



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 09:38 PM EDT

PDB ID : 9PKD / pdb_00009pkd
EMDB ID : EMD-71694
Title : In situ CHX and HHT treated 80S consensus ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-07-14
Resolution : 2.42 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:

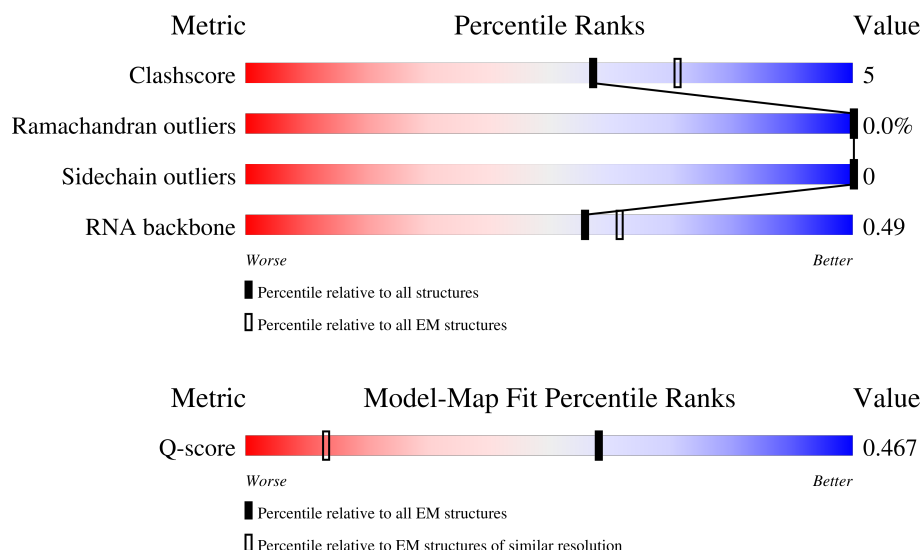
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.42 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	5729 (1.92 - 2.92)

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

Mol	Chain	Length	Quality of chain
1	CI	31	 100%
2	L5	3655	 64% 31%
3	L7	120	 84% 14%

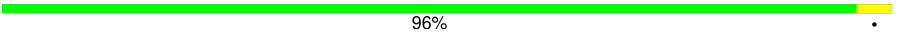
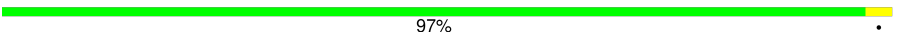
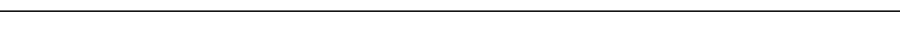
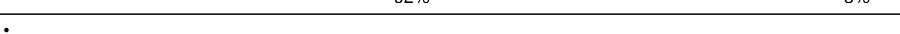
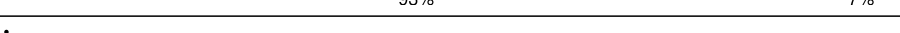
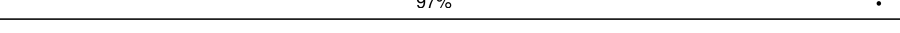
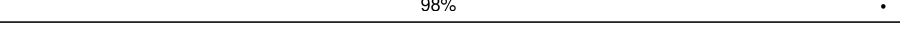
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Mol	Chain	Length	Quality of chain
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	
9	LE	250	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LW	124	
27	LX	120	
28	LY	134	

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Mol	Chain	Length	Quality of chain
29	LZ	135	 96%
30	La	147	 97%
31	Lb	121	 81% 9% 10%
32	Lc	98	 85% 15%
33	Ld	107	 84% 16%
34	Le	128	 91% 9%
35	Lf	109	 91% 9%
36	Lg	114	 94% 6%
37	Lh	122	 88% 12%
38	Li	102	 97%
39	Lj	86	 98%
40	Lk	69	 88% 12%
41	Ll	50	 88% 12%
42	Lm	52	 88% 12%
43	Ln	24	 92% 8%
44	Lo	105	 93% 7%
45	Lp	91	 97%
46	Lr	125	 98%
47	Ls	196	 89% 11%
48	Lt	157	 27% 73% 12% 15%
49	SA	221	 84% 16%
50	SB	214	 5% 76% 24%
51	SC	222	 83% 16%
52	SE	262	 78% 22%
53	SG	237	 8% 74% 26%

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Mol	Chain	Length	Quality of chain
54	SH	189	
55	SI	206	
56	SJ	185	
57	SL	153	
58	SN	150	
59	SO	140	
60	SV	83	
61	SW	129	
62	SX	141	
63	SY	131	
64	Sa	102	
65	Sb	83	
66	Se	58	
67	S2	1740	
68	SR	135	
69	SD	227	
70	SF	189	
71	SK	98	
72	SM	122	
73	SP	121	
74	SQ	144	
75	SS	145	
76	ST	143	
77	SU	104	
78	SZ	75	

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Mol	Chain	Length	Quality of chain
79	Sc	64	
80	Sd	55	
81	Sf	67	
82	Sg	313	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 216861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription factor BTF3.

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

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 7 is a protein called 60S ribosomal protein L4.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called Ribosomal protein uL16-like.

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

- Molecule 14 is a protein called 60S ribosomal protein L11.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called Heparin-binding protein HBp15.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 43 is a protein called 60S ribosomal protein L41.

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

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

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 49 is a protein called 40S ribosomal protein SA.

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

- Molecule 50 is a protein called 40S ribosomal protein S3a.

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

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 53 is a protein called 40S ribosomal protein S6.

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

- Molecule 54 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 55 is a protein called 40S ribosomal protein S8.

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

- Molecule 56 is a protein called 40S ribosomal protein S9.

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

- Molecule 57 is a protein called 40S ribosomal protein S11.

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

- Molecule 58 is a protein called 40S ribosomal protein S13.

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

- Molecule 59 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 61 is a protein called 40S ribosomal protein S15a.

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

- Molecule 62 is a protein called 40S ribosomal protein S23.

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

- Molecule 63 is a protein called 40S ribosomal protein S24.

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

- Molecule 64 is a protein called 40S ribosomal protein S26.

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

- Molecule 65 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 66 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 67 is a RNA chain called 18S rRNA.

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

- Molecule 68 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 69 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 70 is a protein called 40S ribosomal protein S5.

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

- Molecule 71 is a protein called 40S ribosomal protein S10.

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

- Molecule 72 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 73 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 75 is a protein called 40S ribosomal protein S18.

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

- Molecule 76 is a protein called 40S ribosomal protein S19.

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

- Molecule 77 is a protein called 40S ribosomal protein S20.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 79 is a protein called 40S ribosomal protein S28.

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

- Molecule 80 is a protein called 40S ribosomal protein S29.

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

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

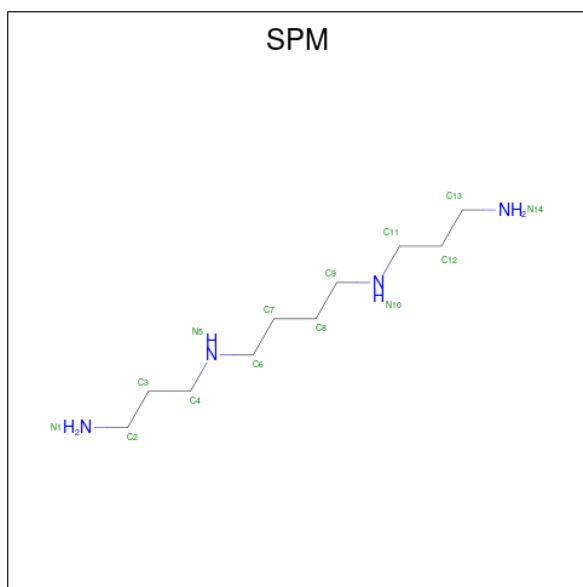
Mol	Chain	Residues	Atoms		AltConf
83	L5	177	Total	Mg	0
			177	177	
83	L7	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
83	L8	5	Total	Mg	0
			5	5	
83	LA	1	Total	Mg	0
			1	1	
83	LI	1	Total	Mg	0
			1	1	
83	LP	1	Total	Mg	0
			1	1	
83	LV	1	Total	Mg	0
			1	1	
83	Le	1	Total	Mg	0
			1	1	
83	Lj	1	Total	Mg	0
			1	1	
83	S2	28	Total	Mg	0
			28	28	

- Molecule 84 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



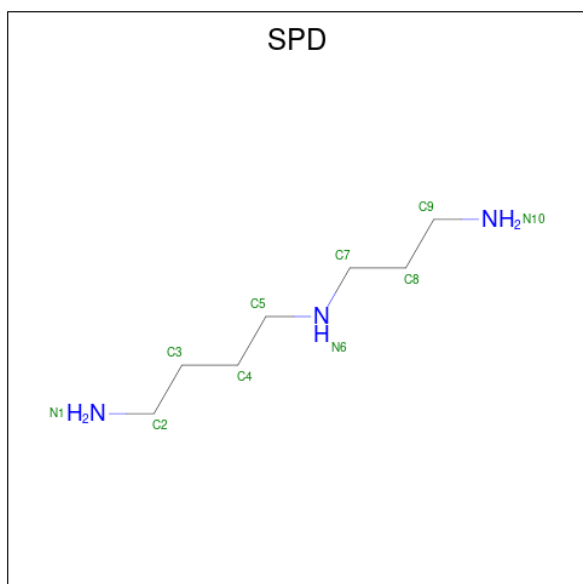
Mol	Chain	Residues	Atoms			AltConf
84	L5	1	Total	C	N	0
			14	10	4	
84	L5	1	Total	C	N	0
			14	10	4	
84	L5	1	Total	C	N	0
			14	10	4	

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

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



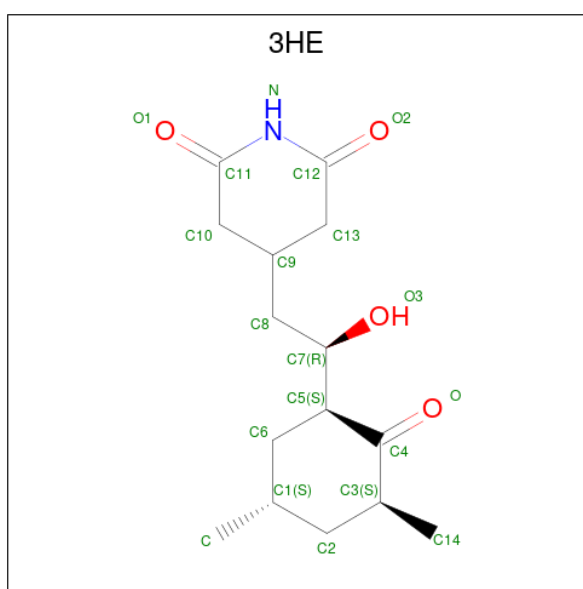
Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	

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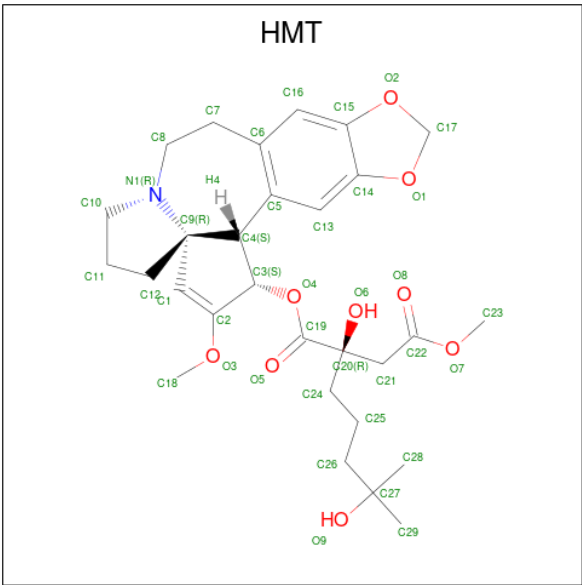
Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	LN	1	Total	C	N	0
			10	7	3	

- Molecule 86 is 4-[(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl]piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
86	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 87 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
87	L5	1	Total	C	N	O	0
			39	29	1	9	

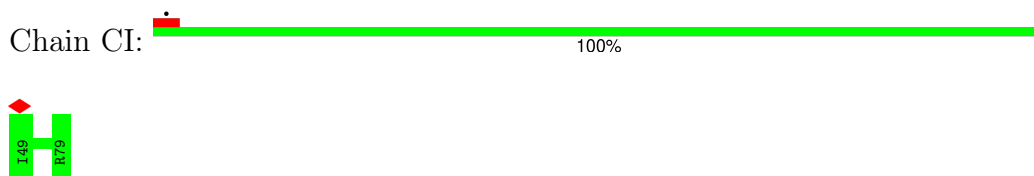
- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

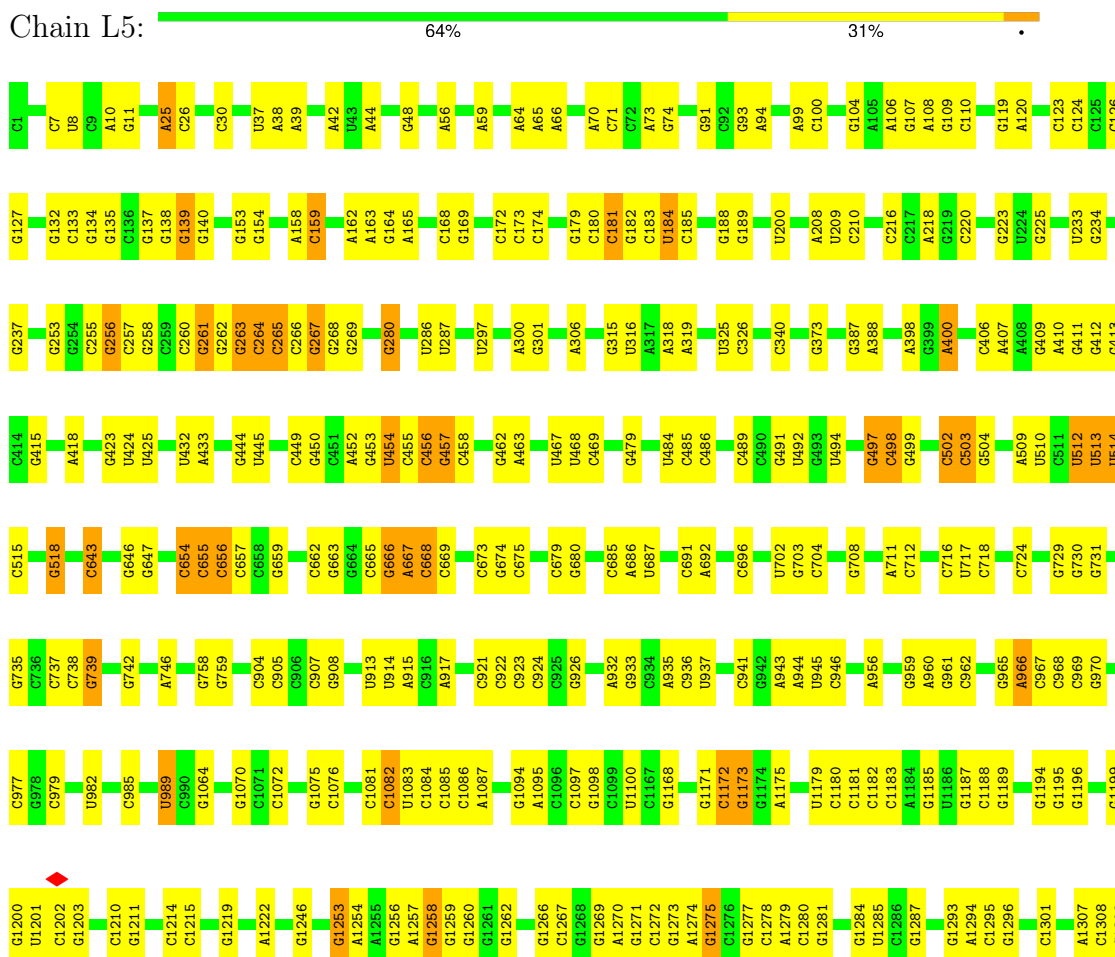
3 Residue-property plots

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

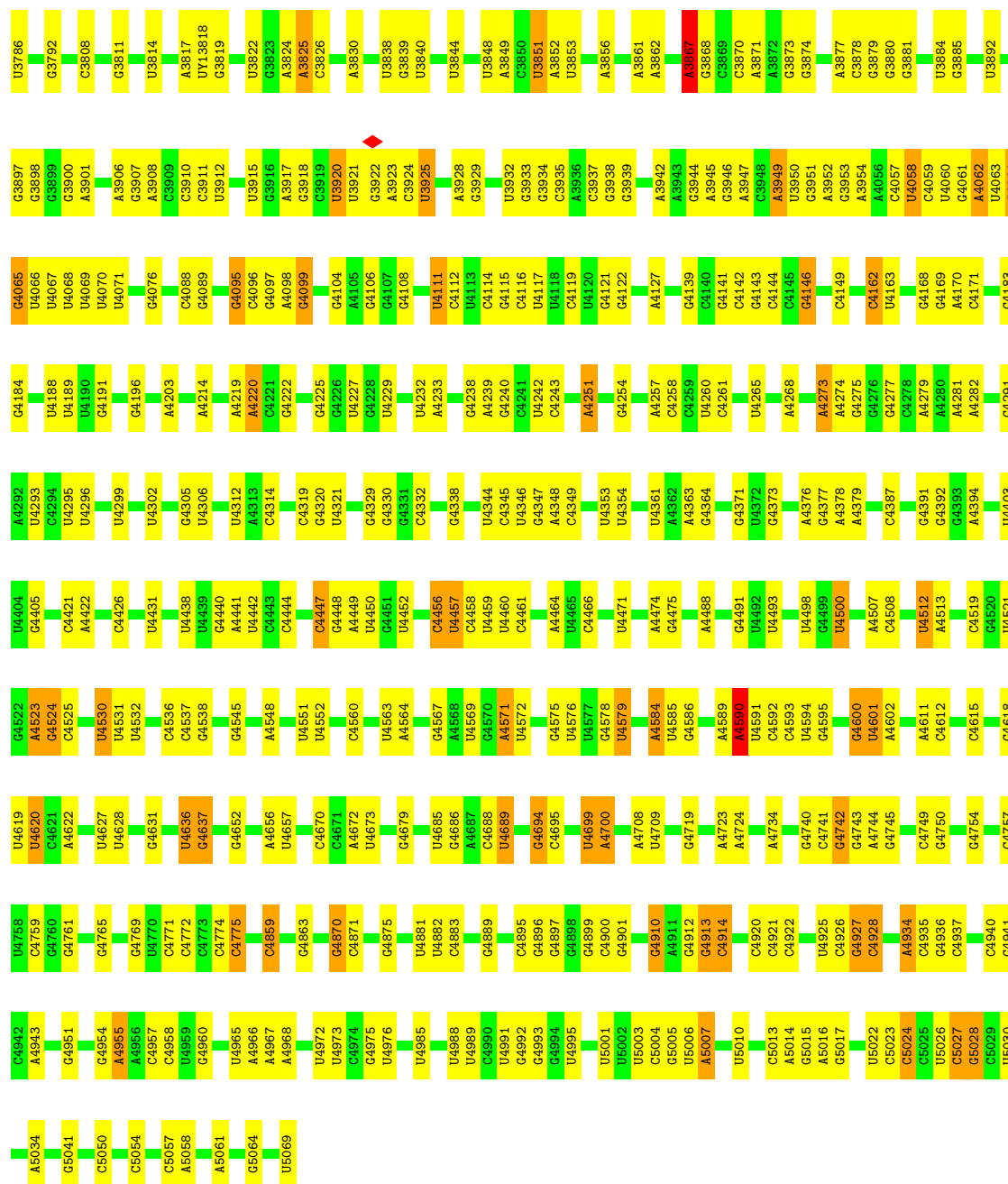
- Molecule 1: Transcription factor BTF3



- Molecule 2: 28S rRNA



G3684	G3685	G3695	G3696	G3697	G3698	C3701	U3707	G3708	G3709	G3710	A3711	A3712	U3713	A3717	A3718	A3719	A3720	U3721	G3722	A3723	A3724	G3725	A3726	A3727	A3728	A3732	A3733	A3736	A3737	A3748	G3753	U3758	A3759	A3760	C3761	U3762	A3763	U3764	G3765	A3766	U3770	A3775	G3776	G3777	C3782	A3785						
G3585	G3586	G3590	G3591	G3594	G3595	G3596	G3597	G3598	A3599	G3600	A3604	C3605	U3606	U3607	A3608	G3609	A3610	A3611	G3615	U3616	G3619	G3626	A3630	A3635	G3636	U3637	G3638	U3639	U3640	U3641	U3644	U3645	A3646	A3647	A3648	A3656	U3657	G3661	A3662	A3663	G3664	G3665	C3670	C3673	G3674	A3675						
A2766	U2769	C2770	G2773	A2787	U2788	A2789	U2790	A2806	C2814	A2815	C2824	A2825	U2826	G2827	U2828	U2829	U2837	G2838	U2839	A2844	G2855	G2856	A2857	C2861	A2864	U2865	G2866	C2867	A2870	G2732	C2733	C2739	G2742	A2743	A2744	A2745	A2746	G2754	U2904	C2905	G2906	U2911	G2912	U2913	A2914	A2915						
U2656	G2662	G2667	G2668	C2669	C2670	C2671	C2672	G2675	A2676	U2687	G2688	G2694	A2695	A2696	C2702	G2706	U2707	U2708	C2709	G2710	G2711	G2714	G2715	G2721	G2724	A2725	G2726	U2730	C2731	C2732	C2733	C2739	G2742	A2743	A2744	A2745	A2746	G2754	U2904	C2905	G2906	U2911	G2912	U2913	A2914	A2915						
U2519	C2520	G2521	A2529	A2537	U2538	C2539	C2540	A2543	G2544	U2545	U2546	U2547	U2554	G2555	G2556	G2557	C2558	G2559	C2560	A2565	G2566	C2567	C2568	C2569	U2570	G2571	C2572	A2573	C2583	A2587	C2588	C2589	A2601	G2602	C2603	C2607	U2611	G2612	C2627	U2632	C2653	G2654	A2641	C2655								
U2413	G2416	A2417	C2422	U2425	U2447	C2448	A2449	G2450	A2453	C2458	C2464	C2465	C2466	C2469	C2470	C2471	G2474	G2475	C2478	G2479	G2483	A2484	U2485	G2486	G2487	C2488	C2489	U2490	C2491	C2492	G2493	U2494	U2495	C2496	C2497	C2498	C2499	G2502	G2503	C2504	C2505	G2506	A2513	A2517	G2518							
C2256	C2257	C2258	G2259	G2262	A2263	C2264	G2265	C2266	U2267	G2270	A2276	C2277	C2289	A2300	C2301	C2302	C2303	G2306	A2313	G2326	G2331	A2332	C2333	C2334	C2335	G2336	G2345	G2348	C2351	A2360	G2361	U2362	A2363	G2364	A2389	A2395	A2396	G2397	G2400	A2401	C2411	A2412										
C2011	A2012	C2016	A2017	C2018	C2019	U2020	G2021	G2024	A2025	A2026	A2029	A2030	G2046	U2047	A2048	G2055	G2056	A2069	G2079	U2080	C2084	G2085	U2090	C2091	G2092	A2093	G2094	C2095	G2096	U2097	G2098	C2101	G2102	G2103	G2106	C2107	C2110	G2111	G2112	C2249	C2250	G2251	G2252	A2253	C2255							
C1921	G1922	G1925	A1802	G1803	A1804	A1805	G1806	G1810	G1821	U1822	G1823	G1824	A1825	G1826	U1834	G1835	G1836	A1837	G1842	G1846	C1847	C1848	G1855	C1856	C1857	A1858	C1859	U1860	U1861	U1862	A1867	A1868	G1869	C1870	A1871	U1882	A1892	A1897	A1907	A1908	G2001	A2002	G2003	U2004	G2005	U2006	G2007					
C1696	G1697	A1698	G1700	A1701	C1702	C1703	C1704	G1705	A1706	G1716	C1717	C1718	A1719	C1720	G1721	U1725	U1726	C1731	G1732	G1733	G1734	C1740	G1741	A1742	A1743	U1744	G1750	G1751	G1752	G1753	U1754	C1755	U1756	U1757	G1758	G1759	G1760	G1761	C1762	C1763	G1764	A1765	A1766	A1767	C1768	U1677	C1678	A1679	G1680	U1683	C1694	U1695
A1563	A1564	A1565	A1566	G1574	G1577	U1578	G1582	U1588	U1589	C1590	U1591	U1596	G1612	A1613	G1617	G1624	G1625	C1628	G1629	A1630	A1631	A1632	G1633	A1634	A1638	U1639	A1503	G1504	C1505	C1509	U1514	A1515	G1516	G1517	A1524	A1534	G1535	U1536	U1537	U1538	C1411	G1412	C1413	G1414	G1415	G1416	C1417					
A1420	C1431	G1432	G1435	G1436	C1437	U1438	C1439	C1442	A1443	U1444	G1446	A1447	G1448	C1449	G1482	C1483	A1497	C1498	G1499	A1500	C1501	A1502	A1503	G1504	C1505	C1509	U1514	A1515	G1516	G1517	A1524	A1534	G1535	U1536	U1537	U1538	C1411	G1412	C1413	G1414	G1415	G1416	C1417									
A1326	C1327	G1328	A1332	A1333	C1337	A1338	A1339	C1340	A1345	C1346	G1347	A1353	G1355	U1356	C1357	G1358	G1359	C1365	G1366	G1367	A1387	G1394	A1397	A1398	G1403	G1404	C1407	G1408	U1409	U1410	U1411	G1412	C1413	G1414	G1415	G1416	C1417															



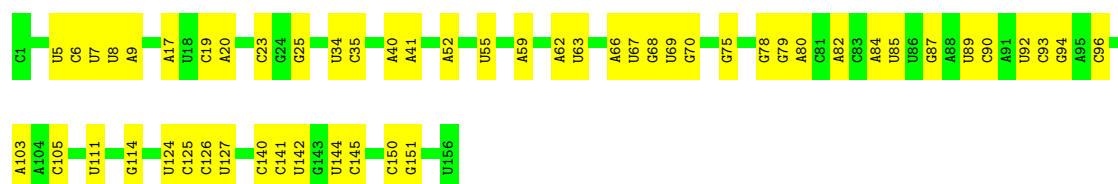
• Molecule 3: 5S rRNA

Chain L7: 84% 14%



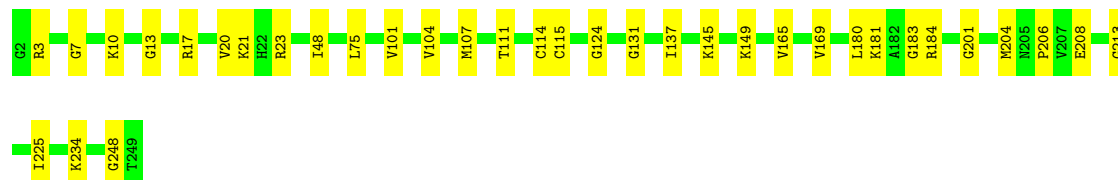
• Molecule 4: 5.8S rRNA

Chain L8: 66% 34%



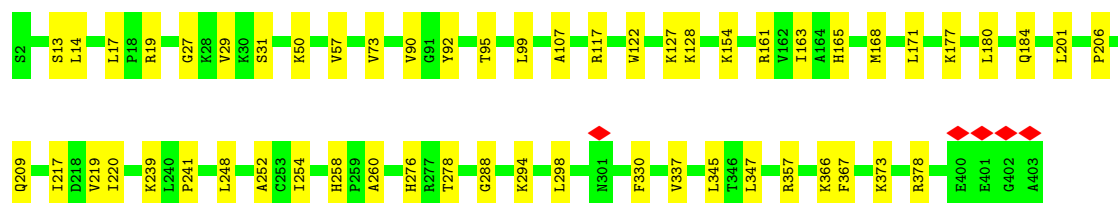
- Molecule 5: 60S ribosomal protein L8

Chain LA: 86% 14%



- Molecule 6: Large ribosomal subunit protein uL3

Chain LB: 86% 14%



- Molecule 7: 60S ribosomal protein L4

Chain LC: 94% 6%



- Molecule 8: Large ribosomal subunit protein uL18

Chain LD: 88% 12%



- Molecule 9: Large ribosomal subunit protein eL6

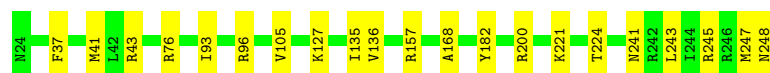
Chain LE: 88% 8%





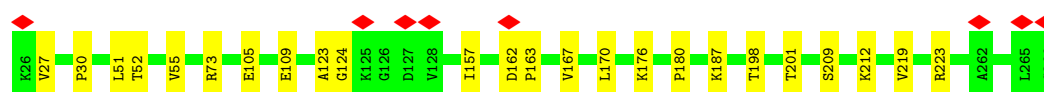
- Molecule 10: 60S ribosomal protein L7

Chain LF: 91% 9%



- Molecule 11: 60S ribosomal protein L7a

Chain LG: 90% 10%



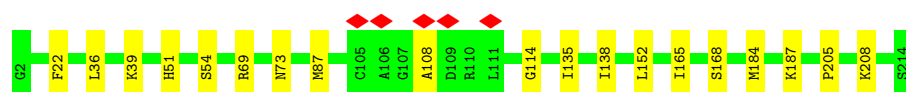
- Molecule 12: 60S ribosomal protein L9

Chain LH: 90% 10%



- Molecule 13: Ribosomal protein uL16-like

Chain LI: 91% 9%



- Molecule 14: 60S ribosomal protein L11

Chain LJ: 88% 9% .



- Molecule 15: Large ribosomal subunit protein eL13

Chain LL: 93% 7%



- Molecule 16: 60S ribosomal protein L14

Chain LM:  87% 13%



- Molecule 17: 60S ribosomal protein L15

Chain LN:  94% 6%



- Molecule 18: 60S ribosomal protein L13a

Chain LO:  88% 12%



- Molecule 19: 60S ribosomal protein L17

Chain LP:  90% 10%



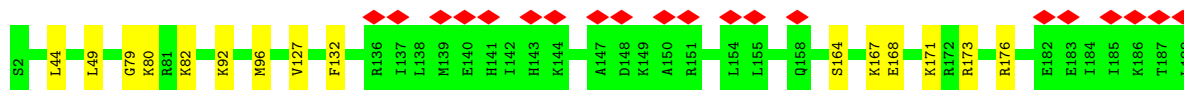
- Molecule 20: 60S ribosomal protein L18

Chain LQ:  93% 7%



- Molecule 21: 60S ribosomal protein L19

Chain LR:  11% 92% 8%

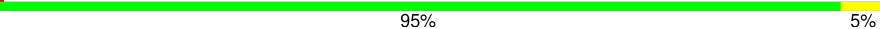


- Molecule 22: 60S ribosomal protein L18a

Chain LS:  94% 6%



- Molecule 23: 60S ribosomal protein L21

Chain LT:  95% 5%

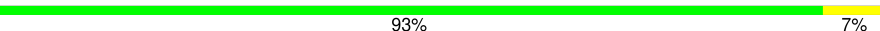


- Molecule 24: Heparin-binding protein HBp15

Chain LU:  92% 8%



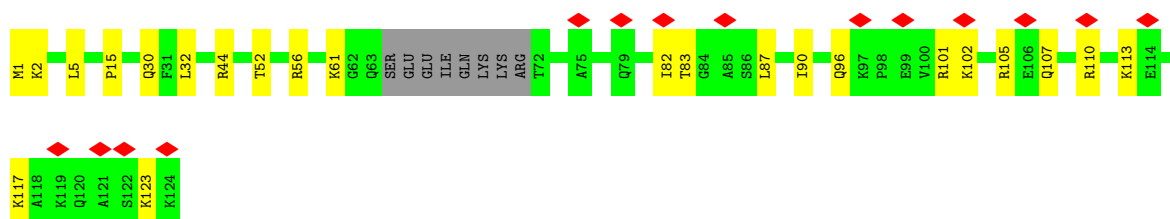
- Molecule 25: 60S ribosomal protein L23

Chain LV:  93% 7%

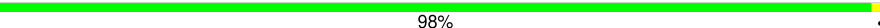


- Molecule 26: Ribosomal protein L24

Chain LW:  11% 75% 19% 6%



- Molecule 27: 60S ribosomal protein L23a

Chain LX:  98%

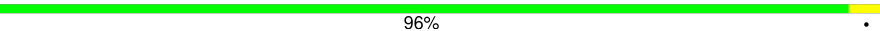


- Molecule 28: 60S ribosomal protein L26

Chain LY:  89% 11%



- Molecule 29: 60S ribosomal protein L27

Chain LZ:  96%



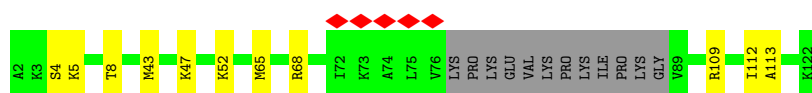
- Molecule 30: 60S ribosomal protein L27a

Chain La: 97%



- Molecule 31: Large ribosomal subunit protein eL29

Chain Lb: 81% 9% 10%



- Molecule 32: 60S ribosomal protein L30

Chain Lc: 85% 15%



- Molecule 33: 60S ribosomal protein L31

Chain Ld: 84% 16%



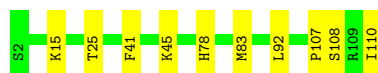
- Molecule 34: 60S ribosomal protein L32

Chain Le: 91% 9%



- Molecule 35: 60S ribosomal protein L35a

Chain Lf: 91% 9%



- Molecule 36: 60S ribosomal protein L34

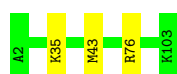
Chain Lg: 94% 6%



- Molecule 37: 60S ribosomal protein L35



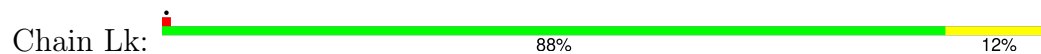
- Molecule 38: 60S ribosomal protein L36



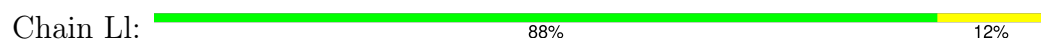
- Molecule 39: 60S ribosomal protein L37



- Molecule 40: 60S ribosomal protein L38



- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Large ribosomal subunit protein eL40



- Molecule 43: 60S ribosomal protein L41





- Molecule 44: 60S ribosomal protein L36a



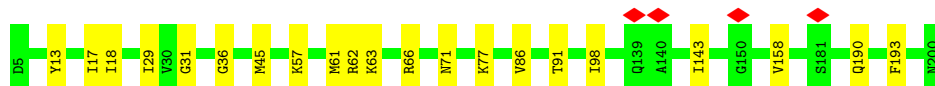
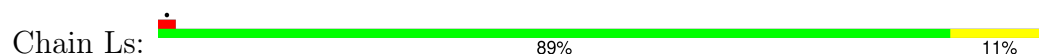
- Molecule 45: 60S ribosomal protein L37a



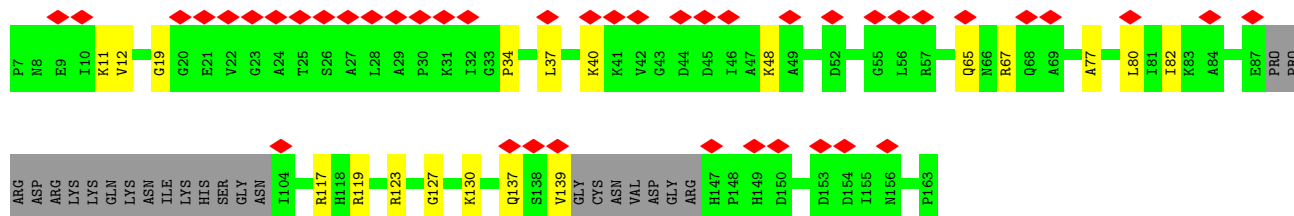
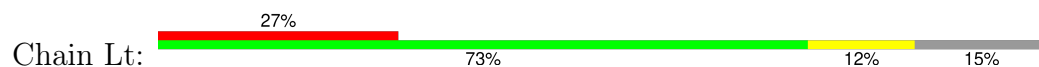
- Molecule 46: 60S ribosomal protein L28



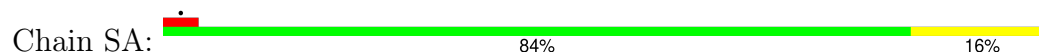
- Molecule 47: 60S acidic ribosomal protein P0

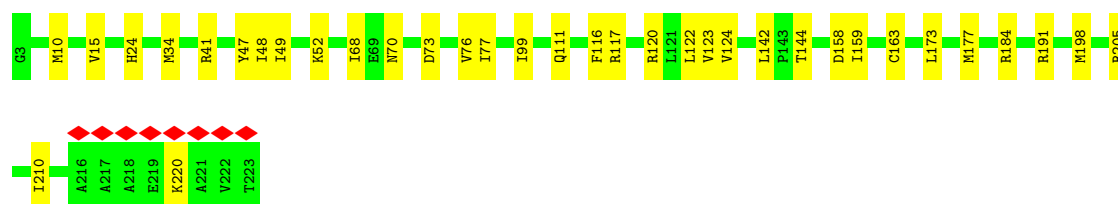


- Molecule 48: Large ribosomal subunit protein uL11

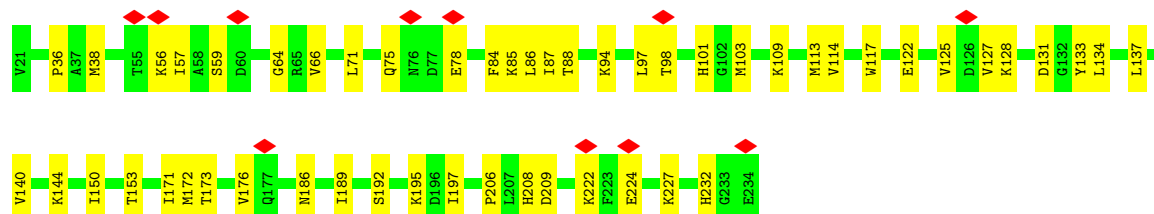
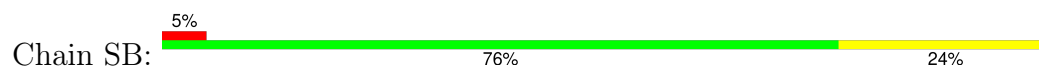


- Molecule 49: 40S ribosomal protein SA

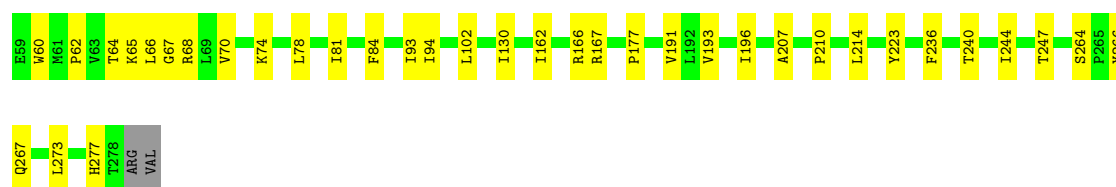
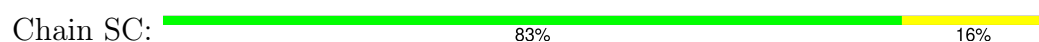




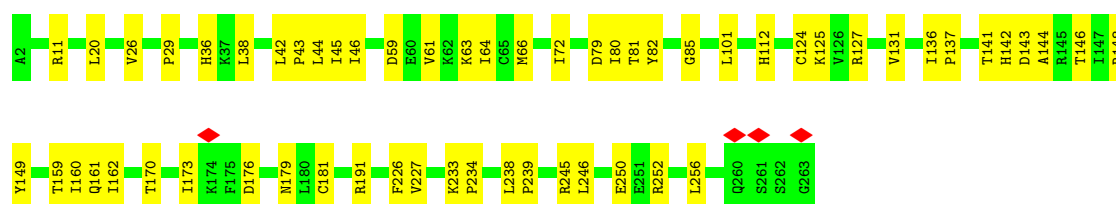
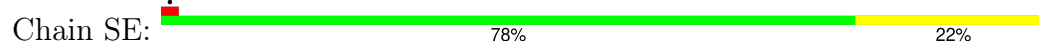
- Molecule 50: 40S ribosomal protein S3a



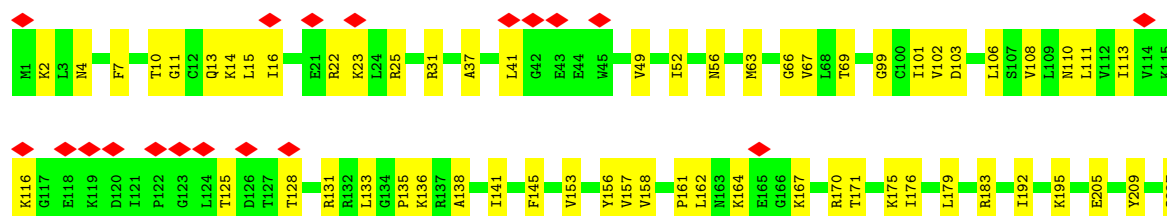
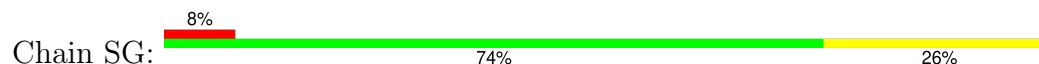
- Molecule 51: 40S ribosomal protein S2

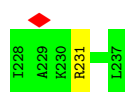


- Molecule 52: Small ribosomal subunit protein eS4, X isoform

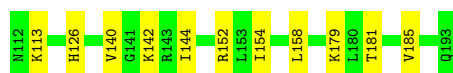
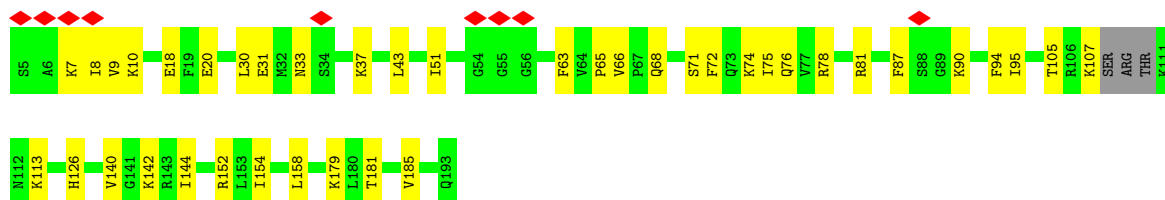
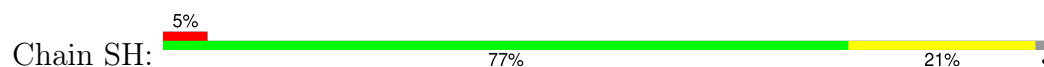


- Molecule 53: 40S ribosomal protein S6

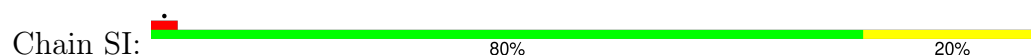




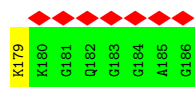
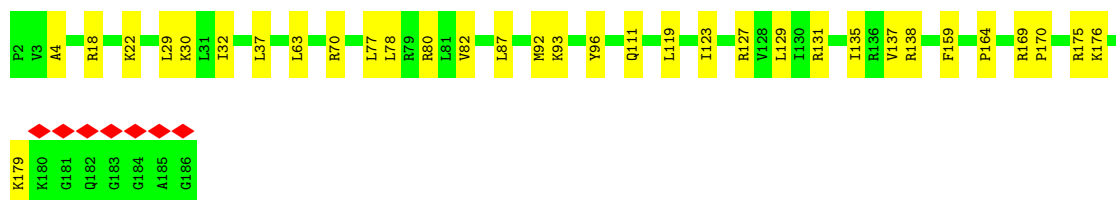
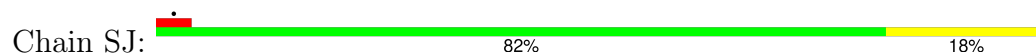
- Molecule 54: Small ribosomal subunit protein eS7



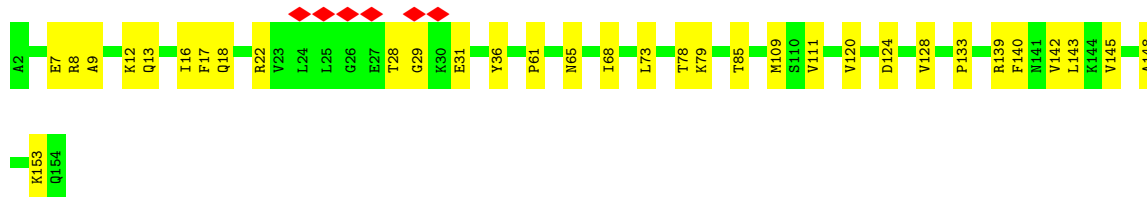
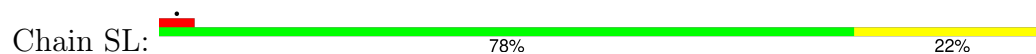
- Molecule 55: 40S ribosomal protein S8



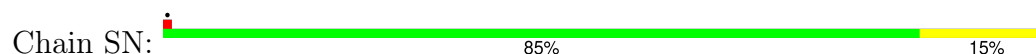
- Molecule 56: 40S ribosomal protein S9



- Molecule 57: 40S ribosomal protein S11

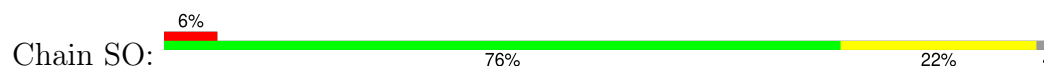


- Molecule 58: 40S ribosomal protein S13

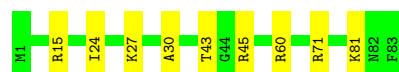




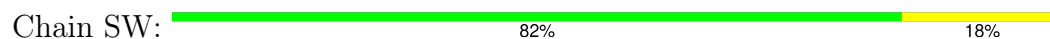
- Molecule 59: Small ribosomal subunit protein uS11



- Molecule 60: Small ribosomal subunit protein eS21



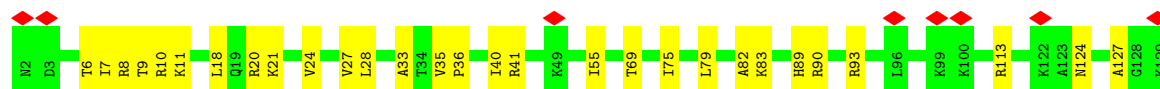
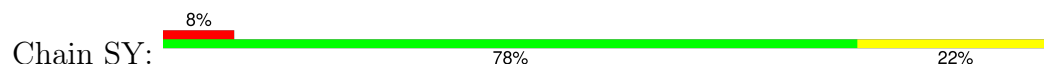
- Molecule 61: 40S ribosomal protein S15a



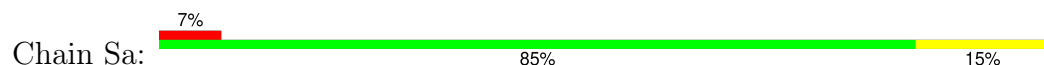
- Molecule 62: 40S ribosomal protein S23

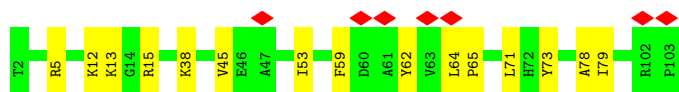


- Molecule 63: 40S ribosomal protein S24

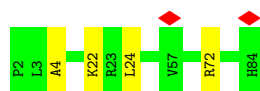


- Molecule 64: 40S ribosomal protein S26

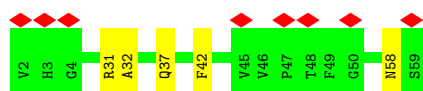




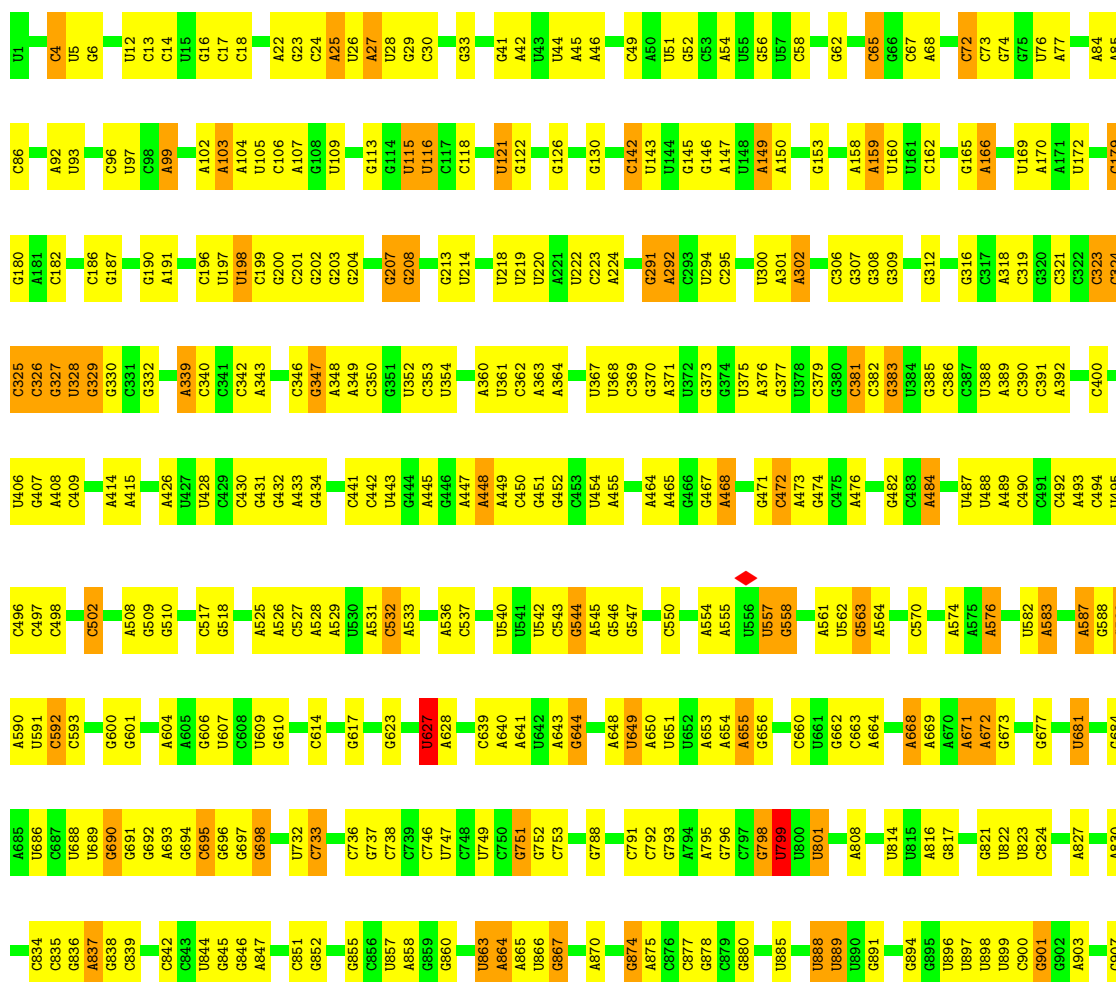
- Molecule 65: Small ribosomal subunit protein eS27

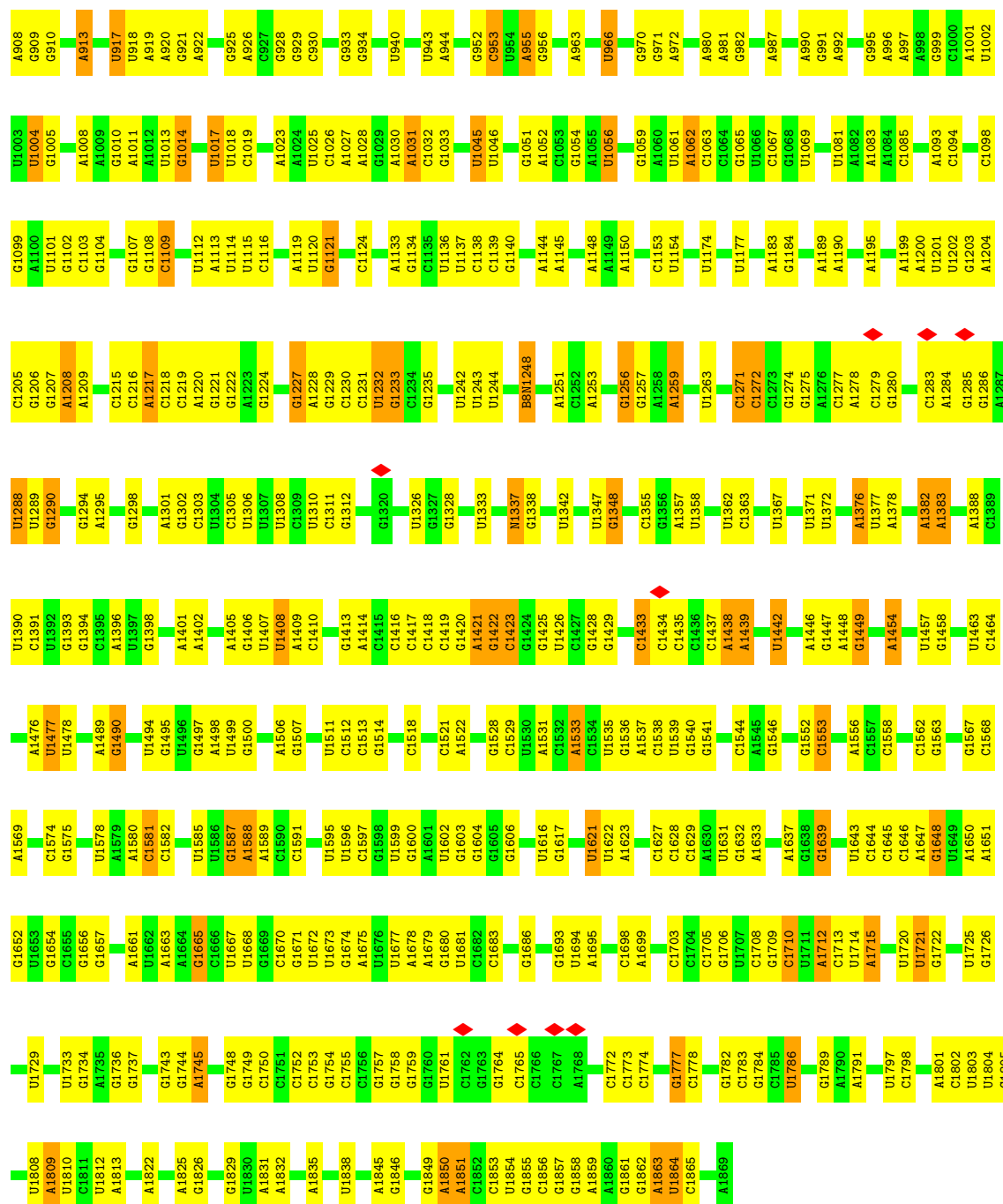


- Molecule 66: Small ribosomal subunit protein eS30

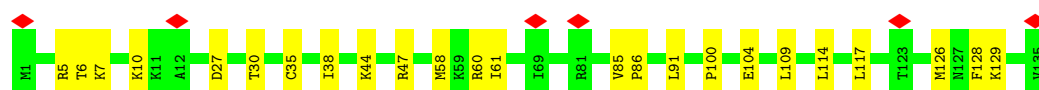
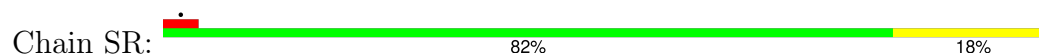


- Molecule 67: 18S rRNA

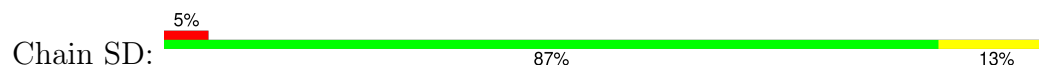


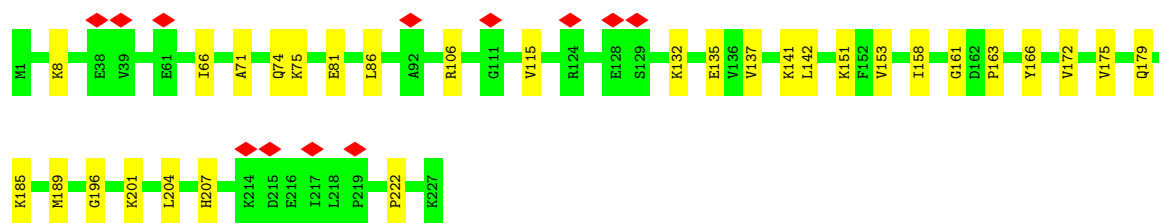


- Molecule 68: Small ribosomal subunit protein eS17

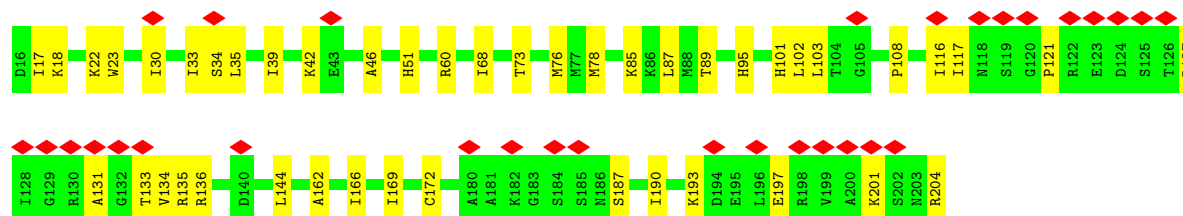
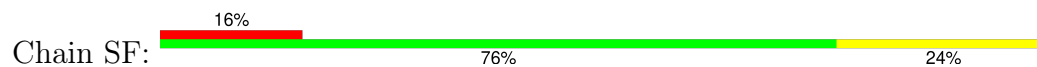


