82:VAL:HG21	15:LG:182:LYS:HD3	1.94	0.48
31:LW:24:ARG:HG2	31:LW:75:TRP:CH2	2.48	0.48
38:Ld:16:LEU:O	38:Ld:20:MET:HG2	2.13	0.48
38:Ld:50:CYS:O	38:Ld:55:ARG:NH2	2.46	0.48
51:S1:5:U:H2'	51:S1:6:G:H8	1.77	0.48
51:S1:769:A:H3'	51:S1:770:A:H8	1.76	0.48
51:S1:1530:G:H5'	51:S1:1542:C:H42	1.78	0.48
51:S1:1624:U:H5	51:S1:1839:G:H1	1.61	0.48
51:S1:2005:U:H2'	51:S1:2006:A:C8	2.47	0.48
64:SI:139:VAL:HG13	64:SI:192:PRO:HB3	1.95	0.48
65:SJ:114:GLU:OE2	65:SJ:117:ARG:NH2	2.46	0.48
88:Sg:222:ASP:HB2	88:Sg:229:LEU:HD11	1.95	0.48
1:L1:718:A:OP2	17:LI:41:ARG:NH1	2.46	0.48
7:L7:34:U:H5''	7:L7:34:U:H6	1.78	0.48
11:LC:268:ALA:HA	11:LC:276:THR:HG22	1.95	0.48
16:LH:72:TYR:OH	16:LH:91:HIS:O	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1916:G:H3'	51:S1:1917:A:H8	1.78	0.48
81:SZ:93:GLU:HB3	81:SZ:98:LYS:HG3	1.94	0.48
1:L1:415:A:H4'	1:L1:416:A:H5'	1.94	0.48
2:L2:1233:U:OP1	50:Lp:61:LYS:NZ	2.47	0.48
10:LB:87:VAL:HG23	10:LB:163:ILE:HG22	1.95	0.48
25:LQ:165:ARG:NH1	25:LQ:168:GLN:OE1	2.46	0.48
37:Lc:109:GLN:HG3	37:Lc:140:VAL:HG12	1.96	0.48
59:SD:76:MET:HE1	59:SD:95:VAL:HG23	1.95	0.48
63:SH:111:SER:HA	63:SH:124:ALA:HA	1.95	0.48
1:L1:606:C:H2'	1:L1:607:C:C6	2.48	0.48
1:L1:1015:G:H21	20:LL:40:HIS:HA	1.78	0.48
8:L8:92:U:H2'	8:L8:93:G:O4'	2.14	0.48
16:LH:79:ARG:HA	16:LH:88:PRO:HD2	1.95	0.48
51:S1:1569:G:O6	74:SS:7:TRP:NE1	2.45	0.48
51:S1:1591:U:H2'	51:S1:1592:U:O4'	2.14	0.48
54:S4:37:A:H3'	54:S4:38:A:H8	1.77	0.48
57:SB:58:TRP:O	57:SB:62:ILE:HG12	2.13	0.48
61:SF:149:VAL:HG21	61:SF:231:ARG:HG3	1.95	0.48
77:SV:122:ARG:HG2	77:SV:122:ARG:HH11	1.78	0.48
1:L1:1049:A:H4'	8:L8:105:A:N3	2.29	0.48
1:L1:1147:A:O2'	1:L1:1150:A:N1	2.47	0.48
6:L6:70:G:H1'	6:L6:71:A:H5'	1.95	0.48
23:LO:212:ASP:O	23:LO:216:GLN:HG3	2.13	0.48
51:S1:809:C:H1'	51:S1:810:G:C8	2.49	0.48
51:S1:1173:A:H1'	51:S1:1235:A:C2	2.49	0.48
51:S1:1572:C:H41	51:S1:1615:G:H1	1.62	0.48
54:S4:55:U:H5	54:S4:57:G:H3'	1.77	0.48
56:SA:207:LEU:HD12	56:SA:208:PRO:HD2	1.95	0.48
58:SC:49:ILE:HD11	58:SC:85:LEU:HD12	1.95	0.48
60:SE:121:MET:HB3	60:SE:138:THR:HB	1.96	0.48
88:Sg:90:ARG:NH1	88:Sg:102:LYS:HD3	2.28	0.48
88:Sg:109:ASP:OD2	88:Sg:127:ARG:NH1	2.47	0.48
2:L2:512:PSU:H2'	2:L2:513:C:C6	2.47	0.48
2:L2:1266:G:H4'	22:LN:4:ARG:HE	1.79	0.48
3:L3:159:C:H2'	3:L3:160:U:O4'	2.13	0.48
16:LH:92:ARG:NH1	16:LH:164:VAL:O	2.40	0.48
51:S1:830:G:H3'	51:S1:831:G:H8	1.79	0.48
51:S1:1883:G:H22	51:S1:1941:A:H3'	1.79	0.48
60:SE:8:ARG:NH1	60:SE:24:PHE:O	2.46	0.48
89:Sh:188:GLU:OE1	89:Sh:188:GLU:N	2.46	0.48
1:L1:155:A:H3'	1:L1:156:A:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1287:C:O2'	2:L2:1288:G:H8	1.96	0.48
5:L5:56:U:H2'	5:L5:57:C:C6	2.48	0.48
11:LC:316:PRO:HD3	11:LC:324:ARG:HH21	1.78	0.48
22:LN:57:LEU:HD12	22:LN:130:ARG:HA	1.96	0.48
33:LY:16:GLY:O	42:Lh:77:ARG:HG3	2.14	0.48
37:Lc:118:LEU:HD21	37:Lc:125:VAL:HG22	1.95	0.48
51:S1:122:A:N1	51:S1:337:U:H5	2.12	0.48
51:S1:939:G:H3'	51:S1:940:C:H6	1.78	0.48
51:S1:1695:C:H5''	68:SM:49:GLY:HA3	1.95	0.48
77:SV:16:VAL:HG11	77:SV:35:ILE:HD11	1.95	0.48
79:SX:33:ARG:O	79:SX:37:GLN:HG3	2.13	0.48
1:L1:223:A:N7	4:L4:10:U:H5	2.10	0.48
1:L1:1185:U:H2'	1:L1:1186:A:O4'	2.14	0.48
2:L2:819:U:H2'	2:L2:820:G:H8	1.78	0.48
3:L3:197:A:H1'	3:L3:199:A:H2'	1.95	0.48
15:LG:65:VAL:O	15:LG:69:ARG:HG2	2.14	0.48
31:LW:69:ALA:HB3	31:LW:78:LEU:HD12	1.94	0.48
51:S1:1114:G:H1	51:S1:1207:U:H3	1.62	0.48
51:S1:1555:A:H61	51:S1:1972:G:H1'	1.79	0.48
51:S1:1800:U:H2'	51:S1:1801:G:O4'	2.13	0.48
51:S1:2198:A:OP2	83:Sb:5:ARG:NH2	2.45	0.48
73:SR:25:ARG:CZ	73:SR:33:MET:HE2	2.43	0.48
88:Sg:20:PRO:HG3	88:Sg:27:ILE:HD12	1.94	0.48
88:Sg:236:SER:HB3	88:Sg:256:ARG:HH11	1.79	0.48
1:L1:720:A:C8	1:L1:721:U:H2'	2.48	0.48
1:L1:1683:C:N4	1:L1:1709:U:H3	2.05	0.48
2:L2:406:G:H2'	2:L2:407:C:C6	2.49	0.48
18:LJ:34:LYS:HE2	18:LJ:34:LYS:HA	1.95	0.48
19:LK:129:ASP:OD1	41:Lg:22:SER:OG	2.25	0.48
39:Le:113:LYS:NZ	39:Le:125:ASN:O	2.47	0.48
51:S1:1133:U:H1'	70:SO:130:THR:HG23	1.96	0.48
66:SK:61:ASP:OD2	66:SK:61:ASP:N	2.47	0.48
2:L2:134:C:H2'	2:L2:135:A:C8	2.48	0.48
2:L2:974:G:H4'	42:Lh:91:ARG:HD2	1.96	0.48
5:L5:55:U:H3	5:L5:61:C:N4	2.09	0.48
6:L6:44:G:H2'	6:L6:45:G:C8	2.48	0.48
10:LB:40:LYS:HG2	10:LB:41:PRO:HD2	1.96	0.48
14:LF:54:LEU:HD11	14:LF:66:SER:HB3	1.95	0.48
15:LG:49[B]:ARG:HE	30:LV:27:ARG:NH2	2.12	0.48
51:S1:1572:C:H2'	51:S1:1573:A:C8	2.49	0.48
56:SA:31:ASP:OD2	56:SA:240:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:SZ:61:GLN:HA	81:SZ:89:LEU:HD13	1.95	0.48
1:L1:212:U:H2'	1:L1:213:G:C8	2.49	0.47
1:L1:1351:C:HO2'	1:L1:1352:C:H6	1.61	0.47
1:L1:1610:C:OP2	28:LT:23:ARG:NH2	2.47	0.47
15:LG:122:LYS:HE2	15:LG:122:LYS:HB2	1.68	0.47
23:LO:192:GLU:O	23:LO:193:LYS:HG2	2.15	0.47
27:LS:153:TYR:HA	27:LS:156:MET:HE3	1.95	0.47
31:LW:108:LEU:HB3	31:LW:113:LYS:HE3	1.95	0.47
51:S1:699:A:H2'	51:S1:700:G:O4'	2.14	0.47
59:SD:59:LEU:HD21	59:SD:92:LEU:HB3	1.96	0.47
88:Sg:239:ASN:N	88:Sg:253:ALA:O	2.47	0.47
89:Sh:187:VAL:HG22	89:Sh:202:VAL:HG12	1.95	0.47
1:L1:1371:OMU:HM23	1:L1:1371:OMU:H1'	1.65	0.47
2:L2:554:C:H3'	2:L2:555:A:H2'	1.96	0.47
10:LB:17:LEU:HD21	10:LB:238:TRP:HH2	1.78	0.47
15:LG:93:LYS:HB3	15:LG:93:LYS:HE3	1.58	0.47
16:LH:85:THR:O	16:LH:86:LYS:HG2	2.14	0.47
40:Lf:10:ILE:HG12	40:Lf:64:THR:HB	1.94	0.47
50:Lp:61:LYS:HZ2	50:Lp:62:ALA:H	1.61	0.47
51:S1:762:A:H1'	51:S1:771:G:H22	1.79	0.47
51:S1:1909:C:H2'	51:S1:1910:C:H6	1.79	0.47
53:S3:47:U:H4'	53:S3:48:C:OP2	2.14	0.47
57:SB:24:MET:CE	77:SV:91:VAL:HB	2.44	0.47
57:SB:37:MET:HE3	57:SB:157:LEU:HD11	1.95	0.47
60:SE:99:MET:HE3	60:SE:99:MET:HB3	1.79	0.47
66:SK:110:LYS:HG3	66:SK:121:LEU:HD23	1.96	0.47
74:SS:7:TRP:CD1	74:SS:8:ARG:HG3	2.48	0.47
84:Sc:36:VAL:HG21	84:Sc:47:VAL:HG21	1.97	0.47
1:L1:130:U:H2'	1:L1:132:A:H62	1.79	0.47
1:L1:320:G:O2'	50:Lp:38:ARG:NH2	2.48	0.47
1:L1:568:U:H4'	1:L1:569:G:C4	2.49	0.47
2:L2:781:G:H2'	2:L2:782:G:C8	2.49	0.47
13:LE:19:ASP:HB3	13:LE:26:THR:HG23	1.97	0.47
27:LS:63:ILE:HD12	36:Lb:27:LEU:CD1	2.45	0.47
66:SK:214:ARG:HA	66:SK:217:LYS:HD2	1.97	0.47
69:SN:82:TYR:C	69:SN:82:TYR:CD1	2.91	0.47
73:SR:31:LEU:HD21	73:SR:68:ILE:HD13	1.97	0.47
88:Sg:127:ARG:HA	88:Sg:152:TRP:HB2	1.95	0.47
1:L1:163:U:H2'	1:L1:164:G:H8	1.76	0.47
1:L1:824:U:O2	1:L1:824:U:O4'	2.31	0.47
1:L1:1357:G:O2'	26:LR:117:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:38:ARG:NH2	22:LN:83:ASP:O	2.38	0.47
44:Lj:52:LYS:HE3	44:Lj:52:LYS:HB2	1.70	0.47
51:S1:1287:U:H2'	51:S1:1288:G:C8	2.50	0.47
51:S1:1851:U:H1'	74:SS:7:TRP:CZ3	2.49	0.47
54:S4:9:A:H61	54:S4:22:G:H3'	1.78	0.47
56:SA:8:ARG:HD2	56:SA:11:LYS:HA	1.94	0.47
81:SZ:69:THR:HG22	81:SZ:76:THR:HG22	1.96	0.47
7:L7:71:A:H3'	31:LW:48:ARG:HG3	1.96	0.47
10:LB:112:VAL:O	10:LB:116:ARG:HG3	2.14	0.47
10:LB:367:ASP:OD2	32:LX:17:HIS:NE2	2.41	0.47
11:LC:178:ASP:HB3	11:LC:206:PRO:HD3	1.95	0.47
24:LP:189:SER:O	24:LP:190:TYR:CD2	2.67	0.47
41:Lg:47:HIS:H	41:Lg:47:HIS:CD2	2.33	0.47
57:SB:97:VAL:O	57:SB:189:ARG:NH1	2.34	0.47
60:SE:148:ASP:O	60:SE:151:THR:OG1	2.32	0.47
70:SO:65:TYR:O	70:SO:68:MET:HG2	2.14	0.47
1:L1:114:G:H4'	21:LM:49:ARG:HG2	1.95	0.47
1:L1:1184:G:OP2	22:LN:98:ARG:NH2	2.47	0.47
5:L5:118:U:O2'	5:L5:119:U:O2	2.29	0.47
6:L6:54:A:H1'	6:L6:55:U:C5	2.49	0.47
9:LA:117:GLU:HG2	9:LA:124:GLY:H	1.80	0.47
19:LK:151:ALA:HB1	41:Lg:14:LEU:HD11	1.96	0.47
27:LS:141:LYS:HD3	27:LS:141:LYS:HA	1.64	0.47
33:LY:76:ASN:OD1	33:LY:77:HIS:N	2.48	0.47
51:S1:580:A:H8	51:S1:584:U:H5''	1.80	0.47
51:S1:846:U:H2'	51:S1:847:A:C8	2.49	0.47
51:S1:1096:C:H2'	51:S1:1097:C:C6	2.49	0.47
51:S1:1917:A:H4'	51:S1:1918:U:H3'	1.96	0.47
54:S4:65:G:H2'	54:S4:66:U:C6	2.49	0.47
57:SB:16:SER:O	57:SB:20:LYS:HG3	2.15	0.47
78:SW:89:ASP:OD1	78:SW:89:ASP:N	2.45	0.47
1:L1:687:C:H2'	1:L1:688:A:C8	2.49	0.47
1:L1:1226:G:H4'	37:Lc:227:LYS:HE3	1.97	0.47
2:L2:516:A:H2'	2:L2:517:A:C8	2.49	0.47
25:LQ:41:VAL:O	25:LQ:45:ILE:HG13	2.14	0.47
35:La:2:SER:O	35:La:47:ARG:NH1	2.43	0.47
38:Ld:48:ASN:C	38:Ld:48:ASN:OD1	2.57	0.47
44:Lj:51:VAL:O	44:Lj:55:LYS:HG2	2.15	0.47
46:Ll:38:ASN:C	46:Ll:40:LYS:H	2.22	0.47
51:S1:617:G:H4'	71:SP:88:ASP:HB3	1.97	0.47
51:S1:784:C:H3'	51:S1:787:G:N1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:788:A:N1	51:S1:832:C:H5	2.12	0.47
51:S1:1810:G:N2	51:S1:1812:A:H3'	2.29	0.47
58:SC:33:PHE:HA	58:SC:51:ALA:HA	1.97	0.47
64:SI:41:LEU:N	64:SI:42:PRO:HD2	2.30	0.47
66:SK:162:TRP:HB3	66:SK:166:ARG:HH21	1.78	0.47
67:SL:135:TRP:CH2	68:SM:73:THR:HG23	2.50	0.47
73:SR:111:ASP:OD1	73:SR:114:ARG:NH2	2.39	0.47
76:SU:93:THR:HG22	76:SU:99:ILE:HG22	1.95	0.47
88:Sg:39:ILE:HG12	88:Sg:60:ARG:HG3	1.97	0.47
1:L1:216:G:O6	34:LZ:140:LYS:HD2	2.15	0.47
1:L1:739:U:H2'	1:L1:740:C:C6	2.49	0.47
2:L2:459:A:N1	2:L2:675:G:H1'	2.30	0.47
2:L2:742:U:H2'	2:L2:743:C:C6	2.50	0.47
2:L2:1003:G:O2'	2:L2:1004:G:H8	1.98	0.47
2:L2:1384:A2M:HM'3	2:L2:1384:A2M:H1'	1.57	0.47
4:L4:49:A:H61	4:L4:60:A:H3'	1.79	0.47
5:L5:62:C:H3'	5:L5:63:G:N2	2.29	0.47
9:LA:117:GLU:HB2	9:LA:162:SER:HB2	1.96	0.47
11:LC:140:GLY:HA2	34:LZ:17:ARG:HD2	1.96	0.47
20:LL:75:LEU:HG	20:LL:111:GLY:HA2	1.96	0.47
26:LR:94:LYS:HE2	26:LR:94:LYS:HB3	1.75	0.47
44:Lj:17:ILE:HG12	44:Lj:29:VAL:HG22	1.96	0.47
49:Lo:67:GLY:HA3	49:Lo:70:THR:O	2.14	0.47
51:S1:547:U:H3'	51:S1:548:G:C8	2.48	0.47
51:S1:927:G:H1	51:S1:959:U:H3	1.63	0.47
51:S1:1723:A:N1	67:SL:35:ILE:N	2.63	0.47
60:SE:119:LYS:HE2	60:SE:140:ASP:OD2	2.15	0.47
60:SE:248:GLN:NE2	60:SE:252:GLU:OE2	2.46	0.47
69:SN:14:TYR:CG	69:SN:83:MET:CE	2.97	0.47
80:SY:20:ARG:NH1	80:SY:38:GLN:OE1	2.48	0.47
88:Sg:12:GLY:HA3	88:Sg:34:ARG:HB3	1.96	0.47
89:Sh:132:HIS:ND1	89:Sh:204:LEU:O	2.38	0.47
1:L1:1658:U:H5''	2:L2:417:G:H5'	1.96	0.47
2:L2:1115:U:H5	23:LO:17:GLN:O	1.98	0.47
4:L4:114:A:H3'	4:L4:115:A:C8	2.49	0.47
11:LC:178:ASP:O	11:LC:182:VAL:HG12	2.15	0.47
14:LF:66:SER:HB2	14:LF:76:ILE:HA	1.96	0.47
51:S1:232:C:H2'	51:S1:233:G:C8	2.50	0.47
51:S1:2086:A:N1	51:S1:2137:U:H5	2.13	0.47
1:L1:1231:G:N2	16:LH:105:MET:SD	2.88	0.47
2:L2:502[A]:A2M:CM'	51:S1:2065:G:H21	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L4:180:C:H1'	5:L5:5:C:H1'	1.97	0.47
20:LL:129:LEU:HG	20:LL:133:LYS:HD2	1.97	0.47
24:LP:16:ARG:HD2	24:LP:18:HIS:O	2.15	0.47
30:LV:134:ASP:O	30:LV:138:THR:HG23	2.15	0.47
43:Li:93:MET:HE2	43:Li:93:MET:CA	2.45	0.47
50:Lp:65:THR:HG22	50:Lp:89:LYS:HG2	1.96	0.47
51:S1:245:A:N1	51:S1:302:U:H5	2.13	0.47
51:S1:1782:G:H5'	68:SM:84:ARG:HH22	1.80	0.47
54:S4:51:U:H3	54:S4:63:G:H1	1.62	0.47
67:SL:141:ARG:O	67:SL:143:ARG:NH1	2.48	0.47
79:SX:53:SER:HB3	79:SX:56:ARG:HH11	1.79	0.47
88:Sg:7:LEU:HD12	88:Sg:41:TRP:CD2	2.50	0.47
2:L2:847:U:H2'	2:L2:848:C:C6	2.49	0.46
4:L4:51:U:H2'	4:L4:52:A:H8	1.80	0.46
23:LO:162:GLY:HA2	23:LO:187:PRO:HD3	1.97	0.46
51:S1:450:A:H2'	51:S1:451:C:C6	2.50	0.46
51:S1:933:G:N2	51:S1:937:C:O2	2.48	0.46
51:S1:946:U:H2'	51:S1:947:U:C6	2.50	0.46
51:S1:1681:A:H3'	51:S1:1682:G:H8	1.80	0.46
57:SB:140:ALA:HB1	57:SB:145:ILE:HB	1.96	0.46
60:SE:83:PHE:CE2	60:SE:84:MET:HG2	2.51	0.46
67:SL:31:ALA:HB1	79:SX:13:LYS:HE3	1.97	0.46
68:SM:47:ILE:HG22	68:SM:49:GLY:H	1.80	0.46
70:SO:71:ALA:HB1	70:SO:112:LEU:HD22	1.96	0.46
82:Sa:71:ILE:HB	82:Sa:75:ILE:HD11	1.97	0.46
88:Sg:33:SER:OG	88:Sg:34:ARG:N	2.47	0.46
88:Sg:38:ALA:HB3	88:Sg:61:LEU:HB2	1.96	0.46
1:L1:235:A2M:H8	1:L1:235:A2M:OP2	2.16	0.46
2:L2:347:A:H2'	2:L2:348:A:C8	2.50	0.46
12:LD:112:ILE:HD13	12:LD:124:ILE:HD11	1.97	0.46
18:LJ:65:LYS:HA	18:LJ:65:LYS:HD2	1.81	0.46
20:LL:61:TYR:OH	50:Lp:38:ARG:NH2	2.48	0.46
24:LP:44:PHE:CD2	24:LP:140:GLY:HA3	2.50	0.46
37:Lc:166:ILE:HD12	37:Lc:171:VAL:HB	1.97	0.46
51:S1:1718:A:H5'	82:Sa:85:ARG:HG2	1.96	0.46
54:S4:38:A:H3'	54:S4:39:U:C6	2.50	0.46
63:SH:24:LEU:HD12	63:SH:103:SER:HA	1.97	0.46
66:SK:153:LYS:O	66:SK:153:LYS:HG3	2.14	0.46
68:SM:16:THR:HG23	68:SM:114:LEU:HB2	1.97	0.46
68:SM:27:LYS:HB2	68:SM:27:LYS:HE3	1.60	0.46
1:L1:460:A:H5''	1:L1:662:C:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:555:U:H2'	1:L1:556:C:C6	2.51	0.46
2:L2:1335:C:C2	2:L2:1337:C:H5'	2.51	0.46
8:L8:26:A:H2'	8:L8:27:A:C8	2.50	0.46
15:LG:134:VAL:HB	15:LG:200:ALA:HB3	1.98	0.46
23:LO:17:GLN:HB2	27:LS:20:ARG:HG2	1.97	0.46
33:LY:44:ALA:HB1	33:LY:112:VAL:HG11	1.98	0.46
40:Lf:96:VAL:HG22	40:Lf:121:ALA:HB3	1.98	0.46
53:S3:23:C:H2'	53:S3:24:U:C6	2.50	0.46
57:SB:176:MET:HE3	57:SB:180:LEU:HG	1.97	0.46
58:SC:79:LYS:HA	58:SC:79:LYS:HD3	1.74	0.46
66:SK:110:LYS:HB2	66:SK:110:LYS:HE3	1.74	0.46
66:SK:110:LYS:HE2	66:SK:179:LEU:O	2.14	0.46
66:SK:119:ILE:HD11	66:SK:166:ARG:HD3	1.97	0.46
73:SR:62:ALA:HA	73:SR:65:LEU:HB2	1.96	0.46
77:SV:35:ILE:HA	77:SV:38:VAL:HG22	1.97	0.46
78:SW:102:ALA:HA	78:SW:111:ALA:HA	1.98	0.46
79:SX:10:ARG:NE	79:SX:14:ARG:O	2.48	0.46
88:Sg:247:ARG:NH2	88:Sg:308:ILE:HG21	2.30	0.46
1:L1:553:A:C8	11:LC:337:THR:HG21	2.50	0.46
1:L1:1259:C:H2'	1:L1:1260:G:C8	2.50	0.46
2:L2:105:A:H2'	2:L2:106:A:C8	2.50	0.46
16:LH:209:PRO:HG2	16:LH:212:ASN:ND2	2.31	0.46
26:LR:75:ASN:HD21	26:LR:145:HIS:HE1	1.62	0.46
39:Le:86:MET:HE3	39:Le:86:MET:HB3	1.77	0.46
51:S1:251:A:H1'	51:S1:784:C:H1'	1.98	0.46
51:S1:2028:C:H5''	67:SL:78:GLY:HA2	1.96	0.46
58:SC:167:VAL:HG22	58:SC:188:MET:HG2	1.98	0.46
1:L1:64:A:N6	1:L1:74:G:H1'	2.30	0.46
1:L1:1436:G:N7	34:LZ:109:ARG:NH2	2.62	0.46
2:L2:447:G:H1'	9:LA:222:PRO:HG2	1.96	0.46
3:L3:22:C:H2'	3:L3:23:U:C6	2.51	0.46
3:L3:204:A:H2'	3:L3:205:A:C8	2.50	0.46
10:LB:302:THR:OG1	10:LB:308:THR:O	2.27	0.46
27:LS:36:VAL:HA	27:LS:64:VAL:HG22	1.98	0.46
29:LU:70:LEU:HD23	29:LU:79:ILE:HG12	1.97	0.46
48:Ln:13:LYS:NZ	51:S1:2177:G:N7	2.63	0.46
51:S1:775:C:H3'	51:S1:776:A:C8	2.50	0.46
51:S1:1961:G:H5'	79:SX:99:GLY:HA2	1.98	0.46
53:S3:54:U:H2'	53:S3:55:U:O4'	2.16	0.46
55:S5:6:U:H2'	55:S5:7:G:C8	2.50	0.46
68:SM:101:PHE:HD1	68:SM:103:MET:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:23:U:H4'	1:L1:24:A:N7	2.30	0.46
1:L1:199:A:N1	34:LZ:140:LYS:NZ	2.63	0.46
1:L1:897:A:N6	51:S1:1218:A:N1	2.63	0.46
2:L2:95:A2M:HM'3	2:L2:95:A2M:H1'	1.77	0.46
3:L3:39:C:H5''	25:LQ:96:MET:SD	2.55	0.46
6:L6:19:C:H2'	6:L6:20:A:C8	2.51	0.46
6:L6:46:C:H5'	19:LK:121:ALA:HB2	1.98	0.46
16:LH:202:LYS:HE3	16:LH:202:LYS:HB3	1.59	0.46
25:LQ:66:MET:HG3	25:LQ:70:LYS:HD2	1.97	0.46
28:LT:88:VAL:O	28:LT:92:MET:HG3	2.16	0.46
31:LW:71:TYR:O	94:LW:201:HOH:O	2.21	0.46
51:S1:157:G:C2	51:S1:158:G:H1'	2.51	0.46
63:SH:8:LEU:HD11	63:SH:36:PRO:HD3	1.97	0.46
2:L2:1087:C:H2'	2:L2:1088:G:C8	2.51	0.46
7:L7:75:OMG:HM23	7:L7:75:OMG:H1'	1.71	0.46
10:LB:165:HIS:HA	10:LB:182:HIS:O	2.15	0.46
11:LC:273:LYS:HA	11:LC:273:LYS:HE3	1.98	0.46
11:LC:354:LYS:HE2	11:LC:354:LYS:HB2	1.69	0.46
16:LH:45:LEU:HD11	16:LH:120:LEU:HB2	1.96	0.46
21:LM:18:VAL:O	21:LM:22:ILE:HG13	2.15	0.46
48:Ln:29:MET:HG3	51:S1:2151:OMG:HM21	1.97	0.46
51:S1:364:G:H3'	51:S1:365:U:H2'	1.98	0.46
51:S1:784:C:H42	51:S1:834:U:H3	1.64	0.46
53:S3:21:A:H3'	53:S3:46:A:N6	2.31	0.46
56:SA:51:THR:HG23	56:SA:56:ILE:HA	1.98	0.46
65:SJ:37:PHE:O	65:SJ:41:MET:HG3	2.15	0.46
77:SV:107:GLN:O	77:SV:111:ARG:HD3	2.16	0.46
78:SW:67:LEU:HD22	78:SW:83:VAL:HG11	1.97	0.46
82:Sa:50:LEU:O	82:Sa:54:VAL:HB	2.16	0.46
88:Sg:35:ASP:OD1	88:Sg:35:ASP:N	2.39	0.46
1:L1:472:U:H2'	1:L1:473:A:C8	2.51	0.46
1:L1:633:U:H4'	1:L1:634:G:H5''	1.98	0.46
1:L1:694:U:H2'	1:L1:695:OMC:C6	2.50	0.46
1:L1:700:A:H2	1:L1:845:OMU:H5	1.79	0.46
1:L1:1004:G:N2	1:L1:1173:G:H2'	2.31	0.46
1:L1:1626:OMG:HM21	1:L1:1755:U:H5'	1.98	0.46
2:L2:403:G:N7	9:LA:152:SER:OG	2.44	0.46
3:L3:71:U:H5''	42:Lh:25:ARG:O	2.16	0.46
8:L8:51:U:OP1	23:LO:94:ASN:ND2	2.48	0.46
10:LB:41:PRO:HA	10:LB:189:ASN:O	2.16	0.46
38:Ld:34:THR:O	38:Ld:38:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1:G:H21	61:SF:192:ALA:H	1.62	0.46
51:S1:955:A:O2'	51:S1:956:A:H8	1.98	0.46
60:SE:165:LYS:HB2	60:SE:165:LYS:HE2	1.78	0.46
67:SL:100:GLN:HB2	67:SL:108:LYS:HE3	1.98	0.46
84:Sc:54:SER:HB3	84:Sc:63:LYS:HE2	1.98	0.46
1:L1:34:C:H4'	1:L1:859:A:C2	2.51	0.46
2:L2:622:G:H2'	2:L2:623:A:C8	2.51	0.46
2:L2:1334:C:H4'	47:Lm:95:VAL:HG11	1.97	0.46
11:LC:194:LYS:HA	11:LC:199:ARG:HA	1.98	0.46
29:LU:51:PHE:HB3	29:LU:70:LEU:HD22	1.98	0.46
31:LW:66:LYS:HB3	31:LW:66:LYS:HE3	1.71	0.46
34:LZ:9:TRP:CZ2	34:LZ:13:ARG:HG3	2.50	0.46
37:Lc:60:LYS:HB3	37:Lc:60:LYS:HE2	1.75	0.46
43:Li:97:LEU:O	43:Li:101:THR:HG23	2.16	0.46
44:Lj:37:CYS:HB2	44:Lj:44:ARG:HD3	1.97	0.46
51:S1:1523:A:H2'	51:S1:1524:G:H8	1.80	0.46
52:S2:37:MIA:H3'	52:S2:38:A:H8	1.80	0.46
54:S4:2:C:H2'	54:S4:3:G:C8	2.50	0.46
57:SB:24:MET:HG3	57:SB:176:MET:HG2	1.97	0.46
69:SN:18:PHE:CD2	69:SN:83:MET:HB3	2.49	0.46
1:L1:1666:G:H4'	1:L1:1667:G:H8	1.80	0.46
2:L2:1278:C:N4	2:L2:1283:A:O2'	2.49	0.46
4:L4:21:C:O2'	5:L5:135:C:N4	2.49	0.46
20:LL:51:GLY:HA2	24:LP:182:ARG:H	1.80	0.46
39:Le:125:ASN:HA	39:Le:168:THR:HG22	1.96	0.46
41:Lg:34:TYR:CE1	41:Lg:136:ARG:HG2	2.51	0.46
51:S1:1:G:H1'	61:SF:191:VAL:HG13	1.98	0.46
51:S1:1539:PSU:HN3	51:S1:1550:OMG:HN1	1.63	0.46
59:SD:76:MET:HE3	59:SD:92:LEU:HA	1.98	0.46
69:SN:94:MET:HB3	69:SN:98:GLN:HB2	1.97	0.46
89:Sh:177:LEU:HD12	89:Sh:183:ALA:HA	1.97	0.46
1:L1:435:G:H22	1:L1:438:A:H5''	1.81	0.45
2:L2:558:A:H2'	2:L2:561:G:H21	1.81	0.45
2:L2:1329:U:H5	2:L2:1350:G:O6	1.99	0.45
10:LB:36:ASP:O	10:LB:190:GLY:HA2	2.17	0.45
23:LO:185:ARG:HD3	23:LO:185:ARG:HA	1.74	0.45
31:LW:81:LYS:HD3	31:LW:81:LYS:HA	1.69	0.45
39:Le:11:LEU:HD22	39:Le:15:LYS:HE2	1.99	0.45
51:S1:1277:A:H62	83:Sb:1:MET:H1	1.64	0.45
51:S1:1862:C:H2'	51:S1:1863:G:C8	2.51	0.45
54:S4:16:U:H2'	54:S4:60:U:H5	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SN:94:MET:HE3	69:SN:95:PRO:HD2	1.99	0.45
72:SQ:50:VAL:HA	72:SQ:53:THR:HG22	1.98	0.45
73:SR:21:VAL:HG13	73:SR:30:ALA:HB1	1.98	0.45
73:SR:67:LYS:HD2	73:SR:71:ILE:CD1	2.46	0.45
1:L1:598:G:H5''	27:LS:137:ILE:HD12	1.97	0.45
1:L1:1640:G:H2'	1:L1:1641:A:C8	2.51	0.45
2:L2:431:C:H5'	9:LA:219:ILE:HD11	1.99	0.45
2:L2:1007:U:H2'	2:L2:1008:C:C6	2.51	0.45
9:LA:79:PRO:HD2	9:LA:82:MET:SD	2.56	0.45
26:LR:70:LYS:O	26:LR:74:ARG:NH2	2.49	0.45
35:La:53:LYS:HD3	35:La:53:LYS:HA	1.70	0.45
51:S1:111:U:H5'	76:SU:82:ARG:HD2	1.97	0.45
51:S1:789:G:OP2	60:SE:173:ARG:NH2	2.49	0.45
51:S1:1579:A:H1'	51:S1:1581:G:N3	2.31	0.45
51:S1:1999:G:H2'	51:S1:2000:U:C6	2.50	0.45
53:S3:56:C:H3'	53:S3:57:A:C8	2.52	0.45
57:SB:51:ILE:HG22	77:SV:108:MET:HE1	1.98	0.45
62:SG:231:LYS:HB2	62:SG:231:LYS:NZ	2.31	0.45
64:SI:117:ARG:HA	64:SI:117:ARG:HD2	1.82	0.45
75:ST:99:ARG:HG2	75:ST:115:LEU:HD21	1.97	0.45
82:Sa:70:LYS:HD3	82:Sa:70:LYS:HA	1.68	0.45
1:L1:234:G:H2'	1:L1:235:A2M:C8	2.47	0.45
1:L1:325:C:H5''	21:LM:170:LYS:O	2.16	0.45
1:L1:352:G:OP2	43:Li:25:ARG:NH2	2.50	0.45
1:L1:830:G:OP1	24:LP:192:ARG:NH2	2.49	0.45
1:L1:973:U:C6	1:L1:978:C:H5'	2.51	0.45
1:L1:1565:A:H2'	1:L1:1566:A:C8	2.51	0.45
1:L1:1629:G:O6	42:Lh:11:ARG:NH2	2.49	0.45
1:L1:1665:A:H2'	1:L1:1667:G:H5'	1.99	0.45
8:L8:27:A:H2'	8:L8:28:A:C8	2.51	0.45
16:LH:209:PRO:O	16:LH:213:VAL:HG23	2.16	0.45
27:LS:39:TYR:CZ	27:LS:63:ILE:HD11	2.51	0.45
31:LW:56:LYS:HE2	31:LW:56:LYS:HB3	1.80	0.45
34:LZ:7:LEU:O	34:LZ:11:LEU:HG	2.15	0.45
41:Lg:74:ARG:HG2	41:Lg:141:PRO:HD3	1.97	0.45
51:S1:260:A:H2'	51:S1:261:A:O4'	2.16	0.45
52:S2:36:A:H3'	52:S2:37:MIA:H8	1.98	0.45
77:SV:33:ARG:HD3	77:SV:36:MET:HE2	1.98	0.45
1:L1:543:G:H1'	1:L1:1392:G:C8	2.52	0.45
9:LA:180:LEU:HD22	49:Lo:18:TYR:HB3	1.97	0.45
10:LB:132:ARG:NH1	10:LB:135:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:181:ARG:HA	25:LQ:181:ARG:HD2	1.77	0.45
49:Lo:67:GLY:HA2	49:Lo:73:THR:HG23	1.98	0.45
51:S1:676:C:H5''	75:ST:5:HIS:CD2	2.52	0.45
51:S1:933:G:H5''	76:SU:43:LYS:HD3	1.99	0.45
51:S1:1017:U:H2'	51:S1:1018:G:C8	2.52	0.45
88:Sg:68:VAL:HG12	88:Sg:84:SER:HB2	1.98	0.45
1:L1:1018:A:N3	27:LS:81:ARG:NH2	2.65	0.45
4:L4:16:G:H3'	4:L4:17:A:H8	1.82	0.45
42:Lh:40:SER:HB2	42:Lh:61:ARG:HG3	1.98	0.45
51:S1:110:G:O2'	76:SU:82:ARG:NH1	2.49	0.45
51:S1:275:A:H1'	51:S1:276:G:H5'	1.99	0.45
51:S1:575:C:H3'	51:S1:576:A:H8	1.82	0.45
51:S1:1663:U:C4'	77:SV:4:ILE:HD11	2.45	0.45
51:S1:1715:C:C6	79:SX:8:ILE:HG12	2.51	0.45
51:S1:1989:A:H2'	51:S1:1990:A:C8	2.52	0.45
51:S1:2178:U:H2'	51:S1:2179:A:C8	2.51	0.45
57:SB:36:ALA:HB1	57:SB:157:LEU:HD12	1.98	0.45
63:SH:45:ARG:HA	63:SH:45:ARG:HD3	1.70	0.45
66:SK:80:ASP:OD1	66:SK:94:LYS:HE3	2.17	0.45
1:L1:289:U:H2'	1:L1:290:G:C8	2.52	0.45
1:L1:1445:G:OP1	34:LZ:26:ARG:NH2	2.49	0.45
1:L1:1671:G:N7	30:LV:37:ARG:NH2	2.60	0.45
1:L1:1680:U:H2'	1:L1:1681:G:C8	2.51	0.45
2:L2:502[A]:A2M:C2	51:S1:2065:G:H22	2.30	0.45
2:L2:777:A:H4'	15:LG:248:ARG:HD2	1.97	0.45
3:L3:72:A:H5'	42:Lh:26:THR:HA	1.99	0.45
5:L5:2:U:O2'	5:L5:3:U:O2	2.34	0.45
19:LK:140:HIS:HD2	19:LK:141:LYS:HD3	1.81	0.45
27:LS:84:THR:HG23	36:Lb:22:LYS:O	2.16	0.45
44:Lj:25:ASN:O	44:Lj:25:ASN:ND2	2.50	0.45
51:S1:639:C:H2'	51:S1:640:A:C8	2.52	0.45
66:SK:69:SER:OG	66:SK:204:GLU:OE1	2.25	0.45
67:SL:85:TYR:O	67:SL:88:ARG:HG2	2.17	0.45
67:SL:89:GLN:HE22	67:SL:125:ALA:HB2	1.82	0.45
73:SR:106:THR:HG23	73:SR:109:ARG:HH22	1.81	0.45
89:Sh:154:MET:HA	89:Sh:154:MET:CE	2.43	0.45
1:L1:412:G:H4'	1:L1:437:A:N1	2.31	0.45
1:L1:675:U:H5''	1:L1:1004:G:H1	1.82	0.45
2:L2:4:C:O2	3:L3:18:A:O2'	2.35	0.45
2:L2:665:A2M:HM'3	2:L2:665:A2M:H1'	1.82	0.45
13:LE:52:ARG:HG2	13:LE:52:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:121:VAL:CG1	21:LM:131:GLU:HG3	2.45	0.45
29:LU:87:LYS:HG2	29:LU:117:TYR:CE2	2.51	0.45
51:S1:1632:C:H2'	51:S1:1633:G:C8	2.51	0.45
81:SZ:4:GLN:OE1	81:SZ:4:GLN:N	2.49	0.45
1:L1:1003:A:OP1	36:Lb:18:ARG:NH2	2.49	0.45
2:L2:1205:A:H1'	2:L2:1206:G:C8	2.52	0.45
13:LE:88:ARG:HB2	13:LE:186:ILE:CG2	2.47	0.45
20:LL:132:LYS:O	20:LL:136:LYS:HG2	2.17	0.45
21:LM:5:MET:O	21:LM:9:GLU:HG2	2.17	0.45
51:S1:258:C:H2'	51:S1:259:C:C6	2.51	0.45
51:S1:1484:A:H2'	51:S1:1485:A:C8	2.52	0.45
51:S1:1701:A:H2'	51:S1:1702:A:C8	2.51	0.45
54:S4:10:G:H1	54:S4:26:A:H1'	1.82	0.45
56:SA:66:PHE:CD2	70:SO:41:SER:HB3	2.52	0.45
58:SC:112:LEU:HD12	58:SC:113:GLN:H	1.82	0.45
66:SK:219:LYS:HZ3	66:SK:220:LYS:HE2	1.80	0.45
88:Sg:61:LEU:HD13	88:Sg:92:TRP:CG	2.52	0.45
89:Sh:152:GLN:HA	89:Sh:155:GLU:OE2	2.17	0.45
1:L1:413:A:H2'	1:L1:414:A:C8	2.51	0.45
1:L1:1202:G:H1'	40:Lf:46:ARG:HH21	1.82	0.45
2:L2:1240:A:H5'	50:Lp:56:PRO:HB3	1.99	0.45
7:L7:22:U:H6	31:LW:18:GLN:HE21	1.65	0.45
10:LB:221:ASP:OD2	10:LB:346:ARG:NH2	2.30	0.45
35:La:17:ASP:O	35:La:21:THR:HG22	2.17	0.45
38:Ld:15:LYS:O	38:Ld:19:VAL:HG23	2.16	0.45
51:S1:994:U:H3	51:S1:1018:G:H1	1.64	0.45
51:S1:2030:G:H4'	63:SH:63:MET:HE1	1.99	0.45
61:SF:107:ARG:NH1	61:SF:109:ARG:HH11	2.14	0.45
64:SI:189:MET:HE3	64:SI:195:GLN:HA	1.98	0.45
71:SP:85:VAL:HA	71:SP:86:PRO:HD3	1.84	0.45
1:L1:626:U:H5''	11:LC:335:ARG:HH21	1.82	0.45
1:L1:1099:A:H2'	22:LN:22:PHE:CZ	2.51	0.45
3:L3:44:C:H4'	42:Lh:31:LEU:HD11	1.98	0.45
9:LA:42:ARG:HG3	9:LA:89:PHE:CE2	2.51	0.45
9:LA:80:GLU:HG3	49:Lo:66:GLY:HA3	1.99	0.45
10:LB:121:ASN:ND2	10:LB:124:GLN:HG3	2.32	0.45
22:LN:90:ARG:HG3	22:LN:134:ILE:HG22	1.99	0.45
23:LO:30:TYR:HA	23:LO:33:ARG:HB3	1.99	0.45
24:LP:196:ARG:HG3	24:LP:196:ARG:NH1	2.32	0.45
26:LR:75:ASN:HD21	26:LR:145:HIS:CE1	2.34	0.45
51:S1:232:C:H2'	51:S1:233:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1586:A:H3'	51:S1:1597:G:C8	2.52	0.45
51:S1:2132:C:H2'	51:S1:2133:G:O4'	2.17	0.45
82:Sa:58:LYS:HD2	82:Sa:58:LYS:HA	1.62	0.45
1:L1:1666:G:N2	15:LG:53:TRP:O	2.50	0.44
3:L3:143:A:H3'	3:L3:144:U:H6	1.83	0.44
13:LE:5:LYS:HE2	13:LE:59:TRP:CH2	2.52	0.44
16:LH:65:GLU:OE2	16:LH:69:LYS:NZ	2.42	0.44
26:LR:46:MET:HA	26:LR:46:MET:HE2	2.00	0.44
51:S1:16:G:H2'	51:S1:17:C:C6	2.52	0.44
51:S1:550:C:H2'	51:S1:551:A:C8	2.52	0.44
51:S1:777:A:H4'	51:S1:778:G:O5'	2.17	0.44
51:S1:1712:G:C6	79:SX:149:PHE:HE1	2.35	0.44
51:S1:1713:C:H2'	51:S1:1714:C:O4'	2.17	0.44
54:S4:51:U:H2'	54:S4:52:G:C8	2.53	0.44
57:SB:51:ILE:HG22	77:SV:108:MET:CE	2.47	0.44
58:SC:98:MET:HG3	58:SC:172:ARG:HH22	1.83	0.44
73:SR:25:ARG:NH2	73:SR:33:MET:HE2	2.32	0.44
73:SR:128:TYR:OH	78:SW:133:VAL:O	2.28	0.44
79:SX:77:ILE:HD13	79:SX:83:VAL:HG12	1.99	0.44
79:SX:118:LYS:HB2	79:SX:118:LYS:HE3	1.66	0.44
1:L1:23:U:OP2	44:Lj:46:ARG:NH2	2.50	0.44
2:L2:1507:U:H2'	2:L2:1508:A:C8	2.52	0.44
3:L3:16:G:N1	3:L3:20:C:H2'	2.29	0.44
3:L3:126:C:H2'	3:L3:127:G:C8	2.51	0.44
26:LR:15:GLU:HG3	26:LR:53:VAL:HG13	2.00	0.44
33:LY:123:GLY:HA2	33:LY:126:MET:HE3	1.98	0.44
51:S1:587:A:H5'	59:SD:170:ARG:NH2	2.32	0.44
51:S1:1248:A:H2'	51:S1:1249:G:C8	2.52	0.44
56:SA:170:ILE:HD11	56:SA:212:LEU:HD11	1.99	0.44
58:SC:160:GLY:O	58:SC:163:HIS:ND1	2.49	0.44
60:SE:140:ASP:OD1	60:SE:140:ASP:N	2.41	0.44
81:SZ:28:PHE:HE1	81:SZ:50:LEU:HD21	1.82	0.44
88:Sg:246:ASN:ND2	88:Sg:247:ARG:HG3	2.32	0.44
1:L1:717:G:N7	17:LI:37:LYS:NZ	2.60	0.44
1:L1:1133:A:P	23:LO:135:LYS:HZ1	2.41	0.44
1:L1:1684:G:H1	1:L1:1708:G:H22	1.65	0.44
2:L2:1246:A:H5'	2:L2:1246:A:C8	2.52	0.44
19:LK:3:LYS:HB3	19:LK:3:LYS:HE3	1.78	0.44
24:LP:175:ASN:HD22	24:LP:178:LYS:H	1.65	0.44
32:LX:56:THR:O	32:LX:60:ARG:HG2	2.18	0.44
51:S1:158:G:H4'	62:SG:15:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:956:A:H2'	51:S1:957:G:H8	1.82	0.44
51:S1:1535:A:H2'	51:S1:1536:A:C8	2.53	0.44
51:S1:1862:C:H2'	51:S1:1863:G:H8	1.83	0.44
51:S1:1889:G:H5''	51:S1:1889:G:H8	1.82	0.44
56:SA:226:ASP:HB3	56:SA:229:ALA:HB3	1.99	0.44
69:SN:61:LEU:HD11	69:SN:82:TYR:HB3	1.98	0.44
73:SR:118:MET:HE1	78:SW:121:HIS:HE1	1.82	0.44
77:SV:119:ARG:HE	77:SV:119:ARG:HB3	1.68	0.44
78:SW:35:LEU:HD22	78:SW:39:GLU:HB2	1.99	0.44
1:L1:911:G:OP1	49:Lo:17:ARG:NH1	2.51	0.44
1:L1:1742:G:H2'	1:L1:1743:A:C8	2.52	0.44
9:LA:96:LEU:HD11	9:LA:107:ILE:HG23	2.00	0.44
13:LE:56:VAL:HG22	13:LE:69:LEU:HD23	1.99	0.44
13:LE:149:ASP:O	13:LE:153:VAL:HG23	2.18	0.44
14:LF:167:LYS:HE3	14:LF:167:LYS:HB3	1.72	0.44
29:LU:87:LYS:HE2	29:LU:117:TYR:CZ	2.52	0.44
40:Lf:105:LYS:HE3	40:Lf:105:LYS:HB2	1.77	0.44
51:S1:1471:U:H2'	51:S1:1472:U:C6	2.52	0.44
51:S1:1513:C:H2'	51:S1:1514:A:C8	2.50	0.44
56:SA:33:VAL:HG22	56:SA:42:GLN:HG3	1.98	0.44
57:SB:40:TYR:CD1	57:SB:56:MET:HE2	2.52	0.44
59:SD:58:LEU:HD11	59:SD:71:GLU:HB3	1.98	0.44
88:Sg:14:VAL:HG21	88:Sg:303:ILE:HG13	1.99	0.44
44:Lj:27:TYR:HA	44:Lj:34:CYS:HA	2.00	0.44
50:Lp:10:MET:HG2	50:Lp:11:HIS:N	2.33	0.44
51:S1:12:PSU:H1'	51:S1:1652:A:N3	2.32	0.44
51:S1:847:A:C2	51:S1:906:U:H5	2.35	0.44
51:S1:1206:C:H5''	75:ST:14:SER:HB2	1.99	0.44
51:S1:1664:G:H1	51:S1:1682:G:H5'	1.82	0.44
53:S3:70:G:N3	53:S3:70:G:H2'	2.32	0.44
64:SI:75:ARG:NH1	64:SI:131:ASP:OD1	2.49	0.44
77:SV:25:ASN:CG	77:SV:26:PHE:N	2.74	0.44
88:Sg:27:ILE:H	88:Sg:27:ILE:HG13	1.59	0.44
88:Sg:105:LYS:HB2	88:Sg:134:TRP:CH2	2.52	0.44
1:L1:627:C:H2'	1:L1:628:C:C6	2.53	0.44
1:L1:1675:A:H3'	1:L1:1676:G:C8	2.49	0.44
11:LC:32:ARG:NH2	11:LC:34:ASP:OD2	2.38	0.44
14:LF:64:VAL:HG11	14:LF:101:ILE:HG21	1.99	0.44
15:LG:113:VAL:HG11	15:LG:127:THR:HG22	1.99	0.44
36:Lb:45:ARG:O	36:Lb:49:LYS:HD3	2.18	0.44
41:Lg:39:LEU:HD11	41:Lg:54:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:2040:C:H2'	51:S1:2041:U:C6	2.53	0.44
58:SC:32:GLY:O	58:SC:52:THR:N	2.38	0.44
63:SH:130:MET:HE2	63:SH:134:ASN:OD1	2.18	0.44
1:L1:147:G:O6	15:LG:139:GLU:HG3	2.17	0.44
1:L1:687:C:H2'	1:L1:688:A:H8	1.83	0.44
2:L2:1105:A:H2'	2:L2:1106:A:O4'	2.18	0.44
2:L2:1397:OMC:HM22	2:L2:1398:C:O4'	2.18	0.44
7:L7:46:G:OP2	46:L1:15:LYS:HG3	2.17	0.44
9:LA:9:ARG:NH2	9:LA:16:TYR:OH	2.51	0.44
11:LC:288:THR:O	11:LC:292:GLN:HG3	2.17	0.44
16:LH:214:GLU:OE1	16:LH:217:LYS:NZ	2.51	0.44
24:LP:165:PRO:HB2	24:LP:196:ARG:HD3	2.00	0.44
28:LT:116:HIS:O	28:LT:148:LEU:HA	2.18	0.44
33:LY:97:ILE:HB	33:LY:108:SER:HB3	1.98	0.44
36:Lb:66:PHE:O	36:Lb:69:LYS:HG3	2.17	0.44
38:Ld:97:VAL:HG12	38:Ld:102:ILE:HG13	1.99	0.44
50:Lp:70:LEU:HD21	50:Lp:91:PHE:CZ	2.52	0.44
51:S1:504:G:H2'	51:S1:505:A:C8	2.53	0.44
51:S1:1801:G:H5'	77:SV:60:ARG:HD3	1.99	0.44
67:SL:10:LYS:HB3	67:SL:102:TYR:CE2	2.53	0.44
77:SV:122:ARG:HG2	77:SV:122:ARG:NH1	2.33	0.44
82:Sa:48:ASP:OD1	82:Sa:49:LYS:N	2.51	0.44
1:L1:412:G:N2	1:L1:414:A:H3'	2.32	0.44
1:L1:955:A2M:HM'3	1:L1:955:A2M:H1'	1.75	0.44
1:L1:1715:U:H2'	1:L1:1716:G:H21	1.83	0.44
2:L2:1299:U:H2'	2:L2:1300:U:C6	2.52	0.44
18:LJ:31:THR:HG21	18:LJ:112:LYS:HG2	1.99	0.44
28:LT:31:GLU:H	28:LT:31:GLU:HG2	1.59	0.44
45:Lk:66:LYS:HB3	45:Lk:66:LYS:HE2	1.59	0.44
51:S1:128:C:H4'	51:S1:129:U:O5'	2.17	0.44
51:S1:1171:A:H2'	51:S1:1172:G:C8	2.53	0.44
58:SC:104:LEU:HB2	58:SC:121:ILE:HG13	2.00	0.44
63:SH:35:VAL:HG21	67:SL:49:THR:HG23	1.99	0.44
70:SO:40:MET:HE3	70:SO:40:MET:HB3	1.82	0.44
71:SP:95:GLU:O	71:SP:98:ASP:HB2	2.18	0.44
79:SX:19:LEU:HD12	79:SX:20:LYS:H	1.83	0.44
1:L1:450:G:H21	1:L1:1532:U:H4'	1.83	0.44
1:L1:1597:G:H1'	2:L2:26:C:H5''	2.00	0.44
2:L2:755:U:H2'	2:L2:756:C:O4'	2.18	0.44
2:L2:809:C:H2'	2:L2:810:G:C8	2.52	0.44
3:L3:20:C:H5	42:Lh:71:HIS:HE2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L4:7:U:OP2	28:LT:9:GLN:OE1	2.36	0.44
34:LZ:123:LYS:HE3	34:LZ:123:LYS:HB3	1.63	0.44
51:S1:966:G:H5'	64:SI:10:LYS:HD3	1.99	0.44
51:S1:1571:A:H3'	51:S1:1572:C:O2	2.18	0.44
57:SB:91:TYR:CZ	57:SB:95:GLN:OE1	2.71	0.44
66:SK:57:ALA:HB2	66:SK:196:GLY:HA2	1.99	0.44
67:SL:104:ASN:OD1	67:SL:107:GLU:HG2	2.18	0.44
73:SR:44:LEU:HD23	73:SR:44:LEU:HA	1.82	0.44
79:SX:8:ILE:CD1	79:SX:154:ARG:HD3	2.45	0.44
1:L1:620:U:H1'	1:L1:621:U:C5	2.53	0.43
1:L1:1276:U:H2'	1:L1:1277:G:C8	2.52	0.43
5:L5:5:C:H2'	5:L5:6:G:O4'	2.19	0.43
6:L6:56:A:H3'	6:L6:57:U:O2	2.18	0.43
22:LN:51:HIS:NE2	22:LN:168:SER:HB2	2.32	0.43
29:LU:96:LYS:HB3	29:LU:96:LYS:HE3	1.67	0.43
34:LZ:35:ASN:HB3	34:LZ:37:ASN:H	1.82	0.43
37:Lc:160:LYS:HD3	37:Lc:252:ILE:HG22	2.00	0.43
47:Lm:83:VAL:HG12	47:Lm:87:LYS:HD2	1.99	0.43
51:S1:587:A:N3	51:S1:590:A:H2'	2.33	0.43
51:S1:1597:G:H4'	51:S1:1598:U:C5	2.53	0.43
53:S3:13:C:O2	53:S3:13:C:H2'	2.18	0.43
64:SI:25:LYS:HB2	64:SI:25:LYS:HE3	1.74	0.43
64:SI:39:GLN:H	64:SI:39:GLN:HG2	1.61	0.43
67:SL:55:MET:O	67:SL:59:THR:HG23	2.17	0.43
68:SM:25:ASN:HB3	68:SM:28:ALA:HB3	2.00	0.43
89:Sh:139:PHE:HB2	89:Sh:174:TYR:CE1	2.53	0.43
1:L1:868:A:O2'	44:Lj:11:ARG:HG2	2.19	0.43
2:L2:957:C:H2'	2:L2:958:A:H8	1.83	0.43
2:L2:1003:G:HO2'	2:L2:1004:G:H8	1.64	0.43
3:L3:19:A:H2	3:L3:215:G:H21	1.63	0.43
3:L3:105:C:H2'	3:L3:106:U:C6	2.53	0.43
5:L5:25:A:H5''	10:LB:179:LYS:HG3	1.99	0.43
36:Lb:31:ASN:OD1	36:Lb:31:ASN:N	2.43	0.43
51:S1:1438:A:C5	51:S1:1439:G:H1'	2.53	0.43
51:S1:2023:C:H2'	51:S1:2024:U:C6	2.53	0.43
88:Sg:46:ASP:N	88:Sg:46:ASP:OD1	2.50	0.43
1:L1:613:C:H2'	1:L1:614:A:C8	2.53	0.43
2:L2:1156:G:O6	27:LS:78:LYS:HE2	2.19	0.43
3:L3:213:G:OP2	33:LY:131:ARG:NH2	2.51	0.43
17:LI:65:CYS:HA	17:LI:66:PRO:HD3	1.90	0.43
18:LJ:108:LYS:HA	18:LJ:108:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LK:148:LEU:HD23	19:LK:148:LEU:HA	1.86	0.43
21:LM:165:THR:O	21:LM:169:ARG:HG3	2.17	0.43
51:S1:1572:C:H5	51:S1:1615:G:H22	1.66	0.43
51:S1:1597:G:H1	51:S1:1602:U:H3	1.67	0.43
51:S1:2025:G:OP2	67:SL:133:LYS:HD3	2.18	0.43
52:S2:34:G:H2'	52:S2:35:A:C8	2.53	0.43
64:SI:143:TRP:CZ3	65:SJ:54:ASP:HB2	2.52	0.43
72:SQ:62:CYS:O	72:SQ:88:LEU:HA	2.19	0.43
1:L1:574:G:O5'	11:LC:324:ARG:HG2	2.18	0.43
1:L1:1741:A:O2'	3:L3:204:A:N1	2.49	0.43
2:L2:578:U:H2'	2:L2:579:C:O4'	2.19	0.43
5:L5:122:U:H2'	5:L5:123:G:C8	2.53	0.43
12:LD:28:SER:HA	12:LD:32:LEU:HB2	1.99	0.43
12:LD:81:LEU:HD12	12:LD:81:LEU:HA	1.88	0.43
15:LG:64:ARG:O	15:LG:68:ARG:HG3	2.19	0.43
16:LH:22:PRO:HG2	16:LH:24:ILE:HD11	2.00	0.43
20:LL:92:LYS:HG3	20:LL:138:GLY:HA3	1.99	0.43
22:LN:84:VAL:HG21	22:LN:144:TYR:CE2	2.53	0.43
48:Ln:34:LYS:HE2	48:Ln:34:LYS:HB2	1.85	0.43
51:S1:192:U:H3	51:S1:233:G:H1	1.67	0.43
51:S1:306:U:H4'	66:SK:64:ASN:HD21	1.83	0.43
51:S1:979:U:H2'	51:S1:980:G:H8	1.83	0.43
51:S1:1916:G:H3'	51:S1:1917:A:C8	2.53	0.43
62:SG:80:ARG:HG2	62:SG:87:THR:HA	2.00	0.43
67:SL:55:MET:HE3	67:SL:55:MET:HB3	1.70	0.43
70:SO:58:ASP:OD1	70:SO:58:ASP:N	2.51	0.43
85:Sd:29:VAL:HA	85:Sd:42:VAL:HG23	2.00	0.43
88:Sg:282:CYS:HB2	88:Sg:298:HIS:CE1	2.53	0.43
1:L1:1776:G:H22	2:L2:6:A:H2	1.65	0.43
2:L2:1202:A:N1	2:L2:1203:A:N6	2.67	0.43
6:L6:68:A:N6	41:Lg:34:TYR:OH	2.51	0.43
7:L7:123:G:H3'	7:L7:138:C:H42	1.83	0.43
9:LA:178:PRO:HG2	49:Lo:26:ALA:HB2	2.00	0.43
15:LG:162:GLU:CD	21:LM:26:ARG:HH22	2.25	0.43
30:LV:69:PRO:HA	30:LV:87:PHE:HA	2.00	0.43
51:S1:195:U:H2'	51:S1:196:C:C6	2.53	0.43
51:S1:263:G:H1	51:S1:274:C:H41	1.66	0.43
51:S1:1586:A:H3'	51:S1:1597:G:H8	1.84	0.43
51:S1:2158[A]:A:O2'	51:S1:2159:A:H5'	2.18	0.43
