



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 09:35 AM EDT

PDB ID : 9P7F / pdb_00009p7f
EMDB ID : EMD-71340
Title : In situ HHT and CHX treated A-P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

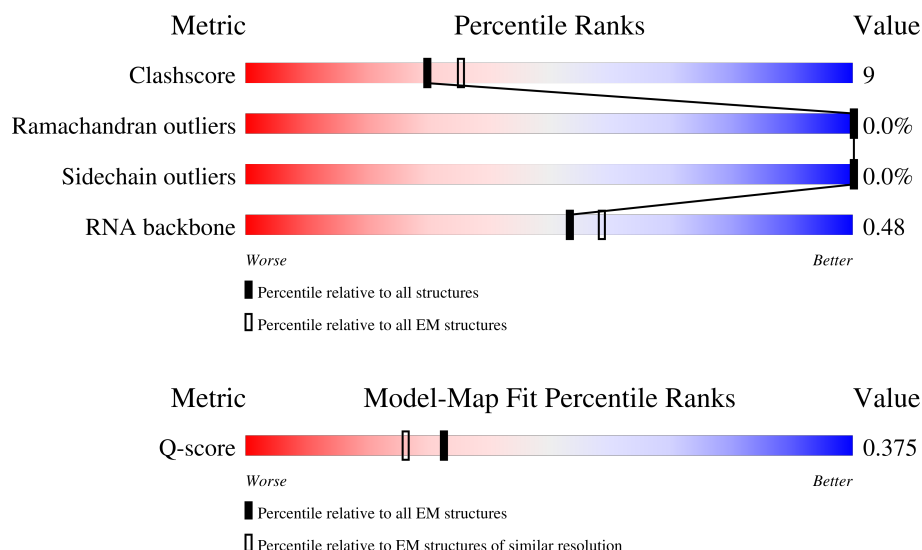
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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	12750 (3.06 - 4.06)

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	SA	221	
2	SB	214	
3	SC	222	

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Mol	Chain	Length	Quality of chain
4	SE	262	
5	SG	237	
6	SH	189	
7	SI	206	
8	SJ	185	
9	SL	153	
10	SN	150	
11	SO	140	
12	SV	83	
13	SW	129	
14	SX	141	
15	SY	131	
16	Sa	102	
17	Sb	83	
18	Se	58	
19	S2	1740	
20	LR	187	
21	LW	124	
22	SR	135	
23	SD	227	
24	SF	189	
25	SK	98	
26	SM	122	
27	SP	121	
28	SQ	144	

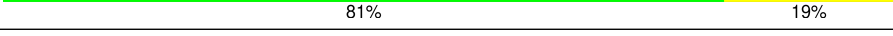
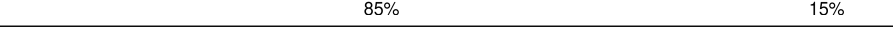
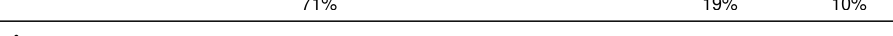
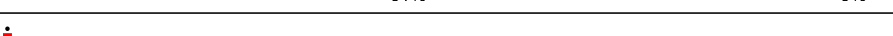
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Mol	Chain	Length	Quality of chain
29	SS	145	
30	ST	143	
31	SU	104	
32	SZ	75	
33	Sc	64	
34	Sd	55	
35	Sf	67	
36	Sg	313	
37	At	71	
38	Pt	74	
39	CI	31	
40	L5	3655	
41	L7	120	
42	L8	156	
43	LA	248	
44	LB	402	
45	LC	368	
46	LD	293	
47	LE	250	
48	LF	225	
49	LG	241	
50	LH	190	
51	LI	213	
52	LJ	176	
53	LL	210	

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Mol	Chain	Length	Quality of chain
54	LM	139	 83%17%
55	LN	203	 85%15%
56	LO	201	 84%16%
57	LP	153	 78%22%
58	LQ	187	 83%17%
59	LS	175	 86%14%
60	LT	159	 85%15%
61	LU	101	 84%16%
62	LV	131	 81%19%
63	LX	120	 88%12%
64	LY	134	 85%15%
65	LZ	135	 84%16%
66	La	147	 87%13%
67	Lb	121	 71%19%10%
68	Lc	98	 85%15%
69	Ld	107	 83%17%
70	Le	128	 91%9%
71	Lf	109	 81%19%
72	Lg	114	 91%9%
73	Lh	122	 83%17%
74	Li	102	 90%10%
75	Lj	86	 84%16%
76	Lk	69	 80%20%
77	Ll	50	 80%20%
78	Lm	52	 83%17%

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Mol	Chain	Length	Quality of chain
79	Ln	24	
80	Lo	105	
81	Lp	91	
82	Lr	125	
83	Ls	196	
84	Lt	157	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 219950 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 40S ribosomal protein SA.

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

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

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

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 5 is a protein called 40S ribosomal protein S6.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 7 is a protein called 40S ribosomal protein S8.

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

- Molecule 8 is a protein called 40S ribosomal protein S9.

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

- Molecule 9 is a protein called 40S ribosomal protein S11.

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

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 12 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 13 is a protein called 40S ribosomal protein S15a.

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

- Molecule 14 is a protein called 40S ribosomal protein S23.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

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

- Molecule 16 is a protein called 40S ribosomal protein S26.

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

- Molecule 17 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 19 is a RNA chain called 18S rRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S2	1740	Total	C	N	O	P	0	0
			36952	16508	6600	12105	1739		

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called Ribosomal protein L24.

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

- Molecule 22 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 24 is a protein called 40S ribosomal protein S5.

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

- Molecule 25 is a protein called 40S ribosomal protein S10.

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

- Molecule 26 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 29 is a protein called 40S ribosomal protein S18.

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

- Molecule 30 is a protein called 40S ribosomal protein S19.

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

- Molecule 31 is a protein called 40S ribosomal protein S20.

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

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 33 is a protein called 40S ribosomal protein S28.

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

- Molecule 34 is a protein called 40S ribosomal protein S29.

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

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 37 is a RNA chain called A site tRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
37	At	71	Total	C	N	O	P	0	0
			1514	677	275	492	70		

- Molecule 38 is a RNA chain called P site tRNA [Homo sapiens].

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

- Molecule 39 is a protein called Transcription factor BTF3.

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

- Molecule 40 is a RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 41 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 42 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 43 is a protein called 60S ribosomal protein L8.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 45 is a protein called 60S ribosomal protein L4.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 47 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 48 is a protein called 60S ribosomal protein L7.

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

- Molecule 49 is a protein called 60S ribosomal protein L7a.

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

- Molecule 50 is a protein called 60S ribosomal protein L9.

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

- Molecule 51 is a protein called Ribosomal protein uL16-like.

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

- Molecule 52 is a protein called 60S ribosomal protein L11.

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

- Molecule 53 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 54 is a protein called 60S ribosomal protein L14.

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

- Molecule 55 is a protein called 60S ribosomal protein L15.

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

- Molecule 56 is a protein called 60S ribosomal protein L13a.

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

- Molecule 57 is a protein called 60S ribosomal protein L17.

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

- Molecule 58 is a protein called 60S ribosomal protein L18.

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

- Molecule 59 is a protein called 60S ribosomal protein L18a.

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

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

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

- Molecule 61 is a protein called Heparin-binding protein HBp15.

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

- Molecule 62 is a protein called 60S ribosomal protein L23.

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

- Molecule 63 is a protein called 60S ribosomal protein L23a.

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

- Molecule 64 is a protein called 60S ribosomal protein L26.

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

- Molecule 65 is a protein called 60S ribosomal protein L27.

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

- Molecule 66 is a protein called 60S ribosomal protein L27a.

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

- Molecule 67 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 68 is a protein called 60S ribosomal protein L30.

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

- Molecule 69 is a protein called 60S ribosomal protein L31.

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

- Molecule 70 is a protein called 60S ribosomal protein L32.

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

- Molecule 71 is a protein called 60S ribosomal protein L35a.

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

- Molecule 72 is a protein called 60S ribosomal protein L34.

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

- Molecule 73 is a protein called 60S ribosomal protein L35.

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

- Molecule 74 is a protein called 60S ribosomal protein L36.

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

- Molecule 75 is a protein called 60S ribosomal protein L37.

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

- Molecule 76 is a protein called 60S ribosomal protein L38.

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

- Molecule 77 is a protein called 60S ribosomal protein L39.

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 79 is a protein called 60S ribosomal protein L41.

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

- Molecule 80 is a protein called 60S ribosomal protein L36a.

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

- Molecule 81 is a protein called 60S ribosomal protein L37a.

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

- Molecule 82 is a protein called 60S ribosomal protein L28.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

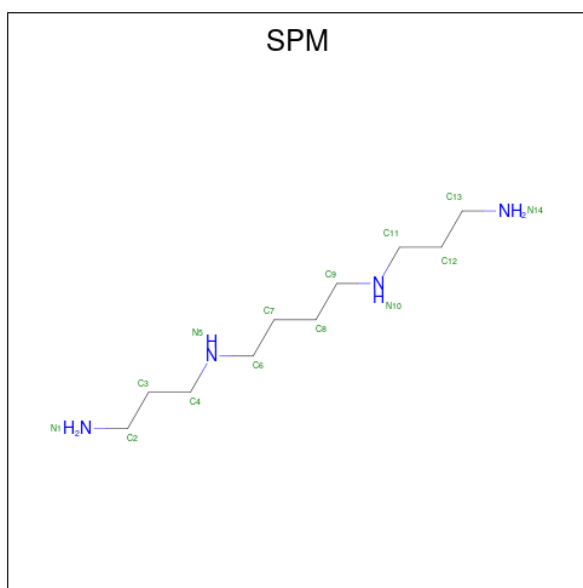
Mol	Chain	Residues	Atoms		AltConf
85	Sa	1	Total	Zn	0
			1	1	
85	Lg	1	Total	Zn	0
			1	1	
85	Lj	1	Total	Zn	0
			1	1	
85	Lm	1	Total	Zn	0
			1	1	
85	Lo	1	Total	Zn	0
			1	1	
85	Lp	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
86	S2	27	Total	Mg	0
			27	27	
86	SS	1	Total	Mg	0
			1	1	
86	L5	178	Total	Mg	0
			178	178	
86	L7	3	Total	Mg	0
			3	3	
86	L8	6	Total	Mg	0
			6	6	
86	LA	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	

- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of

Interest" by depositor).



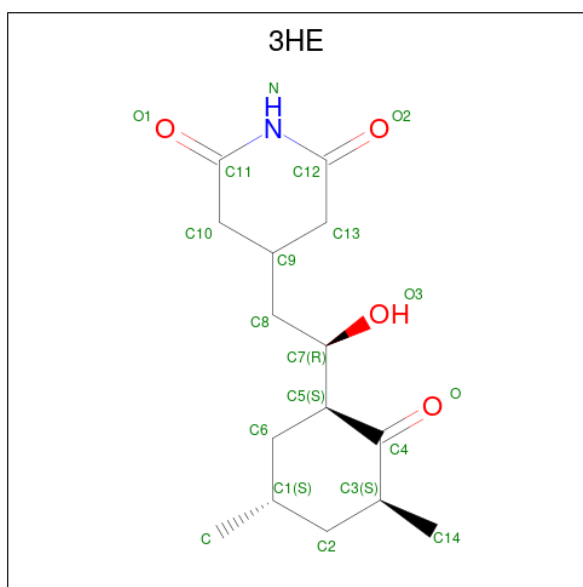
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



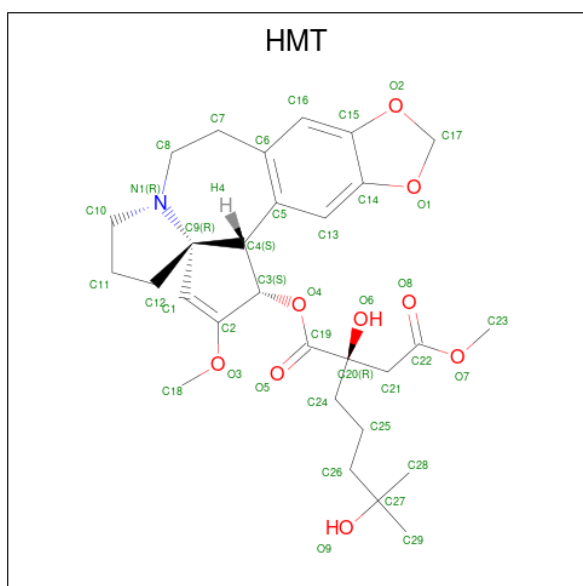
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L8	1	Total	C	N	0
			10	7	3	

- Molecule 89 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
89	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 90 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).