- Molecule 69: Small ribosomal subunit protein uS3

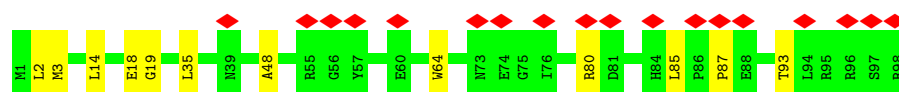
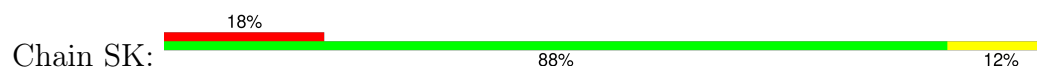




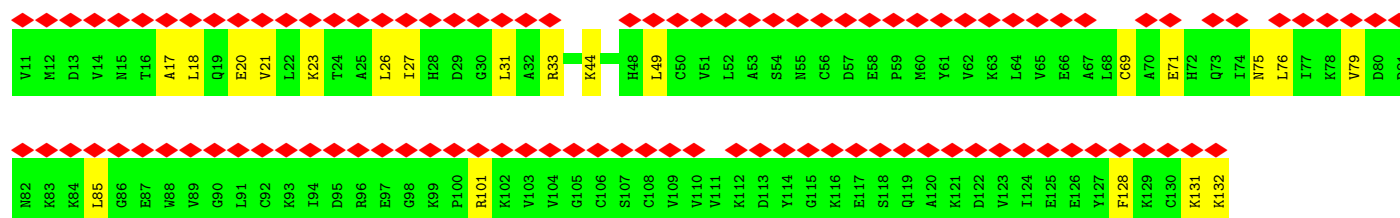
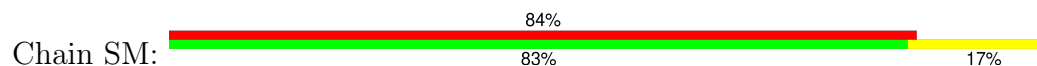
- Molecule 70: 40S ribosomal protein S5



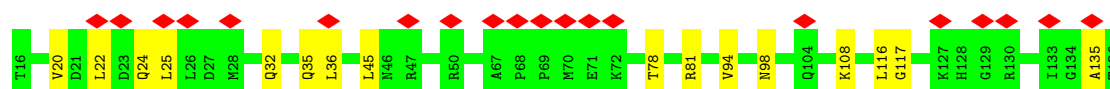
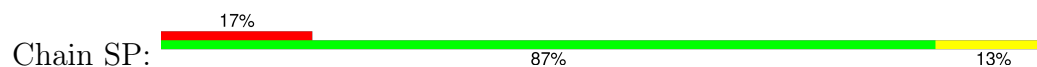
- Molecule 71: 40S ribosomal protein S10



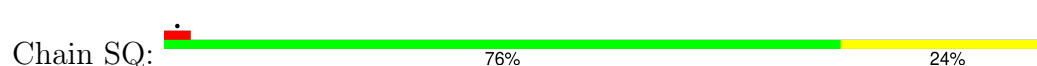
- Molecule 72: Small ribosomal subunit protein eS12

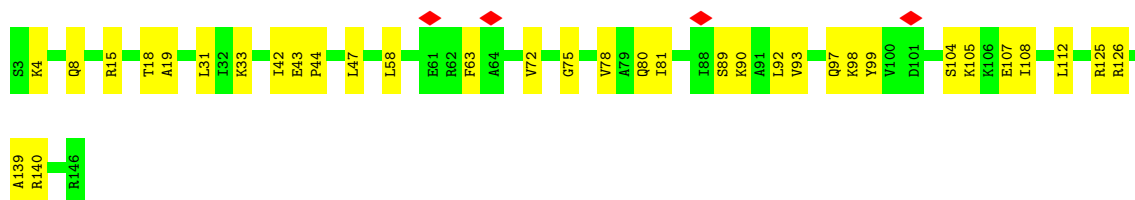


- Molecule 73: Small ribosomal subunit protein uS19

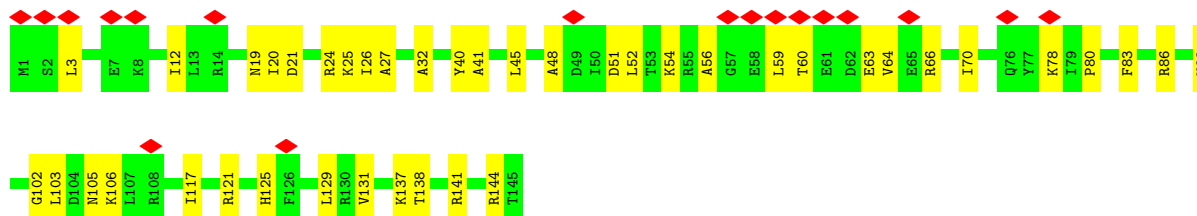


- Molecule 74: Small ribosomal subunit protein uS9

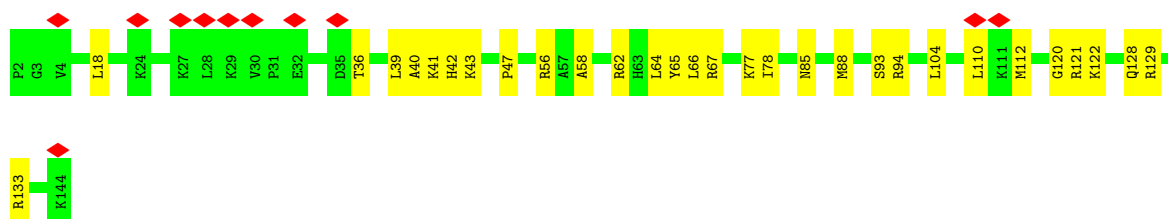
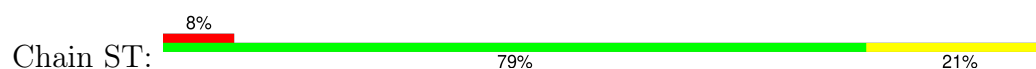




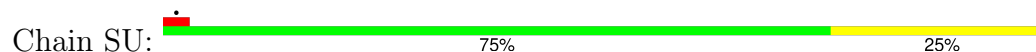
- Molecule 75: 40S ribosomal protein S18



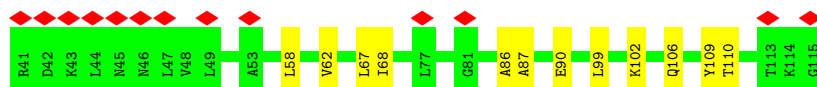
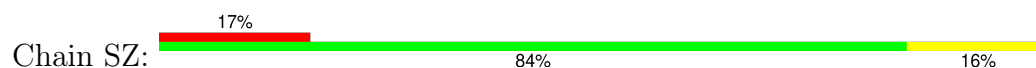
- Molecule 76: 40S ribosomal protein S19



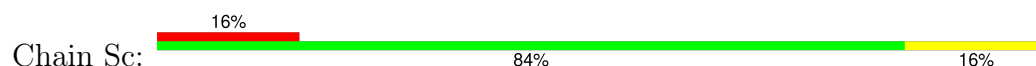
- Molecule 77: 40S ribosomal protein S20

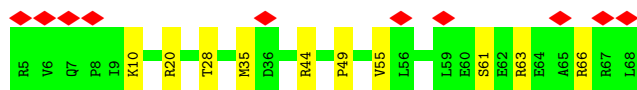


- Molecule 78: Small ribosomal subunit protein eS25



- Molecule 79: 40S ribosomal protein S28





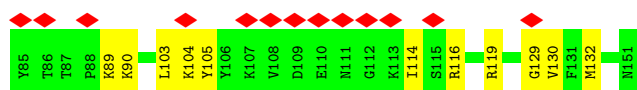
- Molecule 80: 40S ribosomal protein S29

Chain Sd: 82% 18%



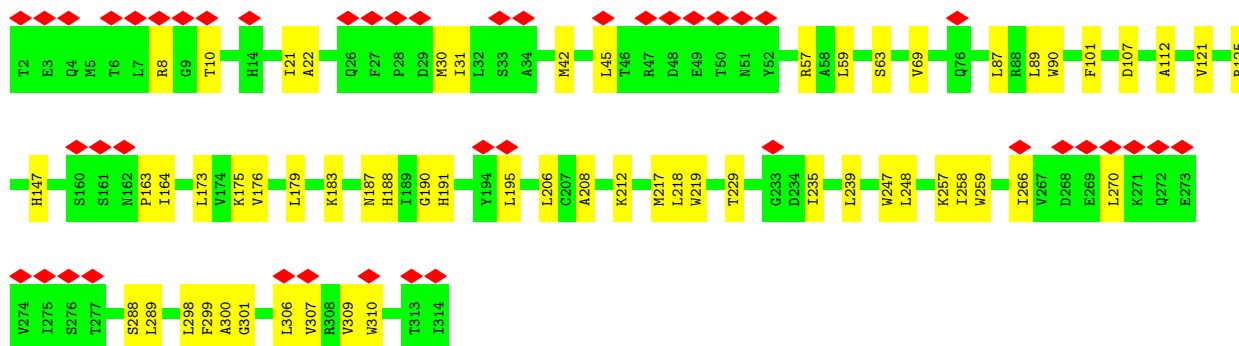
- Molecule 81: Ubiquitin-40S ribosomal protein S27a