53:S3:53:G:H2'	53:S3:53:G:N3	2.34	0.43
57:SB:203:ASP:HA	57:SB:206:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:SV:33:ARG:HD3	77:SV:33:ARG:HA	1.79	0.43
78:SW:24:TYR:HB3	78:SW:32:LEU:HD11	2.00	0.43
78:SW:105:ASN:HB2	78:SW:129:SER:HA	2.00	0.43
87:Sf:78:ARG:HD2	87:Sf:80:PHE:HE1	1.80	0.43
87:Sf:140:CYS:O	87:Sf:144:HIS:N	2.51	0.43
89:Sh:150:LYS:HB2	89:Sh:150:LYS:HE2	1.75	0.43
89:Sh:187:VAL:O	89:Sh:191:ASN:HB2	2.18	0.43
1:L1:31:G:H21	1:L1:49:C:H5	1.67	0.43
2:L2:1004:G:H2'	2:L2:1005:A:C8	2.54	0.43
13:LE:156:GLU:HA	13:LE:159:VAL:HG22	1.99	0.43
37:Lc:230:HIS:CE1	37:Lc:238:GLY:HA3	2.53	0.43
42:Lh:115:LYS:HB2	42:Lh:115:LYS:HE2	1.80	0.43
51:S1:342:C:H1'	60:SE:30:PRO:HG3	1.99	0.43
51:S1:1992:G:H4'	51:S1:1993:A:H8	1.83	0.43
56:SA:62:ARG:NH1	56:SA:92:GLU:OE1	2.51	0.43
58:SC:142:LYS:HD2	58:SC:142:LYS:HA	1.92	0.43
61:SF:107:ARG:HG2	61:SF:107:ARG:HH11	1.84	0.43
61:SF:193:ALA:HB3	61:SF:196:PRO:HD2	2.00	0.43
66:SK:26:LYS:HE2	66:SK:29:LEU:HD21	2.01	0.43
71:SP:32:THR:HG22	71:SP:34:SER:H	1.84	0.43
78:SW:62:VAL:O	78:SW:66:ARG:HG3	2.19	0.43
78:SW:68:ARG:NH2	78:SW:95:GLU:OE1	2.50	0.43
88:Sg:127:ARG:HA	88:Sg:152:TRP:CB	2.48	0.43
1:L1:711:G:H1'	1:L1:839:U:H1'	2.00	0.43
30:LV:120:ASP:C	30:LV:120:ASP:OD1	2.62	0.43
38:Ld:18:LEU:HD13	38:Ld:100:SER:HA	1.99	0.43
40:Lf:33:TRP:O	40:Lf:34:ARG:NH1	2.51	0.43
51:S1:956:A:H2'	51:S1:957:G:C8	2.54	0.43
51:S1:1471:U:H3	51:S1:1480:G:H1	1.67	0.43
57:SB:113:ASN:HB3	57:SB:116:GLN:HG2	2.01	0.43
57:SB:183:ARG:HH11	57:SB:187:ARG:CZ	2.32	0.43
58:SC:169:SER:HB2	58:SC:186:LYS:HG2	2.00	0.43
1:L1:734:U:H2'	1:L1:735:U:C6	2.53	0.43
2:L2:409:U:O2'	9:LA:11:GLY:HA3	2.17	0.43
2:L2:1141:G:N3	2:L2:1141:G:H5''	2.33	0.43
4:L4:18:U:H2'	4:L4:19:C:C6	2.53	0.43
12:LD:93:LEU:O	12:LD:173:ILE:HA	2.19	0.43
13:LE:8:CYS:HB2	13:LE:56:VAL:HG13	2.00	0.43
13:LE:172:ARG:HB3	47:Lm:127:LEU:HD22	2.00	0.43
51:S1:747:C:H2'	51:S1:748:C:O4'	2.18	0.43
51:S1:777:A:H5''	51:S1:779:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:840:A:H2'	51:S1:843:U:O2	2.19	0.43
51:S1:1134:A:H5''	70:SO:127:PRO:HB3	1.99	0.43
51:S1:1724:G:O2'	67:SL:32:GLN:OE1	2.16	0.43
51:S1:2033:U:H2'	51:S1:2034:A:C8	2.54	0.43
59:SD:147:VAL:HG11	59:SD:155:ILE:HD11	2.00	0.43
66:SK:99:ASN:O	66:SK:99:ASN:ND2	2.51	0.43
1:L1:951:G:H1'	1:L1:1739:A:N6	2.34	0.43
5:L5:105:U:O2	5:L5:108:G:H5'	2.19	0.43
13:LE:38:LEU:HD13	13:LE:72:THR:HG23	2.01	0.43
13:LE:88:ARG:HB2	13:LE:186:ILE:HG22	1.99	0.43
23:LO:110:LEU:HD22	23:LO:115:ILE:CG2	2.49	0.43
25:LQ:92:LYS:O	25:LQ:96:MET:HG3	2.19	0.43
27:LS:109:GLU:O	27:LS:113:GLN:HG2	2.18	0.43
51:S1:465:G:H2'	51:S1:466:G:C8	2.54	0.43
66:SK:2:GLY:O	66:SK:24:ARG:NH1	2.52	0.43
69:SN:17:PHE:CE1	69:SN:23:ILE:HG22	2.54	0.43
88:Sg:154:SER:H	88:Sg:171:SER:HA	1.84	0.43
1:L1:434:U:H5	1:L1:438:A:N7	2.17	0.43
1:L1:1086:G:H3'	1:L1:1087:A:C8	2.54	0.43
2:L2:432:U:OP2	9:LA:200:ARG:HD2	2.19	0.43
2:L2:847:U:H3	2:L2:951:G:H1	1.67	0.43
8:L8:87:G:H4'	37:Lc:228:ARG:HB2	2.01	0.43
10:LB:261:HIS:HA	10:LB:262:PRO:C	2.44	0.43
12:LD:43:CYS:SG	12:LD:71:CYS:CB	3.07	0.43
18:LJ:80:ILE:O	18:LJ:124:SER:OG	2.36	0.43
22:LN:189:LYS:O	22:LN:200:ILE:HG12	2.19	0.43
27:LS:17:LYS:HD3	27:LS:22:HIS:HA	2.00	0.43
33:LY:23:ALA:HA	33:LY:45:GLY:HA2	2.01	0.43
37:Lc:165:LYS:HG2	37:Lc:213:TRP:HE3	1.84	0.43
39:Le:53:PHE:O	39:Le:56:VAL:HG23	2.19	0.43
51:S1:580:A:C8	51:S1:584:U:H5''	2.54	0.43
57:SB:1:MET:N	57:SB:59:GLU:O	2.52	0.43
59:SD:126:VAL:HG13	59:SD:130:GLN:NE2	2.34	0.43
62:SG:58:ASP:OD1	62:SG:58:ASP:C	2.62	0.43
63:SH:37:HIS:HE2	67:SL:85:TYR:HE1	1.66	0.43
66:SK:218:LYS:HA	66:SK:218:LYS:HD2	1.71	0.43
88:Sg:1:MET:N	88:Sg:309:SER:OG	2.47	0.43
2:L2:5:A:H2'	2:L2:6:A:C8	2.54	0.42
15:LG:115:GLU:O	15:LG:118:LYS:HG3	2.18	0.42
18:LJ:22:GLY:HA2	18:LJ:37:TYR:CE1	2.54	0.42
33:LY:22:LYS:NZ	33:LY:130:GLN:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Ld:76:ASN:OD1	38:Ld:76:ASN:N	2.51	0.42
40:Lf:56:LYS:H	40:Lf:56:LYS:HG3	1.47	0.42
51:S1:79:A:O2'	51:S1:501:A:N1	2.51	0.42
61:SF:200:LEU:HD23	61:SF:230:LEU:HD21	1.99	0.42
1:L1:3:A:N6	7:L7:169:A:H1'	2.34	0.42
2:L2:1183:C:H2'	2:L2:1184:C:O4'	2.19	0.42
2:L2:1325:A:N3	2:L2:1325:A:H2'	2.34	0.42
2:L2:1391:U:H2'	2:L2:1392:U:H2'	2.01	0.42
2:L2:1485:G:O6	41:Lg:7:HIS:HB3	2.19	0.42
12:LD:28:SER:OG	12:LD:29:GLY:N	2.52	0.42
44:Lj:67:LEU:HD23	44:Lj:67:LEU:HA	1.79	0.42
51:S1:5:U:H2'	51:S1:6:G:C8	2.55	0.42
51:S1:462:G:H5'	62:SG:73:ARG:HH12	1.83	0.42
51:S1:953:U:H2'	51:S1:954:A:O4'	2.20	0.42
54:S4:62:C:H2'	54:S4:63:G:C8	2.54	0.42
82:Sa:67:ASP:OD2	82:Sa:67:ASP:C	2.61	0.42
1:L1:587:G:OP1	37:Lc:66:ARG:NH2	2.52	0.42
2:L2:497:G:N3	53:S3:12:G:H4'	2.34	0.42
2:L2:506:U:O2'	2:L2:507:G:H8	2.02	0.42
2:L2:974:G:O2'	33:LY:134:PHE:O	2.31	0.42
5:L5:61:C:H2'	5:L5:62:C:O4'	2.20	0.42
8:L8:67:C:H1'	23:LO:292:ALA:HB1	2.00	0.42
11:LC:356:LYS:HE3	11:LC:356:LYS:HB3	1.88	0.42
18:LJ:90:LYS:HD3	18:LJ:90:LYS:HA	1.77	0.42
19:LK:100:LYS:O	19:LK:104:VAL:HG13	2.20	0.42
24:LP:82:LYS:HB3	24:LP:82:LYS:HE3	1.59	0.42
59:SD:107:ARG:HH22	59:SD:125:ARG:NH2	2.13	0.42
63:SH:17:LEU:HD23	63:SH:17:LEU:HA	1.84	0.42
63:SH:99:VAL:O	63:SH:103:SER:OG	2.33	0.42
72:SQ:116:LEU:HD23	72:SQ:116:LEU:H	1.84	0.42
88:Sg:78:ASP:HB3	88:Sg:94:LEU:HB2	1.99	0.42
1:L1:599:G:N3	1:L1:599:G:H5''	2.35	0.42
1:L1:696:A:H2'	1:L1:697:A2M:H8	2.02	0.42
1:L1:731:U:H5''	11:LC:43:MET:SD	2.60	0.42
1:L1:1651:U:H1'	1:L1:1654:A:N6	2.34	0.42
1:L1:1684:G:H1	1:L1:1708:G:H1	1.68	0.42
2:L2:73:OMU:HM23	2:L2:73:OMU:H1'	1.87	0.42
2:L2:590:U:H2'	2:L2:591:A2M:C8	2.49	0.42
2:L2:1440:G:H4'	2:L2:1441:C:C6	2.54	0.42
12:LD:112:ILE:HG21	12:LD:118:TYR:HB2	2.02	0.42
16:LH:54:VAL:HG11	16:LH:130:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:65:CYS:HB2	17:LI:70:HIS:O	2.20	0.42
20:LL:110:LEU:O	20:LL:130:ALA:HB2	2.19	0.42
33:LY:98:ASN:OD1	33:LY:99:VAL:N	2.53	0.42
35:La:3:HIS:HB3	35:La:51:ILE:HG13	2.00	0.42
39:Le:98:LYS:HB3	39:Le:98:LYS:HE3	1.79	0.42
51:S1:1019:U:H2'	51:S1:1020:G:O4'	2.20	0.42
51:S1:2021:A2M:HM'3	51:S1:2021:A2M:H1'	1.60	0.42
59:SD:91:LYS:HB2	59:SD:94:TYR:CE1	2.54	0.42
59:SD:93:ASP:OD1	59:SD:93:ASP:N	2.52	0.42
62:SG:211:GLU:OE2	62:SG:214:ARG:NH2	2.52	0.42
64:SI:30:LEU:HD22	64:SI:37:LEU:HD12	2.02	0.42
70:SO:27:PHE:HA	70:SO:91:ARG:HG3	2.02	0.42
72:SQ:55:ASP:OD1	72:SQ:56:CYS:N	2.52	0.42
72:SQ:106:ARG:HB3	72:SQ:109:ALA:HB1	2.02	0.42
79:SX:97:ASN:OD1	79:SX:97:ASN:C	2.62	0.42
88:Sg:235:GLU:HB2	88:Sg:256:ARG:HH12	1.84	0.42
1:L1:254:U:H5	1:L1:258:A:N7	2.17	0.42
1:L1:478:C:H2'	1:L1:479:A:C8	2.54	0.42
2:L2:110:C:H3'	49:Lo:7:LYS:HB2	2.01	0.42
2:L2:481:C:O2'	54:S4:71:G:H5''	2.19	0.42
2:L2:782:G:H3'	2:L2:786:A:N7	2.34	0.42
7:L7:71:A:H2'	31:LW:48:ARG:NH1	2.34	0.42
10:LB:204:LEU:HD12	10:LB:204:LEU:HA	1.86	0.42
11:LC:287:VAL:HA	11:LC:290:ILE:HD12	2.02	0.42
12:LD:31:ARG:O	12:LD:125:TYR:OH	2.28	0.42
13:LE:6:SER:HB2	13:LE:69:LEU:HD11	2.01	0.42
23:LO:88:ILE:HD12	23:LO:249:TYR:CE1	2.54	0.42
23:LO:134:THR:HG22	23:LO:136:LYS:H	1.83	0.42
29:LU:91:LYS:HB2	29:LU:117:TYR:CE2	2.54	0.42
35:La:9:ASP:OD1	35:La:9:ASP:N	2.52	0.42
35:La:109:SER:HA	35:La:112:MET:HE3	2.02	0.42
51:S1:866:G:C6	59:SD:148:ARG:HG3	2.54	0.42
59:SD:58:LEU:HD22	59:SD:68:ARG:HA	2.01	0.42
72:SQ:66:ASP:OD1	72:SQ:67:ASP:N	2.52	0.42
75:ST:32:ASN:O	75:ST:36:MET:HG2	2.19	0.42
76:SU:20:GLU:C	76:SU:22:ALA:H	2.27	0.42
88:Sg:110:VAL:HA	88:Sg:126:GLY:HA2	2.02	0.42
88:Sg:128:ASP:OD2	88:Sg:132:ARG:NH2	2.52	0.42
89:Sh:166:ARG:HA	89:Sh:166:ARG:HD2	1.87	0.42
1:L1:262:C:H5'	31:LW:31:PRO:HD3	2.02	0.42
1:L1:866:G:P	44:Lj:33:ARG:HH22	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1041:U:H4'	27:LS:100:ARG:HB2	2.02	0.42
2:L2:343:U:H2'	2:L2:344:G:H8	1.84	0.42
10:LB:287:ILE:HA	10:LB:331:LEU:HD23	2.01	0.42
23:LO:166:PHE:HA	23:LO:169:LEU:HB3	2.02	0.42
35:La:70:LEU:HD23	35:La:70:LEU:HA	1.87	0.42
35:La:91:LEU:HD23	35:La:91:LEU:HA	1.95	0.42
48:Ln:21:ARG:NH1	51:S1:2182:G:O6	2.52	0.42
51:S1:1177:A:OP1	83:Sb:76:ARG:NH1	2.53	0.42
51:S1:1913:C:H2'	51:S1:1914:U:C6	2.54	0.42
54:S4:52:G:H2'	54:S4:53:G:C8	2.55	0.42
62:SG:121:ASP:OD1	62:SG:121:ASP:N	2.52	0.42
71:SP:14:VAL:HG22	76:SU:112:TYR:HE2	1.84	0.42
88:Sg:122:ILE:O	88:Sg:133:VAL:HA	2.20	0.42
89:Sh:176:TYR:HB2	89:Sh:209:LEU:HD12	2.00	0.42
1:L1:416:A:O4'	31:LW:84:ARG:HD3	2.19	0.42
1:L1:662:C:H2'	1:L1:663:C:C6	2.54	0.42
1:L1:700:A:H4'	24:LP:172:TYR:CE1	2.54	0.42
1:L1:790:C:H4'	37:Lc:38:LYS:HB3	2.02	0.42
1:L1:1764:A:H5''	1:L1:1766:G:OP2	2.19	0.42
2:L2:386:U:H1'	2:L2:1416:U:H5''	2.01	0.42
2:L2:541:A:H2'	2:L2:542:A:C8	2.55	0.42
2:L2:968:U:O2	9:LA:95:PRO:HD3	2.20	0.42
3:L3:71:U:H5	3:L3:150:A:N7	2.18	0.42
5:L5:55:U:H2'	5:L5:56:U:C6	2.55	0.42
12:LD:76:LYS:HA	12:LD:76:LYS:HD3	1.87	0.42
13:LE:90:LYS:HB2	13:LE:182:THR:HG23	2.01	0.42
14:LF:55:LYS:HE3	14:LF:98:THR:HG23	2.00	0.42
14:LF:97:ASP:C	14:LF:99:ALA:H	2.27	0.42
20:LL:74:ASN:OD1	20:LL:112:ASN:HB3	2.20	0.42
23:LO:293:LYS:HA	23:LO:293:LYS:HD2	1.73	0.42
34:LZ:27:MET:HE2	34:LZ:27:MET:HA	2.01	0.42
37:Lc:27:ALA:O	37:Lc:31:GLN:HG3	2.19	0.42
40:Lf:127:LEU:O	40:Lf:128:ARG:HG3	2.19	0.42
41:Lg:42:TYR:OH	41:Lg:126:VAL:O	2.33	0.42
42:Lh:109:LYS:HB3	42:Lh:109:LYS:HE3	1.62	0.42
51:S1:822:U:H2'	51:S1:823:G:C8	2.55	0.42
61:SF:169:LYS:HG2	61:SF:182:VAL:HG13	2.02	0.42
87:Sf:81:THR:HG23	87:Sf:82:LYS:HG3	2.02	0.42
88:Sg:278:LYS:HE3	88:Sg:278:LYS:HB2	1.88	0.42
1:L1:828:U:O2'	2:L2:1147:C:H2'	2.20	0.42
1:L1:1189:C:H4'	2:L2:1303:PSU:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1262:G:H5'	1:L1:1262:G:C8	2.53	0.42
1:L1:1468:U:H2'	1:L1:1469:G:C8	2.55	0.42
1:L1:1668:A:OP2	15:LG:54:PRO:HA	2.20	0.42
2:L2:512:PSU:H2'	2:L2:513:C:H6	1.83	0.42
2:L2:684:C:H2'	2:L2:685:G:O4'	2.20	0.42
3:L3:64:U:H2'	3:L3:65:U:C6	2.54	0.42
4:L4:141:A:H4'	13:LE:70:ASN:HB3	2.02	0.42
21:LM:5:MET:HE2	21:LM:5:MET:HB3	1.92	0.42
26:LR:80:ILE:HG21	26:LR:112:LEU:HD11	2.01	0.42
33:LY:98:ASN:ND2	33:LY:100:SER:OG	2.51	0.42
51:S1:15:U:H2'	51:S1:16:G:O4'	2.19	0.42
51:S1:256:A:H61	51:S1:951:U:H3	1.66	0.42
51:S1:262:U:H2'	51:S1:263:G:H8	1.84	0.42
51:S1:479:A2M:O5'	51:S1:479:A2M:H8	2.20	0.42
51:S1:659:G:H4'	51:S1:661:OMU:H5	2.01	0.42
51:S1:769:A:H3'	51:S1:770:A:C8	2.55	0.42
51:S1:828:G:H2'	51:S1:829:G:C8	2.55	0.42
51:S1:2012:A:H2'	51:S1:2013:G:C8	2.55	0.42
56:SA:173:MET:HE2	56:SA:173:MET:HB3	1.90	0.42
58:SC:91:GLU:OE1	58:SC:91:GLU:N	2.35	0.42
58:SC:130:ALA:HA	58:SC:190:PRO:HD3	2.02	0.42
68:SM:75:ASP:OD1	74:SS:55:LYS:NZ	2.33	0.42
69:SN:84:ARG:HG3	69:SN:89:LEU:HB3	2.02	0.42
70:SO:88:VAL:HB	70:SO:122:ILE:HG23	2.00	0.42
71:SP:88:ASP:OD2	86:Se:15:LYS:HB2	2.19	0.42
80:SY:51:ASN:OD1	80:SY:51:ASN:N	2.46	0.42
1:L1:449:A:H61	7:L7:14:G:H1'	1.84	0.42
1:L1:523:A:N1	1:L1:527:A:H5''	2.34	0.42
1:L1:904:G:N7	49:Lo:2:ALA:N	2.68	0.42
2:L2:530:C:N4	2:L2:554:C:OP2	2.53	0.42
2:L2:954:A:C6	42:Lh:114:MET:CE	3.03	0.42
7:L7:46:G:OP2	46:Ll:15:LYS:NZ	2.52	0.42
11:LC:316:PRO:HG2	11:LC:328:ARG:HH22	1.84	0.42
19:LK:160:ALA:O	19:LK:164:MET:HG3	2.19	0.42
22:LN:200:ILE:HG12	22:LN:200:ILE:H	1.71	0.42
24:LP:46:LYS:O	24:LP:50:GLN:HG3	2.19	0.42
27:LS:87:LYS:HE3	27:LS:87:LYS:HB3	1.79	0.42
27:LS:128:LEU:HD23	27:LS:128:LEU:HA	1.91	0.42
30:LV:94:ASN:HB3	30:LV:97:GLU:HG2	2.02	0.42
35:La:28:GLU:HG3	35:La:51:ILE:HD13	2.02	0.42
51:S1:1917:A:N1	79:SX:111:GLY:HA2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1971:U:H2'	51:S1:1972:G:O4'	2.20	0.42
58:SC:53:LYS:O	58:SC:57:VAL:HG23	2.20	0.42
61:SF:257:GLU:H	61:SF:257:GLU:CD	2.28	0.42
69:SN:22:VAL:HG22	69:SN:74:THR:OG1	2.20	0.42
69:SN:29:ARG:HA	69:SN:29:ARG:HD3	1.85	0.42
73:SR:86:ASN:OD1	73:SR:87:ARG:N	2.53	0.42
1:L1:34:C:H4'	1:L1:859:A:H2	1.84	0.42
1:L1:595:C:H2'	1:L1:596:A:C8	2.54	0.42
1:L1:1201:U:H6	1:L1:1201:U:H2'	1.71	0.42
2:L2:1472:U:H2'	2:L2:1473:C:C6	2.55	0.42
11:LC:291:MET:HG2	24:LP:35:PHE:CD2	2.54	0.42
19:LK:50:VAL:HG23	26:LR:71:LEU:HD13	2.01	0.42
30:LV:60:ILE:HD12	35:La:26:LYS:HE3	2.01	0.42
47:Lm:79:GLU:HB2	47:Lm:82:LEU:HD23	2.02	0.42
48:Ln:22:LEU:HD21	51:S1:2153:A:C5'	2.50	0.42
49:Lo:52:VAL:O	49:Lo:52:VAL:HG13	2.20	0.42
50:Lp:63:LYS:HD2	50:Lp:87:ARG:HH12	1.83	0.42
51:S1:526:G:H2'	51:S1:527:A:C8	2.55	0.42
51:S1:775:C:H3'	51:S1:776:A:H8	1.85	0.42
51:S1:1718:A:O2'	51:S1:1949:A:N6	2.51	0.42
51:S1:1881:G:H2'	51:S1:1882:A:C8	2.54	0.42
51:S1:1942:A:O3'	79:SX:95:LYS:HE2	2.20	0.42
56:SA:117:ARG:HH11	56:SA:117:ARG:HG2	1.83	0.42
60:SE:16:MET:HE1	60:SE:105:ARG:HD2	2.01	0.42
62:SG:32:ARG:HA	62:SG:104:VAL:HA	2.02	0.42
67:SL:53:LYS:HE3	67:SL:53:LYS:HB3	1.80	0.42
73:SR:27:VAL:HG23	73:SR:55:ARG:O	2.20	0.42
73:SR:44:LEU:HD12	73:SR:84:PHE:CE2	2.54	0.42
83:Sb:11:SER:O	83:Sb:11:SER:OG	2.30	0.42
86:Se:26:LYS:HE2	86:Se:26:LYS:HB2	1.66	0.42
88:Sg:67:PHE:O	88:Sg:85:TRP:N	2.52	0.42
9:LA:62:GLU:OE1	9:LA:71:ARG:HD3	2.20	0.41
11:LC:75:ILE:HG12	11:LC:95:CYS:SG	2.59	0.41
15:LG:73:PRO:HG3	21:LM:18:VAL:HA	2.01	0.41
20:LL:110:LEU:HA	20:LL:110:LEU:HD23	1.78	0.41
28:LT:115:LYS:HB3	28:LT:115:LYS:HE3	1.68	0.41
42:Lh:124:LYS:HD3	42:Lh:124:LYS:HA	1.73	0.41
45:Lk:65:LYS:HB3	45:Lk:65:LYS:HE2	1.70	0.41
51:S1:571:A:H2'	51:S1:572:A:O4'	2.20	0.41
51:S1:1708:A:C4'	79:SX:138:ARG:HH12	2.28	0.41
51:S1:1804:C:H2'	51:S1:1805:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:S4:23:A:H2'	54:S4:24:G:C8	2.55	0.41
56:SA:141:VAL:HG22	56:SA:214:ILE:HG12	2.02	0.41
63:SH:130:MET:HA	63:SH:130:MET:HE3	2.02	0.41
66:SK:8:LEU:HB3	66:SK:20:ILE:HG12	2.02	0.41
67:SL:101:LYS:HE3	67:SL:102:TYR:CZ	2.54	0.41
70:SO:54:LYS:HE2	70:SO:69:MET:HB3	2.02	0.41
1:L1:391:A:N1	46:L1:39:GLU:HB3	2.36	0.41
1:L1:1184:G:N2	1:L1:1186:A:H3'	2.35	0.41
1:L1:1588:G:O2'	1:L1:1590:G:OP2	2.38	0.41
2:L2:591:A2M:HM'3	2:L2:591:A2M:H1'	1.92	0.41
3:L3:35:A:H5'	3:L3:35:A:C8	2.55	0.41
3:L3:149:A:H5'	3:L3:150:A:C2	2.55	0.41
5:L5:122:U:H2'	5:L5:123:G:H8	1.84	0.41
7:L7:36:G:OP2	35:La:92:THR:HG23	2.20	0.41
7:L7:94:G:O5'	44:Lj:73:ARG:NH1	2.54	0.41
11:LC:206:PRO:HG2	11:LC:225:LEU:HD12	2.01	0.41
15:LG:51:MET:HE2	15:LG:53:TRP:CE2	2.55	0.41
20:LL:47:LYS:HE3	20:LL:47:LYS:HB2	1.85	0.41
23:LO:170:LYS:HG2	23:LO:201:HIS:CE1	2.54	0.41
28:LT:109:PRO:HA	28:LT:112:MET:HG2	2.01	0.41
30:LV:76:MET:HE3	30:LV:76:MET:HB3	1.91	0.41
37:Lc:37:LYS:O	37:Lc:41:VAL:HG13	2.19	0.41
51:S1:324:U:H4'	51:S1:325:G:C5	2.55	0.41
51:S1:1619:G:H21	51:S1:1849:G:H5'	1.85	0.41
51:S1:2081:G:H1	51:S1:2142:U:H3	1.68	0.41
56:SA:185:GLU:O	56:SA:189:LEU:HG	2.20	0.41
57:SB:70:ALA:HB2	80:SY:42:ALA:HB2	2.02	0.41
63:SH:178:LYS:HA	63:SH:178:LYS:HD2	1.93	0.41
67:SL:107:GLU:O	67:SL:109:ALA:N	2.49	0.41
72:SQ:48:SER:C	72:SQ:50:VAL:H	2.27	0.41
81:SZ:28:PHE:CE1	81:SZ:50:LEU:HD21	2.55	0.41
85:Sd:61:ARG:HD2	85:Sd:75:LEU:HG	2.01	0.41
3:L3:203:A:H2'	3:L3:204:A:C8	2.55	0.41
7:L7:22:U:H5''	31:LW:10:ARG:HG3	2.02	0.41
7:L7:82:C:H1'	7:L7:83:A:N7	2.35	0.41
17:LI:28:LYS:HB2	21:LM:197:ARG:HD3	2.02	0.41
19:LK:141:LYS:HA	19:LK:141:LYS:HD2	1.89	0.41
23:LO:76:MET:CE	23:LO:112:LYS:HD2	2.51	0.41
23:LO:115:ILE:HG23	23:LO:119:PHE:HD2	1.84	0.41
23:LO:164:ARG:O	23:LO:168:VAL:HG23	2.20	0.41
33:LY:34:LYS:HE2	33:LY:34:LYS:HB2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Le:80:LYS:HG3	39:Le:81:PRO:HD2	2.01	0.41
51:S1:263:G:H22	51:S1:274:C:H5	1.68	0.41
51:S1:827:G:H2'	51:S1:828:G:C8	2.55	0.41
51:S1:882:U:H1'	81:SZ:17:PHE:CE2	2.56	0.41
51:S1:1589:G:O6	51:S1:1590:A:N6	2.53	0.41
51:S1:1620:G:H1'	51:S1:1849:G:H5''	2.01	0.41
51:S1:1995:7MG:H2'	51:S1:1996:A:C8	2.55	0.41
56:SA:33:VAL:O	56:SA:234:HIS:HE1	2.02	0.41
58:SC:44:ARG:HE	58:SC:84:GLN:HG3	1.84	0.41
58:SC:137:VAL:HG12	58:SC:141:ILE:HD11	2.02	0.41
70:SO:15:LYS:HE2	70:SO:15:LYS:HB2	1.71	0.41
71:SP:25:LYS:HE3	71:SP:25:LYS:HB3	1.85	0.41
72:SQ:94:ARG:NE	72:SQ:117:LYS:HD2	2.35	0.41
73:SR:60:LEU:HD13	73:SR:65:LEU:HG	2.01	0.41
88:Sg:153:VAL:HA	88:Sg:171:SER:HA	2.03	0.41
1:L1:527:A:H3'	1:L1:528:A:H8	1.85	0.41
1:L1:558:U:H4'	1:L1:559:G:OP2	2.20	0.41
2:L2:1278:C:H2'	2:L2:1279:G:O4'	2.20	0.41
2:L2:1294:G:H4'	2:L2:1294:G:OP1	2.20	0.41
2:L2:1496:G:H2'	2:L2:1497:C:C6	2.55	0.41
4:L4:103:C:H2'	4:L4:104:A:C8	2.55	0.41
5:L5:72:C:H2'	5:L5:73:G:O4'	2.20	0.41
7:L7:21:U:C6	11:LC:195:MET:HE2	2.52	0.41
7:L7:162:A2M:HM'3	7:L7:162:A2M:H1'	1.66	0.41
14:LF:67:GLY:O	14:LF:68:PRO:C	2.61	0.41
15:LG:66:LEU:HD23	15:LG:66:LEU:HA	1.84	0.41
15:LG:191:ILE:HD12	15:LG:193:ARG:HG3	2.02	0.41
51:S1:697:G:H1	51:S1:748:C:H5	1.67	0.41
77:SV:24:LEU:HD13	77:SV:54:THR:CG2	2.50	0.41
1:L1:167:U:H2'	1:L1:168:G:C8	2.55	0.41
6:L6:36:C:H2'	6:L6:37:C:C6	2.55	0.41
9:LA:83:PHE:HB3	49:Lo:64:VAL:HG22	2.03	0.41
11:LC:325:LEU:HD13	11:LC:328:ARG:HH21	1.85	0.41
12:LD:165:PHE:CD2	12:LD:173:ILE:HD11	2.56	0.41
21:LM:157:LYS:O	21:LM:162:ARG:NH1	2.53	0.41
25:LQ:17:CYS:SG	25:LQ:52:ARG:HG3	2.61	0.41
26:LR:26:VAL:HG21	27:LS:140:PRO:HB3	2.01	0.41
34:LZ:105:ASP:O	34:LZ:109:ARG:HG3	2.21	0.41
50:Lp:24:LYS:HE3	50:Lp:24:LYS:HB3	1.67	0.41
51:S1:363:G:H4'	51:S1:367:A:C8	2.55	0.41
51:S1:1859:A:H2'	51:S1:1859:A:N3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S3:51:C:H2'	53:S3:52:G:C8	2.55	0.41
54:S4:39:U:H4'	70:SO:59:ARG:HH12	1.85	0.41
57:SB:138:ARG:O	57:SB:141:SER:OG	2.36	0.41
61:SF:88:LEU:HD12	61:SF:88:LEU:HA	1.89	0.41
66:SK:174:ALA:O	66:SK:178:GLN:HG3	2.20	0.41
80:SY:10:GLU:OE1	80:SY:10:GLU:N	2.52	0.41
86:Se:64:LYS:HA	86:Se:64:LYS:HD2	1.83	0.41
1:L1:71:C:H5'	43:Li:18:HIS:HB3	2.01	0.41
1:L1:470:A:H1'	41:Lg:51:LYS:HD3	2.03	0.41
1:L1:1715:U:H2'	1:L1:1716:G:N2	2.35	0.41
13:LE:12:ILE:HG23	13:LE:16:VAL:HG22	2.03	0.41
16:LH:209:PRO:HG2	16:LH:212:ASN:HD22	1.85	0.41
18:LJ:27:CYS:SG	18:LJ:29:ASP:HB2	2.60	0.41
19:LK:7:ILE:HD11	19:LK:58:PRO:HG3	2.02	0.41
20:LL:75:LEU:HD22	20:LL:115:ILE:HD12	2.03	0.41
51:S1:441:G:P	66:SK:47:ARG:HH22	2.44	0.41
51:S1:895:A:H3'	51:S1:896:A:C8	2.52	0.41
51:S1:1264:C:H2'	51:S1:1265:A:C8	2.56	0.41
51:S1:1555:A:N6	51:S1:1972:G:H1'	2.35	0.41
51:S1:1611:C:H6	51:S1:1611:C:H2'	1.71	0.41
51:S1:1766:G:H5'	79:SX:81:PRO:HG2	2.03	0.41
57:SB:148:ILE:HG12	57:SB:162:ILE:HB	2.03	0.41
59:SD:99:THR:HB	59:SD:101:PRO:HD2	2.01	0.41
68:SM:16:THR:CG2	68:SM:114:LEU:HB2	2.50	0.41
70:SO:24:VAL:HG12	70:SO:86:LEU:HB3	2.02	0.41
72:SQ:105:ARG:HG2	72:SQ:114:LYS:HB3	2.02	0.41
77:SV:14:ARG:HG2	77:SV:69:ILE:HD11	2.03	0.41
77:SV:101:VAL:HB	77:SV:105:THR:HB	2.03	0.41
77:SV:104:LYS:HB2	77:SV:104:LYS:HE2	1.79	0.41
88:Sg:196:TYR:CZ	88:Sg:214:LYS:HB2	2.56	0.41
1:L1:78:C:OP1	21:LM:194:ARG:HD3	2.20	0.41
1:L1:226:C:H2'	1:L1:227:U:C6	2.56	0.41
1:L1:1090:U:H2'	1:L1:1091:A:C8	2.56	0.41
1:L1:1105:A:H5''	2:L2:1064:A:H61	1.86	0.41
2:L2:1253:OMG:H2'	2:L2:1308:5MC:HM51	2.02	0.41
3:L3:154:C:H2'	3:L3:155:A:C8	2.56	0.41
8:L8:31:A:H2'	8:L8:32:C:C6	2.55	0.41
11:LC:164:LYS:HE2	11:LC:164:LYS:HB2	1.93	0.41
26:LR:42:ARG:HA	26:LR:42:ARG:HD2	1.79	0.41
28:LT:43:LYS:HB3	28:LT:43:LYS:HE2	1.67	0.41
38:Ld:38:GLN:HG3	38:Ld:40:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Le:29:SER:O	39:Le:33:ARG:HG3	2.19	0.41
51:S1:558:U:H5	51:S1:587:A:N7	2.19	0.41
51:S1:1579:A:H1'	51:S1:1581:G:C4	2.55	0.41
51:S1:1809:U:H2'	51:S1:1810:G:O4'	2.21	0.41
58:SC:5:SER:O	58:SC:9:MET:HG3	2.20	0.41
58:SC:44:ARG:HE	58:SC:84:GLN:CG	2.34	0.41
60:SE:152:SER:OG	60:SE:155:ASP:OD2	2.31	0.41
61:SF:241:LEU:HD13	80:SY:28:LEU:HD11	2.03	0.41
65:SJ:108:LEU:HD13	65:SJ:119:ARG:NH2	2.35	0.41
72:SQ:43:LEU:HD23	72:SQ:43:LEU:HA	1.85	0.41
73:SR:3:LEU:HD22	73:SR:3:LEU:HA	1.90	0.41
89:Sh:210:GLU:HG2	89:Sh:211:LYS:N	2.35	0.41
1:L1:157:U:H5'	1:L1:158:A:H4'	2.03	0.41
1:L1:391:A:N6	46:L1:35:ILE:HG23	2.35	0.41
1:L1:1186:A:H2'	1:L1:1187:A:C8	2.55	0.41
2:L2:1108:U:H2'	2:L2:1109:C:C6	2.55	0.41
3:L3:24:U:C2	3:L3:27:C:H5	2.39	0.41
10:LB:121:ASN:HD21	10:LB:124:GLN:HG3	1.86	0.41
16:LH:30:LYS:HA	16:LH:58:GLN:HB2	2.01	0.41
17:LI:55:PRO:HD2	35:La:123:TYR:CE2	2.55	0.41
22:LN:4:ARG:NH1	22:LN:99:ILE:HG13	2.35	0.41
51:S1:996:C:H5''	64:SI:59:LYS:CE	2.45	0.41
53:S3:21:A:N1	53:S3:46:A:H2'	2.36	0.41
66:SK:207:GLU:HG3	76:SU:23:TYR:CD2	2.55	0.41
84:Sc:14:ARG:NH1	84:Sc:14:ARG:HG3	2.35	0.41
1:L1:146:U:OP2	15:LG:197:THR:OG1	2.38	0.41
1:L1:213:G:N7	34:LZ:143:ARG:NH2	2.63	0.41
1:L1:248:A:OP2	11:LC:221:ASN:HB2	2.21	0.41
1:L1:513:C:O2'	1:L1:540:A:N7	2.49	0.41
1:L1:835:G:H2'	1:L1:835:G:N3	2.36	0.41
1:L1:989:C:OP2	20:LL:26:ARG:NH1	2.54	0.41
1:L1:1362:G:H5''	1:L1:1363:A:H2'	2.02	0.41
1:L1:1402:U:H2'	1:L1:1403:A:H8	1.85	0.41
2:L2:1185:A2M:HM'3	2:L2:1185:A2M:H1'	1.85	0.41
3:L3:35:A:H5'	3:L3:35:A:H8	1.85	0.41
4:L4:103:C:H2'	4:L4:104:A:H8	1.86	0.41
5:L5:38:U:H5''	10:LB:315:MET:CE	2.51	0.41
6:L6:67:C:OP1	41:Lg:96:ARG:NH2	2.52	0.41
10:LB:310:LYS:NZ	10:LB:366:ILE:O	2.46	0.41
11:LC:34:ASP:OD1	11:LC:34:ASP:N	2.53	0.41
11:LC:107:PHE:CD1	11:LC:107:PHE:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:51:ALA:HA	14:LF:67:GLY:HA3	2.03	0.41
20:LL:101:LEU:HD22	20:LL:123:ALA:HB2	2.03	0.41
23:LO:84:PRO:HA	23:LO:88:ILE:O	2.20	0.41
33:LY:26:VAL:HG11	33:LY:97:ILE:HD11	2.03	0.41
35:La:35:VAL:HG21	35:La:44:ARG:CZ	2.50	0.41
35:La:104:LYS:HB3	35:La:104:LYS:HE3	1.86	0.41
41:Lg:76:CYS:SG	41:Lg:102:ALA:HB1	2.61	0.41
42:Lh:25:ARG:NH2	42:Lh:31:LEU:HB2	2.36	0.41
43:Li:56:LEU:HD12	43:Li:75:TYR:HE2	1.86	0.41
49:Lo:67:GLY:C	49:Lo:69:TYR:H	2.29	0.41
51:S1:52:U:H2'	51:S1:53:G:C8	2.56	0.41
51:S1:99:U:H6	66:SK:21:HIS:HB2	1.85	0.41
51:S1:289:G:H22	51:S1:786:G:P	2.44	0.41
51:S1:755:C:H2'	51:S1:757:C:H5''	2.03	0.41
51:S1:893:A:H2'	51:S1:894:G:C8	2.56	0.41
51:S1:933:G:C5'	76:SU:43:LYS:HD3	2.51	0.41
51:S1:2010:G:H1	51:S1:2026:U:H3	1.69	0.41
56:SA:71:ALA:HB2	56:SA:82:ALA:HA	2.03	0.41
56:SA:183:ILE:O	56:SA:187:VAL:HG13	2.20	0.41
58:SC:55:ARG:HD2	58:SC:55:ARG:N	2.34	0.41
62:SG:45:GLU:H	62:SG:45:GLU:CD	2.28	0.41
63:SH:78:LEU:HD22	63:SH:156:PRO:HD3	2.02	0.41
64:SI:7:LYS:HD3	64:SI:7:LYS:HA	1.61	0.41
70:SO:142:ARG:NH1	70:SO:144:LEU:HD13	2.36	0.41
76:SU:52:LYS:HE3	76:SU:52:LYS:HB2	1.76	0.41
78:SW:75:LYS:HE2	78:SW:75:LYS:HB2	1.78	0.41
80:SY:63:LEU:HD12	80:SY:63:LEU:HA	1.89	0.41
1:L1:525:C:H2'	1:L1:526:A:C8	2.56	0.41
1:L1:898:A:N1	51:S1:1219:G:O2'	2.51	0.41
2:L2:1155:A:C2	20:LL:43:ILE:HG23	2.56	0.41
26:LR:46:MET:HG3	27:LS:146:LEU:HD11	2.03	0.41
26:LR:80:ILE:HG13	26:LR:125:VAL:HA	2.03	0.41
51:S1:41:G:H3'	51:S1:481:A:H62	1.86	0.41
51:S1:114:U:H2'	51:S1:115:C:C6	2.56	0.41
51:S1:231:A:P	51:S1:282:C:H41	2.44	0.41
51:S1:762:A:H1'	51:S1:771:G:N2	2.35	0.41
51:S1:1132:G:H2'	51:S1:1133:U:C6	2.56	0.41
51:S1:1149:G:H1'	51:S1:1154:A:N6	2.36	0.41
51:S1:2198:A:N6	83:Sb:9:GLY:HA3	2.36	0.41
56:SA:32:VAL:HB	56:SA:43:PHE:O	2.21	0.41
56:SA:47:ILE:HD13	70:SO:46:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SC:11:ILE:HD13	58:SC:11:ILE:HA	1.86	0.41
60:SE:95:ARG:HH21	60:SE:112:SER:HA	1.86	0.41
64:SI:193:LYS:HE2	84:Sc:24:ARG:HH12	1.86	0.41
69:SN:25:CYS:SG	69:SN:46:CYS:HB3	2.60	0.41
81:SZ:8:ALA:HB1	81:SZ:37:TRP:CE3	2.56	0.41
89:Sh:178:ASP:OD1	89:Sh:179:SER:N	2.54	0.41
2:L2:502[A]:A2M:N7	51:S1:2160:G:OP2	2.54	0.40
2:L2:601:G:H5''	28:LT:140:MET:O	2.20	0.40
2:L2:1087:C:H2'	2:L2:1088:G:H8	1.86	0.40
4:L4:51:U:H2'	4:L4:52:A:C8	2.56	0.40
4:L4:95:U:H3'	25:LQ:62:ARG:HH22	1.86	0.40
4:L4:184:U:H5'	16:LH:13:GLN:OE1	2.21	0.40
5:L5:38:U:H2'	5:L5:39:G:O4'	2.21	0.40
6:L6:53:U:O4	19:LK:118:ARG:NE	2.50	0.40
9:LA:59:ALA:HB2	9:LA:78:ALA:HB2	2.03	0.40
9:LA:104:LEU:HD11	9:LA:116:VAL:HG13	2.04	0.40
18:LJ:9:LYS:HD2	18:LJ:9:LYS:HA	1.63	0.40
21:LM:57:GLN:HG2	21:LM:139:CYS:SG	2.61	0.40
22:LN:212:MET:HE2	22:LN:212:MET:HB2	1.99	0.40
26:LR:78:VAL:HG22	26:LR:128:VAL:HG23	2.03	0.40
28:LT:113:VAL:O	28:LT:115:LYS:HG2	2.22	0.40
31:LW:71:TYR:C	31:LW:73:LEU:H	2.28	0.40
32:LX:57:ARG:O	32:LX:61:ARG:HG3	2.22	0.40
50:Lp:23:PHE:HB3	50:Lp:72:LEU:HB3	2.03	0.40
51:S1:32:U:O2'	51:S1:643:A:N1	2.53	0.40
51:S1:835:C:H2'	51:S1:836:C:C6	2.55	0.40
51:S1:969:A:C4	64:SI:68:LEU:HD23	2.56	0.40
51:S1:1829:OMG:HM23	51:S1:1829:OMG:H1'	1.76	0.40
51:S1:2159:A:N3	55:S5:9:U:H1'	2.36	0.40
53:S3:14:A:H3'	53:S3:15:G:H8	1.85	0.40
54:S4:55:U:C5	54:S4:57:G:H3'	2.56	0.40
54:S4:72:C:H2'	54:S4:73:A:H5''	2.03	0.40
63:SH:142:LYS:HD3	63:SH:174:TYR:OH	2.21	0.40
64:SI:116:GLN:HG2	64:SI:119:LYS:HG2	2.02	0.40
66:SK:168:ASN:OD1	66:SK:168:ASN:N	2.53	0.40
68:SM:65:THR:O	74:SS:41:ARG:NH1	2.50	0.40
78:SW:59:ARG:HH22	78:SW:62:VAL:HG23	1.86	0.40
88:Sg:230:PHE:HE2	88:Sg:232:ILE:HD11	1.85	0.40
1:L1:675:U:O2'	1:L1:1210:A:N1	2.52	0.40
1:L1:1207:A:C5	1:L1:1372:G:H5'	2.56	0.40
1:L1:1373:A2M:H2'	1:L1:1374:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1290:C:O2'	2:L2:1291:G:H8	2.04	0.40
2:L2:1412:U:H2'	2:L2:1413:PSU:C6	2.56	0.40
8:L8:97:A:O2'	26:LR:122:ASN:OD1	2.39	0.40
13:LE:44:ASP:HB3	13:LE:57:ILE:HB	2.03	0.40
14:LF:177:TYR:OH	19:LK:107:ASP:OD2	2.23	0.40
15:LG:51:MET:HE2	15:LG:51:MET:HB2	1.91	0.40
15:LG:187:LEU:HD23	15:LG:187:LEU:HA	1.97	0.40
16:LH:34:LEU:HA	16:LH:59:LEU:HD22	2.02	0.40
28:LT:16:LYS:O	28:LT:101:ASN:ND2	2.46	0.40
48:Ln:23:LYS:HD2	51:S1:1467:U:H5'	2.03	0.40
51:S1:265:C:H2'	51:S1:266:U:O4'	2.21	0.40
51:S1:489:A:N6	51:S1:509:G:H21	2.19	0.40
51:S1:1165:G:H21	70:SO:43:ARG:HA	1.85	0.40
51:S1:1193:U:H2'	51:S1:1194:C:C6	2.56	0.40
51:S1:1437:A:H2'	51:S1:1438:A:C8	2.56	0.40
51:S1:1652:A:H5'	51:S1:1653:U:OP2	2.21	0.40
51:S1:1956:C:OP2	51:S1:1992:G:N1	2.51	0.40
51:S1:2084:C:H2'	51:S1:2085:A:C8	2.56	0.40
68:SM:56:ARG:HD3	68:SM:56:ARG:HA	1.82	0.40
82:Sa:64:ILE:O	82:Sa:68:ARG:HG2	2.21	0.40
1:L1:214:C:C2'	1:L1:215:U:H5'	2.51	0.40
1:L1:385:G:O2'	7:L7:24:G:N3	2.53	0.40
1:L1:521:G:H2'	1:L1:522:G:C8	2.56	0.40
2:L2:667:OMU:HM23	2:L2:667:OMU:H1'	1.85	0.40
2:L2:1392:U:C4	53:S3:76:A:H2'	2.55	0.40
6:L6:25:U:H6	6:L6:25:U:H2'	1.69	0.40
17:LI:191:LYS:HD2	17:LI:191:LYS:HA	1.93	0.40
21:LM:143:ARG:O	35:La:103:GLU:HB3	2.21	0.40
23:LO:199:LYS:HB3	23:LO:199:LYS:HE3	1.91	0.40
25:LQ:10:LEU:O	25:LQ:14:ILE:HG13	2.21	0.40
29:LU:32:ILE:HB	29:LU:33:PRO:HD3	2.03	0.40
37:Lc:133:MET:HE2	37:Lc:133:MET:HB2	1.83	0.40
40:Lf:3:LYS:HD3	40:Lf:3:LYS:HA	1.74	0.40
51:S1:1186:A:H2'	51:S1:1187:A:C8	2.56	0.40
51:S1:1577:U:O2	51:S1:1582:A:H4'	2.21	0.40
51:S1:1921:A:N3	51:S1:1982:G:O2'	2.53	0.40
57:SB:173:SER:O	57:SB:177:MET:HG2	2.21	0.40
66:SK:77:ARG:HE	66:SK:77:ARG:HB3	1.46	0.40
68:SM:65:THR:HA	68:SM:66:PRO:HD3	1.94	0.40
88:Sg:127:ARG:HD3	88:Sg:152:TRP:CE3	2.56	0.40
1:L1:394:U:H2'	1:L1:395:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1687:G:H22	1:L1:1705:G:H22	1.69	0.40
2:L2:67:G:O6	39:Le:103:LYS:NZ	2.55	0.40
2:L2:1139:U:H2'	2:L2:1140:U:C6	2.56	0.40
6:L6:48:C:C2	14:LF:185:LYS:HD3	2.56	0.40
10:LB:349:MET:HE2	10:LB:349:MET:HB3	1.86	0.40
11:LC:24:PRO:HB2	11:LC:26:VAL:HG12	2.04	0.40
13:LE:130:LYS:HD2	13:LE:130:LYS:HA	1.77	0.40
15:LG:227:SER:O	15:LG:231:ARG:HG3	2.22	0.40
19:LK:113:LEU:O	19:LK:117:ARG:HG2	2.21	0.40
24:LP:34:LYS:HG3	24:LP:49:TYR:CZ	2.56	0.40
31:LW:111:HIS:O	31:LW:115:ILE:HG13	2.22	0.40
51:S1:528:G:H1	51:S1:553:U:H3	1.70	0.40
51:S1:879:A:H2	51:S1:881:U:H4'	1.85	0.40
51:S1:1577:U:H3'	51:S1:1578:G:C8	2.52	0.40
51:S1:1592:U:H6	51:S1:1596:U:C5	2.40	0.40
56:SA:66:PHE:CE2	70:SO:41:SER:HB3	2.56	0.40
56:SA:145:THR:HG22	56:SA:146:LYS:N	2.37	0.40
63:SH:84:GLU:OE2	63:SH:84:GLU:HA	2.20	0.40
65:SJ:50:PHE:HB2	65:SJ:63:VAL:HG22	2.03	0.40
89:Sh:139:PHE:CZ	89:Sh:141:SER:HB2	2.57	0.40
1:L1:246:A:H4'	1:L1:248:A:C8	2.57	0.40
1:L1:307:U:H2'	1:L1:308:A:H8	1.84	0.40
1:L1:1205:G:OP1	41:Lg:46:LEU:HB2	2.22	0.40
1:L1:1733:G:H2'	1:L1:1734:G:O4'	2.22	0.40
2:L2:1409:A:H1'	53:S3:74:C:H5'	2.03	0.40
4:L4:183:C:H2'	4:L4:184:U:O4'	2.21	0.40
14:LF:148:ASP:OD1	14:LF:148:ASP:N	2.54	0.40
16:LH:189:LYS:C	16:LH:191:ALA:H	2.30	0.40
21:LM:201:LEU:O	21:LM:204:ARG:HD3	2.22	0.40
22:LN:189:LYS:HB3	22:LN:189:LYS:HE2	1.83	0.40
26:LR:47:MET:HG2	27:LS:146:LEU:HD22	2.04	0.40
51:S1:58:C:H5''	51:S1:504:G:H1'	2.04	0.40
51:S1:288:A:H5'	62:SG:213:LEU:HD22	2.03	0.40
51:S1:1362:A:OP1	84:Sc:17:ARG:NH2	2.55	0.40
51:S1:1632:C:H2'	51:S1:1633:G:H8	1.86	0.40
51:S1:1797:A:H3'	51:S1:1798:A:C2	2.57	0.40
59:SD:48:LEU:HD23	59:SD:48:LEU:HA	1.90	0.40
61:SF:155:TYR:OH	61:SF:161:GLY:O	2.40	0.40
64:SI:8:LEU:HD23	64:SI:8:LEU:HA	1.91	0.40
85:Sd:26:ILE:HD13	85:Sd:44:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LA	253/260 (97%)	246 (97%)	7 (3%)	0	100	100
10	LB	399/419 (95%)	391 (98%)	8 (2%)	0	100	100
11	LC	364/373 (98%)	352 (97%)	12 (3%)	0	100	100
12	LD	173/188 (92%)	169 (98%)	4 (2%)	0	100	100
13	LE	184/190 (97%)	177 (96%)	7 (4%)	0	100	100
14	LF	145/195 (74%)	138 (95%)	7 (5%)	0	100	100
15	LG	240/264 (91%)	238 (99%)	2 (1%)	0	100	100
16	LH	219/222 (99%)	215 (98%)	4 (2%)	0	100	100
17	LI	206/220 (94%)	202 (98%)	3 (2%)	1 (0%)	24	58
18	LJ	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
19	LK	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
20	LL	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
21	LM	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
22	LN	195/213 (92%)	191 (98%)	4 (2%)	0	100	100
23	LO	284/305 (93%)	279 (98%)	5 (2%)	0	100	100
24	LP	195/198 (98%)	191 (98%)	4 (2%)	0	100	100
25	LQ	199/254 (78%)	199 (100%)	0	0	100	100
26	LR	176/179 (98%)	176 (100%)	0	0	100	100
27	LS	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
28	LT	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
29	LU	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
30	LV	117/145 (81%)	116 (99%)	1 (1%)	0	100	100
31	LW	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
32	LX	81/124 (65%)	78 (96%)	3 (4%)	0	100	100
33	LY	131/134 (98%)	129 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	LZ	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
35	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
36	Lb	66/70 (94%)	62 (94%)	4 (6%)	0	100	100
37	Lc	227/252 (90%)	222 (98%)	5 (2%)	0	100	100
38	Ld	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
39	Le	184/188 (98%)	182 (99%)	2 (1%)	0	100	100
40	Lf	126/133 (95%)	123 (98%)	3 (2%)	0	100	100
41	Lg	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
42	Lh	125/168 (74%)	123 (98%)	2 (2%)	0	100	100
43	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
44	Lj	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
45	Lk	76/83 (92%)	76 (100%)	0	0	100	100
46	Ll	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
47	Lm	49/128 (38%)	49 (100%)	0	0	100	100
48	Ln	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
49	Lo	87/92 (95%)	80 (92%)	5 (6%)	2 (2%)	5	23
50	Lp	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
56	SA	234/264 (89%)	225 (96%)	9 (4%)	0	100	100
57	SB	209/246 (85%)	203 (97%)	6 (3%)	0	100	100
58	SC	210/219 (96%)	208 (99%)	2 (1%)	0	100	100
59	SD	181/190 (95%)	180 (99%)	1 (1%)	0	100	100
60	SE	258/273 (94%)	251 (97%)	7 (3%)	0	100	100
61	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100
62	SG	243/249 (98%)	239 (98%)	4 (2%)	0	100	100
63	SH	178/190 (94%)	176 (99%)	2 (1%)	0	100	100
64	SI	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
65	SJ	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
66	SK	194/220 (88%)	194 (100%)	0	0	100	100
67	SL	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
68	SM	100/116 (86%)	95 (95%)	5 (5%)	0	100	100
69	SN	97/168 (58%)	94 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	SO	134/144 (93%)	129 (96%)	5 (4%)	0	100	100
71	SP	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	SQ	94/141 (67%)	89 (95%)	5 (5%)	0	100	100
73	SR	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
74	SS	54/57 (95%)	54 (100%)	0	0	100	100
75	ST	140/151 (93%)	138 (99%)	2 (1%)	0	100	100
76	SU	151/173 (87%)	147 (97%)	4 (3%)	0	100	100
77	SV	120/143 (84%)	118 (98%)	2 (2%)	0	100	100
78	SW	113/152 (74%)	111 (98%)	2 (2%)	0	100	100
79	SX	150/161 (93%)	147 (98%)	3 (2%)	0	100	100
80	SY	86/164 (52%)	85 (99%)	1 (1%)	0	100	100
81	SZ	128/137 (93%)	126 (98%)	2 (2%)	0	100	100
82	Sa	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
83	Sb	102/112 (91%)	102 (100%)	0	0	100	100
84	Sc	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
85	Sd	64/87 (74%)	63 (98%)	1 (2%)	0	100	100
86	Se	56/66 (85%)	55 (98%)	1 (2%)	0	100	100
87	Sf	40/152 (26%)	38 (95%)	2 (5%)	0	100	100
88	Sg	293/312 (94%)	289 (99%)	4 (1%)	0	100	100
89	Sh	101/235 (43%)	100 (99%)	1 (1%)	0	100	100
All	All	11374/12926 (88%)	11132 (98%)	239 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	Lo	51	ALA
17	LI	66	PRO
49	Lo	52	VAL