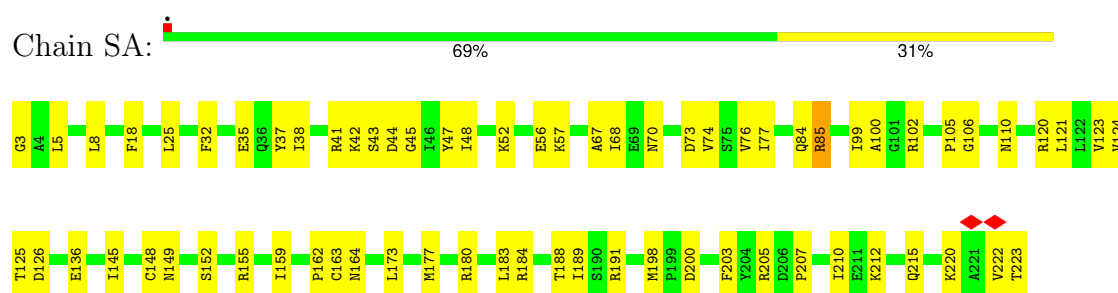


Mol	Chain	Residues	Atoms				AltConf
90	L5	1	Total	C	N	O	0
			39	29	1	9	

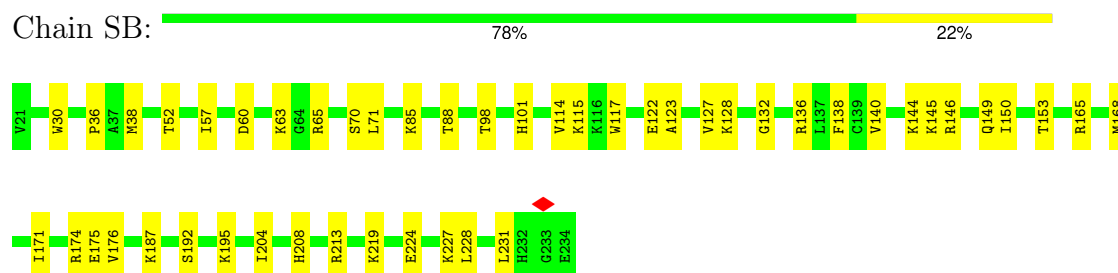
3 Residue-property plots

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: 40S ribosomal protein SA



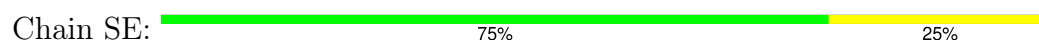
- Molecule 2: 40S ribosomal protein S3a

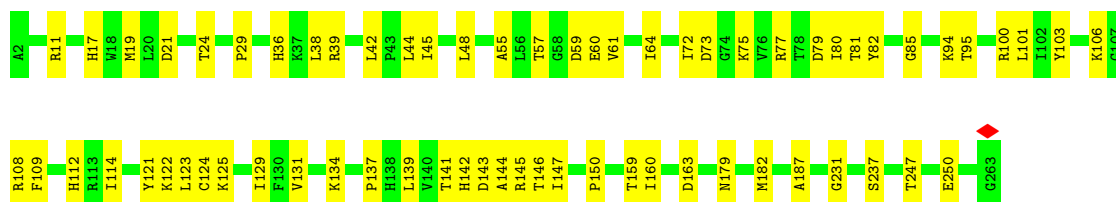


- Molecule 3: 40S ribosomal protein S2



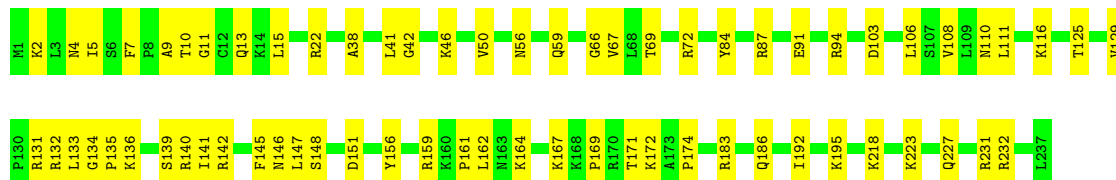
- Molecule 4: Small ribosomal subunit protein eS4, X isoform





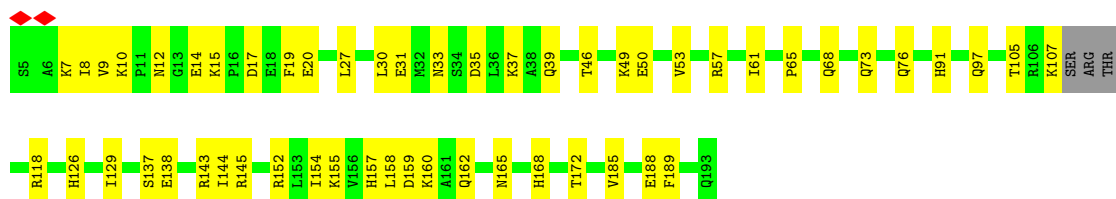
• Molecule 5: 40S ribosomal protein S6

Chain SG: 72% 28%



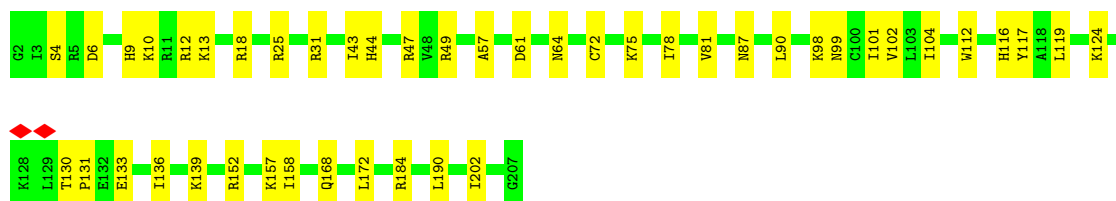
• Molecule 6: Small ribosomal subunit protein eS7

Chain SH: 70% 29%



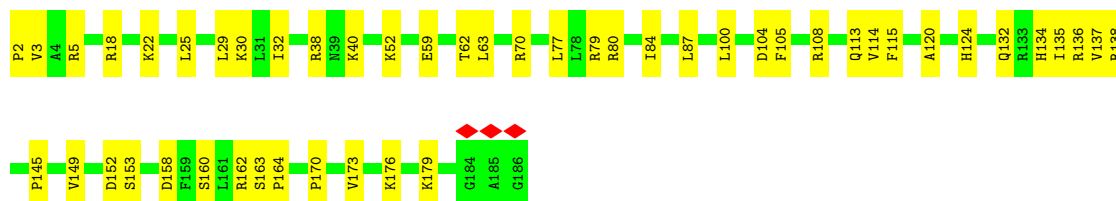
• Molecule 7: 40S ribosomal protein S8

Chain SI: 78% 22%



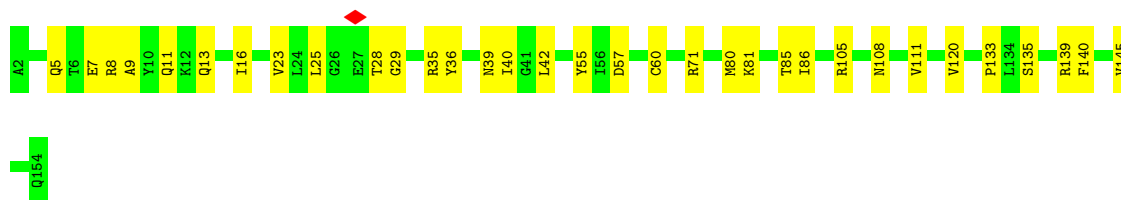
• Molecule 8: 40S ribosomal protein S9

Chain SJ: 74% 26%



• Molecule 9: 40S ribosomal protein S11

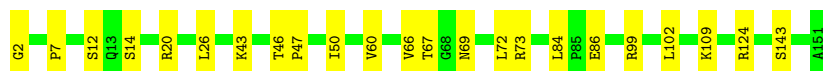
Chain SL:  78% 22%



G154

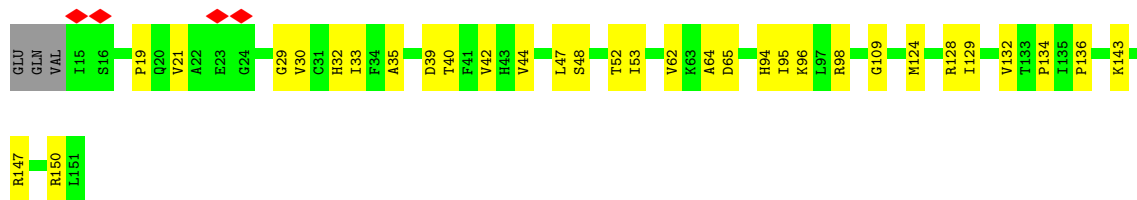
- Molecule 10: 40S ribosomal protein S13

Chain SN:  85% 15%



- Molecule 11: Small ribosomal subunit protein uS11

Chain SO:  75% 23%



R147, R150, L151

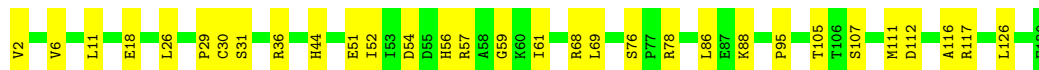
- Molecule 12: Small ribosomal subunit protein eS21

Chain SV:  89% 11%



- Molecule 13: 40S ribosomal protein S15a

Chain SW:  76% 24%

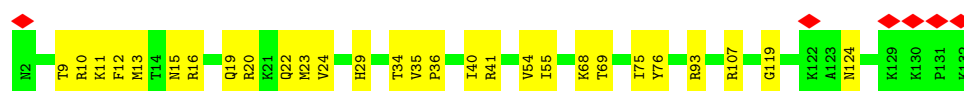
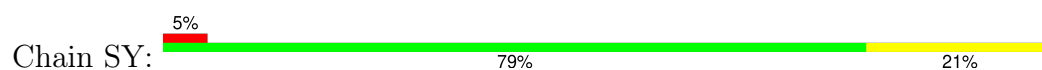


- Molecule 14: 40S ribosomal protein S23

Chain SX:  80% 20%



- Molecule 15: 40S ribosomal protein S24



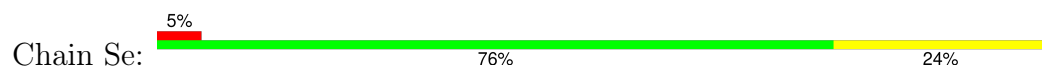
- Molecule 16: 40S ribosomal protein S26