Chain Sf: 19% 84% 16%



- Molecule 82: Receptor of activated protein C kinase 1

Chain Sg: 14% 81% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	463982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0121	Depositor
Map size (Å)	512.64, 512.64, 512.64	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89000005, 0.89000005, 0.89000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, MG, OMC, A2M, UR3, PSU, 6MZ, 4AC, MA6, SPD, ZN, 3HE, B8N, 1MA, 5MC, SPM, OMU, HMT, OMG, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CI	0.17	0/247	0.35	0/323
2	L5	0.30	0/85095	0.32	0/132750
3	L7	0.28	0/2861	0.26	0/4459
4	L8	0.29	0/3631	0.28	0/5657
5	LA	0.30	0/1936	0.44	0/2596
6	LB	0.27	0/3306	0.38	0/4424
7	LC	0.27	0/2981	0.36	0/4002
8	LD	0.22	0/2428	0.32	0/3252
9	LE	0.22	0/1973	0.39	0/2645
10	LF	0.26	0/1905	0.32	0/2539
11	LG	0.23	0/1960	0.38	1/2637 (0.0%)
12	LH	0.22	0/1537	0.33	0/2066
13	LI	0.24	0/1751	0.34	0/2340
14	LJ	0.19	0/1385	0.35	0/1852
15	LL	0.24	0/1732	0.34	0/2315
16	LM	0.26	0/1161	0.37	0/1554
17	LN	0.29	0/1746	0.36	0/2338
18	LO	0.28	0/1682	0.38	0/2250
19	LP	0.27	0/1268	0.36	0/1701
20	LQ	0.29	0/1537	0.36	0/2052
21	LR	0.23	0/1581	0.35	0/2088
22	LS	0.27	0/1493	0.36	0/2003
23	LT	0.24	0/1326	0.31	0/1770
24	LU	0.21	0/839	0.42	0/1126
25	LV	0.25	0/993	0.39	0/1332
26	LW	0.20	0/959	0.36	0/1270
27	LX	0.23	0/1002	0.32	0/1345
28	LY	0.24	0/1132	0.35	0/1504
29	LZ	0.23	0/1130	0.34	0/1507
30	La	0.26	0/1191	0.32	0/1591
31	Lb	0.22	0/889	0.37	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.23	0/774	0.36	0/1038
33	Ld	0.24	0/903	0.33	0/1216
34	Le	0.27	0/1071	0.34	0/1429
35	Lf	0.29	0/895	0.37	0/1198
36	Lg	0.24	0/916	0.33	0/1220
37	Lh	0.22	0/1023	0.34	0/1351
38	Li	0.21	0/843	0.30	0/1115
39	Lj	0.30	0/720	0.39	0/952
40	Lk	0.20	0/575	0.33	0/761
41	Ll	0.25	0/454	0.28	0/599
42	Lm	0.23	0/435	0.34	0/575
43	Ln	0.19	0/231	0.29	0/294
44	Lo	0.25	0/876	0.32	0/1156
45	Lp	0.24	0/718	0.32	0/953
46	Lr	0.26	0/1017	0.35	0/1364
47	Ls	0.12	0/1519	0.31	0/2052
48	Lt	0.16	0/1009	0.43	0/1363
49	SA	0.13	0/1778	0.37	0/2416
50	SB	0.13	0/1765	0.38	0/2362
51	SC	0.15	0/1744	0.38	0/2357
52	SE	0.13	0/2118	0.36	0/2849
53	SG	0.13	0/1946	0.35	0/2590
54	SH	0.16	0/1519	0.41	0/2033
55	SI	0.14	0/1715	0.38	0/2287
56	SJ	0.13	0/1550	0.34	0/2069
57	SL	0.13	0/1268	0.33	0/1696
58	SN	0.13	0/1232	0.32	0/1656
59	SO	0.15	0/1037	0.36	0/1391
60	SV	0.13	0/643	0.33	0/860
61	SW	0.15	0/1051	0.34	0/1406
62	SX	0.14	0/1116	0.36	0/1490
63	SY	0.14	0/1083	0.35	0/1438
64	Sa	0.14	0/836	0.39	0/1121
65	Sb	0.13	0/665	0.35	0/891
66	Se	0.13	0/465	0.37	0/612
67	S2	0.17	2/39755 (0.0%)	0.28	0/61935
68	SR	0.16	0/1105	0.44	0/1484
69	SD	0.12	0/1793	0.31	0/2414
70	SF	0.14	0/1516	0.34	0/2037
71	SK	0.13	0/851	0.36	0/1147
72	SM	0.15	0/950	0.40	0/1275
73	SP	0.15	0/1003	0.38	0/1342
74	SQ	0.16	0/1160	0.40	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SS	0.14	0/1216	0.39	0/1628
76	ST	0.17	0/1131	0.40	0/1515
77	SU	0.18	0/831	0.40	0/1115
78	SZ	0.15	0/604	0.45	0/810
79	Sc	0.13	0/508	0.35	0/680
80	Sd	0.13	0/470	0.30	0/623
81	Sf	0.19	0/560	0.52	0/745
82	Sg	0.13	0/2493	0.36	0/3394
All	All	0.24	2/228113 (0.0%)	0.33	1/334320 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	S2	484	A2M	O3'-P	5.10	1.61	1.56
67	S2	1326	OMU	O3'-P	5.09	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	LG	27	VAL	N-CA-C	-5.26	107.35	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	0	0
2	L5	78444	0	39719	536	0
3	L7	2561	0	1295	10	0
4	L8	3315	0	1685	20	0
5	LA	1898	0	1993	32	0
6	LB	3238	0	3376	41	0
7	LC	2927	0	3104	15	0
8	LD	2382	0	2410	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LE	1935	0	2096	12	0
10	LF	1870	0	1996	16	0
11	LG	1927	0	2074	14	0
12	LH	1518	0	1601	14	0
13	LI	1711	0	1749	13	0
14	LJ	1362	0	1399	10	0
15	LL	1701	0	1818	11	0
16	LM	1138	0	1204	13	0
17	LN	1701	0	1749	11	0
18	LO	1650	0	1794	17	0
19	LP	1242	0	1269	13	0
20	LQ	1513	0	1628	9	0
21	LR	1566	0	1728	12	0
22	LS	1453	0	1490	5	0
23	LT	1298	0	1366	6	0
24	LU	825	0	850	5	0
25	LV	979	0	1039	5	0
26	LW	945	0	1003	17	0
27	LX	985	0	1066	2	0
28	LY	1115	0	1205	10	0
29	LZ	1107	0	1182	4	0
30	La	1162	0	1213	3	0
31	Lb	876	0	948	9	0
32	Lc	764	0	804	9	0
33	Ld	888	0	930	10	0
34	Le	1053	0	1147	8	0
35	Lf	876	0	912	6	0
36	Lg	906	0	998	6	0
37	Lh	1015	0	1148	10	0
38	Li	832	0	917	3	0
39	Lj	705	0	737	2	0
40	Lk	569	0	637	6	0
41	Ll	444	0	483	4	0
42	Lm	429	0	465	4	0
43	Ln	230	0	276	2	0
44	Lo	862	0	929	5	0
45	Lp	708	0	756	3	0
46	Lr	1002	0	1068	2	0
47	Ls	1496	0	1540	13	0
48	Lt	998	0	1032	13	0
49	SA	1741	0	1746	25	0
50	SB	1738	0	1809	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	SC	1707	0	1791	23	0
52	SE	2076	0	2177	37	0
53	SG	1923	0	2089	41	0
54	SH	1497	0	1590	28	0
55	SI	1686	0	1772	31	0
56	SJ	1525	0	1640	23	0
57	SL	1247	0	1323	21	0
58	SN	1208	0	1294	13	0
59	SO	1024	0	1050	23	0
60	SV	636	0	637	7	0
61	SW	1034	0	1080	17	0
62	SX	1098	0	1167	8	0
63	SY	1065	0	1142	22	0
64	Sa	821	0	870	12	0
65	Sb	651	0	672	4	0
66	Se	459	0	503	7	0
67	S2	36953	0	18679	432	0
68	SR	1090	0	1149	17	0
69	SD	1765	0	1865	18	0
70	SF	1495	0	1549	34	0
71	SK	827	0	854	12	0
72	SM	940	0	965	12	0
73	SP	985	0	1031	12	0
74	SQ	1142	0	1213	27	0
75	SS	1198	0	1261	26	0
76	ST	1112	0	1146	21	0
77	SU	821	0	883	18	0
78	SZ	598	0	656	9	0
79	Sc	506	0	536	9	0
80	Sd	459	0	452	11	0
81	Sf	548	0	551	9	0
82	Sg	2436	0	2393	35	0
83	L5	177	0	0	0	0
83	L7	3	0	0	0	0
83	L8	5	0	0	0	0
83	LA	1	0	0	0	0
83	LI	1	0	0	0	0
83	LP	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Lj	1	0	0	0	0
83	S2	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	L5	98	0	182	4	0
85	L5	90	0	171	1	0
85	LN	10	0	19	0	0
86	L5	20	0	23	0	0
87	L5	39	0	39	1	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
All	All	216861	0	162080	1821	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1821) 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)
2:L5:1996:C:H42	2:L5:2000:G:N2	1.55	1.03
2:L5:1629:G:H21	2:L5:1632:A:N6	1.61	0.97
2:L5:1629:G:H21	2:L5:1632:A:H61	1.00	0.95
2:L5:1629:G:N2	2:L5:1632:A:H61	1.65	0.94
2:L5:1996:C:H42	2:L5:2000:G:H22	0.99	0.94
2:L5:1996:C:N4	2:L5:2000:G:H22	1.66	0.93
67:S2:1656:G:H1	67:S2:1668:U:H3	1.13	0.92
67:S2:1417:C:H42	67:S2:1422:G:N2	1.70	0.89
67:S2:1417:C:H42	67:S2:1422:G:H22	0.92	0.88
67:S2:1417:C:N4	67:S2:1422:G:H22	1.72	0.86
2:L5:1759:G:H1	2:L5:1773:U:H3	1.24	0.86
67:S2:1533:A:H62	67:S2:1602:U:H3	1.25	0.85
74:SQ:43:GLU:HG3	74:SQ:44:PRO:HD3	1.55	0.85
74:SQ:44:PRO:HG2	74:SQ:81:ILE:HD11	1.57	0.84
2:L5:5024:C:H41	2:L5:5028:G:H21	1.25	0.83
2:L5:184:U:H3	2:L5:253:G:H1	1.29	0.81
2:L5:1100:U:H3	2:L5:1194:G:H1	1.29	0.80
2:L5:3944:G:H1	2:L5:4069:U:H3	1.28	0.79
76:ST:129:ARG:HD2	76:ST:133:ARG:HH21	1.47	0.79
67:S2:1030:A:H2'	67:S2:1031:A2M:H8	1.63	0.78
2:L5:2557:G:H1	2:L5:2570:U:H3	1.29	0.77
61:SW:53:ILE:HD13	65:Sb:24:LEU:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:1743:G:H21	67:S2:1791:A:H62	1.33	0.76
57:SL:7:GLU:HG2	57:SL:9:ALA:H	1.51	0.76
55:SI:87:ASN:HB3	55:SI:90:LEU:HD23	1.68	0.76
67:S2:1657:G:H1	67:S2:1667:U:H3	1.32	0.75
53:SG:164:LYS:HB2	53:SG:167:LYS:HG2	1.68	0.75
2:L5:2611:A:H5'	2:L5:2688:G:H4'	1.67	0.75
2:L5:184:U:O2	2:L5:253:G:N2	2.21	0.74
2:L5:2458:C:H5''	17:LN:67:ARG:HD2	1.68	0.74
67:S2:1748:G:H1	67:S2:1786:U:H3	1.31	0.74
2:L5:1538:U:H4'	2:L5:1629:G:H5'	1.70	0.74
2:L5:3922[A]:G:H1'	5:LA:3:ARG:HH11	1.51	0.74
2:L5:4242:U:H3	2:L5:4281:A:H2	1.34	0.74
59:SO:52:THR:HG21	67:S2:952:G:H21	1.54	0.73
67:S2:851:C:H5''	67:S2:852:G:H5'	1.71	0.73
2:L5:3937:C:H1'	17:LN:125:SER:HB3	1.71	0.73
2:L5:2007:G:H21	2:L5:2012:A:H62	1.35	0.73
2:L5:1628:C:H2'	2:L5:1629:G:C8	2.24	0.72
52:SE:38:LEU:HD22	67:S2:346:C:H5''	1.71	0.72
54:SH:7:LYS:HE2	54:SH:10:LYS:HB3	1.71	0.72
51:SC:70:VAL:HG11	51:SC:93:ILE:HG12	1.70	0.72
2:L5:3701:OMC:H5	2:L5:3748:A:H62	1.38	0.71
82:Sg:247:TRP:HB3	82:Sg:258:ILE:HD11	1.73	0.71
14:LJ:104:ASN:HD22	14:LJ:133:VAL:HG13	1.56	0.70
77:SU:66:ARG:HH22	77:SU:75:LYS:HD3	1.55	0.70
67:S2:1433:C:H42	77:SU:92:HIS:HD2	1.39	0.70
67:S2:1581:C:H5'	67:S2:1582:C:H5	1.55	0.70
53:SG:116:LYS:HE3	53:SG:125:THR:HG21	1.74	0.70
6:LB:90:VAL:HG23	6:LB:163:ILE:HD11	1.72	0.69
26:LW:82:ILE:HG22	53:SG:131:ARG:HB2	1.74	0.69
67:S2:1854:U:H2'	67:S2:1855:G:H8	1.58	0.69
2:L5:2483:G:H1	2:L5:2495:U:H3	1.39	0.69
47:Ls:18:ILE:HD11	47:Ls:71:ASN:HD21	1.57	0.69
2:L5:2484:A:H62	2:L5:2494:U:H3	1.41	0.68
51:SC:193:VAL:HG11	51:SC:240:THR:HG22	1.75	0.68
49:SA:70:ASN:HB3	49:SA:73:ASP:HB2	1.74	0.68
2:L5:1414:C:H2'	2:L5:1415:G:H8	1.59	0.68
55:SI:56:ARG:HH12	67:S2:379:C:H5''	1.56	0.68
64:Sa:59:PHE:HB2	64:Sa:62:TYR:HB2	1.76	0.68
5:LA:107:MET:HB3	5:LA:111:THR:HG21	1.75	0.68
60:SV:15:ARG:HH21	60:SV:24:ILE:HG21	1.58	0.68
54:SH:154:ILE:HB	54:SH:185:VAL:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4694:G:H4'	12:LH:71:ARG:HH12	1.58	0.67
51:SC:196:ILE:HB	51:SC:223:TYR:HB2	1.76	0.67
67:S2:928:G:H2'	67:S2:929:G:C8	2.29	0.67
75:SS:121:ARG:HG3	75:SS:131:VAL:HB	1.76	0.67
16:LM:15:VAL:HG22	16:LM:50:MET:HE1	1.76	0.67
2:L5:1095:A:H2	2:L5:1200:G:H1	1.43	0.67
2:L5:1435:G:N2	2:L5:1449:C:O2	2.17	0.67
2:L5:1969:G:H4'	47:Ls:36:GLY:HA2	1.77	0.67
2:L5:3611:A:H2	2:L5:5016:A:H8	1.42	0.67
67:S2:1228:A:H2'	67:S2:1229:G:H8	1.59	0.67
84:L5:5292:SPM:H112	18:LO:91:LYS:HD3	1.77	0.67
57:SL:133:PRO:HG2	67:S2:383:G:H21	1.60	0.66
2:L5:1095:A:N1	2:L5:1200:G:O6	2.28	0.66
2:L5:2554:U:O2	2:L5:2764:A:N7	2.28	0.66
19:LP:138:PRO:HB3	19:LP:140:MET:HE2	1.77	0.66
67:S2:116:OMU:HN3	67:S2:347:G:H1	1.44	0.66
12:LH:106:GLN:HB2	12:LH:111:LEU:HB3	1.78	0.66
48:Lt:65:GLN:HG3	48:Lt:67:ARG:H	1.60	0.66
67:S2:677:G:H21	67:S2:1028:A:H62	1.44	0.66
70:SF:34:SER:HA	79:Sc:55:VAL:HG13	1.78	0.66
62:SX:9:THR:HG22	67:S2:681:PSU:H4'	1.77	0.66
57:SL:8:ARG:HH21	67:S2:390:C:H4'	1.61	0.66
19:LP:109:VAL:HA	19:LP:112:LEU:HD13	1.76	0.66
59:SO:33:ILE:HG22	59:SO:42:VAL:HA	1.78	0.65
69:SD:106:ARG:HG3	69:SD:175:VAL:HG22	1.78	0.65
13:LI:205:PRO:HD2	13:LI:208:LYS:HE2	1.77	0.65
67:S2:1398:G:H1'	82:Sg:63:SER:HB2	1.78	0.65
33:Ld:90:ARG:HD3	33:Ld:102:LEU:HD13	1.78	0.65
57:SL:16:ILE:HD11	57:SL:36:TYR:H	1.62	0.65
2:L5:1942:A:H2'	2:L5:1943:A:C8	2.32	0.65
2:L5:4910:G:H4'	6:LB:95:THR:HG22	1.78	0.65
67:S2:1388:A:H61	69:SD:161:GLY:HA3	1.61	0.65
2:L5:2486:G:O6	2:L5:2493:G:O6	2.15	0.64
82:Sg:31:ILE:HG12	82:Sg:45:LEU:HD21	1.77	0.64
49:SA:77:ILE:HG22	49:SA:99:ILE:HB	1.79	0.64
49:SA:99:ILE:HD11	49:SA:117:ARG:HH12	1.62	0.64
82:Sg:208:ALA:HB2	82:Sg:218:LEU:HD13	1.79	0.64
53:SG:227:GLN:HB3	53:SG:231:ARG:HH21	1.62	0.64
7:LC:268:ARG:HH12	7:LC:269:LYS:HE2	1.62	0.64
53:SG:135:PRO:HG2	53:SG:141:ILE:HG22	1.80	0.64
2:L5:4279:A:H5'	2:L5:4281:A:H1'	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4992:G:H2'	2:L5:4993:G:C8	2.33	0.64
2:L5:1628:C:H2'	2:L5:1629:G:H8	1.63	0.64
2:L5:1700:G:H5''	2:L5:1704:C:H42	1.62	0.64
53:SG:183:ARG:HH12	67:S2:316:G:H5''	1.63	0.64
2:L5:3717:A:H2'	2:L5:3718:A2M:H8	1.80	0.63
12:LH:187:VAL:HG12	12:LH:188:GLN:HG3	1.81	0.63
67:S2:1228:A:H2'	67:S2:1229:G:C8	2.33	0.63
51:SC:70:VAL:HG21	51:SC:93:ILE:HG23	1.79	0.63
67:S2:600:G:H2'	67:S2:601:OMG:H8	1.64	0.63
2:L5:4064:C:H2'	2:L5:4065:G:C8	2.34	0.63
55:SI:98:LYS:HB3	67:S2:377:G:H5'	1.80	0.63
63:SY:9:THR:HG22	67:S2:837:A:H61	1.62	0.63
67:S2:1651:A:H2'	67:S2:1652:G:H8	1.64	0.63
73:SP:108:LYS:HD2	75:SS:117:ILE:HG22	1.81	0.63
25:LV:35:LYS:HB2	25:LV:67:LYS:HG3	1.79	0.62
59:SO:102:GLY:H	59:SO:134:PRO:HB2	1.63	0.62
76:ST:39:LEU:HD23	76:ST:56:ARG:HH11	1.64	0.62
71:SK:80:ARG:HH11	71:SK:87:PRO:HA	1.63	0.62
51:SC:65:LYS:HD2	51:SC:273:LEU:HD13	1.79	0.62
53:SG:66:GLY:HA2	67:S2:1745:A:H1'	1.80	0.62
57:SL:85:THR:HG21	67:S2:373:G:H4'	1.81	0.62
67:S2:940:U:H3	67:S2:1002:U:H3	1.46	0.62
2:L5:2351:OMC:HM22	7:LC:95:MET:HG3	1.81	0.62
76:ST:110:LEU:HD23	76:ST:112:MET:HE3	1.82	0.62
78:SZ:68:ILE:HG23	78:SZ:109:TYR:HB2	1.80	0.62
52:SE:79:ASP:HB3	52:SE:82:TYR:HB2	1.81	0.62
67:S2:1289:U:H4'	71:SK:2:LEU:HD21	1.82	0.62
5:LA:137:ILE:HD11	5:LA:149:LYS:HB2	1.82	0.61
6:LB:14:LEU:HD22	6:LB:17:LEU:HD11	1.81	0.61
67:S2:1650:A:H5''	74:SQ:139:ALA:HB2	1.83	0.61
67:S2:1396:A:N7	67:S2:1449:G:O6	2.34	0.61
47:Ls:143:ILE:HD12	47:Ls:158:VAL:HG11	1.83	0.61
53:SG:37:ALA:HA	53:SG:49:VAL:HA	1.83	0.61
61:SW:107:SER:HB2	67:S2:860:G:H21	1.65	0.61
55:SI:22:HIS:HB3	67:S2:433:A:H5''	1.81	0.61
58:SN:55:ARG:HD3	67:S2:1017:U:H5'	1.83	0.61
68:SR:5:ARG:HB2	68:SR:10:LYS:HE3	1.81	0.61
82:Sg:259:TRP:HD1	82:Sg:266:ILE:HA	1.66	0.61
67:S2:1417:C:O2	67:S2:1422:G:O6	2.17	0.61
13:LI:54:SER:HB3	13:LI:135:ILE:HD11	1.82	0.61
67:S2:159:A2M:H2	67:S2:467:G:H21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SX:68:LYS:HB3	62:SX:91:LEU:HD13	1.83	0.61
19:LP:39:MET:HG2	19:LP:43:LYS:HD3	1.83	0.61
55:SI:57:ALA:HB2	55:SI:183:GLY:HA2	1.81	0.61
59:SO:95:ILE:HB	59:SO:129:ILE:HG22	1.82	0.60
62:SX:107:ARG:HG3	62:SX:110:HIS:HB3	1.82	0.60
67:S2:1031:A2M:H2'	67:S2:1032:C:C6	2.36	0.60
67:S2:1277:C:H2'	67:S2:1278:A:H8	1.66	0.60
2:L5:4098:A:H2'	2:L5:4099:G:H4'	1.82	0.60
42:Lm:99:CYS:HB2	42:Lm:114:LYS:HE3	1.83	0.60
54:SH:87:PHE:HB3	54:SH:90:LYS:HG3	1.82	0.60
74:SQ:58:LEU:HD22	74:SQ:108:ILE:HG13	1.83	0.60
76:ST:104:LEU:HD13	76:ST:121:ARG:HD2	1.82	0.60
2:L5:137:G:H2'	2:L5:138:G:H8	1.66	0.60
2:L5:3717:A:H2'	2:L5:3718:A2M:C8	2.32	0.60
33:Ld:64:ILE:HG23	33:Ld:68:LEU:HD23	1.83	0.60
2:L5:512:U:H3	2:L5:647:G:H1	1.48	0.60
2:L5:1704:C:OP1	10:LF:43:ARG:HD3	2.01	0.60
13:LI:36:LEU:HD11	13:LI:69:ARG:HD2	1.83	0.60
73:SP:94:VAL:HG11	73:SP:116:LEU:HD11	1.82	0.60
74:SQ:19:ALA:HB2	74:SQ:75:GLY:HA3	1.84	0.60
2:L5:1503:A:H62	20:LQ:87:THR:HG21	1.65	0.60
54:SH:65:PRO:HG2	54:SH:68:GLN:HB2	1.83	0.60
70:SF:102:LEU:HD21	78:SZ:110:THR:HB	1.83	0.60
26:LW:96:GLN:HB2	26:LW:101:ARG:HE	1.66	0.60
51:SC:191:VAL:HG11	51:SC:236:PHE:HA	1.83	0.59
2:L5:1992:U:H4'	2:L5:1993:C:H5''	1.84	0.59
2:L5:3922[A]:G:H8	5:LA:3:ARG:HD3	1.67	0.59
67:S2:1743:G:N2	67:S2:1791:A:H62	2.00	0.59
2:L5:1726:U:H5'	10:LF:135:ILE:HD11	1.85	0.59
57:SL:61:PRO:HB3	57:SL:68:ILE:HD11	1.83	0.59
59:SO:61:LYS:HZ3	59:SO:76:LEU:HB3	1.68	0.59
2:L5:1996:C:N4	2:L5:2000:G:N2	2.36	0.59
2:L5:3868:G:H22	2:L5:3900:G:H1'	1.68	0.59
6:LB:367:PHE:HB2	26:LW:1:MET:HB2	1.82	0.59
50:SB:224:GLU:HB3	50:SB:227:LYS:HE3	1.85	0.59
52:SE:61:VAL:HA	52:SE:64:ILE:HG22	1.83	0.59
2:L5:1281:G:N1	9:LE:128:HIS:HB2	2.18	0.59
52:SE:191:ARG:HD2	52:SE:245:ARG:HE	1.68	0.59
54:SH:144:ILE:HD11	54:SH:152:ARG:HB3	1.83	0.59
50:SB:84:PHE:HB3	50:SB:86:LEU:HD23	1.84	0.59
54:SH:144:ILE:HD13	54:SH:154:ILE:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SY:124:ASN:HD22	67:S2:84:A:H5''	1.68	0.59
67:S2:1679:A:H2'	70:SF:60:ARG:HD2	1.85	0.59
2:L5:966:A:H5''	2:L5:2092:G:H22	1.67	0.59
2:L5:4441:A:H5''	13:LI:114:GLY:HA2	1.85	0.59
10:LF:105:VAL:HG13	10:LF:136:VAL:HG12	1.84	0.59
61:SW:86:LEU:HD21	61:SW:113:HIS:HB2	1.85	0.59
64:Sa:12:LYS:HG3	64:Sa:15:ARG:HB2	1.83	0.59
70:SF:127:ARG:HH12	79:Sc:66:ARG:HH22	1.51	0.59
77:SU:61:LEU:HB2	77:SU:82:MET:HB3	1.85	0.59
67:S2:557:U:H2'	67:S2:558:G:C8	2.38	0.58
3:L7:49:A:H5''	8:LD:224:SER:HB2	1.85	0.58
53:SG:11:GLY:HA2	67:S2:166:A2M:HM'1	1.84	0.58
78:SZ:99:LEU:HD21	78:SZ:102:LYS:HB2	1.85	0.58
55:SI:72:CYS:HG	55:SI:112:TRP:CG	2.21	0.58
61:SW:111:MET:HE1	61:SW:119:LYS:HD2	1.84	0.58
67:S2:106:C:H2'	67:S2:107:A:H8	1.67	0.58
67:S2:1536:G:H2'	67:S2:1537:A:H8	1.68	0.58
78:SZ:58:LEU:HD12	78:SZ:62:VAL:HG21	1.85	0.58
2:L5:1563:A:H2'	2:L5:1564:A:C8	2.39	0.58
2:L5:4775:C:H41	2:L5:4859:C:H42	1.51	0.58
30:La:72:THR:HG22	30:La:110:LYS:HB3	1.85	0.58
50:SB:57:ILE:HG22	50:SB:59:SER:H	1.68	0.58
50:SB:88:THR:HA	50:SB:98:THR:HA	1.85	0.58
53:SG:162:LEU:HD12	53:SG:170:ARG:HH21	1.69	0.58
57:SL:78:THR:HG22	57:SL:79:LYS:HG3	1.85	0.58
67:S2:1562:C:H2'	67:S2:1563:G:H8	1.68	0.58
67:S2:1829:G:H1'	67:S2:1850:MA6:H2	1.84	0.58
82:Sg:87:LEU:HB2	82:Sg:101:PHE:HB2	1.85	0.58
58:SN:66:VAL:HG13	58:SN:67:THR:HG23	1.84	0.58
75:SS:137:LYS:HG3	75:SS:138:THR:HG23	1.86	0.58
70:SF:30:ILE:HG23	70:SF:117:ILE:HD11	1.85	0.58
28:LY:2:LYS:HD2	28:LY:7:VAL:HG23	1.85	0.58
55:SI:133:GLU:HA	55:SI:136:ILE:HG12	1.84	0.58
63:SY:113:ARG:HG3	63:SY:127:ALA:HB1	1.86	0.58
76:ST:85:ASN:HB3	76:ST:88:MET:HB2	1.85	0.58
52:SE:80:ILE:HG23	52:SE:81:THR:HG23	1.85	0.58
67:S2:694:G:H2'	67:S2:695:C:O4'	2.04	0.58
2:L5:4274:A:H2'	2:L5:4275:G:C8	2.39	0.58
67:S2:115:U:H2'	67:S2:116:OMU:H6	1.85	0.58
2:L5:262:G:H2'	2:L5:263:G:H8	1.69	0.57
2:L5:667:A:H5''	2:L5:668:C:H5''	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:502:C:H3'	2:L5:503:C:H3'	1.86	0.57
53:SG:136:LYS:HB2	67:S2:65:C:H41	1.68	0.57
55:SI:12:ARG:HH21	55:SI:18:ARG:HG3	1.68	0.57
67:S2:981:A:H2'	67:S2:982:G:C8	2.38	0.57
72:SM:26:LEU:HA	72:SM:31:LEU:HD21	1.86	0.57
18:LO:126:VAL:HG13	18:LO:127:VAL:HG13	1.85	0.57
54:SH:113:LYS:HE3	67:S2:798:G:H4'	1.85	0.57
15:LL:64:VAL:HA	15:LL:67:HIS:CD2	2.38	0.57
67:S2:433:A:H2'	67:S2:434:G:C8	2.38	0.57
82:Sg:107:ASP:HB2	82:Sg:125:ARG:HD2	1.85	0.57
2:L5:1326:A2M:H2'	2:L5:1327:C:C6	2.39	0.57
67:S2:1031:A2M:H2'	67:S2:1032:C:H6	1.68	0.57
2:L5:1339:U:H2'	2:L5:1340:OMC:C6	2.38	0.57
3:L7:120:U:H4'	8:LD:262:LYS:HG2	1.86	0.57
49:SA:77:ILE:HD11	49:SA:124:VAL:HG22	1.87	0.57
52:SE:144:ALA:HB3	67:S2:121:OMU:HM23	1.86	0.57
67:S2:639:C:H2'	67:S2:640:A:H8	1.70	0.57
6:LB:165:HIS:HB3	6:LB:180:LEU:HD23	1.87	0.57
67:S2:1464:C:H4'	68:SR:60:ARG:HH11	1.70	0.57
2:L5:2411:C:H2'	2:L5:2412:A:H8	1.69	0.57
12:LH:115:ARG:HD3	12:LH:123:ILE:HD12	1.87	0.57
67:S2:885:U:O2	67:S2:901:G:O6	2.22	0.57
67:S2:1764:G:H5'	67:S2:1765:C:H5''	1.87	0.57
36:Lg:45:ALA:HB3	36:Lg:82:MET:HE2	1.86	0.57
63:SY:55:ILE:HD12	63:SY:75:ILE:HG22	1.85	0.57
6:LB:107:ALA:HB2	6:LB:201:LEU:HD22	1.87	0.56
56:SJ:63:LEU:HD23	56:SJ:70:ARG:HB2	1.87	0.56
67:S2:49:C:H2'	67:S2:472:C:H41	1.69	0.56
2:L5:2007:G:N2	2:L5:2012:A:H62	2.02	0.56
2:L5:2517:A:H5'	36:Lg:62:LYS:HD3	1.87	0.56
53:SG:138:ALA:HB2	53:SG:179:LEU:HD12	1.87	0.56
2:L5:2017:A:HO2'	2:L5:2018:C:H6	1.53	0.56
2:L5:2411:C:H2'	2:L5:2412:A:C8	2.40	0.56
18:LO:54:TYR:CD1	18:LO:145:VAL:HG21	2.40	0.56
67:S2:1729:U:H3	67:S2:1805:G:H1	1.52	0.56
2:L5:1332:C:H2'	2:L5:1333:A:H8	1.70	0.56
60:SV:71:ARG:HH11	65:Sb:4:ALA:HB2	1.69	0.56
67:S2:1259:A:H62	67:S2:1518:C:H3'	1.70	0.56
67:S2:1673:U:H5''	74:SQ:78:VAL:HG12	1.87	0.56
75:SS:56:ALA:HA	75:SS:59:LEU:HD23	1.88	0.56
18:LO:34:VAL:HG22	18:LO:103:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SO:31:CYS:HB2	59:SO:93:LEU:HD22	1.88	0.56
76:ST:65:TYR:HE1	76:ST:128:GLN:HG3	1.71	0.56
67:S2:527:C:H2'	67:S2:528:A:C8	2.41	0.56
67:S2:1004:PSU:H2'	67:S2:1005:G:H8	1.70	0.56
82:Sg:164:ILE:HD11	82:Sg:176:VAL:HB	1.88	0.56
55:SI:57:ALA:HB1	55:SI:60:LEU:HD21	1.86	0.56
67:S2:149:A:H3'	67:S2:150:A:H8	1.71	0.56
61:SW:57:ARG:HD2	67:S2:919:A:H4'	1.88	0.56
67:S2:24:C:HO2'	67:S2:25:A:H8	1.51	0.56
67:S2:28:U:H2'	67:S2:29:G:H8	1.71	0.56
40:Lk:8:ILE:HD11	40:Lk:56:LEU:HD13	1.87	0.56
56:SJ:164:PRO:HB3	56:SJ:170:PRO:HA	1.87	0.56
67:S2:327:G:H5''	67:S2:328:U:C2	2.41	0.56
67:S2:649:PSU:H2'	67:S2:650:A:H8	1.71	0.56
2:L5:1270:A:H8	2:L5:2106:G:H21	1.53	0.56
75:SS:86:ARG:HH21	75:SS:106:LYS:HB3	1.71	0.56
32:Lc:48:LEU:HD13	32:Lc:57:LYS:HG3	1.89	0.55
2:L5:1094:G:O6	2:L5:1201:U:O2	2.24	0.55
6:LB:378:ARG:HE	26:LW:32:LEU:HD21	1.70	0.55
67:S2:640:A:H2'	67:S2:641:A:C8	2.40	0.55
51:SC:67:GLY:HA2	51:SC:70:VAL:HG12	1.88	0.55
68:SR:114:LEU:HB2	68:SR:117:LEU:HG	1.88	0.55
54:SH:74:LYS:HG3	54:SH:75:ILE:HG23	1.89	0.55
67:S2:1337:4AC:H2'	67:S2:1338:G:H8	1.70	0.55
2:L5:1258:G:H2'	2:L5:1259:G:C8	2.41	0.55
8:LD:223:PHE:HB3	8:LD:226:TYR:HB2	1.88	0.55
50:SB:186:ASN:HA	50:SB:189:ILE:HD12	1.88	0.55
51:SC:167:ARG:HB3	51:SC:177:PRO:HB2	1.89	0.55
67:S2:1310:U:H5''	81:Sf:130:VAL:HB	1.87	0.55
67:S2:1720:U:H5''	67:S2:1721:U:H5''	1.88	0.55
23:LT:119:ALA:HA	23:LT:122:LYS:HE3	1.89	0.55
44:Lo:33:LEU:HA	44:Lo:38:LYS:HG2	1.89	0.55
57:SL:73:LEU:HD11	57:SL:109:MET:HE1	1.89	0.55
2:L5:4699:U:H1'	2:L5:4700:A:H5''	1.87	0.55
48:Lt:77:ALA:HB3	48:Lt:80:LEU:HB2	1.89	0.55
52:SE:159:THR:HB	52:SE:173:ILE:HB	1.89	0.55
63:SY:36:PRO:HG3	67:S2:570:C:H4'	1.88	0.55
62:SX:71:ARG:HH21	62:SX:80:LYS:HB3	1.71	0.55
67:S2:874:G:H2'	67:S2:875:A:H8	1.72	0.55
2:L5:1100:U:O4	2:L5:1194:G:O6	2.24	0.55
64:Sa:38:LYS:HB2	64:Sa:71:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:1652:G:H1	67:S2:1672:U:H3	1.54	0.55
2:L5:1759:G:N2	2:L5:1773:U:O2	2.30	0.55
2:L5:5064:G:H21	19:LP:75:GLN:HE22	1.55	0.55
51:SC:210:PRO:HB3	51:SC:240:THR:HG21	1.89	0.55
75:SS:138:THR:HA	75:SS:141:ARG:HH21	1.72	0.55
31:Lb:109:ARG:HA	31:Lb:112:ILE:HG12	1.89	0.54
53:SG:56:ASN:HB2	53:SG:108:VAL:HG22	1.89	0.54
58:SN:103:GLU:HA	58:SN:106:ARG:HH11	1.71	0.54
67:S2:145:G:H2'	67:S2:146:G:C8	2.42	0.54
70:SF:87:LEU:HD11	74:SQ:47:LEU:HD11	1.89	0.54
2:L5:1994:C:H2'	2:L5:1995:G:C8	2.42	0.54
2:L5:4594:U:H2'	2:L5:4595:G:H8	1.73	0.54
2:L5:4743:G:H2'	2:L5:4744:A:C8	2.42	0.54
14:LJ:83:LEU:HD22	14:LJ:132:VAL:HG11	1.88	0.54
67:S2:149:A:N7	67:S2:169:U:O2	2.41	0.54
75:SS:25:LYS:HD3	75:SS:27:ALA:H	1.71	0.54
2:L5:691:C:H2'	2:L5:692:A:C8	2.41	0.54
51:SC:264:SER:HB3	51:SC:267:GLN:HG2	1.90	0.54
67:S2:528:A:H2'	67:S2:529:A:C8	2.43	0.54
67:S2:690:G:H3'	67:S2:691:G:H21	1.71	0.54
67:S2:888:U:H4'	67:S2:889:U:H5'	1.89	0.54
78:SZ:86:ALA:O	78:SZ:90:GLU:HG2	2.08	0.54
2:L5:3736:A:H2'	2:L5:3737:A:C8	2.42	0.54
11:LG:30:PRO:HG2	29:LZ:124:THR:HA	1.89	0.54
32:Lc:38:ILE:HD11	32:Lc:46:VAL:HG21	1.88	0.54
50:SB:125:VAL:HG21	50:SB:173:THR:HB	1.88	0.54
67:S2:996:A:H2'	67:S2:997:A:C8	2.42	0.54
70:SF:131:ALA:HA	70:SF:136:ARG:HG2	1.88	0.54
9:LE:165:LEU:HD11	9:LE:176:THR:HG22	1.90	0.54
56:SJ:127:ARG:HD3	66:Se:31:ARG:HD3	1.90	0.54
67:S2:159:A2M:O5'	67:S2:159:A2M:H8	2.07	0.54
67:S2:414:A:H2'	67:S2:415:A:H8	1.73	0.54
2:L5:268:G:H2'	2:L5:269:G:H8	1.73	0.54
5:LA:20:VAL:HA	5:LA:23:ARG:HG3	1.89	0.54
6:LB:50:LYS:HB2	6:LB:345:LEU:HD11	1.90	0.54
16:LM:38:VAL:HG21	16:LM:50:MET:HB3	1.90	0.54
67:S2:223:C:H2'	67:S2:224:A:C8	2.43	0.54
67:S2:1812:U:H2'	67:S2:1813:A:H8	1.73	0.54
2:L5:1826:G:H4'	31:Lb:43:MET:HE3	1.90	0.54
16:LM:122:ILE:HB	18:LO:189:ILE:HD11	1.90	0.54
66:Se:32:ALA:HB2	67:S2:525:A:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:432:G:H2'	67:S2:433:A:C8	2.42	0.54
2:L5:4967:A:H2'	2:L5:4968:A:H8	1.73	0.54
28:LY:4:ASN:HB3	28:LY:7:VAL:HG22	1.88	0.54
49:SA:76:VAL:HG12	49:SA:123:VAL:HB	1.88	0.54
69:SD:158:ILE:HG23	69:SD:189:MET:HE1	1.90	0.54
70:SF:187:SER:HB3	70:SF:190:ILE:HG12	1.90	0.54
2:L5:261:G:H2'	2:L5:262:G:C8	2.43	0.54
2:L5:654:C:H2'	2:L5:655:C:C6	2.43	0.54
2:L5:5064:G:N2	19:LP:75:GLN:HE22	2.06	0.54
32:Lc:38:ILE:HG21	32:Lc:63:TYR:HB3	1.88	0.54
49:SA:24:HIS:HD2	49:SA:48:ILE:HD12	1.72	0.54
56:SJ:18:ARG:HH21	67:S2:4:C:H1'	1.72	0.54
2:L5:989:U:O2	2:L5:1064:G:N2	2.36	0.53
73:SP:20:VAL:HG11	73:SP:36:LEU:HD21	1.90	0.53
2:L5:717:U:H2'	2:L5:718:C:C6	2.43	0.53
2:L5:1634:A:N7	2:L5:3922[A]:G:H4'	2.23	0.53
21:LR:127:VAL:HG12	21:LR:132:PHE:HD2	1.73	0.53
49:SA:49:ILE:HD13	49:SA:163:CYS:HA	1.90	0.53
58:SN:26:LEU:HD21	58:SN:60:VAL:HG12	1.89	0.53
62:SX:28:LYS:HD2	62:SX:32:LEU:HD22	1.91	0.53
67:S2:1051:G:H2'	67:S2:1052:A:H8	1.72	0.53
2:L5:3641:U:H5	2:L5:3646:A:N7	2.06	0.53
2:L5:4363:A:H5''	44:Lo:36:GLN:HG2	1.90	0.53
9:LE:264:ILE:HD11	9:LE:267:LEU:HD22	1.89	0.53
21:LR:92:LYS:HG2	21:LR:96:MET:HE3	1.91	0.53
59:SO:44:VAL:HG13	59:SO:53:ILE:HB	1.89	0.53
2:L5:262:G:H2'	2:L5:263:G:C8	2.43	0.53
2:L5:2362:U:H2'	2:L5:2363:A2M:H8	1.91	0.53
2:L5:4111:U:H2'	2:L5:4112:C:H5	1.73	0.53
53:SG:135:PRO:HA	67:S2:169:U:H5''	1.90	0.53
59:SO:59:GLY:HA2	59:SO:68:GLU:HG2	1.89	0.53
63:SY:10:ARG:HG3	63:SY:11:LYS:HG2	1.90	0.53
67:S2:1708:C:H2'	67:S2:1709:G:H8	1.73	0.53
2:L5:3867:A2M:H2'	2:L5:3868:G:O4'	2.08	0.53
2:L5:4612:C:C2	12:LH:120:GLU:HB2	2.43	0.53
14:LJ:22:LEU:HD22	14:LJ:128:LEU:HD12	1.89	0.53
50:SB:36:PRO:HB2	50:SB:38:MET:HG2	1.90	0.53
50:SB:66:VAL:HG11	50:SB:85:LYS:HE2	1.90	0.53
2:L5:2745:A:H2'	2:L5:2746:A:C8	2.44	0.53
2:L5:4537:C:H2'	2:L5:4538:G:C8	2.43	0.53
8:LD:62:CYS:HB3	8:LD:105:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LO:166:ILE:HG12	18:LO:169:ARG:HH21	1.73	0.53
71:SK:3:MET:HE1	71:SK:48:ALA:HB2	1.90	0.53
11:LG:180:PRO:HG3	11:LG:219:VAL:HG13	1.90	0.53
52:SE:146:THR:HG21	67:S2:122:G:H21	1.74	0.53
67:S2:1201:U:H2'	67:S2:1202:U:C6	2.44	0.53
67:S2:1677:U:H2'	67:S2:1678:A:H8	1.74	0.53
2:L5:1514:U:H2'	2:L5:1515:A:C8	2.44	0.53
2:L5:3946:G:N2	2:L5:4067:U:O2	2.39	0.53
2:L5:4274:A:H2'	2:L5:4275:G:H8	1.73	0.53
67:S2:508:A:H3'	67:S2:509:OMG:H8	1.74	0.53
2:L5:4251:A:H5''	14:LJ:108:GLY:HA3	1.90	0.53
2:L5:4967:A:H2'	2:L5:4968:A:C8	2.44	0.53
46:Lr:47:LYS:HB2	46:Lr:102:TYR:CZ	2.44	0.53
53:SG:22:ARG:HA	53:SG:25:ARG:HE	1.74	0.53
57:SL:111:VAL:HG12	57:SL:140:PHE:HB2	1.91	0.53
67:S2:1098:C:H2'	67:S2:1099:G:C8	2.44	0.53
72:SM:79:VAL:HG11	72:SM:85:LEU:HB2	1.90	0.53
2:L5:4392:OMG:H2'	2:L5:4447:5MC:HM51	1.91	0.53
54:SH:105:THR:HG23	54:SH:107:LYS:H	1.73	0.53
40:Lk:26:LYS:HB2	40:Lk:69:LEU:HD12	1.91	0.52
67:S2:543:C:H3'	67:S2:544:G:H8	1.74	0.52
67:S2:609:U:H2'	67:S2:610:G:H8	1.74	0.52
2:L5:93:G:H2'	2:L5:94:A:C8	2.45	0.52
2:L5:2745:A:H2'	2:L5:2746:A:H8	1.75	0.52
6:LB:29:VAL:HG12	6:LB:31:SER:H	1.74	0.52
47:Ls:91:THR:HG21	47:Ls:98:ILE:HG13	1.91	0.52
2:L5:3910:C:H2'	2:L5:3911:C:C6	2.44	0.52
6:LB:217:ILE:HD12	6:LB:347:LEU:HB3	1.92	0.52
67:S2:929:G:H2'	67:S2:930:C:O4'	2.08	0.52
67:S2:1536:G:H2'	67:S2:1537:A:C8	2.45	0.52
52:SE:136:ILE:HG21	52:SE:148:ARG:HH11	1.74	0.52
69:SD:8:LYS:HG2	77:SU:61:LEU:HD11	1.91	0.52
2:L5:4260:U:H2'	2:L5:4261:C:C6	2.45	0.52
2:L5:4954:G:H2'	2:L5:4955:A:C8	2.45	0.52
43:Ln:1:MET:HG3	67:S2:1706:G:H5'	1.91	0.52
49:SA:173:LEU:HD13	68:SR:91:LEU:HD12	1.92	0.52
57:SL:13:GLN:HB2	57:SL:16:ILE:HD12	1.91	0.52
79:Sc:20:ARG:HD3	79:Sc:28:THR:HG22	1.90	0.52
2:L5:735:G:H5''	16:LM:70:GLN:HG3	1.91	0.52
2:L5:989:U:H3	2:L5:1064:G:H1	1.58	0.52
2:L5:1366:G:H5''	15:LL:36:ARG:HH12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:3732:A:H2'	2:L5:3733:A:C8	2.44	0.52
16:LM:104:MET:HE3	16:LM:109:ARG:HG2	1.91	0.52
26:LW:102:LYS:HA	26:LW:105:ARG:HG2	1.91	0.52
54:SH:8:ILE:HG13	54:SH:9:VAL:HG23	1.90	0.52
67:S2:808:A:H2	67:S2:855:G:H22	1.58	0.52
67:S2:928:G:H1	67:S2:1013:U:H3	1.57	0.52
67:S2:1528:G:H2'	67:S2:1529:C:C6	2.45	0.52
77:SU:24:LEU:HD22	77:SU:112:VAL:HG12	1.92	0.52
2:L5:711:A:H2'	2:L5:712:C:C6	2.45	0.52
2:L5:4615:C:H5''	6:LB:357:ARG:HD2	1.91	0.52
5:LA:104:VAL:HA	5:LA:107:MET:HE3	1.91	0.52
24:LU:65:ARG:HG2	24:LU:67:LYS:H	1.75	0.52
61:SW:11:LEU:HD12	61:SW:74:VAL:HB	1.91	0.52
67:S2:118:C:H1'	67:S2:445:A:C5	2.45	0.52
67:S2:655:A:H4'	67:S2:656:G:H3'	1.92	0.52
2:L5:1538:U:H2'	2:L5:1539:G:H8	1.74	0.52
2:L5:4281:A:H2'	2:L5:4282:A:H2'	1.91	0.52
15:LL:59:VAL:HG21	15:LL:73:GLY:HA3	1.91	0.52
32:Lc:82:GLY:HA2	32:Lc:91:VAL:HG12	1.91	0.52
53:SG:63:MET:HE1	53:SG:102:VAL:HG12	1.92	0.52
62:SX:68:LYS:HG2	62:SX:91:LEU:HD22	1.92	0.52
67:S2:1423:C:H5	74:SQ:4:LYS:HE3	1.75	0.52
67:S2:1670:C:H2'	67:S2:1671:G:C8	2.45	0.52
76:ST:62:ARG:HH12	76:ST:66:LEU:HD11	1.75	0.52
2:L5:433:A:C2	2:L5:3867:A2M:H4'	2.45	0.52
6:LB:366:LYS:HB3	26:LW:1:MET:HG2	1.92	0.52
51:SC:78:LEU:HD12	51:SC:81:ILE:HD12	1.92	0.52
53:SG:4:ASN:HB3	53:SG:110:ASN:HA	1.92	0.52
54:SH:51:ILE:HG21	54:SH:179:LYS:HG2	1.92	0.52
63:SY:11:LYS:HB2	63:SY:24:VAL:HG12	1.92	0.52
67:S2:115:U:H2'	67:S2:116:OMU:C6	2.40	0.52
67:S2:1144:A:H2'	67:S2:1145:A:C8	2.44	0.52
67:S2:1362:U:H5''	67:S2:1363:C:H5	1.75	0.52
71:SK:64:TRP:HB3	80:Sd:23:VAL:HA	1.90	0.52
82:Sg:206:LEU:HD12	82:Sg:218:LEU:HD12	1.92	0.52
2:L5:1333:A:H2'	2:L5:1334:A:C8	2.45	0.52
50:SB:122:GLU:HG2	50:SB:140:VAL:HG12	1.92	0.52
50:SB:144:LYS:HB2	50:SB:206:PRO:HB2	1.91	0.52
53:SG:13:GLN:HE21	67:S2:153:G:H21	1.58	0.52
67:S2:349:A:H2'	67:S2:350:C:C6	2.45	0.52
69:SD:132:LYS:HB2	69:SD:189:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2491:C:H2'	2:L5:2492:C:C6	2.46	0.51
19:LP:54:GLN:HA	19:LP:83:TRP:CD1	2.45	0.51
53:SG:10:THR:HA	53:SG:128:THR:HG23	1.92	0.51
58:SN:7:PRO:HG3	67:S2:996:A:H5''	1.92	0.51
67:S2:943:U:H2'	67:S2:944:A:H8	1.76	0.51
67:S2:980:A:H2'	67:S2:981:A:C8	2.45	0.51
74:SQ:72:VAL:HG11	74:SQ:80:GLN:HG2	1.91	0.51
6:LB:92:TYR:HB3	6:LB:99:LEU:HD22	1.92	0.51
56:SJ:29:LEU:HD21	66:Se:37:GLN:HG3	1.92	0.51
59:SO:129:ILE:HG13	64:Sa:65:PRO:HG2	1.92	0.51
67:S2:1513:C:H2'	67:S2:1514:G:H8	1.74	0.51
2:L5:99:A:H5''	17:LN:184:ILE:HD12	1.92	0.51
2:L5:491:G:H2'	2:L5:492:U:C6	2.45	0.51
2:L5:1509:C:H5''	30:La:2:PRO:HD3	1.92	0.51
2:L5:4618:OMG:H5'	25:LV:15:ARG:HB2	1.93	0.51
7:LC:298:ILE:HD13	20:LQ:131:PRO:HB3	1.93	0.51
54:SH:142:LYS:HB3	61:SW:54:ASP:HB3	1.92	0.51
64:Sa:5:ARG:HH21	67:S2:1864:U:H3'	1.75	0.51
67:S2:1382:A:H2'	67:S2:1383:A2M:H8	1.92	0.51
75:SS:12:ILE:HD12	75:SS:19:ASN:HB2	1.92	0.51
2:L5:4537:C:H2'	2:L5:4538:G:H8	1.73	0.51
47:Ls:31:GLY:HA2	47:Ls:86:VAL:HG12	1.92	0.51
67:S2:388:U:H2'	67:S2:389:A:H8	1.76	0.51
67:S2:653:A:H2'	67:S2:654:A:O4'	2.11	0.51
67:S2:677:G:N2	67:S2:1028:A:H62	2.07	0.51
67:S2:751:G:H1'	67:S2:793:G:H21	1.76	0.51
67:S2:1644:C:H4'	74:SQ:140:ARG:HB2	1.92	0.51
2:L5:180:C:H2'	2:L5:181:C:H6	1.74	0.51
2:L5:1172:C:H42	2:L5:1188:C:H42	1.58	0.51
2:L5:4162:C:H5	11:LG:73:ARG:HH12	1.59	0.51
28:LY:10:ASP:HB3	28:LY:13:LYS:HB2	1.92	0.51
65:Sb:72:ARG:HH12	67:S2:1120:U:H5'	1.75	0.51
2:L5:2714:G:H2'	2:L5:2715:G:H8	1.75	0.51
2:L5:3898:G:H5'	6:LB:254:ILE:HG13	1.92	0.51
2:L5:3910:C:H2'	2:L5:3911:C:H6	1.76	0.51
57:SL:12:LYS:HD2	57:SL:18:GLN:HE22	1.75	0.51
67:S2:454:U:H2'	67:S2:455:A:H8	1.76	0.51
67:S2:1405:A:H2'	67:S2:1406:G:O4'	2.09	0.51
74:SQ:18:THR:H	74:SQ:126:ARG:HH11	1.57	0.51
2:L5:4188:U:H2'	2:L5:4189:U:C6	2.46	0.51
13:LI:87:MET:HG2	13:LI:138:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:71:LEU:HD21	50:SB:189:ILE:HG23	1.91	0.51
54:SH:140:VAL:HG12	58:SN:19:ARG:HD3	1.93	0.51
61:SW:111:MET:HE3	61:SW:116:ALA:HA	1.92	0.51
67:S2:639:C:H2'	67:S2:640:A:C8	2.45	0.51
67:S2:1417:C:N3	67:S2:1422:G:N1	2.45	0.51
68:SR:27:ASP:HB3	68:SR:30:THR:HB	1.91	0.51
2:L5:325:U:H2'	2:L5:326:C:C6	2.45	0.51
2:L5:2640:G:H2'	2:L5:2641:A:C8	2.46	0.51
2:L5:3922[A]:G:C2	5:LA:208:GLU:HG3	2.46	0.51
2:L5:4742:G:H2'	2:L5:4743:G:H8	1.75	0.51
56:SJ:32:ILE:HG12	56:SJ:37:LEU:HB2	1.93	0.51
67:S2:1801:A:H2'	67:S2:1802:C:C6	2.46	0.51
10:LF:182:TYR:HB3	10:LF:200:ARG:HG3	1.93	0.51
13:LI:152:LEU:HB3	13:LI:165:ILE:HD12	1.92	0.51
14:LJ:146:ARG:HG2	14:LJ:147:ARG:HG3	1.93	0.51
53:SG:145:PHE:HD2	53:SG:156:TYR:HD2	1.58	0.51
67:S2:165:G:H2'	67:S2:166:A2M:H8	1.93	0.51
67:S2:291:G:H2'	67:S2:292:A:C8	2.46	0.51
2:L5:497:G:H21	2:L5:498:C:H5	1.58	0.51
2:L5:1577:G:O2'	2:L5:1612:G:H4'	2.11	0.51
5:LA:206:PRO:HG3	5:LA:213:GLY:HA3	1.92	0.51
31:Lb:5:LYS:HE2	31:Lb:8:THR:HB	1.92	0.51
35:Lf:15:LYS:HB3	35:Lf:25:THR:HG23	1.93	0.51
54:SH:30:LEU:HG	54:SH:33:ASN:HD22	1.75	0.51
67:S2:329:G:H2'	67:S2:330:G:C8	2.46	0.51
67:S2:1562:C:H2'	67:S2:1563:G:C8	2.46	0.51
75:SS:80:PRO:HG2	76:ST:36:THR:HG21	1.91	0.51
2:L5:1308:C:H2'	2:L5:1309:C:C6	2.46	0.50
8:LD:204:VAL:HB	8:LD:236:MET:HE1	1.93	0.50
33:Ld:57:MET:HG2	33:Ld:88:LEU:HD23	1.93	0.50
52:SE:233:LYS:HD2	52:SE:234:PRO:HD2	1.92	0.50
53:SG:23:LYS:HZ2	53:SG:41:LEU:HA	1.76	0.50
64:Sa:79:ILE:HD11	67:S2:1864:U:H5'	1.93	0.50
67:S2:146:G:H2'	67:S2:147:A:C8	2.46	0.50
67:S2:454:U:H2'	67:S2:455:A:C8	2.47	0.50
67:S2:1112:U:O2	67:S2:1121:G:O6	2.29	0.50
73:SP:22:LEU:HA	73:SP:25:LEU:HB2	1.92	0.50
2:L5:1188:C:H2'	2:L5:1189:G:H8	1.75	0.50
2:L5:2765:A:H2'	2:L5:2766:A:C8	2.45	0.50
67:S2:795:A:H2'	67:S2:796:G:C8	2.46	0.50
7:LC:218:ILE:HA	7:LC:229:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LS:161:ARG:HD2	22:LS:164:LYS:HB2	1.92	0.50
37:Lh:80:PRO:HD2	37:Lh:83:LEU:HD12	1.93	0.50
67:S2:1407:U:H2'	67:S2:1408:U:C6	2.46	0.50
74:SQ:97:GLN:HB2	74:SQ:105:LYS:HE3	1.93	0.50
81:Sf:103:LEU:HB2	81:Sf:105:TYR:CE2	2.46	0.50
82:Sg:163:PRO:HB2	82:Sg:179:LEU:HD12	1.92	0.50
2:L5:2539:C:H2'	2:L5:2540:C:C6	2.47	0.50
6:LB:219:VAL:HG11	6:LB:337:VAL:HG13	1.94	0.50
8:LD:211:LEU:HB3	8:LD:219:TYR:HB2	1.94	0.50
26:LW:83:THR:HG22	53:SG:161:PRO:HD2	1.92	0.50
67:S2:1277:C:H2'	67:S2:1278:A:C8	2.45	0.50
67:S2:1447:G:H2'	67:S2:1448:A:C8	2.47	0.50
2:L5:518:G:H1	2:L5:643:C:H2'	1.77	0.50
2:L5:679:C:H2'	2:L5:680:G:H8	1.76	0.50
9:LE:190:HIS:HB3	9:LE:193:PHE:HD2	1.76	0.50
11:LG:176:LYS:HG2	38:Li:43:MET:HE1	1.93	0.50
67:S2:1616:U:H2'	67:S2:1617:G:C8	2.47	0.50
67:S2:1670:C:H2'	67:S2:1671:G:H8	1.77	0.50
75:SS:20:ILE:HG22	75:SS:32:ALA:HB3	1.94	0.50
82:Sg:21:ILE:HG21	82:Sg:299:PHE:HB2	1.94	0.50
2:L5:3615:G:H1'	26:LW:44:ARG:HD3	1.93	0.50
5:LA:248:GLY:HA2	67:S2:1069:U:H5''	1.93	0.50
49:SA:120:ARG:HD2	51:SC:266:TYR:HB3	1.93	0.50
67:S2:1337:4AC:O5'	67:S2:1337:4AC:H6	2.11	0.50
67:S2:1643:U:H2'	67:S2:1644:C:C6	2.47	0.50
2:L5:1175:A:H2	2:L5:1185:G:H22	1.59	0.50
5:LA:201:GLY:HA2	5:LA:204:MET:HE3	1.94	0.50
20:LQ:50:ARG:HH21	20:LQ:140:SER:HB2	1.75	0.50
34:Le:108:ARG:HD2	34:Le:128:ARG:HB2	1.94	0.50
74:SQ:58:LEU:HD21	74:SQ:112:LEU:HG	1.94	0.50
75:SS:125:HIS:CD2	75:SS:131:VAL:HG11	2.46	0.50
2:L5:3949:A:H2	2:L5:4064:C:H42	1.58	0.50
6:LB:168:MET:HE2	6:LB:171:LEU:HD12	1.94	0.50
11:LG:209:SER:HA	11:LG:212:LYS:HG3	1.94	0.50
14:LJ:141:ILE:HA	14:LJ:144:LYS:HD2	1.94	0.50
15:LL:142:GLU:HA	15:LL:146:LEU:HD12	1.93	0.50
57:SL:120:VAL:HG22	57:SL:145:VAL:HG11	1.94	0.50
69:SD:141:LYS:HE2	69:SD:179:GLN:HB3	1.94	0.50
77:SU:80:PHE:HB3	80:Sd:52:PHE:HB3	1.93	0.50
2:L5:2448:G:H2'	2:L5:2449:A:C8	2.47	0.50
2:L5:3922[A]:G:H22	5:LA:204:MET:HG2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:300:U:H2'	67:S2:301:A:C8	2.47	0.50
70:SF:134:VAL:HG12	70:SF:135:ARG:HG2	1.94	0.50
2:L5:1857:C:H2'	2:L5:1858:A:H8	1.76	0.49
2:L5:1867:A:H2'	2:L5:1868:A:C8	2.47	0.49
6:LB:206:PRO:HG2	6:LB:209:GLN:HG3	1.94	0.49
60:SV:30:ALA:O	60:SV:60:ARG:HD3	2.12	0.49
67:S2:388:U:H2'	67:S2:389:A:C8	2.46	0.49
67:S2:1804:U:H2'	67:S2:1805:G:H8	1.77	0.49
26:LW:87:LEU:HD12	26:LW:90:ILE:HD11	1.93	0.49
67:S2:1595:U:H2'	67:S2:1596:U:C6	2.47	0.49
67:S2:1705:C:H2'	67:S2:1706:G:C8	2.47	0.49
76:ST:18:LEU:HD22	76:ST:58:ALA:HA	1.95	0.49
5:LA:101:VAL:HG22	5:LA:165:VAL:HG22	1.94	0.49
50:SB:171:ILE:HD11	50:SB:197:ILE:HA	1.94	0.49
80:Sd:3:HIS:CE1	80:Sd:5:GLN:HB2	2.47	0.49
2:L5:729:G:H5''	10:LF:76:ARG:HD2	1.94	0.49
2:L5:1332:C:H2'	2:L5:1333:A:C8	2.47	0.49
2:L5:1631:A:H2	5:LA:204:MET:HE2	1.78	0.49
16:LM:36:ALA:HB3	16:LM:55:MET:HE1	1.93	0.49
51:SC:68:ARG:HG2	51:SC:277:HIS:HB2	1.92	0.49
53:SG:133:LEU:HD12	67:S2:65:C:C4	2.47	0.49
64:Sa:73:TYR:HB3	64:Sa:78:ALA:HB2	1.95	0.49
67:S2:525:A:H2'	67:S2:526:A:H8	1.76	0.49
67:S2:1337:4AC:H2'	67:S2:1338:G:C8	2.46	0.49
75:SS:63:GLU:HG2	75:SS:66:ARG:HH21	1.76	0.49
82:Sg:212:LYS:HA	82:Sg:235:ILE:HG22	1.93	0.49
82:Sg:217:MET:HG3	82:Sg:229:THR:HG23	1.95	0.49
2:L5:3946:G:H1	2:L5:4067:U:H3	1.60	0.49
17:LN:146:PRO:HB2	37:Lh:104:THR:HG23	1.94	0.49
67:S2:588:G:H4'	67:S2:589:G:H5'	1.93	0.49
67:S2:952:G:H2'	67:S2:953:C:C6	2.48	0.49
78:SZ:99:LEU:HD11	78:SZ:102:LYS:HE2	1.93	0.49
2:L5:3861:A:H2'	2:L5:3862:A:C8	2.47	0.49
2:L5:4345:C:O2'	44:Lo:82:MET:HE3	2.13	0.49
2:L5:4457:PSU:H1'	6:LB:252:ALA:HB3	1.94	0.49
31:Lb:65:MET:HG3	31:Lb:68:ARG:HH12	1.78	0.49
49:SA:77:ILE:HD13	49:SA:122:LEU:HD11	1.94	0.49
54:SH:31:GLU:HA	54:SH:37:LYS:HG3	1.95	0.49
63:SY:41:ARG:HG3	63:SY:55:ILE:HB	1.95	0.49
66:Se:58:ASN:ND2	67:S2:606:G:H1'	2.27	0.49
67:S2:1093:A:H2'	67:S2:1094:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:300:A:H2'	2:L5:301:G:H8	1.78	0.49
2:L5:4474:A:H5''	42:Lm:125:LYS:HG3	1.95	0.49
18:LO:9:LEU:HD23	18:LO:118:MET:HB2	1.94	0.49
67:S2:857:U:H2'	67:S2:858:A:C8	2.47	0.49
2:L5:1199:G:H2'	2:L5:1200:G:C8	2.48	0.49
2:L5:1253:G:H2'	2:L5:1256:G:H5'	1.94	0.49
6:LB:27:GLY:HA2	6:LB:276:HIS:CD2	2.47	0.49
9:LE:261:ILE:HG23	9:LE:267:LEU:HD23	1.94	0.49
49:SA:184:ARG:HB3	49:SA:191:ARG:NE	2.28	0.49
52:SE:59:ASP:O	52:SE:63:LYS:HG3	2.12	0.49
67:S2:1139:C:H2'	67:S2:1140:G:O4'	2.13	0.49
71:SK:80:ARG:NH1	71:SK:87:PRO:HA	2.28	0.49
2:L5:1733:G:N3	2:L5:4214:A:H2'	2.28	0.49
6:LB:161:ARG:HG2	6:LB:184:GLN:HA	1.95	0.49
55:SI:141:ARG:HD3	55:SI:145:ILE:HG21	1.94	0.49
67:S2:12:U:H2'	67:S2:13:C:C6	2.47	0.49
67:S2:85:A:H2'	67:S2:86:C:H6	1.78	0.49
67:S2:562:U:H2'	67:S2:563:G:C8	2.48	0.49
67:S2:1854:U:H2'	67:S2:1855:G:C8	2.44	0.49
81:Sf:119:ARG:HB3	81:Sf:132:MET:HB2	1.94	0.49
2:L5:1503:A:H4'	2:L5:1504:G:H5'	1.95	0.49
2:L5:1767:A:H2'	2:L5:1769:G:H5''	1.94	0.49
2:L5:3951:G:H1'	2:L5:4062:A:H61	1.77	0.49
2:L5:4935:C:H2'	2:L5:4936:G:C8	2.48	0.49
5:LA:13:GLY:O	5:LA:17:ARG:HG3	2.13	0.49
10:LF:127:LYS:HB2	23:LT:133:ALA:HB3	1.95	0.49
49:SA:198:MET:HE3	68:SR:85:VAL:HG13	1.94	0.49
50:SB:128:LYS:HE3	50:SB:134:LEU:HD13	1.95	0.49
58:SN:5:HIS:HB3	58:SN:117:LEU:HD13	1.94	0.49
67:S2:925:G:H2'	67:S2:926:A:H8	1.77	0.49
67:S2:1499:U:H2'	67:S2:1500:G:H8	1.77	0.49
2:L5:280:G:H5''	17:LN:14:LYS:HE2	1.94	0.48
2:L5:1914:C:H4'	18:LO:89:PRO:HD3	1.95	0.48
67:S2:1714:U:H2'	67:S2:1715:A:C8	2.48	0.48
2:L5:4440:G:H5'	13:LI:108:ALA:HB2	1.95	0.48
2:L5:4775:C:N4	2:L5:4859:C:H42	2.11	0.48
67:S2:1347:U:H2'	67:S2:1348:G:N3	2.28	0.48
2:L5:702:U:H2'	2:L5:703:G:O4'	2.12	0.48
12:LH:95:VAL:HG12	42:Lm:82:LEU:HD13	1.95	0.48
17:LN:200:LEU:HD22	17:LN:204:ARG:HH11	1.79	0.48
21:LR:164:SER:HA	21:LR:167:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SG:67:VAL:HG12	53:SG:69:THR:HG22	1.95	0.48
67:S2:746:C:H2'	67:S2:747:U:C6	2.48	0.48
67:S2:907:G:H2'	67:S2:908:A:C8	2.47	0.48
67:S2:1103:C:H2'	67:S2:1104:G:C8	2.47	0.48
75:SS:12:ILE:HG22	75:SS:21:ASP:HA	1.95	0.48
3:L7:119:U:C2	8:LD:261:VAL:HG11	2.48	0.48
14:LJ:95:ARG:HD2	14:LJ:177:GLY:HA3	1.94	0.48
50:SB:75:GLN:HB2	50:SB:78:GLU:HB2	1.95	0.48
51:SC:166:ARG:HB3	51:SC:247:THR:HB	1.95	0.48
67:S2:186:C:H2'	67:S2:187:G:C8	2.48	0.48
67:S2:382:C:H2'	67:S2:383:G:C8	2.47	0.48
67:S2:1010:G:H2'	67:S2:1011:A:H8	1.79	0.48
67:S2:1393:G:H2'	67:S2:1394:G:C8	2.49	0.48
2:L5:162:A:H2'	2:L5:163:A:C8	2.49	0.48
2:L5:432:U:H1'	84:L5:5292:SPM:H82	1.95	0.48
2:L5:2676:A:OP2	2:L5:2676:A:H8	1.96	0.48
2:L5:3732:A:H2'	2:L5:3733:A:H8	1.77	0.48
8:LD:156:GLY:HA2	8:LD:181:PRO:HG3	1.95	0.48
23:LT:44:GLY:HA2	23:LT:95:HIS:HB3	1.94	0.48
44:Lo:4:VAL:HG23	44:Lo:93:LEU:HD23	1.95	0.48
51:SC:102:LEU:HD23	51:SC:130:ILE:HD12	1.95	0.48
74:SQ:90:LYS:HA	74:SQ:93:VAL:HG22	1.95	0.48
2:L5:737:C:C5	2:L5:739:G:H5''	2.49	0.48
2:L5:907:C:H2'	2:L5:908:G:H8	1.79	0.48
2:L5:1632:A:N6	2:L5:3922[A]:G:P	2.86	0.48
2:L5:2520:C:H2'	2:L5:2521:G:H8	1.78	0.48
4:L8:90:C:H1'	28:LY:24:HIS:HB3	1.96	0.48
4:L8:141:C:H2'	4:L8:142:U:C6	2.49	0.48
18:LO:168:TYR:CE2	18:LO:172:LYS:HD2	2.48	0.48
67:S2:17:C:H2'	67:S2:18:C:C6	2.48	0.48
67:S2:1802:C:H2'	67:S2:1803:U:C6	2.48	0.48
2:L5:457:G:H2'	2:L5:458:C:C6	2.49	0.48
2:L5:2696:A:H62	40:Lk:35:LYS:NZ	2.10	0.48
50:SB:97:LEU:HD23	50:SB:232:HIS:CG	2.49	0.48
2:L5:1307:A:H2'	2:L5:1308:C:C6	2.48	0.48
2:L5:2102:G:H1'	2:L5:2103:G:C8	2.48	0.48
2:L5:2492:C:H2'	2:L5:2493:G:H8	1.79	0.48
2:L5:2870:A:H2'	2:L5:2871:A:C8	2.48	0.48
2:L5:3726:A:H2'	2:L5:3727:A:C8	2.49	0.48
69:SD:163:PRO:HA	69:SD:166:TYR:CZ	2.49	0.48
73:SP:81:ARG:HB2	73:SP:117:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:ST:64:LEU:HD12	76:ST:122:LYS:HA	1.95	0.48
82:Sg:42:MET:SD	82:Sg:57:ARG:HB2	2.54	0.48
2:L5:1411:C:H2'	2:L5:1412:G:C8	2.49	0.48
2:L5:1629:G:H22	2:L5:3922[A]:G:N2	2.11	0.48
4:L8:8:U:H2'	4:L8:9:A:C8	2.49	0.48
8:LD:64:ILE:HD13	8:LD:109:LEU:HD22	1.95	0.48
55:SI:101:ILE:HD12	55:SI:172:LEU:HD13	1.95	0.48
67:S2:1568:C:H2'	67:S2:1569:A:C8	2.49	0.48
2:L5:318:A:H2'	2:L5:319:A:C8	2.49	0.48
2:L5:1259:G:H2'	2:L5:1260:G:H8	1.79	0.48
2:L5:3861:A:H2'	2:L5:3862:A:H8	1.79	0.48
55:SI:25:ARG:HA	67:S2:448:A:H5''	1.94	0.48
56:SJ:119:LEU:HD13	56:SJ:135:ILE:HD11	1.96	0.48
57:SL:124:ASP:HA	57:SL:148:ALA:HB2	1.96	0.48
67:S2:223:C:H2'	67:S2:224:A:H8	1.78	0.48
67:S2:1208:A:H2'	67:S2:1209:A:H8	1.79	0.48
2:L5:418:A:C2	4:L8:17:A:H1'	2.49	0.47
2:L5:1971:C:H2'	2:L5:1972:G:C8	2.49	0.47
2:L5:3661:G:H4'	2:L5:3662:A:H5'	1.96	0.47
2:L5:3880:G:H2'	2:L5:3881:G:C8	2.48	0.47
52:SE:141:THR:HG23	52:SE:143:ASP:H	1.79	0.47
53:SG:2:LYS:HD3	53:SG:15:LEU:HD21	1.95	0.47
56:SJ:111:GLN:HE21	56:SJ:123:ILE:HG13	1.78	0.47
70:SF:35:LEU:O	70:SF:39:ILE:HG12	2.13	0.47
73:SP:32:GLN:HA	73:SP:35:GLN:HG2	1.95	0.47
2:L5:1095:A:N1	2:L5:1200:G:C6	2.82	0.47
2:L5:1677:PSU:H4'	2:L5:1680:G:C2	2.49	0.47
2:L5:4220:6MZ:O5'	2:L5:4220:6MZ:H8	2.14	0.47
2:L5:5006:U:H4'	2:L5:5007:A:H5'	1.96	0.47
8:LD:182:GLY:HA2	8:LD:194:VAL:HG23	1.97	0.47
55:SI:139:LYS:HE2	55:SI:139:LYS:HB2	1.65	0.47
67:S2:600:G:H2'	67:S2:601:OMG:C8	2.48	0.47
67:S2:656:G:H5'	67:S2:662:G:N2	2.29	0.47
67:S2:991:G:C6	67:S2:1134:G:H4'	2.48	0.47
67:S2:1661:A:H8	80:Sd:14:PHE:HB2	1.79	0.47
77:SU:19:ARG:HE	77:SU:92:HIS:CD2	2.32	0.47
2:L5:162:A:H2'	2:L5:163:A:H8	1.79	0.47
2:L5:1662:C:H2'	2:L5:1663:C:C6	2.49	0.47
2:L5:4260:U:H2'	2:L5:4261:C:H6	1.79	0.47
4:L8:96:C:H5''	37:Lh:66:LYS:HG2	1.96	0.47
41:Ll:42:ARG:HG3	41:Ll:47:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SJ:137:VAL:HG12	56:SJ:138:ARG:HG2	1.96	0.47
63:SY:90:ARG:HA	63:SY:93:ARG:HD2	1.96	0.47
67:S2:468:A2M:HM'3	67:S2:468:A2M:H1'	1.72	0.47
70:SF:60:ARG:HH21	79:Sc:49:PRO:HA	1.79	0.47
82:Sg:8:ARG:HB3	82:Sg:309:VAL:HG13	1.97	0.47
2:L5:1933:G:H2'	2:L5:1934:A:C8	2.49	0.47
2:L5:3766:A:H1'	67:S2:1708:C:H1'	1.96	0.47
2:L5:3917:A:H2'	2:L5:3918:G:H8	1.79	0.47
2:L5:4594:U:H2'	2:L5:4595:G:C8	2.49	0.47
2:L5:4637:OMG:HM23	2:L5:4637:OMG:H1'	1.70	0.47
3:L7:110:G:H2'	3:L7:111:C:C6	2.49	0.47
10:LF:93:ILE:HG21	10:LF:247:MET:HE3	1.96	0.47
12:LH:102:ASN:HB2	12:LH:115:ARG:HB2	1.96	0.47
52:SE:26:VAL:HG22	56:SJ:4:ALA:HB2	1.96	0.47
52:SE:246:LEU:HB2	52:SE:250:GLU:HG3	1.96	0.47
63:SY:35:VAL:HG13	63:SY:40:ILE:HD11	1.96	0.47
67:S2:1298:G:H4'	73:SP:78:THR:HA	1.97	0.47
67:S2:1438:A:H2'	67:S2:1439:A:C8	2.49	0.47
67:S2:1648:G:H5''	74:SQ:125:ARG:HB2	1.95	0.47
81:Sf:89:LYS:HG2	81:Sf:90:LYS:O	2.14	0.47
2:L5:158:A:H5''	2:L5:159:C:H2'	1.96	0.47
28:LY:126:ARG:HG2	28:LY:130:LYS:HE2	1.97	0.47
29:LZ:50:PRO:HD3	29:LZ:68:ILE:HG12	1.95	0.47
52:SE:29:PRO:HA	67:S2:496:C:H5'	1.97	0.47
58:SN:46:THR:HB	58:SN:86:GLU:HG3	1.97	0.47
67:S2:432:G:H2'	67:S2:433:A:H8	1.78	0.47
67:S2:1305:C:H2'	67:S2:1306:U:C6	2.49	0.47
2:L5:423:G:H5'	19:LP:26:PHE:HZ	1.79	0.47
2:L5:513:U:H3'	2:L5:514:U:H4'	1.96	0.47
2:L5:1097:C:H2'	2:L5:1098:G:C8	2.49	0.47
2:L5:1468:C:H2'	2:L5:1469:C:C6	2.49	0.47
2:L5:3765:G:H21	2:L5:3766:A:N6	2.13	0.47
50:SB:85:LYS:HB2	50:SB:101:HIS:HB3	1.96	0.47
53:SG:157:VAL:HG11	53:SG:176:ILE:HD13	1.97	0.47
59:SO:43:HIS:CD2	59:SO:55:ARG:HB2	2.50	0.47
67:S2:1136:U:H2'	67:S2:1137:U:C6	2.49	0.47
67:S2:1539:U:H4'	76:ST:47:PRO:HA	1.96	0.47
81:Sf:114:ILE:HD11	81:Sf:116:ARG:NH1	2.29	0.47
2:L5:138:G:H2'	2:L5:139:G:H8	1.80	0.47
2:L5:1565:A:C5	2:L5:1566:C:H1'	2.49	0.47
2:L5:1617:G:H1'	2:L5:2513:A:N6	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1629:G:N1	2:L5:3922[A]:G:C4	2.72	0.47
2:L5:1788:A:H2'	13:LI:22:PHE:CZ	2.50	0.47
2:L5:2303:C:H5''	34:Le:104:SER:HB3	1.96	0.47
2:L5:2412:A:H2'	2:L5:2413:U:C6	2.49	0.47
2:L5:3720:G:H22	2:L5:3733:A:H2	1.61	0.47
2:L5:3923:A:H2'	2:L5:3924:C:C6	2.49	0.47
55:SI:103:LEU:HD13	55:SI:170:LYS:HE2	1.97	0.47
56:SJ:129:LEU:HD21	56:SJ:159:PHE:HE1	1.78	0.47
64:Sa:79:ILE:HD13	67:S2:1863:A:H1'	1.96	0.47
67:S2:5:U:H2'	67:S2:6:G:H8	1.79	0.47
67:S2:300:U:H2'	67:S2:301:A:H8	1.78	0.47
67:S2:414:A:H2'	67:S2:415:A:C8	2.50	0.47
67:S2:1446:A:H5''	77:SU:58:THR:HG23	1.97	0.47
67:S2:1777:G:H2'	67:S2:1778:C:H6	1.80	0.47
67:S2:1804:U:H2'	67:S2:1805:G:C8	2.50	0.47
70:SF:133:THR:HG22	70:SF:134:VAL:HG23	1.96	0.47
2:L5:444:G:H2'	2:L5:445:U:C6	2.49	0.47
2:L5:1414:C:H2'	2:L5:1415:G:C8	2.46	0.47
2:L5:1907:A:H2'	2:L5:1908:A:C8	2.50	0.47
2:L5:2568:C:H2'	2:L5:2569:G:C8	2.50	0.47
2:L5:2744:A:H2'	2:L5:2745:A:C8	2.49	0.47
2:L5:4459:U:H2'	2:L5:4460:U:C6	2.49	0.47
2:L5:4530:UR3:H2'	2:L5:4531:U:H2'	1.96	0.47
18:LO:81:TRP:HB2	18:LO:104:VAL:HG21	1.97	0.47
33:Ld:22:THR:HG23	33:Ld:122:VAL:HG13	1.96	0.47
54:SH:43:LEU:HD12	54:SH:72:PHE:CE2	2.49	0.47
55:SI:130:THR:HA	55:SI:133:GLU:HG3	1.96	0.47
67:S2:1217:A:H2'	67:S2:1218:C:C6	2.50	0.47
67:S2:1628:C:H2'	67:S2:1629:C:C6	2.50	0.47
67:S2:1665:G:C6	76:ST:88:MET:HE1	2.49	0.47
70:SF:101:HIS:HB2	70:SF:108:PRO:HG3	1.97	0.47
82:Sg:288:SER:HB3	82:Sg:301:GLY:H	1.80	0.47
2:L5:25:A:H2'	2:L5:26:C:H6	1.80	0.47
2:L5:1968:G:H2'	2:L5:1969:G:C8	2.50	0.47
2:L5:2018:C:H2'	2:L5:2019:C:C6	2.50	0.47
2:L5:2483:G:O6	2:L5:2495:U:O4	2.33	0.47
2:L5:4601:U:H2'	2:L5:4602:A:H8	1.79	0.47
2:L5:4611:A:H2'	2:L5:4612:C:H6	1.80	0.47
12:LH:4:ILE:HG12	12:LH:61:TRP:CH2	2.50	0.47
67:S2:1597:C:H4'	67:S2:1603:G:O6	2.14	0.47
2:L5:665:C:H4'	2:L5:666:G:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1504:G:H2'	2:L5:1505:C:C6	2.50	0.47
2:L5:4239:A:H2'	2:L5:4240:G:C8	2.49	0.47
6:LB:258:HIS:HA	6:LB:260:ALA:N	2.29	0.47
67:S2:656:G:H21	67:S2:663:C:H5''	1.79	0.47
67:S2:1203:G:H2'	67:S2:1204:A:C8	2.50	0.47
67:S2:1506:A:H4'	67:S2:1507:G:H3'	1.97	0.47
68:SR:58:MET:HA	68:SR:61:ILE:HG22	1.97	0.47
2:L5:425:U:H4'	19:LP:6:LEU:HD21	1.97	0.46
2:L5:4723:A:H2'	2:L5:4724:A:C8	2.50	0.46
5:LA:180:LEU:HD22	45:Lp:18:TYR:HB3	1.97	0.46
26:LW:52:THR:O	26:LW:56:ARG:HG2	2.14	0.46
28:LY:22:PRO:HD2	28:LY:25:ILE:HD11	1.97	0.46
63:SY:33:ALA:HB2	67:S2:582:U:H1'	1.96	0.46
67:S2:27:A2M:HM'3	67:S2:27:A2M:H1'	1.53	0.46
67:S2:864:A:H2'	67:S2:865:A:C8	2.50	0.46
75:SS:40:TYR:HA	75:SS:83:PHE:HE2	1.80	0.46
2:L5:153:G:H2'	2:L5:154:G:H8	1.79	0.46
2:L5:457:G:H2'	2:L5:458:C:H6	1.80	0.46
26:LW:2:LYS:HE3	26:LW:15:PRO:HB3	1.97	0.46
35:Lf:45:LYS:NZ	35:Lf:108:SER:HA	2.31	0.46
49:SA:111:GLN:HA	49:SA:116:PHE:CG	2.51	0.46
56:SJ:29:LEU:HB3	66:Se:42:PHE:HE2	1.80	0.46
2:L5:44:A:H5''	84:L5:5264:SPM:H81	1.96	0.46
2:L5:267:G:H2'	2:L5:268:G:H8	1.79	0.46
2:L5:1702:C:H2'	2:L5:1703:C:C6	2.50	0.46
9:LE:222:LEU:HB2	9:LE:237:LYS:HD2	1.97	0.46
19:LP:17:SER:HB2	19:LP:98:ALA:HB2	1.96	0.46
50:SB:103:MET:HE3	50:SB:103:MET:HB3	1.81	0.46
50:SB:109:LYS:O	50:SB:113:MET:HG3	2.15	0.46
51:SC:64:THR:HG22	51:SC:66:LEU:H	1.80	0.46
52:SE:161:GLN:HG3	52:SE:170:THR:HB	1.97	0.46
53:SG:103:ASP:H	53:SG:106:LEU:HD13	1.81	0.46
59:SO:78:ALA:HB1	59:SO:119:LEU:HG	1.97	0.46
70:SF:68:ILE:HD11	70:SF:116:ILE:HG13	1.97	0.46
73:SP:20:VAL:HG23	73:SP:24:GLN:HE21	1.79	0.46
75:SS:51:ASP:HB3	75:SS:54:LYS:HE3	1.97	0.46
2:L5:2764:A:H2'	2:L5:2765:A:H8	1.78	0.46
2:L5:3585:G:H2'	2:L5:3586:G:H8	1.80	0.46
2:L5:3758:U:H2'	2:L5:3765:G:N2	2.31	0.46
43:Ln:1:MET:HB2	43:Ln:6:ARG:HG3	1.97	0.46
48:Lt:19:GLY:HA2	48:Lt:48:LYS:HZ3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SW:69:LEU:HD21	61:SW:72:CYS:HB3	1.97	0.46
67:S2:525:A:H2'	67:S2:526:A:C8	2.51	0.46
2:L5:37:U:H2'	2:L5:38:A:O4'	2.16	0.46
2:L5:2400:G:H21	36:Lg:6:THR:HG22	1.81	0.46
2:L5:4196:OMG:HM23	2:L5:4196:OMG:H1'	1.68	0.46
2:L5:4524:G:C2	6:LB:252:ALA:HB1	2.51	0.46
49:SA:122:LEU:HB3	49:SA:144:THR:HG22	1.96	0.46
70:SF:127:ARG:HB3	70:SF:136:ARG:HB2	1.97	0.46
82:Sg:10:THR:HB	82:Sg:306:LEU:HD21	1.97	0.46
2:L5:400:A2M:H1'	2:L5:400:A2M:HM'3	1.60	0.46
7:LC:169:LEU:O	7:LC:173:LYS:HG2	2.15	0.46
17:LN:140:LYS:HD3	17:LN:140:LYS:HA	1.70	0.46
37:Lh:89:ARG:O	37:Lh:93:ARG:HG2	2.16	0.46
52:SE:181:CYS:HA	52:SE:227:VAL:HA	1.97	0.46
54:SH:66:VAL:HG11	67:S2:913:A:N3	2.30	0.46
64:Sa:45:VAL:HG22	64:Sa:64:LEU:HD21	1.97	0.46
67:S2:323:C:H2'	67:S2:327:G:H1	1.79	0.46
67:S2:509:OMG:H2'	67:S2:510:G:H8	1.80	0.46
67:S2:1010:G:H2'	67:S2:1011:A:C8	2.51	0.46
2:L5:223:G:H4'	2:L5:225:G:N7	2.30	0.46
2:L5:1172:C:O2'	2:L5:1173:G:H8	1.99	0.46
2:L5:1278:C:H2'	2:L5:1279:A:O4'	2.16	0.46
2:L5:1754:U:H1'	8:LD:3:PHE:HZ	1.80	0.46
2:L5:3697:U:H5''	2:L5:3698:G:H5'	1.97	0.46
2:L5:4345:C:H2'	2:L5:4346:U:C6	2.51	0.46
2:L5:4966:A:H5''	6:LB:128:LYS:HG3	1.96	0.46
4:L8:75:OMG:HM23	4:L8:75:OMG:H1'	1.76	0.46
25:LV:43:LYS:HE2	25:LV:62:MET:HE3	1.97	0.46
59:SO:129:ILE:HD11	64:Sa:65:PRO:HD2	1.97	0.46
65:Sb:22:LYS:HG2	67:S2:921:G:C2	2.50	0.46
67:S2:5:U:H2'	67:S2:6:G:C8	2.51	0.46
67:S2:1457:U:H2'	67:S2:1458:G:C8	2.50	0.46
67:S2:1853:C:H2'	67:S2:1854:U:C6	2.51	0.46
67:S2:1856:C:H2'	67:S2:1857:G:C8	2.51	0.46
69:SD:66:ILE:HD11	69:SD:86:LEU:HB3	1.98	0.46
74:SQ:18:THR:H	74:SQ:126:ARG:NH1	2.14	0.46
2:L5:1700:G:H5'	2:L5:1702:C:OP2	2.15	0.46
2:L5:2607:C:O5'	21:LR:96:MET:HE1	2.16	0.46
2:L5:4344:U:H2'	2:L5:4345:C:C6	2.51	0.46
2:L5:4622:A:H4'	6:LB:13:SER:HB2	1.97	0.46
2:L5:4934:A:H2'	2:L5:4935:C:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4965:U:H4'	2:L5:4966:A:H5'	1.98	0.46
16:LM:24:LEU:HD11	16:LM:86:TRP:CG	2.51	0.46
32:Lc:51:ASN:HB2	32:Lc:77:ASN:HB2	1.96	0.46
47:Ls:62:ARG:HB3	47:Ls:66:ARG:HH12	1.80	0.46
48:Lt:117:ARG:HE	48:Lt:119:ARG:H	1.62	0.46
67:S2:1004:PSU:H2'	67:S2:1005:G:C8	2.49	0.46
67:S2:1567:G:H2'	67:S2:1568:C:C6	2.51	0.46
2:L5:1994:C:H2'	2:L5:1995:G:H8	1.81	0.46
2:L5:2351:OMC:HM23	2:L5:2351:OMC:H1'	1.70	0.46
2:L5:3848:U:H2'	2:L5:3849:A:C8	2.50	0.46
2:L5:3856:A:H5''	19:LP:83:TRP:O	2.16	0.46
4:L8:70:G:H5''	28:LY:27:ARG:CZ	2.46	0.46
6:LB:288:GLY:HA3	6:LB:330:PHE:CE1	2.50	0.46
10:LF:41:MET:HE2	31:Lb:113:ALA:HB2	1.97	0.46
67:S2:484:A2M:H8	67:S2:484:A2M:O5'	2.16	0.46
67:S2:1031:A2M:HM'3	67:S2:1031:A2M:H1'	1.52	0.46
67:S2:1733:U:H2'	67:S2:1734:G:O4'	2.16	0.46
2:L5:2521:G:H4'	36:Lg:26:PRO:HD2	1.97	0.46
11:LG:167:VAL:HG12	11:LG:170:LEU:HD12	1.98	0.46
11:LG:187:LYS:HB2	11:LG:198:THR:HG23	1.98	0.46
57:SL:68:ILE:HG12	57:SL:143:LEU:HD11	1.98	0.46
67:S2:1289:U:H2'	67:S2:1290:G:C8	2.51	0.46
2:L5:1696:C:H5'	2:L5:1719:A:H1'	1.97	0.45
50:SB:150:ILE:HG12	67:S2:1124:C:H5''	1.98	0.45
67:S2:1421:A:H3'	67:S2:1422:G:C8	2.51	0.45
82:Sg:30:MET:HE3	82:Sg:30:MET:HB3	1.87	0.45
2:L5:1870:C:H2'	2:L5:1871:A2M:H8	1.98	0.45
2:L5:4913:G:H4'	2:L5:4914:C:O5'	2.16	0.45
84:L5:5292:SPM:H31	84:L5:5292:SPM:H62	1.73	0.45
6:LB:154:LYS:HE2	6:LB:154:LYS:HB2	1.72	0.45
15:LL:110:LEU:O	15:LL:114:VAL:HG13	2.17	0.45
39:Lj:67:LEU:HD23	39:Lj:67:LEU:HA	1.84	0.45
52:SE:112:HIS:HE1	52:SE:238:LEU:O	1.99	0.45
67:S2:159:A2M:HM'3	67:S2:159:A2M:H1'	1.53	0.45
67:S2:649:PSU:H2'	67:S2:650:A:C8	2.51	0.45
67:S2:1271:C:H42	67:S2:1511:U:H3	1.64	0.45
67:S2:1845:A:H2'	67:S2:1846:G:C8	2.51	0.45
71:SK:80:ARG:HD3	71:SK:85:LEU:HB2	1.98	0.45
77:SU:40:ILE:O	77:SU:44:LYS:HG2	2.16	0.45
2:L5:71:C:H1'	15:LL:62:PRO:O	2.16	0.45
2:L5:179:G:H2'	2:L5:180:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1195:G:H2'	2:L5:1196:G:C8	2.52	0.45
2:L5:1869:G:C6	85:L5:5285:SPD:H32	2.51	0.45
2:L5:2870:A:H2'	2:L5:2871:A:H8	1.81	0.45
2:L5:4584:A:H2'	2:L5:4585:U:O4'	2.16	0.45
2:L5:4591:U:H2'	2:L5:4592:C:C6	2.51	0.45
7:LC:266:THR:HG22	7:LC:267:TRP:H	1.81	0.45
10:LF:243:LEU:HG	10:LF:247:MET:HE2	1.97	0.45
32:Lc:47:ILE:HD12	32:Lc:94:LEU:HD11	1.99	0.45
47:Ls:13:TYR:O	47:Ls:17:ILE:HG12	2.16	0.45
63:SY:9:THR:HG22	67:S2:837:A:N6	2.31	0.45
63:SY:27:VAL:HG22	63:SY:69:THR:HB	1.99	0.45
67:S2:12:U:H2'	67:S2:13:C:H6	1.81	0.45
67:S2:207:G:H3'	67:S2:208:G:H8	1.81	0.45
70:SF:18:LYS:HE2	70:SF:22:LYS:HA	1.98	0.45
2:L5:256:G:H2'	2:L5:257:C:C6	2.51	0.45
2:L5:2864:A:H2'	2:L5:2865:U:C6	2.52	0.45
2:L5:3954:A:H1'	2:L5:4058:U:H5'	1.99	0.45
2:L5:5004:C:H2'	2:L5:5005:G:O4'	2.16	0.45
4:L8:52:A:H5'	41:L1:21:ARG:HD3	1.97	0.45
5:LA:48:ILE:HG22	45:Lp:54:ILE:HG12	1.97	0.45
16:LM:96:GLU:O	16:LM:100:ARG:HG2	2.17	0.45
32:Lc:99:PRO:HD3	32:Lc:104:ILE:HD12	1.99	0.45
41:L1:12:PHE:CE2	41:L1:51:LEU:HD22	2.50	0.45
49:SA:158:ASP:HB2	49:SA:159:ILE:HD12	1.99	0.45
50:SB:192:SER:HA	50:SB:195:LYS:HD2	1.98	0.45
67:S2:352:U:H2'	67:S2:353:C:C6	2.52	0.45
67:S2:391:C:H2'	67:S2:392:A:H8	1.81	0.45
67:S2:1476:A:H4'	67:S2:1477:U:H5''	1.99	0.45
82:Sg:22:ALA:HB2	82:Sg:69:VAL:HG13	1.97	0.45
2:L5:2520:C:H2'	2:L5:2521:G:C8	2.51	0.45
2:L5:2667:C:O4'	21:LR:96:MET:HG2	2.15	0.45
2:L5:4302:U:H4'	23:LT:5:LYS:HD3	1.99	0.45
11:LG:157:ILE:HA	11:LG:201:THR:HG22	1.98	0.45
33:Ld:23:ARG:HG2	33:Ld:121:ASN:HA	1.99	0.45
49:SA:52:LYS:HB2	68:SR:109:LEU:HD13	1.99	0.45
67:S2:532:C:H2'	67:S2:533:A:H8	1.82	0.45
67:S2:644:OMG:HM23	67:S2:644:OMG:H1'	1.73	0.45
67:S2:917:U:H2'	67:S2:918:U:C6	2.52	0.45
67:S2:1221:G:H2'	67:S2:1222:G:C8	2.51	0.45
67:S2:1591:C:H5'	70:SF:85:LYS:HE3	1.98	0.45
72:SM:44:LYS:HE3	81:Sf:129:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SQ:104:SER:HA	74:SQ:107:GLU:HG3	1.99	0.45
2:L5:691:C:H2'	2:L5:692:A:H8	1.82	0.45
49:SA:68:ILE:HG22	49:SA:70:ASN:H	1.81	0.45
55:SI:76:THR:HG21	55:SI:104:ILE:HD12	1.98	0.45
60:SV:43:THR:HG23	60:SV:45:ARG:HB2	1.99	0.45
67:S2:348:A:H2'	67:S2:349:A:C8	2.52	0.45
67:S2:1457:U:H2'	67:S2:1458:G:H8	1.82	0.45
67:S2:1535:U:P	70:SF:169:ILE:HG12	2.57	0.45
69:SD:222:PRO:HB3	82:Sg:190:GLY:HA3	1.99	0.45
2:L5:257:C:H2'	2:L5:258:G:C8	2.51	0.45
2:L5:3718:A2M:H2'	2:L5:3719:A:O4'	2.17	0.45
2:L5:3727:A:H2'	2:L5:3728:A:C8	2.52	0.45
2:L5:4688:C:H2'	2:L5:4689:PSU:C6	2.51	0.45
58:SN:91:LEU:HB3	58:SN:122:ILE:HG12	1.99	0.45
67:S2:51:U:H2'	67:S2:52:G:H8	1.82	0.45
68:SR:7:LYS:HE2	68:SR:7:LYS:HB2	1.77	0.45
72:SM:18:LEU:HA	72:SM:21:VAL:HB	1.98	0.45
2:L5:1095:A:C2	2:L5:1200:G:N1	2.77	0.45
2:L5:1613:A:H5''	5:LA:183:GLY:CA	2.47	0.45
2:L5:1632:A:H3'	2:L5:1632:A:N3	2.32	0.45
2:L5:1846:G:H2'	2:L5:1847:C:C6	2.51	0.45
2:L5:1976:G:H22	48:Lt:139:VAL:HG11	1.81	0.45
2:L5:3873:G:H2'	2:L5:3874:G:C8	2.52	0.45
2:L5:4232:U:H5''	44:Lo:3:ASN:O	2.17	0.45
2:L5:4934:A:H2'	2:L5:4935:C:C6	2.52	0.45
17:LN:159:ARG:HB3	17:LN:164:LEU:HB2	1.99	0.45
29:LZ:41:ALA:HB2	29:LZ:77:TYR:HE1	1.81	0.45
51:SC:74:LYS:HD3	51:SC:74:LYS:HA	1.84	0.45
67:S2:656:G:N2	67:S2:663:C:H5''	2.32	0.45
67:S2:1433:C:N4	77:SU:51:LYS:HD2	2.32	0.45
74:SQ:31:LEU:HD11	74:SQ:33:LYS:HE3	1.98	0.45
2:L5:1084:C:H2'	2:L5:1085:C:H6	1.82	0.45
2:L5:1346:C:H2'	2:L5:1347:G:H8	1.81	0.45
2:L5:1982:G:H2'	2:L5:1983:A:O4'	2.17	0.45
48:Lt:127:GLY:HA2	48:Lt:130:LYS:HE2	1.98	0.45
49:SA:10:MET:HE2	49:SA:15:VAL:HG22	1.99	0.45
56:SJ:131:ARG:HD2	56:SJ:131:ARG:HA	1.78	0.45
59:SO:147:ARG:HH22	67:S2:1854:U:P	2.40	0.45
2:L5:1327:C:H2'	2:L5:1328:G:C8	2.52	0.45
2:L5:2671:C:H2'	2:L5:2672:C:C6	2.52	0.45
2:L5:2903:G:H1'	2:L5:2904:U:H5	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4345:C:H2'	2:L5:4346:U:H6	1.82	0.45
2:L5:4585:U:H2'	2:L5:4586:G:C8	2.52	0.45
57:SL:17:PHE:CD2	67:S2:222:U:H5''	2.51	0.45
67:S2:1227:G:H5''	67:S2:1639:G7M:O6	2.17	0.45
67:S2:1680:G:H2'	67:S2:1681:U:C6	2.52	0.45
2:L5:172:C:H4'	2:L5:173:C:H5'	1.99	0.44
2:L5:268:G:H2'	2:L5:269:G:C8	2.50	0.44
2:L5:424:U:H2'	2:L5:425:U:C6	2.52	0.44
2:L5:1857:C:H2'	2:L5:1858:A:C8	2.51	0.44
2:L5:2492:C:H2'	2:L5:2493:G:C8	2.52	0.44
2:L5:4508:C:N3	2:L5:4512:U:H5	2.15	0.44
2:L5:4743:G:H2'	2:L5:4744:A:H8	1.79	0.44
11:LG:105:GLU:HB2	11:LG:109:GLU:HG3	1.99	0.44
30:La:36:GLY:HA3	30:La:40:HIS:CE1	2.52	0.44
52:SE:149:TYR:CD2	53:SG:205:GLU:HB3	2.52	0.44
59:SO:15:ILE:HG12	59:SO:16:SER:H	1.81	0.44
63:SY:8:ARG:HD3	63:SY:8:ARG:HA	1.85	0.44
63:SY:89:HIS:HB3	67:S2:574:A:H4'	1.99	0.44
67:S2:1512:C:H2'	67:S2:1513:C:C6	2.53	0.44
82:Sg:191:HIS:CG	82:Sg:195:LEU:HD21	2.52	0.44
82:Sg:239:LEU:HD11	82:Sg:248:LEU:HD21	1.99	0.44
2:L5:99:A:H2'	2:L5:100:C:O2	2.17	0.44
8:LD:89:LYS:HE2	8:LD:229:ASN:HB2	1.99	0.44
20:LQ:59:PRO:HG3	20:LQ:143:ARG:HA	1.99	0.44
37:Lh:107:GLN:O	37:Lh:111:GLU:HG3	2.17	0.44
52:SE:160:ILE:HD12	52:SE:162:ILE:HD11	1.99	0.44
59:SO:34:PHE:HB3	59:SO:41:PHE:HB2	2.00	0.44
68:SR:35:CYS:HA	68:SR:38:ILE:HG12	1.98	0.44
68:SR:100:PRO:O	68:SR:104:GLU:HG2	2.16	0.44
2:L5:1697:G:H22	2:L5:2084:C:P	2.39	0.44
2:L5:4063:U:H2'	2:L5:4064:C:C6	2.53	0.44
5:LA:114:CYS:HB3	5:LA:165:VAL:HB	2.00	0.44
12:LH:41:ILE:HG22	12:LH:43:VAL:HG13	1.99	0.44
22:LS:93:MET:HE1	22:LS:117:HIS:CE1	2.53	0.44
50:SB:94:LYS:HA	50:SB:94:LYS:HD2	1.87	0.44
63:SY:9:THR:H	67:S2:837:A:H61	1.64	0.44
67:S2:909:G:H2'	67:S2:910:G:C8	2.52	0.44
67:S2:1644:C:H2'	67:S2:1645:C:C6	2.53	0.44
68:SR:6:THR:HG22	68:SR:7:LYS:H	1.82	0.44
2:L5:1317:U:H2'	2:L5:1318:C:C6	2.52	0.44
2:L5:1356:U:H2'	2:L5:1357:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2020:U:H2'	2:L5:2021:G:H8	1.82	0.44
2:L5:2326:G:H5''	34:Le:127:ALA:HB1	1.99	0.44
2:L5:4536:OMC:HM22	2:L5:4537:C:O4'	2.17	0.44
2:L5:4742:G:H2'	2:L5:4743:G:C8	2.52	0.44
51:SC:207:ALA:HB2	67:S2:4:C:H4'	1.98	0.44
52:SE:252:ARG:O	52:SE:256:LEU:HG	2.17	0.44
67:S2:441:C:H2'	67:S2:442:C:C6	2.53	0.44
67:S2:995:G:H22	67:S2:997:A:H3'	1.82	0.44
67:S2:1101:U:H2'	67:S2:1102:G:H8	1.82	0.44
67:S2:1279:C:H2'	67:S2:1280:G:H8	1.82	0.44
67:S2:1406:G:H2'	67:S2:1407:U:C6	2.53	0.44
75:SS:41:ALA:O	75:SS:45:LEU:HG	2.18	0.44
82:Sg:188:HIS:HD1	82:Sg:219:TRP:CG	2.35	0.44
2:L5:1503:A:N6	20:LQ:87:THR:HG21	2.31	0.44
2:L5:1645:C:H2'	2:L5:1646:A:C8	2.52	0.44
2:L5:3707:U:H2'	2:L5:3708:C:C6	2.52	0.44
2:L5:3911:C:H2'	2:L5:3912:U:H6	1.82	0.44
2:L5:4524:G:N3	6:LB:252:ALA:HB1	2.32	0.44
18:LO:88:LEU:HD12	18:LO:99:LEU:HD13	2.00	0.44
48:Lt:37:LEU:HA	48:Lt:40:LYS:HE3	2.00	0.44
51:SC:94:ILE:HD13	51:SC:162:ILE:HG13	1.99	0.44
52:SE:131:VAL:HA	52:SE:137:PRO:HA	1.99	0.44
67:S2:26:U:H2'	67:S2:27:A2M:H8	1.98	0.44
67:S2:1062:A:H2'	67:S2:1063:C:C6	2.52	0.44
74:SQ:15:ARG:HG2	74:SQ:126:ARG:HH12	1.82	0.44
2:L5:138:G:H2'	2:L5:139:G:C8	2.52	0.44
2:L5:2017:A:O2'	2:L5:2018:C:H6	2.01	0.44
2:L5:2335:C:H2'	2:L5:2336:G:H8	1.82	0.44
2:L5:4563:U:H2'	2:L5:4564:A:H8	1.82	0.44
2:L5:4590:A2M:HM'3	2:L5:4590:A2M:H1'	1.77	0.44
4:L8:8:U:H2'	4:L8:9:A:H8	1.81	0.44
14:LJ:42:GLN:HG2	14:LJ:117:ILE:HD12	1.98	0.44
34:Le:98:GLU:HG2	34:Le:123:THR:OG1	2.17	0.44
39:Lj:85:LYS:HB3	39:Lj:85:LYS:HE3	1.75	0.44
53:SG:161:PRO:HA	53:SG:171:THR:HA	1.99	0.44
56:SJ:176:LYS:HA	56:SJ:179:LYS:HG2	1.99	0.44
67:S2:554:A:O2'	67:S2:555:A:H8	2.01	0.44
67:S2:1144:A:H5'	67:S2:1355:C:H41	1.83	0.44
70:SF:162:ALA:HB2	70:SF:172:CYS:SG	2.57	0.44
78:SZ:58:LEU:HD21	78:SZ:87:ALA:HB1	1.99	0.44
2:L5:1968:G:H2'	2:L5:1969:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:3932:U:H2'	2:L5:3933:G:C8	2.53	0.44
2:L5:5027:C:O2'	2:L5:5028:G:H5''	2.17	0.44
26:LW:123:LYS:HG3	67:S2:321:C:OP2	2.17	0.44
33:Ld:29:ILE:O	33:Ld:33:ILE:HG12	2.17	0.44
52:SE:176:ASP:H	52:SE:179:ASN:HD22	1.66	0.44
55:SI:148:LYS:HD3	55:SI:152:ARG:HH11	1.82	0.44
67:S2:508:A:H3'	67:S2:509:OMG:C8	2.52	0.44
67:S2:1651:A:H2'	67:S2:1652:G:C8	2.47	0.44
67:S2:1797:U:H2'	67:S2:1798:C:C6	2.52	0.44
71:SK:64:TRP:CD2	80:Sd:23:VAL:HG22	2.53	0.44
72:SM:23:LYS:O	72:SM:27:ILE:HG12	2.18	0.44
82:Sg:173:LEU:HD11	82:Sg:187:ASN:HB3	2.00	0.44
2:L5:1084:C:H2'	2:L5:1085:C:C6	2.53	0.44
2:L5:1340:OMC:HM23	2:L5:1340:OMC:H1'	1.78	0.44
2:L5:3760:A:H4'	2:L5:3761:C:H5''	1.99	0.44
2:L5:4619:U:H2'	2:L5:4620:OMU:H6	1.99	0.44
4:L8:78:G:H2'	4:L8:79:G:C8	2.52	0.44
5:LA:131:GLY:H	5:LA:169:VAL:HG13	1.82	0.44
5:LA:180:LEU:HD21	45:Lp:22:LEU:HB3	1.99	0.44
8:LD:179:ARG:HD3	8:LD:179:ARG:HA	1.70	0.44
9:LE:95:PRO:HA	9:LE:104:THR:HG22	2.00	0.44
9:LE:149:ILE:HD12	9:LE:271:LEU:HD21	1.99	0.44
21:LR:167:LYS:HE2	21:LR:167:LYS:HB3	1.75	0.44
26:LW:113:LYS:HD2	26:LW:117:LYS:HE3	1.99	0.44
33:Ld:53:ALA:HA	33:Ld:88:LEU:HD21	2.00	0.44
38:Li:76:ARG:HA	38:Li:76:ARG:HD3	1.79	0.44
51:SC:60:TRP:CZ2	51:SC:62:PRO:HB3	2.51	0.44
52:SE:112:HIS:CE1	52:SE:239:PRO:HA	2.53	0.44
53:SG:31:ARG:HG2	53:SG:101:ILE:HG13	1.99	0.44
67:S2:1051:G:H2'	67:S2:1052:A:C8	2.52	0.44
67:S2:1391:OMC:HM23	67:S2:1391:OMC:H1'	1.81	0.44
67:S2:1627:C:H5''	76:ST:41:LYS:HD2	1.99	0.44
67:S2:1858:G:H2'	67:S2:1859:A:H8	1.82	0.44
2:L5:3925:OMU:HM23	2:L5:3925:OMU:H1'	1.84	0.44
4:L8:67:U:H2'	4:L8:68:G:H8	1.83	0.44
10:LF:37:PHE:HZ	31:Lb:113:ALA:HB1	1.83	0.44
26:LW:56:ARG:HH21	26:LW:61:LYS:HB3	1.82	0.44
26:LW:82:ILE:HD11	53:SG:158:VAL:HG21	1.99	0.44
67:S2:198:U:H2'	67:S2:199:C:H2'	1.99	0.44
67:S2:533:A:H61	67:S2:550:C:H42	1.66	0.44
67:S2:1709:G:H2'	67:S2:1710:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:1749:G:H2'	67:S2:1750:C:C6	2.53	0.44
67:S2:1801:A:H2'	67:S2:1802:C:H6	1.82	0.44
77:SU:67:LYS:HG2	77:SU:78:ASP:HB2	2.00	0.44
2:L5:2730:U:H2'	2:L5:2731:C:C6	2.53	0.43
6:LB:29:VAL:HA	6:LB:220:ILE:HD13	1.99	0.43
7:LC:154:VAL:HG11	7:LC:174:LEU:HD11	1.99	0.43
36:Lg:33:LEU:HD23	36:Lg:33:LEU:HA	1.85	0.43
52:SE:149:TYR:HB3	53:SG:209:TYR:HB2	2.00	0.43
67:S2:102:A:H4'	67:S2:104:A:C8	2.52	0.43
67:S2:301:A:H2'	67:S2:302:A:O4'	2.18	0.43
67:S2:1511:U:H2'	67:S2:1512:C:C6	2.53	0.43
67:S2:1713:C:H2'	67:S2:1714:U:C6	2.53	0.43
79:Sc:44:ARG:HA	79:Sc:44:ARG:HD2	1.85	0.43
2:L5:655:C:H2'	2:L5:656:C:C6	2.53	0.43
2:L5:1590:C:H4'	2:L5:2857:A:H5'	2.01	0.43
2:L5:2079:G:H2'	2:L5:2080:U:C6	2.53	0.43
2:L5:2276:A:H2'	2:L5:2277:C:O4'	2.18	0.43
3:L7:63:C:H5'	3:L7:64:G:H5''	2.00	0.43
16:LM:118:MET:HG2	18:LO:192:TYR:CZ	2.53	0.43
50:SB:117:TRP:HB3	50:SB:153:THR:HA	1.99	0.43
67:S2:1390:U:H2'	67:S2:1391:OMC:C6	2.53	0.43
69:SD:71:ALA:O	69:SD:75:LYS:HG3	2.18	0.43
2:L5:1468:C:H2'	2:L5:1469:C:H6	1.83	0.43
2:L5:1802:A:H5''	2:L5:1803:G:H5'	2.00	0.43
2:L5:2558:C:H2'	2:L5:2559:G:C8	2.54	0.43
2:L5:3619:G:H4'	21:LR:79:GLY:O	2.18	0.43
2:L5:3722:G:H2'	2:L5:3723:A:H8	1.83	0.43
2:L5:3723:A:H2'	2:L5:3724:A:C8	2.54	0.43
2:L5:4769:G:H5''	18:LO:176:ARG:HD3	2.00	0.43
10:LF:157:ARG:HE	10:LF:248:ASN:HB2	1.82	0.43
26:LW:5:LEU:HD12	26:LW:30:GLN:NE2	2.33	0.43
37:Lh:73:TYR:HB3	37:Lh:79:LYS:HG2	2.00	0.43
48:Lt:82:ILE:HG12	48:Lt:137:GLN:HG2	1.99	0.43
49:SA:41:ARG:HD2	49:SA:47:TYR:CZ	2.53	0.43
55:SI:125:LYS:HB2	55:SI:128:LYS:HZ1	1.83	0.43
59:SO:61:LYS:NZ	59:SO:76:LEU:HB3	2.32	0.43
67:S2:142:C:H42	67:S2:329:G:H5''	1.84	0.43
67:S2:929:G:N2	67:S2:1104:G:H4'	2.33	0.43
67:S2:1221:G:H2'	67:S2:1222:G:H8	1.83	0.43
67:S2:1284:A:C8	72:SM:33:ARG:HG3	2.53	0.43
67:S2:1808:U:H2'	67:S2:1809:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SF:42:LYS:HA	70:SF:42:LYS:HD3	1.75	0.43
2:L5:106:A:H2'	2:L5:107:G:O4'	2.18	0.43
2:L5:1086:C:H2'	2:L5:1087:A:H8	1.84	0.43
2:L5:1410:U:H3	31:Lb:52:LYS:NZ	2.17	0.43
2:L5:3606:U:H2'	2:L5:3607:U:C6	2.54	0.43
21:LR:44:LEU:HD22	21:LR:49:LEU:HD12	2.01	0.43
50:SB:114:VAL:HG11	67:S2:987:A:H2'	2.00	0.43
67:S2:201:C:H3'	67:S2:202:G:H21	1.84	0.43
67:S2:342:C:H2'	67:S2:343:A:H8	1.83	0.43
67:S2:867:OMG:HM23	67:S2:867:OMG:H1'	1.86	0.43
70:SF:103:LEU:HD22	78:SZ:67:LEU:HD22	2.00	0.43
70:SF:201:LYS:HG3	70:SF:204:ARG:HE	1.83	0.43
73:SP:45:LEU:HD23	73:SP:45:LEU:HA	1.88	0.43
2:L5:1500:A:H5''	2:L5:1501:C:H5''	2.01	0.43
2:L5:1960:A:C8	47:Ls:63:LYS:HE2	2.54	0.43
2:L5:2017:A:H2'	2:L5:2017:A:OP2	2.19	0.43
4:L8:40:A:H2'	4:L8:41:A:C8	2.53	0.43
5:LA:7:GLY:HA2	5:LA:10:LYS:HG3	2.01	0.43
11:LG:51:LEU:O	11:LG:55:VAL:HG23	2.18	0.43
19:LP:126:ARG:CZ	19:LP:140:MET:HE1	2.49	0.43
55:SI:141:ARG:CZ	67:S2:191:A:H5''	2.48	0.43
63:SY:6:THR:HG23	63:SY:28:LEU:HD13	2.00	0.43
64:Sa:13:LYS:HD3	64:Sa:13:LYS:HA	1.80	0.43
67:S2:430:C:H2'	67:S2:431:G:H8	1.82	0.43
67:S2:1693:G:H2'	67:S2:1694:U:C6	2.53	0.43
69:SD:172:VAL:HG22	69:SD:185:LYS:HG2	2.00	0.43
77:SU:20:ILE:HG13	77:SU:116:ILE:HG22	1.99	0.43
81:Sf:103:LEU:HG	81:Sf:104:LYS:H	1.83	0.43
2:L5:173:C:H2'	2:L5:174:C:C6	2.54	0.43
2:L5:2568:C:H2'	2:L5:2569:G:H8	1.84	0.43
2:L5:2864:A:H2'	2:L5:2865:U:H6	1.84	0.43
2:L5:4219:A:H2'	2:L5:4220:6MZ:C8	2.49	0.43
9:LE:119:GLU:HG3	34:Le:7:LEU:HD22	1.99	0.43
12:LH:51:LYS:HG3	12:LH:52:LYS:N	2.34	0.43
13:LI:39:LYS:HE3	13:LI:39:LYS:HB2	1.81	0.43
18:LO:61:ARG:HA	18:LO:70:PRO:HD2	1.99	0.43
22:LS:69:GLU:HG3	22:LS:71:SER:H	1.83	0.43
52:SE:45:ILE:HG13	52:SE:61:VAL:HG11	2.00	0.43
56:SJ:169:ARG:HH12	56:SJ:175:ARG:NE	2.16	0.43
67:S2:1109:C:C4	68:SR:126:MET:HE2	2.53	0.43
67:S2:1603:G:N2	75:SS:24:ARG:HH21	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:7:C:H2'	2:L5:8:U:C6	2.54	0.43
2:L5:208:A:C2	2:L5:233:U:H5''	2.54	0.43
2:L5:1307:A:H2'	2:L5:1308:C:H6	1.84	0.43
2:L5:1613:A:H5''	5:LA:183:GLY:HA2	2.00	0.43
2:L5:1942:A:H2'	2:L5:1943:A:H8	1.77	0.43
2:L5:4344:U:H2'	2:L5:4345:C:H6	1.84	0.43
6:LB:57:VAL:HG22	6:LB:73:VAL:HG22	2.00	0.43
6:LB:220:ILE:HG12	6:LB:278:THR:HG23	1.99	0.43
13:LI:51:HIS:CD2	13:LI:168:SER:HB3	2.53	0.43
40:Lk:24:LYS:HD3	40:Lk:69:LEU:HD21	2.01	0.43
47:Ls:45:MET:HE1	48:Lt:123:ARG:HG2	2.00	0.43
53:SG:69:THR:O	53:SG:99:GLY:HA3	2.18	0.43
67:S2:16:G:H2'	67:S2:17:C:C6	2.54	0.43
67:S2:1271:C:N4	67:S2:1511:U:H3	2.16	0.43
2:L5:737:C:C4	2:L5:739:G:H5''	2.53	0.43
2:L5:1962:A:H2	2:L5:2024:G:H21	1.65	0.43
2:L5:2267:U:OP1	46:Lr:37:SER:HB2	2.19	0.43
2:L5:2474:G:H2'	2:L5:2502:G:N2	2.34	0.43
2:L5:4095:G:H2'	2:L5:4096:C:C6	2.54	0.43
3:L7:4:U:H2'	3:L7:5:A:H8	1.84	0.43
8:LD:181:PRO:HD2	8:LD:195:HIS:CD2	2.54	0.43
9:LE:223:ARG:HA	9:LE:224:LYS:HA	1.72	0.43
11:LG:123:ALA:HA	11:LG:124:GLY:HA2	1.74	0.43
21:LR:173:ARG:O	21:LR:176:ARG:HD3	2.19	0.43
47:Ls:29:ILE:HG13	47:Ls:190:GLN:HB2	2.00	0.43
50:SB:131:ASP:HB3	50:SB:133:TYR:HD1	1.83	0.43
55:SI:184:ARG:HD2	67:S2:219:U:H1'	2.01	0.43
67:S2:1189:A:H2'	67:S2:1190:A:H8	1.84	0.43
72:SM:69:CYS:SG	72:SM:76:LEU:HB2	2.58	0.43
2:L5:1345:A:H2'	2:L5:1346:C:C6	2.53	0.43
2:L5:1359:G:H4'	17:LN:203:TYR:HB2	2.00	0.43
2:L5:1629:G:N2	2:L5:1632:A:N6	2.39	0.43
2:L5:1743:A:O4'	8:LD:15:ARG:HD2	2.19	0.43
2:L5:2029:A:H2'	2:L5:2030:A:C8	2.54	0.43
2:L5:2543:A:H2	2:L5:2773:G:H22	1.65	0.43
4:L8:144:U:H2'	4:L8:145:C:C6	2.54	0.43
11:LG:162:ASP:HB3	11:LG:163:PRO:HD3	2.00	0.43
11:LG:180:PRO:HD3	11:LG:223:ARG:HH21	1.84	0.43
13:LI:73:ASN:HB2	13:LI:87:MET:HE1	2.01	0.43
33:Ld:33:ILE:HD11	33:Ld:45:ALA:HA	2.00	0.43
52:SE:36:HIS:CE1	52:SE:85:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SL:65:ASN:HB2	67:S2:294:U:C4	2.54	0.43
59:SO:56:VAL:HG23	59:SO:60:MET:SD	2.59	0.43
67:S2:54:A:H3'	67:S2:451:G:H22	1.83	0.43
67:S2:96:C:H2'	67:S2:97:U:C6	2.53	0.43
67:S2:496:C:H2'	67:S2:497:C:H6	1.84	0.43
69:SD:115:VAL:HG21	69:SD:142:LEU:HD22	2.00	0.43
2:L5:264:C:H2'	2:L5:265:C:C4	2.54	0.43
2:L5:2743:A:H2'	2:L5:2744:A:C8	2.54	0.43
2:L5:2824:OMC:HM23	2:L5:2824:OMC:H1'	1.68	0.43
2:L5:3664:G:H2'	2:L5:3665:G:H8	1.84	0.43
2:L5:4069:U:H2'	2:L5:4070:U:H6	1.84	0.43
2:L5:4277:G:H5''	23:LT:17:ARG:HG2	2.01	0.43
13:LI:36:LEU:HD21	13:LI:69:ARG:NH1	2.34	0.43
24:LU:80:LYS:HG2	24:LU:110:TYR:CE2	2.54	0.43
34:Le:35:TRP:CZ2	34:Le:56:PRO:HD2	2.54	0.43
40:Lk:25:ILE:HD13	40:Lk:57:LYS:HZ3	1.83	0.43
52:SE:66:MET:HG3	67:S2:502:C:O4'	2.19	0.43
55:SI:23:LYS:HB3	55:SI:23:LYS:HE2	1.73	0.43
55:SI:119:LEU:HD21	55:SI:153:LYS:HE2	2.01	0.43
67:S2:698:G:H5'	67:S2:733:C:N3	2.34	0.43
67:S2:943:U:H2'	67:S2:944:A:C8	2.54	0.43
67:S2:1232:PSU:H2'	67:S2:1233:G:C8	2.53	0.43
67:S2:1533:A:N6	67:S2:1602:U:H3	2.05	0.43
67:S2:1599:U:C4	70:SF:166:ILE:HA	2.53	0.43
67:S2:1708:C:C2	67:S2:1709:G:C8	3.07	0.43
67:S2:1745:A:H62	67:S2:1789:G:H21	1.66	0.43
69:SD:74:GLN:NE2	69:SD:81:GLU:HA	2.33	0.43
75:SS:98:VAL:HG13	75:SS:103:LEU:HD12	2.01	0.43
75:SS:129:LEU:HD23	75:SS:144:ARG:HH21	1.83	0.43
82:Sg:21:ILE:HG12	82:Sg:288:SER:OG	2.18	0.43
82:Sg:147:HIS:CD2	82:Sg:175:LYS:HD2	2.54	0.43
2:L5:260:C:H2'	2:L5:261:G:C8	2.54	0.42
2:L5:2654:C:H2'	2:L5:2655:C:H6	1.84	0.42
3:L7:16:A:H2'	3:L7:17:C:C6	2.53	0.42
35:Lf:41:PHE:HE1	35:Lf:110:ILE:HD13	1.84	0.42
38:Li:35:LYS:HB3	38:Li:35:LYS:HE3	1.79	0.42
42:Lm:93:LYS:HD3	42:Lm:102:ARG:HD3	2.01	0.42
48:Lt:34:PRO:HA	48:Lt:37:LEU:HD22	2.01	0.42
63:SY:18:LEU:HB2	63:SY:20:ARG:HD3	2.01	0.42
64:Sa:53:ILE:HD13	64:Sa:53:ILE:HA	1.89	0.42
67:S2:367:U:H4'	67:S2:371:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:816:A:H2'	67:S2:817:G:O4'	2.19	0.42
67:S2:1230:C:H2'	67:S2:1231:C:C6	2.53	0.42
67:S2:1328:OMG:HM23	67:S2:1328:OMG:H1'	1.75	0.42
67:S2:1383:A2M:H1'	67:S2:1383:A2M:HM'3	1.61	0.42
70:SF:144:LEU:HD23	79:Sc:49:PRO:HB2	2.00	0.42
70:SF:193:LYS:O	70:SF:197:GLU:HG2	2.19	0.42
75:SS:25:LYS:HE2	75:SS:52:LEU:O	2.18	0.42
75:SS:26:ILE:HA	75:SS:56:ALA:HB2	2.01	0.42
76:ST:62:ARG:NH1	76:ST:66:LEU:HD11	2.33	0.42
77:SU:35:VAL:O	77:SU:39:LEU:HD23	2.19	0.42
82:Sg:112:ALA:HB3	82:Sg:121:VAL:HG12	2.01	0.42
2:L5:4507:A:H2'	2:L5:4508:C:C6	2.54	0.42
2:L5:5015:G:H2'	2:L5:5016:A:C2	2.54	0.42
7:LC:109:ARG:O	7:LC:109:ARG:HG2	2.18	0.42
21:LR:168:GLU:HA	21:LR:171:LYS:HG2	2.01	0.42
49:SA:198:MET:HE1	68:SR:86:PRO:HG2	2.02	0.42
67:S2:1103:C:H2'	67:S2:1104:G:H8	1.83	0.42
2:L5:1461:C:H2'	2:L5:1462:A:C8	2.54	0.42
2:L5:1725:U:H2'	2:L5:1726:U:H6	1.84	0.42
2:L5:1751:A:H2'	2:L5:1752:G:C8	2.54	0.42
2:L5:1824:G:H5''	23:LT:35:LYS:HE2	2.01	0.42
2:L5:2090:U:H4'	2:L5:2091:C:H3'	2.00	0.42
2:L5:3607:U:H2'	2:L5:3608:A:C8	2.55	0.42
2:L5:3610:A:H2'	2:L5:3611:A:H8	1.84	0.42
2:L5:3848:U:H2'	2:L5:3849:A:H8	1.84	0.42
2:L5:4069:U:H2'	2:L5:4070:U:C6	2.55	0.42
2:L5:4685:U:H2'	2:L5:4686:G:C8	2.54	0.42
2:L5:5057:C:H2'	2:L5:5058:A:C8	2.55	0.42
7:LC:45:ARG:HG3	7:LC:238:LEU:HD22	2.00	0.42
47:Ls:77:LYS:HE2	47:Ls:193:PHE:HE1	1.84	0.42
55:SI:206:LYS:HD2	55:SI:206:LYS:HA	1.85	0.42
63:SY:21:LYS:HD2	63:SY:75:ILE:HD11	2.00	0.42
67:S2:323:C:H5'	67:S2:324:C:OP1	2.18	0.42
67:S2:495:U:H2'	67:S2:496:C:O4'	2.19	0.42
67:S2:671:A:H4'	67:S2:672:A:H5''	2.02	0.42
67:S2:1845:A:H2'	67:S2:1846:G:H8	1.84	0.42
79:Sc:44:ARG:NH2	79:Sc:63:ARG:HD2	2.34	0.42
82:Sg:42:MET:HG2	82:Sg:57:ARG:H	1.84	0.42
2:L5:163:A:H2'	2:L5:164:G:H8	1.83	0.42
2:L5:2844:A:O2'	2:L5:4631:G:H4'	2.19	0.42
2:L5:3920:PSU:H2'	2:L5:3921:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4070:U:H2'	2:L5:4071:U:C6	2.54	0.42
2:L5:4088:C:H2'	2:L5:4089:G:C8	2.55	0.42
2:L5:4954:G:H2'	2:L5:4955:A:H8	1.82	0.42
3:L7:55:A:H4'	14:LJ:155:HIS:HB2	2.01	0.42
11:LG:52:THR:HG22	27:LX:41:ARG:HG3	2.01	0.42
22:LS:4:SER:HB3	22:LS:111:ARG:HH22	1.84	0.42
33:Ld:114:PHE:HA	33:Ld:117:LEU:HD12	2.02	0.42
54:SH:63:PHE:HA	54:SH:95:ILE:O	2.19	0.42
2:L5:267:G:H2'	2:L5:268:G:C8	2.54	0.42
2:L5:1431:C:H2'	2:L5:1432:G:O4'	2.20	0.42
2:L5:2019:C:H2'	2:L5:2020:U:C6	2.54	0.42
2:L5:2489:C:H4'	2:L5:2491:C:H42	1.83	0.42
2:L5:4870:G:H5''	16:LM:91:TRP:CD2	2.55	0.42
4:L8:6:C:H2'	4:L8:7:U:H6	1.83	0.42
10:LF:243:LEU:O	10:LF:247:MET:HB2	2.19	0.42
15:LL:46:ILE:O	15:LL:46:ILE:HG13	2.19	0.42
15:LL:194:ILE:HD12	15:LL:194:ILE:HA	1.90	0.42
56:SJ:93:LYS:HB2	56:SJ:96:TYR:CD2	2.55	0.42
67:S2:389:A:H2'	67:S2:390:C:C6	2.54	0.42
67:S2:1054:G:C6	67:S2:1065:G:C6	3.08	0.42
2:L5:1081:C:C2'	2:L5:1082:C:H5'	2.50	0.42
2:L5:4523:A2M:HM'3	2:L5:4523:A2M:H1'	1.84	0.42
6:LB:258:HIS:HA	6:LB:260:ALA:H	1.84	0.42
6:LB:294:LYS:HD3	6:LB:298:LEU:HD11	2.01	0.42
15:LL:18:TRP:CD1	15:LL:18:TRP:H	2.37	0.42
34:Le:76:LYS:HD2	34:Le:98:GLU:CD	2.45	0.42
52:SE:127:ARG:HD2	52:SE:142:HIS:HA	2.01	0.42
54:SH:158:LEU:HD23	54:SH:158:LEU:HA	1.88	0.42
67:S2:145:G:H2'	67:S2:146:G:H8	1.84	0.42
67:S2:339:A:H2'	67:S2:340:C:H5	1.84	0.42
67:S2:1235:G:H21	73:SP:135:ALA:HB2	1.84	0.42
67:S2:1263:U:H4'	80:Sd:27:ARG:HD2	2.01	0.42
74:SQ:98:LYS:HE2	74:SQ:98:LYS:HB2	1.91	0.42
2:L5:126:C:H2'	2:L5:127:G:H8	1.84	0.42
2:L5:513:U:H3	2:L5:515:C:H3'	1.85	0.42
2:L5:515:C:H41	2:L5:647:G:H21	1.66	0.42
2:L5:724:C:OP1	7:LC:350:ARG:HD3	2.20	0.42
2:L5:1346:C:H2'	2:L5:1347:G:C8	2.54	0.42
2:L5:2101:C:H2'	2:L5:2102:G:C8	2.54	0.42
2:L5:3610:A:H2'	2:L5:3611:A:C8	2.54	0.42
2:L5:3656:A:H2'	2:L5:3657:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4088:C:H2'	2:L5:4089:G:H8	1.85	0.42
10:LF:221:LYS:HA	10:LF:221:LYS:HD3	1.86	0.42
17:LN:142:ILE:HG23	17:LN:148:THR:HG22	2.02	0.42
24:LU:112:LEU:HD23	24:LU:112:LEU:H	1.85	0.42
53:SG:170:ARG:HG3	67:S2:72:C:N3	2.35	0.42
59:SO:75:MET:HG3	59:SO:118:ALA:HB2	2.01	0.42
63:SY:7:ILE:HD12	63:SY:27:VAL:HG12	2.02	0.42
67:S2:587:A:H5'	67:S2:592:C:H41	1.84	0.42
67:S2:1025:U:H2'	67:S2:1026:C:O4'	2.19	0.42
79:Sc:10:LYS:HE3	79:Sc:61:SER:OG	2.20	0.42
81:Sf:90:LYS:HD2	81:Sf:90:LYS:HA	1.74	0.42
2:L5:444:G:H2'	2:L5:445:U:H6	1.85	0.42
2:L5:455:C:O2'	2:L5:456:C:H5'	2.19	0.42
2:L5:1541:C:H5''	5:LA:21:LYS:HG2	2.01	0.42
2:L5:1564:A:H2'	2:L5:1565:A:C8	2.55	0.42
2:L5:2519:U:H1'	2:L5:2520:C:C6	2.55	0.42
2:L5:3825:A2M:H2'	2:L5:3826:C:O4'	2.19	0.42
2:L5:4139:G:H1'	2:L5:4146:G:N1	2.35	0.42
2:L5:4273:A:H2'	2:L5:4274:A:C8	2.55	0.42
4:L8:89:U:H2'	4:L8:90:C:C6	2.54	0.42
4:L8:92:U:H2'	4:L8:93:C:O4'	2.20	0.42
5:LA:145:LYS:HA	5:LA:145:LYS:HD3	1.85	0.42
15:LL:48:PRO:HG3	37:Lh:118:LYS:HE2	2.01	0.42
52:SE:43:PRO:HG2	52:SE:46:ILE:HG12	2.01	0.42
54:SH:43:LEU:HD11	54:SH:71:SER:HB2	2.02	0.42
55:SI:125:LYS:HB2	55:SI:128:LYS:NZ	2.35	0.42
56:SJ:77:LEU:HA	56:SJ:80:ARG:HE	1.84	0.42
56:SJ:169:ARG:HD2	56:SJ:169:ARG:HA	1.87	0.42
67:S2:381:C:H2'	67:S2:382:C:C6	2.55	0.42
67:S2:496:C:H2'	67:S2:497:C:C6	2.55	0.42
67:S2:1777:G:H2'	67:S2:1778:C:C6	2.54	0.42
71:SK:14:LEU:HD22	71:SK:35:LEU:HD13	2.02	0.42
71:SK:19:GLY:H	71:SK:93:THR:HG23	1.84	0.42
74:SQ:8:GLN:HG3	74:SQ:99:TYR:CE1	2.55	0.42
2:L5:318:A:H2'	2:L5:319:A:H8	1.83	0.42
2:L5:937:U:C6	16:LM:46:ARG:HD2	2.55	0.42
2:L5:1847:C:H2'	2:L5:1848:C:C6	2.54	0.42
2:L5:2264:C:H2'	2:L5:2265:G:O4'	2.20	0.42
2:L5:2498:C:H2'	2:L5:2499:C:H6	1.84	0.42
2:L5:3599:A:H2'	2:L5:3600:G:C8	2.54	0.42
2:L5:4578:G:H2'	2:L5:4579:PSU:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LF:241:ASN:O	10:LF:245:ARG:HG2	2.20	0.42
59:SO:101:GLY:HA3	59:SO:134:PRO:HD2	2.02	0.42
67:S2:582:U:H2'	67:S2:583:A:H5''	2.01	0.42
71:SK:64:TRP:CD1	80:Sd:23:VAL:HG13	2.55	0.42
72:SM:17:ALA:O	72:SM:20:GLU:HG3	2.20	0.42
72:SM:49:LEU:HG	72:SM:75:ASN:HB3	2.02	0.42
74:SQ:90:LYS:HB3	74:SQ:90:LYS:HE2	1.82	0.42
2:L5:1629:G:C8	2:L5:1629:G:O5'	2.72	0.42
2:L5:1631:A:C2	5:LA:204:MET:HE2	2.55	0.42
2:L5:1972:G:C6	2:L5:1973:G:C6	3.08	0.42
2:L5:2256:C:H2'	2:L5:2257:C:O4'	2.20	0.42
2:L5:3911:C:H2'	2:L5:3912:U:C6	2.54	0.42
6:LB:239:LYS:HE3	6:LB:248:LEU:HD13	2.02	0.42
12:LH:107:GLU:O	12:LH:107:GLU:HG2	2.19	0.42
17:LN:200:LEU:HD22	17:LN:204:ARG:NH1	2.35	0.42
18:LO:189:ILE:HD13	18:LO:189:ILE:HA	1.91	0.42
35:Lf:45:LYS:HA	35:Lf:107:PRO:HD2	2.01	0.42
35:Lf:78:HIS:O	35:Lf:83:MET:HB2	2.20	0.42
52:SE:42:LEU:HD12	52:SE:101:LEU:HD21	2.02	0.42
52:SE:136:ILE:HG23	52:SE:149:TYR:CE1	2.55	0.42
67:S2:1136:U:H2'	67:S2:1137:U:H6	1.84	0.42
67:S2:1631:U:H2'	67:S2:1632:G:O4'	2.19	0.42
70:SF:17:ILE:HG21	70:SF:46:ALA:HB1	2.01	0.42
82:Sg:257:LYS:HE3	82:Sg:259:TRP:HZ2	1.85	0.42
2:L5:2891:U:H2'	2:L5:2892:C:O4'	2.20	0.41
2:L5:3684:G:H2'	2:L5:3685:C:C6	2.55	0.41
2:L5:4238:G:H2'	2:L5:4239:A:C8	2.55	0.41
2:L5:4347:G:H2'	2:L5:4348:A:C8	2.55	0.41
2:L5:4593:C:H2'	2:L5:4594:U:H6	1.85	0.41
4:L8:66:A:H2'	4:L8:67:U:C6	2.54	0.41
6:LB:117:ARG:HA	6:LB:177:LYS:HD2	2.02	0.41
9:LE:224:LYS:HG2	9:LE:227:HIS:HB3	2.02	0.41
20:LQ:154:LYS:HE2	20:LQ:154:LYS:HB3	1.81	0.41
49:SA:220:LYS:HA	49:SA:220:LYS:HD3	1.94	0.41
50:SB:64:GLY:HA2	50:SB:87:ILE:HD11	2.02	0.41
50:SB:208:HIS:CD2	50:SB:209:ASP:HB2	2.54	0.41
53:SG:52:ILE:HA	53:SG:111:LEU:HD23	2.02	0.41
56:SJ:77:LEU:HA	56:SJ:80:ARG:HG2	2.02	0.41
62:SX:46:HIS:CD2	62:SX:103:ALA:HB2	2.55	0.41
67:S2:24:C:O2'	67:S2:25:A:H8	2.01	0.41
67:S2:27:A2M:H2'	67:S2:28:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:443:U:O4	67:S2:447:A:N7	2.53	0.41
67:S2:648:A:H2'	67:S2:649:PSU:C6	2.55	0.41
67:S2:1256:G:H1	80:Sd:31:ILE:HG12	1.85	0.41
67:S2:1553:C:H41	80:Sd:22:ARG:CZ	2.33	0.41
67:S2:1736:G:H2'	67:S2:1737:G:C8	2.55	0.41
69:SD:196:GLY:HA3	69:SD:201:LYS:HG2	2.01	0.41
70:SF:73:THR:O	70:SF:89:THR:HG21	2.19	0.41
73:SP:81:ARG:NH1	73:SP:98:ASN:HA	2.34	0.41
76:ST:77:LYS:HB2	76:ST:94:ARG:NH2	2.35	0.41
2:L5:454:U:H2'	2:L5:455:C:O4'	2.20	0.41
2:L5:758:G:H4'	12:LH:51:LYS:HE3	2.02	0.41
2:L5:2570:U:H2'	2:L5:2571:C:C6	2.55	0.41
2:L5:4066:U:H2'	2:L5:4067:U:H6	1.85	0.41
32:Lc:23:LYS:HB3	32:Lc:23:LYS:HE3	1.83	0.41
34:Le:89:LEU:HD13	34:Le:118:LEU:HD22	2.02	0.41
48:Lt:119:ARG:NH2	48:Lt:123:ARG:HH12	2.18	0.41
51:SC:214:LEU:HD22	51:SC:244:ILE:HD11	2.02	0.41
51:SC:264:SER:H	51:SC:267:GLN:HE21	1.68	0.41
53:SG:7:PHE:HB2	53:SG:113:ILE:HD13	2.02	0.41
54:SH:18:GLU:C	54:SH:20:GLU:H	2.28	0.41
57:SL:28:THR:HA	57:SL:29:GLY:HA2	1.61	0.41
58:SN:47:PRO:HA	58:SN:50:ILE:HD12	2.01	0.41
61:SW:6:VAL:HG12	61:SW:34:ILE:HD11	2.02	0.41
67:S2:179:C:H3'	67:S2:180:G:H8	1.85	0.41
67:S2:1205:C:H2'	67:S2:1206:G:H8	1.86	0.41
67:S2:1540:G:H2'	67:S2:1541:G:H8	1.85	0.41
67:S2:1569:A:H5'	76:ST:41:LYS:HD3	2.02	0.41
67:S2:1647:A:N1	67:S2:1675:A:H5''	2.35	0.41
68:SR:44:LYS:O	68:SR:47:ARG:HG2	2.20	0.41
68:SR:128:PHE:CD2	68:SR:129:LYS:HG3	2.55	0.41
74:SQ:63:PHE:CZ	74:SQ:92:LEU:HD22	2.55	0.41
2:L5:286:U:H2'	2:L5:287:U:C6	2.55	0.41
2:L5:921:C:H2'	2:L5:922:C:C6	2.55	0.41
2:L5:979:C:OP2	9:LE:66:LYS:HD3	2.19	0.41
2:L5:1333:A:H2'	2:L5:1334:A:H8	1.83	0.41
2:L5:2640:G:H2'	2:L5:2641:A:H8	1.84	0.41
2:L5:3928:A:H2'	2:L5:3929:G:O4'	2.20	0.41
2:L5:3932:U:H2'	2:L5:3933:G:H8	1.85	0.41
3:L7:23:A:H2'	3:L7:24:C:C6	2.55	0.41
12:LH:61:TRP:CZ3	16:LM:33:GLN:HG3	2.55	0.41
20:LQ:3:VAL:HG13	20:LQ:5:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LV:37:LEU:HD23	25:LV:65:VAL:HG12	2.02	0.41
52:SE:125:LYS:HB2	52:SE:226:PHE:CD1	2.56	0.41
53:SG:141:ILE:HD11	53:SG:153:VAL:HG13	2.01	0.41
54:SH:30:LEU:HB3	54:SH:37:LYS:HZ2	1.85	0.41
55:SI:36:THR:HG22	55:SI:96:LEU:HD12	2.02	0.41
66:Se:58:ASN:HD21	67:S2:606:G:H1'	1.83	0.41
67:S2:1656:G:O6	67:S2:1668:U:O4	2.39	0.41
69:SD:204:LEU:HB2	69:SD:207:HIS:HB2	2.02	0.41
70:SF:22:LYS:HG3	70:SF:23:TRP:CD2	2.56	0.41
70:SF:95:HIS:CD2	78:SZ:106:GLN:HB3	2.55	0.41
72:SM:128:PHE:HA	72:SM:131:LYS:HG2	2.02	0.41
2:L5:1199:G:H2'	2:L5:1200:G:H8	1.86	0.41
2:L5:1855:G:OP1	31:Lb:4:SER:HB2	2.20	0.41
2:L5:2696:A:H62	40:Lk:35:LYS:HZ2	1.69	0.41
2:L5:2732:G:H2'	2:L5:2733:C:C6	2.55	0.41
8:LD:33:ARG:O	8:LD:37:VAL:HG22	2.21	0.41
8:LD:150:LEU:HD12	14:LJ:146:ARG:HG3	2.03	0.41
35:Lf:92:LEU:HD23	35:Lf:92:LEU:HA	1.90	0.41
37:Lh:52:LYS:HD3	37:Lh:52:LYS:HA	1.74	0.41
49:SA:205:ARG:NH2	49:SA:210:ILE:HG13	2.34	0.41
53:SG:136:LYS:HB2	67:S2:65:C:N4	2.34	0.41
55:SI:12:ARG:HH12	67:S2:103:A:H5'	1.85	0.41
57:SL:133:PRO:HB3	57:SL:139:ARG:NH1	2.35	0.41
59:SO:61:LYS:HD2	59:SO:61:LYS:HA	1.75	0.41
63:SY:79:LEU:HG	63:SY:83:LYS:HE2	2.03	0.41
67:S2:543:C:H3'	67:S2:544:G:C8	2.54	0.41
67:S2:1018:U:H2'	67:S2:1019:C:H6	1.85	0.41
67:S2:1098:C:H2'	67:S2:1099:G:H8	1.85	0.41
82:Sg:89:LEU:HB2	82:Sg:101:PHE:HE1	1.85	0.41
82:Sg:289:LEU:HD11	82:Sg:298:LEU:HD21	2.03	0.41
2:L5:2267:U:C6	2:L5:2270:G:H4'	2.56	0.41
2:L5:2465:C:H2'	2:L5:2466:G:O4'	2.20	0.41
2:L5:2521:G:H5'	2:L5:2640:G:H1'	2.03	0.41
2:L5:2765:A:H2'	2:L5:2766:A:H8	1.86	0.41
2:L5:3917:A:H2'	2:L5:3918:G:C8	2.56	0.41
2:L5:4460:U:H2'	2:L5:4461:C:C6	2.55	0.41
2:L5:4957:C:H2'	2:L5:4958:C:C6	2.55	0.41
5:LA:131:GLY:N	5:LA:169:VAL:HG13	2.35	0.41
8:LD:209:ARG:O	8:LD:213:GLU:HG2	2.21	0.41
47:Ls:31:GLY:N	47:Ls:190:GLN:HG2	2.36	0.41
52:SE:44:LEU:HD21	52:SE:72:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SW:45:GLY:O	61:SW:68:ARG:HD2	2.20	0.41
67:S2:85:A:H2'	67:S2:86:C:C6	2.55	0.41
67:S2:509:OMG:H2'	67:S2:510:G:C8	2.56	0.41
67:S2:544:G:H2'	67:S2:545:A:C8	2.56	0.41
67:S2:955:A:N3	67:S2:956:G:H1'	2.35	0.41
67:S2:1376:A:H2'	67:S2:1377:U:O4'	2.20	0.41
67:S2:1588:A:H2'	67:S2:1589:A:C8	2.56	0.41
82:Sg:59:LEU:HD23	82:Sg:90:TRP:CD2	2.55	0.41
2:L5:1274:A:O2'	2:L5:1275:G:H8	2.03	0.41
2:L5:1403:G:N2	2:L5:1404:G:N2	2.69	0.41
2:L5:2389:A:H4'	33:Ld:70:LYS:HG3	2.02	0.41
2:L5:2422:OMC:HM23	2:L5:2422:OMC:H1'	1.82	0.41
2:L5:4450:U:H2'	87:L5:5295:HMT:H1	2.02	0.41
2:L5:4458:C:H2'	2:L5:4459:U:C6	2.55	0.41
2:L5:4935:C:H2'	2:L5:4936:G:H8	1.83	0.41
7:LC:150:LEU:HA	7:LC:150:LEU:HD12	1.79	0.41
22:LS:15:ARG:HD2	22:LS:25:PRO:HG2	2.01	0.41
28:LY:47:MET:HG3	28:LY:115:ARG:HH21	1.86	0.41
37:Lh:95:LEU:HB3	37:Lh:99:GLU:HG3	2.03	0.41
50:SB:137:LEU:HB3	50:SB:172:MET:HE3	2.02	0.41
54:SH:76:GLN:HG3	54:SH:94:PHE:HD2	1.86	0.41
56:SJ:82:VAL:HG12	56:SJ:87:LEU:HB3	2.02	0.41
58:SN:89:TYR:CE1	58:SN:150:VAL:HG23	2.56	0.41
67:S2:325:C:H3'	67:S2:326:C:H4'	2.02	0.41
67:S2:627:OMU:H6	67:S2:627:OMU:H2'	1.86	0.41
67:S2:1311:C:H2'	67:S2:1312:G:C8	2.56	0.41
69:SD:137:VAL:HG22	69:SD:151:LYS:HG3	2.02	0.41
71:SK:64:TRP:CE3	80:Sd:23:VAL:HG22	2.56	0.41
72:SM:71:GLU:CD	81:Sf:114:ILE:HB	2.45	0.41
75:SS:48:ALA:HB2	75:SS:70:ILE:HG13	2.02	0.41
2:L5:2018:C:H2'	2:L5:2019:C:H6	1.85	0.41
2:L5:2495:U:H2'	2:L5:2496:G:C8	2.56	0.41
2:L5:3851:PSU:H2'	2:L5:3852:A:O4'	2.21	0.41
2:L5:3922[A]:G:C5	5:LA:208:GLU:HB2	2.55	0.41
2:L5:4523:A2M:H5''	2:L5:4524:G:H5'	2.03	0.41
2:L5:4563:U:H2'	2:L5:4564:A:C8	2.55	0.41
2:L5:4571:A2M:H2'	2:L5:4572:U:H6	1.85	0.41
2:L5:4627:U:H4'	6:LB:373:LYS:HE2	2.03	0.41
4:L8:5:U:H2'	4:L8:6:C:H6	1.86	0.41
6:LB:17:LEU:HD23	6:LB:17:LEU:HA	1.84	0.41
7:LC:315:LYS:HD2	10:LF:168:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LQ:25:LEU:O	20:LQ:29:VAL:HG23	2.20	0.41
25:LV:42:VAL:HB	25:LV:45:ILE:HG13	2.01	0.41
32:Lc:65:MET:HE3	32:Lc:65:MET:HB3	1.96	0.41
55:SI:192:GLY:O	55:SI:196:GLU:HG3	2.21	0.41
61:SW:28:ARG:HD3	67:S2:921:G:C5	2.56	0.41
61:SW:119:LYS:HG3	61:SW:121:THR:HG22	2.03	0.41
2:L5:263:G:H3'	2:L5:264:C:C6	2.56	0.41
2:L5:1514:U:H2'	2:L5:1515:A:H8	1.83	0.41
2:L5:1978:C:H2'	2:L5:1979:A:O4'	2.21	0.41
2:L5:3785:A2M:H2	2:L5:4551:U:O2	2.21	0.41
2:L5:3934:G:H2'	2:L5:3935:C:C6	2.55	0.41
5:LA:225:ILE:HG12	5:LA:234:LYS:HA	2.03	0.41
6:LB:14:LEU:HA	6:LB:17:LEU:HG	2.03	0.41
8:LD:108:ARG:CZ	8:LD:253:TYR:HB2	2.50	0.41
8:LD:289:ARG:O	8:LD:292:GLU:HG3	2.20	0.41
15:LL:111:GLN:HA	15:LL:114:VAL:HG22	2.03	0.41
24:LU:39:PHE:HD2	24:LU:70:ILE:HD12	1.86	0.41
48:Lt:12:VAL:HG11	48:Lt:65:GLN:H	1.85	0.41
50:SB:56:LYS:HB3	50:SB:56:LYS:HE3	1.94	0.41
55:SI:84:ASN:HD22	55:SI:100:CYS:HB3	1.86	0.41
57:SL:22:ARG:HH21	57:SL:31:GLU:HG2	1.86	0.41
61:SW:28:ARG:NH2	67:S2:1093:A:H5''	2.36	0.41
67:S2:28:U:H2'	67:S2:29:G:C8	2.54	0.41
67:S2:494:C:N4	67:S2:509:OMG:HN22	2.18	0.41
67:S2:1409:A:H2'	67:S2:1410:C:C6	2.56	0.41
67:S2:1562:C:H4'	76:ST:120:GLY:N	2.35	0.41
69:SD:75:LYS:NZ	71:SK:18:GLU:HG3	2.36	0.41
76:ST:40:ALA:HB3	76:ST:43:LYS:HG3	2.02	0.41
2:L5:10:A:H2'	2:L5:11:G:C8	2.56	0.41
2:L5:139:G:H2'	2:L5:140:G:H8	1.86	0.41
2:L5:468:U:C6	2:L5:469:C:H5	2.39	0.41
2:L5:654:C:H4'	7:LC:269:LYS:HE2	2.03	0.41
2:L5:1588:U:H2'	2:L5:1589:C:C6	2.56	0.41
2:L5:1634:A:C5	2:L5:3922[A]:G:P	3.14	0.41
2:L5:1700:G:H5''	2:L5:1704:C:N4	2.31	0.41
2:L5:1984:A:H5'	2:L5:1986:U:P	2.61	0.41
2:L5:2602:G:H2'	2:L5:2603:C:C6	2.56	0.41
2:L5:2611:A:H2'	2:L5:2612:G:C8	2.55	0.41
2:L5:2656:U:H5''	29:LZ:38:TYR:HB3	2.02	0.41
2:L5:2909:C:H1'	2:L5:3585:G:H1	1.85	0.41
2:L5:3867:A2M:HM'3	2:L5:3880:G:N2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4456:OMC:HM21	6:LB:241:PRO:HD3	2.02	0.41
2:L5:4578:G:H2'	2:L5:4579:PSU:C6	2.55	0.41
2:L5:4585:U:H2'	2:L5:4586:G:H8	1.86	0.41
2:L5:4627:U:H5''	6:LB:373:LYS:HG2	2.02	0.41
2:L5:4749:C:H2'	2:L5:4750:G:O4'	2.21	0.41
2:L5:5003:U:H2'	2:L5:5004:C:C6	2.55	0.41
5:LA:75:LEU:HD12	5:LA:75:LEU:HA	1.90	0.41
5:LA:181:LYS:HB2	5:LA:184:ARG:HG3	2.01	0.41
5:LA:234:LYS:H	5:LA:234:LYS:HG2	1.74	0.41
6:LB:19:ARG:HA	6:LB:19:ARG:HD3	1.93	0.41
8:LD:83:LEU:HB3	8:LD:88:VAL:HG13	2.02	0.41
16:LM:119:ARG:HG3	18:LO:189:ILE:HG23	2.02	0.41
19:LP:105:LYS:HB3	19:LP:105:LYS:HE2	1.90	0.41
20:LQ:43:PHE:CD2	20:LQ:133:GLY:HA3	2.55	0.41
21:LR:80:LYS:HD2	21:LR:80:LYS:HA	1.82	0.41
21:LR:82:LYS:HA	21:LR:82:LYS:HD2	1.90	0.41
24:LU:23:LEU:HD23	24:LU:110:TYR:HB2	2.02	0.41
26:LW:107:GLN:HA	26:LW:110:ARG:HG3	2.02	0.41
47:Ls:57:LYS:O	47:Ls:61:MET:HG2	2.21	0.41
49:SA:122:LEU:HB2	49:SA:142:LEU:HD21	2.01	0.41
50:SB:127:VAL:HG21	50:SB:176:VAL:HB	2.02	0.41
50:SB:222:LYS:HD2	50:SB:222:LYS:HA	1.91	0.41
51:SC:84:PHE:HA	60:SV:15:ARG:NH1	2.35	0.41
55:SI:154:LYS:HB3	55:SI:154:LYS:HE3	1.92	0.41
56:SJ:30:LYS:HG2	66:Se:42:PHE:CE2	2.56	0.41
57:SL:128:VAL:HG12	57:SL:142:VAL:HA	2.03	0.41
58:SN:131:THR:HG22	58:SN:132:LYS:HE2	2.03	0.41
59:SO:95:ILE:HG21	59:SO:116:LEU:HD12	2.02	0.41
59:SO:134:PRO:HB3	67:S2:944:A:H5''	2.02	0.41
67:S2:497:C:H2'	67:S2:498:C:C6	2.56	0.41
67:S2:1183:A:H2'	67:S2:1184:G:H8	1.86	0.41
67:S2:1202:U:H2'	67:S2:1203:G:C8	2.55	0.41
67:S2:1204:A:H2'	67:S2:1205:C:C6	2.56	0.41
67:S2:1279:C:H2'	67:S2:1280:G:C8	2.55	0.41
67:S2:1587:G:C5	76:ST:78:ILE:HD11	2.56	0.41
67:S2:1621:U:O2'	67:S2:1622:U:H2'	2.21	0.41
68:SR:44:LYS:HA	68:SR:47:ARG:HG2	2.03	0.41
70:SF:76:MET:HE3	70:SF:76:MET:HB3	1.97	0.41
72:SM:132:LYS:HD3	72:SM:132:LYS:HA	1.77	0.41
74:SQ:89:SER:HB2	74:SQ:112:LEU:HD13	2.03	0.41
75:SS:60:THR:O	75:SS:64:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:SU:51:LYS:HB2	77:SU:90:ASP:HB2	2.02	0.41
2:L5:662:C:H2'	2:L5:663:G:C8	2.56	0.41
2:L5:1403:G:N2	2:L5:1415:G:C4	2.89	0.41
2:L5:2490:U:H3'	2:L5:2491:C:C6	2.56	0.41
2:L5:3870:C:H2'	2:L5:3871:A:C8	2.55	0.41
5:LA:115:CYS:SG	5:LA:124:GLY:HA3	2.61	0.41
52:SE:11:ARG:HH11	52:SE:20:LEU:HB3	1.86	0.41
52:SE:141:THR:HG23	52:SE:143:ASP:N	2.36	0.41
54:SH:78:ARG:HH12	54:SH:81:ARG:HD2	1.85	0.41
55:SI:12:ARG:NH1	67:S2:103:A:H5'	2.36	0.41
56:SJ:22:LYS:HA	56:SJ:22:LYS:HD2	1.73	0.41
56:SJ:78:LEU:HB3	56:SJ:92:MET:SD	2.61	0.41
58:SN:102:LEU:HD13	58:SN:111:ALA:HB3	2.03	0.41
60:SV:27:LYS:HD3	60:SV:27:LYS:HA	1.85	0.41
67:S2:527:C:H2'	67:S2:528:A:H8	1.85	0.41
67:S2:874:G:H2'	67:S2:875:A:C8	2.53	0.41
67:S2:1674:G:P	74:SQ:78:VAL:HG11	2.61	0.41
67:S2:1709:G:H2'	67:S2:1710:C:C6	2.56	0.41
67:S2:1712:A:N6	67:S2:1822:A:H61	2.19	0.41
2:L5:462:G:H2'	2:L5:463:A:C8	2.56	0.40
2:L5:1705:G:H2'	2:L5:1706:A:O4'	2.20	0.40
7:LC:76:ILE:HG12	7:LC:96:CYS:SG	2.61	0.40
19:LP:137:ASN:HD22	19:LP:137:ASN:HA	1.67	0.40
53:SG:175:LYS:HD2	67:S2:77:A:H2	1.86	0.40
54:SH:33:ASN:HD21	54:SH:37:LYS:HE3	1.86	0.40
67:S2:51:U:H2'	67:S2:52:G:C8	2.56	0.40
67:S2:142:C:N4	67:S2:329:G:H5''	2.37	0.40
67:S2:517:OMC:H2'	67:S2:518:G:O4'	2.21	0.40
67:S2:561:A:H2'	67:S2:562:U:C6	2.56	0.40
67:S2:1217:A:H2'	67:S2:1218:C:H6	1.84	0.40
67:S2:1454:A:C2	67:S2:1476:A:H1'	2.57	0.40
67:S2:1736:G:H2'	67:S2:1737:G:H8	1.86	0.40
77:SU:48:LEU:HG	77:SU:93:SER:HB3	2.02	0.40
2:L5:153:G:H2'	2:L5:154:G:C8	2.56	0.40
2:L5:168:C:H2'	2:L5:169:G:C8	2.56	0.40
2:L5:716:C:OP1	7:LC:317:ASN:HB2	2.21	0.40
2:L5:4600:G:H4'	2:L5:4601:U:O5'	2.21	0.40
4:L8:19:C:H2'	4:L8:20:A:C8	2.55	0.40
12:LH:92:MET:HE2	12:LH:179:ILE:HG22	2.03	0.40
27:LX:82:THR:HG21	37:Lh:37:THR:HG22	2.03	0.40
28:LY:76:LYS:HE2	41:LI:31:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Lg:60:ARG:HD2	36:Lg:60:ARG:HA	1.77	0.40
53:SG:14:LYS:HE2	53:SG:16:ILE:HD11	2.03	0.40
53:SG:192:ILE:HD12	53:SG:195:LYS:HD2	2.02	0.40
54:SH:33:ASN:ND2	54:SH:37:LYS:HE3	2.36	0.40
54:SH:126:HIS:CE1	54:SH:181:THR:HG23	2.56	0.40
55:SI:57:ALA:HB1	55:SI:60:LEU:CD2	2.51	0.40
57:SL:153:LYS:HA	57:SL:153:LYS:HD3	1.82	0.40
61:SW:20:ARG:HD2	61:SW:20:ARG:HA	1.96	0.40
63:SY:79:LEU:HD12	63:SY:82:ALA:HB3	2.04	0.40
67:S2:342:C:H2'	67:S2:343:A:C8	2.56	0.40
67:S2:845:G:H2'	67:S2:846:G:C8	2.56	0.40
67:S2:1114:U:O2'	67:S2:1115:U:H2'	2.22	0.40
67:S2:1538:C:H2'	67:S2:1539:U:C6	2.55	0.40
67:S2:1748:G:O6	67:S2:1786:U:O4	2.39	0.40
67:S2:1858:G:H2'	67:S2:1859:A:C8	2.56	0.40
75:SS:3:LEU:HD23	75:SS:3:LEU:H	1.85	0.40
75:SS:78:LYS:HA	75:SS:78:LYS:HD3	1.87	0.40
77:SU:27:ARG:HD3	77:SU:82:MET:HE3	2.03	0.40
77:SU:46:LYS:HD3	77:SU:100:GLN:HB3	2.02	0.40
77:SU:49:LYS:HE3	77:SU:49:LYS:HB3	1.91	0.40
80:Sd:10:HIS:HA	80:Sd:11:PRO:HD3	1.94	0.40
2:L5:123:C:H2'	2:L5:124:C:H6	1.86	0.40
2:L5:180:C:H2'	2:L5:181:C:C6	2.55	0.40
2:L5:674:G:H2'	2:L5:675:C:C6	2.56	0.40
2:L5:1662:C:H2'	2:L5:1663:C:H6	1.86	0.40
2:L5:4169:G:H4'	2:L5:4171:C:C2	2.56	0.40
6:LB:122:TRP:CE2	6:LB:127:LYS:HE3	2.57	0.40
10:LF:96:ARG:HH12	10:LF:224:THR:HG22	1.86	0.40
28:LY:111:LEU:HD23	28:LY:111:LEU:HA	1.92	0.40
54:SH:144:ILE:HG23	61:SW:52:ILE:HB	2.02	0.40
59:SO:118:ALA:HA	59:SO:121:ARG:HG2	2.04	0.40
60:SV:81:LYS:HA	60:SV:81:LYS:HD3	1.96	0.40
61:SW:94:LEU:HD21	61:SW:102:ILE:HG13	2.03	0.40
62:SX:137:LYS:HZ3	67:S2:30:C:H4'	1.86	0.40
67:S2:22:A:H2'	67:S2:23:G:H8	1.86	0.40
67:S2:159:A2M:C2	67:S2:467:G:H21	2.31	0.40
67:S2:218:U:H2'	67:S2:219:U:C6	2.56	0.40
67:S2:489:A:H2'	67:S2:490:C:C6	2.57	0.40
67:S2:799:OMU:HM23	67:S2:799:OMU:H1'	1.91	0.40
67:S2:1059:G:N2	67:S2:1829:G:H4'	2.36	0.40
67:S2:1490:OMG:HM23	67:S2:1490:OMG:H1'	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:S2:1587:G:N7	76:ST:67:ARG:HD3	2.36	0.40
67:S2:1803:U:H2'	67:S2:1804:U:C6	2.57	0.40
69:SD:135:GLU:HB2	69:SD:153:VAL:HG23	2.03	0.40
70:SF:51:HIS:CE1	74:SQ:78:VAL:HG21	2.56	0.40
70:SF:121:PRO:HA	70:SF:193:LYS:HG3	2.03	0.40
74:SQ:42:ILE:HD12	74:SQ:42:ILE:HA	1.94	0.40
2:L5:264:C:H2'	2:L5:265:C:C5	2.57	0.40
2:L5:423:G:H2'	2:L5:424:U:C6	2.57	0.40
2:L5:3762:U:H3'	2:L5:3763:A:H8	1.87	0.40
2:L5:4320:G:H2'	2:L5:4321:U:C6	2.57	0.40
3:L7:4:U:H2'	3:L7:5:A:C8	2.56	0.40
13:LI:184:MET:HA	13:LI:187:LYS:HE2	2.02	0.40
48:Lt:11:LYS:HA	48:Lt:11:LYS:HD2	1.81	0.40
49:SA:34:MET:HE3	49:SA:34:MET:HB3	1.91	0.40
52:SE:124:CYS:HB3	52:SE:141:THR:OG1	2.22	0.40
67:S2:375:U:H2'	67:S2:376:A:C8	2.57	0.40
70:SF:33:ILE:HD11	79:Sc:35:MET:HE1	2.04	0.40
70:SF:78:MET:HE2	70:SF:78:MET:HB3	1.91	0.40
82:Sg:183:LYS:HD2	82:Sg:183:LYS:HA	1.90	0.40
82:Sg:300:ALA:C	82:Sg:307:VAL:HG23	2.47	0.40
2:L5:4920:C:H2'	2:L5:4921:C:H6	1.86	0.40
2:L5:4927:G:H5''	2:L5:4928:C:C5	2.57	0.40
4:L8:140:C:H2'	4:L8:141:C:C6	2.56	0.40
8:LD:66:TYR:HE2	8:LD:68:ARG:HE	1.68	0.40
18:LO:47:PHE:HA	18:LO:136:ALA:HB2	2.02	0.40
31:Lb:43:MET:HE2	31:Lb:47:LYS:NZ	2.37	0.40
49:SA:173:LEU:O	49:SA:177:MET:HG2	2.21	0.40
67:S2:1013:U:H2'	67:S2:1014:G:H8	1.86	0.40
67:S2:1199:A:H2'	67:S2:1200:A:C8	2.57	0.40
67:S2:1218:C:H2'	67:S2:1219:C:C6	2.56	0.40
67:S2:1235:G:N2	73:SP:135:ALA:HB2	2.37	0.40
67:S2:1425:G:H2'	67:S2:1426:U:C6	2.56	0.40
67:S2:1671:G:H2'	67:S2:1672:U:H6	1.87	0.40
75:SS:102:GLY:HA2	75:SS:105:ASN:ND2	2.37	0.40
76:ST:42:HIS:HB3	76:ST:93:SER:HB3	2.04	0.40
82:Sg:270:LEU:HD13	82:Sg:310:TRP:CD2	2.56	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	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
5	LA	246/248 (99%)	231 (94%)	15 (6%)	0	100	100
6	LB	400/402 (100%)	385 (96%)	15 (4%)	0	100	100
7	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
8	LD	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
9	LE	236/250 (94%)	223 (94%)	13 (6%)	0	100	100
10	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
11	LG	239/241 (99%)	228 (95%)	11 (5%)	0	100	100
12	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
13	LI	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
14	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
15	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
16	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
17	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
18	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
19	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	LQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
21	LR	183/187 (98%)	180 (98%)	3 (2%)	0	100	100
22	LS	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
23	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
24	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
25	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
26	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
27	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
28	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
30	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
31	Lb	105/121 (87%)	103 (98%)	2 (2%)	0	100	100
32	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
33	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
34	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
35	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
36	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
37	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
38	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
39	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
40	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
41	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	Lm	50/52 (96%)	50 (100%)	0	0	100	100
43	Ln	22/24 (92%)	22 (100%)	0	0	100	100
44	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
45	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
46	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
47	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
48	Lt	128/157 (82%)	113 (88%)	15 (12%)	0	100	100
49	SA	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
50	SB	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
51	SC	218/222 (98%)	209 (96%)	9 (4%)	0	100	100
52	SE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
53	SG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
54	SH	182/189 (96%)	168 (92%)	14 (8%)	0	100	100
55	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
56	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
57	SL	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
58	SN	148/150 (99%)	148 (100%)	0	0	100	100
59	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
61	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
62	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
63	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
64	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
65	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
66	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
68	SR	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
69	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
70	SF	187/189 (99%)	174 (93%)	13 (7%)	0	100	100
71	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
72	SM	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	23
73	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
74	SQ	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
75	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
76	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
77	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
78	SZ	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
79	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
80	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
81	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
82	Sg	311/313 (99%)	296 (95%)	15 (5%)	0	100	100
All	All	11670/11907 (98%)	11235 (96%)	434 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	SM	101	ARG