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	
9	LA	197/204 (97%)	193 (98%)	4 (2%)	48	75
10	LB	329/351 (94%)	322 (98%)	7 (2%)	47	74
11	LC	289/301 (96%)	282 (98%)	7 (2%)	43	72
12	LD	131/162 (81%)	127 (97%)	4 (3%)	35	66
13	LE	164/172 (95%)	157 (96%)	7 (4%)	26	58
14	LF	122/153 (80%)	116 (95%)	6 (5%)	22	54
15	LG	196/221 (89%)	195 (100%)	1 (0%)	81	89
16	LH	181/188 (96%)	173 (96%)	8 (4%)	25	58
17	LI	170/183 (93%)	168 (99%)	2 (1%)	63	82
18	LJ	105/111 (95%)	102 (97%)	3 (3%)	37	68
19	LK	136/145 (94%)	133 (98%)	3 (2%)	45	73
20	LL	113/114 (99%)	110 (97%)	3 (3%)	39	70
21	LM	178/180 (99%)	174 (98%)	4 (2%)	45	73
22	LN	168/179 (94%)	160 (95%)	8 (5%)	23	55
23	LO	210/242 (87%)	208 (99%)	2 (1%)	68	83
24	LP	162/164 (99%)	157 (97%)	5 (3%)	35	66
25	LQ	169/198 (85%)	165 (98%)	4 (2%)	43	72
26	LR	157/159 (99%)	152 (97%)	5 (3%)	34	65
27	LS	128/134 (96%)	118 (92%)	10 (8%)	11	37
28	LT	128/143 (90%)	126 (98%)	2 (2%)	55	78
29	LU	92/114 (81%)	88 (96%)	4 (4%)	26	58
30	LV	100/124 (81%)	98 (98%)	2 (2%)	48	75
31	LW	101/122 (83%)	98 (97%)	3 (3%)	36	67
32	LX	74/104 (71%)	73 (99%)	1 (1%)	59	80
33	LY	111/116 (96%)	110 (99%)	1 (1%)	70	85
34	LZ	113/118 (96%)	111 (98%)	2 (2%)	51	76
35	La	114/118 (97%)	111 (97%)	3 (3%)	40	70
36	Lb	56/58 (97%)	54 (96%)	2 (4%)	31	63
37	Lc	191/209 (91%)	189 (99%)	2 (1%)	68	83
38	Ld	85/89 (96%)	80 (94%)	5 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Le	154/158 (98%)	149 (97%)	5 (3%)	34	65
40	Lf	111/115 (96%)	108 (97%)	3 (3%)	39	70
41	Lg	120/121 (99%)	118 (98%)	2 (2%)	53	77
42	Lh	107/146 (73%)	104 (97%)	3 (3%)	38	69
43	Li	84/88 (96%)	83 (99%)	1 (1%)	63	82
44	Lj	68/70 (97%)	67 (98%)	1 (2%)	57	79
45	Lk	57/74 (77%)	57 (100%)	0	100	100
46	Ll	46/47 (98%)	46 (100%)	0	100	100
47	Lm	41/113 (36%)	39 (95%)	2 (5%)	22	54
48	Ln	30/32 (94%)	28 (93%)	2 (7%)	15	44
49	Lo	69/74 (93%)	68 (99%)	1 (1%)	59	80
50	Lp	82/92 (89%)	80 (98%)	2 (2%)	43	72
56	SA	205/222 (92%)	199 (97%)	6 (3%)	37	68
57	SB	175/202 (87%)	173 (99%)	2 (1%)	65	82
58	SC	170/184 (92%)	166 (98%)	4 (2%)	43	72
59	SD	158/164 (96%)	156 (99%)	2 (1%)	61	81
60	SE	216/225 (96%)	214 (99%)	2 (1%)	70	85
61	SF	174/208 (84%)	171 (98%)	3 (2%)	53	77
62	SG	201/208 (97%)	192 (96%)	9 (4%)	24	57
63	SH	150/159 (94%)	149 (99%)	1 (1%)	76	87
64	SI	179/186 (96%)	175 (98%)	4 (2%)	45	73
65	SJ	110/111 (99%)	107 (97%)	3 (3%)	39	70
66	SK	162/176 (92%)	158 (98%)	4 (2%)	42	71
67	SL	116/120 (97%)	109 (94%)	7 (6%)	17	48
68	SM	92/104 (88%)	91 (99%)	1 (1%)	65	82
69	SN	86/128 (67%)	84 (98%)	2 (2%)	44	72
70	SO	101/113 (89%)	97 (96%)	4 (4%)	28	60
71	SP	113/117 (97%)	106 (94%)	7 (6%)	16	46
72	SQ	56/120 (47%)	55 (98%)	1 (2%)	51	76
73	SR	105/130 (81%)	102 (97%)	3 (3%)	37	68
74	SS	46/49 (94%)	45 (98%)	1 (2%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	ST	125/132 (95%)	120 (96%)	5 (4%)	28	60
76	SU	134/152 (88%)	128 (96%)	6 (4%)	24	57
77	SV	96/126 (76%)	95 (99%)	1 (1%)	68	83
78	SW	97/130 (75%)	93 (96%)	4 (4%)	27	60
79	SX	122/131 (93%)	120 (98%)	2 (2%)	55	78
80	SY	71/116 (61%)	69 (97%)	2 (3%)	38	69
81	SZ	111/118 (94%)	107 (96%)	4 (4%)	31	63
82	Sa	64/95 (67%)	58 (91%)	6 (9%)	8	30
83	Sb	85/93 (91%)	80 (94%)	5 (6%)	18	48
84	Sc	75/76 (99%)	72 (96%)	3 (4%)	28	60
85	Sd	48/75 (64%)	44 (92%)	4 (8%)	10	35
86	Se	50/54 (93%)	49 (98%)	1 (2%)	48	75
87	Sf	19/126 (15%)	19 (100%)	0	100	100
88	Sg	258/265 (97%)	244 (95%)	14 (5%)	20	51
89	Sh	85/177 (48%)	82 (96%)	3 (4%)	32	63
All	All	9494/10798 (88%)	9226 (97%)	268 (3%)	38	69