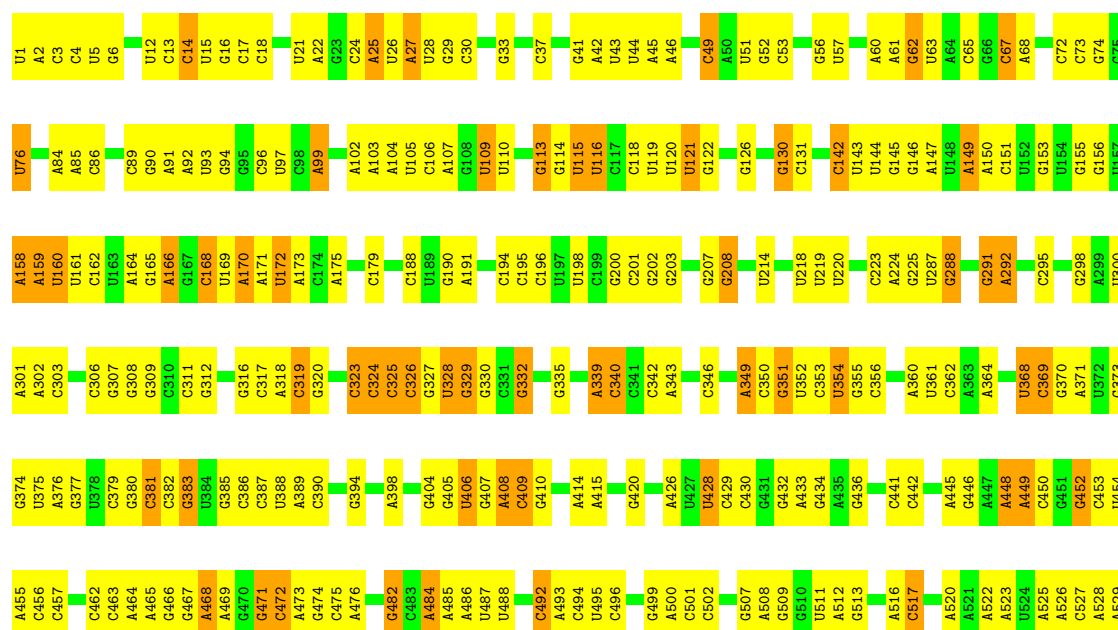
- Molecule 17: Small ribosomal subunit protein eS27



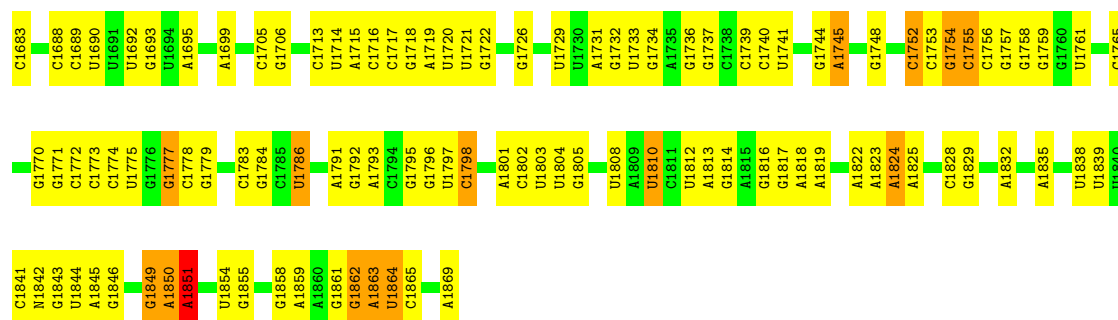
- Molecule 18: Small ribosomal subunit protein eS30



- Molecule 19: 18S rRNA [Homo sapiens]

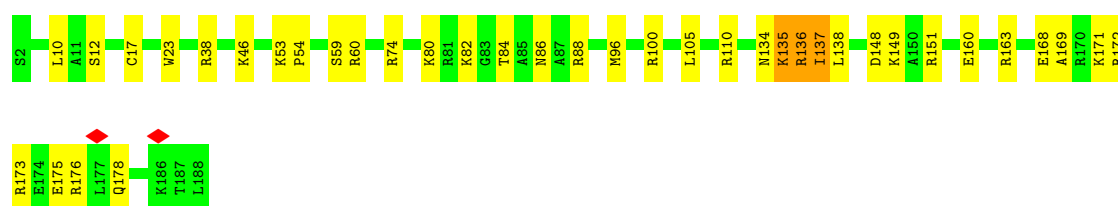


A1620	G1560	A1480	G1334	A1259	G1184	A1113	G1033	A962	G894	U820	U681	A605	U530
U1621	U1551	G1481	G1335	A1260	G1187	U1114	G1037	A963	G895	G821	U682	G606	A531
A1623	G1552	C1482	N1337	C1261	U1115	U1116	U1038	A964	U896	U822	U683	U607	C532
U1624	U1555	G1487	G1338	C1264	U1192	C1117	U966	U965	U897	U823	G684	U899	A533
C1628	U1556	A1488	U1342	G1269	A1194	C1118	U969	U966	U898	A825	A685	G610	G534
C1629	C1557	A1489	U1343	G1270	A1195	U1119	G370	U969	U899	A826	U686	A536	G535
A1630	U1558	G1490	U1344	C1271	U1120	U1121	G371	G370	C900	A827	C614	C614	A537
U1631	C1559	G1491	G1345	A1272	G1198	C1122	U1045	U969	C900	G828	C615	C615	U540
C1632	U1560	C1492	U1346	C1273	G1199	A1123	U1046	U969	G901	G829	A616	A616	U541
A1633	A1561	U1493	U1347	C1274	A1200	C1124	C973	U969	A903	A830	G691	G617	C542
A1634	C1562	U1494	G1348	G1275	A1201	C1125	C974	U969	A908	C834	C692	G620	U543
C1635	G1563	U1495	G1349	A1276	U1202	G1126	G375	G370	G909	C835	G693	G620	C544
G1636	U1566	U1496	U1350	C1277	U1203	C1127	A980	G370	G910	C836	C694	G623	A545
A1637	C1567	G1497	G1351	A1278	A1204	C1128	A981	U969	C911	G837	C695	G623	A546
G1638	U1568	U1498	U1352	C1279	U1205	C1129	G982	U969	C912	G838	C696	U627	G547
C1639	C1569	G1499	U1353	C1280	G1207	G1130	U989	U969	C913	G839	C697	A628	C548
A1640	U1569	U1500	G1354	G1281	A1208	C1131	A991	U969	A913	C840	C730	A629	C549
A1641	G1570	C1501	C1355	G1282	U1208	G1132	A992	U969	A916	G841	G731	U630	C550
U1642	U1571	G1502	G1356	A1282	C1208	C1133	G993	U969	U917	G842	C732	U631	U551
U1643	G1572	A1506	A1357	A1283	C1215	C1078	A996	U969	A918	C843	C733	A634	U556
C1644	C1573	G1507	U1358	A1284	C1216	C1079	A997	U969	U919	G844	C734	G635	U557
U1647	G1575	U1508	U1359	G1285	A1217	A1080	A998	U969	A920	U844	G735	G635	G558
G1648	U1576	A1509	G1360	G1286	C1218	U1081	C1000	U969	A921	U845	C736	G635	G559
U1649	A1579	U1509	U1361	A1287	C1219	C1067	C1000	U969	A922	G846	G737	G635	A560
A1650	C1580	G1512	U1362	U1288	A1220	G1068	U1002	U969	A923	C851	U749	C638	A561
A1651	C1581	C1482	C1363	U1289	G1221	U1069	U1003	U969	G924	G852	C750	A640	U562
G1652	C1582	G1514	U1367	G1290	C1222	C1078	U1004	U969	G925	U847	C751	A641	G563
U1653	U1585	G1517	U1371	G1294	A1223	C1079	G1005	U969	A926	G848	C752	U642	A564
C1654	U1586	U1518	U1372	A1295	U1225	A1080	U1005	U969	A927	G849	C753	G644	G565
G1655	C1587	C1373	C1373	A1296	C1226	U1081	C1006	U969	G928	G850	C754	C645	C568
C1656	A1588	G1374	G1374	G1297	C1227	C1083	C1007	U969	G929	U851	C755	U647	A569
U1657	U1589	C1375	C1375	A1301	G1228	A1084	U1008	U969	A1001	C852	C756	A648	C570
G1658	C1593	A1376	U1377	G1302	C1230	C1085	U1009	U969	A1002	A864	C757	A649	U573
U1659	A1594	U1378	A1378	C1303	C1231	C1088	U1010	U969	A1003	A865	C758	A650	A574
C1660	U1595	A1379	A1379	U1304	U1232	U1089	U1011	U969	A1004	U866	C759	A651	A575
U1661	G1596	U1380	U1380	C1305	G1233	C1090	U1012	U969	A1005	U867	C760	A652	A576
A1662	C1597	A1382	A1382	U1306	C1234	C1091	U1013	U969	A1006	U868	C761	A653	A577
C1663	U1598	C1383	C1383	U1307	G1235	U1092	U1014	U969	A1007	U869	C762	A654	A578
A1664	A1599	U1384	U1384	U1308	C1236	G1093	U1015	U969	A1008	U870	C763	A655	A579
C1665	U1600	C1385	G1385	U1309	C1237	U1094	U1016	U969	A1009	U871	C764	G662	U591
U1667	A1601	G1456	G1386	C1311	G1245	C1095	U1017	U969	A1010	U872	C765	C663	C592
U1668	U1602	U1457	A1388	G1312	A1241	C1096	U1018	U969	A1011	U873	C766	A664	A590
C1669	G1603	G1458	U1389	A1313	U1242	U1096	U1019	U969	A1012	U874	C767	U658	G586
A1670	G1604	C1459	C1391	U1314	U1243	G1097	U1020	U969	A1013	A875	C768	G659	A587
G1671	G1605	G1461	U1392	C1317	U1244	U1098	U1021	U969	A1014	C876	C769	G660	G588
U1672	C1606	U1462	G1393	G1318	G1245	U1099	U1022	U969	U945	C877	C770	U661	G589
U1673	A1607	U1463	G1394	U1319	B81248	A1100	C951	U969	U946	U878	C771	G662	A590
G1674	U1608	C1464	U1394	U1319	U1172	A1101	C952	U969	U947	C879	C772	C663	U591
U1675	C1609	U1467	A1401	U1320	U1173	U1102	C953	U969	U948	U880	C773	A664	C592
U1676	G1610	C1468	A1402	U1321	U1174	C1103	C954	U969	U949	A809	C774	G665	A595
U1677	U1611	U1469	C1403	U1322	G1175	G1104	U954	U969	U950	A810	C775	U666	U596
A1678	A1614	C1470	U1404	C1323	G1176	U1107	A955	U969	A957	A811	C776	U667	U597
A1679	U1615	G1473	U1405	U1324	U1177	G1108	U956	U969	G958	A812	C777	A668	G600
U1680	G1616	U1474	A1406	C1325	U1178	C1109	U957	U969	G959	A813	C778	A669	G601
U1681	U1617	A1475	U1407	G1256	G1179	U1112	U960	U969	U960	U814	C779	A670	G602
C1682	U1618	C1476	A1476	A1258	A1182	U1112	U961	U969	G961	A818	C780	A671	C603
												A672	A604



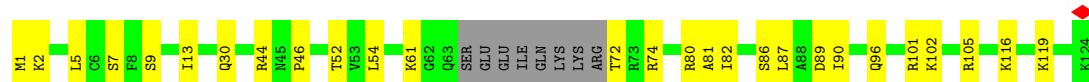
- Molecule 20: 60S ribosomal protein L19