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Le	114/114 (100%)	114 (100%)	0	100	100
35	Lf	88/88 (100%)	88 (100%)	0	100	100
36	Lg	98/98 (100%)	98 (100%)	0	100	100
37	Lh	109/109 (100%)	109 (100%)	0	100	100
38	Li	86/86 (100%)	86 (100%)	0	100	100
39	Lj	73/73 (100%)	73 (100%)	0	100	100
40	Lk	64/64 (100%)	64 (100%)	0	100	100
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	48 (100%)	0	100	100
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	74/74 (100%)	74 (100%)	0	100	100
46	Lr	109/109 (100%)	109 (100%)	0	100	100
47	Ls	162/164 (99%)	162 (100%)	0	100	100
48	Lt	107/130 (82%)	107 (100%)	0	100	100
49	SA	183/183 (100%)	183 (100%)	0	100	100
50	SB	195/195 (100%)	195 (100%)	0	100	100
51	SC	186/188 (99%)	186 (100%)	0	100	100
52	SE	224/224 (100%)	224 (100%)	0	100	100
53	SG	207/207 (100%)	207 (100%)	0	100	100
54	SH	166/169 (98%)	166 (100%)	0	100	100
55	SI	178/178 (100%)	178 (100%)	0	100	100
56	SJ	161/161 (100%)	161 (100%)	0	100	100
57	SL	137/137 (100%)	137 (100%)	0	100	100
58	SN	130/130 (100%)	130 (100%)	0	100	100
59	SO	107/110 (97%)	107 (100%)	0	100	100
60	SV	67/67 (100%)	67 (100%)	0	100	100
61	SW	112/112 (100%)	112 (100%)	0	100	100
62	SX	113/113 (100%)	113 (100%)	0	100	100
63	SY	113/113 (100%)	113 (100%)	0	100	100
64	Sa	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	Sb	75/75 (100%)	75 (100%)	0	100	100
66	Se	47/47 (100%)	47 (100%)	0	100	100
68	SR	122/122 (100%)	122 (100%)	0	100	100
69	SD	190/190 (100%)	190 (100%)	0	100	100
70	SF	159/159 (100%)	159 (100%)	0	100	100
71	SK	89/89 (100%)	89 (100%)	0	100	100
72	SM	102/104 (98%)	102 (100%)	0	100	100
73	SP	107/107 (100%)	107 (100%)	0	100	100
74	SQ	119/119 (100%)	119 (100%)	0	100	100
75	SS	126/126 (100%)	126 (100%)	0	100	100
76	ST	113/113 (100%)	113 (100%)	0	100	100
77	SU	94/94 (100%)	94 (100%)	0	100	100
78	SZ	66/66 (100%)	66 (100%)	0	100	100
79	Sc	57/57 (100%)	57 (100%)	0	100	100
80	Sd	48/48 (100%)	48 (100%)	0	100	100
81	Sf	60/60 (100%)	60 (100%)	0	100	100
82	Sg	272/272 (100%)	272 (100%)	0	100	100
All	All	10147/10221 (99%)	10147 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
5	LA	132	ASN
6	LB	145	GLN
6	LB	203	GLN
6	LB	354	GLN
7	LC	187	GLN
7	LC	329	ASN
11	LG	112	GLN
11	LG	208	ASN
12	LH	98	HIS
12	LH	138	GLN
13	LI	59	GLN
13	LI	73	ASN