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	LA	18	VAL
9	LA	157	SER
9	LA	161	THR
9	LA	185	SER
10	LB	44	THR
10	LB	87	VAL
10	LB	171	LEU
10	LB	211	ASP
10	LB	307	LEU
10	LB	323	THR
10	LB	398	GLU
11	LC	6	SER
11	LC	56	LEU
11	LC	84	SER
11	LC	124	VAL
11	LC	182	VAL
11	LC	271	VAL

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Mol	Chain	Res	Type
11	LC	333	VAL
12	LD	20	CYS
12	LD	46	THR
12	LD	58	THR
12	LD	157	THR
13	LE	6	SER
13	LE	16	VAL
13	LE	17	THR
13	LE	56	VAL
13	LE	83	VAL
13	LE	137	SER
13	LE	182	THR
14	LF	81	SER
14	LF	84	VAL
14	LF	95	SER
14	LF	98	THR
14	LF	108	ARG
14	LF	113	LYS
15	LG	66	LEU
16	LH	30	LYS
16	LH	64	THR
16	LH	82	THR
16	LH	85	THR
16	LH	137	VAL
16	LH	155	THR
16	LH	169	SER
16	LH	184	SER
17	LI	68	VAL
17	LI	202	THR
18	LJ	41	VAL
18	LJ	53	SER
18	LJ	114	SER
19	LK	4	SER
19	LK	70	SER
19	LK	137	VAL
20	LL	8	CYS
20	LL	39	HIS
20	LL	79	SER
21	LM	61	VAL
21	LM	106	LEU
21	LM	117	ASN
21	LM	155	VAL

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Mol	Chain	Res	Type
22	LN	8	CYS
22	LN	15	LYS
22	LN	43	VAL
22	LN	51	HIS
22	LN	125	VAL
22	LN	137	SER
22	LN	166	VAL
22	LN	189	LYS
23	LO	42	THR
23	LO	261	SER
24	LP	14	VAL
24	LP	57	SER
24	LP	115	SER
24	LP	162	SER
24	LP	186	THR
25	LQ	13	SER
25	LQ	27	ASN
25	LQ	55	VAL
25	LQ	116	ASP
26	LR	62	SER
26	LR	65	VAL
26	LR	93	VAL
26	LR	150	SER
26	LR	173	THR
27	LS	4	SER
27	LS	46	SER
27	LS	61	THR
27	LS	64	VAL
27	LS	66	ASN
27	LS	68	THR
27	LS	80	VAL
27	LS	84	THR
27	LS	131	SER
27	LS	132	SER
28	LT	11	SER
28	LT	75	GLU
29	LU	5	ARG
29	LU	70	LEU
29	LU	76	VAL
29	LU	118	GLN
30	LV	34	GLN
30	LV	144	LEU

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Mol	Chain	Res	Type
31	LW	91	THR
31	LW	99	SER
31	LW	118	ARG
32	LX	29	THR
33	LY	29	SER
34	LZ	14	GLN
34	LZ	93	SER
35	La	9	ASP
35	La	14	SER
35	La	43	THR
36	Lb	5	LYS
36	Lb	7	HIS
37	Lc	56	LEU
37	Lc	62	SER
38	Ld	7	SER
38	Ld	26	VAL
38	Ld	41	SER
38	Ld	90	CYS
38	Ld	92	LEU
39	Le	102	SER
39	Le	168	THR
39	Le	170	ILE
39	Le	171	SER
39	Le	177	SER
40	Lf	15	THR
40	Lf	56	LYS
40	Lf	87	VAL
41	Lg	21	THR
41	Lg	125	SER
42	Lh	12	MET
42	Lh	24	VAL
42	Lh	62	HIS
43	Li	50	LEU
44	Lj	43	SER
47	Lm	81	THR
47	Lm	105	VAL
48	Ln	33	SER
48	Ln	34	LYS
49	Lo	41	PHE
50	Lp	2	VAL
50	Lp	88	THR
56	SA	46	THR

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Mol	Chain	Res	Type
56	SA	86	VAL
56	SA	109	THR
56	SA	110	ASP
56	SA	139	LEU
56	SA	194	VAL
57	SB	10	VAL
57	SB	33	GLN
58	SC	159	SER
58	SC	174	CYS
58	SC	203	LEU
58	SC	206	VAL
59	SD	121	VAL
59	SD	126	VAL
60	SE	151	THR
60	SE	242	LEU
61	SF	205	VAL
61	SF	208	VAL
61	SF	248	SER
62	SG	13	VAL
62	SG	22	VAL
62	SG	75	SER
62	SG	101	ARG
62	SG	104	VAL
62	SG	121	ASP
62	SG	142	SER
62	SG	236	VAL
62	SG	237	HIS
63	SH	111	SER
64	SI	9	ARG
64	SI	17	SER
64	SI	109	VAL
64	SI	147	THR
65	SJ	30	SER
65	SJ	81	CYS
65	SJ	83	THR
66	SK	77	ARG
66	SK	81	VAL
66	SK	88	ASN
66	SK	169	HIS
67	SL	9	LEU
67	SL	12	VAL
67	SL	33	CYS

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Mol	Chain	Res	Type
67	SL	45	ILE
67	SL	75	VAL
67	SL	100	GLN
67	SL	142	THR
68	SM	107	VAL
69	SN	44	VAL
69	SN	46	CYS
70	SO	29	SER
70	SO	45	THR
70	SO	93	VAL
70	SO	133	THR
71	SP	2	THR
71	SP	21	ARG
71	SP	72	VAL
71	SP	100	VAL
71	SP	102	VAL
71	SP	105	PHE
71	SP	115	ILE
72	SQ	112	VAL
73	SR	3	LEU
73	SR	34	VAL
73	SR	104	VAL
74	SS	9	SER
75	ST	30	SER
75	ST	48	SER
75	ST	53	GLU
75	ST	87	ASP
75	ST	107	THR
76	SU	13	VAL
76	SU	16	THR
76	SU	21	LYS
76	SU	44	SER
76	SU	101	ILE
76	SU	153	ASN
77	SV	8	THR
78	SW	67	LEU
78	SW	69	GLU
78	SW	74	VAL
78	SW	99	SER
79	SX	106	VAL
79	SX	126	VAL
80	SY	4	ILE

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Mol	Chain	Res	Type
80	SY	55	THR
81	SZ	19	VAL
81	SZ	27	GLN
81	SZ	76	THR
81	SZ	85	ASP
82	Sa	36	LEU
82	Sa	40	VAL
82	Sa	50	LEU
82	Sa	84	CYS
82	Sa	92	VAL
82	Sa	98	THR
83	Sb	21	LYS
83	Sb	32	THR
83	Sb	42	VAL
83	Sb	87	THR
83	Sb	88	VAL
84	Sc	27	GLN
84	Sc	45	THR
84	Sc	60	CYS
85	Sd	33	THR
85	Sd	38	ASN
85	Sd	42	VAL
85	Sd	78	THR
86	Se	45	LEU
88	Sg	27	ILE
88	Sg	64	HIS
88	Sg	104	LEU
88	Sg	111	LEU
88	Sg	115	PHE
88	Sg	123	VAL
88	Sg	178	VAL
88	Sg	198	SER
88	Sg	200	VAL
88	Sg	209	CYS
88	Sg	260	VAL
88	Sg	268	VAL
88	Sg	272	LEU
88	Sg	305	VAL
89	Sh	140	VAL
89	Sh	156	LEU
89	Sh	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116)

such sidechains are listed below:

Mol	Chain	Res	Type
9	LA	86	GLN
9	LA	115	ASN
10	LB	121	ASN
10	LB	167	GLN
10	LB	215	GLN
10	LB	275	HIS
10	LB	282	GLN
11	LC	49	GLN
11	LC	145	ASN
11	LC	212	ASN
11	LC	257	GLN
11	LC	314	GLN
12	LD	97	ASN
12	LD	111	HIS
13	LE	11	GLN
13	LE	101	ASN
13	LE	162	GLN
14	LF	72	ASN
14	LF	152	GLN
14	LF	154	GLN
15	LG	77	ASN
16	LH	74	GLN
16	LH	143	GLN
16	LH	163	HIS
16	LH	187	HIS
17	LI	6	ASN
17	LI	18	ASN
17	LI	38	HIS
17	LI	119	GLN
18	LJ	77	ASN
19	LK	40	ASN
20	LL	11	GLN
20	LL	112	ASN
21	LM	99	GLN
21	LM	112	ASN
21	LM	158	HIS
22	LN	73	ASN
22	LN	210	ASN
23	LO	35	GLN
23	LO	94	ASN
23	LO	120	GLN
23	LO	231	GLN

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Mol	Chain	Res	Type
24	LP	18	HIS
25	LQ	134	ASN
26	LR	75	ASN
26	LR	85	GLN
27	LS	66	ASN
28	LT	9	GLN
28	LT	133	HIS
29	LU	54	ASN
30	LV	39	HIS
30	LV	133	HIS
31	LW	16	HIS
31	LW	110	HIS
33	LY	130	GLN
35	La	3	HIS
36	Lb	11	ASN
36	Lb	17	HIS
36	Lb	50	HIS
37	Lc	120	GLN
37	Lc	226	GLN
39	Le	161	ASN
39	Le	172	ASN
40	Lf	21	HIS
41	Lg	60	ASN
41	Lg	113	ASN
42	Lh	29	ASN
42	Lh	41	GLN
43	Li	18	HIS
46	Li	19	GLN
56	SA	103	HIS
56	SA	151	GLN
57	SB	95	GLN
58	SC	73	GLN
58	SC	74	GLN
58	SC	144	GLN
59	SD	3	ASN
60	SE	47	ASN
60	SE	142	HIS
60	SE	160	ASN
60	SE	206	HIS
61	SF	114	ASN
61	SF	147	ASN
62	SG	149	ASN

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Mol	Chain	Res	Type
63	SH	87	HIS
63	SH	96	GLN
63	SH	165	ASN
64	SI	89	HIS
64	SI	181	HIS
64	SI	191	ASN
64	SI	196	GLN
66	SK	35	ASN
66	SK	169	HIS
66	SK	194	GLN
67	SL	44	GLN
67	SL	100	GLN
68	SM	72	ASN
69	SN	98	GLN
71	SP	77	ASN
74	SS	3	HIS
74	SS	47	ASN
75	ST	7	ASN
76	SU	24	GLN
76	SU	104	ASN
76	SU	113	GLN
77	SV	48	ASN
79	SX	45	ASN
79	SX	94	ASN
79	SX	150	GLN
81	SZ	119	ASN
83	Sb	7	ASN
83	Sb	27	ASN
84	Sc	20	HIS
84	Sc	86	HIS
86	Se	60	GLN
88	Sg	239	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1648/1782 (92%)	574 (34%)	54 (3%)
2	L2	1139/1526 (74%)	374 (32%)	38 (3%)
3	L3	178/216 (82%)	67 (37%)	7 (3%)
4	L4	183/184 (99%)	60 (32%)	5 (2%)
5	L5	119/135 (88%)	37 (31%)	6 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	S1	1812/2204 (82%)	636 (35%)	50 (2%)
52	S2	11/76 (14%)	6 (54%)	1 (9%)
53	S3	69/77 (89%)	28 (40%)	2 (2%)
54	S4	62/76 (81%)	37 (59%)	2 (3%)
55	S5	10/13 (76%)	4 (40%)	1 (10%)
6	L6	70/73 (95%)	40 (57%)	5 (7%)
7	L7	162/171 (94%)	58 (35%)	5 (3%)
8	L8	118/123 (95%)	28 (23%)	2 (1%)
All	All	5581/6656 (83%)	1949 (34%)	178 (3%)

All (1949) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	7	C
1	L1	10	A
1	L1	16	G
1	L1	19	G
1	L1	20	G
1	L1	24	A
1	L1	29	C
1	L1	32	A
1	L1	38	A
1	L1	39	G
1	L1	41	A
1	L1	47	C
1	L1	53	G
1	L1	56	G
1	L1	57	G
1	L1	58	A
1	L1	63	A
1	L1	64	A
1	L1	65	A
1	L1	69	A2M
1	L1	70	C
1	L1	71	C
1	L1	72	G
1	L1	74	G
1	L1	84	G
1	L1	86	G
1	L1	87	A
1	L1	91	G

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Mol	Chain	Res	Type
1	L1	98	A
1	L1	104	G
1	L1	109	A
1	L1	110	A
1	L1	116	U
1	L1	119	C
1	L1	120	G
1	L1	121	A
1	L1	123	U
1	L1	126	G
1	L1	131	U
1	L1	133	C
1	L1	134	A
1	L1	135	A
1	L1	136	G
1	L1	141	U
1	L1	142	G
1	L1	143	A
1	L1	144	G
1	L1	146	U
1	L1	147	G
1	L1	154	A
1	L1	155	A
1	L1	156	A
1	L1	158	A
1	L1	160	C
1	L1	161	A
1	L1	162	U
1	L1	166	G
1	L1	167	U
1	L1	170	U
1	L1	171	U
1	L1	176	C
1	L1	182	U
1	L1	188	A
1	L1	191	U
1	L1	192	C
1	L1	195	G
1	L1	199	A
1	L1	200	A
1	L1	201	A
1	L1	202	G