Chain LR: 80% 19%



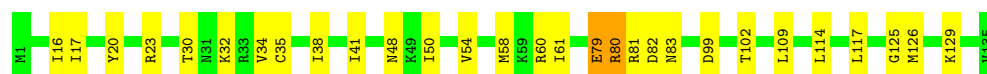
- Molecule 21: Ribosomal protein L24

Chain LW: 72% 22% 6%



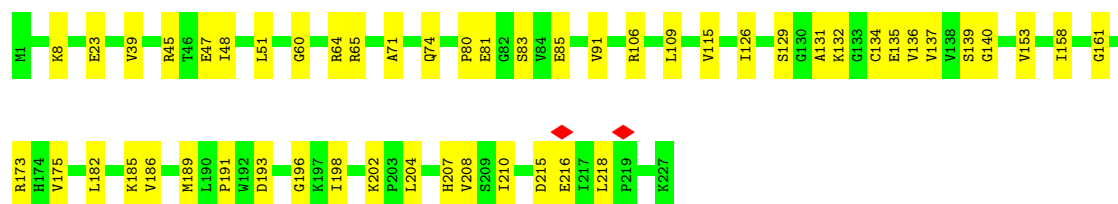
- Molecule 22: Small ribosomal subunit protein eS17

Chain SR: 79% 20%



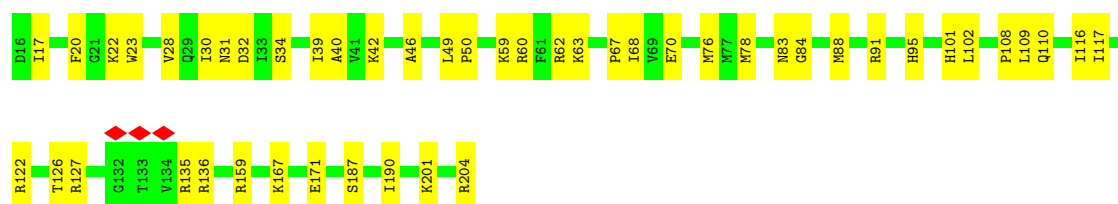
- Molecule 23: Small ribosomal subunit protein uS3

Chain SD: 78% 22%

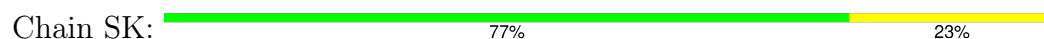


- Molecule 24: 40S ribosomal protein S5

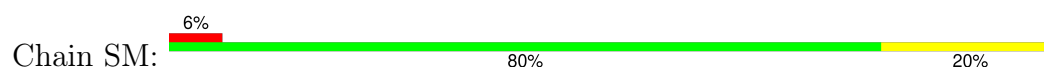
Chain SF: 75% 25%



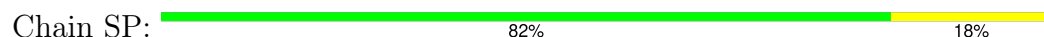
- Molecule 25: 40S ribosomal protein S10



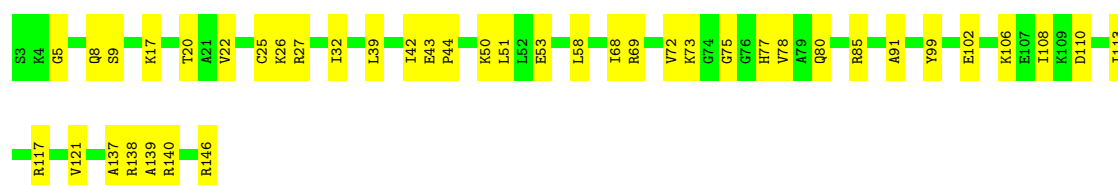
- Molecule 26: Small ribosomal subunit protein eS12



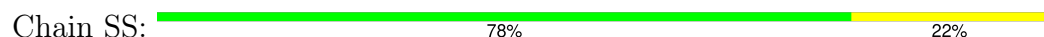
- Molecule 27: Small ribosomal subunit protein uS19



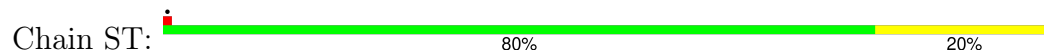
- Molecule 28: Small ribosomal subunit protein uS9



- Molecule 29: 40S ribosomal protein S18



- Molecule 30: 40S ribosomal protein S19





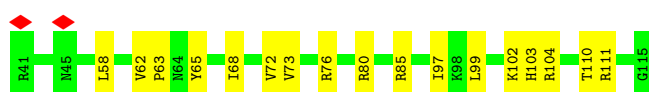
- Molecule 31: 40S ribosomal protein S20

Chain SU:



- Molecule 32: Small ribosomal subunit protein eS25

Chain SZ:



- Molecule 33: 40S ribosomal protein S28

Chain Sc:



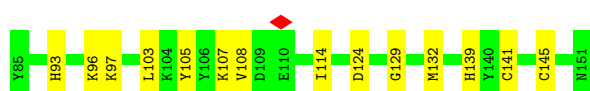
- Molecule 34: 40S ribosomal protein S29

Chain Sd:



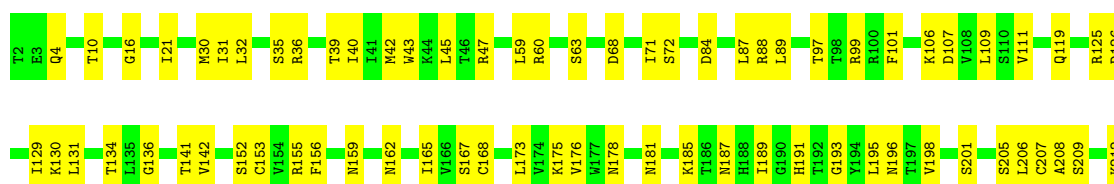
- Molecule 35: Ubiquitin-40S ribosomal protein S27a

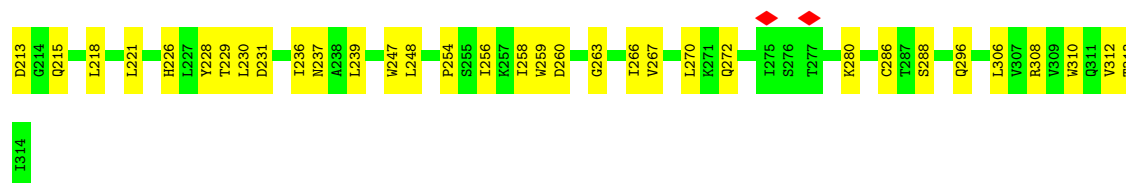
Chain Sf:



- Molecule 36: Receptor of activated protein C kinase 1

Chain Sg:





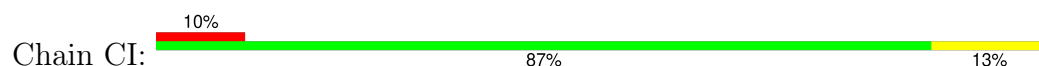
• Molecule 37: A site tRNA [Homo sapiens]



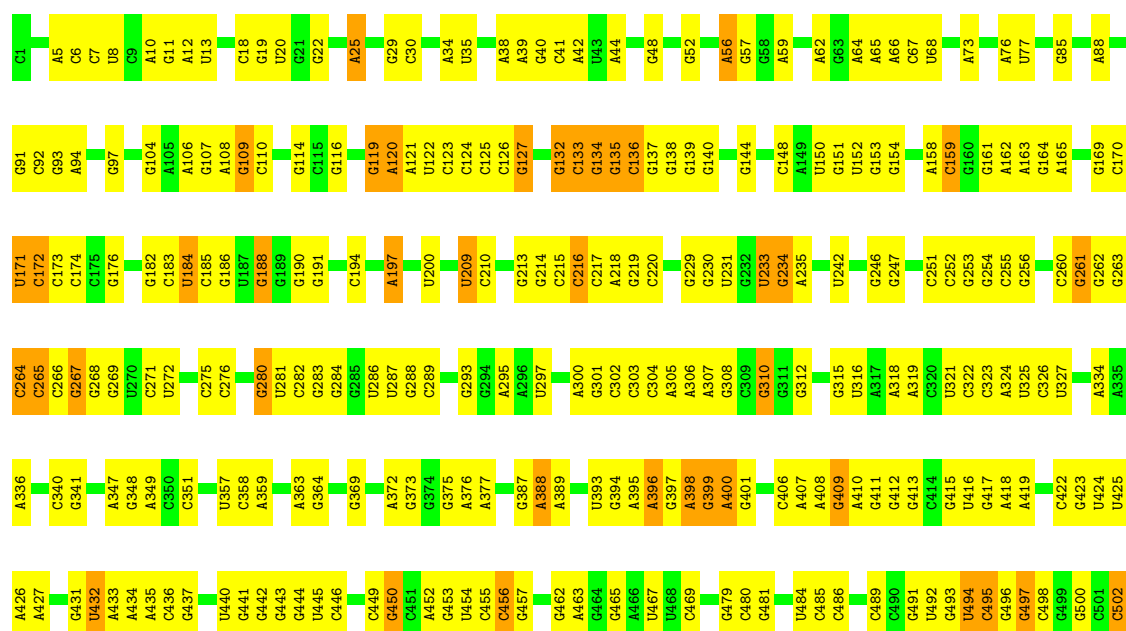
• Molecule 38: P site tRNA [Homo sapiens]



• Molecule 39: Transcription factor BTF3

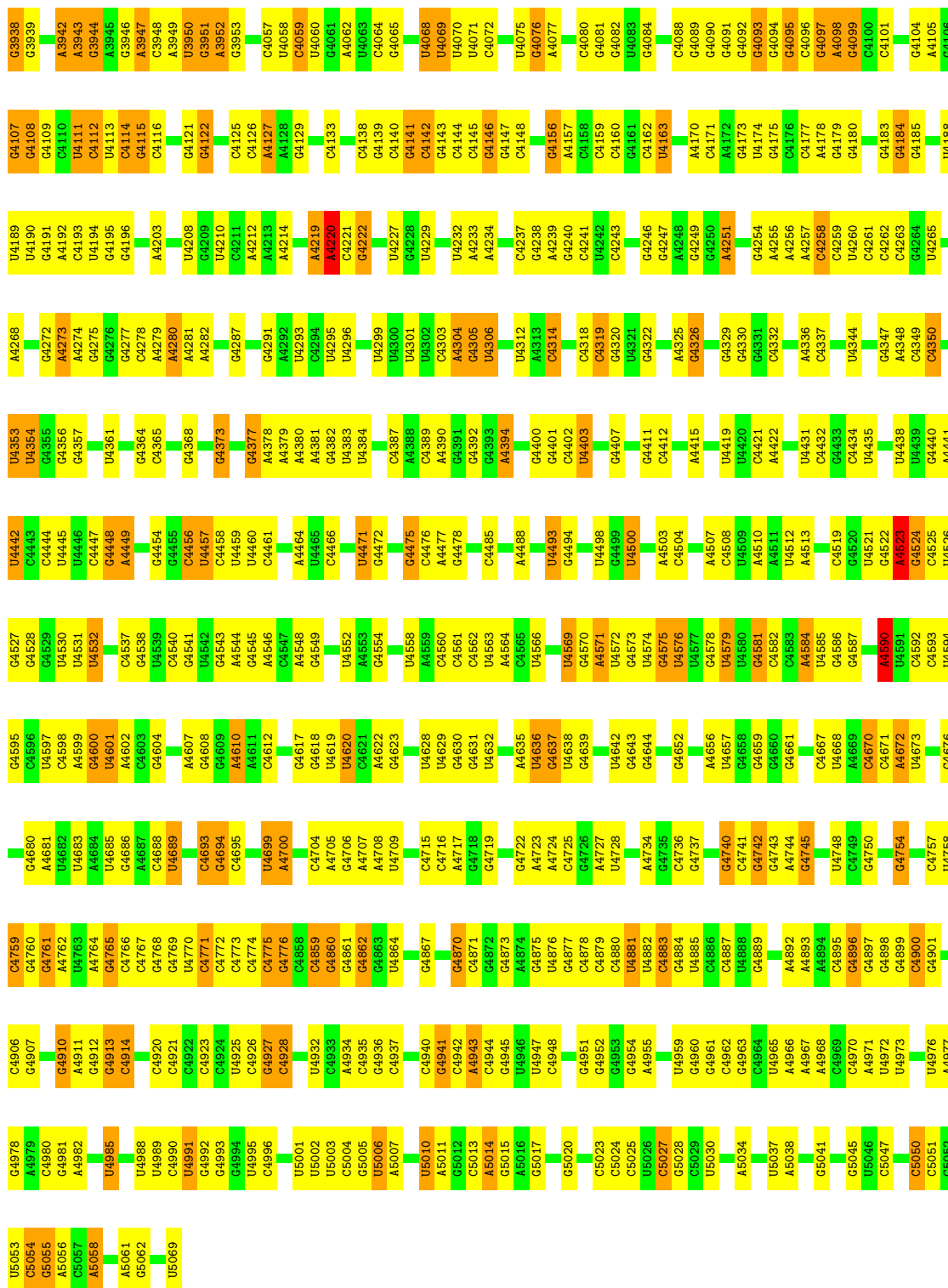


• Molecule 40: 28S rRNA [Homo sapiens]