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Mol	Chain	Res	Type
13	LI	147	HIS
14	LJ	65	ASN
15	LL	205	GLN
16	LM	34	ASN
17	LN	199	GLN
18	LO	50	ASN
18	LO	199	HIS
19	LP	75	GLN
19	LP	133	HIS
20	LQ	21	GLN
20	LQ	57	ASN
20	LQ	162	HIS
22	LS	108	GLN
23	LT	144	ASN
24	LU	50	ASN
24	LU	94	ASN
25	LV	77	HIS
27	LX	93	ASN
27	LX	125	ASN
28	LY	14	ASN
28	LY	61	HIS
30	La	34	ASN
30	La	67	GLN
31	Lb	49	HIS
32	Lc	72	HIS
34	Le	23	HIS
34	Le	52	GLN
35	Lf	20	ASN
35	Lf	21	GLN
37	Lh	98	HIS
38	Li	15	HIS
46	Lr	21	ASN
46	Lr	30	ASN
50	SB	158	HIS
51	SC	115	GLN
51	SC	267	GLN
52	SE	50	ASN
52	SE	112	HIS
53	SG	105	ASN
53	SG	227	GLN
54	SH	12	ASN
55	SI	9	HIS

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Mol	Chain	Res	Type
57	SL	11	GLN
57	SL	13	GLN
57	SL	18	GLN
57	SL	19	ASN
59	SO	32	HIS
60	SV	35	ASN
61	SW	24	GLN
62	SX	16	HIS
62	SX	20	GLN
62	SX	31	HIS
63	SY	124	ASN
65	Sb	65	GLN
69	SD	57	ASN
69	SD	179	GLN
69	SD	226	GLN
70	SF	137	GLN
72	SM	15	ASN
72	SM	119	GLN
73	SP	79	HIS
73	SP	104	GLN
76	ST	10	ASN
77	SU	18	HIS
77	SU	92	HIS
81	Sf	139	HIS
82	Sg	4	GLN
82	Sg	56	GLN
82	Sg	64	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L5	3643/3655 (99%)	725 (19%)	12 (0%)
3	L7	119/120 (99%)	7 (5%)	0
4	L8	155/156 (99%)	23 (14%)	0
67	S2	1714/1740 (98%)	390 (22%)	6 (0%)
All	All	5631/5671 (99%)	1145 (20%)	18 (0%)

All (1145) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L5	25	A

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Mol	Chain	Res	Type
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G
2	L5	56	A
2	L5	59	A
2	L5	64	A
2	L5	65	A
2	L5	66	A
2	L5	70	A
2	L5	73	A
2	L5	74	G
2	L5	91	G
2	L5	104	G
2	L5	108	A
2	L5	109	G
2	L5	110	C
2	L5	119	G
2	L5	120	A
2	L5	132	G
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	139	G
2	L5	159	C
2	L5	165	A
2	L5	181	C
2	L5	182	G
2	L5	183	C
2	L5	184	U
2	L5	185	C
2	L5	188	G
2	L5	189	G
2	L5	200	U
2	L5	209	U
2	L5	210	C
2	L5	216	C
2	L5	218	A
2	L5	220	C
2	L5	234	G
2	L5	237	G
2	L5	255	C

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Mol	Chain	Res	Type
2	L5	256	G
2	L5	261	G
2	L5	263	G
2	L5	264	C
2	L5	265	C
2	L5	266	C
2	L5	267	G
2	L5	280	G
2	L5	297	U
2	L5	306	A
2	L5	315	G
2	L5	316	U
2	L5	340	C
2	L5	373	G
2	L5	387	G
2	L5	388	A
2	L5	407	A
2	L5	409	G
2	L5	410	A
2	L5	411	G
2	L5	412	G
2	L5	413	G
2	L5	415	G
2	L5	449	C
2	L5	450	G
2	L5	452	A
2	L5	453	G
2	L5	454	U
2	L5	456	C
2	L5	457	G
2	L5	467	U
2	L5	479	G
2	L5	484	U
2	L5	485	C
2	L5	486	C
2	L5	489	C
2	L5	494	U
2	L5	497	G
2	L5	498	C
2	L5	499	G
2	L5	502	C
2	L5	503	C

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Mol	Chain	Res	Type
2	L5	504	G
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	513	U
2	L5	514	U
2	L5	518	G
2	L5	643	C
2	L5	646	G
2	L5	654	C
2	L5	655	C
2	L5	656	C
2	L5	657	C
2	L5	659	G
2	L5	666	G
2	L5	667	A
2	L5	668	C
2	L5	669	C
2	L5	673	C
2	L5	685	C
2	L5	686	A
2	L5	687	U
2	L5	696	C
2	L5	704	C
2	L5	708	G
2	L5	730	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	742	G
2	L5	746	A
2	L5	759	G
2	L5	904	C
2	L5	905	C
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	917	A
2	L5	923	C
2	L5	924	C
2	L5	926	G
2	L5	932	A

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Mol	Chain	Res	Type
2	L5	933	G
2	L5	935	A
2	L5	936	C
2	L5	941	C
2	L5	943	A
2	L5	944	A
2	L5	945	U
2	L5	946	C
2	L5	956	A
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	966	A
2	L5	967	C
2	L5	968	C
2	L5	969	C
2	L5	970	G
2	L5	977	C
2	L5	982	U
2	L5	985	C
2	L5	989	U
2	L5	1070	G
2	L5	1072	C
2	L5	1075	G
2	L5	1076	C
2	L5	1082	C
2	L5	1083	U
2	L5	1168	G
2	L5	1171	G
2	L5	1172	C
2	L5	1173	G
2	L5	1179	U
2	L5	1180	C
2	L5	1181	C
2	L5	1182	C
2	L5	1183	C
2	L5	1187	G
2	L5	1202	C
2	L5	1203	G
2	L5	1210	C

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Mol	Chain	Res	Type
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1219	G
2	L5	1222	A
2	L5	1246	G
2	L5	1253	G
2	L5	1254	A
2	L5	1257	A
2	L5	1258	G
2	L5	1262	G
2	L5	1266	G
2	L5	1267	C
2	L5	1269	G
2	L5	1271	G
2	L5	1272	C
2	L5	1273	G
2	L5	1275	G
2	L5	1277	G
2	L5	1280	C
2	L5	1284	G
2	L5	1285	U
2	L5	1287	G
2	L5	1293	G
2	L5	1294	A
2	L5	1295	C
2	L5	1296	G
2	L5	1301	C
2	L5	1312	A
2	L5	1313	C
2	L5	1314	C
2	L5	1326	A2M
2	L5	1337	A
2	L5	1354	A
2	L5	1359	G
2	L5	1365	C
2	L5	1366	G
2	L5	1367	C
2	L5	1387	A
2	L5	1394	G
2	L5	1397	A
2	L5	1398	A

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Mol	Chain	Res	Type
2	L5	1404	G
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1411	C
2	L5	1414	C
2	L5	1416	G
2	L5	1417	C
2	L5	1420	A
2	L5	1437	C
2	L5	1438	U
2	L5	1439	C
2	L5	1442	C
2	L5	1443	A
2	L5	1444	G
2	L5	1446	C
2	L5	1447	C
2	L5	1482	G
2	L5	1483	C
2	L5	1497	A
2	L5	1498	G
2	L5	1502	G
2	L5	1517	G
2	L5	1524	A2M
2	L5	1534	A2M
2	L5	1537	A
2	L5	1547	A
2	L5	1564	A
2	L5	1566	C
2	L5	1574	G
2	L5	1578	U
2	L5	1591	U
2	L5	1596	U
2	L5	1624	G
2	L5	1625	OMG
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1640	C
2	L5	1641	G
2	L5	1642	A

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Mol	Chain	Res	Type
2	L5	1654	G
2	L5	1661	C
2	L5	1676	C
2	L5	1677	PSU
2	L5	1678	C
2	L5	1680	G
2	L5	1694	C
2	L5	1697	G
2	L5	1699	A
2	L5	1700	G
2	L5	1701	A
2	L5	1702	C
2	L5	1703	C
2	L5	1704	C
2	L5	1705	G
2	L5	1717	C
2	L5	1718	C
2	L5	1719	A
2	L5	1721	G
2	L5	1731	C
2	L5	1734	G
2	L5	1740	C
2	L5	1742	A
2	L5	1750	G
2	L5	1753	G
2	L5	1755	C
2	L5	1757	U
2	L5	1758	G
2	L5	1761	G
2	L5	1762	C
2	L5	1763	C
2	L5	1764	G
2	L5	1765	A
2	L5	1766	A
2	L5	1767	A
2	L5	1768	C
2	L5	1770	A
2	L5	1787	A
2	L5	1804	A
2	L5	1806	G
2	L5	1810	G
2	L5	1821	G

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Mol	Chain	Res	Type
2	L5	1822	U
2	L5	1834	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1855	G
2	L5	1869	G
2	L5	1882	U
2	L5	1892	A
2	L5	1897	A
2	L5	1917	A
2	L5	1918	U
2	L5	1919	G
2	L5	1920	C
2	L5	1921	C
2	L5	1922	G
2	L5	1925	G
2	L5	1931	C
2	L5	1932	A
2	L5	1936	C
2	L5	1948	G
2	L5	1951	G
2	L5	1961	G
2	L5	1962	A
2	L5	1974	U
2	L5	1975	G
2	L5	1978	C
2	L5	1980	U
2	L5	1981	G
2	L5	1982	G
2	L5	1984	A
2	L5	1985	G
2	L5	1986	U
2	L5	1991	A
2	L5	1993	C
2	L5	1997	U
2	L5	1998	A
2	L5	1999	A
2	L5	2001	G
2	L5	2002	A
2	L5	2003	G
2	L5	2004	U

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Mol	Chain	Res	Type
2	L5	2005	G
2	L5	2011	C
2	L5	2016	C
2	L5	2017	A
2	L5	2018	C
2	L5	2021	G
2	L5	2024	G
2	L5	2026	A
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A
2	L5	2084	C
2	L5	2085	G
2	L5	2092	G
2	L5	2093	A
2	L5	2095	A
2	L5	2097	U
2	L5	2098	G
2	L5	2101	C
2	L5	2102	G
2	L5	2107	C
2	L5	2110	C
2	L5	2112	G
2	L5	2250	C
2	L5	2252	G
2	L5	2254	G
2	L5	2256	C
2	L5	2259	G
2	L5	2262	G
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2306	G
2	L5	2313	A
2	L5	2331	G
2	L5	2333	G
2	L5	2345	G
2	L5	2348	G
2	L5	2351	OMC
2	L5	2360	A

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Mol	Chain	Res	Type
2	L5	2364	OMG
2	L5	2395	A
2	L5	2397	G
2	L5	2401	A2M
2	L5	2417	A
2	L5	2425	U
2	L5	2447	U
2	L5	2450	G
2	L5	2453	A
2	L5	2464	C
2	L5	2465	C
2	L5	2469	C
2	L5	2471	G
2	L5	2474	G
2	L5	2475	G
2	L5	2478	C
2	L5	2479	G
2	L5	2483	G
2	L5	2484	A
2	L5	2485	U
2	L5	2487	G
2	L5	2488	C
2	L5	2489	C
2	L5	2490	U
2	L5	2491	C
2	L5	2494	U
2	L5	2504	C
2	L5	2505	C
2	L5	2506	G
2	L5	2513	A
2	L5	2518	G
2	L5	2519	U
2	L5	2520	C
2	L5	2529	A
2	L5	2537	A
2	L5	2544	G
2	L5	2546	G
2	L5	2547	G
2	L5	2554	U
2	L5	2555	G
2	L5	2560	C
2	L5	2565	A

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Mol	Chain	Res	Type
2	L5	2567	G
2	L5	2573	A
2	L5	2583	C
2	L5	2587	A
2	L5	2589	C
2	L5	2601	A
2	L5	2602	G
2	L5	2627	C
2	L5	2653	C
2	L5	2662	G
2	L5	2669	C
2	L5	2675	G
2	L5	2676	A
2	L5	2687	U
2	L5	2694	G
2	L5	2695	A
2	L5	2696	A
2	L5	2702	C
2	L5	2706	G
2	L5	2707	U
2	L5	2708	U
2	L5	2710	C
2	L5	2711	G
2	L5	2721	G
2	L5	2724	G
2	L5	2726	G
2	L5	2739	C
2	L5	2742	G
2	L5	2743	A
2	L5	2754	G
2	L5	2761	U
2	L5	2763	U
2	L5	2769	U
2	L5	2770	C
2	L5	2788	U
2	L5	2790	U
2	L5	2806	A
2	L5	2814	C
2	L5	2815	A2M
2	L5	2826	U
2	L5	2827	G
2	L5	2829	U

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Mol	Chain	Res	Type
2	L5	2838	G
2	L5	2855	G
2	L5	2867	C
2	L5	2877	G
2	L5	2900	U
2	L5	2901	G
2	L5	2902	G
2	L5	2903	G
2	L5	2904	U
2	L5	2905	C
2	L5	2907	G
2	L5	2908	U
2	L5	3590	G
2	L5	3591	C
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3604	A
2	L5	3605	C
2	L5	3616	U
2	L5	3626	G
2	L5	3630	A
2	L5	3635	A
2	L5	3644	U
2	L5	3646	A
2	L5	3648	A
2	L5	3662	A
2	L5	3664	G
2	L5	3670	C
2	L5	3673	C
2	L5	3674	G
2	L5	3701	OMC
2	L5	3710	G
2	L5	3711	A
2	L5	3713	U
2	L5	3727	A
2	L5	3753	G
2	L5	3760	A
2	L5	3764	U
2	L5	3770	U
2	L5	3775	A

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Mol	Chain	Res	Type
2	L5	3776	G
2	L5	3777	G
2	L5	3785	A2M
2	L5	3786	U
2	L5	3792	OMG
2	L5	3811	G
2	L5	3814	U
2	L5	3817	A
2	L5	3819	G
2	L5	3824	A
2	L5	3838	U
2	L5	3839	G
2	L5	3840	U
2	L5	3867	A2M
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3885	G
2	L5	3892	U
2	L5	3897	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3938	G
2	L5	3939	G
2	L5	3942	A
2	L5	3945	A
2	L5	3947	A
2	L5	3949	A
2	L5	3950	U
2	L5	3952	A
2	L5	3953	G
2	L5	4057	C
2	L5	4058	U
2	L5	4059	C
2	L5	4060	U
2	L5	4061	G
2	L5	4062	A
2	L5	4064	C
2	L5	4065	G

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Mol	Chain	Res	Type
2	L5	4068	U
2	L5	4076	G
2	L5	4095	G
2	L5	4097	G
2	L5	4099	G
2	L5	4104	G
2	L5	4106	G
2	L5	4108	G
2	L5	4111	U
2	L5	4114	C
2	L5	4115	G
2	L5	4116	C
2	L5	4117	U
2	L5	4119	C
2	L5	4121	G
2	L5	4122	G
2	L5	4127	A
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4144	C
2	L5	4146	G
2	L5	4149	C
2	L5	4162	C
2	L5	4163	U
2	L5	4168	G
2	L5	4170	A
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4203	A
2	L5	4222	G
2	L5	4225	G
2	L5	4229	U
2	L5	4233	A
2	L5	4243	C
2	L5	4251	A
2	L5	4254	G
2	L5	4257	A
2	L5	4258	C
2	L5	4265	U
2	L5	4268	A

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Mol	Chain	Res	Type
2	L5	4273	A
2	L5	4291	G
2	L5	4295	U
2	L5	4305	G
2	L5	4314	C
2	L5	4319	C
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C
2	L5	4338	G
2	L5	4349	C
2	L5	4354	U
2	L5	4364	G
2	L5	4371	G
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4379	A
2	L5	4387	C
2	L5	4391	G
2	L5	4394	A
2	L5	4405	G
2	L5	4421	C
2	L5	4422	A
2	L5	4426	C
2	L5	4438	U
2	L5	4444	C
2	L5	4448	G
2	L5	4449	A
2	L5	4452	U
2	L5	4464	A
2	L5	4466	C
2	L5	4475	G
2	L5	4488	A
2	L5	4491	G
2	L5	4500	PSU
2	L5	4512	U
2	L5	4513	A
2	L5	4519	C
2	L5	4524	G
2	L5	4525	C

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Mol	Chain	Res	Type
2	L5	4545	G
2	L5	4548	A
2	L5	4560	C
2	L5	4567	G
2	L5	4569	U
2	L5	4575	G
2	L5	4584	A
2	L5	4589	A
2	L5	4590	A2M
2	L5	4600	G
2	L5	4601	U
2	L5	4636	PSU
2	L5	4637	OMG
2	L5	4652	G
2	L5	4656	A
2	L5	4657	U
2	L5	4670	C
2	L5	4672	A
2	L5	4679	G
2	L5	4694	G
2	L5	4695	C
2	L5	4700	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4734	A
2	L5	4740	G
2	L5	4741	C
2	L5	4742	G
2	L5	4745	G
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4761	G
2	L5	4765	G
2	L5	4771	C
2	L5	4772	C
2	L5	4774	C
2	L5	4775	C
2	L5	4859	C
2	L5	4863	G
2	L5	4870	G

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Mol	Chain	Res	Type
2	L5	4871	C
2	L5	4875	G
2	L5	4881	U
2	L5	4882	U
2	L5	4883	C
2	L5	4889	G
2	L5	4895	C
2	L5	4896	G
2	L5	4897	G
2	L5	4899	G
2	L5	4900	C
2	L5	4901	G
2	L5	4910	G
2	L5	4912	G
2	L5	4914	C
2	L5	4922	C
2	L5	4925	U
2	L5	4926	C
2	L5	4927	G
2	L5	4928	C
2	L5	4934	A
2	L5	4937	C
2	L5	4940	C
2	L5	4941	G
2	L5	4943	A
2	L5	4951	G
2	L5	4955	A
2	L5	4960	G
2	L5	4975	G
2	L5	4976	U
2	L5	4985	U
2	L5	4988	U
2	L5	4989	U
2	L5	4991	U
2	L5	4995	U
2	L5	5007	A
2	L5	5013	C
2	L5	5014	A
2	L5	5017	G
2	L5	5022	U
2	L5	5023	C
2	L5	5024	C

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Mol	Chain	Res	Type
2	L5	5026	U
2	L5	5027	C
2	L5	5028	G
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5061	A
2	L5	5069	U
3	L7	33	U
3	L7	38	U
3	L7	53	U
3	L7	54	A
3	L7	64	G
3	L7	100	A
3	L7	110	G
4	L8	23	C
4	L8	25	G
4	L8	34	U
4	L8	35	C
4	L8	59	A
4	L8	62	A
4	L8	63	U
4	L8	80	A
4	L8	82	A
4	L8	84	A
4	L8	85	U
4	L8	87	G
4	L8	94	G
4	L8	103	A
4	L8	105	C
4	L8	111	U
4	L8	114	G
4	L8	124	U
4	L8	125	C
4	L8	126	C
4	L8	127	U
4	L8	150	C
4	L8	151	G
67	S2	4	C
67	S2	14	C

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Mol	Chain	Res	Type
67	S2	25	A
67	S2	33	G
67	S2	41	G
67	S2	42	A
67	S2	44	U
67	S2	45	A
67	S2	46	A
67	S2	56	G
67	S2	58	C
67	S2	62	G
67	S2	65	C
67	S2	67	C
67	S2	68	A
67	S2	72	C
67	S2	73	C
67	S2	74	G
67	S2	76	U
67	S2	92	A
67	S2	99	A2M
67	S2	103	A
67	S2	113	G
67	S2	115	U
67	S2	126	G
67	S2	130	G
67	S2	142	C
67	S2	143	U
67	S2	149	A
67	S2	158	A
67	S2	160	U
67	S2	162	C
67	S2	170	A
67	S2	179	C
67	S2	182	C
67	S2	190	G
67	S2	196	C
67	S2	197	U
67	S2	198	U
67	S2	200	G
67	S2	203	G
67	S2	204	G
67	S2	207	G
67	S2	208	G

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Mol	Chain	Res	Type
67	S2	213	G
67	S2	214	U
67	S2	220	U
67	S2	291	G
67	S2	292	A
67	S2	295	C
67	S2	302	A
67	S2	306	C
67	S2	307	G
67	S2	308	G
67	S2	309	G
67	S2	312	G
67	S2	318	A
67	S2	319	C
67	S2	323	C
67	S2	324	C
67	S2	325	C
67	S2	326	C
67	S2	327	G
67	S2	328	U
67	S2	329	G
67	S2	332	G
67	S2	339	A
67	S2	347	G
67	S2	360	A
67	S2	361	U
67	S2	362	C
67	S2	363	A
67	S2	364	A
67	S2	368	U
67	S2	369	C
67	S2	370	G
67	S2	381	C
67	S2	383	G
67	S2	385	G
67	S2	386	C
67	S2	400	C
67	S2	407	G
67	S2	408	A
67	S2	409	C
67	S2	426	A
67	S2	448	A

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Mol	Chain	Res	Type
67	S2	449	A
67	S2	450	C
67	S2	452	G
67	S2	464	A
67	S2	465	A
67	S2	471	G
67	S2	472	C
67	S2	473	A
67	S2	474	G
67	S2	476	A
67	S2	482	G
67	S2	487	U
67	S2	488	U
67	S2	492	C
67	S2	493	A
67	S2	502	C
67	S2	531	A
67	S2	532	C
67	S2	536	A
67	S2	537	C
67	S2	540	U
67	S2	542	U
67	S2	544	G
67	S2	546	G
67	S2	547	G
67	S2	557	U
67	S2	558	G
67	S2	563	G
67	S2	564	A
67	S2	576	A2M
67	S2	583	A
67	S2	587	A
67	S2	589	G
67	S2	590	A
67	S2	591	U
67	S2	592	C
67	S2	593	C
67	S2	604	A
67	S2	607	U
67	S2	614	C
67	S2	617	G
67	S2	623	G

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Mol	Chain	Res	Type
67	S2	627	OMU
67	S2	628	A
67	S2	643	A
67	S2	644	OMG
67	S2	655	A
67	S2	660	C
67	S2	664	A
67	S2	668	A2M
67	S2	669	A
67	S2	671	A
67	S2	672	A
67	S2	673	G
67	S2	684	G
67	S2	688	U
67	S2	689	U
67	S2	690	G
67	S2	692	G
67	S2	693	A
67	S2	695	C
67	S2	696	G
67	S2	697	G
67	S2	698	G
67	S2	732	U
67	S2	733	C
67	S2	736	C
67	S2	737	G
67	S2	738	C
67	S2	749	U
67	S2	751	G
67	S2	752	G
67	S2	753	C
67	S2	788	G
67	S2	791	C
67	S2	792	C
67	S2	798	G
67	S2	799	OMU
67	S2	801	PSU
67	S2	821	G
67	S2	822	U
67	S2	823	U
67	S2	824	C
67	S2	827	A

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Mol	Chain	Res	Type
67	S2	830	A
67	S2	834	C
67	S2	835	C
67	S2	836	G
67	S2	837	A
67	S2	838	G
67	S2	839	C
67	S2	842	C
67	S2	844	U
67	S2	847	A
67	S2	863	PSU
67	S2	864	A
67	S2	867	OMG
67	S2	870	A
67	S2	874	G
67	S2	877	C
67	S2	878	G
67	S2	880	G
67	S2	888	U
67	S2	889	U
67	S2	891	G
67	S2	894	G
67	S2	896	U
67	S2	897	U
67	S2	898	U
67	S2	899	U
67	S2	900	C
67	S2	901	G
67	S2	903	A
67	S2	913	A
67	S2	917	U
67	S2	920	A
67	S2	922	A
67	S2	933	G
67	S2	934	G
67	S2	953	C
67	S2	955	A
67	S2	963	A
67	S2	966	PSU
67	S2	970	G
67	S2	971	G
67	S2	972	A

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Mol	Chain	Res	Type
67	S2	990	A
67	S2	992	A
67	S2	999	G
67	S2	1001	A
67	S2	1008	A
67	S2	1014	G
67	S2	1017	U
67	S2	1023	A
67	S2	1027	A
67	S2	1033	G
67	S2	1045	PSU
67	S2	1056	PSU
67	S2	1061	U
67	S2	1062	A
67	S2	1067	C
67	S2	1083	A
67	S2	1085	C
67	S2	1107	G
67	S2	1108	G
67	S2	1109	C
67	S2	1113	A
67	S2	1116	C
67	S2	1119	A
67	S2	1121	G
67	S2	1133	A
67	S2	1138	C
67	S2	1148	A
67	S2	1150	A
67	S2	1153	C
67	S2	1154	U
67	S2	1195	A
67	S2	1207	G
67	S2	1208	A
67	S2	1215	C
67	S2	1216	C
67	S2	1217	A
67	S2	1220	A
67	S2	1224	G
67	S2	1227	G
67	S2	1233	G
67	S2	1242	U
67	S2	1243	U

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Mol	Chain	Res	Type
67	S2	1248	B8N
67	S2	1251	A
67	S2	1253	A
67	S2	1256	G
67	S2	1257	G
67	S2	1259	A
67	S2	1271	C
67	S2	1272	OMC
67	S2	1274	G
67	S2	1275	G
67	S2	1283	C
67	S2	1285	G
67	S2	1286	G
67	S2	1288	OMU
67	S2	1290	G
67	S2	1294	G
67	S2	1295	A
67	S2	1301	A
67	S2	1302	G
67	S2	1303	C
67	S2	1308	U
67	S2	1333	U
67	S2	1342	U
67	S2	1348	G
67	S2	1357	A
67	S2	1358	U
67	S2	1371	U
67	S2	1372	U
67	S2	1376	A
67	S2	1378	A
67	S2	1382	A
67	S2	1401	A
67	S2	1402	A
67	S2	1408	U
67	S2	1413	G
67	S2	1414	A
67	S2	1416	C
67	S2	1418	C
67	S2	1419	C
67	S2	1420	G
67	S2	1421	A
67	S2	1422	G

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Mol	Chain	Res	Type
67	S2	1423	C
67	S2	1428	G
67	S2	1429	G
67	S2	1433	C
67	S2	1435	C
67	S2	1437	C
67	S2	1438	A
67	S2	1439	A
67	S2	1442	OMU
67	S2	1449	G
67	S2	1454	A
67	S2	1463	U
67	S2	1477	U
67	S2	1478	U
67	S2	1489	A
67	S2	1490	OMG
67	S2	1494	U
67	S2	1495	G
67	S2	1497	G
67	S2	1498	A
67	S2	1521	C
67	S2	1522	A
67	S2	1531	A
67	S2	1533	A
67	S2	1544	C
67	S2	1546	G
67	S2	1552	G
67	S2	1553	C
67	S2	1556	A
67	S2	1558	C
67	S2	1574	C
67	S2	1575	G
67	S2	1578	U
67	S2	1580	A
67	S2	1581	C
67	S2	1585	U
67	S2	1587	G
67	S2	1588	A
67	S2	1600	G
67	S2	1604	G
67	S2	1606	G
67	S2	1621	U

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Mol	Chain	Res	Type
67	S2	1623	A
67	S2	1633	A
67	S2	1637	A
67	S2	1646	C
67	S2	1648	G
67	S2	1654	G
67	S2	1663	A
67	S2	1665	G
67	S2	1683	C
67	S2	1686	G
67	S2	1695	A
67	S2	1698	C
67	S2	1699	A
67	S2	1710	C
67	S2	1712	A
67	S2	1715	A
67	S2	1721	U
67	S2	1722	G
67	S2	1725	U
67	S2	1726	G
67	S2	1744	G
67	S2	1745	A
67	S2	1752	C
67	S2	1753	C
67	S2	1754	G
67	S2	1755	C
67	S2	1757	G
67	S2	1758	G
67	S2	1759	G
67	S2	1761	U
67	S2	1772	C
67	S2	1773	C
67	S2	1774	C
67	S2	1777	G
67	S2	1782	G
67	S2	1783	C
67	S2	1784	G
67	S2	1786	U
67	S2	1809	A
67	S2	1810	U
67	S2	1825	A
67	S2	1826	G

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Mol	Chain	Res	Type
67	S2	1831	A
67	S2	1835	A
67	S2	1838	U
67	S2	1849	G
67	S2	1851	MA6
67	S2	1861	G
67	S2	1862	G
67	S2	1863	A
67	S2	1864	U
67	S2	1865	C

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	406	C
2	L5	914	U
2	L5	1082	C
2	L5	1633	G
2	L5	1977	C
2	L5	2416	G
2	L5	2675	G
2	L5	2760	G
2	L5	3673	C
2	L5	4600	G
2	L5	4699	U
2	L5	4913	G
67	S2	291	G
67	S2	531	A
67	S2	563	G
67	S2	688	U
67	S2	1434	C
67	S2	1477	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
67	OMG	S2	683	67	23,26,27	0.49	0	32,38,41	0.53	0
67	OMG	S2	644	67	23,26,27	0.44	0	32,38,41	0.49	0
2	OMG	L5	1625	2	23,26,27	0.54	0	32,38,41	0.51	0
2	OMC	L5	2861	2	19,22,23	0.62	0	25,31,34	0.84	2 (8%)
2	A2M	L5	2401	2	22,25,26	1.11	1 (4%)	30,36,39	1.58	7 (23%)
2	OMC	L5	3869	2	19,22,23	0.63	0	25,31,34	0.65	0
2	OMG	L5	4494	2	23,26,27	0.56	0	32,38,41	0.51	0
2	PSU	L5	3851	2	18,21,22	1.04	1 (5%)	21,30,33	1.93	4 (19%)
2	PSU	L5	4973	2	18,21,22	1.06	2 (11%)	21,30,33	2.01	5 (23%)
67	OMC	S2	174	67	19,22,23	0.49	0	25,31,34	0.69	0
67	A2M	S2	99	83,67	22,25,26	1.19	1 (4%)	30,36,39	1.58	8 (26%)
4	PSU	L8	69	4	18,21,22	1.09	1 (5%)	21,30,33	2.00	5 (23%)
67	PSU	S2	866	67	18,21,22	1.15	1 (5%)	21,30,33	1.94	4 (19%)
67	OMC	S2	1703	67	19,22,23	0.53	0	25,31,34	0.72	1 (4%)
67	PSU	S2	1244	67	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
2	PSU	L5	2632	2	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
2	PSU	L5	2839	2	18,21,22	1.11	2 (11%)	21,30,33	1.88	4 (19%)
2	A2M	L5	2363	83,2	22,25,26	1.20	2 (9%)	30,36,39	1.56	9 (30%)
67	OMC	S2	1272	67	19,22,23	0.52	0	25,31,34	0.94	2 (8%)
2	PSU	L5	5010	2	18,21,22	1.08	2 (11%)	21,30,33	1.91	4 (19%)
2	A2M	L5	4523	83,2	22,25,26	1.23	3 (13%)	30,36,39	1.58	7 (23%)
2	PSU	L5	4576	2	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
2	PSU	L5	4628	2	18,21,22	0.98	1 (5%)	21,30,33	1.88	4 (19%)
2	OMU	L5	4306	2	19,22,23	3.19	7 (36%)	25,31,34	1.73	4 (16%)
67	A2M	S2	1031	67	22,25,26	1.18	1 (4%)	30,36,39	1.50	7 (23%)
2	OMC	L5	2804	2	19,22,23	0.66	0	25,31,34	0.60	0
67	OMU	S2	116	67	19,22,23	3.36	7 (36%)	25,31,34	1.72	5 (20%)
2	OMU	L5	4620	2	19,22,23	3.17	7 (36%)	25,31,34	1.76	5 (20%)
67	A2M	S2	576	67	22,25,26	1.25	2 (9%)	30,36,39	1.52	6 (20%)
67	6MZ	S2	1832	83,67	26,26,26	2.81	4 (15%)	36,39,39	2.13	10 (27%)
2	A2M	L5	2787	2	22,25,26	1.11	1 (4%)	30,36,39	1.46	7 (23%)
67	PSU	S2	1177	67	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
2	PSU	L5	3853	83,2	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
2	A2M	L5	1323	2	22,25,26	1.22	3 (13%)	30,36,39	1.63	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L5	4571	2	22,25,26	1.27	2 (9%)	30,36,39	1.61	9 (30%)
2	1MA	L5	1322	83,2	21,25,26	0.64	0	30,37,40	0.83	2 (6%)
2	OMG	L5	2364	83,2	23,26,27	0.58	0	32,38,41	0.43	0
67	A2M	S2	159	67	22,25,26	1.16	2 (9%)	30,36,39	1.49	7 (23%)
67	PSU	S2	651	67	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
67	OMC	S2	1391	67	19,22,23	0.49	0	25,31,34	0.68	0
67	PSU	S2	1045	67	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
67	A2M	S2	468	67	22,25,26	1.27	1 (4%)	30,36,39	1.57	7 (23%)
2	PSU	L5	3920	83,2	18,21,22	1.07	2 (11%)	21,30,33	1.93	5 (23%)
2	A2M	L5	2815	2	22,25,26	1.12	2 (9%)	30,36,39	1.55	9 (30%)
67	A2M	S2	1383	67	22,25,26	1.20	1 (4%)	30,36,39	1.62	6 (20%)
2	A2M	L5	400	2	22,25,26	1.24	2 (9%)	30,36,39	1.59	8 (26%)
2	A2M	L5	3825	2	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
67	PSU	S2	93	67	18,21,22	1.11	1 (5%)	21,30,33	1.79	4 (19%)
67	OMG	S2	509	67	23,26,27	0.46	0	32,38,41	0.51	0
67	PSU	S2	966	83,67	18,21,22	1.15	1 (5%)	21,30,33	1.86	4 (19%)
2	OMC	L5	2824	2	19,22,23	0.62	0	25,31,34	0.69	0
67	OMU	S2	627	67	19,22,23	3.39	7 (36%)	25,31,34	1.81	5 (20%)
67	PSU	S2	109	67	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
67	A2M	S2	166	67	22,25,26	1.29	1 (4%)	30,36,39	1.63	7 (23%)
2	OMC	L5	3808	2	19,22,23	0.69	0	25,31,34	0.84	1 (4%)
2	OMG	L5	4499	2	23,26,27	0.54	0	32,38,41	0.47	0
2	5MC	L5	3782	83,2	19,22,23	0.70	0	26,32,35	0.81	1 (3%)
2	OMG	L5	3627	2	23,26,27	0.55	0	32,38,41	0.61	0
2	PSU	L5	4431	2	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
2	OMG	L5	4392	2	23,26,27	0.59	0	32,38,41	0.45	0
67	A2M	S2	27	67	22,25,26	1.23	1 (4%)	30,36,39	1.55	7 (23%)
2	A2M	L5	1524	2	22,25,26	1.25	2 (9%)	30,36,39	1.51	7 (23%)
2	OMC	L5	4536	2	19,22,23	0.65	0	25,31,34	0.68	0
2	OMG	L5	4618	2	23,26,27	0.61	0	32,38,41	0.49	0
67	PSU	S2	1367	67	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
2	OMG	L5	3792	2	23,26,27	0.56	0	32,38,41	0.51	0
2	PSU	L5	4552	2	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
2	PSU	L5	3884	2	18,21,22	1.11	2 (11%)	21,30,33	1.98	4 (19%)
2	OMC	L5	3887	2	19,22,23	0.65	0	25,31,34	0.69	0
2	PSU	L5	1683	2	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
2	PSU	L5	4403	2	18,21,22	1.06	2 (11%)	21,30,33	2.04	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4972	2	18,21,22	1.07	1 (5%)	21,30,33	1.94	4 (19%)
2	OMU	L5	4498	2	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
2	PSU	L5	1792	2	18,21,22	1.03	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	1744	83,2	18,21,22	1.05	1 (5%)	21,30,33	2.00	5 (23%)
2	PSU	L5	4442	2	18,21,22	1.06	1 (5%)	21,30,33	1.99	6 (28%)
67	B8N	S2	1248	67	25,29,30	3.28	7 (28%)	28,42,45	1.95	8 (28%)
2	PSU	L5	4361	2	18,21,22	1.05	1 (5%)	21,30,33	1.94	4 (19%)
2	PSU	L5	1677	2	18,21,22	1.04	1 (5%)	21,30,33	1.92	5 (23%)
67	OMU	S2	1288	67	19,22,23	3.43	7 (36%)	25,31,34	1.73	5 (20%)
2	A2M	L5	3785	83,2	22,25,26	1.15	1 (4%)	30,36,39	1.62	10 (33%)
67	PSU	S2	1004	67	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
4	OMG	L8	75	4	23,26,27	0.53	0	32,38,41	0.48	0
2	A2M	L5	1871	83,2	22,25,26	1.23	2 (9%)	30,36,39	1.67	7 (23%)
2	PSU	L5	4353	2	18,21,22	1.05	1 (5%)	21,30,33	1.96	4 (19%)
67	OMG	S2	1490	67	23,26,27	0.52	0	32,38,41	0.55	0
67	4AC	S2	1337	67	21,24,25	0.37	0	28,34,37	0.66	1 (3%)
2	PSU	L5	1860	2	18,21,22	1.06	1 (5%)	21,30,33	1.81	4 (19%)
2	OMG	L5	2876	2	23,26,27	0.57	0	32,38,41	0.51	0
2	OMU	L5	3925	2	19,22,23	3.17	7 (36%)	25,31,34	1.83	5 (20%)
2	OMG	L5	1316	2	23,26,27	0.65	0	32,38,41	0.58	0
67	OMC	S2	517	67	19,22,23	0.51	0	25,31,34	0.72	0
67	PSU	S2	686	67	18,21,22	1.14	1 (5%)	21,30,33	1.87	4 (19%)
67	OMU	S2	354	67	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
67	G7M	S2	1639	67	23,26,27	2.67	8 (34%)	34,39,42	2.57	11 (32%)
67	PSU	S2	681	67	18,21,22	1.05	1 (5%)	21,30,33	1.87	4 (19%)
2	5MC	L5	4447	2	19,22,23	0.91	1 (5%)	26,32,35	0.87	0
67	PSU	S2	406	67	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
67	MA6	S2	1850	67	23,26,27	1.29	2 (8%)	33,38,41	3.35	12 (36%)
67	OMU	S2	428	67	19,22,23	3.39	7 (36%)	25,31,34	1.79	5 (20%)
2	OMG	L5	2424	2	23,26,27	0.57	0	32,38,41	0.41	0
2	OMG	L5	3899	2	23,26,27	0.64	0	32,38,41	0.53	0
67	OMU	S2	1442	67	19,22,23	3.45	7 (36%)	25,31,34	1.77	4 (16%)
2	A2M	L5	398	2	22,25,26	1.16	1 (4%)	30,36,39	1.58	7 (23%)
2	A2M	L5	3830	2	22,25,26	1.16	1 (4%)	30,36,39	1.59	7 (23%)
2	PSU	L5	4521	83,2	18,21,22	1.09	2 (11%)	21,30,33	1.99	5 (23%)
2	OMG	L5	3744	2	23,26,27	0.54	0	32,38,41	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L5	1326	2	22,25,26	1.15	2 (9%)	30,36,39	1.50	9 (30%)
2	PSU	L5	1536	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
67	OMG	S2	601	67	23,26,27	0.47	0	32,38,41	0.49	0
2	PSU	L5	4296	2	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
2	OMG	L5	1522	2	23,26,27	0.60	0	32,38,41	0.66	0
2	PSU	L5	3639	2	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
2	PSU	L5	4500	2	18,21,22	1.12	2 (11%)	21,30,33	2.02	5 (23%)
4	PSU	L8	55	4	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
2	PSU	L5	1582	2	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
2	A2M	L5	3718	2	22,25,26	1.13	1 (4%)	30,36,39	1.53	6 (20%)
2	A2M	L5	3867	2	22,25,26	1.22	2 (9%)	30,36,39	1.53	7 (23%)
67	PSU	S2	1232	67	18,21,22	1.14	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4493	2	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)
67	OMU	S2	121	67	19,22,23	3.39	7 (36%)	25,31,34	1.78	5 (20%)
2	6MZ	L5	4220	2	22,25,26	3.96	12 (54%)	29,36,39	2.35	10 (34%)
2	OMG	L5	4196	2	23,26,27	0.55	0	32,38,41	0.44	0
2	OMU	L5	2837	2	19,22,23	3.26	7 (36%)	25,31,34	1.94	4 (16%)
2	PSU	L5	3844	2	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
67	A2M	S2	668	83,67	22,25,26	1.28	2 (9%)	30,36,39	1.58	6 (20%)
2	PSU	L5	4471	2	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
2	OMG	L5	4637	2	23,26,27	0.57	0	32,38,41	0.49	0
2	PSU	L5	4299	2	18,21,22	1.06	2 (11%)	21,30,33	1.86	4 (19%)
2	UR3	L5	4530	2	19,22,23	2.67	7 (36%)	26,32,35	1.58	3 (11%)
67	PSU	S2	801	67	18,21,22	1.16	1 (5%)	21,30,33	1.80	4 (19%)
2	PSU	L5	1782	2	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
67	MA6	S2	1851	67	23,26,27	1.26	2 (8%)	33,38,41	3.38	12 (36%)
2	OMC	L5	3701	2	19,22,23	0.72	0	25,31,34	1.75	4 (16%)
2	PSU	L5	4457	2	18,21,22	1.07	2 (11%)	21,30,33	2.03	4 (19%)
2	PSU	L5	4532	2	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
2	OMC	L5	2365	83,2	19,22,23	0.64	0	25,31,34	0.61	0
2	PSU	L5	1781	2	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
2	A2M	L5	4590	2	22,25,26	1.18	2 (9%)	30,36,39	1.57	6 (20%)
2	OMC	L5	3841	2	19,22,23	0.68	0	25,31,34	0.61	0
2	PSU	L5	4636	2	18,21,22	1.10	2 (11%)	21,30,33	2.17	7 (33%)
2	OMG	L5	4370	2	23,26,27	0.54	0	32,38,41	0.51	0
67	PSU	S2	1174	67	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	OMG	S2	436	67	23,26,27	0.47	0	32,38,41	0.54	0
67	OMU	S2	799	67	19,22,23	3.42	7 (36%)	25,31,34	1.79	5 (20%)
2	OMG	L5	4228	2	23,26,27	0.61	0	32,38,41	0.74	0
67	PSU	S2	1056	67	18,21,22	1.07	1 (5%)	21,30,33	1.85	4 (19%)
2	OMU	L5	4227	2	19,22,23	3.26	7 (36%)	25,31,34	1.88	5 (20%)
2	PSU	L5	1862	2	18,21,22	1.03	1 (5%)	21,30,33	1.97	4 (19%)
67	PSU	S2	105	67	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
67	PSU	S2	1081	67	18,21,22	1.06	1 (5%)	21,30,33	2.01	6 (28%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	1.96	4 (19%)
67	4AC	S2	1842	67	21,24,25	0.39	0	28,34,37	0.49	0
2	PSU	L5	3637	2	18,21,22	1.06	1 (5%)	21,30,33	2.05	5 (23%)
67	OMC	S2	462	67	19,22,23	0.52	0	25,31,34	0.57	0
67	OMU	S2	172	67	19,22,23	3.38	7 (36%)	25,31,34	1.84	5 (20%)
2	PSU	L5	4293	2	18,21,22	1.05	2 (11%)	21,30,33	1.93	4 (19%)
67	PSU	S2	649	67	18,21,22	1.14	1 (5%)	21,30,33	1.86	4 (19%)
67	PSU	S2	814	67	18,21,22	1.08	1 (5%)	21,30,33	1.73	4 (19%)
67	PSU	S2	863	67	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
67	OMG	S2	867	67	23,26,27	0.51	0	32,38,41	0.52	0
2	OMC	L5	2422	83,2	19,22,23	0.66	0	25,31,34	0.70	0
2	OMC	L5	1340	2	19,22,23	0.68	0	25,31,34	0.84	0
67	OMU	S2	1326	67	19,22,23	3.40	7 (36%)	25,31,34	1.80	5 (20%)
2	OMC	L5	4456	2	19,22,23	0.71	0	25,31,34	0.75	1 (4%)
2	OMG	L5	4623	2	23,26,27	0.58	0	32,38,41	0.57	0
67	A2M	S2	484	67	22,25,26	1.21	2 (9%)	30,36,39	1.52	8 (26%)
2	PSU	L5	3822	2	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
2	PSU	L5	4673	83,2	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
2	UY1	L5	3818	2	19,22,23	4.78	10 (52%)	21,31,34	1.96	5 (23%)
2	A2M	L5	1534	83,2	22,25,26	1.25	2 (9%)	30,36,39	1.57	9 (30%)
2	PSU	L5	4689	2	18,21,22	1.10	2 (11%)	21,30,33	1.85	4 (19%)
67	PSU	S2	1046	67	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	3695	2	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
2	PSU	L5	4312	2	18,21,22	1.07	2 (11%)	21,30,33	1.89	4 (19%)
2	PSU	L5	5001	2	18,21,22	1.05	1 (5%)	21,30,33	1.97	4 (19%)
67	OMG	S2	1328	67	23,26,27	0.44	0	32,38,41	0.45	0
2	OMC	L5	2351	83,2	19,22,23	0.72	0	25,31,34	1.01	2 (8%)

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
67	OMG	S2	683	67	-	0/9/27/28	0/3/3/3
67	OMG	S2	644	67	-	4/9/27/28	0/3/3/3
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	2401	2	-	2/9/27/28	0/3/3/3
2	OMC	L5	3869	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4494	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	3851	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
67	OMC	S2	174	67	-	0/9/27/28	0/2/2/2
67	A2M	S2	99	83,67	-	3/9/27/28	0/3/3/3
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
67	PSU	S2	866	67	-	2/7/25/26	0/2/2/2
67	OMC	S2	1703	67	-	0/9/27/28	0/2/2/2
67	PSU	S2	1244	67	-	1/7/25/26	0/2/2/2
2	PSU	L5	2632	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2363	83,2	-	1/9/27/28	0/3/3/3
67	OMC	S2	1272	67	-	2/9/27/28	0/2/2/2
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4523	83,2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
67	A2M	S2	1031	67	-	1/9/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
67	OMU	S2	116	67	-	0/9/27/28	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
67	A2M	S2	576	67	-	3/9/27/28	0/3/3/3
67	6MZ	S2	1832	83,67	-	6/12/28/28	0/3/3/3
2	A2M	L5	2787	2	-	5/9/27/28	0/3/3/3
67	PSU	S2	1177	67	-	0/7/25/26	0/2/2/2
2	PSU	L5	3853	83,2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1323	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
2	1MA	L5	1322	83,2	-	2/7/25/26	0/3/3/3
2	OMG	L5	2364	83,2	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	A2M	S2	159	67	-	1/9/27/28	0/3/3/3
67	PSU	S2	651	67	-	0/7/25/26	0/2/2/2
67	OMC	S2	1391	67	-	0/9/27/28	0/2/2/2
67	PSU	S2	1045	67	-	2/7/25/26	0/2/2/2
67	A2M	S2	468	67	-	1/9/27/28	0/3/3/3
2	PSU	L5	3920	83,2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2815	2	-	2/9/27/28	0/3/3/3
67	A2M	S2	1383	67	-	3/9/27/28	0/3/3/3
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	93	67	-	0/7/25/26	0/2/2/2
67	OMG	S2	509	67	-	0/9/27/28	0/3/3/3
67	PSU	S2	966	83,67	-	0/7/25/26	0/2/2/2
2	OMC	L5	2824	2	-	1/9/27/28	0/2/2/2
67	OMU	S2	627	67	-	6/9/27/28	0/2/2/2
67	PSU	S2	109	67	-	0/7/25/26	0/2/2/2
67	A2M	S2	166	67	-	0/9/27/28	0/3/3/3
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4499	2	-	1/9/27/28	0/3/3/3
2	5MC	L5	3782	83,2	-	1/7/25/26	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
67	A2M	S2	27	67	-	1/9/27/28	0/3/3/3
2	A2M	L5	1524	2	-	2/9/27/28	0/3/3/3
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4618	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	1367	67	-	0/7/25/26	0/2/2/2
2	OMG	L5	3792	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3887	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1792	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	1744	83,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
67	B8N	S2	1248	67	-	4/16/34/35	0/2/2/2
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	1677	2	-	2/7/25/26	0/2/2/2
67	OMU	S2	1288	67	-	3/9/27/28	0/2/2/2
2	A2M	L5	3785	83,2	-	1/9/27/28	0/3/3/3
67	PSU	S2	1004	67	-	0/7/25/26	0/2/2/2
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
2	A2M	L5	1871	83,2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
67	OMG	S2	1490	67	-	2/9/27/28	0/3/3/3
67	4AC	S2	1337	67	-	1/11/29/30	0/2/2/2
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2876	2	-	0/9/27/28	0/3/3/3
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
67	OMC	S2	517	67	-	0/9/27/28	0/2/2/2
67	PSU	S2	686	67	-	0/7/25/26	0/2/2/2
67	OMU	S2	354	67	-	0/9/27/28	0/2/2/2
67	G7M	S2	1639	67	-	2/7/25/26	0/3/3/3
67	PSU	S2	681	67	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	2	-	3/7/25/26	0/2/2/2
67	PSU	S2	406	67	-	0/7/25/26	0/2/2/2
67	MA6	S2	1850	67	-	0/11/29/30	0/3/3/3
67	OMU	S2	428	67	-	4/9/27/28	0/2/2/2
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	3899	2	-	2/9/27/28	0/3/3/3
67	OMU	S2	1442	67	-	2/9/27/28	0/2/2/2
2	A2M	L5	398	2	-	1/9/27/28	0/3/3/3
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4521	83,2	-	0/7/25/26	0/2/2/2
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1326	2	-	3/9/27/28	0/3/3/3
2	PSU	L5	1536	2	-	2/7/25/26	0/2/2/2
67	OMG	S2	601	67	-	0/9/27/28	0/3/3/3
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	L5	3867	2	-	2/9/27/28	0/3/3/3
67	PSU	S2	1232	67	-	0/7/25/26	0/2/2/2
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2
67	OMU	S2	121	67	-	0/9/27/28	0/2/2/2
2	6MZ	L5	4220	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	4196	2	-	1/9/27/28	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
67	A2M	S2	668	83,67	-	2/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	2	-	3/9/27/28	0/3/3/3
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
67	PSU	S2	801	67	-	2/7/25/26	0/2/2/2
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
67	MA6	S2	1851	67	-	2/11/29/30	0/3/3/3
2	OMC	L5	3701	2	-	6/9/27/28	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2365	83,2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1781	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	3/9/27/28	0/3/3/3
2	OMC	L5	3841	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4636	2	-	1/7/25/26	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	1174	67	-	0/7/25/26	0/2/2/2
67	OMG	S2	436	67	-	0/9/27/28	0/3/3/3
67	OMU	S2	799	67	-	2/9/27/28	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	1056	67	-	2/7/25/26	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
67	PSU	S2	105	67	-	0/7/25/26	0/2/2/2
67	PSU	S2	1081	67	-	1/7/25/26	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
67	4AC	S2	1842	67	-	0/11/29/30	0/2/2/2
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
67	OMC	S2	462	67	-	1/9/27/28	0/2/2/2
67	OMU	S2	172	67	-	0/9/27/28	0/2/2/2
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	PSU	S2	649	67	-	2/7/25/26	0/2/2/2
67	PSU	S2	814	67	-	0/7/25/26	0/2/2/2
67	PSU	S2	863	67	-	2/7/25/26	0/2/2/2
67	OMG	S2	867	67	-	3/9/27/28	0/3/3/3
2	OMC	L5	2422	83,2	-	2/9/27/28	0/2/2/2
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
67	OMU	S2	1326	67	-	0/9/27/28	0/2/2/2
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
67	A2M	S2	484	67	-	0/9/27/28	0/3/3/3
2	PSU	L5	3822	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4673	83,2	-	0/7/25/26	0/2/2/2
2	UY1	L5	3818	2	-	3/9/27/28	0/2/2/2
2	A2M	L5	1534	83,2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
67	PSU	S2	1046	67	-	1/7/25/26	0/2/2/2
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
67	OMG	S2	1328	67	-	1/9/27/28	0/3/3/3
2	OMC	L5	2351	83,2	-	4/9/27/28	0/2/2/2