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Mol	Chain	Res	Type
1	L1	203	C
1	L1	204	A
1	L1	205	A
1	L1	206	A
1	L1	209	C
1	L1	212	U
1	L1	215	U
1	L1	216	G
1	L1	218	A
1	L1	219	U
1	L1	220	A
1	L1	222	A
1	L1	223	A
1	L1	225	C
1	L1	226	C
1	L1	230	A
1	L1	233	U
1	L1	234	G
1	L1	235	A2M
1	L1	236	G
1	L1	237	U
1	L1	240	U
1	L1	243	G
1	L1	248	A
1	L1	249	G
1	L1	250	A
1	L1	251	A
1	L1	256	U
1	L1	264	U
1	L1	268	G
1	L1	272	U
1	L1	273	A
1	L1	280	A
1	L1	281	G
1	L1	283	G
1	L1	293	C
1	L1	301	A
1	L1	305	A2M
1	L1	306	G
1	L1	322	A
1	L1	323	U
1	L1	324	G

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Mol	Chain	Res	Type
1	L1	332	A
1	L1	335	U
1	L1	336	U
1	L1	337	G
1	L1	342	G
1	L1	343	U
1	L1	344	A
1	L1	348	G
1	L1	357	A
1	L1	367	A
1	L1	368	G
1	L1	369	A
1	L1	371	U
1	L1	373	G
1	L1	374	G
1	L1	376	A
1	L1	377	G
1	L1	378	A
1	L1	382	A
1	L1	383	U
1	L1	392	A
1	L1	406	A
1	L1	408	G
1	L1	409	U
1	L1	410	U
1	L1	413	A
1	L1	414	A
1	L1	416	A
1	L1	417	G
1	L1	419	A
1	L1	431	G
1	L1	434	U
1	L1	438	A
1	L1	439	U
1	L1	443	A
1	L1	444	C
1	L1	447	G
1	L1	448	A
1	L1	454	U
1	L1	461	G
1	L1	463	C
1	L1	464	A

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Mol	Chain	Res	Type
1	L1	471	G
1	L1	477	C
1	L1	484	A
1	L1	485	A
1	L1	486	C
1	L1	487	G
1	L1	488	G
1	L1	494	A
1	L1	495	C
1	L1	496	C
1	L1	500	C
1	L1	502	U
1	L1	503	A
1	L1	510	PSU
1	L1	511	A
1	L1	512	U
1	L1	518	C
1	L1	520	G
1	L1	522	G
1	L1	525	C
1	L1	527	A
1	L1	534	G
1	L1	535	C
1	L1	537	G
1	L1	539	C
1	L1	541	A
1	L1	542	C
1	L1	546	G
1	L1	547	U
1	L1	551	A
1	L1	553	A
1	L1	554	A
1	L1	555	U
1	L1	557	U
1	L1	558	U
1	L1	559	G
1	L1	563	C
1	L1	564	U
1	L1	565	U
1	L1	568	U
1	L1	569	G
1	L1	571	A

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Mol	Chain	Res	Type
1	L1	572	A
1	L1	573	U
1	L1	574	G
1	L1	575	A
1	L1	576	G
1	L1	577	C
1	L1	578	G
1	L1	580	A
1	L1	584	U
1	L1	585	U
1	L1	586	U
1	L1	587	G
1	L1	589	G
1	L1	592	G
1	L1	597	C
1	L1	606	C
1	L1	609	C
1	L1	610	A
1	L1	611	C
1	L1	612	G
1	L1	613	C
1	L1	616	U
1	L1	617	G
1	L1	620	U
1	L1	621	U
1	L1	622	C
1	L1	623	U
1	L1	625	C
1	L1	627	C
1	L1	631	G
1	L1	632	A
1	L1	633	U
1	L1	634	G
1	L1	635	C
1	L1	644	G
1	L1	649	U
1	L1	650	G
1	L1	651	G
1	L1	652	A
1	L1	653	A
1	L1	655	U
1	L1	662	C

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Mol	Chain	Res	Type
1	L1	663	C
1	L1	664	C
1	L1	666	C
1	L1	668	C
1	L1	669	C
1	L1	678	A2M
1	L1	681	A2M
1	L1	684	G
1	L1	685	A
1	L1	692	A
1	L1	709	A
1	L1	710	G
1	L1	717	G
1	L1	718	A
1	L1	719	U
1	L1	722	G
1	L1	729	A
1	L1	736	C
1	L1	737	U
1	L1	743	A
1	L1	750	G
1	L1	752	G
1	L1	753	A
1	L1	760	A
1	L1	762	A
1	L1	763	U
1	L1	764	G
1	L1	770	G
1	L1	771	U
1	L1	778	C
1	L1	783	G
1	L1	789	U
1	L1	790	C
1	L1	792	G
1	L1	794	U
1	L1	795	U
1	L1	803	C
1	L1	807	C
1	L1	810	C
1	L1	818	C
1	L1	823	G
1	L1	824	U

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Mol	Chain	Res	Type
1	L1	825	G
1	L1	828	U
1	L1	832	G
1	L1	835	G
1	L1	836	G
1	L1	838	G
1	L1	839	U
1	L1	849	U
1	L1	850	G
1	L1	851	G
1	L1	852	A
1	L1	856	OMG
1	L1	859	A
1	L1	867	A
1	L1	868	A
1	L1	869	C
1	L1	877	G
1	L1	886	G
1	L1	893	G
1	L1	894	G
1	L1	896	G
1	L1	897	A
1	L1	900	C
1	L1	905	G
1	L1	912	C
1	L1	925	U
1	L1	930	U
1	L1	935	A
1	L1	946	G
1	L1	947	A
1	L1	948	U
1	L1	957	C
1	L1	958	G
1	L1	959	OMG
1	L1	965	A
1	L1	966	A
1	L1	967	G
1	L1	968	A
1	L1	971	C
1	L1	972	A
1	L1	973	U
1	L1	974	C

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Mol	Chain	Res	Type
1	L1	975	G
1	L1	976	A
1	L1	985	G
1	L1	988	G
1	L1	989	C
1	L1	995	C
1	L1	1000	C
1	L1	1003	A
1	L1	1010	OMC
1	L1	1011	PSU
1	L1	1013	A
1	L1	1015	G
1	L1	1016	A
1	L1	1017	PSU
1	L1	1022	G
1	L1	1025	G
1	L1	1029	G
1	L1	1031	A
1	L1	1032	G
1	L1	1035	G
1	L1	1036	U
1	L1	1037	A
1	L1	1044	G
1	L1	1045	G
1	L1	1047	A
1	L1	1049	A
1	L1	1052	A
1	L1	1053	A
1	L1	1056	G
1	L1	1089	C
1	L1	1090	U
1	L1	1092	U
1	L1	1096	C
1	L1	1097	A
1	L1	1098	A
1	L1	1100	C
1	L1	1101	U
1	L1	1102	U
1	L1	1108	G
1	L1	1110	G
1	L1	1116	A
1	L1	1121	G

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Mol	Chain	Res	Type
1	L1	1122	U
1	L1	1123	G
1	L1	1128	A
1	L1	1129	G
1	L1	1134	C
1	L1	1135	U
1	L1	1136	G
1	L1	1138	A
1	L1	1141	G
1	L1	1144	G
1	L1	1146	A
1	L1	1147	A
1	L1	1148	A
1	L1	1149	G
1	L1	1150	A
1	L1	1154	G
1	L1	1155	A
1	L1	1156	A
1	L1	1159	A
1	L1	1161	A
1	L1	1162	G
1	L1	1163	G
1	L1	1164	C
1	L1	1165	A
1	L1	1169	A
1	L1	1170	G
1	L1	1171	PSU
1	L1	1172	G
1	L1	1174	G
1	L1	1175	C
1	L1	1176	C
1	L1	1177	PSU
1	L1	1178	U
1	L1	1179	C
1	L1	1182	C
1	L1	1186	A
1	L1	1188	G
1	L1	1192	A
1	L1	1198	C
1	L1	1201	U
1	L1	1202	G
1	L1	1205	G

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Mol	Chain	Res	Type
1	L1	1207	A
1	L1	1210	A
1	L1	1211	A
1	L1	1212	C
1	L1	1216	U
1	L1	1219	G
1	L1	1223	U
1	L1	1225	U
1	L1	1229	G
1	L1	1235	A
1	L1	1238	C
1	L1	1239	U
1	L1	1240	U
1	L1	1242	U
1	L1	1243	G
1	L1	1248	C
1	L1	1251	U
1	L1	1253	U
1	L1	1254	C
1	L1	1258	A
1	L1	1261	U
1	L1	1262	G
1	L1	1263	A
1	L1	1264	A
1	L1	1265	A
1	L1	1266	A
1	L1	1270	U
1	L1	1271	G
1	L1	1276	U
1	L1	1349	A
1	L1	1351	C
1	L1	1352	C
1	L1	1364	A
1	L1	1365	A
1	L1	1367	U
1	L1	1368	G
1	L1	1369	G
1	L1	1371	OMU
1	L1	1373	A2M
1	L1	1375	G
1	L1	1378	U
1	L1	1379	A

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Mol	Chain	Res	Type
1	L1	1387	U
1	L1	1388	U
1	L1	1389	A
1	L1	1390	G
1	L1	1391	U
1	L1	1393	A
1	L1	1395	U
1	L1	1396	G
1	L1	1400	A
1	L1	1401	U
1	L1	1402	U
1	L1	1404	U
1	L1	1412	G
1	L1	1413	U
1	L1	1414	A
1	L1	1416	G
1	L1	1420	G
1	L1	1421	G
1	L1	1422	A
1	L1	1423	A
1	L1	1426	A
1	L1	1427	A
1	L1	1429	U
1	L1	1435	A
1	L1	1438	A
1	L1	1439	A
1	L1	1444	A
1	L1	1445	G
1	L1	1455	U
1	L1	1456	G
1	L1	1464	G
1	L1	1479	A
1	L1	1480	C
1	L1	1481	G
1	L1	1482	A
1	L1	1483	A
1	L1	1485	C
1	L1	1488	A
1	L1	1489	U
1	L1	1490	G
1	L1	1495	G
1	L1	1497	G

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Mol	Chain	Res	Type
1	L1	1504	A
1	L1	1505	U
1	L1	1507	G
1	L1	1509	C
1	L1	1518	A
1	L1	1519	G
1	L1	1520	U
1	L1	1521	G
1	L1	1526	U
1	L1	1527	OMC
1	L1	1528	PSU
1	L1	1536	C
1	L1	1540	OMG
1	L1	1545	G
1	L1	1546	A
1	L1	1547	U
1	L1	1557	A
1	L1	1558	U
1	L1	1560	U
1	L1	1561	A
1	L1	1565	A
1	L1	1566	A
1	L1	1569	U
1	L1	1570	G
1	L1	1574	C
1	L1	1575	G
1	L1	1582	A
1	L1	1586	G
1	L1	1590	G
1	L1	1605	G
1	L1	1607	C
1	L1	1608	A
1	L1	1612	G
1	L1	1613	C
1	L1	1616	U
1	L1	1627	U
1	L1	1628	U
1	L1	1631	U
1	L1	1632	C
1	L1	1654	A
1	L1	1655	U
1	L1	1656	C

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Mol	Chain	Res	Type
1	L1	1660	U
1	L1	1661	U
1	L1	1662	G
1	L1	1663	U
1	L1	1666	G
1	L1	1667	G
1	L1	1668	A
1	L1	1671	G
1	L1	1672	U
1	L1	1675	A
1	L1	1676	G
1	L1	1683	C
1	L1	1713	A
1	L1	1715	U
1	L1	1716	G
1	L1	1726	G
1	L1	1727	A
1	L1	1729	A
1	L1	1734	G
1	L1	1737	A
1	L1	1739	A
1	L1	1740	G
1	L1	1742	G
1	L1	1743	A
1	L1	1744	A
1	L1	1747	U
1	L1	1750	G
1	L1	1753	U
1	L1	1756	A
1	L1	1757	U
1	L1	1758	U
1	L1	1759	C
1	L1	1762	A
1	L1	1763	A
1	L1	1764	A
1	L1	1766	G
1	L1	1770	U
1	L1	1771	U
1	L1	1772	G
1	L1	1773	C
1	L1	1774	A
2	L2	5	A

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Mol	Chain	Res	Type
2	L2	13	A
2	L2	22	A
2	L2	24	C
2	L2	25	A
2	L2	26	C
2	L2	29	C
2	L2	30	A
2	L2	33	A
2	L2	41	A
2	L2	42	A
2	L2	47	A
2	L2	61	C
2	L2	62	A
2	L2	63	U
2	L2	68	A
2	L2	69	A
2	L2	75	C
2	L2	76	A
2	L2	80	A
2	L2	83	G
2	L2	85	A
2	L2	90	G
2	L2	96	U
2	L2	110	C
2	L2	118	G
2	L2	123	G
2	L2	125	C
2	L2	130	A
2	L2	137	A
2	L2	340	A
2	L2	342	U
2	L2	343	U
2	L2	348	A
2	L2	349	C
2	L2	358	G
2	L2	359	OMC
2	L2	365	G
2	L2	366	C
2	L2	368	G
2	L2	372	A
2	L2	377	A
2	L2	386	U

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Mol	Chain	Res	Type
2	L2	388	A
2	L2	390	A
2	L2	391	A
2	L2	392	C
2	L2	404	A
2	L2	406	G
2	L2	414	G
2	L2	415	U
2	L2	421	A
2	L2	423	A
2	L2	426	G
2	L2	427	C
2	L2	434	A
2	L2	435	U
2	L2	438	C
2	L2	439	U
2	L2	443	OMC
2	L2	444	A
2	L2	447	G
2	L2	451	U
2	L2	452	G
2	L2	463	U
2	L2	478	A
2	L2	489	A
2	L2	492	G
2	L2	495	G
2	L2	503	C
2	L2	506	U
2	L2	507	G
2	L2	508	A
2	L2	511	C
2	L2	512	PSU
2	L2	515	U
2	L2	518	G
2	L2	519	G
2	L2	527	A2M
2	L2	528	U
2	L2	529	G
2	L2	530	C
2	L2	534	OMG
2	L2	544	U
2	L2	550	C

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Mol	Chain	Res	Type
2	L2	551	G
2	L2	552	C
2	L2	553	G
2	L2	554	C
2	L2	556	U
2	L2	559	A
2	L2	561	G
2	L2	570	A2M
2	L2	571	G
2	L2	580	U
2	L2	581	G
2	L2	582	U
2	L2	601	G
2	L2	602	A
2	L2	610	G
2	L2	616	G
2	L2	619	A
2	L2	620	C
2	L2	621	G
2	L2	623	A
2	L2	624	C
2	L2	629	A
2	L2	632	G
2	L2	635	A
2	L2	636	A
2	L2	637	G
2	L2	639	G
2	L2	643	A
2	L2	647	A
2	L2	648	A
2	L2	649	G
2	L2	650	A
2	L2	651	C
2	L2	652	C
2	L2	657	U
2	L2	658	G
2	L2	664	G
2	L2	665	A2M
2	L2	668	C
2	L2	685	G
2	L2	686	OMG
2	L2	688	G

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Mol	Chain	Res	Type
2	L2	695	G
2	L2	696	A
2	L2	697	G
2	L2	698	G
2	L2	745	G
2	L2	746	A
2	L2	747	A
2	L2	749	G
2	L2	750	U
2	L2	751	U
2	L2	752	G
2	L2	758	C
2	L2	760	U
2	L2	768	G
2	L2	769	A
2	L2	772	A
2	L2	778	A
2	L2	779	U
2	L2	780	G
2	L2	782	G
2	L2	783	U
2	L2	784	U
2	L2	785	U
2	L2	787	G
2	L2	789	G
2	L2	793	U
2	L2	797	C
2	L2	799	G
2	L2	800	G
2	L2	802	PSU
2	L2	803	A
2	L2	804	U
2	L2	806	C
2	L2	808	C
2	L2	810	G
2	L2	811	U
2	L2	812	C
2	L2	818	U
2	L2	819	U
2	L2	823	A
2	L2	824	G
2	L2	849	C

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Mol	Chain	Res	Type
2	L2	851	C
2	L2	954	A
2	L2	955	C
2	L2	963	U
2	L2	964	G
2	L2	965	C
2	L2	970	A
2	L2	971	A
2	L2	973	U
2	L2	979	A
2	L2	984	G
2	L2	986	U
2	L2	998	G
2	L2	999	U
2	L2	1001	C
2	L2	1002	C
2	L2	1004	G
2	L2	1006	G
2	L2	1011	G
2	L2	1012	U
2	L2	1017	A
2	L2	1019	A
2	L2	1020	C
2	L2	1021	A
2	L2	1033	G
2	L2	1034	G
2	L2	1041	G
2	L2	1046	OMG
2	L2	1053	A
2	L2	1055	A
2	L2	1062	A
2	L2	1064	A
2	L2	1075	G
2	L2	1078	OMG
2	L2	1079	U
2	L2	1083	A
2	L2	1084	A
2	L2	1085	G
2	L2	1093	C
2	L2	1096	U
2	L2	1101	A
2	L2	1102	C

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Mol	Chain	Res	Type
2	L2	1104	G
2	L2	1105	A
2	L2	1108	U
2	L2	1111	C
2	L2	1115	U
2	L2	1116	A
2	L2	1117	G
2	L2	1118	A
2	L2	1121	A
2	L2	1123	A
2	L2	1129	A
2	L2	1130	A
2	L2	1131	A
2	L2	1132	A
2	L2	1133	G
2	L2	1137	G
2	L2	1140	U
2	L2	1141	G
2	L2	1142	A
2	L2	1143	U
2	L2	1147	C
2	L2	1148	G
2	L2	1154	C
2	L2	1155	A
2	L2	1156	G
2	L2	1157	U
2	L2	1158	A
2	L2	1162	A
2	L2	1171	G
2	L2	1172	C
2	L2	1176	A
2	L2	1178	C
2	L2	1179	A
2	L2	1180	A
2	L2	1181	G
2	L2	1189	A
2	L2	1193	U
2	L2	1199	A
2	L2	1200	A
2	L2	1201	G
2	L2	1203	A
2	L2	1204	U

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Mol	Chain	Res	Type
2	L2	1206	G
2	L2	1207	G
2	L2	1209	A
2	L2	1215	A
2	L2	1216	A
2	L2	1219	A
2	L2	1221	U
2	L2	1226	C
2	L2	1229	OMG
2	L2	1233	U
2	L2	1234	G
2	L2	1237	A
2	L2	1238	G
2	L2	1239	A
2	L2	1240	A
2	L2	1241	U
2	L2	1245	U
2	L2	1246	A
2	L2	1248	OMC
2	L2	1252	G
2	L2	1255	A
2	L2	1256	U
2	L2	1260	U
2	L2	1262	G
2	L2	1264	PSU
2	L2	1265	PSU
2	L2	1266	G
2	L2	1270	C
2	L2	1271	G
2	L2	1276	A
2	L2	1278	C
2	L2	1283	A
2	L2	1285	A
2	L2	1288	G
2	L2	1289	A
2	L2	1290	C
2	L2	1291	G
2	L2	1294	G
2	L2	1295	C
2	L2	1297	U
2	L2	1298	U
2	L2	1305	C

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Mol	Chain	Res	Type
2	L2	1309	G
2	L2	1313	U
2	L2	1314	C
2	L2	1324	U
2	L2	1325	A
2	L2	1327	C
2	L2	1329	U
2	L2	1332	C
2	L2	1336	G
2	L2	1337	C
2	L2	1342	G
2	L2	1347	U
2	L2	1348	A
2	L2	1349	A
2	L2	1350	G
2	L2	1356	G
2	L2	1361	U
2	L2	1371	G
2	L2	1373	C
2	L2	1374	A
2	L2	1376	G
2	L2	1379	A
2	L2	1380	C
2	L2	1381	G
2	L2	1385	G
2	L2	1388	G
2	L2	1389	G
2	L2	1391	U
2	L2	1408	C
2	L2	1409	A
2	L2	1410	G
2	L2	1416	U
2	L2	1421	C
2	L2	1423	C
2	L2	1425	A
2	L2	1426	C
2	L2	1427	U
2	L2	1428	U
2	L2	1430	G
2	L2	1433	G
2	L2	1434	G
2	L2	1436	A

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Mol	Chain	Res	Type
2	L2	1437	A
2	L2	1438	U
2	L2	1439	U
2	L2	1440	G
2	L2	1441	C
2	L2	1443	A
2	L2	1444	G
2	L2	1445	A
2	L2	1446	A
2	L2	1447	A
2	L2	1448	A
2	L2	1449	A
2	L2	1450	G
2	L2	1453	U
2	L2	1454	A
2	L2	1455	U
2	L2	1456	C
2	L2	1457	C
2	L2	1459	U
2	L2	1461	C
2	L2	1462	A
2	L2	1463	A
2	L2	1464	A
2	L2	1465	G
2	L2	1474	G
2	L2	1479	G
2	L2	1484	U
2	L2	1485	G
2	L2	1486	G
2	L2	1494	G
2	L2	1498	G
2	L2	1506	G
2	L2	1510	A
2	L2	1511	U
2	L2	1512	G
2	L2	1513	G
2	L2	1514	U
3	L3	6	G
3	L3	15	C
3	L3	16	G
3	L3	17	A
3	L3	19	A

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Mol	Chain	Res	Type
3	L3	20	C
3	L3	21	A
3	L3	22	C
3	L3	24	U
3	L3	25	G
3	L3	26	C
3	L3	34	C
3	L3	35	A
3	L3	36	A
3	L3	39	C
3	L3	41	A
3	L3	45	U
3	L3	46	C
3	L3	48	C
3	L3	49	A
3	L3	51	G
3	L3	52	G
3	L3	59	U
3	L3	61	C
3	L3	63	U
3	L3	64	U
3	L3	70	A
3	L3	71	U
3	L3	74	U
3	L3	99	U
3	L3	109	U
3	L3	110	U
3	L3	111	A
3	L3	112	C
3	L3	113	U
3	L3	114	U
3	L3	117	C
3	L3	121	U
3	L3	124	U
3	L3	125	U
3	L3	129	A
3	L3	130	G
3	L3	131	C
3	L3	132	G
3	L3	136	G
3	L3	142	G
3	L3	143	A

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Mol	Chain	Res	Type
3	L3	146	G
3	L3	149	A
3	L3	150	A
3	L3	151	A
3	L3	169	A
3	L3	173	U
3	L3	182	U
3	L3	187	U
3	L3	192	G
3	L3	193	C
3	L3	194	A
3	L3	195	U
3	L3	196	U
3	L3	199	A
3	L3	200	G
3	L3	202	A
3	L3	210	G
3	L3	213	G
3	L3	214	U
3	L3	216	U
4	L4	7	U
4	L4	8	U
4	L4	9	G
4	L4	10	U
4	L4	11	G
4	L4	16	G
4	L4	18	U
4	L4	19	C
4	L4	20	U
4	L4	24	A
4	L4	31	G
4	L4	39	A
4	L4	40	G
4	L4	50	G
4	L4	51	U
4	L4	58	G
4	L4	60	A
4	L4	61	A
4	L4	62	C
4	L4	67	A
4	L4	76	C
4	L4	77	U

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Mol	Chain	Res	Type
4	L4	83	U
4	L4	84	U
4	L4	85	C
4	L4	86	U
4	L4	87	G
4	L4	89	G
4	L4	90	G
4	L4	97	G
4	L4	102	G
4	L4	106	G
4	L4	108	G
4	L4	114	A
4	L4	115	A
4	L4	120	U
4	L4	121	C
4	L4	128	U
4	L4	132	U
4	L4	133	C
4	L4	137	G
4	L4	143	C
4	L4	144	G
4	L4	145	C
4	L4	149	U
4	L4	150	A
4	L4	151	A
4	L4	153	C
4	L4	154	C
4	L4	157	A
4	L4	158	A
4	L4	159	G
4	L4	163	A
4	L4	166	C
4	L4	168	A
4	L4	169	A
4	L4	170	G
4	L4	173	C
4	L4	178	G
4	L4	180	C
5	L5	3	U
5	L5	6	G
5	L5	15	C
5	L5	23	A

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Mol	Chain	Res	Type
5	L5	24	G
5	L5	26	A
5	L5	27	C
5	L5	29	U
5	L5	30	G
5	L5	39	G
5	L5	45	A
5	L5	50	C
5	L5	51	A
5	L5	52	U
5	L5	53	G
5	L5	54	C
5	L5	61	C
5	L5	64	G
5	L5	65	U
5	L5	68	G
5	L5	73	G
5	L5	86	G
5	L5	88	C
5	L5	92	A
5	L5	99	G
5	L5	105	U
5	L5	106	G
5	L5	107	A
5	L5	108	G
5	L5	109	G
5	L5	113	G
5	L5	117	A
5	L5	118	U
5	L5	119	U
5	L5	120	C
5	L5	126	C
5	L5	135	C
6	L6	7	A
6	L6	10	C
6	L6	11	G
6	L6	14	A
6	L6	15	C
6	L6	22	G
6	L6	23	A
6	L6	24	C
6	L6	25	U

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Mol	Chain	Res	Type
6	L6	26	G
6	L6	29	G
6	L6	31	U
6	L6	32	U
6	L6	33	G
6	L6	39	U
6	L6	40	C
6	L6	41	G
6	L6	42	A
6	L6	43	A
6	L6	44	G
6	L6	48	C
6	L6	49	C
6	L6	50	A
6	L6	51	A
6	L6	52	G
6	L6	53	U
6	L6	54	A
6	L6	56	A
6	L6	57	U
6	L6	58	U
6	L6	62	G
6	L6	64	U
6	L6	65	C
6	L6	67	C
6	L6	68	A
6	L6	69	A
6	L6	70	G
6	L6	71	A
6	L6	72	C
6	L6	73	A
7	L7	3	C
7	L7	5	U
7	L7	12	A
7	L7	15	G
7	L7	16	A
7	L7	17	U
7	L7	18	G
7	L7	19	A
7	L7	22	U
7	L7	31	A
7	L7	32	U

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Mol	Chain	Res	Type
7	L7	33	U
7	L7	34	U
7	L7	38	U
7	L7	51	A
7	L7	53	A
7	L7	59	A
7	L7	61	A
7	L7	62	A
7	L7	63	G
7	L7	67	U
7	L7	68	A
7	L7	69	PSU
7	L7	71	A
7	L7	72	A
7	L7	77	A
7	L7	80	A
7	L7	81	U
7	L7	82	C
7	L7	84	U
7	L7	87	A
7	L7	88	A
7	L7	89	U
7	L7	94	G
7	L7	95	A
7	L7	96	A
7	L7	100	U
7	L7	103	A
7	L7	104	A
7	L7	105	C
7	L7	107	C
7	L7	110	A
7	L7	112	G
7	L7	115	G
7	L7	116	C
7	L7	120	G
7	L7	124	A
7	L7	125	A
7	L7	127	C
7	L7	128	U
7	L7	153	C
7	L7	156	A
7	L7	157	U

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Mol	Chain	Res	Type
7	L7	158	U
7	L7	164	U
7	L7	167	C
7	L7	169	A
7	L7	170	A
8	L8	6	A
8	L8	11	G
8	L8	14	C
8	L8	21	G
8	L8	22	A
8	L8	25	G
8	L8	26	A
8	L8	30	C
8	L8	37	U
8	L8	39	C
8	L8	42	U
8	L8	45	G
8	L8	46	A
8	L8	52	G
8	L8	57	U
8	L8	58	A
8	L8	59	A
8	L8	67	C
8	L8	68	A
8	L8	76	U
8	L8	80	U
8	L8	93	G
8	L8	94	A
8	L8	101	G
8	L8	104	A
8	L8	113	U
8	L8	114	G
8	L8	117	G
51	S1	3	U
51	S1	8	OMU
51	S1	17	C
51	S1	25	C
51	S1	26	A
51	S1	34	G
51	S1	40	A
51	S1	42	G
51	S1	45	U

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Mol	Chain	Res	Type
51	S1	46	U
51	S1	47	A
51	S1	61	C
51	S1	62	A
51	S1	65	A
51	S1	66	U
51	S1	67	C
51	S1	68	A
51	S1	82	A
51	S1	98	A2M
51	S1	102	A
51	S1	103	A
51	S1	109	C
51	S1	110	G
51	S1	112	A
51	S1	113	A
51	S1	114	U
51	S1	117	G
51	S1	119	C
51	S1	122	A
51	S1	128	C
51	S1	129	U
51	S1	133	G
51	S1	144	A
51	S1	145	A
51	S1	146	U
51	S1	147	U
51	S1	148	G
51	S1	151	U
51	S1	152	A
51	S1	158	G
51	S1	162	A
51	S1	164	C
51	S1	165	G
51	S1	167	C
51	S1	168	A
51	S1	170	G
51	S1	176	A
51	S1	181	A
51	S1	182	A
51	S1	192	U
51	S1	194	U

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Mol	Chain	Res	Type
51	S1	195	U
51	S1	198	C
51	S1	199	C
51	S1	227	U
51	S1	228	G
51	S1	232	C
51	S1	234	C
51	S1	235	C
51	S1	237	A
51	S1	238	G
51	S1	246	A
51	S1	249	A
51	S1	252	G
51	S1	253	U
51	S1	255	A
51	S1	256	A
51	S1	257	A
51	S1	264	C
51	S1	265	C
51	S1	275	A
51	S1	276	G
51	S1	277	U
51	S1	278	A
51	S1	279	A
51	S1	281	A
51	S1	282	C
51	S1	285	A
51	S1	286	G
51	S1	287	C
51	S1	288	A
51	S1	289	G
51	S1	290	U
51	S1	295	A
51	S1	296	C
51	S1	297	U
51	S1	298	C
51	S1	306	U
51	S1	308	C
51	S1	309	G
51	S1	310	U
51	S1	315	A
51	S1	316	A

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Mol	Chain	Res	Type
51	S1	321	G
51	S1	322	C
51	S1	323	U
51	S1	324	U
51	S1	325	G
51	S1	326	U
51	S1	327	U
51	S1	328	C
51	S1	329	C
51	S1	330	G
51	S1	332	C
51	S1	340	G
51	S1	341	A
51	S1	343	G
51	S1	352	C
51	S1	356	A
51	S1	357	U
51	S1	358	C
51	S1	360	G
51	S1	363	G
51	S1	364	G
51	S1	365	U
51	S1	367	A
51	S1	376	U
51	S1	377	A
51	S1	378	G
51	S1	379	U
51	S1	381	G
51	S1	382	A
51	S1	388	A
51	S1	395	U
51	S1	396	G
51	S1	403	G
51	S1	404	C
51	S1	405	G
51	S1	423	U
51	S1	432	G
51	S1	433	G
51	S1	443	A
51	S1	444	A
51	S1	445	U
51	S1	446	A

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Mol	Chain	Res	Type
51	S1	447	G
51	S1	450	A
51	S1	451	C
51	S1	452	C
51	S1	454	C
51	S1	455	PSU
51	S1	456	U
51	S1	460	C
51	S1	461	G
51	S1	462	G
51	S1	464	G
51	S1	466	G
51	S1	467	C
51	S1	469	G
51	S1	473	G
51	S1	474	C
51	S1	476	C
51	S1	477	G
51	S1	478	C
51	S1	481	A
51	S1	482	U
51	S1	487	C
51	S1	488	A
51	S1	491	G
51	S1	495	A
51	S1	496	A
51	S1	497	A
51	S1	505	A
51	S1	507	G
51	S1	508	A
51	S1	512	A2M
51	S1	516	A
51	S1	517	A
51	S1	523	A
51	S1	525	A
51	S1	527	A
51	S1	547	U
51	S1	551	A
51	S1	552	U
51	S1	555	C
51	S1	556	A
51	S1	559	G

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Mol	Chain	Res	Type
51	S1	561	G
51	S1	565	U
51	S1	566	A
51	S1	572	A
51	S1	574	C
51	S1	575	C
51	S1	576	A
51	S1	577	U
51	S1	579	C
51	S1	580	A
51	S1	584	U
51	S1	585	C
51	S1	587	A
51	S1	588	G
51	S1	589	U
51	S1	590	A
51	S1	591	A
51	S1	593	A
51	S1	594	A
51	S1	598	G
51	S1	605	A
51	S1	608	C
51	S1	611	G
51	S1	612	U
51	S1	614	C
51	S1	617	G
51	S1	618	C
51	S1	620	C
51	S1	626	G
51	S1	627	U
51	S1	628	A
51	S1	629	A
51	S1	632	C
51	S1	643	A
51	S1	655	U
51	S1	660	U
51	S1	667	U
51	S1	668	A2M
51	S1	669	A
51	S1	670	A
51	S1	671	G
51	S1	672	G

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Mol	Chain	Res	Type
51	S1	673	G
51	S1	675	U
51	S1	678	U
51	S1	679	A
51	S1	686	C
51	S1	687	U
51	S1	688	G
51	S1	690	G
51	S1	695	G
51	S1	697	G
51	S1	698	C
51	S1	699	A
51	S1	700	G
51	S1	701	G
51	S1	749	U
51	S1	750	U
51	S1	755	C
51	S1	757	C
51	S1	759	U
51	S1	760	G
51	S1	761	A
51	S1	775	C
51	S1	778	G
51	S1	782	C
51	S1	783	A
51	S1	784	C
51	S1	786	G
51	S1	788	A
51	S1	789	G
51	S1	790	U
51	S1	791	G
51	S1	793	G
51	S1	810	G
51	S1	811	C
51	S1	812	A
51	S1	814	G
51	S1	815	U
51	S1	816	C
51	S1	817	A
51	S1	818	U
51	S1	819	G
51	S1	825	C

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Mol	Chain	Res	Type
51	S1	826	A
51	S1	827	G
51	S1	830	G
51	S1	831	G
51	S1	833	G
51	S1	834	U
51	S1	835	C
51	S1	838	U
51	S1	841	U
51	S1	844	U
51	S1	845	U
51	S1	853	A
51	S1	856	A
51	S1	863	C
51	S1	866	G
51	S1	867	A
51	S1	868	C
51	S1	872	A
51	S1	877	U
51	S1	881	U
51	S1	882	U
51	S1	883	G
51	S1	886	U
51	S1	887	U
51	S1	890	A
51	S1	892	U
51	S1	893	A
51	S1	895	A
51	S1	904	G
51	S1	905	A
51	S1	907	A
51	S1	913	G
51	S1	914	G
51	S1	916	G
51	S1	918	A
51	S1	919	G
51	S1	920	C
51	S1	922	U
51	S1	923	C
51	S1	925	A
51	S1	926	G
51	S1	927	G