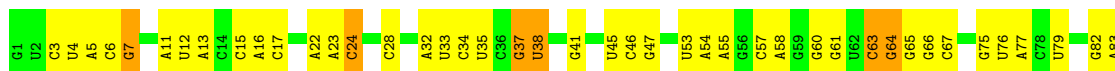


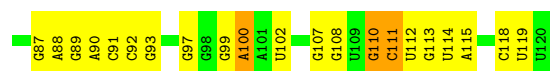
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U1949	A1871	U1800	C1718	G1629	G1517	A1437	G1355	A1278	C1197	U982	G912	G504
U1950	A1872	A1801	A1719	A1630	A1518	U1438	G1356	C1280	G1198	G982	U913	G505
G1951	A1873	A1802	C1720	A1632	C1521	C1439	G1357	G1281	G1199	C985	U914	G506
G1961	C1874	G1803	G1721	G1633	C1522	U1440	G1358	G1284	U1200	C986	A915	G507
A1962	C1875	A1804	G1722	A1634	A1523	C1441	G1359	G1287	U1202	U989	A917	G508
C1963	U1876	A1805	U1727	C1635	A1524	C1442	G1360	G1287	G1203	U989	G918	A509
A1964	G1877	G1806	U1728	C1636	A1525	A1443	U1364	G1292	C1204	U989	U702	U510
G1965	C1878	G1807	A1729	A1637	A1526	U1444	G1365	C1292	G1205	G1070	G703	U511
C1966	C1879	A1808	U1730	A1637	A1527	U1445	G1366	C1292	G1206	C1071	G704	U512
A1967	G1880	G1811	C1731	G1640	A1534	C1447	C1367	A1294	C1207	C1072	G709	U513
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C1973	G1890	C1820	A1743	C1655	A1547	A1459	G1377	C1305	G1215	U1083	G715	G520
U1974	A1891	G1821	U1744	C1655	A1547	C1460	C1378	C1305	G1215	C1084	G716	G642
G1975	C1892	U1822	G1745	C1656	A1553	C1461	C1379	C1306	G1219	C1085	U717	G643
C1976	G1893	G1823	U1749	U1660	A1554	C1462	G1380	C1307	G1219	C1086	C719	G644
G1977	C1894	G1824	G1750	C1661	A1554	C1463	G1381	C1308	A1222	A1087	C724	G647
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G1985	C1914	A1837	G1761	C1676	C1574	C1474	A1392	C1321	G1244	C1097	G942	A660
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G2000	A1932	C1856	A1779	C1692	C1612	G1498	C1417	C1340	A1263	C1181	G957	C677
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G2005	G1937	C1860	A1787	C1698	U1616	G1510	G1424	C1346	U1186	G1185	G961	G681
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C2010	A1942	U1866	U1792	C1703	G1626	U1514	G1431	C1352	G1274	C977	C907	A686
A2012	A1943	G1869	U1792	C1704	G1627	A1515	G1432	G1353	G1275	G1194	G908	U687
C2014										G1195	G978	C691
												A692

C3869	C3870	A3799	A3800	A3711	A3712	G3626	A2879	G2726	G2649	G2559	G2479	G2094	U2015
A3871	A3872	U3805	A3630	A3717	A2881	A3630	U2880	C2727	G2650	C2560	G2483	A2095	C2016
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A3876	C3809	G3636	G3636	G3722	A2885	C2804	C2804	U2734	C2655	G2569	G2487	G2099	C2019
A3877	G3810	U3637	U3637	A3723	G2888	C2805	C2806	G2736	G2668	U2570	C2488	A2100	U2020
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G3879	C3812	U3639	U3639	G3725	G2890	G2808	G2809	G2740	G2663	C2579	U2490	G2102	C2023
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G3926	U3786	U3695	U3695	A3785	G3615	C2861	C2861	G2781	C2716	G2545	U2469	C2084	C2084
U3927	G3787	C3696	C3696	G3786	U3616	G2862	G2862	G2782	G2717	U2546	C2470	U2293	G2085
A3928	C3788	U3697	U3697	G3787	G3617	U2869	U2869	G2783	C2718	G2547	G2471	G2294	A2088
G3929	C3789	G3698	G3698	G3788	G3618	A2870	A2870	G2784	C2719	A2641	G2474	G2295	G2089
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G3933	A3861	G3701	G3701	G3792	G3619	G2872	G2872	G2786	G2721	G2643	G2476	G2297	C2091
G3934	A3862	A3702	A3702	U3796	G3620	G2873	G2873	G2787	G2722	A2647	A2477	G2300	G2092
C3937	A3867	G3710	G3710	U3798	A3624	G2874	G2874	G2788	G2723	A2648	G2478	A2300	G2093
	G3868				G3625	G2875	G2875	G2789	A2649	G2648		G2301	

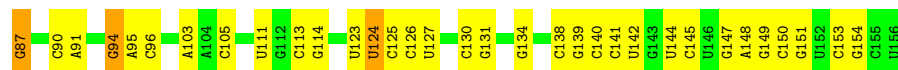
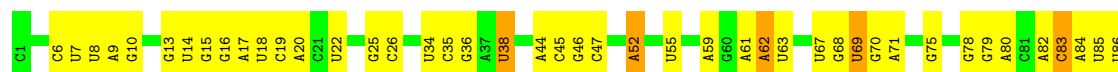


Chain L7:

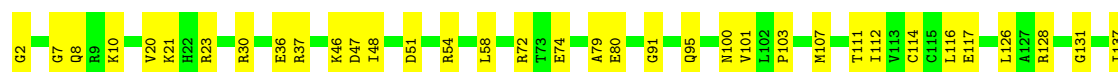




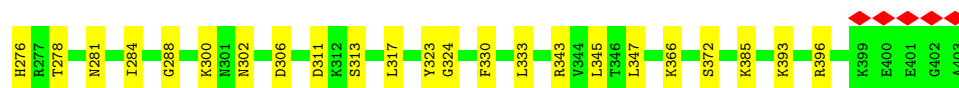
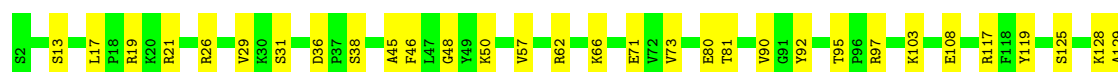
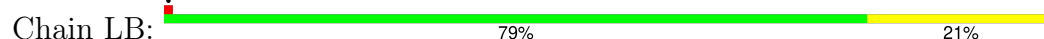
- Molecule 42: 5.8S rRNA [Homo sapiens]



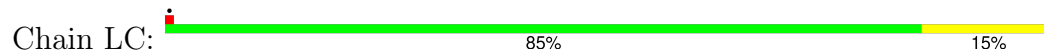
- Molecule 43: 60S ribosomal protein L8



- Molecule 44: Large ribosomal subunit protein uL3

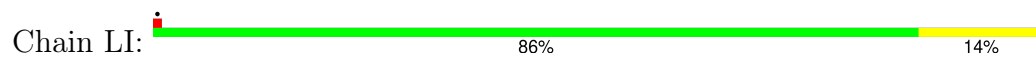


- Molecule 45: 60S ribosomal protein L4

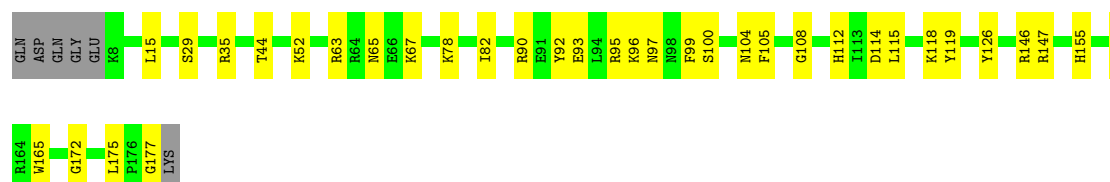
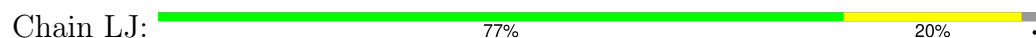


- Molecule 46: Large ribosomal subunit protein uL18

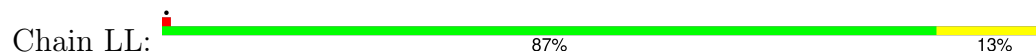
- Molecule 51: Ribosomal protein uL16-like



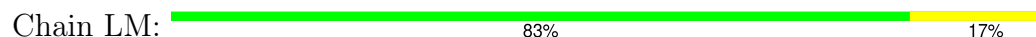
- Molecule 52: 60S ribosomal protein L11



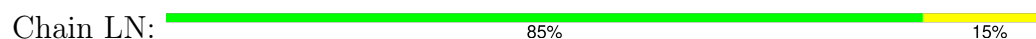
- Molecule 53: Large ribosomal subunit protein eL13



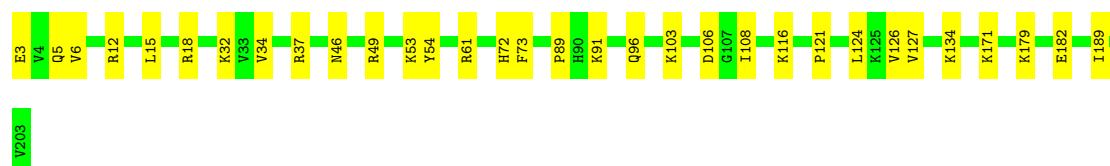
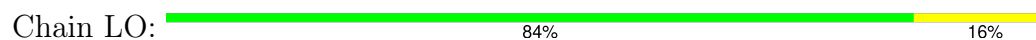
- Molecule 54: 60S ribosomal protein L14