All (304) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	S2	1832	6MZ	C6-N6	12.68	1.48	1.34
2	L5	3818	UY1	C6-C5	12.48	1.49	1.35
2	L5	4220	6MZ	C6-N6	11.99	1.47	1.34
2	L5	3818	UY1	C2-N1	11.36	1.51	1.36
67	S2	1288	OMU	C2-N1	8.76	1.52	1.38
67	S2	1442	OMU	C2-N1	8.64	1.52	1.38
67	S2	799	OMU	C2-N1	8.56	1.51	1.38
2	L5	4220	6MZ	C3'-C2'	-8.49	1.30	1.53
67	S2	121	OMU	C2-N1	8.35	1.51	1.38
67	S2	627	OMU	C2-N1	8.35	1.51	1.38
67	S2	428	OMU	C2-N1	8.33	1.51	1.38
67	S2	1326	OMU	C2-N1	8.32	1.51	1.38
67	S2	172	OMU	C2-N1	8.27	1.51	1.38
67	S2	116	OMU	C2-N1	8.23	1.51	1.38
67	S2	354	OMU	C2-N1	8.20	1.51	1.38
2	L5	2837	OMU	C2-N1	8.08	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4227	OMU	C2-N1	7.91	1.50	1.38
67	S2	1248	B8N	C6-N1	7.91	1.55	1.36
67	S2	1248	B8N	C4-N3	-7.75	1.26	1.40
2	L5	4306	OMU	C2-N1	7.74	1.50	1.38
2	L5	4498	OMU	C2-N1	7.67	1.50	1.38
2	L5	3925	OMU	C2-N1	7.66	1.50	1.38
2	L5	4620	OMU	C2-N1	7.63	1.50	1.38
2	L5	3818	UY1	C2-N3	7.58	1.50	1.37
67	S2	1326	OMU	C2-N3	7.07	1.50	1.38
67	S2	1442	OMU	C2-N3	7.05	1.50	1.38
67	S2	1248	B8N	C4-C5	7.02	1.63	1.47
67	S2	116	OMU	C2-N3	7.02	1.50	1.38
67	S2	428	OMU	C2-N3	7.01	1.50	1.38
67	S2	172	OMU	C2-N3	7.00	1.50	1.38
67	S2	799	OMU	C2-N3	6.96	1.50	1.38
67	S2	627	OMU	C2-N3	6.95	1.50	1.38
67	S2	121	OMU	C2-N3	6.94	1.50	1.38
67	S2	1288	OMU	C2-N3	6.92	1.50	1.38
67	S2	354	OMU	C2-N3	6.81	1.49	1.38
67	S2	1639	G7M	C4-N3	6.77	1.49	1.34
2	L5	4227	OMU	C2-N3	6.59	1.49	1.38
2	L5	2837	OMU	C2-N3	6.54	1.49	1.38
2	L5	4498	OMU	C2-N3	6.53	1.49	1.38
2	L5	4620	OMU	C2-N3	6.43	1.49	1.38
2	L5	4306	OMU	C2-N3	6.42	1.49	1.38
2	L5	3925	OMU	C2-N3	6.36	1.49	1.38
2	L5	4530	UR3	C2-N1	6.26	1.47	1.38
2	L5	4530	UR3	C6-C5	6.14	1.49	1.35
67	S2	1326	OMU	C6-C5	5.96	1.48	1.35
67	S2	1248	B8N	C2-N1	5.96	1.56	1.39
67	S2	1442	OMU	C6-C5	5.95	1.48	1.35
67	S2	428	OMU	C6-C5	5.92	1.48	1.35
67	S2	799	OMU	C6-C5	5.88	1.48	1.35
67	S2	627	OMU	C6-C5	5.88	1.48	1.35
67	S2	172	OMU	C6-C5	5.88	1.48	1.35
67	S2	121	OMU	C6-C5	5.87	1.48	1.35
67	S2	1288	OMU	C6-C5	5.87	1.48	1.35
67	S2	354	OMU	C6-C5	5.77	1.48	1.35
67	S2	116	OMU	C6-C5	5.74	1.48	1.35
2	L5	4227	OMU	C6-C5	5.72	1.48	1.35
2	L5	3925	OMU	O4-C4	-5.71	1.13	1.24
2	L5	4498	OMU	O4-C4	-5.71	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4306	OMU	O4-C4	-5.70	1.13	1.24
2	L5	4530	UR3	C2-N3	5.66	1.50	1.39
2	L5	4620	OMU	O4-C4	-5.66	1.13	1.24
2	L5	2837	OMU	O4-C4	-5.64	1.13	1.24
2	L5	4306	OMU	C6-C5	5.61	1.48	1.35
2	L5	4498	OMU	C6-C5	5.60	1.48	1.35
2	L5	2837	OMU	C6-C5	5.59	1.48	1.35
67	S2	1248	B8N	C6-C5	5.58	1.43	1.35
2	L5	4227	OMU	O4-C4	-5.58	1.13	1.24
2	L5	3925	OMU	C6-C5	5.56	1.48	1.35
67	S2	1639	G7M	C2-N3	5.55	1.46	1.33
67	S2	354	OMU	O4-C4	-5.54	1.13	1.24
2	L5	4620	OMU	C6-C5	5.54	1.47	1.35
67	S2	799	OMU	O4-C4	-5.46	1.13	1.24
67	S2	121	OMU	O4-C4	-5.42	1.13	1.24
67	S2	1442	OMU	O4-C4	-5.42	1.13	1.24
67	S2	627	OMU	O4-C4	-5.41	1.14	1.24
67	S2	116	OMU	O4-C4	-5.41	1.14	1.24
67	S2	428	OMU	O4-C4	-5.39	1.14	1.24
67	S2	1288	OMU	O4-C4	-5.39	1.14	1.24
67	S2	1326	OMU	O4-C4	-5.36	1.14	1.24
67	S2	172	OMU	O4-C4	-5.35	1.14	1.24
2	L5	3818	UY1	C6-N1	5.20	1.44	1.36
67	S2	1639	G7M	C2-N2	4.93	1.45	1.34
2	L5	4220	6MZ	O4'-C1'	-4.79	1.30	1.42
2	L5	4220	6MZ	O4'-C4'	4.66	1.55	1.45
67	S2	1639	G7M	C5-N7	-4.47	1.34	1.39
67	S2	627	OMU	C4-N3	4.46	1.46	1.38
67	S2	116	OMU	C4-N3	4.45	1.46	1.38
67	S2	1326	OMU	C4-N3	4.45	1.46	1.38
67	S2	1442	OMU	C4-N3	4.44	1.46	1.38
67	S2	172	OMU	C4-N3	4.43	1.46	1.38
67	S2	428	OMU	C4-N3	4.43	1.46	1.38
67	S2	799	OMU	C4-N3	4.40	1.46	1.38
2	L5	3818	UY1	C4-N3	4.36	1.47	1.38
2	L5	4220	6MZ	C5'-C4'	-4.36	1.38	1.51
67	S2	354	OMU	C4-N3	4.31	1.46	1.38
67	S2	121	OMU	C4-N3	4.30	1.46	1.38
67	S2	1288	OMU	C4-N3	4.29	1.46	1.38
2	L5	4498	OMU	C4-N3	4.07	1.45	1.38
2	L5	4227	OMU	C4-N3	4.05	1.45	1.38
2	L5	2837	OMU	C4-N3	3.96	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	S2	1639	G7M	C5-C6	3.89	1.54	1.43
67	S2	966	PSU	C6-C5	3.87	1.39	1.35
67	S2	801	PSU	C6-C5	3.87	1.39	1.35
2	L5	4620	OMU	C4-N3	3.82	1.45	1.38
67	S2	866	PSU	C6-C5	3.82	1.39	1.35
67	S2	1004	PSU	C6-C5	3.80	1.39	1.35
67	S2	1367	PSU	C6-C5	3.79	1.39	1.35
67	S2	1232	PSU	C6-C5	3.78	1.39	1.35
67	S2	686	PSU	C6-C5	3.78	1.39	1.35
2	L5	4306	OMU	C4-N3	3.77	1.45	1.38
67	S2	93	PSU	C6-C5	3.76	1.39	1.35
67	S2	1046	PSU	C6-C5	3.75	1.39	1.35
2	L5	3925	OMU	C4-N3	3.72	1.45	1.38
67	S2	1244	PSU	C6-C5	3.71	1.39	1.35
67	S2	649	PSU	C6-C5	3.71	1.39	1.35
2	L5	3818	UY1	O4-C4	-3.69	1.16	1.23
67	S2	651	PSU	C6-C5	3.69	1.39	1.35
67	S2	814	PSU	C6-C5	3.66	1.39	1.35
67	S2	1045	PSU	C6-C5	3.63	1.39	1.35
67	S2	1248	B8N	C1'-C5	3.62	1.58	1.50
67	S2	109	PSU	C6-C5	3.62	1.39	1.35
67	S2	406	PSU	C6-C5	3.61	1.39	1.35
67	S2	105	PSU	C6-C5	3.61	1.39	1.35
67	S2	1174	PSU	C6-C5	3.57	1.39	1.35
67	S2	863	PSU	C6-C5	3.53	1.39	1.35
67	S2	1177	PSU	C6-C5	3.52	1.39	1.35
2	L5	1871	A2M	O5'-C5'	-3.51	1.34	1.44
67	S2	1056	PSU	C6-C5	3.50	1.39	1.35
2	L5	400	A2M	O5'-C5'	-3.48	1.34	1.44
2	L5	3825	A2M	O5'-C5'	-3.48	1.34	1.44
2	L5	3844	PSU	C6-C5	3.47	1.39	1.35
2	L5	3830	A2M	O5'-C5'	-3.46	1.34	1.44
2	L5	1323	A2M	O5'-C5'	-3.45	1.34	1.44
2	L5	4220	6MZ	C5-N7	-3.45	1.32	1.39
2	L5	3785	A2M	O5'-C5'	-3.44	1.34	1.44
2	L5	4571	A2M	O5'-C5'	-3.43	1.34	1.44
2	L5	2815	A2M	O5'-C5'	-3.42	1.34	1.44
2	L5	2401	A2M	O5'-C5'	-3.41	1.34	1.44
67	S2	668	A2M	O5'-C5'	-3.40	1.34	1.44
2	L5	1534	A2M	O5'-C5'	-3.38	1.34	1.44
67	S2	468	A2M	O5'-C5'	-3.38	1.34	1.44
2	L5	4493	PSU	C6-C5	3.38	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4500	PSU	C6-C5	3.38	1.39	1.35
67	S2	1081	PSU	C6-C5	3.37	1.39	1.35
2	L5	1326	A2M	O5'-C5'	-3.37	1.34	1.44
2	L5	1524	A2M	O5'-C5'	-3.36	1.34	1.44
2	L5	4220	6MZ	C5-C4	-3.35	1.33	1.39
67	S2	99	A2M	O5'-C5'	-3.35	1.34	1.44
2	L5	4431	PSU	C6-C5	3.35	1.39	1.35
2	L5	3818	UY1	O2-C2	-3.33	1.16	1.23
2	L5	3867	A2M	O5'-C5'	-3.33	1.34	1.44
2	L5	3718	A2M	O5'-C5'	-3.33	1.34	1.44
2	L5	2787	A2M	O5'-C5'	-3.32	1.34	1.44
2	L5	5010	PSU	C6-C5	3.32	1.39	1.35
2	L5	2632	PSU	C6-C5	3.31	1.39	1.35
2	L5	4523	A2M	O5'-C5'	-3.31	1.34	1.44
2	L5	3822	PSU	C6-C5	3.30	1.38	1.35
2	L5	4296	PSU	C6-C5	3.30	1.38	1.35
2	L5	4590	A2M	O5'-C5'	-3.30	1.34	1.44
67	S2	681	PSU	C6-C5	3.29	1.38	1.35
67	S2	576	A2M	O5'-C5'	-3.29	1.34	1.44
2	L5	4471	PSU	C6-C5	3.29	1.38	1.35
2	L5	2363	A2M	O5'-C5'	-3.28	1.34	1.44
67	S2	1031	A2M	O5'-C5'	-3.28	1.34	1.44
2	L5	4972	PSU	C6-C5	3.27	1.38	1.35
2	L5	398	A2M	O5'-C5'	-3.27	1.34	1.44
4	L8	55	PSU	C6-C5	3.27	1.38	1.35
2	L5	2839	PSU	C6-C5	3.26	1.38	1.35
2	L5	4576	PSU	C6-C5	3.26	1.38	1.35
67	S2	166	A2M	O5'-C5'	-3.25	1.34	1.44
67	S2	27	A2M	O5'-C5'	-3.25	1.34	1.44
2	L5	1781	PSU	C6-C5	3.24	1.38	1.35
2	L5	4532	PSU	C6-C5	3.24	1.38	1.35
2	L5	4312	PSU	C6-C5	3.23	1.38	1.35
2	L5	4689	PSU	C6-C5	3.21	1.38	1.35
2	L5	1860	PSU	C6-C5	3.21	1.38	1.35
4	L8	69	PSU	C6-C5	3.21	1.38	1.35
67	S2	1850	MA6	C6-N6	3.19	1.45	1.36
2	L5	4579	PSU	C6-C5	3.19	1.38	1.35
67	S2	1383	A2M	O5'-C5'	-3.19	1.34	1.44
2	L5	1782	PSU	C6-C5	3.19	1.38	1.35
2	L5	3695	PSU	C6-C5	3.17	1.38	1.35
2	L5	4353	PSU	C6-C5	3.17	1.38	1.35
67	S2	484	A2M	O5'-C5'	-3.17	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	3818	UY1	C1'-C5	3.16	1.57	1.50
2	L5	1683	PSU	C6-C5	3.16	1.38	1.35
67	S2	1851	MA6	C6-N6	3.15	1.45	1.36
2	L5	4552	PSU	C6-C5	3.15	1.38	1.35
2	L5	1862	PSU	C6-C5	3.14	1.38	1.35
2	L5	4636	PSU	C6-C5	3.13	1.38	1.35
2	L5	4521	PSU	C6-C5	3.12	1.38	1.35
2	L5	4973	PSU	C6-C5	3.11	1.38	1.35
2	L5	3884	PSU	C6-C5	3.11	1.38	1.35
2	L5	4361	PSU	C6-C5	3.11	1.38	1.35
2	L5	1792	PSU	C6-C5	3.09	1.38	1.35
2	L5	3637	PSU	C6-C5	3.09	1.38	1.35
2	L5	4293	PSU	C6-C5	3.09	1.38	1.35
67	S2	159	A2M	O5'-C5'	-3.08	1.35	1.44
2	L5	1744	PSU	C6-C5	3.08	1.38	1.35
2	L5	3851	PSU	C6-C5	3.08	1.38	1.35
2	L5	3639	PSU	C6-C5	3.08	1.38	1.35
2	L5	3853	PSU	C6-C5	3.07	1.38	1.35
67	S2	1832	6MZ	C5-C4	-3.07	1.33	1.39
2	L5	4299	PSU	C6-C5	3.07	1.38	1.35
2	L5	5001	PSU	C6-C5	3.06	1.38	1.35
67	S2	1832	6MZ	C5-N7	-3.05	1.33	1.39
2	L5	4673	PSU	C6-C5	3.05	1.38	1.35
2	L5	4442	PSU	C6-C5	3.04	1.38	1.35
2	L5	4220	6MZ	C8-N9	-3.03	1.32	1.37
2	L5	1582	PSU	C6-C5	2.99	1.38	1.35
2	L5	4457	PSU	C6-C5	2.99	1.38	1.35
2	L5	3920	PSU	C6-C5	2.96	1.38	1.35
2	L5	4403	PSU	C6-C5	2.96	1.38	1.35
2	L5	1536	PSU	C6-C5	2.94	1.38	1.35
2	L5	4220	6MZ	C2'-C1'	2.94	1.62	1.53
67	S2	428	OMU	C5-C4	2.91	1.50	1.43
67	S2	1442	OMU	C5-C4	2.90	1.50	1.43
67	S2	172	OMU	C5-C4	2.90	1.50	1.43
67	S2	1326	OMU	C5-C4	2.89	1.50	1.43
67	S2	627	OMU	C5-C4	2.88	1.50	1.43
67	S2	799	OMU	C5-C4	2.86	1.49	1.43
67	S2	1288	OMU	C5-C4	2.81	1.49	1.43
2	L5	1677	PSU	C6-C5	2.81	1.38	1.35
67	S2	121	OMU	C6-N1	2.80	1.44	1.38
67	S2	1639	G7M	C2-N1	2.80	1.44	1.37
67	S2	121	OMU	C5-C4	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	S2	1288	OMU	C6-N1	2.78	1.44	1.38
67	S2	1442	OMU	C6-N1	2.77	1.44	1.38
67	S2	354	OMU	C5-C4	2.75	1.49	1.43
67	S2	799	OMU	C6-N1	2.74	1.44	1.38
2	L5	4628	PSU	C6-C5	2.72	1.38	1.35
67	S2	354	OMU	C6-N1	2.70	1.44	1.38
67	S2	116	OMU	C5-C4	2.70	1.49	1.43
67	S2	1832	6MZ	C8-N9	-2.70	1.33	1.37
67	S2	1326	OMU	C6-N1	2.69	1.44	1.38
67	S2	428	OMU	C6-N1	2.69	1.44	1.38
67	S2	627	OMU	C6-N1	2.69	1.44	1.38
2	L5	4227	OMU	C5-C4	2.67	1.49	1.43
2	L5	4571	A2M	O4'-C4'	-2.67	1.39	1.45
2	L5	4220	6MZ	O3'-C3'	2.63	1.49	1.43
2	L5	4530	UR3	O2-C2	-2.63	1.17	1.22
67	S2	172	OMU	C6-N1	2.61	1.44	1.38
67	S2	1639	G7M	O6-C6	-2.60	1.18	1.23
67	S2	116	OMU	C6-N1	2.59	1.44	1.38
2	L5	1524	A2M	O4'-C4'	-2.59	1.39	1.45
2	L5	2363	A2M	O4'-C4'	-2.59	1.39	1.45
2	L5	2837	OMU	C5-C4	2.57	1.49	1.43
2	L5	3925	OMU	C5-C4	2.54	1.49	1.43
2	L5	4498	OMU	C5-C4	2.54	1.49	1.43
2	L5	4220	6MZ	C6-N1	-2.50	1.31	1.35
2	L5	1534	A2M	O4'-C4'	-2.48	1.39	1.45
2	L5	1323	A2M	O4'-C4'	-2.47	1.39	1.45
67	S2	1639	G7M	C6-N1	2.47	1.43	1.38
2	L5	4306	OMU	C5-C4	2.46	1.49	1.43
2	L5	4227	OMU	C6-N1	2.46	1.43	1.38
2	L5	2837	OMU	C6-N1	2.44	1.43	1.38
2	L5	4306	OMU	C6-N1	2.44	1.43	1.38
2	L5	4530	UR3	C6-N1	2.44	1.43	1.38
2	L5	4498	OMU	C6-N1	2.43	1.43	1.38
67	S2	668	A2M	O4'-C4'	-2.42	1.39	1.45
2	L5	4620	OMU	C5-C4	2.42	1.49	1.43
2	L5	3925	OMU	C6-N1	2.36	1.43	1.38
2	L5	4620	OMU	C6-N1	2.34	1.43	1.38
2	L5	3884	PSU	C4-C5	-2.31	1.37	1.44
67	S2	1850	MA6	C5-C4	-2.30	1.35	1.39
2	L5	4447	5MC	C4-N3	-2.29	1.30	1.34
67	S2	1851	MA6	C5-C4	-2.28	1.35	1.39
2	L5	400	A2M	O4'-C4'	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	2839	PSU	C4-C5	-2.25	1.38	1.44
2	L5	1871	A2M	O4'-C4'	-2.23	1.40	1.45
2	L5	1326	A2M	O4'-C4'	-2.22	1.40	1.45
2	L5	3818	UY1	O4'-C1'	-2.21	1.40	1.43
2	L5	4523	A2M	O4'-C4'	-2.21	1.40	1.45
2	L5	1323	A2M	O3'-C3'	-2.20	1.37	1.43
2	L5	3867	A2M	O4'-C4'	-2.19	1.40	1.45
2	L5	4530	UR3	C5-C4	2.18	1.49	1.43
2	L5	4689	PSU	C4-C5	-2.16	1.38	1.44
2	L5	3920	PSU	C4-C5	-2.14	1.38	1.44
67	S2	576	A2M	C5-C4	2.12	1.42	1.39
2	L5	4523	A2M	O3'-C3'	-2.11	1.37	1.43
2	L5	4521	PSU	C4-C5	-2.10	1.38	1.44
2	L5	4530	UR3	C3U-N3	2.09	1.50	1.47
2	L5	3695	PSU	C4-C5	-2.09	1.38	1.44
2	L5	4457	PSU	C4-C5	-2.09	1.38	1.44
2	L5	4293	PSU	C4-C5	-2.06	1.38	1.44
2	L5	3825	A2M	O4'-C4'	-2.06	1.40	1.45
2	L5	1582	PSU	C4-C5	-2.06	1.38	1.44
2	L5	3818	UY1	C4-C5	2.05	1.50	1.44
2	L5	4220	6MZ	C4-N9	-2.05	1.33	1.37
2	L5	4636	PSU	C4-C5	-2.05	1.38	1.44
2	L5	3639	PSU	C4-C5	-2.05	1.38	1.44
2	L5	4973	PSU	C4-C5	-2.05	1.38	1.44
2	L5	4500	PSU	C4-C5	-2.04	1.38	1.44
2	L5	4590	A2M	O4'-C4'	-2.03	1.40	1.45
2	L5	4312	PSU	C4-C5	-2.03	1.38	1.44
2	L5	4552	PSU	C4-C5	-2.03	1.38	1.44
2	L5	4576	PSU	C4-C5	-2.02	1.38	1.44
2	L5	5010	PSU	C4-C5	-2.01	1.38	1.44
2	L5	2815	A2M	O4'-C4'	-2.01	1.40	1.45
67	S2	159	A2M	C5-C4	2.00	1.42	1.39
67	S2	1248	B8N	O4'-C1'	-2.00	1.41	1.43
2	L5	4299	PSU	C4-C5	-2.00	1.38	1.44
2	L5	4403	PSU	C4-C5	-2.00	1.38	1.44
67	S2	484	A2M	C5-C4	2.00	1.42	1.39

All (691) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	1851	MA6	N1-C6-N6	-11.93	102.32	116.86
67	S2	1850	MA6	N1-C6-N6	-11.90	102.36	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	1850	MA6	C5-C6-N6	8.02	138.02	125.33
67	S2	1851	MA6	C5-C6-N6	7.89	137.82	125.33
67	S2	1639	G7M	C1'-N9-C8	-7.36	101.88	126.74
67	S2	1639	G7M	C1'-N9-C4	7.35	148.19	126.49
2	L5	4227	OMU	C4-N3-C2	-5.90	119.29	126.61
2	L5	2837	OMU	C4-N3-C2	-5.84	119.36	126.61
2	L5	4220	6MZ	N1-C2-N3	-5.80	119.80	128.58
2	L5	4498	OMU	C4-N3-C2	-5.79	119.43	126.61
67	S2	172	OMU	C4-N3-C2	-5.68	119.56	126.61
67	S2	1832	6MZ	N1-C2-N3	-5.67	119.99	128.58
67	S2	627	OMU	C4-N3-C2	-5.62	119.63	126.61
2	L5	3925	OMU	C4-N3-C2	-5.62	119.63	126.61
67	S2	354	OMU	C4-N3-C2	-5.58	119.69	126.61
67	S2	428	OMU	C4-N3-C2	-5.54	119.73	126.61
67	S2	1851	MA6	N1-C2-N3	-5.53	120.21	128.58
67	S2	1326	OMU	C4-N3-C2	-5.50	119.78	126.61
67	S2	1850	MA6	N1-C2-N3	-5.50	120.26	128.58
2	L5	3637	PSU	N1-C2-N3	5.48	120.95	115.17
67	S2	1850	MA6	N9-C8-N7	-5.47	106.18	113.94
67	S2	799	OMU	C4-N3-C2	-5.44	119.86	126.61
2	L5	4636	PSU	C4-N3-C2	-5.42	118.91	126.37
2	L5	4530	UR3	C4-N3-C2	-5.41	120.22	124.58
2	L5	3701	OMC	C1'-N1-C2	5.40	130.36	118.44
67	S2	1442	OMU	C4-N3-C2	-5.39	119.92	126.61
67	S2	1851	MA6	N9-C8-N7	-5.31	106.40	113.94
2	L5	4636	PSU	N1-C2-N3	5.29	120.75	115.17
2	L5	4306	OMU	C4-N3-C2	-5.20	120.15	126.61
2	L5	4457	PSU	C4-N3-C2	-5.17	119.25	126.37
2	L5	3637	PSU	C4-N3-C2	-5.15	119.28	126.37
2	L5	1683	PSU	N1-C2-N3	5.15	120.60	115.17
67	S2	121	OMU	C4-N3-C2	-5.13	120.25	126.61
2	L5	4403	PSU	N1-C2-N3	5.12	120.57	115.17
2	L5	1677	PSU	C4-N3-C2	-5.11	119.33	126.37
2	L5	1582	PSU	C4-N3-C2	-5.10	119.34	126.37
2	L5	4457	PSU	N1-C2-N3	5.10	120.55	115.17
2	L5	4620	OMU	C4-N3-C2	-5.09	120.30	126.61
67	S2	1248	B8N	C5-C4-N3	5.07	125.36	116.15
2	L5	4353	PSU	C4-N3-C2	-5.06	119.40	126.37
4	L8	69	PSU	C4-N3-C2	-5.06	119.40	126.37
2	L5	1744	PSU	N1-C2-N3	5.05	120.49	115.17
2	L5	4552	PSU	N1-C2-N3	5.05	120.49	115.17
2	L5	4500	PSU	N1-C2-N3	5.04	120.49	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4521	PSU	N1-C2-N3	5.04	120.49	115.17
2	L5	4973	PSU	C4-N3-C2	-5.04	119.43	126.37
2	L5	4442	PSU	N1-C2-N3	5.03	120.48	115.17
2	L5	4579	PSU	N1-C2-N3	5.03	120.48	115.17
2	L5	4973	PSU	N1-C2-N3	5.03	120.48	115.17
2	L5	4521	PSU	C4-N3-C2	-5.02	119.45	126.37
2	L5	3851	PSU	N1-C2-N3	5.01	120.46	115.17
2	L5	3884	PSU	N1-C2-N3	5.01	120.46	115.17
2	L5	3695	PSU	C4-N3-C2	-5.01	119.48	126.37
67	S2	1081	PSU	C4-N3-C2	-5.01	119.48	126.37
2	L5	4403	PSU	C4-N3-C2	-5.00	119.48	126.37
2	L5	3822	PSU	N1-C2-N3	5.00	120.44	115.17
2	L5	5001	PSU	N1-C2-N3	5.00	120.44	115.17
67	S2	116	OMU	C4-N3-C2	-5.00	120.41	126.61
4	L8	69	PSU	N1-C2-N3	4.99	120.43	115.17
2	L5	1792	PSU	C4-N3-C2	-4.98	119.51	126.37
2	L5	4500	PSU	C4-N3-C2	-4.98	119.52	126.37
2	L5	3695	PSU	N1-C2-N3	4.98	120.42	115.17
2	L5	1862	PSU	C4-N3-C2	-4.98	119.52	126.37
2	L5	4296	PSU	C4-N3-C2	-4.97	119.52	126.37
2	L5	4972	PSU	C4-N3-C2	-4.97	119.52	126.37
2	L5	4293	PSU	C4-N3-C2	-4.97	119.52	126.37
2	L5	5001	PSU	C4-N3-C2	-4.97	119.53	126.37
2	L5	4576	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	4673	PSU	N1-C2-N3	4.96	120.40	115.17
67	S2	1081	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	4552	PSU	C4-N3-C2	-4.96	119.54	126.37
2	L5	3639	PSU	N1-C2-N3	4.95	120.39	115.17
2	L5	4493	PSU	N1-C2-N3	4.95	120.39	115.17
67	S2	866	PSU	C4-N3-C2	-4.95	119.56	126.37
2	L5	4361	PSU	N1-C2-N3	4.95	120.39	115.17
2	L5	3818	UY1	C4-N3-C2	-4.95	119.56	126.37
2	L5	1862	PSU	N1-C2-N3	4.95	120.38	115.17
67	S2	1288	OMU	C4-N3-C2	-4.94	120.48	126.61
2	L5	4471	PSU	N1-C2-N3	4.93	120.37	115.17
2	L5	1744	PSU	C4-N3-C2	-4.93	119.58	126.37
2	L5	4361	PSU	C4-N3-C2	-4.92	119.59	126.37
2	L5	4442	PSU	C4-N3-C2	-4.92	119.59	126.37
2	L5	4353	PSU	N1-C2-N3	4.92	120.35	115.17
67	S2	1832	6MZ	N9-C8-N7	-4.91	106.97	113.94
2	L5	4972	PSU	N1-C2-N3	4.91	120.34	115.17
2	L5	3822	PSU	C4-N3-C2	-4.91	119.61	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3851	PSU	C4-N3-C2	-4.91	119.61	126.37
67	S2	1177	PSU	C4-N3-C2	-4.91	119.61	126.37
67	S2	105	PSU	N1-C2-N3	4.88	120.32	115.17
2	L5	4296	PSU	N1-C2-N3	4.88	120.31	115.17
2	L5	3920	PSU	C4-N3-C2	-4.87	119.66	126.37
2	L5	4576	PSU	C4-N3-C2	-4.87	119.66	126.37
2	L5	4431	PSU	N1-C2-N3	4.87	120.30	115.17
2	L5	1782	PSU	C4-N3-C2	-4.87	119.67	126.37
2	L5	3920	PSU	N1-C2-N3	4.87	120.30	115.17
2	L5	3884	PSU	C4-N3-C2	-4.86	119.67	126.37
67	S2	863	PSU	C4-N3-C2	-4.85	119.69	126.37
2	L5	1683	PSU	C4-N3-C2	-4.85	119.69	126.37
2	L5	1582	PSU	N1-C2-N3	4.84	120.28	115.17
2	L5	1677	PSU	N1-C2-N3	4.84	120.28	115.17
67	S2	1045	PSU	N1-C2-N3	4.83	120.26	115.17
2	L5	1792	PSU	N1-C2-N3	4.83	120.26	115.17
2	L5	5010	PSU	N1-C2-N3	4.83	120.26	115.17
2	L5	1536	PSU	C4-N3-C2	-4.83	119.72	126.37
2	L5	4579	PSU	C4-N3-C2	-4.82	119.73	126.37
2	L5	4312	PSU	N1-C2-N3	4.82	120.25	115.17
2	L5	4431	PSU	C4-N3-C2	-4.82	119.73	126.37
67	S2	1045	PSU	C4-N3-C2	-4.82	119.74	126.37
2	L5	1782	PSU	N1-C2-N3	4.81	120.24	115.17
67	S2	109	PSU	C4-N3-C2	-4.81	119.75	126.37
2	L5	1781	PSU	N1-C2-N3	4.80	120.23	115.17
67	S2	866	PSU	N1-C2-N3	4.79	120.22	115.17
2	L5	4299	PSU	N1-C2-N3	4.79	120.22	115.17
2	L5	4532	PSU	C4-N3-C2	-4.78	119.78	126.37
67	S2	1232	PSU	C4-N3-C2	-4.78	119.78	126.37
2	L5	4628	PSU	C4-N3-C2	-4.78	119.78	126.37
67	S2	406	PSU	C4-N3-C2	-4.78	119.78	126.37
2	L5	1536	PSU	N1-C2-N3	4.78	120.21	115.17
2	L5	4532	PSU	N1-C2-N3	4.78	120.21	115.17
2	L5	4293	PSU	N1-C2-N3	4.77	120.19	115.17
67	S2	1177	PSU	N1-C2-N3	4.76	120.19	115.17
2	L5	4493	PSU	C4-N3-C2	-4.76	119.82	126.37
67	S2	651	PSU	C4-N3-C2	-4.76	119.82	126.37
2	L5	4628	PSU	N1-C2-N3	4.75	120.18	115.17
67	S2	1046	PSU	N1-C2-N3	4.75	120.18	115.17
67	S2	651	PSU	N1-C2-N3	4.75	120.18	115.17
67	S2	109	PSU	N1-C2-N3	4.75	120.18	115.17
67	S2	681	PSU	N1-C2-N3	4.74	120.17	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	1174	PSU	N1-C2-N3	4.74	120.17	115.17
2	L5	4673	PSU	C4-N3-C2	-4.74	119.84	126.37
4	L8	55	PSU	N1-C2-N3	4.74	120.17	115.17
67	S2	863	PSU	N1-C2-N3	4.73	120.16	115.17
2	L5	2632	PSU	N1-C2-N3	4.73	120.16	115.17
67	S2	406	PSU	N1-C2-N3	4.73	120.16	115.17
67	S2	1851	MA6	C5-C4-N3	-4.73	120.21	126.72
2	L5	5010	PSU	C4-N3-C2	-4.73	119.86	126.37
67	S2	1232	PSU	N1-C2-N3	4.72	120.15	115.17
67	S2	1174	PSU	C4-N3-C2	-4.72	119.87	126.37
67	S2	105	PSU	C4-N3-C2	-4.72	119.88	126.37
67	S2	1244	PSU	C4-N3-C2	-4.71	119.88	126.37
67	S2	1832	6MZ	C5-C4-N3	-4.71	120.23	126.72
2	L5	4689	PSU	N1-C2-N3	4.71	120.14	115.17
67	S2	1367	PSU	N1-C2-N3	4.71	120.13	115.17
2	L5	2839	PSU	N1-C2-N3	4.70	120.13	115.17
67	S2	686	PSU	N1-C2-N3	4.70	120.12	115.17
2	L5	3844	PSU	N1-C2-N3	4.69	120.12	115.17
67	S2	686	PSU	C4-N3-C2	-4.69	119.91	126.37
67	S2	966	PSU	N1-C2-N3	4.69	120.11	115.17
67	S2	1004	PSU	N1-C2-N3	4.68	120.11	115.17
2	L5	1781	PSU	C4-N3-C2	-4.68	119.92	126.37
67	S2	649	PSU	N1-C2-N3	4.67	120.10	115.17
67	S2	1244	PSU	N1-C2-N3	4.67	120.10	115.17
67	S2	649	PSU	C4-N3-C2	-4.67	119.93	126.37
2	L5	2632	PSU	C4-N3-C2	-4.67	119.94	126.37
67	S2	1004	PSU	C4-N3-C2	-4.67	119.94	126.37
4	L8	55	PSU	C4-N3-C2	-4.66	119.95	126.37
67	S2	1056	PSU	C4-N3-C2	-4.66	119.95	126.37
2	L5	1860	PSU	N1-C2-N3	4.66	120.08	115.17
67	S2	1056	PSU	N1-C2-N3	4.65	120.08	115.17
2	L5	4312	PSU	C4-N3-C2	-4.65	119.97	126.37
2	L5	3639	PSU	C4-N3-C2	-4.65	119.97	126.37
67	S2	681	PSU	C4-N3-C2	-4.65	119.97	126.37
2	L5	3853	PSU	C4-N3-C2	-4.64	119.98	126.37
2	L5	3853	PSU	N1-C2-N3	4.64	120.06	115.17
2	L5	4299	PSU	C4-N3-C2	-4.64	119.98	126.37
2	L5	1871	A2M	C3'-C2'-C1'	-4.63	93.95	102.81
2	L5	4471	PSU	C4-N3-C2	-4.62	120.00	126.37
67	S2	966	PSU	C4-N3-C2	-4.61	120.02	126.37
67	S2	93	PSU	C4-N3-C2	-4.59	120.06	126.37
67	S2	1367	PSU	C4-N3-C2	-4.58	120.06	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	1046	PSU	C4-N3-C2	-4.57	120.07	126.37
67	S2	93	PSU	N1-C2-N3	4.57	119.98	115.17
67	S2	801	PSU	N1-C2-N3	4.56	119.98	115.17
2	L5	4220	6MZ	N9-C8-N7	-4.56	107.47	113.94
67	S2	1248	B8N	C4-N3-C2	-4.54	120.03	125.62
67	S2	801	PSU	C4-N3-C2	-4.48	120.19	126.37
67	S2	1639	G7M	C2-N3-C4	4.46	119.97	112.30
67	S2	1850	MA6	C4-N9-C8	4.45	110.41	105.74
2	L5	1860	PSU	C4-N3-C2	-4.44	120.25	126.37
67	S2	814	PSU	N1-C2-N3	4.43	119.84	115.17
2	L5	2839	PSU	C4-N3-C2	-4.39	120.32	126.37
2	L5	4220	6MZ	C5-C4-N3	-4.35	120.72	126.72
2	L5	3844	PSU	C4-N3-C2	-4.33	120.41	126.37
2	L5	3818	UY1	N1-C2-N3	4.30	119.70	115.17
2	L5	3701	OMC	C1'-N1-C6	-4.29	111.61	120.78
2	L5	3830	A2M	C3'-C2'-C1'	-4.24	94.70	102.81
67	S2	814	PSU	C4-N3-C2	-4.21	120.57	126.37
67	S2	1850	MA6	C5-C4-N3	-4.21	120.92	126.72
2	L5	2837	OMU	N3-C2-N1	4.18	120.34	114.89
2	L5	4689	PSU	C4-N3-C2	-4.17	120.62	126.37
67	S2	1639	G7M	C5-C6-N1	4.13	120.37	111.84
67	S2	1383	A2M	C3'-C2'-C1'	-4.12	94.92	102.81
67	S2	121	OMU	N3-C2-N1	4.09	120.21	114.89
2	L5	4220	6MZ	C9-N6-C6	-4.03	119.11	122.85
2	L5	4523	A2M	C3'-C2'-C1'	-4.03	95.10	102.81
2	L5	4227	OMU	N3-C2-N1	4.01	120.12	114.89
67	S2	1851	MA6	C4-N9-C8	3.96	109.90	105.74
67	S2	1639	G7M	C5-C4-N3	-3.93	120.72	128.15
67	S2	354	OMU	N3-C2-N1	3.92	119.99	114.89
2	L5	3925	OMU	N3-C2-N1	3.91	119.98	114.89
2	L5	4498	OMU	N3-C2-N1	3.89	119.95	114.89
67	S2	172	OMU	N3-C2-N1	3.86	119.92	114.89
67	S2	1326	OMU	N3-C2-N1	3.86	119.92	114.89
2	L5	4227	OMU	C5-C4-N3	3.85	120.19	114.80
2	L5	4498	OMU	C5-C4-N3	3.82	120.15	114.80
67	S2	1442	OMU	N3-C2-N1	3.80	119.84	114.89
2	L5	4530	UR3	C5-C4-N3	3.77	120.01	115.04
2	L5	398	A2M	C3'-C2'-C1'	-3.77	95.59	102.81
67	S2	428	OMU	N3-C2-N1	3.76	119.78	114.89
67	S2	799	OMU	N3-C2-N1	3.74	119.77	114.89
67	S2	1851	MA6	C4-C5-C6	3.74	119.77	115.91
2	L5	4306	OMU	N3-C2-N1	3.73	119.75	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	627	OMU	N3-C2-N1	3.73	119.75	114.89
2	L5	3925	OMU	C5-C4-N3	3.72	120.01	114.80
2	L5	4620	OMU	N3-C2-N1	3.72	119.73	114.89
2	L5	2837	OMU	C5-C4-N3	3.68	119.95	114.80
67	S2	627	OMU	C5-C4-N3	3.66	119.93	114.80
2	L5	3867	A2M	C2'-C1'-N9	3.65	119.75	113.75
67	S2	1288	OMU	N3-C2-N1	3.65	119.64	114.89
2	L5	2401	A2M	O3'-C3'-C2'	3.65	121.39	111.19
67	S2	166	A2M	O3'-C3'-C2'	3.64	121.36	111.19
67	S2	354	OMU	C5-C4-N3	3.62	119.87	114.80
2	L5	3825	A2M	C3'-C2'-C1'	-3.62	95.88	102.81
67	S2	799	OMU	C5-C4-N3	3.60	119.84	114.80
67	S2	1850	MA6	C2-N1-C6	3.57	120.54	111.83
67	S2	428	OMU	C5-C4-N3	3.57	119.80	114.80
67	S2	1248	B8N	N3-C2-N1	3.55	121.05	116.72
2	L5	398	A2M	O3'-C3'-C2'	3.53	121.08	111.19
67	S2	166	A2M	C3'-C2'-C1'	-3.53	96.04	102.81
67	S2	1383	A2M	O3'-C3'-C2'	3.53	121.06	111.19
2	L5	3718	A2M	C3'-C2'-C1'	-3.52	96.07	102.81
2	L5	4590	A2M	C3'-C2'-C1'	-3.52	96.08	102.81
67	S2	172	OMU	C5-C4-N3	3.51	119.72	114.80
67	S2	116	OMU	N3-C2-N1	3.50	119.45	114.89
67	S2	1326	OMU	C5-C4-N3	3.48	119.68	114.80
67	S2	1442	OMU	C5-C4-N3	3.48	119.68	114.80
2	L5	4306	OMU	C5-C4-N3	3.48	119.67	114.80
67	S2	1850	MA6	C4-C5-C6	3.45	119.48	115.91
2	L5	2787	A2M	O3'-C3'-C2'	3.45	120.85	111.19
67	S2	1851	MA6	N3-C4-N9	3.44	133.02	127.17
67	S2	1832	6MZ	C2-N3-C4	3.43	120.20	111.83
67	S2	1851	MA6	C2-N1-C6	3.42	120.19	111.83
67	S2	468	A2M	O3'-C3'-C2'	3.42	120.76	111.19
2	L5	4620	OMU	C5-C4-N3	3.42	119.59	114.80
2	L5	4689	PSU	C6-N1-C2	-3.42	119.52	122.69
2	L5	1323	A2M	C2'-C1'-N9	3.41	119.37	113.75
2	L5	2401	A2M	C3'-C2'-C1'	-3.41	96.28	102.81
67	S2	1832	6MZ	C4-N9-C8	3.38	109.29	105.74
67	S2	116	OMU	C5-C4-N3	3.37	119.52	114.80
2	L5	2815	A2M	C2'-C1'-N9	3.37	119.29	113.75
67	S2	576	A2M	O3'-C3'-C2'	3.37	120.61	111.19
67	S2	1639	G7M	O6-C6-C5	-3.36	120.51	128.01
67	S2	1248	B8N	C1'-C5-C4	3.36	122.70	117.61
67	S2	99	A2M	O3'-C3'-C2'	3.35	120.56	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1534	A2M	C3'-C2'-C1'	-3.34	96.41	102.81
2	L5	1871	A2M	O3'-C3'-C2'	3.33	120.51	111.19
67	S2	1832	6MZ	N3-C4-N9	3.28	132.75	127.17
67	S2	1851	MA6	C5-N7-C8	3.27	108.59	103.45
67	S2	1288	OMU	C5-C4-N3	3.26	119.37	114.80
67	S2	1851	MA6	C2-N3-C4	3.25	119.76	111.83
67	S2	1639	G7M	N9-C4-N3	3.24	132.43	125.95
2	L5	4220	6MZ	C2-N3-C4	3.24	119.74	111.83
2	L5	4571	A2M	O3'-C3'-C2'	3.24	120.25	111.19
2	L5	1524	A2M	O3'-C3'-C2'	3.23	120.21	111.19
2	L5	1323	A2M	O3'-C3'-C2'	3.22	120.21	111.19
67	S2	99	A2M	C3'-C2'-C1'	-3.22	96.65	102.81
2	L5	1536	PSU	O2-C2-N1	-3.21	119.47	122.79
67	S2	121	OMU	C5-C4-N3	3.21	119.30	114.80
2	L5	3830	A2M	O3'-C3'-C2'	3.21	120.16	111.19
67	S2	1850	MA6	C5-N7-C8	3.18	108.44	103.45
2	L5	4220	6MZ	C4-N9-C8	3.17	109.07	105.74
67	S2	468	A2M	C3'-C2'-C1'	-3.17	96.74	102.81
2	L5	1683	PSU	O2-C2-N1	-3.16	119.53	122.79
67	S2	1850	MA6	N3-C4-N9	3.15	132.52	127.17
67	S2	116	OMU	O4-C4-C5	-3.15	119.74	125.16
67	S2	159	A2M	O3'-C3'-C2'	3.13	119.94	111.19
67	S2	1832	6MZ	C5-N7-C8	3.13	108.36	103.45
2	L5	4500	PSU	O2-C2-N1	-3.12	119.57	122.79
2	L5	1862	PSU	O2-C2-N1	-3.12	119.57	122.79
2	L5	4571	A2M	C3'-C2'-C1'	-3.10	96.87	102.81
2	L5	2351	OMC	C1'-N1-C2	3.09	125.26	118.44
2	L5	4636	PSU	C6-C5-C4	3.08	120.25	118.17
2	L5	2363	A2M	C2'-C1'-N9	3.08	118.81	113.75
2	L5	3718	A2M	O3'-C3'-C2'	3.07	119.78	111.19
67	S2	1639	G7M	CN7-N7-C5	3.06	130.61	126.80
2	L5	4220	6MZ	N3-C4-N9	3.06	132.36	127.17
2	L5	4403	PSU	O2-C2-N1	-3.05	119.64	122.79
2	L5	4523	A2M	O3'-C3'-C2'	3.05	119.72	111.19
2	L5	4552	PSU	O2-C2-N1	-3.05	119.65	122.79
2	L5	4457	PSU	O2-C2-N1	-3.04	119.65	122.79
2	L5	400	A2M	O3'-C3'-C2'	3.04	119.69	111.19
2	L5	2815	A2M	O3'-C3'-C2'	3.03	119.67	111.19
2	L5	1326	A2M	C2'-C1'-N9	3.02	118.72	113.75
67	S2	668	A2M	O3'-C3'-C2'	3.02	119.64	111.19
2	L5	3701	OMC	O2-C2-N3	-3.02	117.57	122.33
67	S2	1832	6MZ	C4-C5-C6	3.01	119.28	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3818	UY1	C6-C5-C4	3.01	120.21	118.17
2	L5	2837	OMU	O4-C4-C5	-3.01	119.97	125.16
67	S2	1850	MA6	C2-N3-C4	3.01	119.17	111.83
67	S2	27	A2M	C3'-C2'-C1'	-3.00	97.06	102.81
67	S2	627	OMU	O4-C4-C5	-3.00	119.98	125.16
67	S2	1081	PSU	O2-C2-N1	-3.00	119.69	122.79
4	L8	69	PSU	O2-C2-N1	-3.00	119.70	122.79
2	L5	4973	PSU	O2-C2-N1	-3.00	119.70	122.79
2	L5	4498	OMU	O4-C4-C5	-3.00	120.00	125.16
2	L5	3825	A2M	O3'-C3'-C2'	2.99	119.56	111.19
67	S2	1004	PSU	O2-C2-N1	-2.99	119.71	122.79
2	L5	5001	PSU	O2-C2-N1	-2.98	119.71	122.79
67	S2	1639	G7M	C2-N1-C6	-2.98	119.70	125.11
67	S2	668	A2M	C4-N9-C1'	-2.98	119.67	126.63
2	L5	3785	A2M	O3'-C3'-C2'	2.98	119.52	111.19
2	L5	3822	PSU	O2-C2-N1	-2.97	119.72	122.79
2	L5	1744	PSU	O2-C2-N1	-2.97	119.73	122.79
67	S2	484	A2M	O3'-C3'-C2'	2.97	119.50	111.19
2	L5	2363	A2M	C3'-C2'-C1'	-2.97	97.13	102.81
67	S2	1045	PSU	O2-C2-N1	-2.97	119.73	122.79
2	L5	1871	A2M	C4-N9-C1'	-2.97	119.69	126.63
67	S2	27	A2M	C4-N9-C1'	-2.97	119.70	126.63
67	S2	1031	A2M	O3'-C3'-C2'	2.96	119.46	111.19
67	S2	172	OMU	O4-C4-C5	-2.95	120.07	125.16
2	L5	3785	A2M	C4'-O4'-C1'	-2.95	102.95	109.47
67	S2	354	OMU	O4-C4-C5	-2.95	120.08	125.16
67	S2	428	OMU	O4-C4-C5	-2.94	120.08	125.16
2	L5	2839	PSU	C6-N1-C2	-2.94	119.96	122.69
2	L5	4227	OMU	O4-C4-C5	-2.94	120.09	125.16
67	S2	668	A2M	O4'-C1'-C2'	2.94	111.65	106.59
67	S2	1046	PSU	O2-C2-N1	-2.94	119.76	122.79
2	L5	4620	OMU	O4-C4-C5	-2.94	120.10	125.16
2	L5	400	A2M	C3'-C2'-C1'	-2.93	97.19	102.81
67	S2	99	A2M	C4-N9-C1'	-2.93	119.78	126.63
2	L5	4576	PSU	O2-C2-N1	-2.92	119.77	122.79
67	S2	27	A2M	O3'-C3'-C2'	2.92	119.37	111.19
67	S2	105	PSU	O2-C2-N1	-2.92	119.78	122.79
2	L5	2839	PSU	O2-C2-N1	-2.91	119.78	122.79
67	S2	1326	OMU	O4-C4-C5	-2.91	120.14	125.16
2	L5	3884	PSU	O2-C2-N1	-2.91	119.79	122.79
2	L5	5010	PSU	O2-C2-N1	-2.91	119.79	122.79
67	S2	799	OMU	O4-C4-C5	-2.91	120.15	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	406	PSU	O2-C2-N1	-2.91	119.79	122.79
2	L5	4590	A2M	C4-N9-C1'	-2.91	119.84	126.63
67	S2	1232	PSU	O2-C2-N1	-2.91	119.79	122.79
67	S2	166	A2M	C4-N9-C1'	-2.90	119.84	126.63
67	S2	468	A2M	C4-N9-C1'	-2.90	119.86	126.63
2	L5	4579	PSU	O2-C2-N1	-2.89	119.81	122.79
2	L5	4293	PSU	O2-C2-N1	-2.89	119.81	122.79
2	L5	3925	OMU	O4-C4-C5	-2.89	120.18	125.16
2	L5	4361	PSU	O2-C2-N1	-2.89	119.81	122.79
2	L5	1683	PSU	C6-N1-C2	-2.88	120.02	122.69
2	L5	4532	PSU	O2-C2-N1	-2.88	119.82	122.79
67	S2	863	PSU	O2-C2-N1	-2.87	119.83	122.79
67	S2	1442	OMU	O4-C4-C5	-2.87	120.22	125.16
2	L5	3884	PSU	C6-N1-C2	-2.86	120.03	122.69
2	L5	1326	A2M	O3'-C3'-C2'	2.86	119.20	111.19
2	L5	4579	PSU	C6-N1-C2	-2.86	120.03	122.69
2	L5	4296	PSU	O2-C2-N1	-2.85	119.85	122.79
2	L5	4353	PSU	O2-C2-N1	-2.85	119.85	122.79
2	L5	3844	PSU	C6-N1-C2	-2.84	120.06	122.69
67	S2	1244	PSU	O2-C2-N1	-2.84	119.86	122.79
67	S2	576	A2M	C3'-C2'-C1'	-2.83	97.39	102.81
67	S2	484	A2M	C4-N9-C1'	-2.83	120.02	126.63
67	S2	1383	A2M	C4-N9-C1'	-2.82	120.03	126.63
2	L5	1323	A2M	C3'-C2'-C1'	-2.82	97.41	102.81
67	S2	651	PSU	O2-C2-N1	-2.82	119.88	122.79
67	S2	866	PSU	O2-C2-N1	-2.82	119.88	122.79
67	S2	686	PSU	O2-C2-N1	-2.82	119.88	122.79
67	S2	1367	PSU	O2-C2-N1	-2.82	119.89	122.79
67	S2	1056	PSU	O2-C2-N1	-2.81	119.89	122.79
2	L5	4431	PSU	O2-C2-N1	-2.81	119.89	122.79
2	L5	1677	PSU	O2-C2-N1	-2.81	119.89	122.79
2	L5	3853	PSU	O2-C2-N1	-2.81	119.89	122.79
2	L5	4571	A2M	C4-N9-C1'	-2.79	120.11	126.63
67	S2	814	PSU	C6-N1-C2	-2.78	120.11	122.69
67	S2	27	A2M	C1'-N9-C8	2.78	133.27	127.09
2	L5	4500	PSU	C6-N1-C2	-2.78	120.11	122.69
2	L5	4628	PSU	O2-C2-N1	-2.78	119.92	122.79
67	S2	1046	PSU	C6-N1-C2	-2.78	120.11	122.69
67	S2	1272	OMC	C1'-N1-C2	2.78	124.57	118.44
2	L5	4471	PSU	C6-N1-C2	-2.78	120.11	122.69
2	L5	4636	PSU	O2-C2-N1	-2.78	119.92	122.79
67	S2	484	A2M	C1'-N9-C8	2.78	133.25	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L8	55	PSU	O2-C2-N1	-2.77	119.93	122.79
2	L5	3639	PSU	C6-N1-C2	-2.77	120.12	122.69
67	S2	1288	OMU	C1'-N1-C2	2.76	122.56	117.59
2	L5	3695	PSU	O2-C2-N1	-2.76	119.94	122.79
67	S2	1288	OMU	O4-C4-C5	-2.76	120.41	125.16
67	S2	109	PSU	O2-C2-N1	-2.76	119.94	122.79
2	L5	1782	PSU	O2-C2-N1	-2.76	119.95	122.79
2	L5	4689	PSU	O2-C2-N1	-2.75	119.95	122.79
2	L5	3851	PSU	O2-C2-N1	-2.75	119.95	122.79
2	L5	4442	PSU	O2-C2-N1	-2.75	119.95	122.79
2	L5	3830	A2M	C4-N9-C1'	-2.75	120.21	126.63
2	L5	1871	A2M	C1'-N9-C8	2.74	133.19	127.09
2	L5	4673	PSU	C6-N1-C2	-2.74	120.14	122.69
67	S2	121	OMU	O4-C4-C5	-2.74	120.43	125.16
2	L5	3825	A2M	C4-N9-C1'	-2.74	120.22	126.63
2	L5	4590	A2M	C1'-N9-C8	2.74	133.18	127.09
2	L5	4312	PSU	O2-C2-N1	-2.74	119.96	122.79
2	L5	4220	6MZ	C5-N7-C8	2.74	107.75	103.45
2	L5	2632	PSU	O2-C2-N1	-2.74	119.97	122.79
2	L5	4523	A2M	C4-N9-C1'	-2.73	120.24	126.63
2	L5	4220	6MZ	C4-C5-C6	2.73	119.05	116.78
2	L5	1860	PSU	C6-N1-C2	-2.73	120.16	122.69
67	S2	668	A2M	C1'-N9-C8	2.73	133.15	127.09
67	S2	1031	A2M	C4-N9-C1'	-2.73	120.26	126.63
2	L5	4306	OMU	O4-C4-C5	-2.72	120.47	125.16
2	L5	4471	PSU	O2-C2-N1	-2.72	119.98	122.79
67	S2	1174	PSU	O2-C2-N1	-2.72	119.98	122.79
2	L5	4673	PSU	O2-C2-N1	-2.72	119.98	122.79
2	L5	5010	PSU	C6-N1-C2	-2.71	120.18	122.69
67	S2	99	A2M	C1'-N9-C8	2.71	133.10	127.09
2	L5	3701	OMC	O2-C2-N1	2.70	124.20	118.90
67	S2	1177	PSU	O2-C2-N1	-2.70	120.00	122.79
2	L5	4312	PSU	C6-N1-C2	-2.70	120.19	122.69
2	L5	3808	OMC	C1'-N1-C2	2.70	124.39	118.44
2	L5	4972	PSU	O2-C2-N1	-2.69	120.01	122.79
67	S2	681	PSU	C6-N1-C2	-2.69	120.20	122.69
2	L5	1534	A2M	C2'-C1'-N9	2.69	118.17	113.75
2	L5	3718	A2M	C1'-N9-C8	2.68	133.05	127.09
2	L5	1582	PSU	O2-C2-N1	-2.68	120.02	122.79
2	L5	3818	UY1	O2-C2-N1	-2.67	120.03	122.79
2	L5	3785	A2M	C4-N9-C1'	-2.66	120.40	126.63
2	L5	3818	UY1	C6-N1-C2	-2.66	120.22	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1781	PSU	O2-C2-N1	-2.66	120.04	122.79
2	L5	1744	PSU	C6-N1-C2	-2.66	120.22	122.69
2	L5	4493	PSU	O2-C2-N1	-2.66	120.05	122.79
2	L5	2861	OMC	C1'-N1-C2	2.66	124.31	118.44
2	L5	2363	A2M	C4-N9-C1'	-2.65	120.42	126.63
67	S2	468	A2M	C1'-N9-C8	2.65	132.99	127.09
2	L5	4552	PSU	C6-N1-C2	-2.65	120.23	122.69
2	L5	2401	A2M	C4-N9-C1'	-2.65	120.43	126.63
2	L5	3920	PSU	O2-C2-N1	-2.65	120.06	122.79
67	S2	966	PSU	O2-C2-N1	-2.65	120.06	122.79
2	L5	3639	PSU	O2-C2-N1	-2.65	120.06	122.79
2	L5	4493	PSU	C6-N1-C2	-2.64	120.24	122.69
67	S2	105	PSU	C6-N1-C2	-2.64	120.24	122.69
2	L5	3844	PSU	O2-C2-N1	-2.64	120.06	122.79
2	L5	1524	A2M	O4'-C1'-C2'	2.64	111.13	106.59
2	L5	400	A2M	C4-N9-C1'	-2.63	120.47	126.63
67	S2	1383	A2M	C1'-N9-C8	2.63	132.94	127.09
2	L5	4590	A2M	O3'-C3'-C2'	2.63	118.55	111.19
67	S2	649	PSU	O2-C2-N1	-2.63	120.07	122.79
67	S2	1031	A2M	C1'-N9-C8	2.63	132.93	127.09
2	L5	1534	A2M	C4-N9-C1'	-2.63	120.49	126.63
2	L5	3830	A2M	C1'-N9-C8	2.63	132.92	127.09
2	L5	1536	PSU	C6-N1-C2	-2.62	120.26	122.69
2	L5	3825	A2M	C1'-N9-C8	2.62	132.91	127.09
2	L5	1781	PSU	C6-N1-C2	-2.61	120.27	122.69
2	L5	398	A2M	C4-N9-C1'	-2.61	120.54	126.63
67	S2	814	PSU	O2-C2-N1	-2.61	120.10	122.79
67	S2	166	A2M	C1'-N9-C8	2.61	132.88	127.09
2	L5	400	A2M	C2'-C1'-N9	2.60	118.04	113.75
67	S2	1174	PSU	C6-N1-C2	-2.60	120.28	122.69
2	L5	1792	PSU	O2-C2-N1	-2.60	120.11	122.79
2	L5	4628	PSU	C6-N1-C2	-2.59	120.28	122.69
2	L5	1326	A2M	C3'-C2'-C1'	-2.59	97.84	102.81
67	S2	801	PSU	C6-N1-C2	-2.59	120.29	122.69
2	L5	4299	PSU	C6-N1-C2	-2.59	120.29	122.69
67	S2	93	PSU	O2-C2-N1	-2.59	120.12	122.79
2	L5	4571	A2M	C1'-N9-C8	2.58	132.83	127.09
4	L8	55	PSU	C6-N1-C2	-2.58	120.29	122.69
67	S2	1639	G7M	CN7-N7-C8	-2.58	120.88	124.79
2	L5	4403	PSU	C6-N1-C2	-2.58	120.30	122.69
2	L5	3822	PSU	C6-N1-C2	-2.57	120.30	122.69
67	S2	484	A2M	O4'-C1'-C2'	2.57	111.01	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	1367	PSU	C6-N1-C2	-2.57	120.31	122.69
2	L5	3637	PSU	C6-N1-C2	-2.56	120.31	122.69
2	L5	2363	A2M	C1'-N9-C8	2.56	132.78	127.09
67	S2	1004	PSU	C6-N1-C2	-2.56	120.32	122.69
2	L5	1534	A2M	C1'-N9-C8	2.56	132.78	127.09
2	L5	2815	A2M	C3'-C2'-C1'	-2.56	97.91	102.81
2	L5	1323	A2M	O4'-C1'-C2'	2.56	110.99	106.59
67	S2	1056	PSU	C6-N1-C2	-2.55	120.33	122.69
67	S2	681	PSU	O2-C2-N1	-2.55	120.16	122.79
2	L5	4431	PSU	C6-N1-C2	-2.54	120.33	122.69
2	L5	1860	PSU	O2-C2-N1	-2.54	120.17	122.79
2	L5	3718	A2M	C4-N9-C1'	-2.54	120.70	126.63
2	L5	398	A2M	C1'-N9-C8	2.53	132.72	127.09
67	S2	159	A2M	C1'-N9-C8	2.53	132.72	127.09
67	S2	576	A2M	C4-N9-C1'	-2.53	120.72	126.63
2	L5	4442	PSU	C6-N1-C2	-2.52	120.35	122.69
67	S2	686	PSU	C6-N1-C2	-2.52	120.35	122.69
67	S2	801	PSU	O2-C2-N1	-2.52	120.19	122.79
2	L5	4523	A2M	C1'-N9-C8	2.51	132.68	127.09
2	L5	400	A2M	C1'-N9-C8	2.51	132.67	127.09
67	S2	406	PSU	C6-N1-C2	-2.51	120.36	122.69
2	L5	3920	PSU	C6-N1-C2	-2.51	120.36	122.69
67	S2	159	A2M	C4-N9-C1'	-2.51	120.77	126.63
2	L5	4973	PSU	C6-N1-C2	-2.51	120.37	122.69
67	S2	649	PSU	C6-N1-C2	-2.50	120.37	122.69
67	S2	1832	6MZ	C9-N6-C6	-2.50	120.53	122.85
2	L5	4576	PSU	C6-N1-C2	-2.49	120.38	122.69
67	S2	1232	PSU	C6-N1-C2	-2.49	120.38	122.69
2	L5	2401	A2M	C1'-N9-C8	2.49	132.63	127.09
67	S2	1248	B8N	O4-C4-N3	-2.49	115.94	119.99
2	L5	2632	PSU	C6-N1-C2	-2.49	120.38	122.69
2	L5	4521	PSU	O2-C2-N1	-2.49	120.22	122.79
2	L5	3695	PSU	C6-N1-C2	-2.49	120.38	122.69
2	L5	5001	PSU	C6-N1-C2	-2.49	120.38	122.69
67	S2	1244	PSU	C6-N1-C2	-2.48	120.39	122.69
2	L5	1534	A2M	O3'-C3'-C4'	-2.48	103.97	111.08
2	L5	3867	A2M	O3'-C3'-C2'	2.47	118.11	111.19
2	L5	2363	A2M	O3'-C3'-C2'	2.47	118.11	111.19
67	S2	1045	PSU	C6-N1-C2	-2.47	120.40	122.69
67	S2	484	A2M	O4'-C4'-C3'	2.46	110.04	105.15
2	L5	4532	PSU	C6-N1-C2	-2.46	120.41	122.69
67	S2	966	PSU	C6-N1-C2	-2.45	120.41	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	159	A2M	C3'-C2'-C1'	-2.45	98.11	102.81
2	L5	4521	PSU	C6-N1-C2	-2.45	120.42	122.69
2	L5	4457	PSU	C6-N1-C2	-2.45	120.42	122.69
2	L5	1524	A2M	C4-N9-C1'	-2.45	120.91	126.63
2	L5	2787	A2M	O4'-C1'-C2'	2.44	110.79	106.59
4	L8	69	PSU	C6-N1-C2	-2.44	120.43	122.69
67	S2	1851	MA6	C1'-N9-C8	-2.44	121.68	127.09
2	L5	3851	PSU	C6-N1-C2	-2.43	120.43	122.69
67	S2	651	PSU	C6-N1-C2	-2.43	120.44	122.69
2	L5	1782	PSU	C6-N1-C2	-2.43	120.44	122.69
2	L5	4299	PSU	O2-C2-N1	-2.41	120.31	122.79
2	L5	1323	A2M	C4-N9-C1'	-2.40	121.01	126.63
67	S2	1639	G7M	N9-C8-N7	-2.40	106.64	112.48
67	S2	1081	PSU	C6-N1-C2	-2.40	120.46	122.69
2	L5	3867	A2M	C4-N9-C1'	-2.40	121.02	126.63
67	S2	1031	A2M	C3'-C2'-C1'	-2.40	98.22	102.81
67	S2	576	A2M	C1'-N9-C8	2.39	132.40	127.09
67	S2	866	PSU	C6-N1-C2	-2.39	120.47	122.69
67	S2	863	PSU	C6-N1-C2	-2.39	120.48	122.69
2	L5	3867	A2M	C3'-C2'-C1'	-2.38	98.24	102.81
2	L5	4361	PSU	C6-N1-C2	-2.38	120.48	122.69
2	L5	1524	A2M	C1'-N9-C8	2.37	132.35	127.09
67	S2	1850	MA6	C1'-N9-C8	-2.36	121.85	127.09
67	S2	1248	B8N	O4'-C1'-C2'	2.36	108.42	105.15
2	L5	1322	1MA	N1-C6-N6	2.36	125.64	119.71
67	S2	109	PSU	C6-N1-C2	-2.36	120.50	122.69
2	L5	3785	A2M	C1'-N9-C8	2.35	132.32	127.09
2	L5	1323	A2M	C1'-N9-C8	2.35	132.31	127.09
2	L5	4972	PSU	C6-N1-C2	-2.35	120.51	122.69
67	S2	1177	PSU	C6-N1-C2	-2.35	120.51	122.69
2	L5	2363	A2M	O4'-C1'-C2'	2.34	110.62	106.59
67	S2	93	PSU	C6-N1-C2	-2.34	120.52	122.69
2	L5	1871	A2M	C6-C5-C4	-2.34	113.98	117.18
67	S2	1337	4AC	N4-C4-N3	2.34	117.66	113.87
67	S2	172	OMU	O2-C2-N1	-2.33	119.76	122.80
2	L5	1862	PSU	C6-N1-C2	-2.32	120.53	122.69
2	L5	4571	A2M	C2'-C1'-N9	2.32	117.56	113.75
2	L5	4590	A2M	C6-C5-C4	-2.32	114.02	117.18
2	L5	3853	PSU	C6-N1-C2	-2.31	120.55	122.69
67	S2	27	A2M	O4'-C1'-C2'	2.31	110.56	106.59
67	S2	1031	A2M	O4'-C1'-C2'	2.30	110.54	106.59
2	L5	3785	A2M	C3'-C2'-C1'	-2.30	98.41	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4571	A2M	O4'-C1'-C2'	2.30	110.54	106.59
2	L5	3867	A2M	C1'-N9-C8	2.29	132.18	127.09
2	L5	1534	A2M	O3'-C3'-C2'	2.29	117.59	111.19
2	L5	1524	A2M	C4'-O4'-C1'	-2.28	104.42	109.47
2	L5	2815	A2M	C1'-N9-C8	2.27	132.13	127.09
67	S2	799	OMU	C1'-N1-C2	2.27	121.66	117.59
67	S2	99	A2M	C6-C5-C4	-2.26	114.09	117.18
2	L5	2815	A2M	C4-N9-C1'	-2.26	121.35	126.63
2	L5	400	A2M	C6-C5-C4	-2.26	114.10	117.18
67	S2	668	A2M	C6-C5-C4	-2.25	114.10	117.18
2	L5	4403	PSU	O4'-C1'-C2'	2.25	108.27	105.15
2	L5	4636	PSU	O4'-C1'-C2'	2.25	108.26	105.15
2	L5	3785	A2M	C2-N1-C6	-2.25	115.04	118.73
67	S2	1248	B8N	O4-C4-C5	-2.24	118.70	122.58
67	S2	27	A2M	C6-C5-C4	-2.24	114.12	117.18
2	L5	1326	A2M	C1'-N9-C8	2.23	132.05	127.09
2	L5	2787	A2M	C4-N9-C1'	-2.23	121.42	126.63
2	L5	1792	PSU	C6-N1-C2	-2.23	120.62	122.69
2	L5	4296	PSU	C6-N1-C2	-2.23	120.62	122.69
67	S2	1832	6MZ	C5-C6-N1	2.22	120.54	118.15
2	L5	3822	PSU	O4'-C1'-C2'	2.22	108.23	105.15
67	S2	99	A2M	C5-C6-N1	2.21	123.13	117.51
2	L5	4571	A2M	C6-C5-C4	-2.21	114.16	117.18
2	L5	3785	A2M	O4'-C1'-N9	2.21	112.34	108.09
2	L5	4498	OMU	O2-C2-N1	-2.21	119.92	122.80
67	S2	468	A2M	C6-C5-C4	-2.21	114.16	117.18
67	S2	116	OMU	C1'-N1-C2	2.21	121.56	117.59
2	L5	3825	A2M	C6-C5-C4	-2.21	114.17	117.18
2	L5	3830	A2M	C6-C5-C4	-2.20	114.17	117.18
2	L5	3785	A2M	C5-C6-N1	2.20	123.11	117.51
2	L5	4456	OMC	C1'-N1-C2	2.20	123.31	118.44
2	L5	3637	PSU	C6-C5-C4	2.20	119.66	118.17
2	L5	2815	A2M	O4'-C1'-C2'	2.20	110.37	106.59
2	L5	4442	PSU	C6-C5-C4	2.20	119.66	118.17
2	L5	1677	PSU	C6-N1-C2	-2.20	120.65	122.69
2	L5	3925	OMU	O2-C2-N1	-2.20	119.94	122.80
2	L5	4353	PSU	C6-N1-C2	-2.20	120.65	122.69
2	L5	1326	A2M	C4-N9-C1'	-2.19	121.51	126.63
2	L5	4220	6MZ	C5-C6-N1	2.19	120.50	118.15
67	S2	1081	PSU	C6-C5-C4	2.19	119.65	118.17
2	L5	400	A2M	O4'-C1'-C2'	2.19	110.36	106.59
67	S2	166	A2M	C6-C5-C4	-2.19	114.19	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4590	A2M	C2'-C1'-N9	2.18	117.34	113.75
67	S2	1031	A2M	C6-C5-C4	-2.18	114.21	117.18
2	L5	4530	UR3	C6-N1-C2	-2.17	120.02	121.80
2	L5	1524	A2M	C6-C5-C4	-2.16	114.22	117.18
2	L5	2363	A2M	C6-C5-C4	-2.16	114.23	117.18
2	L5	3637	PSU	O2-C2-N1	-2.16	120.56	122.79
2	L5	1534	A2M	C6-C5-C4	-2.16	114.23	117.18
2	L5	2787	A2M	C1'-N9-C8	2.15	131.87	127.09
2	L5	3785	A2M	O4'-C4'-C3'	2.15	109.42	105.15
67	S2	1272	OMC	C1'-N1-C6	-2.15	116.19	120.78
67	S2	1383	A2M	C6-C5-C4	-2.15	114.25	117.18
67	S2	99	A2M	C2-N1-C6	-2.14	115.22	118.73
2	L5	1744	PSU	C6-C5-C4	2.14	119.62	118.17
2	L5	4523	A2M	C6-C5-C4	-2.14	114.26	117.18
2	L5	2401	A2M	C6-C5-C4	-2.14	114.26	117.18
2	L5	1322	1MA	CM1-N1-C6	-2.14	116.84	120.15
2	L5	3785	A2M	C6-C5-C4	-2.13	114.27	117.18
2	L5	4293	PSU	C6-N1-C2	-2.13	120.72	122.69
2	L5	4523	A2M	C2-N1-C6	-2.13	115.23	118.73
2	L5	1582	PSU	C6-N1-C2	-2.12	120.72	122.69
2	L5	1323	A2M	C6-C5-C4	-2.12	114.28	117.18
67	S2	1367	PSU	C6-C5-C4	2.12	119.60	118.17
2	L5	4403	PSU	C6-C5-C4	2.12	119.60	118.17
2	L5	2351	OMC	C1'-N1-C6	-2.12	116.26	120.78
2	L5	4442	PSU	O4'-C1'-C2'	2.12	108.08	105.15
2	L5	4500	PSU	C6-C5-C4	2.12	119.60	118.17
67	S2	576	A2M	C6-C5-C4	-2.12	114.29	117.18
4	L8	69	PSU	O4'-C1'-C2'	2.11	108.08	105.15
2	L5	4636	PSU	C6-N1-C2	-2.11	120.73	122.69
2	L5	1871	A2M	C4'-O4'-C1'	-2.11	104.81	109.47
2	L5	398	A2M	C5-C6-N1	2.10	122.85	117.51
2	L5	4571	A2M	C5-C6-N1	2.10	122.85	117.51
2	L5	3782	5MC	C1'-N1-C6	-2.10	117.69	121.15
2	L5	4523	A2M	C5-C6-N1	2.10	122.85	117.51
67	S2	1326	OMU	O2-C2-N1	-2.10	120.06	122.80
2	L5	3825	A2M	C5-C6-N1	2.10	122.84	117.51
67	S2	1031	A2M	C5-C6-N1	2.10	122.84	117.51
67	S2	1703	OMC	C1'-N1-C2	2.10	123.07	118.44
2	L5	398	A2M	C6-C5-C4	-2.09	114.32	117.18
67	S2	166	A2M	C5-C6-N1	2.09	122.83	117.51
2	L5	4521	PSU	C6-C5-C4	2.09	119.59	118.17
2	L5	2363	A2M	C5-C6-N1	2.09	122.82	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	627	OMU	O2-C2-N1	-2.09	120.08	122.80
2	L5	400	A2M	C5-C6-N1	2.08	122.80	117.51
2	L5	2401	A2M	C5-C6-N1	2.08	122.80	117.51
2	L5	1323	A2M	C5-C6-N1	2.08	122.80	117.51
67	S2	99	A2M	O4'-C1'-C2'	2.08	110.17	106.59
67	S2	121	OMU	C6-N1-C2	-2.08	118.47	121.00
2	L5	3867	A2M	C2-N1-C6	-2.08	115.32	118.73
2	L5	2815	A2M	C6-C5-C4	-2.08	114.34	117.18
2	L5	3867	A2M	C6-C5-C4	-2.07	114.35	117.18
2	L5	1323	A2M	C2-N1-C6	-2.07	115.32	118.73
2	L5	1534	A2M	C2-N1-C6	-2.07	115.32	118.73
67	S2	484	A2M	C6-C5-C4	-2.07	114.35	117.18
2	L5	1534	A2M	C5-C6-N1	2.07	122.77	117.51
2	L5	398	A2M	C2-N1-C6	-2.07	115.34	118.73
2	L5	1326	A2M	C5-C6-N1	2.06	122.75	117.51
67	S2	159	A2M	C2-N1-C6	-2.06	115.34	118.73
2	L5	3830	A2M	C5-C6-N1	2.06	122.75	117.51
67	S2	354	OMU	O2-C2-N1	-2.06	120.11	122.80
67	S2	468	A2M	C5-C6-N1	2.06	122.75	117.51
2	L5	4227	OMU	O2-C2-N1	-2.06	120.11	122.80
2	L5	3920	PSU	O4'-C1'-C2'	2.06	108.00	105.15
2	L5	2815	A2M	C2-N1-C6	-2.06	115.35	118.73
2	L5	4571	A2M	C2-N1-C6	-2.06	115.35	118.73
2	L5	2787	A2M	C5-C6-N1	2.05	122.73	117.51
2	L5	1677	PSU	C6-C5-C4	2.05	119.56	118.17
67	S2	109	PSU	C6-C5-C4	2.05	119.56	118.17
2	L5	2815	A2M	C5-C6-N1	2.05	122.73	117.51
67	S2	1248	B8N	C31-N3-C4	2.05	120.08	117.18
2	L5	2363	A2M	C2-N1-C6	-2.05	115.36	118.73
67	S2	1081	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L5	2787	A2M	C2-N1-C6	-2.05	115.37	118.73
2	L5	1326	A2M	C2-N1-C6	-2.05	115.37	118.73
2	L5	4636	PSU	C5-C6-N1	-2.05	119.30	122.14
2	L5	1871	A2M	C5-C6-N1	2.04	122.70	117.51
67	S2	1383	A2M	C5-C6-N1	2.04	122.70	117.51
2	L5	4973	PSU	C6-C5-C4	2.04	119.55	118.17
67	S2	428	OMU	O2-C2-N1	-2.04	120.14	122.80
67	S2	159	A2M	C2'-C1'-N9	2.04	117.11	113.75
2	L5	1326	A2M	C6-C5-C4	-2.04	114.40	117.18
2	L5	3825	A2M	C2-N1-C6	-2.04	115.39	118.73
2	L5	2401	A2M	C2-N1-C6	-2.04	115.39	118.73
67	S2	159	A2M	O4'-C1'-C2'	2.03	110.09	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	2861	OMC	C1'-N1-C6	-2.03	116.44	120.78
67	S2	576	A2M	C5-C6-N1	2.03	122.66	117.51
67	S2	27	A2M	C5-C6-N1	2.02	122.65	117.51
67	S2	468	A2M	O4'-C1'-C2'	2.02	110.07	106.59
2	L5	3718	A2M	C2-N1-C6	-2.02	115.41	118.73
2	L5	1524	A2M	C5-C6-N1	2.02	122.64	117.51
2	L5	3825	A2M	C2'-C1'-N9	2.02	117.07	113.75
2	L5	3718	A2M	C6-C5-C4	-2.02	114.42	117.18
67	S2	484	A2M	C5-C6-N1	2.01	122.62	117.51
2	L5	1326	A2M	O4'-C1'-C2'	2.01	110.05	106.59
2	L5	4620	OMU	O2-C2-N1	-2.01	120.18	122.80
67	S2	109	PSU	O4'-C1'-C2'	2.01	107.93	105.15
67	S2	166	A2M	C2-N1-C6	-2.00	115.44	118.73
2	L5	3830	A2M	C4'-O4'-C1'	-2.00	105.04	109.47
67	S2	668	A2M	C5-C6-N1	2.00	122.60	117.51
67	S2	484	A2M	C2-N1-C6	-2.00	115.44	118.73
2	L5	2787	A2M	C6-C5-C4	-2.00	114.44	117.18