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Mol	Chain	Res	Type
51	S1	930	A
51	S1	935	U
51	S1	936	U
51	S1	944	U
51	S1	945	G
51	S1	951	U
51	S1	952	U
51	S1	955	A
51	S1	956	A
51	S1	958	G
51	S1	959	U
51	S1	962	A
51	S1	964	U
51	S1	966	G
51	S1	969	A
51	S1	970	U
51	S1	971	U
51	S1	972	A
51	S1	973	U
51	S1	1093	C
51	S1	1101	A
51	S1	1102	G
51	S1	1103	G
51	S1	1105	A
51	S1	1107	G
51	S1	1109	A
51	S1	1115	G
51	S1	1116	U
51	S1	1117	A
51	S1	1119	U
51	S1	1123	G
51	S1	1130	A
51	S1	1133	U
51	S1	1139	G
51	S1	1145	A
51	S1	1150	U
51	S1	1161	G
51	S1	1175	G
51	S1	1180	A
51	S1	1181	C
51	S1	1182	A
51	S1	1187	A

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Mol	Chain	Res	Type
51	S1	1197	C
51	S1	1198	A
51	S1	1207	U
51	S1	1210	C
51	S1	1211	U
51	S1	1213	A
51	S1	1217	A
51	S1	1218	A
51	S1	1232	G
51	S1	1235	A
51	S1	1236	U
51	S1	1239	A
51	S1	1240	A
51	S1	1248	A
51	S1	1250	A
51	S1	1251	A
51	S1	1256	U
51	S1	1268	C
51	S1	1270	G
51	S1	1271	C
51	S1	1272	A
51	S1	1273	A
51	S1	1274	A
51	S1	1275	C
51	S1	1277	A
51	S1	1278	U
51	S1	1290	A
51	S1	1296	G
51	S1	1298	U
51	S1	1359	C
51	S1	1360	U
51	S1	1361	U
51	S1	1362	A
51	S1	1365	U
51	S1	1371	U
51	S1	1398	C
51	S1	1399	G
51	S1	1400	G
51	S1	1408	C
51	S1	1414	A
51	S1	1431	A
51	S1	1442	U

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Mol	Chain	Res	Type
51	S1	1443	U
51	S1	1444	G
51	S1	1446	G
51	S1	1448	U
51	S1	1449	U
51	S1	1452	A
51	S1	1460	G
51	S1	1461	G
51	S1	1466	G
51	S1	1467	U
51	S1	1469	C
51	S1	1478	OMG
51	S1	1489	A
51	S1	1490	A
51	S1	1502	G
51	S1	1507	G
51	S1	1510	C
51	S1	1516	G
51	S1	1517	A
51	S1	1518	C
51	S1	1537	U
51	S1	1538	U
51	S1	1539	PSU
51	S1	1542	C
51	S1	1543	B8N
51	S1	1546	A
51	S1	1548	A
51	S1	1551	G
51	S1	1552	G
51	S1	1554	A
51	S1	1559	U
51	S1	1564	G
51	S1	1569	G
51	S1	1570	G
51	S1	1576	A
51	S1	1577	U
51	S1	1579	A
51	S1	1582	A
51	S1	1583	U
51	S1	1587	C
51	S1	1591	U
51	S1	1594	A

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Mol	Chain	Res	Type
51	S1	1595	G
51	S1	1597	G
51	S1	1598	U
51	S1	1603	U
51	S1	1605	U
51	S1	1606	C
51	S1	1608	A
51	S1	1609	U
51	S1	1611	C
51	S1	1612	C
51	S1	1613	C
51	S1	1614	U
51	S1	1615	G
51	S1	1616	A
51	S1	1622	G
51	S1	1625	G
51	S1	1627	A
51	S1	1636	U
51	S1	1637	A
51	S1	1638	U
51	S1	1643	G
51	S1	1649	G
51	S1	1650	U
51	S1	1652	A
51	S1	1653	U
51	S1	1658	U
51	S1	1666	U
51	S1	1667	U
51	S1	1673	A
51	S1	1677	G
51	S1	1680	G
51	S1	1686	C
51	S1	1689	G
51	S1	1690	C
51	S1	1693	C
51	S1	1697	G
51	S1	1698	U
51	S1	1699	A
51	S1	1702	A
51	S1	1704	U
51	S1	1705	C
51	S1	1708	A

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Mol	Chain	Res	Type
51	S1	1709	A
51	S1	1712	G
51	S1	1713	C
51	S1	1715	C
51	S1	1716	A
51	S1	1717	U
51	S1	1718	A
51	S1	1719	G
51	S1	1720	G
51	S1	1724	G
51	S1	1725	C
51	S1	1761	C
51	S1	1762	A
51	S1	1766	G
51	S1	1767	G
51	S1	1768	U
51	S1	1769	C
51	S1	1770	G
51	S1	1772	A
51	S1	1778	C
51	S1	1781	U
51	S1	1784	G
51	S1	1789	U
51	S1	1790	C
51	S1	1793	U
51	S1	1794	U
51	S1	1795	G
51	S1	1799	U
51	S1	1801	G
51	S1	1803	A
51	S1	1810	G
51	S1	1814	U
51	S1	1816	U
51	S1	1819	G
51	S1	1824	C
51	S1	1826	G
51	S1	1827	C
51	S1	1828	A
51	S1	1829	OMG
51	S1	1832	C
51	S1	1833	OMU
51	S1	1835	U

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Mol	Chain	Res	Type
51	S1	1836	G
51	S1	1838	U
51	S1	1845	C
51	S1	1846	A
51	S1	1847	A
51	S1	1848	U
51	S1	1851	U
51	S1	1858	G
51	S1	1859	A
51	S1	1861	A
51	S1	1862	C
51	S1	1867	A
51	S1	1872	A
51	S1	1873	A
51	S1	1874	U
51	S1	1875	G
51	S1	1880	U
51	S1	1882	A
51	S1	1884	A
51	S1	1887	A
51	S1	1888	A
51	S1	1889	G
51	S1	1890	A
51	S1	1891	A
51	S1	1892	A
51	S1	1893	A
51	S1	1906	G
51	S1	1907	A
51	S1	1908	A
51	S1	1909	C
51	S1	1913	C
51	S1	1916	G
51	S1	1917	A
51	S1	1918	U
51	S1	1919	C
51	S1	1920	A
51	S1	1923	A
51	S1	1928	G
51	S1	1929	G
51	S1	1931	G
51	S1	1933	A
51	S1	1934	A

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Mol	Chain	Res	Type
51	S1	1938	C
51	S1	1939	G
51	S1	1943	U
51	S1	1944	C
51	S1	1948	U
51	S1	1949	A
51	S1	1950	G
51	S1	1953	C
51	S1	1956	C
51	S1	1957	U
51	S1	1958	U
51	S1	1961	G
51	S1	1962	A
51	S1	1963	C
51	S1	1969	A
51	S1	1976	U
51	S1	1981	G
51	S1	1985	G
51	S1	1988	C
51	S1	1989	A
51	S1	1995	7MG
51	S1	1998	U
51	S1	2004	G
51	S1	2005	U
51	S1	2010	G
51	S1	2015	U
51	S1	2016	C
51	S1	2020	A
51	S1	2021	A2M
51	S1	2027	G
51	S1	2031	A
51	S1	2036	G
51	S1	2038	C
51	S1	2039	C
51	S1	2040	C
51	S1	2042	G
51	S1	2053	A
51	S1	2054	C
51	S1	2064	C
51	S1	2070	U
51	S1	2079	U
51	S1	2083	G

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Mol	Chain	Res	Type
51	S1	2084	C
51	S1	2092	G
51	S1	2093	U
51	S1	2097	C
51	S1	2099	G
51	S1	2100	A
51	S1	2101	C
51	S1	2118	G
51	S1	2119	C
51	S1	2120	C
51	S1	2121	C
51	S1	2124	A
51	S1	2125	A
51	S1	2134	A
51	S1	2136	A
51	S1	2137	U
51	S1	2157	A
51	S1	2159	A
51	S1	2160	G
51	S1	2163	G
51	S1	2165	A
51	S1	2166	A
51	S1	2169	A
51	S1	2170	G
51	S1	2171	G
51	S1	2172	U
51	S1	2173	A
51	S1	2178	U
51	S1	2180	G
51	S1	2183	G
51	S1	2185	MA6
51	S1	2186	C
51	S1	2195	G
51	S1	2196	G
51	S1	2197	G
51	S1	2198	A
51	S1	2199	C
51	S1	2202	PSU
51	S1	2203	U
52	S2	31	A
52	S2	34	G
52	S2	35	A

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Mol	Chain	Res	Type
52	S2	36	A
52	S2	37	MIA
52	S2	38	A
53	S3	3	C
53	S3	7	G
53	S3	8	U
53	S3	9	G
53	S3	11	A
53	S3	22	G
53	S3	31	G
53	S3	42	G
53	S3	46	A
53	S3	47	U
53	S3	48	C
53	S3	49	G
53	S3	52	G
53	S3	53	G
53	S3	54	U
53	S3	55	U
53	S3	58	A
53	S3	62	C
53	S3	63	G
53	S3	64	G
53	S3	66	C
53	S3	68	C
53	S3	70	G
53	S3	71	C
53	S3	73	A
53	S3	74	C
53	S3	75	C
53	S3	76	A
54	S4	5	G
54	S4	6	G
54	S4	8	U
54	S4	9	A
54	S4	11	C
54	S4	14	A
54	S4	22	G
54	S4	23	A
54	S4	25	C
54	S4	26	A
54	S4	27	G

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Mol	Chain	Res	Type
54	S4	30	G
54	S4	31	A
54	S4	32	U
54	S4	38	A
54	S4	40	C
54	S4	41	C
54	S4	42	C
54	S4	43	C
54	S4	44	G
54	S4	45	U
54	S4	46	G
54	S4	50	U
54	S4	51	U
54	S4	53	G
54	S4	54	U
54	S4	55	U
54	S4	56	C
54	S4	58	A
54	S4	59	U
54	S4	61	C
54	S4	65	G
54	S4	69	G
54	S4	70	C
54	S4	73	A
54	S4	75	C
54	S4	76	A
55	S5	2	A
55	S5	5	A
55	S5	7	G
55	S5	8	U

All (178) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	38	A
1	L1	63	A
1	L1	92	C
1	L1	120	G
1	L1	141	U
1	L1	161	A
1	L1	170	U
1	L1	191	U

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Mol	Chain	Res	Type
1	L1	200	A
1	L1	208	C
1	L1	233	U
1	L1	415	A
1	L1	543	G
1	L1	563	C
1	L1	574	G
1	L1	575	A
1	L1	576	G
1	L1	582	U
1	L1	584	U
1	L1	610	A
1	L1	760	A
1	L1	823	G
1	L1	824	U
1	L1	835	G
1	L1	836	G
1	L1	851	G
1	L1	947	A
1	L1	967	G
1	L1	1012	C
1	L1	1031	A
1	L1	1044	G
1	L1	1051	C
1	L1	1096	C
1	L1	1114	A
1	L1	1121	G
1	L1	1200	A
1	L1	1209	G
1	L1	1211	A
1	L1	1261	U
1	L1	1387	U
1	L1	1390	G
1	L1	1412	G
1	L1	1413	U
1	L1	1439	A
1	L1	1479	A
1	L1	1519	G
1	L1	1565	A
1	L1	1574	C
1	L1	1612	G
1	L1	1662	G

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Mol	Chain	Res	Type
1	L1	1669	A
1	L1	1673	G
1	L1	1726	G
1	L1	1742	G
2	L2	25	A
2	L2	29	C
2	L2	41	A
2	L2	62	A
2	L2	68	A
2	L2	414	G
2	L2	443	OMC
2	L2	507	G
2	L2	551	G
2	L2	623	A
2	L2	695	G
2	L2	696	A
2	L2	748	C
2	L2	777	A
2	L2	998	G
2	L2	1083	A
2	L2	1101	A
2	L2	1116	A
2	L2	1131	A
2	L2	1136	U
2	L2	1141	G
2	L2	1156	G
2	L2	1170	U
2	L2	1203	A
2	L2	1246	A
2	L2	1293	C
2	L2	1297	U
2	L2	1313	U
2	L2	1324	U
2	L2	1349	A
2	L2	1388	G
2	L2	1437	A
2	L2	1439	U
2	L2	1454	A
2	L2	1461	C
2	L2	1484	U
2	L2	1485	G
2	L2	1512	G

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Mol	Chain	Res	Type
3	L3	19	A
3	L3	34	C
3	L3	35	A
3	L3	112	C
3	L3	113	U
3	L3	149	A
3	L3	193	C
4	L4	33	G
4	L4	76	C
4	L4	83	U
4	L4	127	G
4	L4	149	U
5	L5	26	A
5	L5	49	G
5	L5	51	A
5	L5	106	G
5	L5	125	U
5	L5	134	C
6	L6	41	G
6	L6	50	A
6	L6	51	A
6	L6	64	U
6	L6	71	A
7	L7	21	U
7	L7	71	A
7	L7	93	C
7	L7	95	A
7	L7	104	A
8	L8	45	G
8	L8	113	U
51	S1	102	A
51	S1	128	C
51	S1	145	A
51	S1	234	C
51	S1	236	C
51	S1	237	A
51	S1	276	G
51	S1	281	A
51	S1	294	G
51	S1	307	C
51	S1	328	C
51	S1	366	G

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Mol	Chain	Res	Type
51	S1	443	A
51	S1	516	A
51	S1	550	C
51	S1	579	C
51	S1	588	G
51	S1	589	U
51	S1	620	C
51	S1	628	A
51	S1	656	G
51	S1	687	U
51	S1	777	A
51	S1	789	G
51	S1	814	G
51	S1	889	A
51	S1	904	G
51	S1	913	G
51	S1	958	G
51	S1	1209	C
51	S1	1360	U
51	S1	1460	G
51	S1	1608	A
51	S1	1672	C
51	S1	1724	G
51	S1	1761	C
51	S1	1767	G
51	S1	1827	C
51	S1	1873	A
51	S1	1889	G
51	S1	1908	A
51	S1	1915	U
51	S1	1919	C
51	S1	1994	G
51	S1	2035	C
51	S1	2053	A
51	S1	2099	G
51	S1	2119	C
51	S1	2157	A
51	S1	2171	G
52	S2	34	G
53	S3	47	U
53	S3	74	C
54	S4	13	C

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Mol	Chain	Res	Type
54	S4	58	A
55	S5	7	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

162 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	$\# Z > 2$
2	OMC	L2	1397	2	19,22,23	0.29	0	25,31,34	0.57	0
51	OMC	S1	1866	51	19,22,23	0.30	0	25,31,34	0.47	0
51	OMU	S1	661	51	19,22,23	0.21	0	25,31,34	0.40	0
7	PSU	L7	74	90,7	18,21,22	0.92	1 (5%)	21,30,33	0.65	0
1	A2M	L1	305	1	22,25,26	0.23	0	30,36,39	0.67	2 (6%)
1	PSU	L1	1171	1	18,21,22	0.94	1 (5%)	21,30,33	0.69	0
51	PSU	S1	1156	51	18,21,22	0.92	1 (5%)	21,30,33	0.66	0
2	PSU	L2	512	2	18,21,22	0.93	1 (5%)	21,30,33	0.77	0
2	OMU	L2	73	2	19,22,23	0.24	0	25,31,34	0.43	0
2	OMG	L2	71	2	23,26,27	0.30	0	32,38,41	0.53	0
51	OMU	S1	1621	51	19,22,23	0.23	0	25,31,34	0.46	0
51	OMG	S1	1478	51	23,26,27	0.32	0	32,38,41	0.43	0
1	PSU	L1	1528	1	18,21,22	0.92	1 (5%)	21,30,33	0.56	0
51	A2M	S1	2021	51	22,25,26	0.20	0	30,36,39	0.43	0
2	OMC	L2	14	1,2	19,22,23	0.29	0	25,31,34	0.34	0
2	PSU	L2	662	2,92	18,21,22	0.93	1 (5%)	21,30,33	0.67	0
1	A2M	L1	678	1,2	22,25,26	0.20	0	30,36,39	0.34	0
2	A2M	L2	95	2	22,25,26	0.20	0	30,36,39	0.37	0
2	OMG	L2	655	2	23,26,27	0.34	0	32,38,41	0.45	0
1	PSU	L1	1177	1	18,21,22	0.92	1 (5%)	21,30,33	0.55	0
2	OMC	L2	1159	2	19,22,23	0.30	0	25,31,34	0.46	0
51	PSU	S1	1246	51	18,21,22	0.92	1 (5%)	21,30,33	0.62	0
7	OMG	L7	75	7	23,26,27	0.31	0	32,38,41	0.48	0
2	A2M	L2	1185	2	22,25,26	0.22	0	30,36,39	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	L1	1010	1,92	19,22,23	0.32	0	25,31,34	0.40	0
1	PSU	L1	1529	1	18,21,22	0.93	1 (5%)	21,30,33	0.75	0
1	A2M	L1	235	1	22,25,26	0.17	0	30,36,39	0.42	0
2	PSU	L2	437	2	18,21,22	0.90	1 (5%)	21,30,33	0.69	0
51	OMC	S1	38	51	19,22,23	0.30	0	25,31,34	0.53	0
2	OMC	L2	443	91,90,2	19,22,23	0.36	0	25,31,34	0.52	0
2	PSU	L2	1060	2	18,21,22	0.94	1 (5%)	21,30,33	0.87	1 (4%)
51	PSU	S1	1192	51	18,21,22	0.91	1 (5%)	21,30,33	0.57	0
2	A2M	L2	572	2	22,25,26	0.20	0	30,36,39	0.58	0
2	5MC	L2	1308	2	19,22,23	0.75	1 (5%)	26,32,35	0.62	1 (3%)
2	PSU	L2	1194	2	18,21,22	0.92	1 (5%)	21,30,33	0.64	0
2	A2M	L2	502[A]	2,51	22,25,26	0.28	0	30,36,39	0.76	2 (6%)
1	A2M	L1	927	1	22,25,26	0.20	0	30,36,39	0.33	0
2	PSU	L2	593	2	18,21,22	0.92	1 (5%)	21,30,33	0.60	0
2	PSU	L2	1284	2	18,21,22	0.91	1 (5%)	21,30,33	0.58	0
2	PSU	L2	1264	2	18,21,22	0.91	1 (5%)	21,30,33	0.79	1 (4%)
51	PSU	S1	2202	51	18,21,22	0.91	1 (5%)	21,30,33	0.60	0
51	OMG	S1	600	51	23,26,27	0.30	0	32,38,41	0.38	0
2	A2M	L2	604	1,2	22,25,26	0.19	0	30,36,39	0.39	0
1	A2M	L1	955	1	22,25,26	0.20	0	30,36,39	0.42	0
1	PSU	L1	940	1	18,21,22	0.93	1 (5%)	21,30,33	0.78	1 (4%)
1	A2M	L1	858	1	22,25,26	0.21	0	30,36,39	0.57	0
2	PSU	L2	1058	2	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
1	A2M	L1	681	1	22,25,26	0.19	0	30,36,39	0.33	0
7	A2M	L7	43	7	22,25,26	0.23	0	30,36,39	0.53	0
2	5MC	L2	524	2,92	19,22,23	0.82	1 (5%)	26,32,35	0.50	0
2	PSU	L2	1213	2	18,21,22	0.90	1 (5%)	21,30,33	0.70	0
2	PSU	L2	1318	2	18,21,22	0.90	1 (5%)	21,30,33	0.68	0
51	PSU	S1	1533	51	18,21,22	0.93	1 (5%)	21,30,33	0.75	0
51	PSU	S1	2048	51	18,21,22	0.94	1 (5%)	21,30,33	0.70	0
2	PSU	L2	1403	2	18,21,22	0.92	1 (5%)	21,30,33	0.75	0
2	PSU	L2	1303	2	18,21,22	0.89	1 (5%)	21,30,33	0.77	0
1	PSU	L1	1181	1	18,21,22	0.91	1 (5%)	21,30,33	0.78	1 (4%)
2	PSU	L2	565	2	18,21,22	0.92	1 (5%)	21,30,33	0.64	0
51	OMG	S1	1647	51	23,26,27	0.31	0	32,38,41	0.55	0
2	OMG	L2	1078	2	23,26,27	0.34	0	32,38,41	0.53	1 (3%)
1	OMC	L1	1527	1	19,22,23	0.31	0	25,31,34	0.36	0
1	OMG	L1	1190	1	23,26,27	0.32	0	32,38,41	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	L2	1359	2	19,22,23	0.22	0	25,31,34	0.53	0
2	PSU	L2	597	2	18,21,22	0.92	1 (5%)	21,30,33	0.69	0
2	A2M	L2	1372	2	22,25,26	0.21	0	30,36,39	0.60	1 (3%)
2	A2M	L2	591	2	22,25,26	0.19	0	30,36,39	0.39	0
7	PSU	L7	69	92,7	18,21,22	0.91	1 (5%)	21,30,33	0.79	0
1	OMG	L1	1524	1	23,26,27	0.36	0	32,38,41	0.63	1 (3%)
2	OMG	L2	534	2	23,26,27	0.30	0	32,38,41	0.34	0
2	PSU	L2	1265	2	18,21,22	0.92	1 (5%)	21,30,33	0.75	0
2	PSU	L2	78	2	18,21,22	0.93	1 (5%)	21,30,33	0.80	1 (4%)
2	PSU	L2	626	2	18,21,22	0.93	1 (5%)	21,30,33	0.63	0
52	MIA	S2	37	52	28,31,32	0.56	1 (3%)	38,44,47	3.69	1 (2%)
2	PSU	L2	1144	2	18,21,22	0.88	1 (5%)	21,30,33	0.68	0
2	OMG	L2	1229	2	23,26,27	0.33	0	32,38,41	0.40	0
51	MA6	S1	2185	90,51	23,26,27	0.28	0	33,38,41	0.63	1 (3%)
51	PSU	S1	2046	51	18,21,22	0.94	1 (5%)	21,30,33	0.78	0
51	PSU	S1	33	51	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
1	PSU	L1	1664	1	18,21,22	0.92	1 (5%)	21,30,33	0.63	0
51	OMU	S1	29	51	19,22,23	0.22	0	25,31,34	0.59	0
2	A2M	L2	665	2	22,25,26	0.19	0	30,36,39	0.33	0
2	OMG	L2	1517	2	23,26,27	0.32	0	32,38,41	0.44	0
1	PSU	L1	239	1	18,21,22	0.94	1 (5%)	21,30,33	0.64	0
51	5MC	S1	2061	51	19,22,23	0.76	1 (5%)	26,32,35	0.56	0
2	OMG	L2	1253	2	23,26,27	0.31	0	32,38,41	0.35	0
2	PSU	L2	1152	2	18,21,22	0.92	1 (5%)	21,30,33	0.67	0
2	A2M	L2	570	1,2	22,25,26	0.23	0	30,36,39	0.49	0
2	PSU	L2	472	2	18,21,22	0.90	1 (5%)	21,30,33	0.68	0
51	OMC	S1	18	51	19,22,23	0.31	0	25,31,34	0.43	0
51	OMU	S1	8	51	19,22,23	0.26	0	25,31,34	0.57	0
51	OMG	S1	2151	51	23,26,27	0.31	0	32,38,41	0.50	0
1	OMG	L1	1626	1	23,26,27	0.32	0	32,38,41	0.42	0
1	PSU	L1	422	1	18,21,22	0.92	1 (5%)	21,30,33	0.68	0
51	7MG	S1	1995	53,51	23,26,27	0.98	1 (4%)	27,39,42	0.77	1 (3%)
1	A2M	L1	1539	1,2,92	22,25,26	0.21	0	30,36,39	0.32	0
1	OMU	L1	1659	1,92	19,22,23	0.23	0	25,31,34	0.42	0
2	OMC	L2	359	2	19,22,23	0.28	0	25,31,34	0.42	0
1	PSU	L1	1017	1	18,21,22	0.93	1 (5%)	21,30,33	0.78	0
1	A2M	L1	407	1	22,25,26	0.21	0	30,36,39	0.52	0
1	1MA	L1	677	1	21,25,26	0.42	0	30,37,40	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	L2	667	2	19,22,23	0.22	0	25,31,34	0.62	0
2	A2M	L2	527	2	22,25,26	0.26	0	30,36,39	0.47	0
51	PSU	S1	455	51	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
1	PSU	L1	1011	1,2	18,21,22	0.88	1 (5%)	21,30,33	0.77	1 (4%)
2	OMG	L2	1231	2	23,26,27	0.32	0	32,38,41	0.47	0
51	A2M	S1	668	92,51	22,25,26	0.21	0	30,36,39	0.45	0
51	PSU	S1	1657	51	18,21,22	0.90	1 (5%)	21,30,33	0.62	0
51	A2M	S1	479	51	22,25,26	0.20	0	30,36,39	0.37	0
1	OMU	L1	1107	1	19,22,23	0.22	0	25,31,34	0.61	0
51	OMG	S1	1829	92,51	23,26,27	0.32	0	32,38,41	0.38	0
2	PSU	L2	500	2	18,21,22	0.91	1 (5%)	21,30,33	0.63	0
2	PSU	L2	802	2,92	18,21,22	0.92	1 (5%)	21,30,33	0.62	0
51	B8N	S1	1543	-	25,29,30	0.96	2 (8%)	28,42,45	0.83	1 (3%)
1	OMU	L1	1039	1	19,22,23	0.22	0	25,31,34	0.55	0
51	A2M	S1	512	51	22,25,26	0.19	0	30,36,39	0.54	0
51	OMG	S1	1623	51	23,26,27	0.30	0	32,38,41	0.34	0
51	PSU	S1	1539	51	18,21,22	0.92	1 (5%)	21,30,33	0.65	0
2	A2M	L2	502[B]	2	22,25,26	0.30	0	30,36,39	0.67	1 (3%)
2	OMG	L2	1046	2,53	23,26,27	0.32	0	32,38,41	0.36	0
1	A2M	L1	1373	1	22,25,26	0.21	0	30,36,39	0.42	0
2	OMC	L2	1317	2	19,22,23	0.29	0	25,31,34	0.34	0
1	OMU	L1	1371	1	19,22,23	0.30	0	25,31,34	1.02	1 (4%)
2	OMC	L2	583	2	19,22,23	0.30	0	25,31,34	0.43	0
2	OMG	L2	686	2	23,26,27	0.31	0	32,38,41	0.50	0
1	OMG	L1	1540	1,90,2	23,26,27	0.32	0	32,38,41	0.33	0
51	OMG	S1	1550	51	23,26,27	0.33	0	32,38,41	0.43	0
1	OMG	L1	856	1	23,26,27	0.33	0	32,38,41	0.55	1 (3%)
1	OMU	L1	847	1	19,22,23	0.22	0	25,31,34	0.52	0
51	PSU	S1	1841	51	18,21,22	0.93	1 (5%)	21,30,33	0.68	0
1	OMU	L1	845	1	19,22,23	0.32	0	25,31,34	0.88	0
2	PSU	L2	1382	2,92	18,21,22	0.92	1 (5%)	21,30,33	0.73	0
2	OMC	L2	1248	2	19,22,23	0.30	0	25,31,34	0.50	0
51	PSU	S1	12	51	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
51	OMU	S1	1833	51	19,22,23	0.23	0	25,31,34	0.38	0
3	OMU	L3	13	3	19,22,23	0.25	0	25,31,34	0.52	0
7	A2M	L7	162	1,7	22,25,26	0.19	0	30,36,39	0.30	0
1	PSU	L1	774	1	18,21,22	0.92	1 (5%)	21,30,33	0.79	1 (4%)
2	OMG	L2	1360	2	23,26,27	0.33	0	32,38,41	0.38	0
51	PSU	S1	1566	51	18,21,22	0.92	1 (5%)	21,30,33	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PSU	L7	101	7	18,21,22	0.91	1 (5%)	21,30,33	0.79	1 (4%)
51	OMC	S1	2140	51	19,22,23	0.31	0	25,31,34	0.53	0
2	OMU	L2	1419	2	19,22,23	0.22	0	25,31,34	0.33	0
1	A2M	L1	697	1	22,25,26	0.20	0	30,36,39	0.46	0
1	PSU	L1	1533	1,2	18,21,22	0.92	1 (5%)	21,30,33	0.67	0
51	MA6	S1	2184	90,51	23,26,27	0.28	0	33,38,41	0.65	1 (3%)
1	OMC	L1	695	1	19,22,23	0.31	0	25,31,34	0.46	0
51	A2M	S1	98	92,51	22,25,26	0.20	0	30,36,39	0.47	0
2	OMU	L2	1077	2	19,22,23	0.22	0	25,31,34	0.42	0
2	A2M	L2	382	2	22,25,26	0.20	0	30,36,39	0.34	0
1	PSU	L1	510	1	18,21,22	0.95	1 (5%)	21,30,33	0.63	0
2	A2M	L2	1384	2,92	22,25,26	0.19	0	30,36,39	0.52	0
51	OMU	S1	1979	51	19,22,23	0.23	0	25,31,34	0.41	0
2	PSU	L2	510	2	18,21,22	0.92	1 (5%)	21,30,33	0.66	0
51	5MC	S1	1544	51	19,22,23	0.73	1 (5%)	26,32,35	0.49	0
51	OMG	S1	1865	51	23,26,27	0.31	0	32,38,41	0.50	0
4	OMG	L4	74	4	23,26,27	0.31	0	32,38,41	0.34	0
2	OMU	L2	560	91,2	19,22,23	0.23	0	25,31,34	1.03	1 (4%)
2	PSU	L2	1413	90,2	18,21,22	0.93	1 (5%)	21,30,33	0.75	1 (4%)
2	OMG	L2	641	2	23,26,27	0.30	0	32,38,41	0.58	0
1	OMG	L1	959	1	23,26,27	0.34	0	32,38,41	0.72	1 (3%)
1	A2M	L1	69	1	22,25,26	0.25	0	30,36,39	0.48	0
2	A2M	L2	628	2	22,25,26	0.20	0	30,36,39	0.39	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
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
51	OMC	S1	1866	51	-	0/9/27/28	0/2/2/2
51	OMU	S1	661	51	-	0/9/27/28	0/2/2/2
7	PSU	L7	74	90,7	-	0/7/25/26	0/2/2/2
1	A2M	L1	305	1	-	2/9/27/28	0/3/3/3
1	PSU	L1	1171	1	-	2/7/25/26	0/2/2/2
51	PSU	S1	1156	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	512	2	-	2/7/25/26	0/2/2/2
2	OMU	L2	73	2	-	0/9/27/28	0/2/2/2
2	OMG	L2	71	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	OMU	S1	1621	51	-	0/9/27/28	0/2/2/2
51	OMG	S1	1478	51	-	1/9/27/28	0/3/3/3
1	PSU	L1	1528	1	-	2/7/25/26	0/2/2/2
51	A2M	S1	2021	51	-	2/9/27/28	0/3/3/3
2	OMC	L2	14	1,2	-	0/9/27/28	0/2/2/2
2	PSU	L2	662	2,92	-	0/7/25/26	0/2/2/2
1	A2M	L1	678	1,2	-	4/9/27/28	0/3/3/3
2	A2M	L2	95	2	-	1/9/27/28	0/3/3/3
2	OMG	L2	655	2	-	1/9/27/28	0/3/3/3
1	PSU	L1	1177	1	-	2/7/25/26	0/2/2/2
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1246	51	-	0/7/25/26	0/2/2/2
7	OMG	L7	75	7	-	1/9/27/28	0/3/3/3
2	A2M	L2	1185	2	-	2/9/27/28	0/3/3/3
1	OMC	L1	1010	1,92	-	2/9/27/28	0/2/2/2
1	PSU	L1	1529	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	235	1	-	2/9/27/28	0/3/3/3
2	PSU	L2	437	2	-	0/7/25/26	0/2/2/2
51	OMC	S1	38	51	-	0/9/27/28	0/2/2/2
2	OMC	L2	443	91,90,2	-	4/9/27/28	0/2/2/2
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	1192	51	-	0/7/25/26	0/2/2/2
2	A2M	L2	572	2	-	0/9/27/28	0/3/3/3
2	5MC	L2	1308	2	-	4/7/25/26	0/2/2/2
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	502[A]	2,51	-	3/9/27/28	0/3/3/3
1	A2M	L1	927	1	-	0/9/27/28	0/3/3/3
2	PSU	L2	593	2	-	2/7/25/26	0/2/2/2
2	PSU	L2	1284	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1264	2	-	2/7/25/26	0/2/2/2
51	PSU	S1	2202	51	-	1/7/25/26	0/2/2/2
51	OMG	S1	600	51	-	1/9/27/28	0/3/3/3
2	A2M	L2	604	1,2	-	0/9/27/28	0/3/3/3
1	A2M	L1	955	1	-	1/9/27/28	0/3/3/3
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	858	1	-	3/9/27/28	0/3/3/3
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	681	1	-	3/9/27/28	0/3/3/3
7	A2M	L7	43	7	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	L2	524	2,92	-	1/7/25/26	0/2/2/2
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1318	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	1533	51	-	0/7/25/26	0/2/2/2
51	PSU	S1	2048	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1181	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	565	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1647	51	-	0/9/27/28	0/3/3/3
2	OMG	L2	1078	2	-	2/9/27/28	0/3/3/3
1	OMC	L1	1527	1	-	1/9/27/28	0/2/2/2
1	OMG	L1	1190	1	-	0/9/27/28	0/3/3/3
2	OMU	L2	1359	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	1372	2	-	0/9/27/28	0/3/3/3
2	A2M	L2	591	2	-	0/9/27/28	0/3/3/3
7	PSU	L7	69	92,7	-	0/7/25/26	0/2/2/2
1	OMG	L1	1524	1	-	3/9/27/28	0/3/3/3
2	OMG	L2	534	2	-	2/9/27/28	0/3/3/3
2	PSU	L2	1265	2	-	1/7/25/26	0/2/2/2
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
52	MIA	S2	37	52	-	4/15/33/34	0/3/3/3
2	PSU	L2	1144	2	-	2/7/25/26	0/2/2/2
2	OMG	L2	1229	2	-	2/9/27/28	0/3/3/3
51	MA6	S1	2185	90,51	-	4/11/29/30	0/3/3/3
51	PSU	S1	2046	51	-	0/7/25/26	0/2/2/2
51	PSU	S1	33	51	-	0/7/25/26	0/2/2/2
1	PSU	L1	1664	1	-	0/7/25/26	0/2/2/2
51	OMU	S1	29	51	-	1/9/27/28	0/2/2/2
2	A2M	L2	665	2	-	3/9/27/28	0/3/3/3
2	OMG	L2	1517	2	-	0/9/27/28	0/3/3/3
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
51	5MC	S1	2061	51	-	2/7/25/26	0/2/2/2
2	OMG	L2	1253	2	-	0/9/27/28	0/3/3/3
2	PSU	L2	1152	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	570	1,2	-	5/9/27/28	0/3/3/3
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
51	OMC	S1	18	51	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	OMU	S1	8	51	-	6/9/27/28	0/2/2/2
51	OMG	S1	2151	51	-	2/9/27/28	0/3/3/3
1	OMG	L1	1626	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
51	7MG	S1	1995	53,51	-	0/7/37/38	0/3/3/3
1	A2M	L1	1539	1,2,92	-	0/9/27/28	0/3/3/3
1	OMU	L1	1659	1,92	-	0/9/27/28	0/2/2/2
2	OMC	L2	359	2	-	2/9/27/28	0/2/2/2
1	PSU	L1	1017	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	407	1	-	0/9/27/28	0/3/3/3
1	1MA	L1	677	1	-	2/7/25/26	0/3/3/3
2	OMU	L2	667	2	-	1/9/27/28	0/2/2/2
2	A2M	L2	527	2	-	3/9/27/28	0/3/3/3
51	PSU	S1	455	51	-	1/7/25/26	0/2/2/2
1	PSU	L1	1011	1,2	-	0/7/25/26	0/2/2/2
2	OMG	L2	1231	2	-	0/9/27/28	0/3/3/3
51	A2M	S1	668	92,51	-	3/9/27/28	0/3/3/3
51	PSU	S1	1657	51	-	2/7/25/26	0/2/2/2
51	A2M	S1	479	51	-	0/9/27/28	0/3/3/3
1	OMU	L1	1107	1	-	1/9/27/28	0/2/2/2
51	OMG	S1	1829	92,51	-	2/9/27/28	0/3/3/3
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	802	2,92	-	2/7/25/26	0/2/2/2
51	B8N	S1	1543	-	-	6/16/34/35	0/2/2/2
1	OMU	L1	1039	1	-	0/9/27/28	0/2/2/2
51	A2M	S1	512	51	-	2/9/27/28	0/3/3/3
51	OMG	S1	1623	51	-	0/9/27/28	0/3/3/3
51	PSU	S1	1539	51	-	2/7/25/26	0/2/2/2
2	A2M	L2	502[B]	2	-	2/9/27/28	0/3/3/3
2	OMG	L2	1046	2,53	-	3/9/27/28	0/3/3/3
1	A2M	L1	1373	1	-	2/9/27/28	0/3/3/3
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
1	OMU	L1	1371	1	-	5/9/27/28	0/2/2/2
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
2	OMG	L2	686	2	-	2/9/27/28	0/3/3/3
1	OMG	L1	1540	1,90,2	-	2/9/27/28	0/3/3/3
51	OMG	S1	1550	51	-	0/9/27/28	0/3/3/3
1	OMG	L1	856	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
51	PSU	S1	1841	51	-	0/7/25/26	0/2/2/2
1	OMU	L1	845	1	-	4/9/27/28	0/2/2/2
2	PSU	L2	1382	2,92	-	0/7/25/26	0/2/2/2
2	OMC	L2	1248	2	-	1/9/27/28	0/2/2/2
51	PSU	S1	12	51	-	0/7/25/26	0/2/2/2
51	OMU	S1	1833	51	-	1/9/27/28	0/2/2/2
3	OMU	L3	13	3	-	1/9/27/28	0/2/2/2
7	A2M	L7	162	1,7	-	1/9/27/28	0/3/3/3
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
2	OMG	L2	1360	2	-	1/9/27/28	0/3/3/3
51	PSU	S1	1566	51	-	0/7/25/26	0/2/2/2
7	PSU	L7	101	7	-	0/7/25/26	0/2/2/2
51	OMC	S1	2140	51	-	0/9/27/28	0/2/2/2
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
1	A2M	L1	697	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	1533	1,2	-	0/7/25/26	0/2/2/2
51	MA6	S1	2184	90,51	-	3/11/29/30	0/3/3/3
1	OMC	L1	695	1	-	0/9/27/28	0/2/2/2
51	A2M	S1	98	92,51	-	2/9/27/28	0/3/3/3
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2
2	A2M	L2	382	2	-	0/9/27/28	0/3/3/3
1	PSU	L1	510	1	-	2/7/25/26	0/2/2/2
2	A2M	L2	1384	2,92	-	1/9/27/28	0/3/3/3
51	OMU	S1	1979	51	-	1/9/27/28	0/2/2/2
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
51	5MC	S1	1544	51	-	1/7/25/26	0/2/2/2
51	OMG	S1	1865	51	-	0/9/27/28	0/3/3/3
4	OMG	L4	74	4	-	2/9/27/28	0/3/3/3
2	OMU	L2	560	91,2	-	3/9/27/28	0/2/2/2
2	PSU	L2	1413	90,2	-	0/7/25/26	0/2/2/2
2	OMG	L2	641	2	-	0/9/27/28	0/3/3/3
1	OMG	L1	959	1	-	3/9/27/28	0/3/3/3
1	A2M	L1	69	1	-	0/9/27/28	0/3/3/3
2	A2M	L2	628	2	-	0/9/27/28	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1995	7MG	C5-N7	3.87	1.40	1.35
1	L1	510	PSU	C6-C5	3.69	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1171	PSU	C6-C5	3.64	1.39	1.35
51	S1	455	PSU	C6-C5	3.61	1.39	1.35
51	S1	2048	PSU	C6-C5	3.60	1.39	1.35
51	S1	33	PSU	C6-C5	3.60	1.39	1.35
51	S1	1841	PSU	C6-C5	3.59	1.39	1.35
1	L1	1177	PSU	C6-C5	3.59	1.39	1.35
51	S1	1156	PSU	C6-C5	3.58	1.39	1.35
51	S1	2046	PSU	C6-C5	3.58	1.39	1.35
2	L2	802	PSU	C6-C5	3.57	1.39	1.35
51	S1	1533	PSU	C6-C5	3.57	1.39	1.35
51	S1	1539	PSU	C6-C5	3.57	1.39	1.35
1	L1	239	PSU	C6-C5	3.56	1.39	1.35
51	S1	1566	PSU	C6-C5	3.56	1.39	1.35
2	L2	1265	PSU	C6-C5	3.55	1.39	1.35
1	L1	1533	PSU	C6-C5	3.55	1.39	1.35
2	L2	1413	PSU	C6-C5	3.55	1.39	1.35
2	L2	1060	PSU	C6-C5	3.55	1.39	1.35
2	L2	1382	PSU	C6-C5	3.55	1.39	1.35
2	L2	78	PSU	C6-C5	3.54	1.39	1.35
2	L2	1152	PSU	C6-C5	3.54	1.39	1.35
1	L1	1181	PSU	C6-C5	3.53	1.39	1.35
2	L2	597	PSU	C6-C5	3.53	1.39	1.35
2	L2	626	PSU	C6-C5	3.53	1.39	1.35
2	L2	593	PSU	C6-C5	3.53	1.39	1.35
7	L7	74	PSU	C6-C5	3.53	1.39	1.35
51	S1	2202	PSU	C6-C5	3.53	1.39	1.35
2	L2	662	PSU	C6-C5	3.52	1.39	1.35
2	L2	1058	PSU	C6-C5	3.52	1.39	1.35
2	L2	565	PSU	C6-C5	3.52	1.39	1.35
1	L1	1528	PSU	C6-C5	3.52	1.39	1.35
2	L2	1284	PSU	C6-C5	3.52	1.39	1.35
51	S1	12	PSU	C6-C5	3.51	1.39	1.35
1	L1	1664	PSU	C6-C5	3.51	1.39	1.35
2	L2	500	PSU	C6-C5	3.51	1.39	1.35
1	L1	1017	PSU	C6-C5	3.51	1.39	1.35
7	L7	69	PSU	C6-C5	3.51	1.39	1.35
1	L1	940	PSU	C6-C5	3.51	1.39	1.35
2	L2	1403	PSU	C6-C5	3.50	1.39	1.35
2	L2	1194	PSU	C6-C5	3.50	1.39	1.35
1	L1	774	PSU	C6-C5	3.49	1.39	1.35
2	L2	510	PSU	C6-C5	3.49	1.39	1.35
7	L7	101	PSU	C6-C5	3.49	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1529	PSU	C6-C5	3.49	1.39	1.35
51	S1	1246	PSU	C6-C5	3.49	1.39	1.35
51	S1	1657	PSU	C6-C5	3.49	1.39	1.35
2	L2	1264	PSU	C6-C5	3.48	1.39	1.35
1	L1	422	PSU	C6-C5	3.48	1.39	1.35
2	L2	512	PSU	C6-C5	3.47	1.39	1.35
2	L2	1303	PSU	C6-C5	3.47	1.39	1.35
51	S1	1192	PSU	C6-C5	3.47	1.39	1.35
1	L1	1011	PSU	C6-C5	3.46	1.39	1.35
2	L2	1318	PSU	C6-C5	3.46	1.39	1.35
2	L2	472	PSU	C6-C5	3.45	1.39	1.35
2	L2	1213	PSU	C6-C5	3.43	1.39	1.35
2	L2	437	PSU	C6-C5	3.42	1.39	1.35
2	L2	1144	PSU	C6-C5	3.38	1.39	1.35
2	L2	524	5MC	C5-C4	-3.28	1.41	1.44
51	S1	2061	5MC	C5-C4	-3.04	1.41	1.44
2	L2	1308	5MC	C5-C4	-2.95	1.41	1.44
51	S1	1544	5MC	C5-C4	-2.90	1.41	1.44
51	S1	1543	B8N	C4-C5	-2.79	1.41	1.47
51	S1	1543	B8N	C6-C5	2.79	1.39	1.35
52	S2	37	MIA	C2-S10	2.07	1.77	1.75