- Molecule 55: 60S ribosomal protein L15

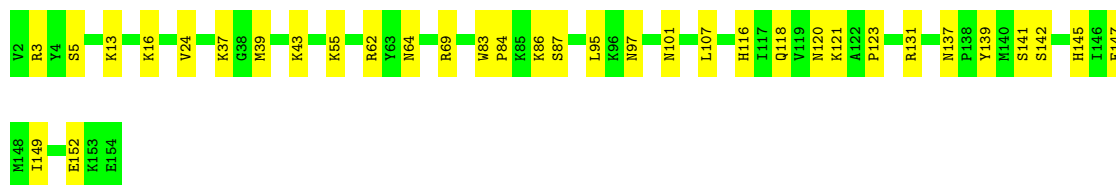


- Molecule 56: 60S ribosomal protein L13a



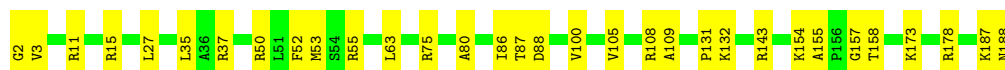
- Molecule 57: 60S ribosomal protein L17

Chain LP:  78% 22%



- Molecule 58: 60S ribosomal protein L18

Chain LQ:  83% 17%



- Molecule 59: 60S ribosomal protein L18a

Chain LS:  86% 14%



- Molecule 60: 60S ribosomal protein L21

Chain LT:  85% 15%



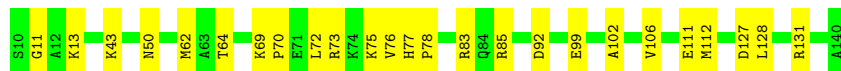
- Molecule 61: Heparin-binding protein HBp15

Chain LU:  84% 16%



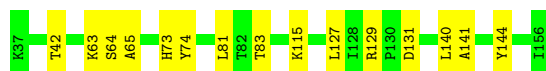
- Molecule 62: 60S ribosomal protein L23

Chain LV:  81% 19%



- Molecule 63: 60S ribosomal protein L23a

Chain LX:  88% 12%



- Molecule 64: 60S ribosomal protein L26

Chain LY:  85% 15%



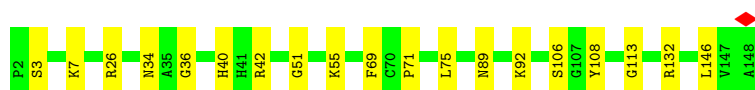
- Molecule 65: 60S ribosomal protein L27

Chain LZ:  84% 16%



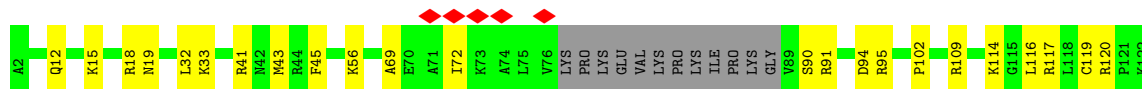
- Molecule 66: 60S ribosomal protein L27a

Chain La:  87% 13%



- Molecule 67: Large ribosomal subunit protein eL29

Chain Lb:  71% 19% 10%



- Molecule 68: 60S ribosomal protein L30

Chain Lc:  85% 15%



- Molecule 69: 60S ribosomal protein L31

Chain Ld:  83% 17%



- Molecule 70: 60S ribosomal protein L32

Chain Le:  91% 9%

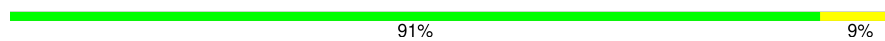


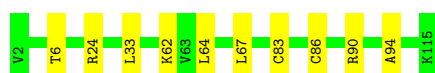
- Molecule 71: 60S ribosomal protein L35a

Chain Lf:  81% 19%



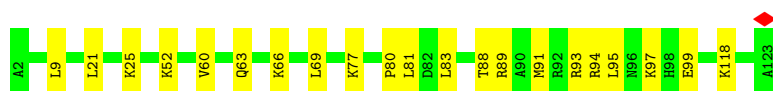
- Molecule 72: 60S ribosomal protein L34

Chain Lg:  91% 9%



- Molecule 73: 60S ribosomal protein L35

Chain Lh:  83% 17%



- Molecule 74: 60S ribosomal protein L36

Chain Li:  90% 10%



- Molecule 75: 60S ribosomal protein L37

Chain Lj:  84% 16%



- Molecule 76: 60S ribosomal protein L38

Chain Lk:  80% 20%



- Molecule 77: 60S ribosomal protein L39

Chain Ll:  80% 20%



- Molecule 78: Large ribosomal subunit protein eL40

Chain Lm: 83% 17%



- Molecule 79: 60S ribosomal protein L41

Chain Ln: 83% 17%



- Molecule 80: 60S ribosomal protein L36a

Chain Lo: 80% 20%



- Molecule 81: 60S ribosomal protein L37a

Chain Lp: 92% 8%



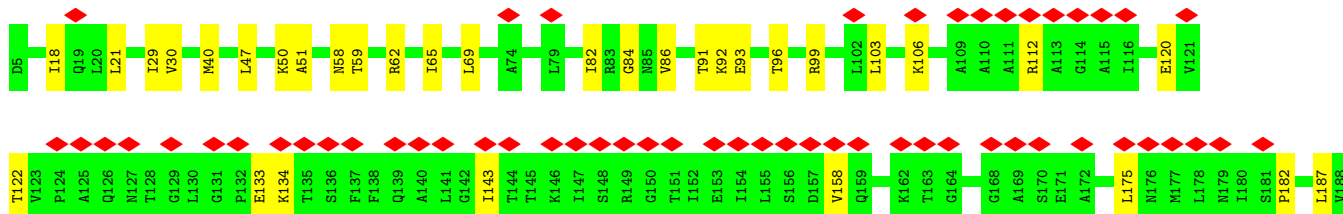
- Molecule 82: 60S ribosomal protein L28

Chain Lr: 89% 11%



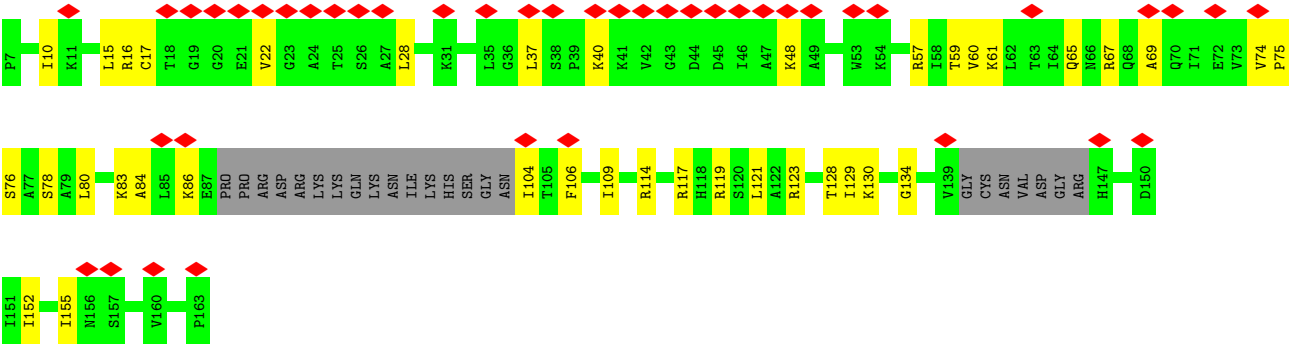
- Molecule 83: 60S acidic ribosomal protein P0

Chain Ls: 29% 82% 18%





- Molecule 84: Large ribosomal subunit protein uL11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.562	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.0758	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	SA	0.17	0/1778	0.37	0/2416
2	SB	0.11	0/1765	0.28	0/2362
3	SC	0.16	0/1744	0.32	0/2357
4	SE	0.12	0/2118	0.32	0/2849
5	SG	0.11	0/1946	0.30	0/2590
6	SH	0.13	0/1519	0.35	0/2033
7	SI	0.12	0/1715	0.33	0/2287
8	SJ	0.11	0/1550	0.31	0/2069
9	SL	0.11	0/1268	0.29	0/1696
10	SN	0.10	0/1232	0.26	0/1656
11	SO	0.12	0/1037	0.32	0/1391
12	SV	0.13	0/643	0.33	0/860
13	SW	0.13	0/1051	0.29	0/1406
14	SX	0.13	0/1116	0.33	0/1490
15	SY	0.12	0/1083	0.33	0/1438
16	Sa	0.12	0/836	0.30	0/1121
17	Sb	0.14	0/665	0.34	0/891
18	Se	0.13	0/465	0.35	0/612
19	S2	0.17	1/39756 (0.0%)	0.28	0/61939
20	LR	0.21	0/1582	0.41	0/2091
21	LW	0.12	0/959	0.29	0/1270
22	SR	0.24	0/1105	0.48	0/1484
23	SD	0.12	0/1793	0.26	0/2414
24	SF	0.10	0/1516	0.27	0/2037
25	SK	0.12	0/851	0.31	0/1147
26	SM	0.10	0/950	0.34	0/1275
27	SP	0.11	0/1003	0.30	0/1342
28	SQ	0.12	0/1160	0.34	0/1553
29	SS	0.11	0/1216	0.33	0/1628
30	ST	0.11	0/1131	0.28	0/1515
31	SU	0.13	0/831	0.33	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SZ	0.13	0/604	0.37	0/810
33	Sc	0.13	0/508	0.31	0/680
34	Sd	0.12	0/470	0.27	0/623
35	Sf	0.14	0/560	0.43	0/745
36	Sg	0.12	0/2493	0.33	0/3394
37	At	0.11	0/1692	0.24	0/2634
38	Pt	0.12	0/1761	0.25	0/2741
39	CI	0.08	0/247	0.27	0/323
40	L5	0.17	0/85098	0.28	0/132762
41	L7	0.14	0/2861	0.24	0/4459
42	L8	0.14	0/3631	0.27	0/5657
43	LA	0.15	0/1936	0.35	0/2596
44	LB	0.13	0/3306	0.30	0/4424
45	LC	0.14	0/2981	0.30	0/4002
46	LD	0.13	0/2428	0.28	0/3252
47	LE	0.14	0/1973	0.37	0/2645
48	LF	0.13	0/1905	0.24	0/2539
49	LG	0.12	0/1960	0.32	0/2637
50	LH	0.12	0/1537	0.30	0/2066
51	LI	0.12	0/1751	0.27	0/2340
52	LJ	0.12	0/1385	0.32	0/1852
53	LL	0.13	0/1732	0.29	0/2315
54	LM	0.12	0/1161	0.28	0/1554
55	LN	0.13	0/1746	0.27	0/2338
56	LO	0.14	0/1682	0.29	0/2250
57	LP	0.13	0/1268	0.31	0/1701
58	LQ	0.14	0/1537	0.29	0/2052
59	LS	0.14	0/1493	0.28	0/2003
60	LT	0.12	0/1326	0.26	0/1770
61	LU	0.12	0/839	0.34	0/1126
62	LV	0.13	0/993	0.30	0/1332
63	LX	0.12	0/1002	0.28	0/1345
64	LY	0.12	0/1132	0.28	0/1504
65	LZ	0.13	0/1130	0.29	0/1507
66	La	0.14	0/1191	0.28	0/1591
67	Lb	0.12	0/889	0.31	0/1175
68	Lc	0.13	0/774	0.31	0/1038
69	Ld	0.12	0/903	0.29	0/1216
70	Le	0.13	0/1071	0.26	0/1429
71	Lf	0.13	0/895	0.28	0/1198
72	Lg	0.12	0/916	0.27	0/1220
73	Lh	0.10	0/1023	0.25	0/1351
74	Li	0.11	0/843	0.26	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.13	0/720	0.31	0/952
76	Lk	0.12	0/575	0.31	0/761
77	Ll	0.12	0/454	0.22	0/599
78	Lm	0.14	0/435	0.35	0/575
79	Ln	0.10	0/231	0.24	0/294
80	Lo	0.13	0/876	0.27	0/1156
81	Lp	0.12	0/718	0.28	0/953
82	Lr	0.12	0/1017	0.30	0/1364
83	Ls	0.15	0/1519	0.33	0/2052
84	Lt	0.16	0/1009	0.44	0/1363
All	All	0.15	1/231571 (0.0%)	0.29	0/339714