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L8	75	OMG	C1'-C2'-O2'-CM2
2	L5	400	A2M	C1'-C2'-O2'-CM'
2	L5	1326	A2M	O4'-C4'-C5'-O5'
2	L5	1625	OMG	O4'-C4'-C5'-O5'
2	L5	2351	OMC	C1'-C2'-O2'-CM2
2	L5	2787	A2M	C1'-C2'-O2'-CM'
2	L5	2824	OMC	C1'-C2'-O2'-CM2
2	L5	3701	OMC	O4'-C4'-C5'-O5'
2	L5	3792	OMG	O4'-C4'-C5'-O5'
2	L5	4196	OMG	C1'-C2'-O2'-CM2
2	L5	4590	A2M	O4'-C4'-C5'-O5'
2	L5	4637	OMG	O4'-C4'-C5'-O5'
2	L5	4637	OMG	C1'-C2'-O2'-CM2
67	S2	27	A2M	C1'-C2'-O2'-CM'
67	S2	99	A2M	C1'-C2'-O2'-CM'
67	S2	159	A2M	C1'-C2'-O2'-CM'
67	S2	462	OMC	C1'-C2'-O2'-CM2
67	S2	644	OMG	O4'-C4'-C5'-O5'
67	S2	644	OMG	C1'-C2'-O2'-CM2
67	S2	863	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
67	S2	863	PSU	O4'-C4'-C5'-O5'
67	S2	1031	A2M	C1'-C2'-O2'-CM'
67	S2	1248	B8N	O4'-C4'-C5'-O5'
67	S2	1272	OMC	O4'-C4'-C5'-O5'
67	S2	1288	OMU	O4'-C4'-C5'-O5'
67	S2	1328	OMG	C1'-C2'-O2'-CM2
67	S2	1337	4AC	N3-C4-N4-C7
67	S2	1383	A2M	C1'-C2'-O2'-CM'
67	S2	1490	OMG	C1'-C2'-O2'-CM2
67	S2	1832	6MZ	C5-C6-N6-C9
67	S2	1832	6MZ	N1-C6-N6-C9
67	S2	1832	6MZ	C5'-O5'-P-OP2
67	S2	1832	6MZ	C5'-O5'-P-OP3
2	L5	3701	OMC	C2'-C1'-N1-C2
2	L5	1323	A2M	O4'-C4'-C5'-O5'
2	L5	1326	A2M	C3'-C4'-C5'-O5'
2	L5	1536	PSU	C3'-C4'-C5'-O5'
2	L5	1536	PSU	O4'-C4'-C5'-O5'
2	L5	1625	OMG	C3'-C4'-C5'-O5'
2	L5	2364	OMG	O4'-C4'-C5'-O5'
2	L5	2401	A2M	C3'-C4'-C5'-O5'
2	L5	2815	A2M	O4'-C4'-C5'-O5'
2	L5	3701	OMC	C3'-C4'-C5'-O5'
2	L5	3867	A2M	C3'-C4'-C5'-O5'
2	L5	4500	PSU	O4'-C4'-C5'-O5'
2	L5	4590	A2M	C3'-C4'-C5'-O5'
67	S2	867	OMG	C3'-C4'-C5'-O5'
67	S2	1045	PSU	C3'-C4'-C5'-O5'
67	S2	1045	PSU	O4'-C4'-C5'-O5'
67	S2	1272	OMC	C3'-C4'-C5'-O5'
67	S2	1288	OMU	C3'-C4'-C5'-O5'
2	L5	3701	OMC	C2'-C1'-N1-C6
2	L5	1677	PSU	C3'-C4'-C5'-O5'
2	L5	1677	PSU	O4'-C4'-C5'-O5'
2	L5	2401	A2M	O4'-C4'-C5'-O5'
2	L5	3867	A2M	O4'-C4'-C5'-O5'
2	L5	3899	OMG	C3'-C4'-C5'-O5'
2	L5	4500	PSU	C3'-C4'-C5'-O5'
67	S2	99	A2M	O4'-C4'-C5'-O5'
67	S2	1442	OMU	O4'-C4'-C5'-O5'
67	S2	428	OMU	C2'-C1'-N1-C6
67	S2	627	OMU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	L5	4637	OMG	C3'-C4'-C5'-O5'
67	S2	1248	B8N	C3'-C4'-C5'-O5'
2	L5	1323	A2M	C3'-C4'-C5'-O5'
2	L5	3792	OMG	C3'-C4'-C5'-O5'
67	S2	627	OMU	O4'-C4'-C5'-O5'
67	S2	644	OMG	C3'-C4'-C5'-O5'
67	S2	668	A2M	O4'-C4'-C5'-O5'
67	S2	801	PSU	C3'-C4'-C5'-O5'
67	S2	428	OMU	C2'-C1'-N1-C2
2	L5	1524	A2M	O4'-C4'-C5'-O5'
2	L5	2364	OMG	C3'-C4'-C5'-O5'
2	L5	2815	A2M	C3'-C4'-C5'-O5'
2	L5	3899	OMG	O4'-C4'-C5'-O5'
67	S2	668	A2M	C3'-C4'-C5'-O5'
67	S2	867	OMG	O4'-C4'-C5'-O5'
67	S2	576	A2M	O4'-C4'-C5'-O5'
67	S2	1442	OMU	C3'-C4'-C5'-O5'
67	S2	1832	6MZ	C5'-O5'-P-OP1
2	L5	1524	A2M	C3'-C4'-C5'-O5'
67	S2	99	A2M	C3'-C4'-C5'-O5'
67	S2	576	A2M	C3'-C4'-C5'-O5'
2	L5	3818	UY1	C4'-C5'-O5'-P
67	S2	627	OMU	C2'-C1'-N1-C2
67	S2	799	OMU	C3'-C4'-C5'-O5'
67	S2	1248	B8N	N34-C33-C34-O36
2	L5	2787	A2M	C2'-C1'-N9-C8
2	L5	2787	A2M	C3'-C4'-C5'-O5'
67	S2	801	PSU	O4'-C4'-C5'-O5'
67	S2	1639	G7M	O4'-C4'-C5'-O5'
67	S2	1639	G7M	C3'-C4'-C5'-O5'
67	S2	1248	B8N	C31-C32-C33-C34
2	L5	4590	A2M	C4'-C5'-O5'-P
67	S2	1851	MA6	C5-C6-N6-C10
2	L5	2422	OMC	C3'-C4'-C5'-O5'
67	S2	627	OMU	C3'-C4'-C5'-O5'
67	S2	428	OMU	O4'-C1'-N1-C6
67	S2	627	OMU	O4'-C1'-N1-C6
2	L5	3782	5MC	O4'-C4'-C5'-O5'
67	S2	428	OMU	O4'-C1'-N1-C2
67	S2	1046	PSU	O4'-C4'-C5'-O5'
67	S2	1832	6MZ	C4'-C5'-O5'-P
2	L5	4447	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	L5	1534	A2M	C4'-C5'-O5'-P
2	L5	2422	OMC	O4'-C4'-C5'-O5'
67	S2	576	A2M	C4'-C5'-O5'-P
2	L5	4447	5MC	C2'-C1'-N1-C6
2	L5	3818	UY1	O4'-C1'-C5-C4
67	S2	649	PSU	O4'-C1'-C5-C4
67	S2	866	PSU	O4'-C1'-C5-C4
2	L5	2787	A2M	C2'-C1'-N9-C4
67	S2	627	OMU	O4'-C1'-N1-C2
67	S2	1056	PSU	C3'-C4'-C5'-O5'
2	L5	1326	A2M	C4'-C5'-O5'-P
67	S2	1081	PSU	C4'-C5'-O5'-P
2	L5	3701	OMC	O4'-C1'-N1-C6
2	L5	4500	PSU	C4'-C5'-O5'-P
67	S2	1851	MA6	C4'-C5'-O5'-P
2	L5	398	A2M	O4'-C4'-C5'-O5'
2	L5	1792	PSU	O4'-C4'-C5'-O5'
67	S2	799	OMU	O4'-C4'-C5'-O5'
2	L5	3844	PSU	C4'-C5'-O5'-P
67	S2	644	OMG	C4'-C5'-O5'-P
67	S2	1490	OMG	C4'-C5'-O5'-P
2	L5	1340	OMC	C1'-C2'-O2'-CM2
67	S2	468	A2M	C1'-C2'-O2'-CM'
2	L5	3818	UY1	O4'-C1'-C5-C6
2	L5	4636	PSU	O4'-C1'-C5-C6
67	S2	649	PSU	O4'-C1'-C5-C6
67	S2	866	PSU	O4'-C1'-C5-C6
2	L5	4494	OMG	C3'-C2'-O2'-CM2
2	L5	4499	OMG	C3'-C2'-O2'-CM2
2	L5	4447	5MC	O4'-C1'-N1-C2
67	S2	1244	PSU	O4'-C4'-C5'-O5'
2	L5	3701	OMC	O4'-C1'-N1-C2
2	L5	1322	1MA	C2'-C1'-N9-C8
2	L5	2351	OMC	O4'-C4'-C5'-O5'
67	S2	1056	PSU	O4'-C4'-C5'-O5'
67	S2	1383	A2M	C3'-C4'-C5'-O5'
67	S2	867	OMG	C4'-C5'-O5'-P
2	L5	2351	OMC	C2'-C1'-N1-C6
2	L5	2363	A2M	C3'-C2'-O2'-CM'
2	L5	3785	A2M	C3'-C2'-O2'-CM'
2	L5	2632	PSU	C3'-C4'-C5'-O5'
67	S2	1383	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L5	2787	A2M	O4'-C1'-N9-C8
2	L5	2351	OMC	C2'-C1'-N1-C2
67	S2	1288	OMU	C2'-C1'-N1-C2
2	L5	1322	1MA	C2'-C1'-N9-C4

There are no ring outliers.

60 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	S2	644	OMG	1	0
2	L5	3851	PSU	1	0
2	L5	2363	A2M	1	0
2	L5	4523	A2M	2	0
67	S2	1031	A2M	4	0
67	S2	116	OMU	3	0
2	L5	4620	OMU	1	0
2	L5	4571	A2M	1	0
67	S2	159	A2M	4	0
67	S2	1391	OMC	2	0
67	S2	468	A2M	1	0
2	L5	3920	PSU	1	0
67	S2	1383	A2M	2	0
2	L5	400	A2M	1	0
2	L5	3825	A2M	1	0
67	S2	509	OMG	5	0
2	L5	2824	OMC	1	0
67	S2	627	OMU	1	0
67	S2	166	A2M	2	0
2	L5	4392	OMG	1	0
67	S2	27	A2M	3	0
2	L5	4536	OMC	1	0
2	L5	4618	OMG	1	0
2	L5	1677	PSU	1	0
2	L5	3785	A2M	1	0
67	S2	1004	PSU	2	0
4	L8	75	OMG	1	0
2	L5	1871	A2M	1	0
67	S2	1490	OMG	1	0
67	S2	1337	4AC	3	0
2	L5	3925	OMU	1	0
67	S2	517	OMC	1	0
67	S2	1639	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	S2	681	PSU	1	0
2	L5	4447	5MC	1	0
67	S2	1850	MA6	1	0
2	L5	1326	A2M	1	0
67	S2	601	OMG	2	0
2	L5	3718	A2M	3	0
2	L5	3867	A2M	3	0
67	S2	1232	PSU	1	0
67	S2	121	OMU	1	0
2	L5	4220	6MZ	2	0
2	L5	4196	OMG	1	0
2	L5	4637	OMG	1	0
2	L5	4530	UR3	1	0
2	L5	3701	OMC	1	0
2	L5	4457	PSU	1	0
2	L5	4590	A2M	1	0
67	S2	799	OMU	1	0
2	L5	4579	PSU	2	0
67	S2	649	PSU	3	0
67	S2	867	OMG	1	0
2	L5	2422	OMC	1	0
2	L5	1340	OMC	2	0
2	L5	4456	OMC	1	0
67	S2	484	A2M	1	0
2	L5	4689	PSU	1	0
67	S2	1328	OMG	1	0
2	L5	2351	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 244 ligands modelled in this entry, 225 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.86	0
85	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.87	0
87	HMT	L5	5295	-	41,43,43	0.52	0	43,66,66	0.67	1 (2%)
85	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	1.01	0
85	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.92	0
84	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.01	0
84	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	1.01	0
84	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.94	0
85	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.84	0
84	SPM	L5	5267	-	13,13,13	0.37	0	12,12,12	1.09	0
84	SPM	L5	5291	-	13,13,13	0.36	0	12,12,12	0.97	0
85	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.84	0
85	SPD	L5	5289	-	9,9,9	0.31	0	8,8,8	0.86	0
84	SPM	L5	5292	-	13,13,13	0.36	0	12,12,12	0.85	0
85	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.84	0
84	SPM	L5	5288	-	13,13,13	0.36	0	12,12,12	0.97	0
85	SPD	L5	5290	-	9,9,9	0.34	0	8,8,8	0.82	0
85	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.83	0
86	3HE	L5	5294	-	21,21,21	0.52	0	23,30,30	0.83	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
85	SPD	LN	301	-	-	3/7/7/7	-
85	SPD	L5	5286	-	-	3/7/7/7	-
87	HMT	L5	5295	-	-	0/27/74/74	0/5/5/5
85	SPD	L5	5261	-	-	0/7/7/7	-
85	SPD	L5	5284	-	-	5/7/7/7	-
84	SPM	L5	5264	-	-	6/11/11/11	-
84	SPM	L5	5259	-	-	3/11/11/11	-
84	SPM	L5	5263	-	-	4/11/11/11	-
85	SPD	L5	5285	-	-	0/7/7/7	-
84	SPM	L5	5267	-	-	3/11/11/11	-
84	SPM	L5	5291	-	-	6/11/11/11	-
85	SPD	L5	5282	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5289	-	-	2/7/7/7	-
84	SPM	L5	5292	-	-	5/11/11/11	-
85	SPD	L5	5287	-	-	1/7/7/7	-
84	SPM	L5	5288	-	-	4/11/11/11	-
85	SPD	L5	5290	-	-	4/7/7/7	-
85	SPD	L5	5283	-	-	4/7/7/7	-
86	3HE	L5	5294	-	-	4/8/36/36	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5295	HMT	C3-O4-C19	2.27	120.81	117.24

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	L5	5294	3HE	C6-C5-C7-C8
85	L5	5283	SPD	C3-C4-C5-N6
85	L5	5286	SPD	C3-C4-C5-N6
84	L5	5291	SPM	C7-C8-C9-N10
84	L5	5291	SPM	C2-C3-C4-N5
84	L5	5292	SPM	N10-C11-C12-C13
84	L5	5264	SPM	C2-C3-C4-N5
85	L5	5284	SPD	N6-C7-C8-C9
85	L5	5284	SPD	C3-C4-C5-N6
84	L5	5292	SPM	C8-C9-N10-C11
84	L5	5291	SPM	N10-C11-C12-C13
84	L5	5264	SPM	C6-C7-C8-C9
84	L5	5264	SPM	N1-C2-C3-C4
84	L5	5288	SPM	C12-C11-N10-C9
84	L5	5291	SPM	C7-C6-N5-C4
85	L5	5290	SPD	C8-C7-N6-C5
85	L5	5286	SPD	N6-C7-C8-C9
86	L5	5294	3HE	C7-C8-C9-C10
84	L5	5267	SPM	C6-C7-C8-C9
85	L5	5284	SPD	C2-C3-C4-C5
84	L5	5259	SPM	C6-C7-C8-C9
84	L5	5292	SPM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
84	L5	5263	SPM	C6-C7-C8-C9
84	L5	5288	SPM	C8-C9-N10-C11
84	L5	5263	SPM	C11-C12-C13-N14
84	L5	5288	SPM	N1-C2-C3-C4
85	L5	5283	SPD	C7-C8-C9-N10
85	L5	5290	SPD	C7-C8-C9-N10
86	L5	5294	3HE	C7-C8-C9-C13
84	L5	5259	SPM	C3-C4-N5-C6
84	L5	5288	SPM	C7-C6-N5-C4
85	L5	5290	SPD	C4-C5-N6-C7
85	L5	5282	SPD	C2-C3-C4-C5
85	LN	301	SPD	C3-C4-C5-N6
85	L5	5289	SPD	C2-C3-C4-C5
84	L5	5292	SPM	C11-C12-C13-N14
85	L5	5284	SPD	C7-C8-C9-N10
85	L5	5286	SPD	C8-C7-N6-C5
84	L5	5291	SPM	C6-C7-C8-C9
85	L5	5283	SPD	N1-C2-C3-C4
84	L5	5264	SPM	C8-C9-N10-C11
84	L5	5292	SPM	C7-C6-N5-C4
84	L5	5259	SPM	N5-C6-C7-C8
84	L5	5267	SPM	C2-C3-C4-N5
85	L5	5290	SPD	N1-C2-C3-C4
85	L5	5283	SPD	C8-C7-N6-C5
85	L5	5287	SPD	C8-C7-N6-C5
85	LN	301	SPD	C4-C5-N6-C7
84	L5	5263	SPM	C3-C4-N5-C6
84	L5	5267	SPM	N10-C11-C12-C13
86	L5	5294	3HE	C4-C5-C7-O3
85	LN	301	SPD	C2-C3-C4-C5
85	L5	5284	SPD	C4-C5-N6-C7
84	L5	5264	SPM	N5-C6-C7-C8
84	L5	5263	SPM	N1-C2-C3-C4
84	L5	5291	SPM	C8-C9-N10-C11
85	L5	5289	SPD	C7-C8-C9-N10
84	L5	5264	SPM	C7-C8-C9-N10

There are no ring outliers.

4 monomers are involved in 6 short contacts:

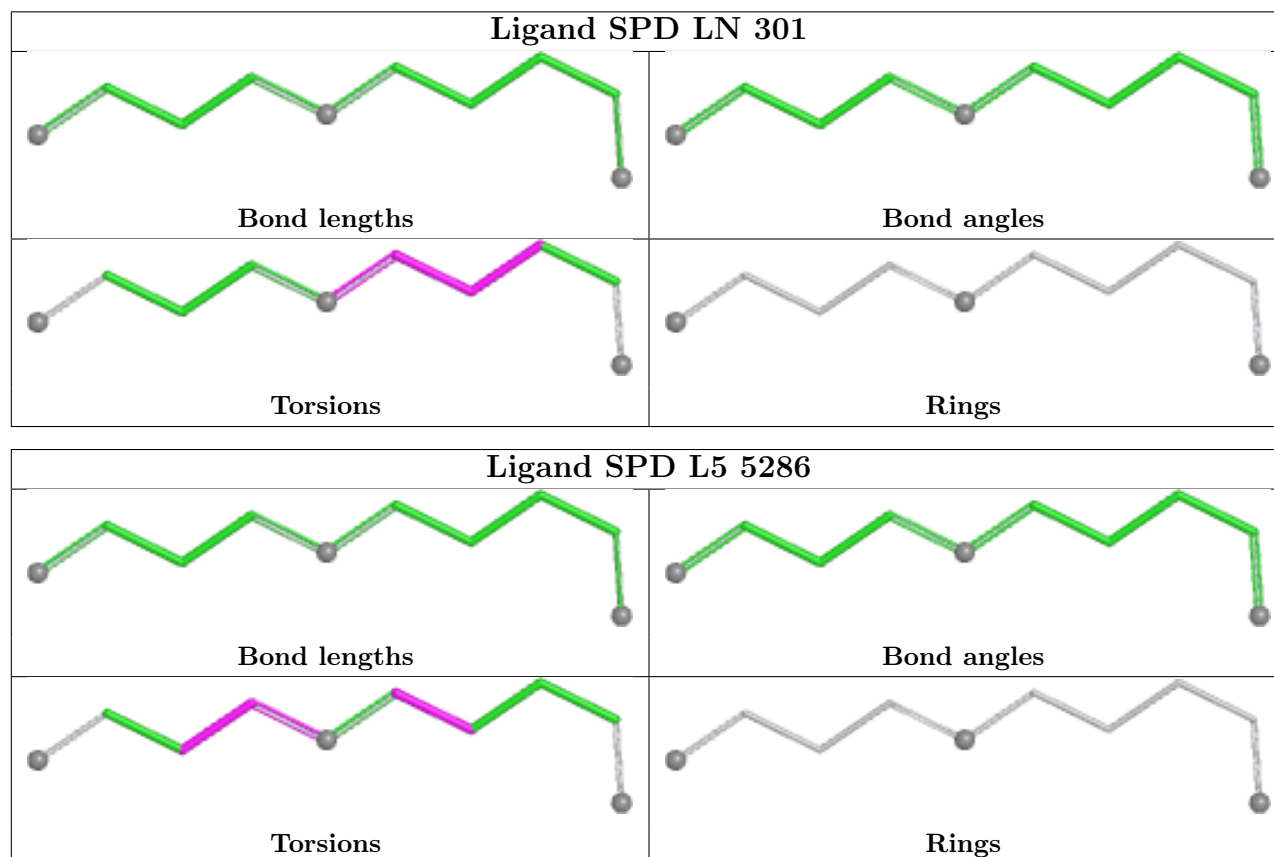
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5295	HMT	1	0

Continued on next page...

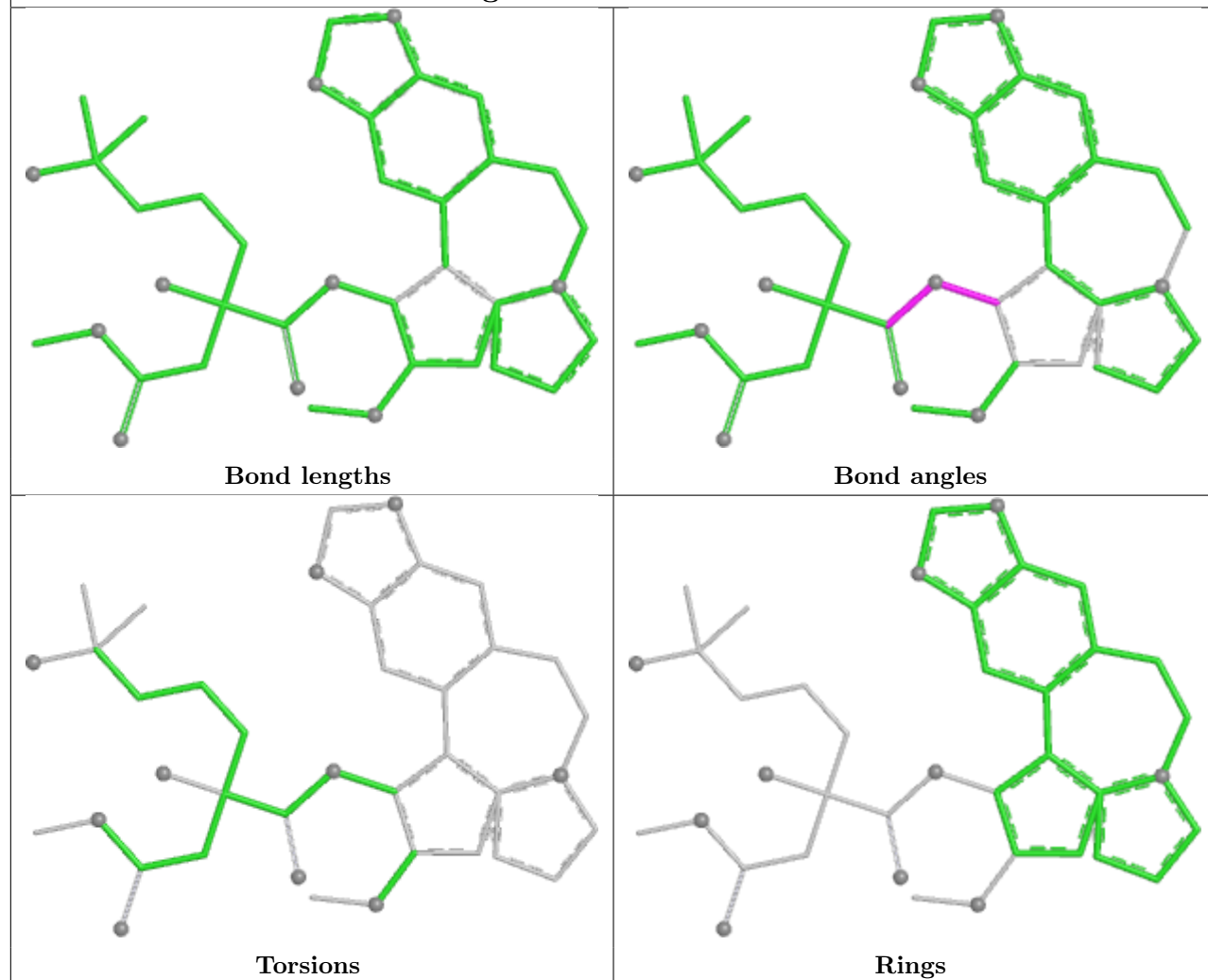
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	L5	5264	SPM	1	0
85	L5	5285	SPD	1	0
84	L5	5292	SPM	3	0

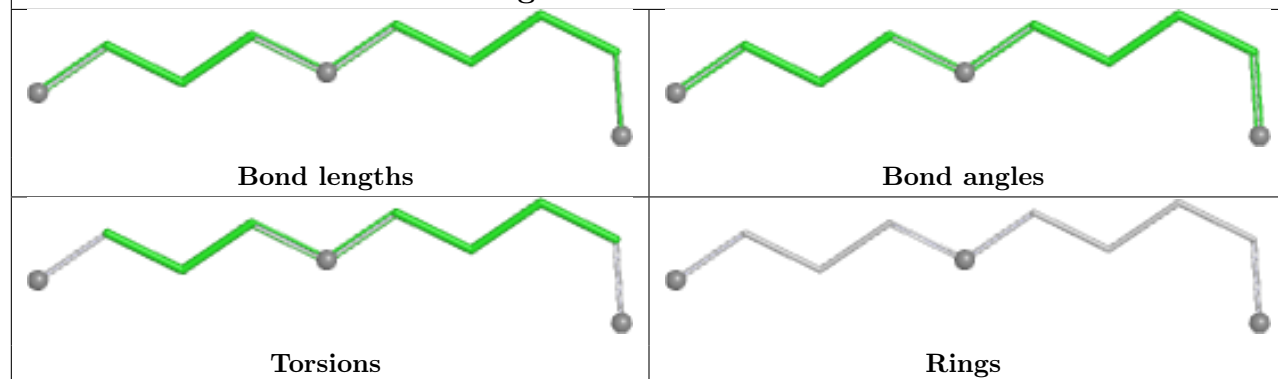
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

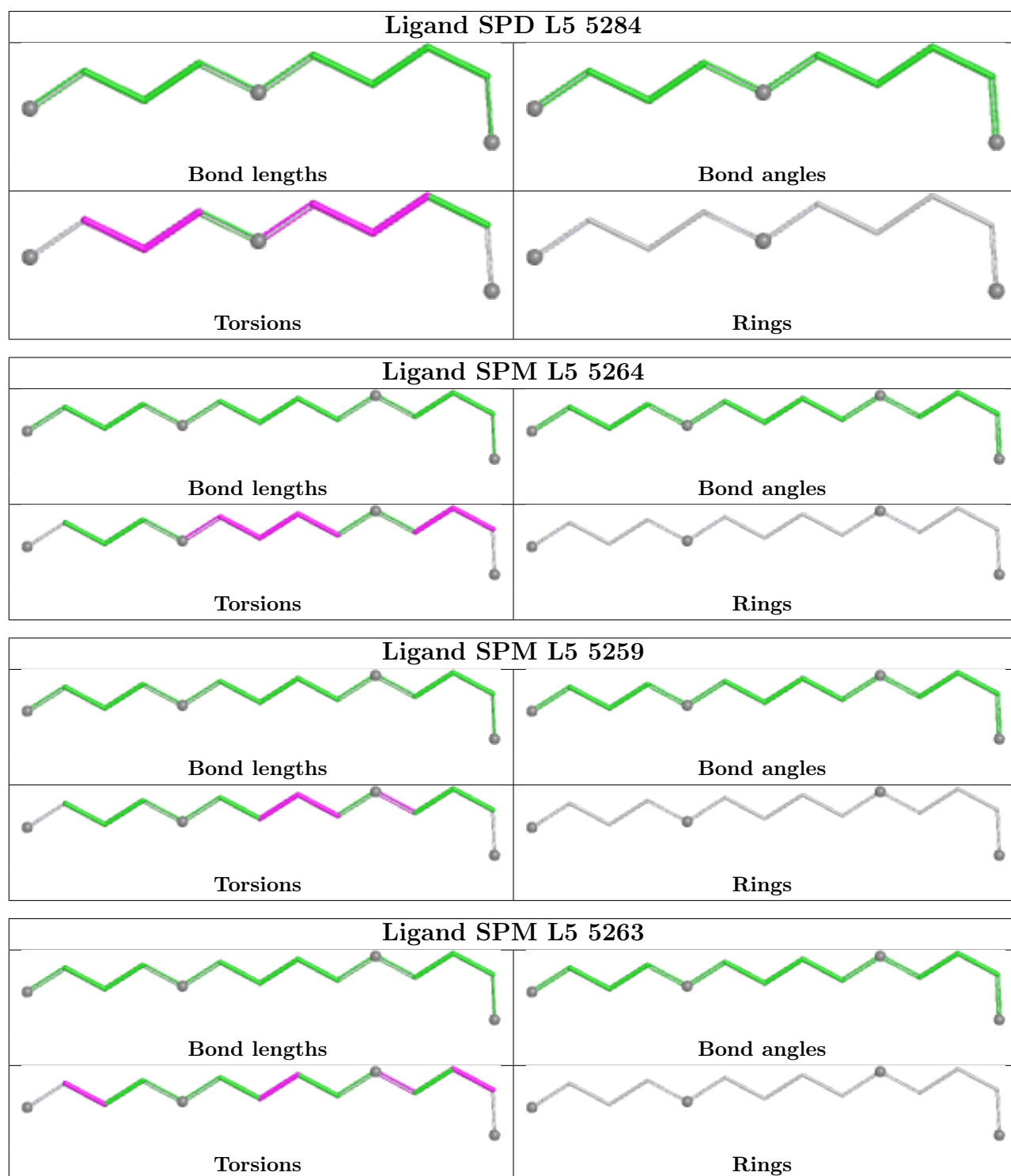


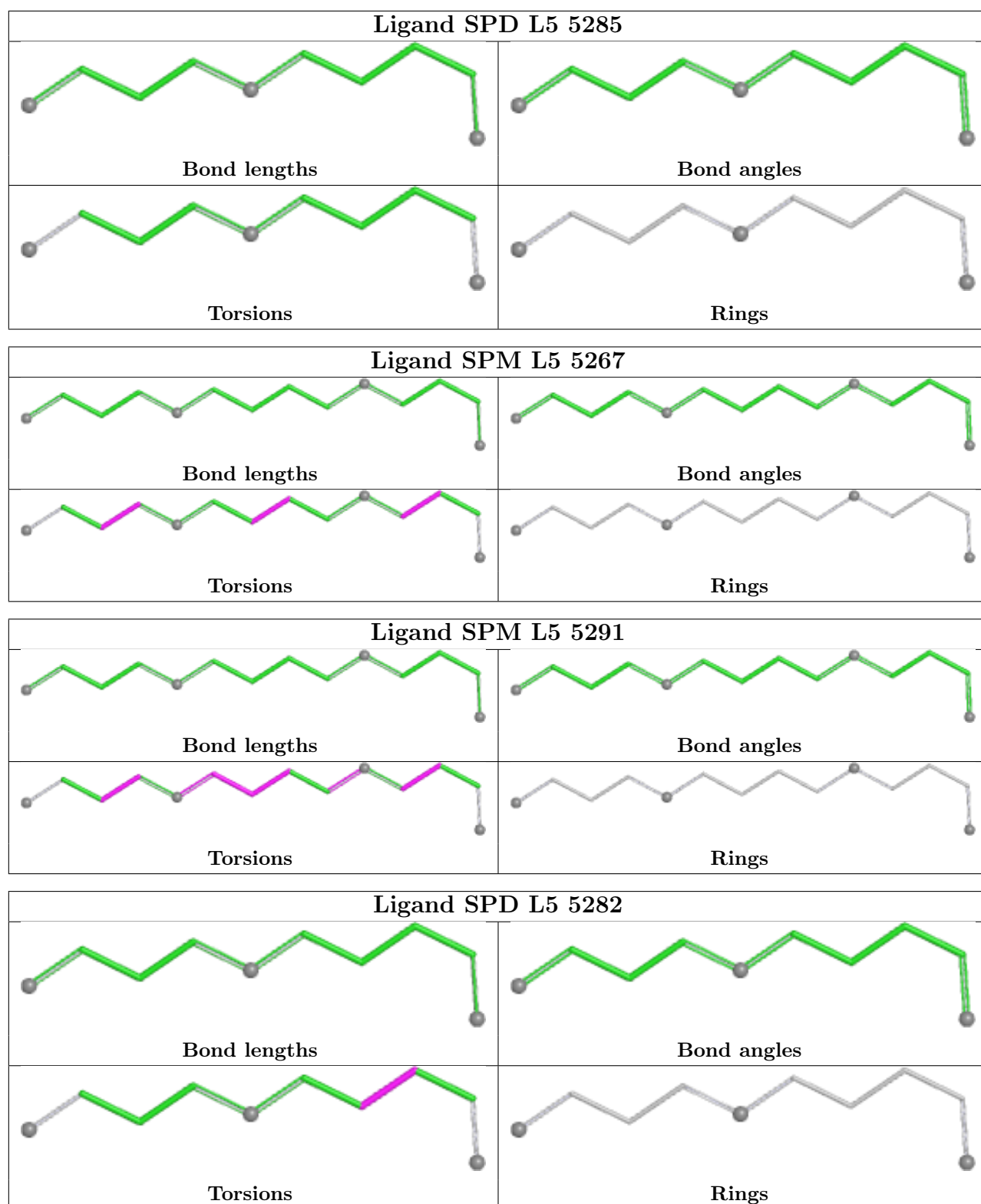
Ligand HMT L5 5295

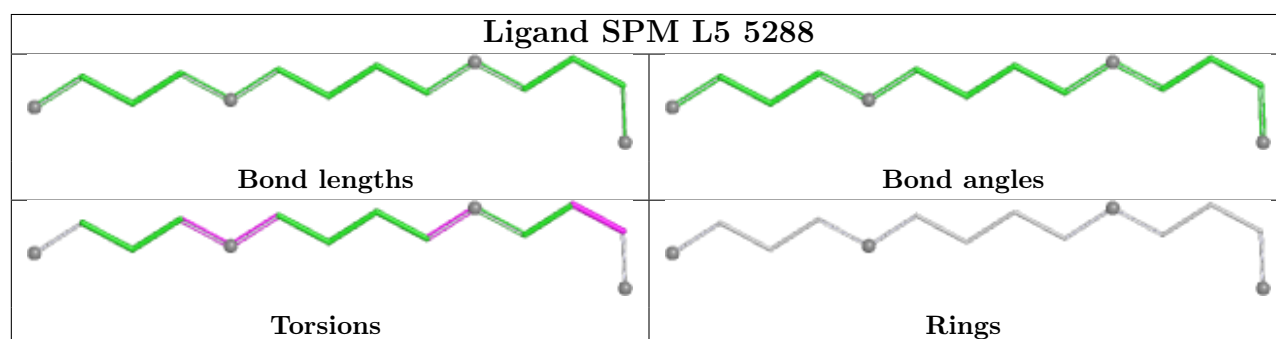
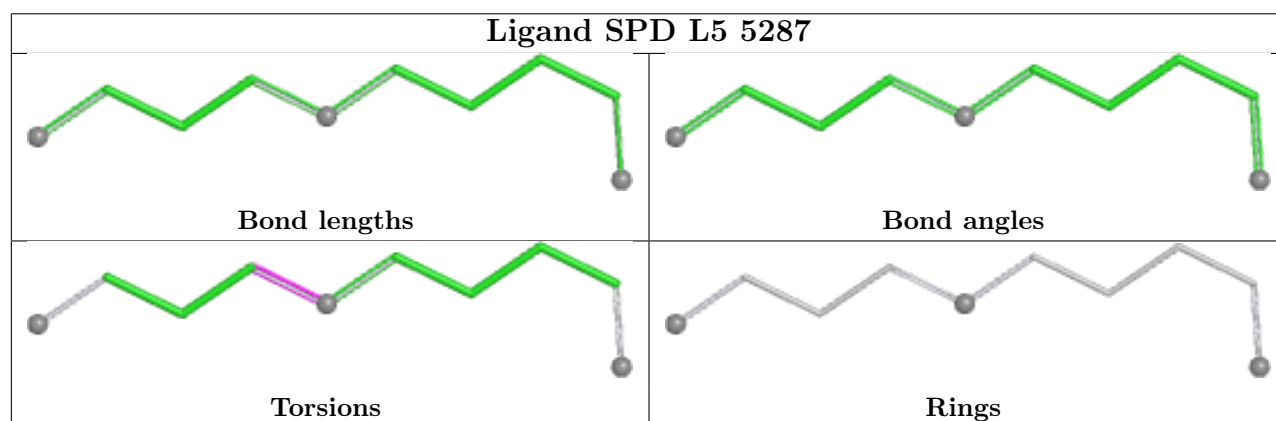
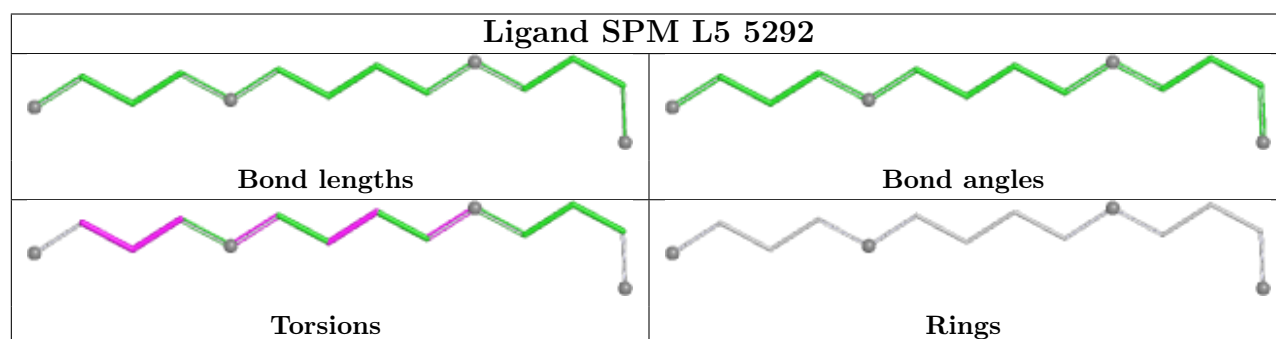
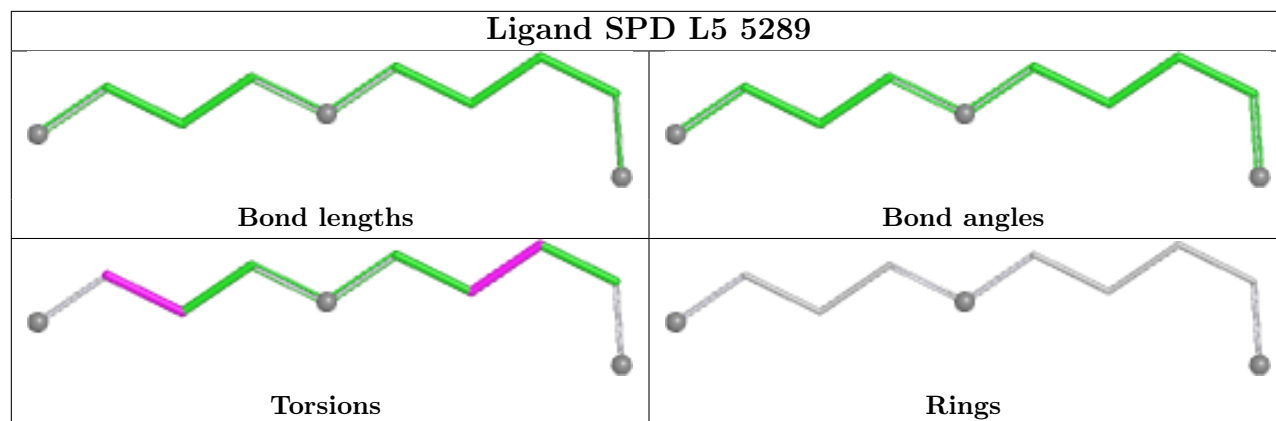