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	37	MIA	C11-S10-C2	22.55	119.17	102.25
2	L2	560	OMU	O3'-C3'-C4'	3.41	120.86	111.08
51	S1	2185	MA6	C2-N1-C6	2.79	118.65	111.83
1	L1	959	OMG	O2'-C2'-C1'	2.73	114.17	108.99
51	S1	2184	MA6	C2-N1-C6	2.72	118.49	111.83
1	L1	1524	OMG	O2'-C2'-C1'	2.71	114.13	108.99
2	L2	1060	PSU	C2'-C3'-C4'	-2.59	97.60	102.61
2	L2	502[A]	A2M	O3'-C3'-C2'	2.35	117.78	111.19
2	L2	78	PSU	C2'-C3'-C4'	-2.30	98.16	102.61
2	L2	502[A]	A2M	O2'-C2'-C1'	2.29	113.34	108.99
1	L1	1011	PSU	C3'-C2'-C1'	2.26	104.36	101.69
7	L7	101	PSU	C3'-C2'-C1'	2.24	104.33	101.69
51	S1	1995	7MG	C4-C5-N7	2.24	108.03	105.38
1	L1	305	A2M	O2'-C2'-C1'	2.22	113.20	108.99
1	L1	1181	PSU	C2'-C3'-C4'	-2.14	98.48	102.61
51	S1	1543	B8N	C1'-C5-C4	2.13	120.84	117.61
2	L2	1264	PSU	C3'-C2'-C1'	2.13	104.20	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1371	OMU	C1'-N1-C2	2.07	121.31	117.59
2	L2	502[B]	A2M	O3'-C3'-C2'	2.06	116.94	111.19
2	L2	1372	A2M	C2'-C1'-N9	-2.05	110.37	113.75
1	L1	774	PSU	C2'-C3'-C4'	-2.05	98.65	102.61
1	L1	856	OMG	C2'-C1'-N9	-2.02	110.40	114.24
2	L2	1078	OMG	C3'-C2'-C1'	-2.02	98.94	102.81
2	L2	1413	PSU	C2'-C3'-C4'	-2.02	98.71	102.61
1	L1	305	A2M	C3'-C2'-C1'	-2.01	98.95	102.81
2	L2	1308	5MC	C5-C6-N1	-2.01	121.13	123.31
1	L1	940	PSU	C2'-C3'-C4'	-2.00	98.74	102.61

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L7	75	OMG	C1'-C2'-O2'-CM2
7	L7	162	A2M	C1'-C2'-O2'-CM'
1	L1	235	A2M	O4'-C4'-C5'-O5'
1	L1	510	PSU	C2'-C1'-C5-C4
1	L1	678	A2M	O4'-C4'-C5'-O5'
1	L1	678	A2M	C1'-C2'-O2'-CM'
1	L1	681	A2M	O4'-C4'-C5'-O5'
1	L1	845	OMU	O4'-C1'-N1-C2
1	L1	845	OMU	O4'-C1'-N1-C6
1	L1	845	OMU	C1'-C2'-O2'-CM2
1	L1	955	A2M	C1'-C2'-O2'-CM'
1	L1	959	OMG	C1'-C2'-O2'-CM2
1	L1	1010	OMC	O4'-C4'-C5'-O5'
1	L1	1371	OMU	O4'-C1'-N1-C2
1	L1	1371	OMU	O4'-C1'-N1-C6
1	L1	1371	OMU	C1'-C2'-O2'-CM2
1	L1	1524	OMG	C1'-C2'-O2'-CM2
1	L1	1540	OMG	O4'-C4'-C5'-O5'
2	L2	95	A2M	C1'-C2'-O2'-CM'
2	L2	443	OMC	C2'-C1'-N1-C6
2	L2	527	A2M	O4'-C4'-C5'-O5'
2	L2	534	OMG	O4'-C4'-C5'-O5'
2	L2	686	OMG	O4'-C4'-C5'-O5'
2	L2	1046	OMG	O4'-C4'-C5'-O5'
2	L2	1046	OMG	C1'-C2'-O2'-CM2
2	L2	1185	A2M	C1'-C2'-O2'-CM'
2	L2	1229	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L2	1265	PSU	O4'-C1'-C5-C6
2	L2	1384	A2M	C1'-C2'-O2'-CM'
51	S1	29	OMU	C1'-C2'-O2'-CM2
51	S1	668	A2M	O4'-C4'-C5'-O5'
51	S1	668	A2M	C3'-C4'-C5'-O5'
51	S1	1543	B8N	O4'-C4'-C5'-O5'
51	S1	1657	PSU	O4'-C1'-C5-C6
51	S1	1829	OMG	C1'-C2'-O2'-CM2
51	S1	1979	OMU	C1'-C2'-O2'-CM2
51	S1	2021	A2M	C1'-C2'-O2'-CM'
51	S1	2184	MA6	C5-C6-N6-C10
51	S1	2185	MA6	C5-C6-N6-C10
51	S1	2202	PSU	O4'-C1'-C5-C6
52	S2	37	MIA	O4'-C4'-C5'-O5'
52	S2	37	MIA	C3'-C4'-C5'-O5'
52	S2	37	MIA	N1-C2-S10-C11
52	S2	37	MIA	N3-C2-S10-C11
51	S1	1543	B8N	N34-C33-C34-O36
2	L2	443	OMC	C2'-C1'-N1-C2
1	L1	235	A2M	C3'-C4'-C5'-O5'
1	L1	678	A2M	C3'-C4'-C5'-O5'
1	L1	681	A2M	C3'-C4'-C5'-O5'
1	L1	1171	PSU	C3'-C4'-C5'-O5'
1	L1	1540	OMG	C3'-C4'-C5'-O5'
2	L2	534	OMG	C3'-C4'-C5'-O5'
2	L2	802	PSU	C3'-C4'-C5'-O5'
2	L2	802	PSU	O4'-C4'-C5'-O5'
2	L2	1229	OMG	C3'-C4'-C5'-O5'
51	S1	8	OMU	C3'-C4'-C5'-O5'
51	S1	512	A2M	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C3'-C4'-C5'-O5'
1	L1	305	A2M	O4'-C4'-C5'-O5'
1	L1	305	A2M	C3'-C4'-C5'-O5'
1	L1	1017	PSU	C3'-C4'-C5'-O5'
1	L1	1171	PSU	O4'-C4'-C5'-O5'
1	L1	1371	OMU	C3'-C4'-C5'-O5'
1	L1	1371	OMU	O4'-C4'-C5'-O5'
2	L2	502[A]	A2M	O4'-C4'-C5'-O5'
2	L2	502[A]	A2M	C3'-C4'-C5'-O5'
2	L2	527	A2M	C3'-C4'-C5'-O5'
2	L2	665	A2M	C3'-C4'-C5'-O5'
2	L2	686	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L2	1144	PSU	O4'-C4'-C5'-O5'
2	L2	1264	PSU	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C4'-C5'-O5'
51	S1	98	A2M	O4'-C4'-C5'-O5'
51	S1	1539	PSU	O4'-C4'-C5'-O5'
51	S1	2184	MA6	N1-C6-N6-C10
51	S1	2185	MA6	N1-C6-N6-C10
2	L2	1308	5MC	C2'-C1'-N1-C6
51	S1	8	OMU	C2'-C1'-N1-C6
1	L1	1010	OMC	C3'-C4'-C5'-O5'
2	L2	512	PSU	C3'-C4'-C5'-O5'
1	L1	1017	PSU	O4'-C4'-C5'-O5'
2	L2	502[B]	A2M	O4'-C4'-C5'-O5'
2	L2	502[B]	A2M	C3'-C4'-C5'-O5'
2	L2	570	A2M	O4'-C4'-C5'-O5'
2	L2	570	A2M	C3'-C4'-C5'-O5'
2	L2	665	A2M	O4'-C4'-C5'-O5'
2	L2	1046	OMG	C3'-C4'-C5'-O5'
2	L2	1144	PSU	C3'-C4'-C5'-O5'
4	L4	74	OMG	C3'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C2
51	S1	8	OMU	C2'-C1'-N1-C2
1	L1	1524	OMG	O4'-C4'-C5'-O5'
1	L1	1528	PSU	O4'-C4'-C5'-O5'
2	L2	512	PSU	O4'-C4'-C5'-O5'
2	L2	593	PSU	C3'-C4'-C5'-O5'
2	L2	1078	OMG	O4'-C4'-C5'-O5'
51	S1	512	A2M	C3'-C4'-C5'-O5'
51	S1	2184	MA6	C5-C6-N6-C9
51	S1	2185	MA6	C5-C6-N6-C9
2	L2	560	OMU	C3'-C4'-C5'-O5'
2	L2	1078	OMG	C3'-C4'-C5'-O5'
2	L2	1264	PSU	C3'-C4'-C5'-O5'
51	S1	1539	PSU	C3'-C4'-C5'-O5'
1	L1	1373	A2M	O4'-C4'-C5'-O5'
1	L1	1524	OMG	C3'-C4'-C5'-O5'
51	S1	98	A2M	C3'-C4'-C5'-O5'
2	L2	667	OMU	C1'-C2'-O2'-CM2
1	L1	1177	PSU	C3'-C4'-C5'-O5'
1	L1	1373	A2M	C3'-C4'-C5'-O5'
51	S1	2061	5MC	C3'-C4'-C5'-O5'
2	L2	359	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	L4	74	OMG	O4'-C4'-C5'-O5'
51	S1	2151	OMG	C3'-C4'-C5'-O5'
2	L2	570	A2M	C2'-C1'-N9-C8
51	S1	8	OMU	O4'-C1'-N1-C6
51	S1	1543	B8N	N3-C31-C32-C33
2	L2	1308	5MC	O4'-C1'-N1-C2
1	L1	959	OMG	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C4'-C5'-O5'-P
51	S1	2061	5MC	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C1'-N1-C2
2	L2	1308	5MC	O4'-C1'-N1-C6
2	L2	655	OMG	C3'-C2'-O2'-CM2
1	L1	681	A2M	C4'-C5'-O5'-P
2	L2	560	OMU	C4'-C5'-O5'-P
51	S1	1833	OMU	C4'-C5'-O5'-P
1	L1	510	PSU	O4'-C1'-C5-C4
51	S1	1657	PSU	O4'-C1'-C5-C4
1	L1	1528	PSU	C3'-C4'-C5'-O5'
51	S1	2185	MA6	C4'-C5'-O5'-P
2	L2	443	OMC	O4'-C1'-N1-C6
2	L2	1248	OMC	C4'-C5'-O5'-P
2	L2	359	OMC	O4'-C4'-C5'-O5'
1	L1	858	A2M	O4'-C1'-N9-C8
1	L1	1107	OMU	C3'-C2'-O2'-CM2
51	S1	1478	OMG	C4'-C5'-O5'-P
51	S1	600	OMG	O4'-C4'-C5'-O5'
2	L2	443	OMC	O4'-C1'-N1-C2
1	L1	677	1MA	C2'-C1'-N9-C4
2	L2	502[A]	A2M	C4'-C5'-O5'-P
2	L2	560	OMU	O4'-C4'-C5'-O5'
51	S1	1544	5MC	O4'-C4'-C5'-O5'
2	L2	570	A2M	C2'-C1'-N9-C4
51	S1	668	A2M	C2'-C1'-N9-C8
1	L1	677	1MA	C2'-C1'-N9-C8
2	L2	665	A2M	C1'-C2'-O2'-CM'
51	S1	18	OMC	C1'-C2'-O2'-CM2
1	L1	678	A2M	C4'-C5'-O5'-P
51	S1	1829	OMG	C4'-C5'-O5'-P
1	L1	858	A2M	C3'-C4'-C5'-O5'
1	L1	858	A2M	O4'-C1'-N9-C4
1	L1	1527	OMC	C3'-C2'-O2'-CM2
2	L2	1360	OMG	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
51	S1	2021	A2M	C3'-C2'-O2'-CM'
1	L1	1177	PSU	C4'-C5'-O5'-P
1	L1	959	OMG	C3'-C4'-C5'-O5'
2	L2	570	A2M	O4'-C1'-N9-C8
51	S1	2151	OMG	O4'-C4'-C5'-O5'
3	L3	13	OMU	C4'-C5'-O5'-P
2	L2	1185	A2M	C4'-C5'-O5'-P
51	S1	455	PSU	C4'-C5'-O5'-P
2	L2	527	A2M	C2'-C1'-N9-C8
2	L2	524	5MC	O4'-C4'-C5'-O5'
2	L2	593	PSU	O4'-C4'-C5'-O5'
51	S1	1543	B8N	N34-C33-C34-O35
1	L1	845	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L2	1397	OMC	1	0
51	S1	661	OMU	1	0
2	L2	512	PSU	2	0
2	L2	73	OMU	1	0
51	S1	2021	A2M	1	0
2	L2	95	A2M	1	0
2	L2	655	OMG	1	0
7	L7	75	OMG	1	0
2	L2	1185	A2M	2	0
1	L1	235	A2M	2	0
2	L2	1060	PSU	1	0
2	L2	1308	5MC	1	0
2	L2	502[A]	A2M	6	0
51	S1	2202	PSU	1	0
1	L1	955	A2M	1	0
7	L7	43	A2M	1	0
2	L2	1213	PSU	1	0
2	L2	1318	PSU	1	0
2	L2	1303	PSU	1	0
1	L1	1527	OMC	1	0
2	L2	591	A2M	3	0
52	S2	37	MIA	2	0
2	L2	665	A2M	2	0
51	S1	2061	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L2	1253	OMG	1	0
51	S1	2151	OMG	1	0
1	L1	1626	OMG	1	0
51	S1	1995	7MG	1	0
1	L1	1539	A2M	1	0
2	L2	667	OMU	1	0
51	S1	479	A2M	1	0
51	S1	1829	OMG	1	0
51	S1	1539	PSU	1	0
1	L1	1373	A2M	1	0
1	L1	1371	OMU	2	0
51	S1	1550	OMG	1	0
1	L1	845	OMU	3	0
51	S1	12	PSU	1	0
7	L7	162	A2M	1	0
1	L1	697	A2M	1	0
1	L1	1533	PSU	1	0
51	S1	2184	MA6	1	0
1	L1	695	OMC	1	0
2	L2	382	A2M	1	0
2	L2	1384	A2M	1	0
2	L2	1413	PSU	1	0
1	L1	959	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 299 ligands modelled in this entry, 299 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
51	S1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	1543:B8N	O3'	1544:5MC	P	3.91
1	S1	1542:C	O3'	1543:B8N	P	3.22

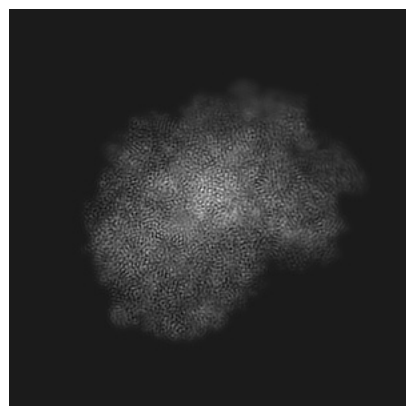
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19582. These allow visual inspection of the internal detail of the map and identification of artifacts.

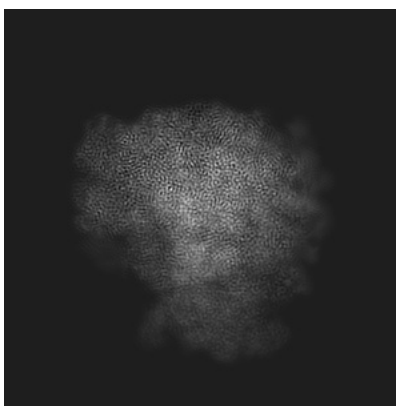
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

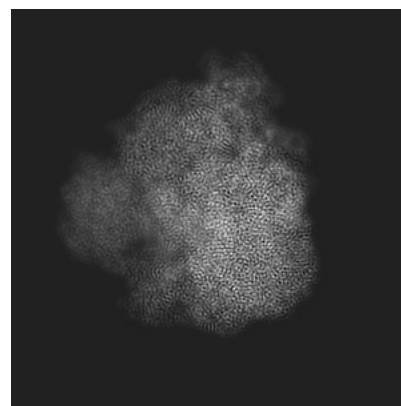
6.1.1 Primary map



X

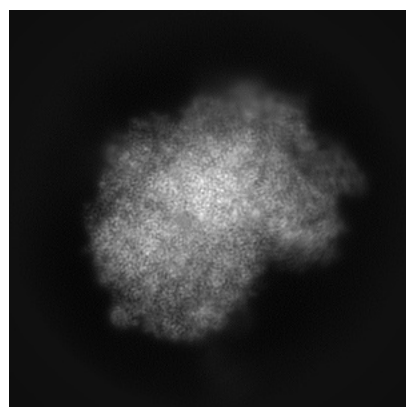


Y

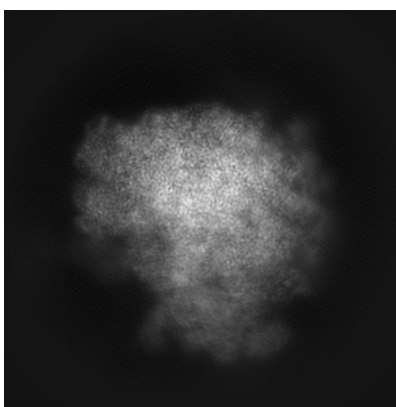


Z

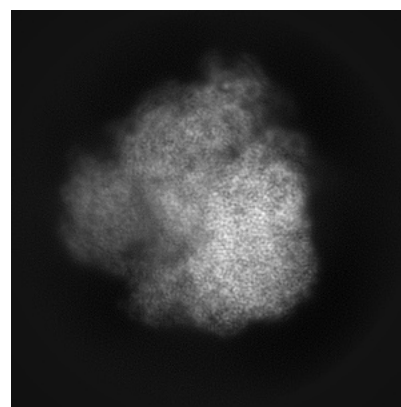
6.1.2 Raw map



X



Y

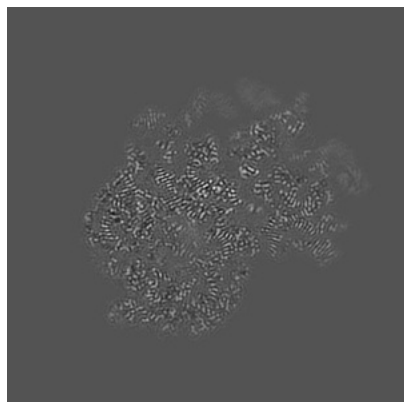


Z

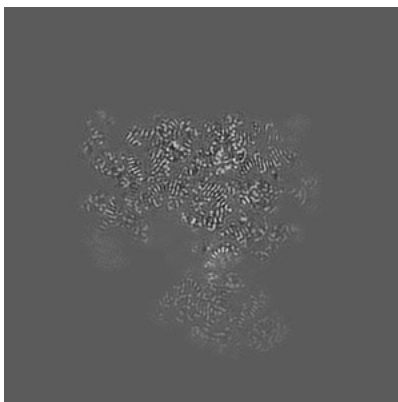
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

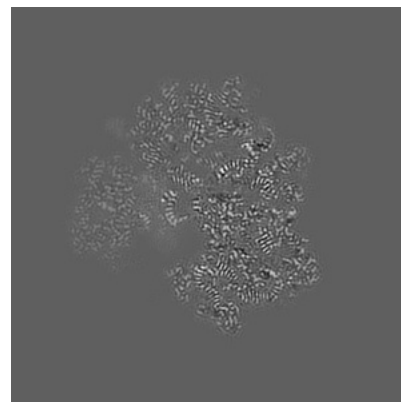
6.2.1 Primary map



X Index: 240

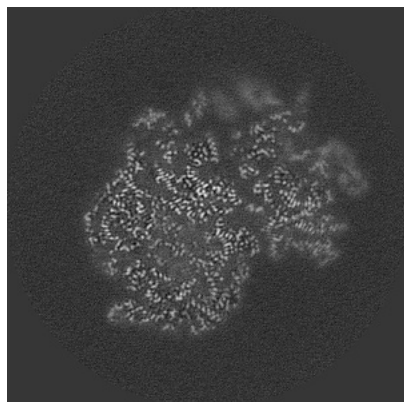


Y Index: 240

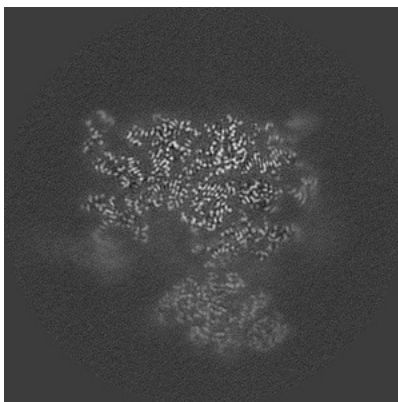


Z Index: 240

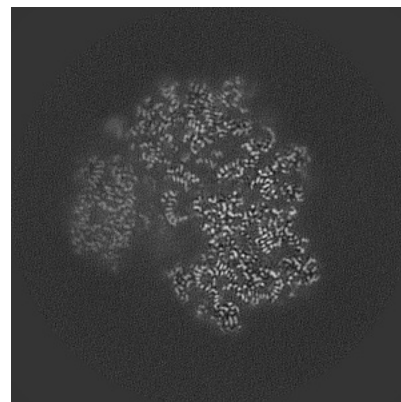
6.2.2 Raw map



X Index: 240



Y Index: 240

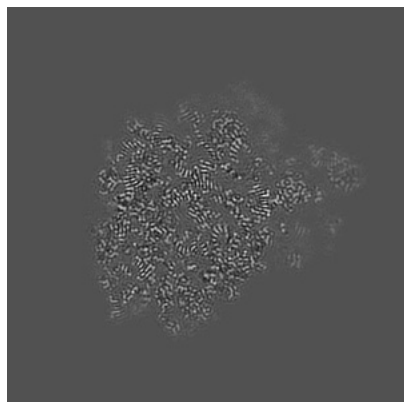


Z Index: 240

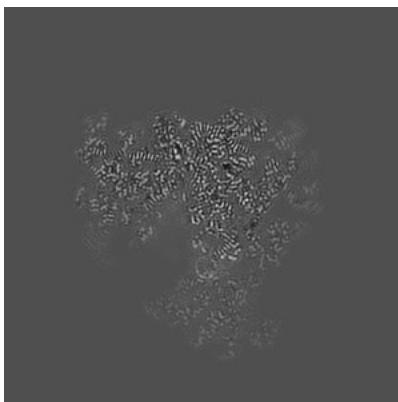
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

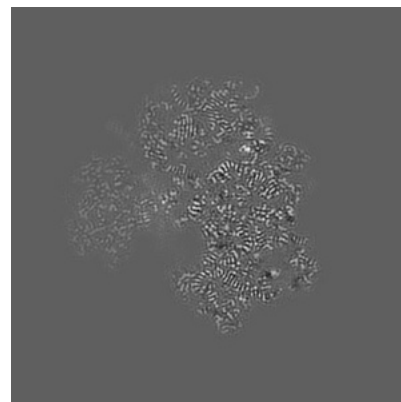
6.3.1 Primary map



X Index: 286

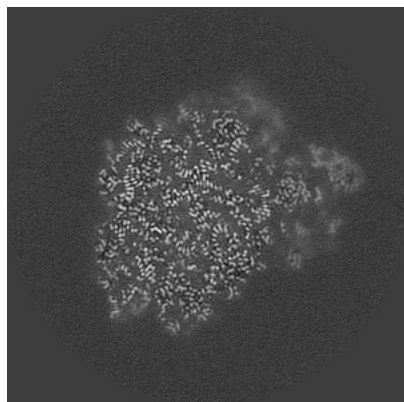


Y Index: 230

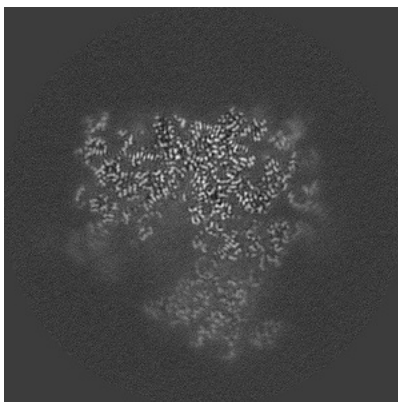


Z Index: 245

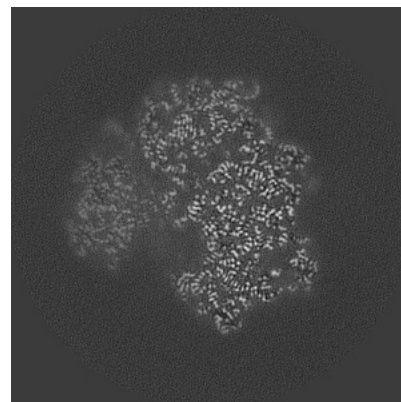
6.3.2 Raw map



X Index: 286



Y Index: 230

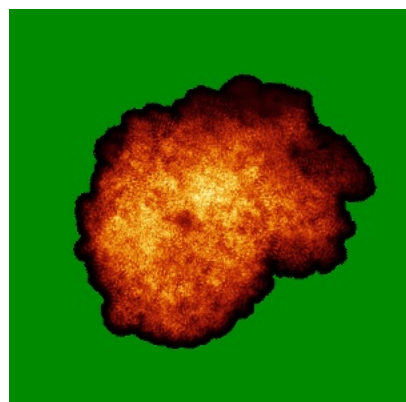


Z Index: 245

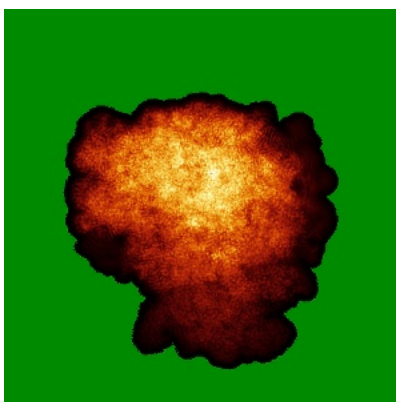
The images above show the largest variance slices of the map in three orthogonal directions.