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	SA	0	2
20	LR	0	1
22	SR	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	668	A2M	O3'-P	5.21	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	LR	136	ARG	Sidechain
1	SA	205	ARG	Sidechain
1	SA	85	ARG	Sidechain
22	SR	80	ARG	Sidechain
22	SR	81	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SA	1741	0	1744	50	0
2	SB	1738	0	1809	35	0
3	SC	1707	0	1791	34	0
4	SE	2076	0	2177	48	0
5	SG	1923	0	2089	61	0
6	SH	1497	0	1590	34	0
7	SI	1686	0	1772	33	0
8	SJ	1525	0	1640	40	0
9	SL	1247	0	1323	24	0
10	SN	1208	0	1294	18	0
11	SO	1024	0	1050	24	0
12	SV	636	0	637	6	0
13	SW	1034	0	1080	23	0
14	SX	1098	0	1167	23	0
15	SY	1065	0	1142	21	0
16	Sa	821	0	870	21	0
17	Sb	651	0	670	17	0
18	Se	459	0	503	12	0
19	S2	36952	0	18678	751	0
20	LR	1566	0	1729	29	0
21	LW	945	0	1003	25	0
22	SR	1090	0	1149	21	0
23	SD	1765	0	1865	37	0
24	SF	1495	0	1549	33	0
25	SK	827	0	854	17	0
26	SM	940	0	965	17	0
27	SP	985	0	1031	17	0
28	SQ	1142	0	1213	29	0
29	SS	1198	0	1261	25	0
30	ST	1112	0	1146	23	0
31	SU	821	0	883	24	0
32	SZ	598	0	656	14	0
33	Sc	506	0	536	7	0
34	Sd	459	0	449	19	0
35	Sf	548	0	553	14	0
36	Sg	2436	0	2391	64	0
37	At	1514	0	770	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Pt	1576	0	803	25	0
39	CI	247	0	283	4	0
40	L5	78444	0	39715	1358	0
41	L7	2561	0	1295	47	0
42	L8	3315	0	1685	57	0
43	LA	1898	0	1993	52	0
44	LB	3238	0	3376	62	0
45	LC	2927	0	3104	46	0
46	LD	2382	0	2410	40	0
47	LE	1935	0	2096	42	0
48	LF	1870	0	1996	26	0
49	LG	1927	0	2074	24	0
50	LH	1518	0	1601	20	0
51	LI	1711	0	1749	21	0
52	LJ	1362	0	1399	22	0
53	LL	1701	0	1818	22	0
54	LM	1138	0	1204	17	0
55	LN	1701	0	1749	25	0
56	LO	1650	0	1794	27	0
57	LP	1242	0	1269	27	0
58	LQ	1513	0	1628	25	0
59	LS	1453	0	1490	19	0
60	LT	1298	0	1366	22	0
61	LU	825	0	850	12	0
62	LV	979	0	1039	15	0
63	LX	985	0	1066	11	0
64	LY	1115	0	1205	14	0
65	LZ	1107	0	1182	16	0
66	La	1162	0	1213	16	0
67	Lb	876	0	948	18	0
68	Lc	764	0	804	8	0
69	Ld	888	0	930	11	0
70	Le	1053	0	1147	9	0
71	Lf	876	0	912	15	0
72	Lg	906	0	998	8	0
73	Lh	1015	0	1148	19	0
74	Li	832	0	917	8	0
75	Lj	705	0	737	11	0
76	Lk	569	0	637	8	0
77	Ll	444	0	483	10	0
78	Lm	429	0	465	6	0
79	Ln	230	0	276	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Lo	862	0	929	15	0
81	Lp	708	0	756	8	0
82	Lr	1002	0	1068	10	0
83	Ls	1496	0	1540	22	0
84	Lt	998	0	1032	27	0
85	Lg	1	0	0	0	0
85	Lj	1	0	0	0	0
85	Lm	1	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	1	0	0	0	0
85	Sa	1	0	0	0	0
86	L5	178	0	0	0	0
86	L7	3	0	0	0	0
86	L8	6	0	0	0	0
86	LA	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	S2	27	0	0	0	0
86	SS	1	0	0	0	0
87	L5	98	0	182	7	0
88	L5	90	0	171	3	0
88	L8	10	0	19	2	0
89	L5	20	0	23	0	0
90	L5	39	0	39	1	0
All	All	219950	0	163642	3404	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 9.