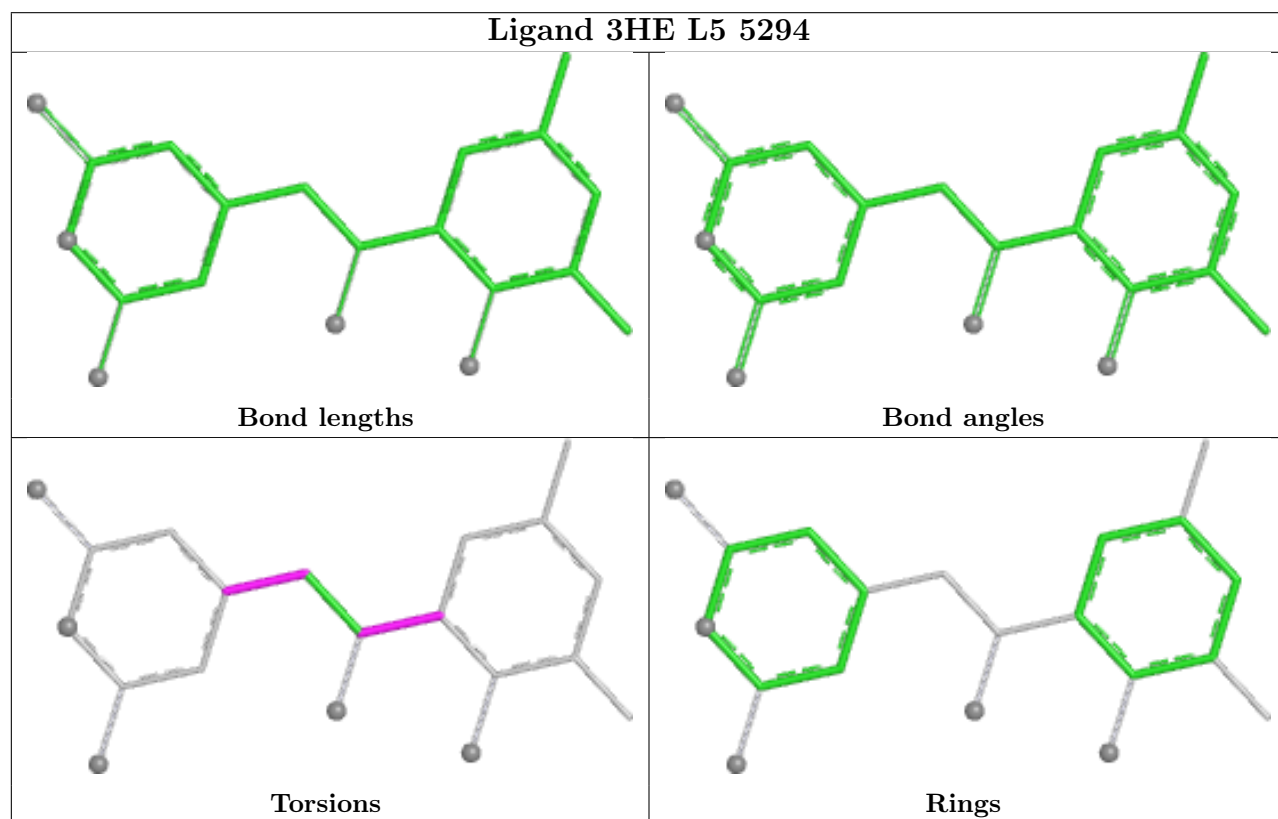
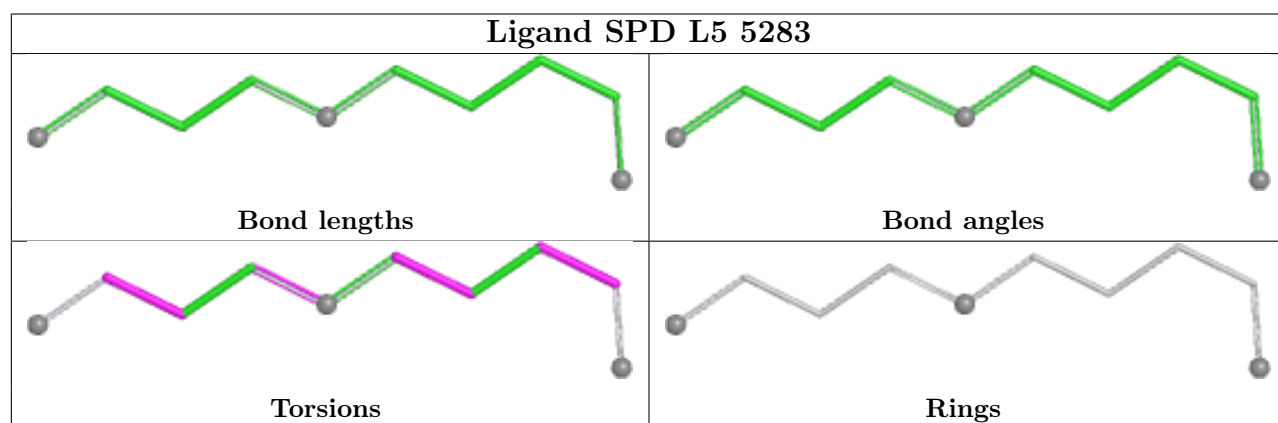
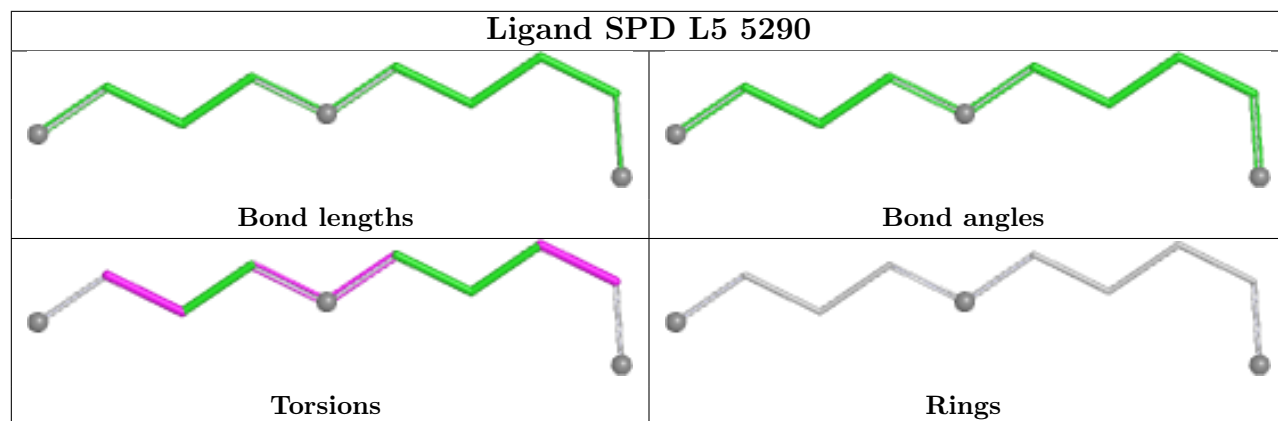
Ligand SPD L5 5261











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L5	12
67	S2	6
21	LR	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.26
1	L5	3921:U	O3'	3922[A]:G	P	26.93
1	L5	3922[A]:G	O3'	3923:A	P	26.05
1	L5	2910:G	O3'	3584:C	P	21.20
1	L5	1706:A	O3'	1716:G	P	20.85
1	L5	760:G	O3'	903:C	P	17.32
1	L5	519:C	O3'	642:G	P	15.61
1	L5	4776:G	O3'	4858:C	P	15.45
1	L5	2112:G	O3'	2249:C	P	15.01
1	S2	698:G	O3'	730:C	P	13.72
1	L5	3954:A	O3'	4056:A	P	13.14
1	S2	739:C	O3'	746:C	P	12.95
1	L5	990:C	O3'	1064:G	P	12.94
1	L5	1222:A	O3'	1234:G	P	9.70
1	S2	225:G	O3'	287:U	P	7.11
1	L5	1100:U	O3'	1167:C	P	6.98
1	S2	1210:G	O3'	1211:G	P	4.41
1	LR	134:ASN	C	135:LYS	N	4.36
1	S2	1831:A	O3'	1832:6MZ	P	3.23

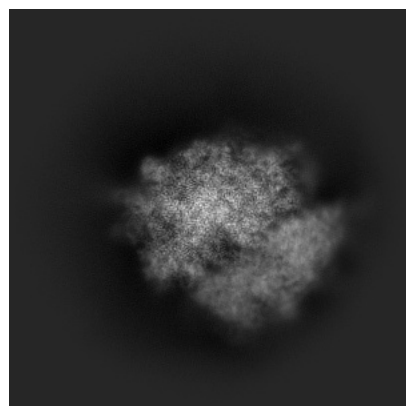
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71694. These allow visual inspection of the internal detail of the map and identification of artifacts.

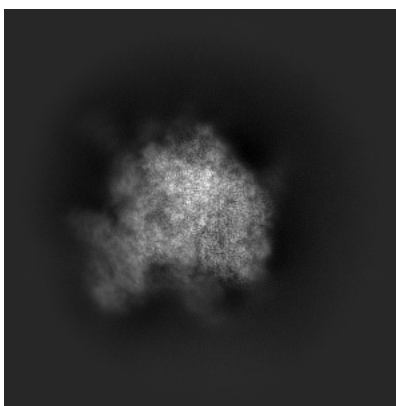
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

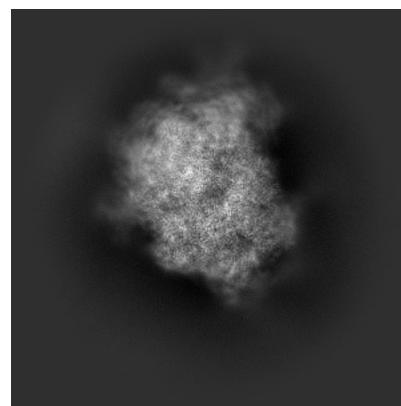
6.1.1 Primary map



X

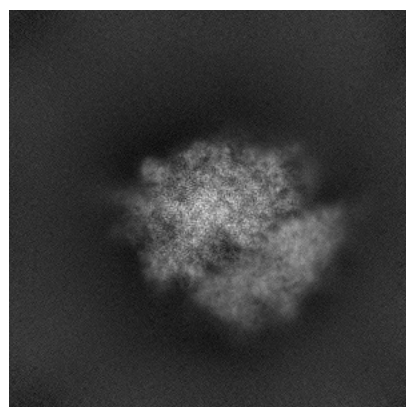


Y

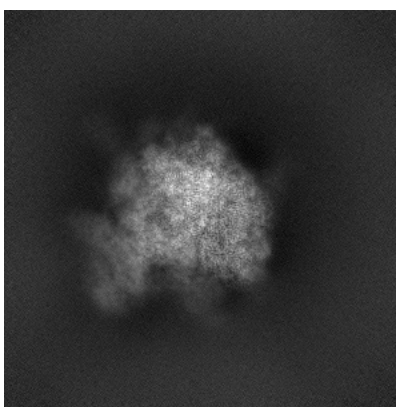


Z

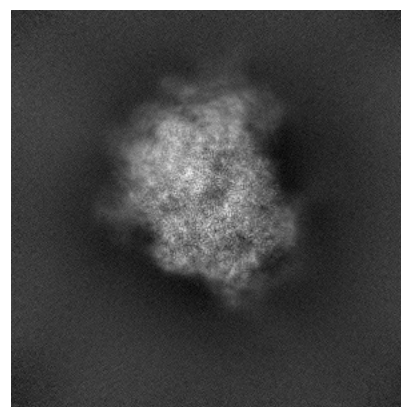
6.1.2 Raw map



X



Y

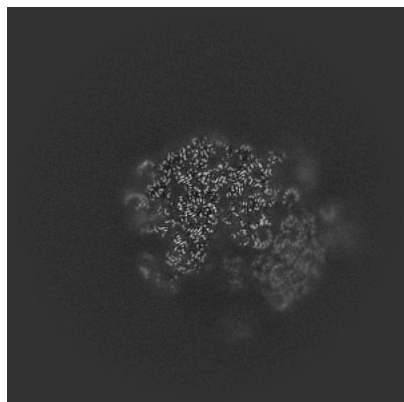


Z

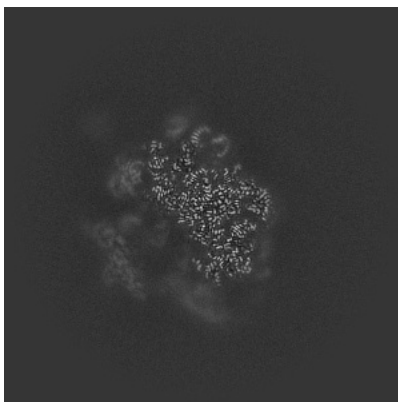
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

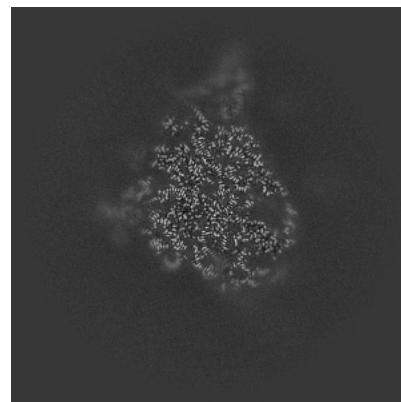
6.2.1 Primary map



X Index: 288

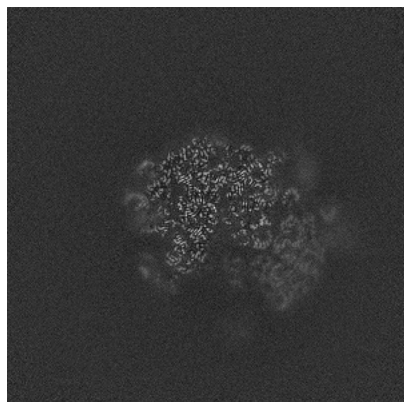


Y Index: 288

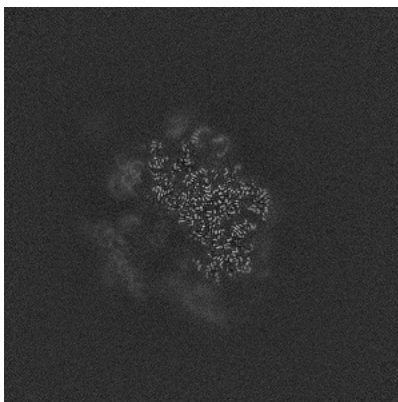


Z Index: 288

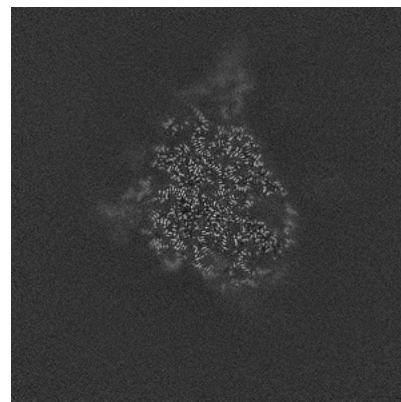
6.2.2 Raw map



X Index: 288



Y Index: 288

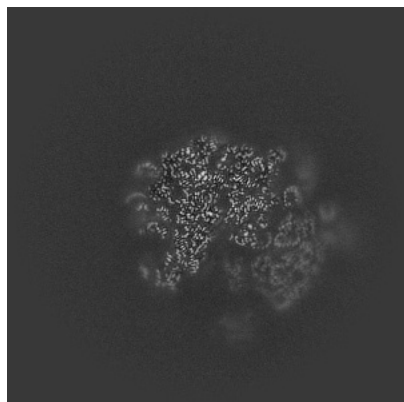


Z Index: 288

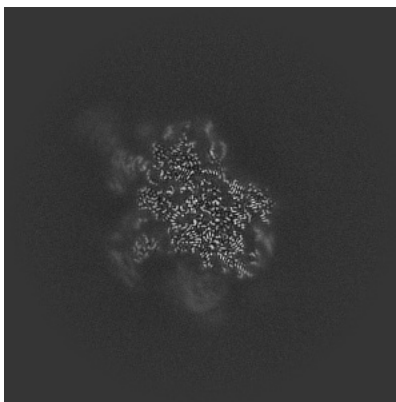
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

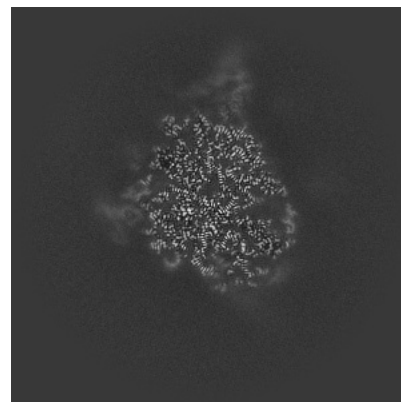
6.3.1 Primary map



X Index: 285

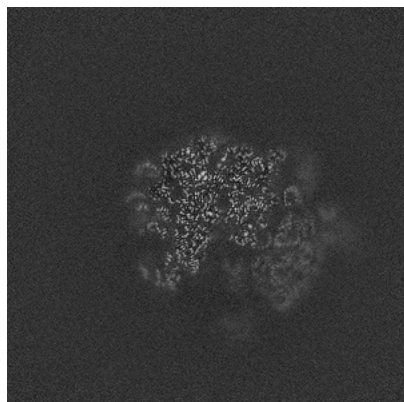


Y Index: 272

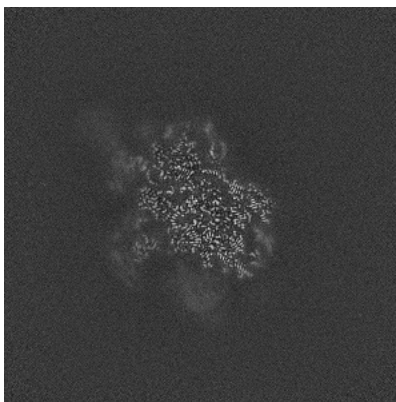


Z Index: 290

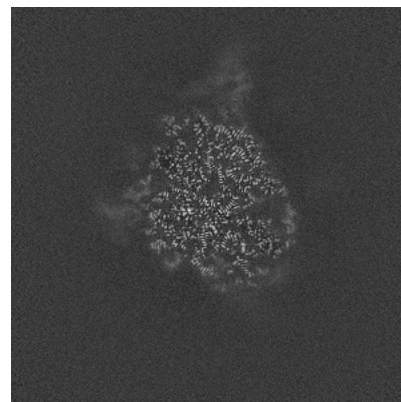
6.3.2 Raw map



X Index: 285



Y Index: 272

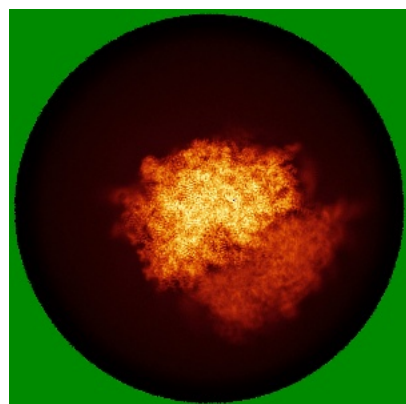


Z Index: 290

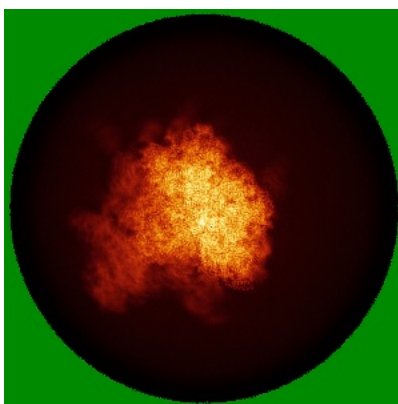
The images above show the largest variance slices of the map in three orthogonal directions.

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

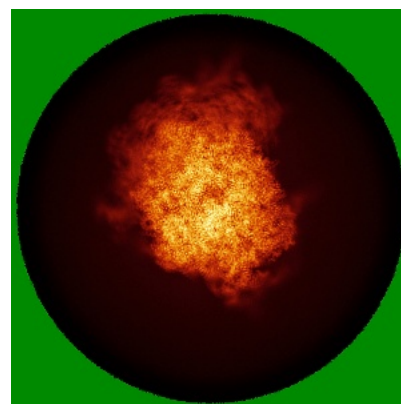
6.4.1 Primary map



X

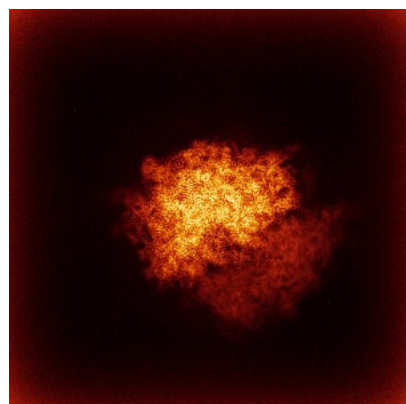


Y

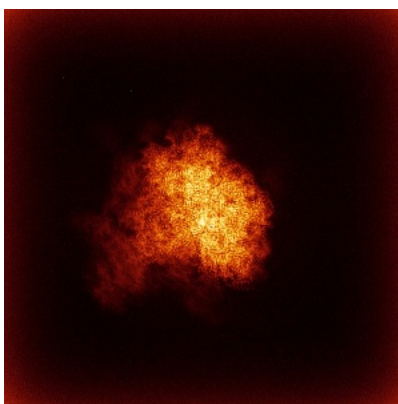


Z

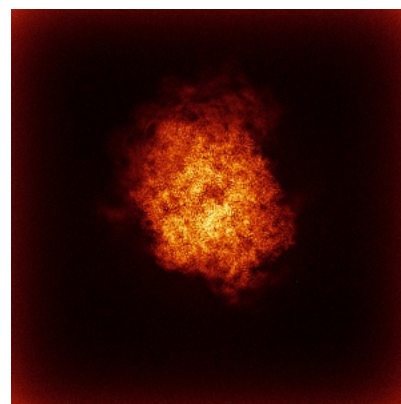
6.4.2 Raw map



X



Y

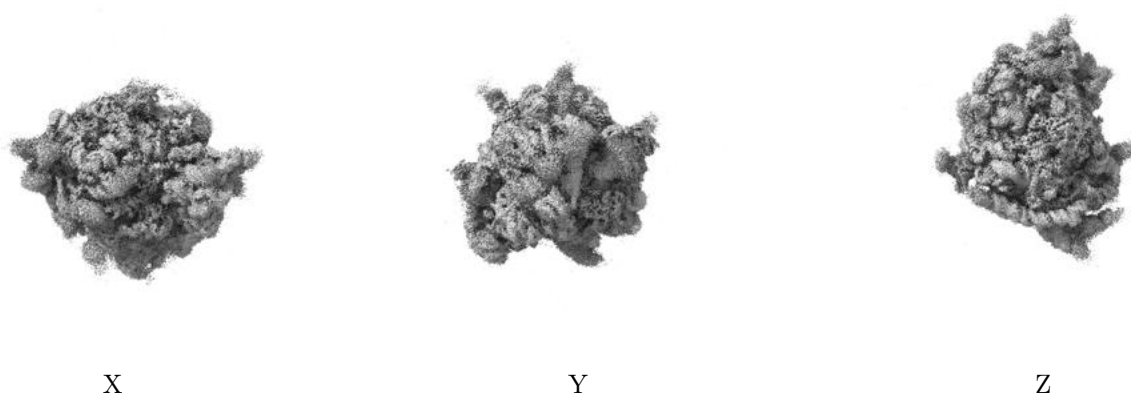


Z

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.

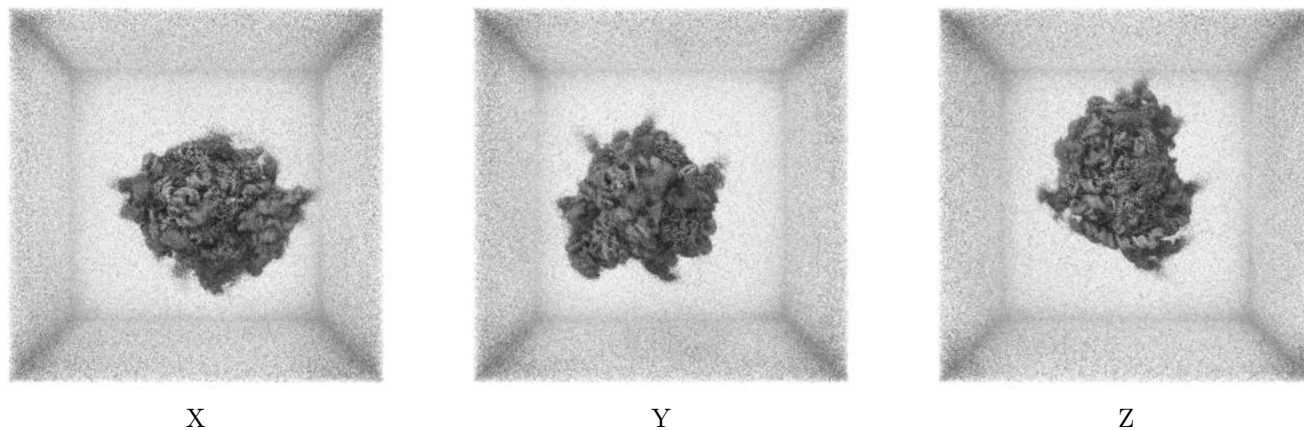
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0121. 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.

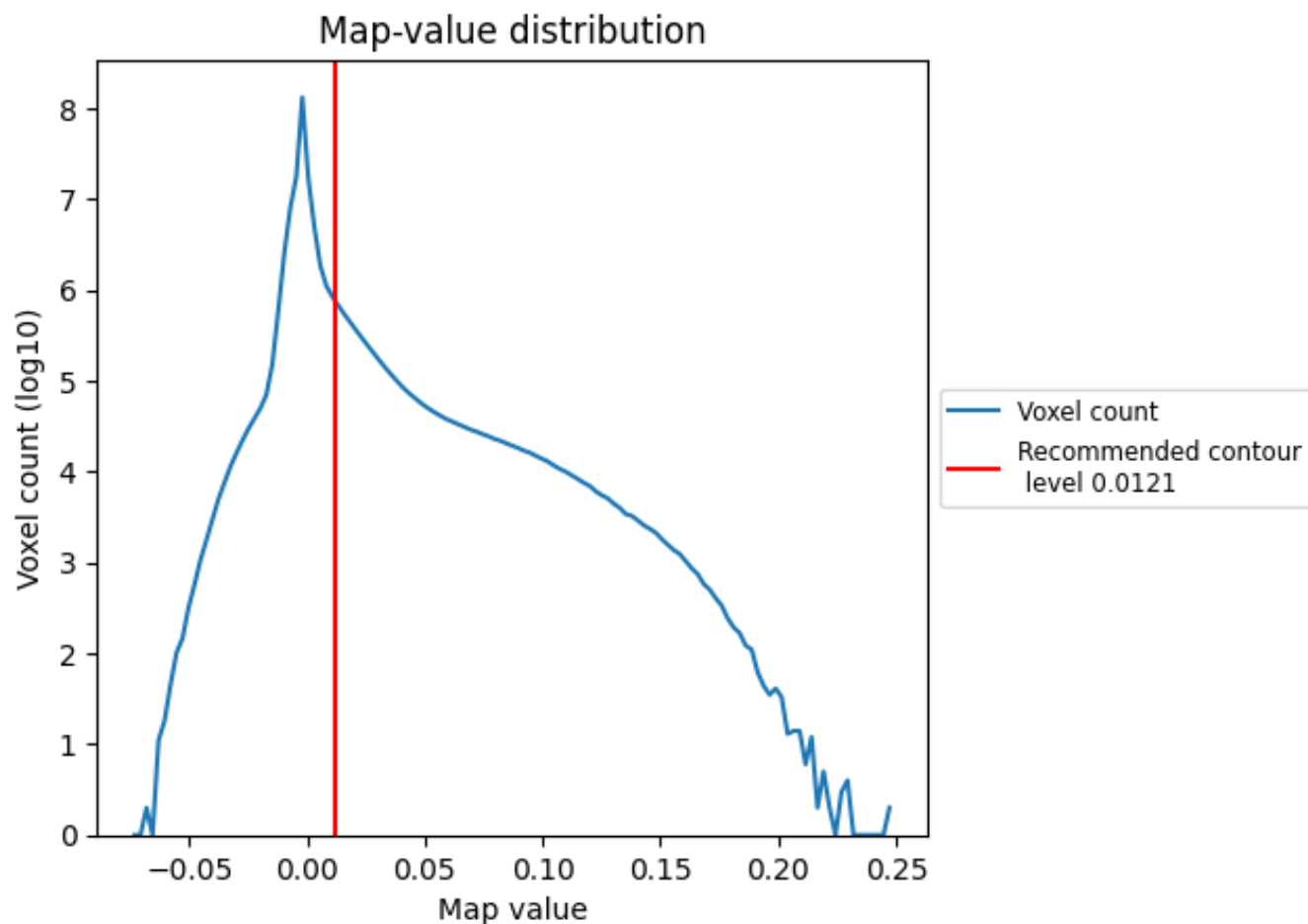
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

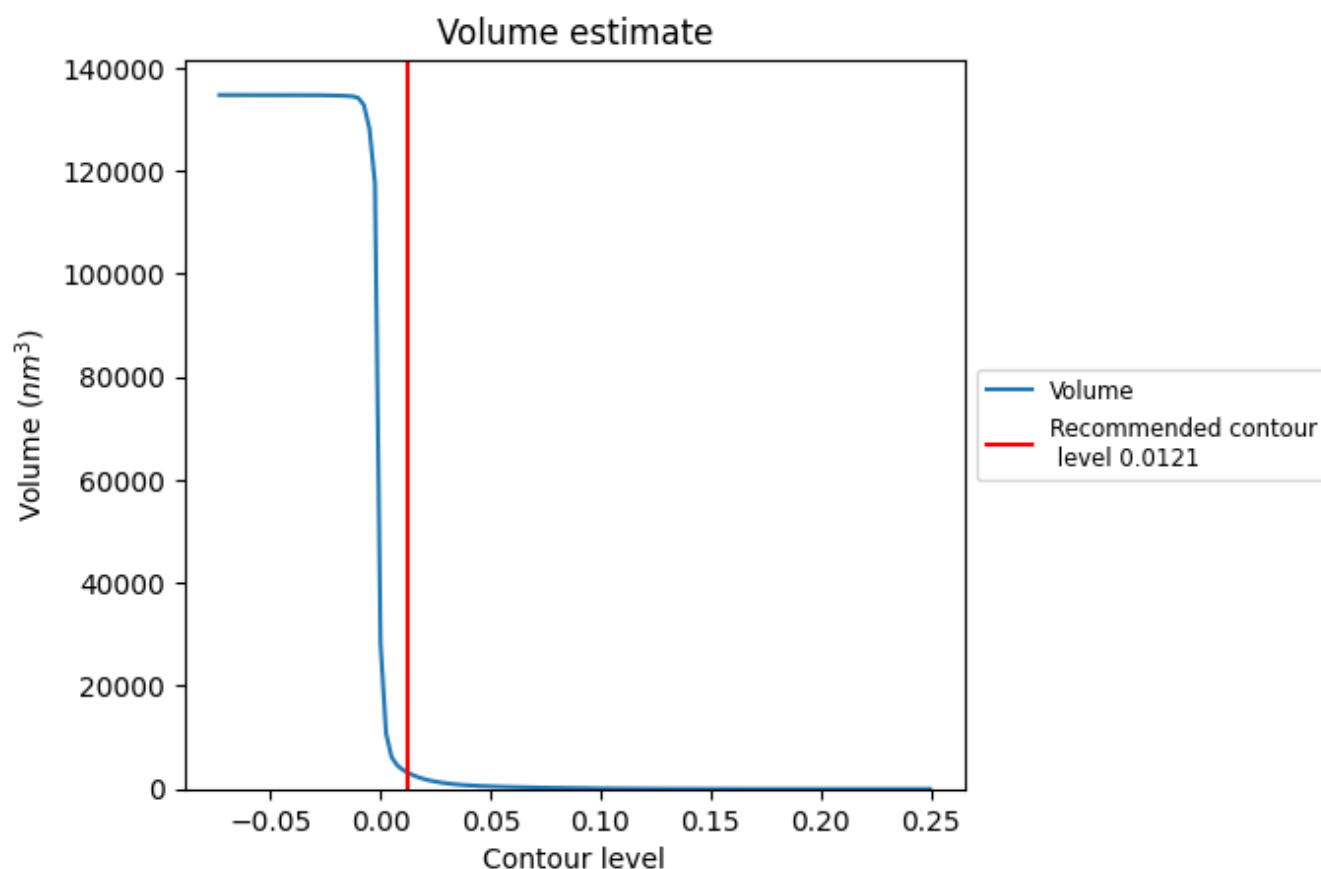
This section contains the results of statistical analysis of the map.

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.

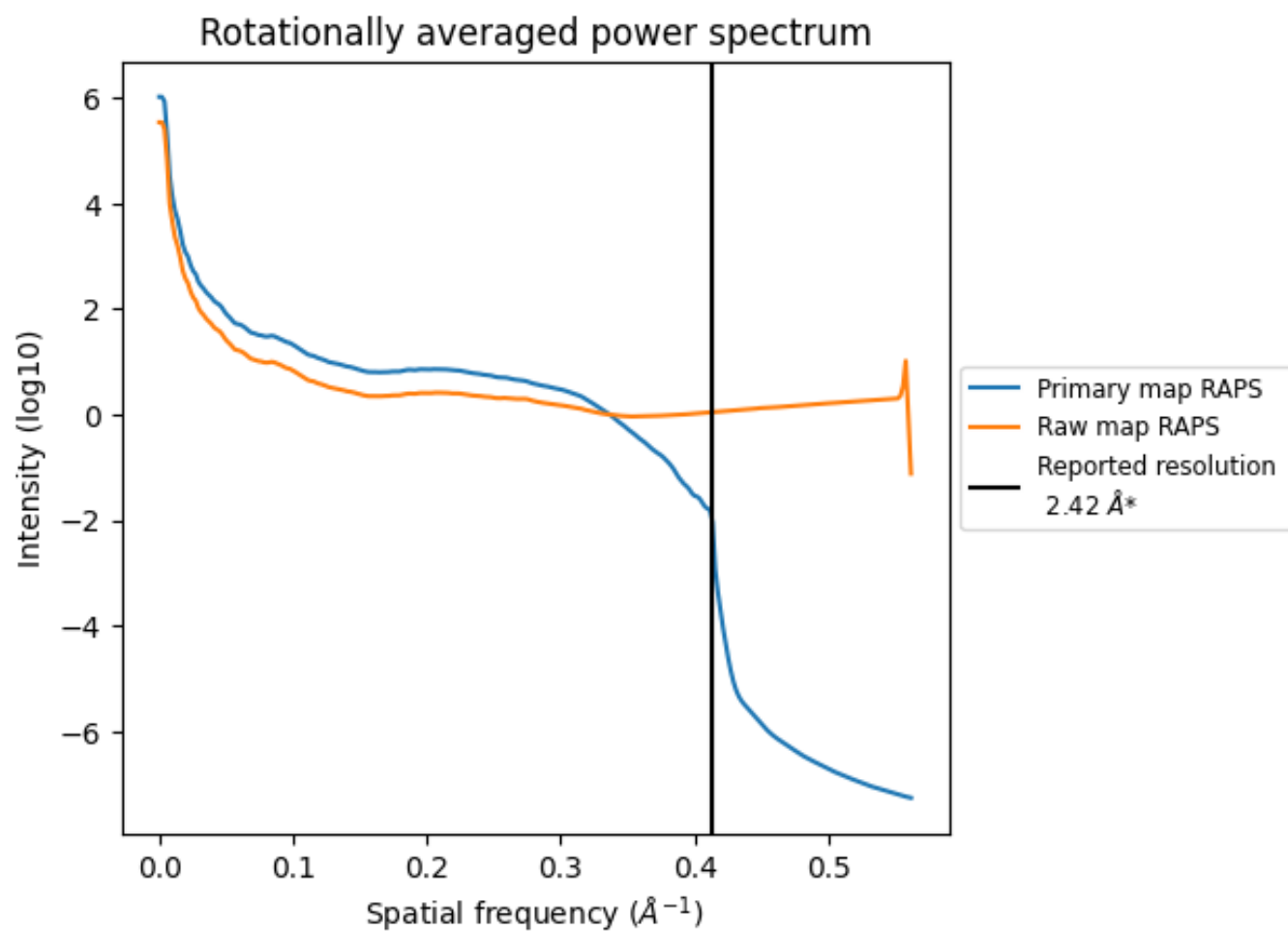
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3242 nm³; this corresponds to an approximate mass of 2929 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 ⓘ

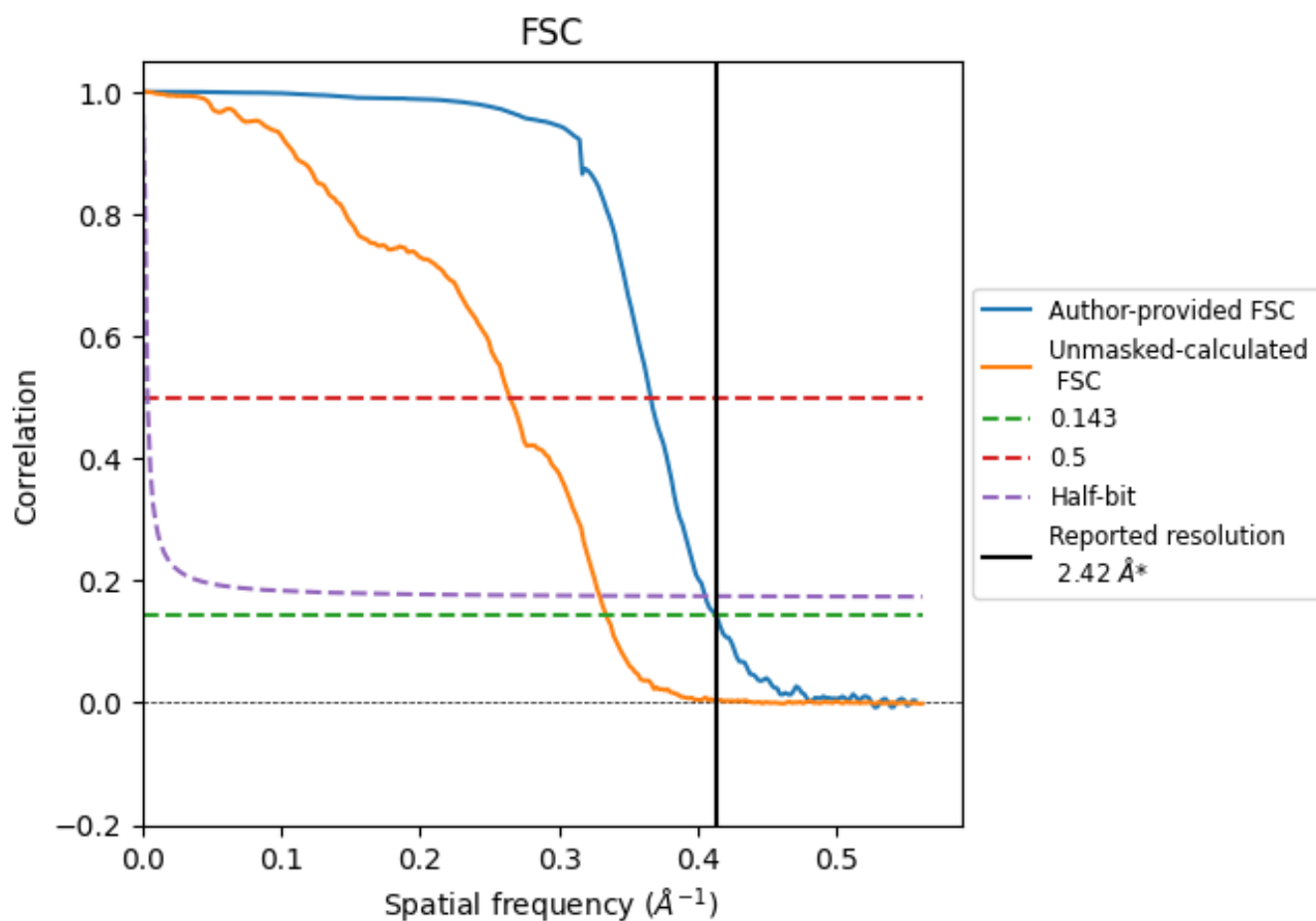


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

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 0.413 $\text{\AA}^{-1}$

8.2 Resolution estimates

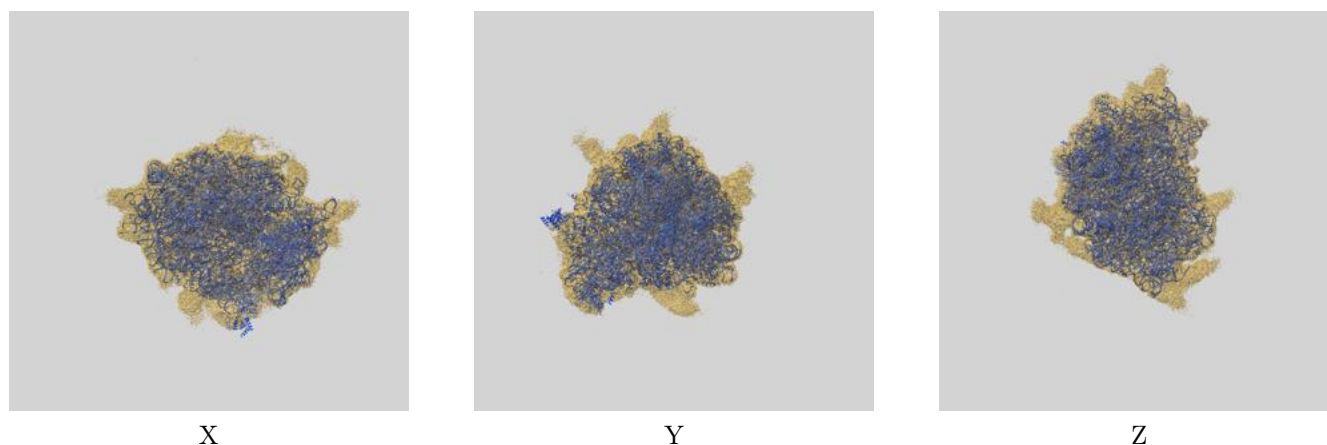
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.73	2.47
Unmasked-calculated*	2.99	3.78	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

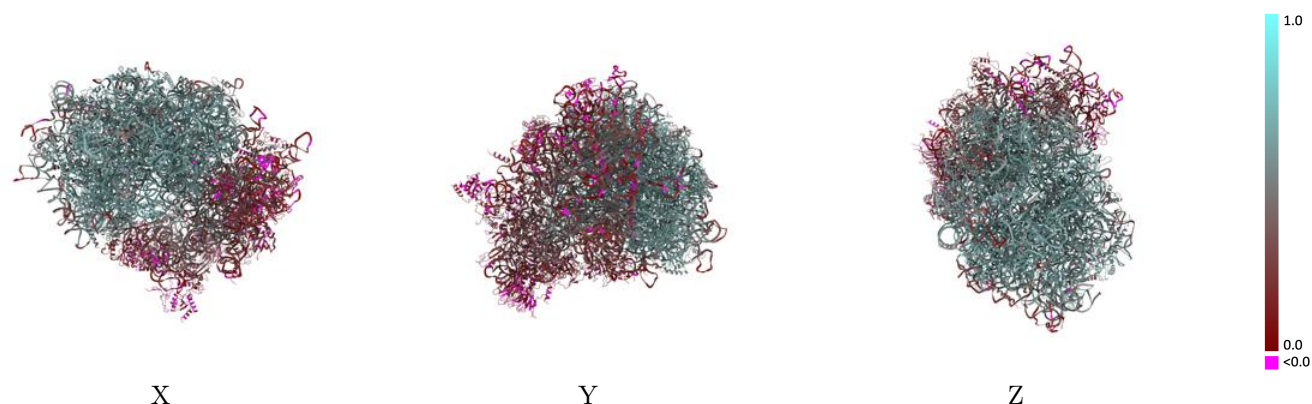
This section contains information regarding the fit between EMDB map EMD-71694 and PDB model 9PKD. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



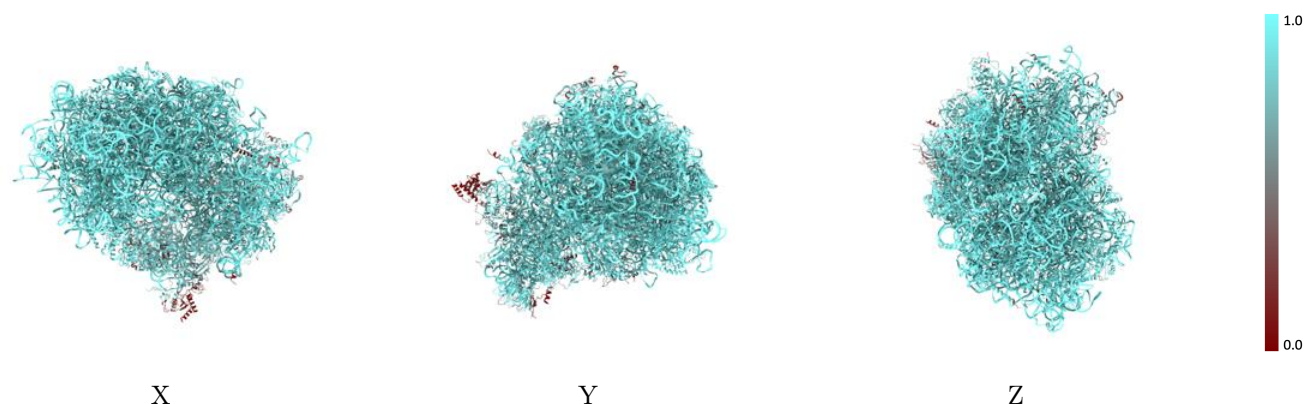
The images above show the 3D surface view of the map at the recommended contour level 0.0121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



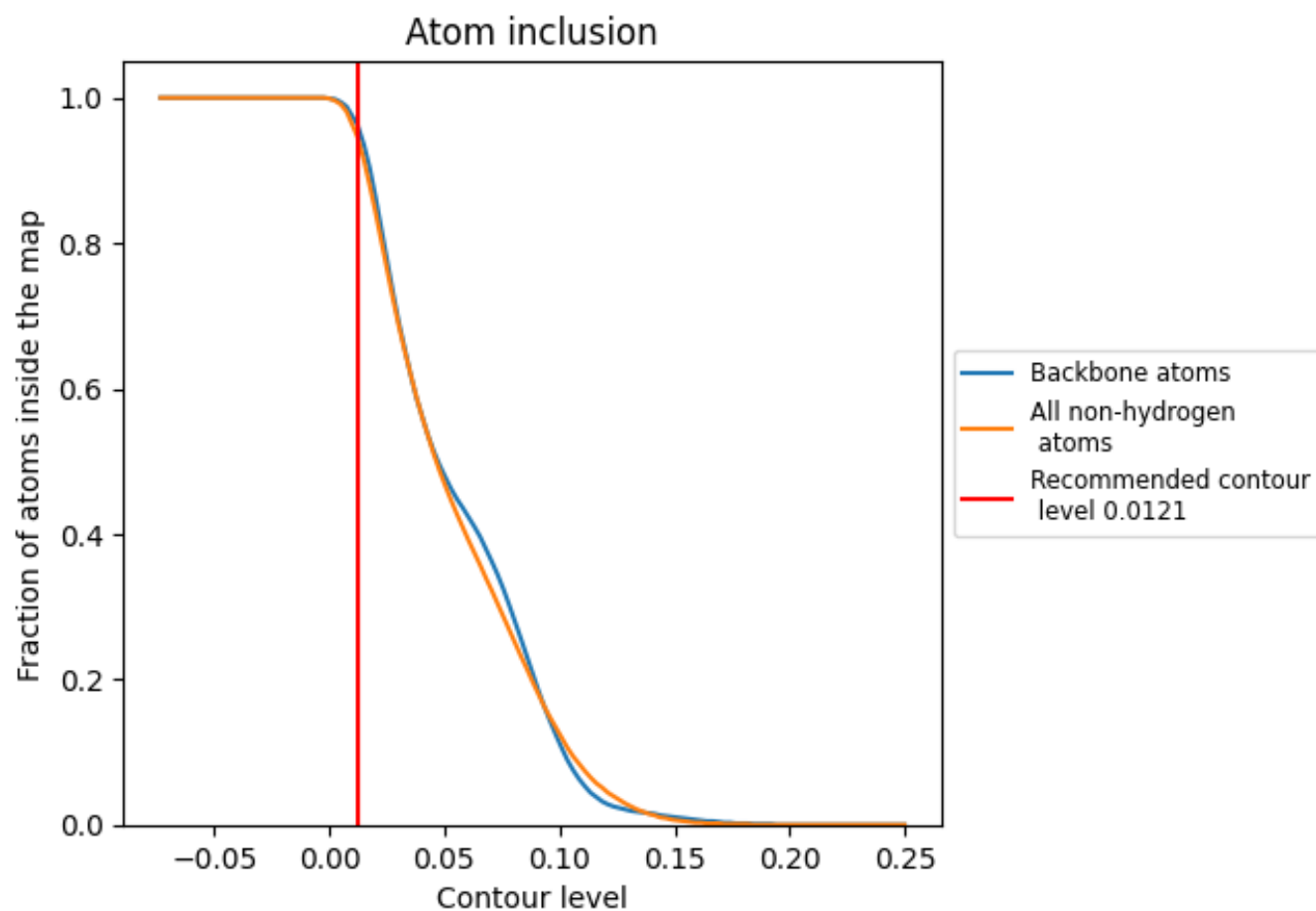
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0121).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.0121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.4670
CI	 0.8450	 0.4780
L5	 0.9910	 0.5720
L7	 0.9990	 0.6220
L8	 0.9940	 0.5970
LA	 0.9900	 0.6300
LB	 0.9700	 0.6130
LC	 0.9750	 0.6150
LD	 0.9740	 0.5750
LE	 0.9600	 0.5510
LF	 0.9860	 0.6220
LG	 0.9420	 0.5510
LH	 0.9780	 0.6000
LI	 0.9540	 0.6020
LJ	 0.9480	 0.5350
LL	 0.9470	 0.5880
LM	 0.9770	 0.5950
LN	 0.9960	 0.6480
LO	 0.9770	 0.6200
LP	 0.9820	 0.6280
LQ	 0.9870	 0.6390
LR	 0.8560	 0.4710
LS	 0.9910	 0.6370
LT	 0.9700	 0.6010
LU	 0.9650	 0.5190
LV	 0.9830	 0.6260
LW	 0.8090	 0.3530
LX	 0.9700	 0.5960
LY	 0.9810	 0.6010
LZ	 0.9820	 0.5890
La	 0.9860	 0.6380
Lb	 0.9340	 0.5360
Lc	 0.9590	 0.5730
Ld	 0.9760	 0.5960
Le	 0.9860	 0.6310



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Chain	Atom inclusion	Q-score
Lf	 0.9910	 0.6430
Lg	 0.9770	 0.6060
Lh	 0.9690	 0.5910
Li	 0.9720	 0.5920
Lj	 0.9910	 0.6360
Lk	 0.9390	 0.5410
Ll	 0.9860	 0.6110
Lm	 0.9710	 0.6100
Ln	 0.9670	 0.5760
Lo	 0.9690	 0.6110
Lp	 0.9700	 0.6120
Lr	 0.9860	 0.6210
Ls	 0.8250	 0.2460
Lt	 0.5890	 0.0920
S2	 0.9740	 0.3110
SA	 0.8580	 0.2770
SB	 0.8060	 0.2350
SC	 0.9060	 0.3520
SD	 0.7900	 0.2240
SE	 0.8930	 0.2160
SF	 0.7670	 0.1720
SG	 0.7880	 0.1060
SH	 0.8460	 0.2520
SI	 0.8830	 0.3260
SJ	 0.8790	 0.2710
SK	 0.7030	 0.1780
SL	 0.8700	 0.3580
SM	 0.1700	 0.0590
SN	 0.9100	 0.3620
SO	 0.8490	 0.2250
SP	 0.7560	 0.1180
SQ	 0.8930	 0.1810
SR	 0.8200	 0.1840
SS	 0.7440	 0.1380
ST	 0.8220	 0.1690
SU	 0.8770	 0.2660
SV	 0.9100	 0.3090
SW	 0.9420	 0.4030
SX	 0.8680	 0.3790
SY	 0.8110	 0.1160
SZ	 0.7000	 0.1110
Sa	 0.8680	 0.3030

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Chain	Atom inclusion	Q-score
Sb	 0.8810	 0.2990
Sc	 0.7610	 0.1830
Sd	 0.9120	 0.2900
Se	 0.7700	 0.1900
Sf	 0.7000	 0.0760
Sg	 0.7580	 0.1020