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

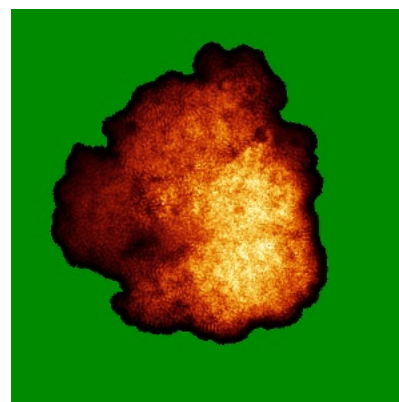
6.4.1 Primary map



X

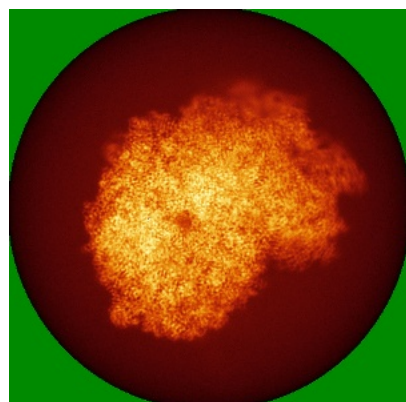


Y

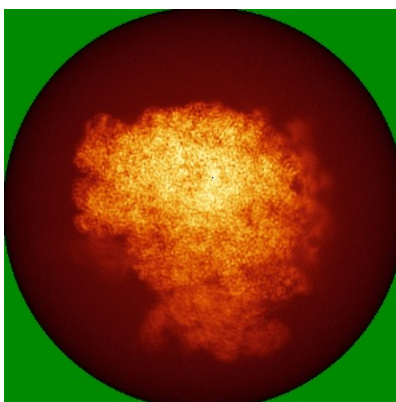


Z

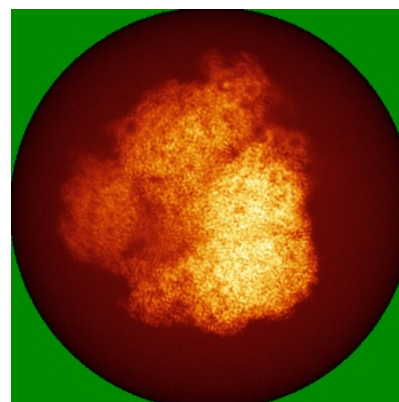
6.4.2 Raw map



X



Y

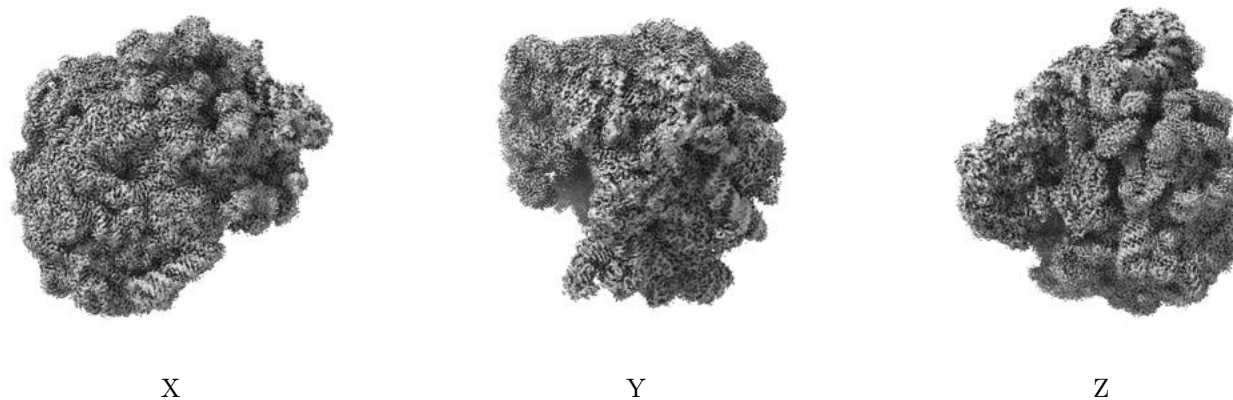


Z

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.

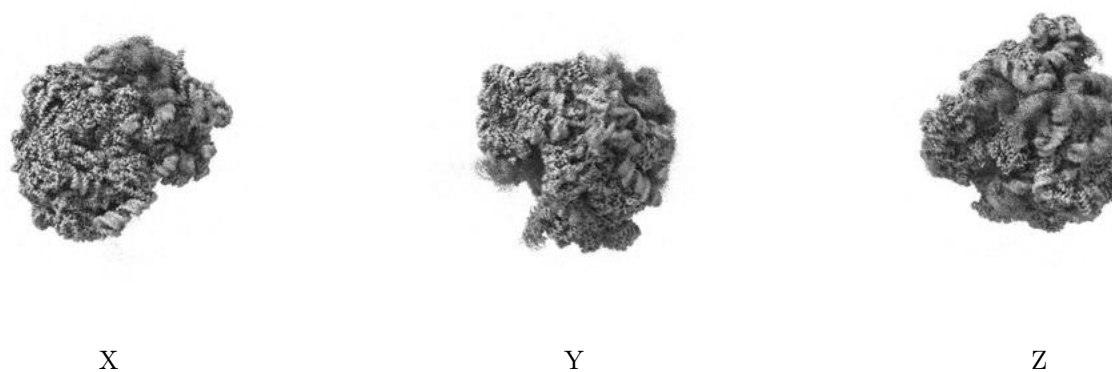
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

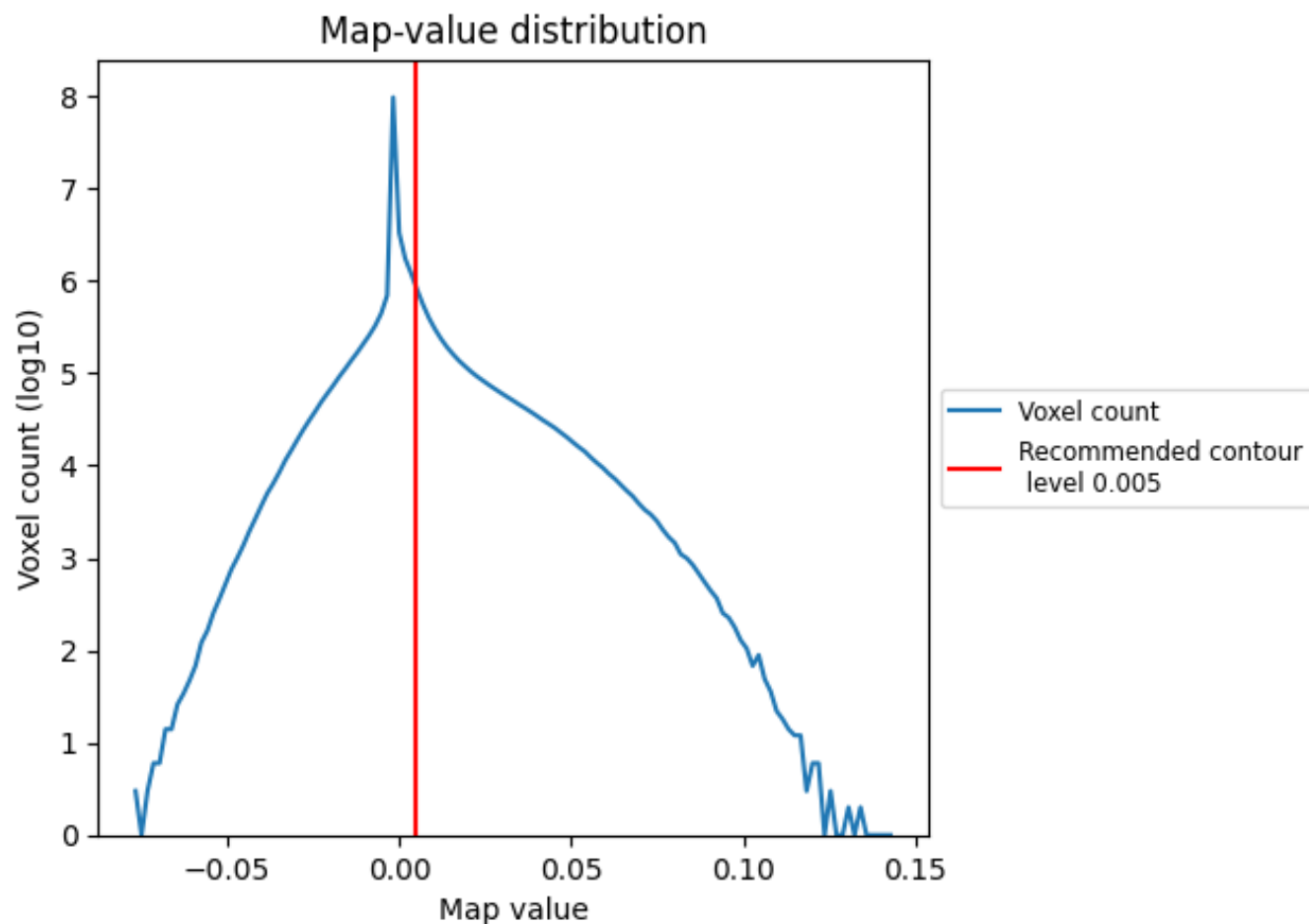
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

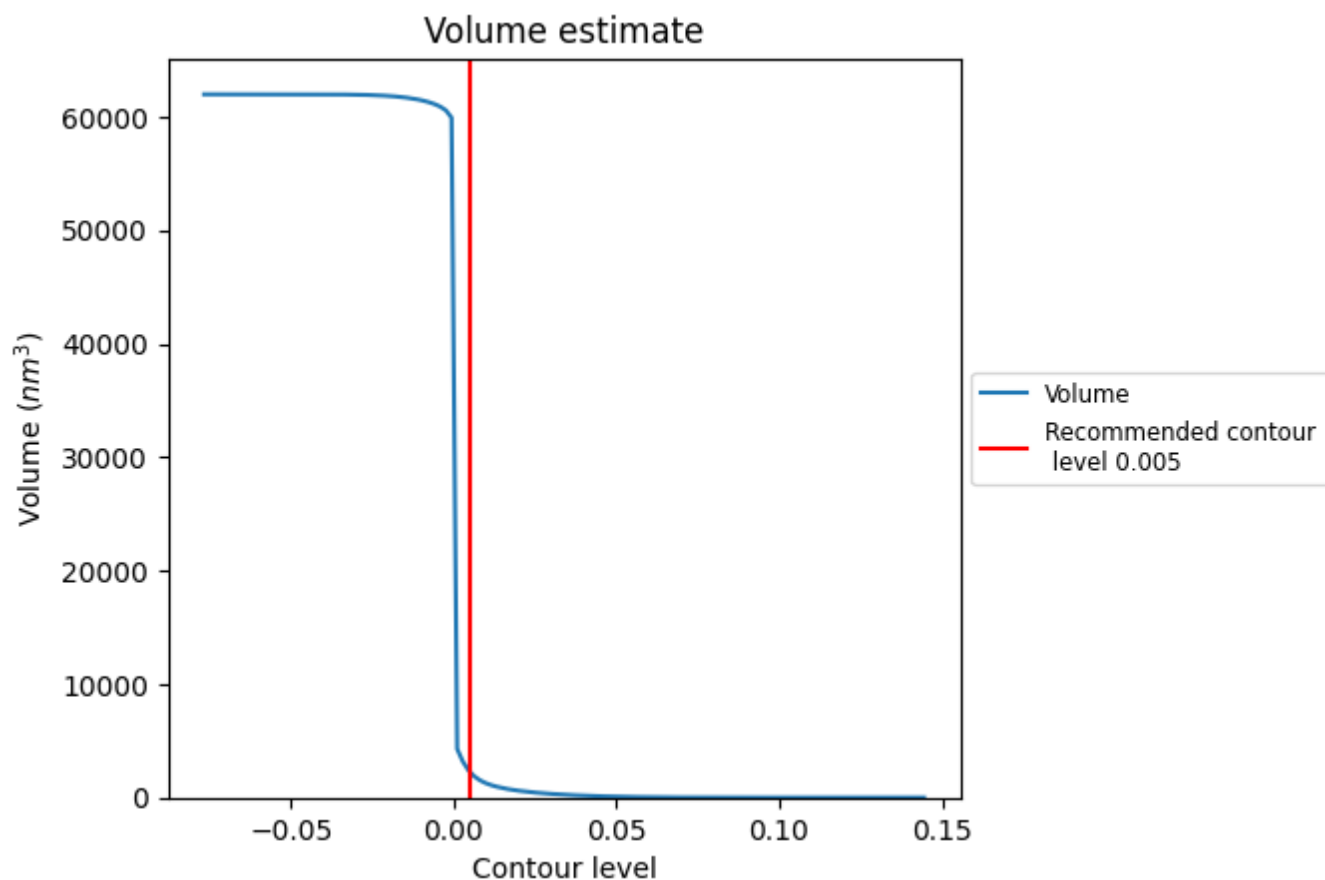
This section contains the results of statistical analysis of the map.

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.

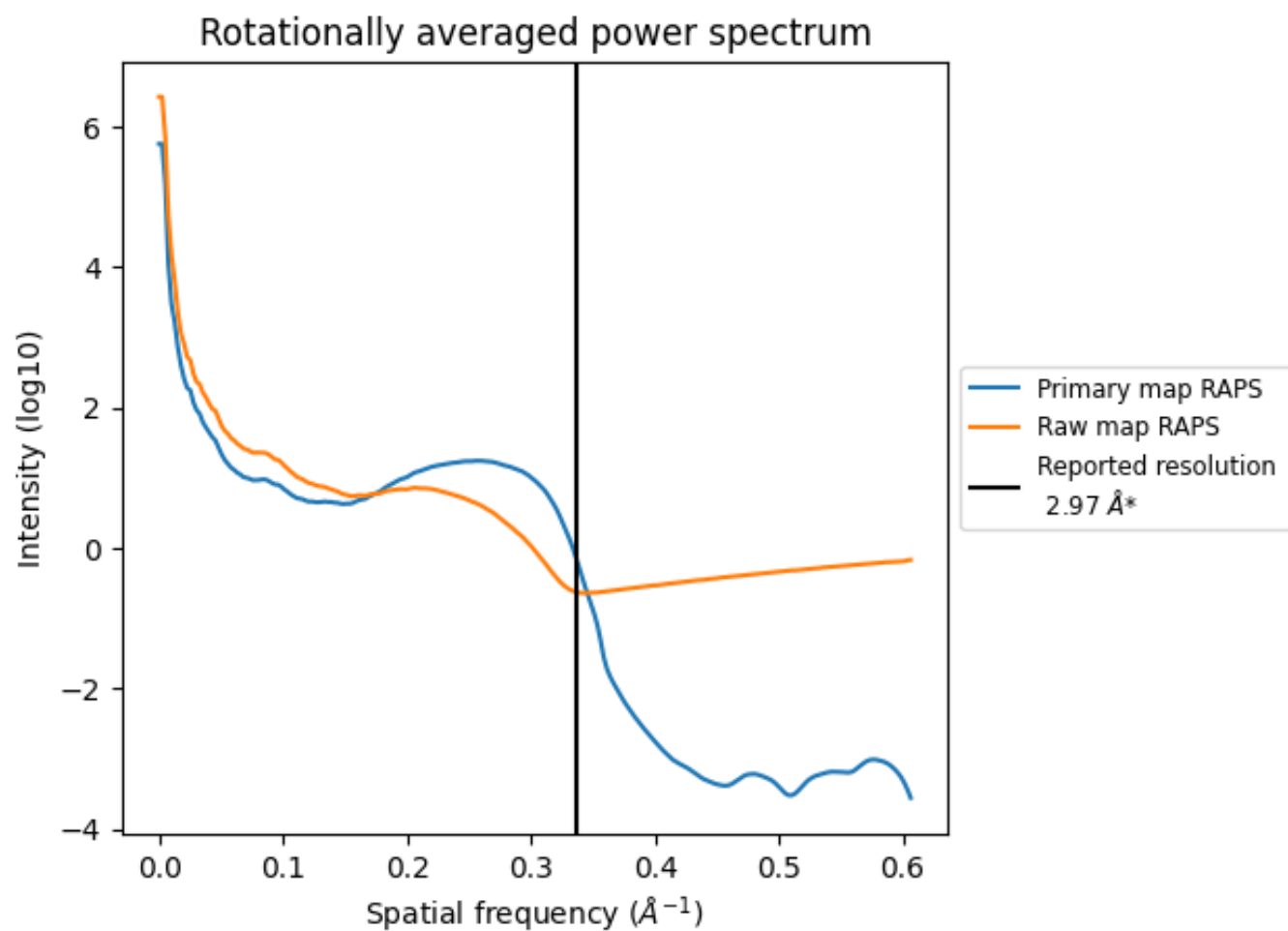
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2282 nm³; this corresponds to an approximate mass of 2062 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

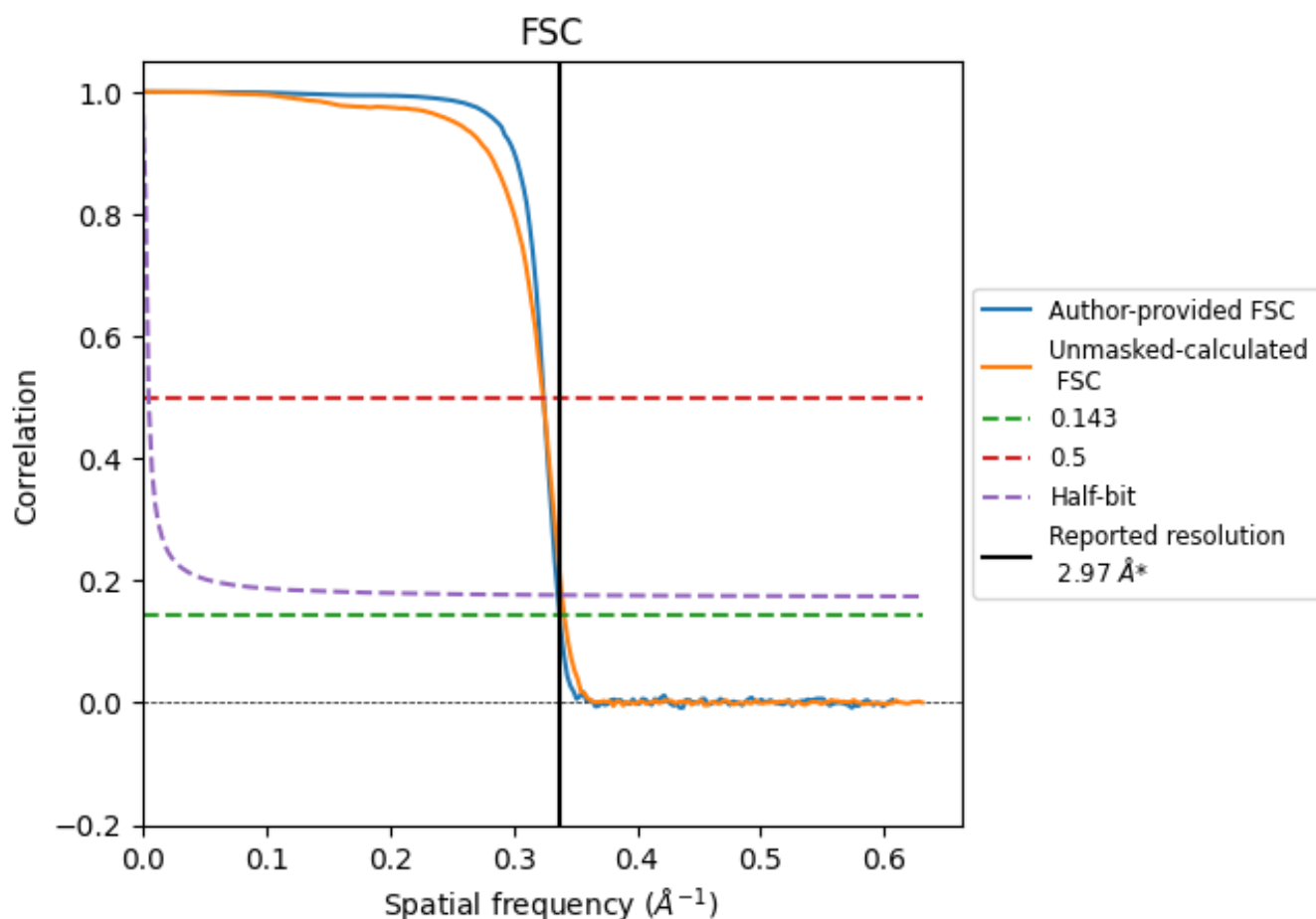


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

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 0.337 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

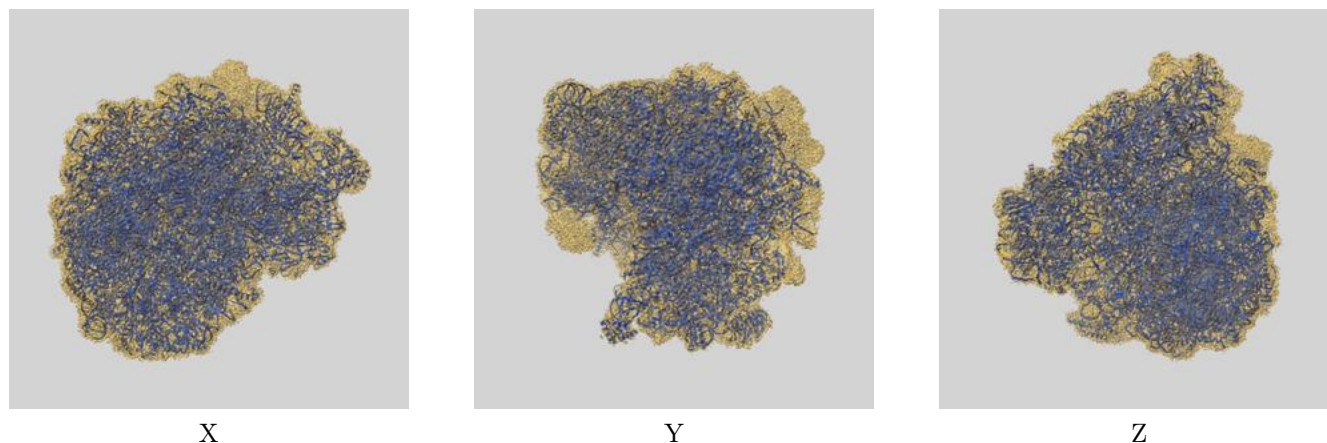
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.96	3.08	2.98
Unmasked-calculated*	2.93	3.09	2.95

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

9 Map-model fit [i](#)

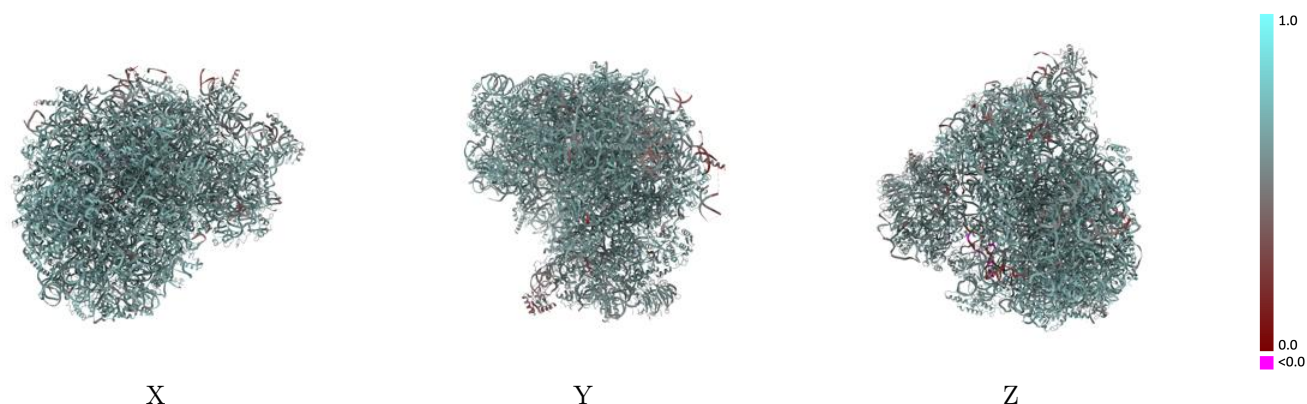
This section contains information regarding the fit between EMDB map EMD-19582 and PDB model 8RXX. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



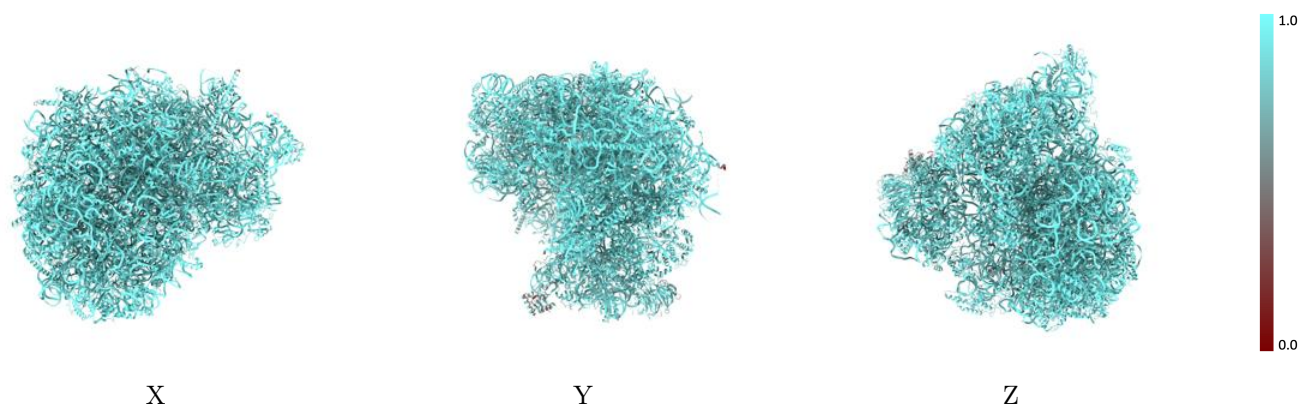
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



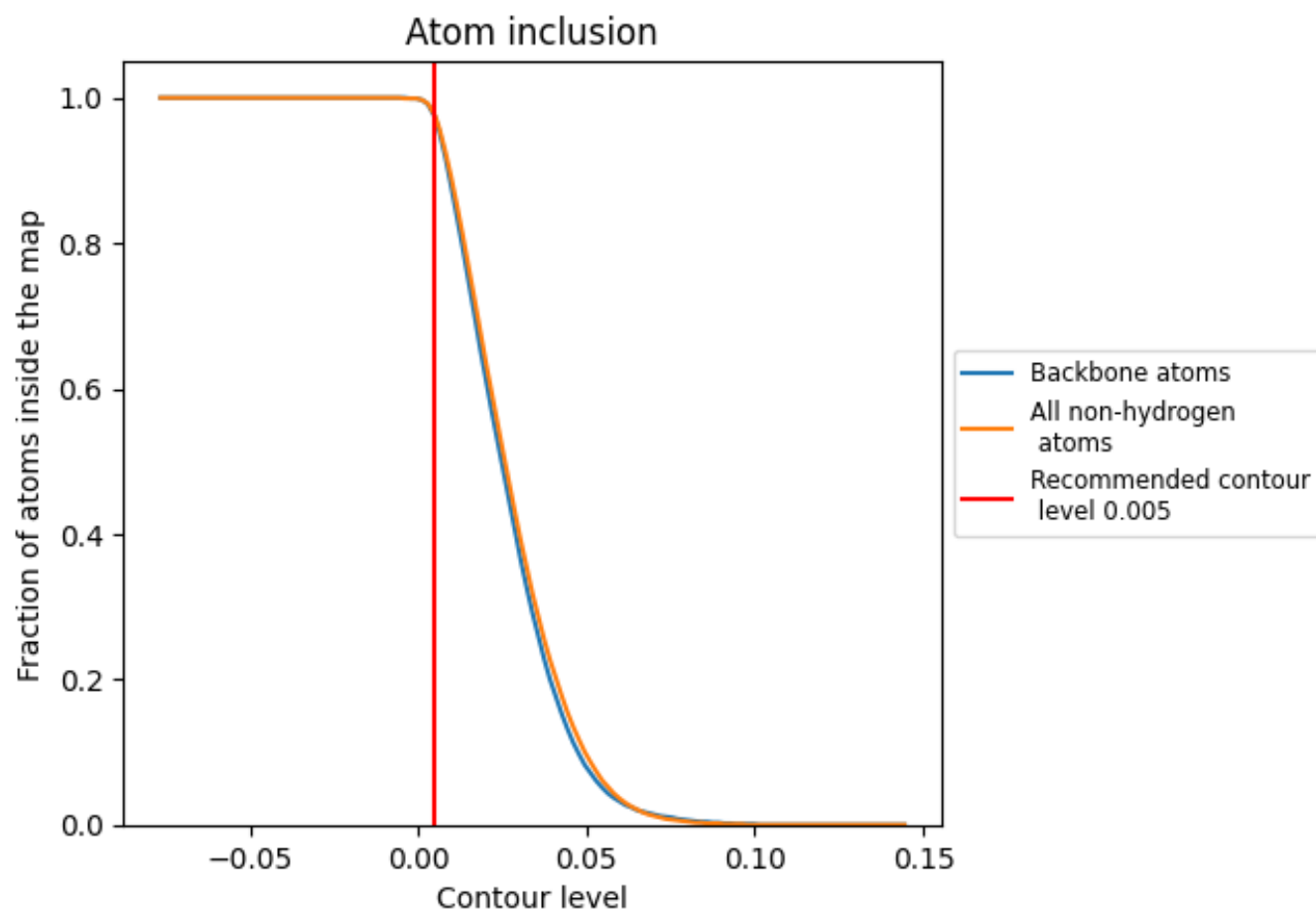
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6010
L1	 0.9900	 0.6160
L2	 0.9860	 0.6050
L3	 0.9830	 0.6020
L4	 0.9940	 0.6220
L5	 0.9820	 0.6000
L6	 0.9780	 0.5990
L7	 0.9900	 0.6210
L8	 0.9950	 0.6100
LA	 0.9940	 0.6460
LB	 0.9910	 0.6410
LC	 0.9910	 0.6370
LD	 0.9760	 0.5850
LE	 0.9810	 0.6230
LF	 0.9760	 0.6200
LG	 0.9710	 0.6130
LH	 0.9880	 0.6360
LI	 0.9870	 0.6360
LJ	 0.9930	 0.6370
LK	 0.9860	 0.6210
LL	 0.9890	 0.6450
LM	 0.9950	 0.6450
LN	 0.9650	 0.6080
LO	 0.9740	 0.6110
LP	 0.9950	 0.6380
LQ	 0.9780	 0.6010
LR	 0.9890	 0.6360
LS	 0.9910	 0.6280
LT	 0.9960	 0.6440
LU	 0.9790	 0.6120
LV	 0.9860	 0.6370
LW	 0.9910	 0.6410
LX	 0.9740	 0.6200
LY	 0.9780	 0.6200
LZ	 0.9900	 0.6370



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Chain	Atom inclusion	Q-score
La	 0.9870	 0.6300
Lb	 0.9810	 0.6270
Lc	 0.9880	 0.6380
Ld	 0.9810	 0.6110
Le	 0.9780	 0.6260
Lf	 0.9910	 0.6360
Lg	 0.9940	 0.6480
Lh	 0.9710	 0.6140
Li	 0.9600	 0.6060
Lj	 0.9920	 0.6440
Lk	 0.9810	 0.6310
Ll	 0.9930	 0.6460
Lm	 0.9820	 0.6220
Ln	 0.9930	 0.6020
Lo	 0.9930	 0.6290
Lp	 0.9920	 0.6370
S1	 0.9780	 0.5780
S2	 0.9390	 0.3690
S3	 0.9900	 0.4260
S4	 0.8410	 0.2800
S5	 1.0000	 0.5370
SA	 0.9570	 0.6080
SB	 0.9720	 0.6000
SC	 0.8880	 0.5730
SD	 0.9630	 0.6020
SE	 0.9810	 0.6170
SF	 0.9770	 0.6140
SG	 0.9670	 0.5930
SH	 0.9320	 0.5810
SI	 0.9820	 0.6100
SJ	 0.9870	 0.6230
SK	 0.9920	 0.6190
SL	 0.9600	 0.5890
SM	 0.8980	 0.5670
SN	 0.8740	 0.5500
SO	 0.9680	 0.6110
SP	 0.9770	 0.6090
SQ	 0.5140	 0.3640
SR	 0.8760	 0.5510
SS	 0.9450	 0.5940
ST	 0.9810	 0.6140
SU	 0.9930	 0.6310

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Chain	Atom inclusion	Q-score
SV	 0.9300	 0.5740
SW	 0.8330	 0.5420
SX	 0.9560	 0.5760
SY	 0.9660	 0.5940
SZ	 0.9710	 0.6020
Sa	 0.8930	 0.5580
Sb	 0.9750	 0.6120
Sc	 0.9800	 0.6050
Sd	 0.9070	 0.5710
Se	 0.9070	 0.5600
Sf	 0.7700	 0.4760
Sg	 0.8350	 0.5300
Sh	 0.9290	 0.5350