All (3404) 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)
40:L5:1095:A:C2	40:L5:1200:G:N1	2.25	1.02
40:L5:1095:A:H2	40:L5:1200:G:H1	1.01	0.98
40:L5:2483:G:H1	40:L5:2495:U:H3	1.09	0.98
40:L5:1095:A:H2	40:L5:1200:G:N1	1.57	0.98
40:L5:4601:U:H3	40:L5:4610:A:H62	1.01	0.97
19:S2:1166:G:H1	19:S2:1193:U:H3	1.13	0.96
19:S2:1417:C:H42	19:S2:1422:G:H22	1.15	0.94
40:L5:1759:G:H1	40:L5:1773:U:H3	0.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:925:G:H1	19:S2:1017:U:H3	0.93	0.87
40:L5:1629:G:H1	43:LA:208:GLU:HG2	1.39	0.87
19:S2:878:G:H1	19:S2:908:A:H2	1.21	0.84
40:L5:4601:U:H3	40:L5:4610:A:N6	1.74	0.84
40:L5:450:G:H1	40:L5:1297:U:H3	1.24	0.83
19:S2:1096:G:H1	19:S2:1136:U:H3	1.24	0.82
40:L5:4421:C:H42	40:L5:4475:G:H22	1.25	0.82
40:L5:4638:U:H3	40:L5:4661:G:H1	1.28	0.82
40:L5:4748:U:H3	40:L5:4952:G:H1	1.26	0.81
1:SA:148:CYS:N	1:SA:163:CYS:SG	2.54	0.81
19:S2:1752:C:C4	19:S2:1779:G:N2	2.49	0.80
19:S2:1033:G:H1	19:S2:1080:A:HO2'	1.28	0.79
40:L5:1176:C:N3	40:L5:1184:A:N6	2.32	0.78
19:S2:146:G:H1	19:S2:173:A:H61	1.30	0.77
19:S2:822:U:H3	19:S2:826:A:H62	1.34	0.76
40:L5:4421:C:H42	40:L5:4475:G:N2	1.84	0.76
19:S2:1656:G:H1	19:S2:1668:U:H3	1.32	0.76
40:L5:2520:C:O2	40:L5:2640:G:N2	2.19	0.76
19:S2:1351:G:H1	19:S2:1360:U:H3	1.33	0.75
19:S2:1729:U:H3	19:S2:1805:G:H1	1.33	0.75
4:SE:79:ASP:HB3	4:SE:82:TYR:HB2	1.68	0.75
19:S2:1650:A:H5''	28:SQ:139:ALA:HB2	1.69	0.75
84:Lt:16:ARG:HE	84:Lt:17:CYS:H	1.33	0.75
40:L5:4421:C:N4	40:L5:4475:G:H22	1.84	0.75
40:L5:2557:G:H1	40:L5:2570:U:H3	1.34	0.74
40:L5:4745:G:H1	40:L5:4955:A:H61	1.33	0.74
1:SA:148:CYS:SG	1:SA:163:CYS:N	2.60	0.74
20:LR:134:ASN:H	20:LR:137:ILE:HD11	1.52	0.74
40:L5:1974:U:H4'	40:L5:1975:G:H3'	1.68	0.74
40:L5:5002:U:H3	40:L5:5045:G:H1	1.34	0.74
40:L5:1273:G:N7	67:Lb:117:ARG:NH1	2.36	0.74
40:L5:3937:C:H1'	55:LN:125:SER:HB3	1.70	0.74
19:S2:106:C:H2'	19:S2:107:A:H8	1.52	0.73
37:At:50:U:H3	37:At:64:G:H1	1.36	0.73
40:L5:1095:A:N1	40:L5:1200:G:O6	2.22	0.72
40:L5:2611:A:H5'	40:L5:2688:G:H4'	1.70	0.72
19:S2:110:U:H3	19:S2:351:G:H1	1.34	0.72
40:L5:262:G:H2'	40:L5:263:G:H8	1.54	0.72
36:Sg:10:THR:HB	36:Sg:306:LEU:HD21	1.69	0.72
40:L5:3868:G:H22	40:L5:3900:G:H1'	1.54	0.72
19:S2:639:C:H2'	19:S2:640:A:H8	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1461:G:H3'	19:S2:1463:U:H3	1.56	0.71
19:S2:1652:G:H1	19:S2:1672:U:H3	1.38	0.71
29:SS:45:LEU:HD22	29:SS:50:ILE:HD11	1.73	0.71
40:L5:4887:C:H42	40:L5:4932:U:H3	1.36	0.71
40:L5:4126:C:H5''	40:L5:4127:A:H5''	1.72	0.71
36:Sg:247:TRP:HB3	36:Sg:258:ILE:HD11	1.73	0.71
11:SO:95:ILE:HB	11:SO:129:ILE:HG22	1.70	0.71
19:S2:1752:C:N4	19:S2:1779:G:N2	2.39	0.71
40:L5:1414:C:H2'	40:L5:1415:G:H8	1.56	0.71
19:S2:508:A:H3'	19:S2:509:OMG:H8	1.55	0.71
40:L5:2780:C:H2'	40:L5:2781:G:H8	1.56	0.70
19:S2:878:G:O6	19:S2:908:A:N1	2.24	0.70
1:SA:41:ARG:HE	1:SA:45:GLY:HA2	1.57	0.70
40:L5:512:U:H3	40:L5:647:G:H1	1.39	0.70
40:L5:1976:G:O6	40:L5:1990:A:N1	2.25	0.70
11:SO:52:THR:HG21	19:S2:952:G:H21	1.56	0.70
40:L5:2845:A:H61	40:L5:3843:C:H42	1.40	0.70
19:S2:851:C:H5''	19:S2:852:G:H5'	1.74	0.70
19:S2:864:A:H2'	19:S2:865:A:H8	1.56	0.70
19:S2:928:G:H2'	19:S2:929:G:C8	2.27	0.69
19:S2:43:U:OP2	19:S2:485:A:N6	2.21	0.69
40:L5:4546:A:N7	43:LA:215:ASN:ND2	2.40	0.69
41:L7:28:C:H1'	41:L7:54:A:H61	1.57	0.69
34:Sd:21:CYS:SG	34:Sd:39:CYS:N	2.64	0.69
37:At:18:G:O6	37:At:55:U:O2	2.11	0.69
40:L5:3780:G:H1	40:L5:3814:U:H3	1.40	0.69
40:L5:2702:C:OP1	61:LU:101:ARG:NH2	2.25	0.69
40:L5:1759:G:N2	40:L5:1773:U:O2	2.22	0.69
72:Lg:83:CYS:SG	72:Lg:86:CYS:HB2	2.32	0.69
13:SW:2:VAL:N	19:S2:1091:C:HO2'	1.91	0.69
40:L5:3824:A:H3'	40:L5:3825:A2M:H8	1.73	0.69
40:L5:323:C:H2'	40:L5:324:A:H8	1.58	0.69
19:S2:1417:C:O2	19:S2:1422:G:O6	2.11	0.69
19:S2:159:A2M:H2	19:S2:467:G:H21	1.58	0.68
19:S2:15:U:O2'	19:S2:669:A:N6	2.27	0.68
34:Sd:39:CYS:HB2	34:Sd:42:CYS:HB2	1.76	0.68
3:SC:173:LYS:HD3	12:SV:3:ASN:HA	1.75	0.68
76:Lk:13:LEU:HA	76:Lk:16:ARG:HG2	1.75	0.68
19:S2:557:U:H2'	19:S2:558:G:C8	2.29	0.68
19:S2:1748:G:H1	19:S2:1786:U:H3	1.42	0.68
29:SS:63:GLU:HG2	29:SS:66:ARG:HH21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:664:G:N2	40:L5:666:G:O6	2.27	0.68
40:L5:3641:U:OP2	40:L5:3646:A:N6	2.27	0.68
36:Sg:87:LEU:HB2	36:Sg:101:PHE:HB2	1.76	0.68
87:L5:5292:SPM:H112	56:LO:91:LYS:HD3	1.75	0.68
1:SA:125:THR:HG22	1:SA:126:ASP:H	1.58	0.68
14:SX:64:SER:HB3	19:S2:614:C:H1'	1.76	0.68
40:L5:1984:A:N7	40:L5:2010:A:O2'	2.27	0.68
2:SB:192:SER:HA	2:SB:195:LYS:HD2	1.76	0.67
7:SI:98:LYS:HB3	19:S2:377:G:H5'	1.75	0.67
84:Lt:76:SER:O	84:Lt:114:ARG:NH2	2.27	0.67
44:LB:90:VAL:HG23	44:LB:163:ILE:HD11	1.77	0.67
17:Sb:20:LYS:NZ	19:S2:1016:U:OP2	2.26	0.67
40:L5:4992:G:H2'	40:L5:4993:G:C8	2.30	0.67
84:Lt:123:ARG:HB2	84:Lt:128:THR:HG21	1.76	0.67
3:SC:193:VAL:HG11	3:SC:240:THR:HG22	1.76	0.67
40:L5:2093:A:N3	40:L5:2094:G:N1	2.43	0.67
6:SH:7:LYS:NZ	6:SH:15:LYS:O	2.28	0.67
17:Sb:65:GLN:HB2	17:Sb:72:ARG:HB3	1.76	0.67
51:LI:54:SER:HB3	51:LI:135:ILE:HD11	1.75	0.67
40:L5:40:G:N2	40:L5:4380:A:N7	2.43	0.67
1:SA:38:ILE:HD11	1:SA:47:TYR:HB3	1.78	0.66
40:L5:505:G:H1	40:L5:653:U:H3	1.42	0.66
17:Sb:56:CYS:HB2	17:Sb:59:CYS:H	1.60	0.66
42:L8:134:G:H5''	63:LX:63:LYS:HD2	1.77	0.66
4:SE:100:ARG:HB2	4:SE:114:ILE:HD13	1.77	0.66
7:SI:124:LYS:NZ	40:L5:5025:C:OP2	2.28	0.66
40:L5:679:C:H2'	40:L5:680:G:H8	1.61	0.66
3:SC:196:ILE:HB	3:SC:223:TYR:HB2	1.76	0.66
37:At:23:C:H2'	37:At:24:A:H8	1.60	0.66
40:L5:4373:G:N7	80:Lo:61:LYS:NZ	2.43	0.66
40:L5:4537:C:H2'	40:L5:4538:G:H8	1.61	0.66
40:L5:308:G:OP2	40:L5:308:G:N2	2.27	0.66
4:SE:19:MET:SD	4:SE:108:ARG:NH1	2.68	0.66
6:SH:144:ILE:HD13	6:SH:154:ILE:HG13	1.78	0.66
5:SG:42:GLY:O	5:SG:46:LYS:NZ	2.28	0.66
57:LP:118:GLN:HE21	57:LP:120:ASN:HD21	1.42	0.66
41:L7:23:A:N3	41:L7:118:C:O2'	2.27	0.65
6:SH:154:ILE:HB	6:SH:185:VAL:HG22	1.77	0.65
26:SM:96:ARG:NH2	26:SM:100:PRO:O	2.29	0.65
31:SU:66:ARG:HH12	31:SU:75:LYS:HD3	1.62	0.65
6:SH:30:LEU:HG	6:SH:33:ASN:HD22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1403:C:N4	19:S2:1433:C:OP1	2.29	0.65
27:SP:18:ARG:NH1	29:SS:88:LYS:O	2.29	0.65
40:L5:1326:A2M:H2'	40:L5:1327:C:C6	2.31	0.65
40:L5:3594:C:O2	40:L5:3597:G:N2	2.30	0.65
32:SZ:68:ILE:HD11	32:SZ:73:VAL:HB	1.79	0.65
40:L5:4122:G:H4'	72:Lg:90:ARG:HG2	1.79	0.65
42:L8:90:C:H1'	64:LY:24:HIS:HB3	1.77	0.65
19:S2:1756:C:N4	19:S2:1775:U:O4	2.30	0.65
37:At:23:C:H2'	37:At:24:A:C8	2.31	0.65
19:S2:1844:U:OP1	79:Ln:11:ARG:NH2	2.30	0.65
40:L5:1995:G:N2	84:Lt:121:LEU:O	2.30	0.65
32:SZ:58:LEU:HD12	32:SZ:62:VAL:HG21	1.79	0.65
40:L5:300:A:H2'	40:L5:301:G:H8	1.61	0.65
40:L5:3672:G:OP2	40:L5:3672:G:N2	2.29	0.65
47:LE:281:ILE:HD12	47:LE:286:LEU:HD11	1.78	0.65
19:S2:146:G:H1	19:S2:173:A:N6	1.95	0.65
19:S2:1546:G:H22	19:S2:1655:C:H1'	1.63	0.64
19:S2:1603:G:H21	29:SS:24:ARG:HH21	1.45	0.64
1:SA:198:MET:HE1	1:SA:200:ASP:HB2	1.78	0.64
41:L7:92:C:H2'	41:L7:93:G:H8	1.62	0.64
1:SA:102:ARG:HH21	1:SA:105:PRO:HD3	1.63	0.64
40:L5:2870:A:OP2	40:L5:2879:A:N6	2.30	0.64
84:Lt:37:LEU:HA	84:Lt:40:LYS:HE3	1.80	0.64
3:SC:68:ARG:HG2	3:SC:277:HIS:HB2	1.78	0.64
6:SH:144:ILE:HD11	6:SH:152:ARG:HB3	1.80	0.64
19:S2:874:G:H2'	19:S2:875:A:H8	1.62	0.64
40:L5:758:G:H4'	50:LH:51:LYS:HE3	1.80	0.64
5:SG:146:ASN:O	21:LW:101:ARG:NH1	2.31	0.64
19:S2:191:A:N6	19:S2:208:G:O2'	2.30	0.64
40:L5:1094:G:O6	40:L5:1201:U:O2	2.15	0.64
40:L5:4523:A2M:H5''	40:L5:4524:G:H5'	1.79	0.64
40:L5:2845:A:H61	40:L5:3843:C:N4	1.96	0.64
40:L5:4101:C:O2'	40:L5:4109:G:O6	2.16	0.64
84:Lt:16:ARG:HH22	84:Lt:28:LEU:HB3	1.61	0.64
13:SW:107:SER:HB2	19:S2:860:G:H21	1.62	0.64
40:L5:1870:C:H2'	40:L5:1871:A2M:H8	1.79	0.64
3:SC:182:CYS:HB2	13:SW:95:PRO:HB2	1.80	0.63
5:SG:2:LYS:HD3	5:SG:15:LEU:HD21	1.80	0.63
29:SS:67:VAL:HG12	29:SS:71:MET:HE2	1.80	0.63
40:L5:4558:U:OP2	44:LB:246:ARG:NH2	2.30	0.63
47:LE:264:ILE:HD11	47:LE:267:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Lr:46:ARG:O	82:Lr:70:GLN:NE2	2.30	0.63
5:SG:56:ASN:OD1	19:S2:155:G:N2	2.31	0.63
19:S2:1403:C:OP2	19:S2:1405:A:N6	2.30	0.63
19:S2:1536:G:H2'	19:S2:1537:A:H8	1.62	0.63
19:S2:1850:MA6:H2'	19:S2:1851:MA6:H8	1.80	0.63
40:L5:174:C:OP1	53:LL:129:ARG:NH2	2.31	0.63
40:L5:4272:G:N2	40:L5:4272:G:OP2	2.30	0.63
15:SY:36:PRO:HG3	19:S2:570:C:H4'	1.79	0.63
19:S2:668:A2M:H2'	19:S2:669:A:N7	2.14	0.63
2:SB:60:ASP:HA	2:SB:63:LYS:HD2	1.79	0.63
6:SH:8:ILE:HG13	6:SH:9:VAL:HG23	1.79	0.63
8:SJ:80:ARG:NH2	19:S2:818:A:OP1	2.32	0.63
17:Sb:26:GLN:NE2	19:S2:921:G:OP2	2.31	0.63
19:S2:1513:C:H2'	19:S2:1514:G:H8	1.63	0.63
50:LH:106:GLN:HB2	50:LH:111:LEU:HB3	1.79	0.63
40:L5:1700:G:H5''	40:L5:1704:C:H42	1.64	0.63
40:L5:3659:G:OP1	43:LA:241:ARG:NH1	2.31	0.63
40:L5:4088:C:H2'	40:L5:4089:G:H8	1.64	0.63
75:Lj:2:THR:HG22	75:Lj:4:GLY:H	1.63	0.63
16:Sa:59:PHE:HB2	16:Sa:62:TYR:HB2	1.81	0.63
19:S2:603:C:N4	19:S2:620:G:O6	2.32	0.63
21:LW:1:MET:HG3	44:LB:366:LYS:HB3	1.81	0.63
40:L5:327:U:O2'	74:Li:30:ARG:NH1	2.31	0.63
40:L5:1332:C:H2'	40:L5:1333:A:H8	1.64	0.63
19:S2:885:U:O2	19:S2:901:G:O6	2.17	0.63
40:L5:1646:A:O2'	75:Lj:49:TRP:O	2.17	0.63
40:L5:4304:A:OP2	40:L5:4305:G:N2	2.32	0.63
5:SG:186:GLN:NE2	19:S2:332:G:O6	2.32	0.63
19:S2:690:G:H3'	19:S2:691:G:H21	1.64	0.63
19:S2:1752:C:N3	19:S2:1779:G:N1	2.46	0.63
40:L5:1743:A:N1	40:L5:1789:C:O2'	2.29	0.63
40:L5:3722:G:H2'	40:L5:3723:A:H8	1.64	0.63
40:L5:4174:U:H2'	40:L5:4175:G:H8	1.63	0.63
4:SE:11:ARG:NH1	4:SE:24:THR:OG1	2.27	0.63
22:SR:20:TYR:HD2	22:SR:23:ARG:HG3	1.63	0.62
40:L5:1683:PSU:H2'	40:L5:1684:A:H8	1.64	0.62
40:L5:4280:A:OP2	46:LD:23:ARG:NH2	2.32	0.62
19:S2:1536:G:H2'	19:S2:1537:A:C8	2.34	0.62
40:L5:2601:A:N6	40:L5:2744:A:OP2	2.31	0.62
40:L5:2613:C:OP1	72:Lg:24:ARG:NH2	2.32	0.62
53:LL:209:LYS:HG3	53:LL:210:LYS:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:SX:64:SER:OG	19:S2:1824:A:N6	2.33	0.62
21:LW:2:LYS:NZ	62:LV:92:ASP:O	2.33	0.62
40:L5:4745:G:H1	40:L5:4955:A:N6	1.96	0.62
45:LC:317:ASN:HD22	45:LC:320:LYS:HD3	1.64	0.62
3:SC:194:ARG:NH1	19:S2:1156:U:O4	2.33	0.62
19:S2:149:A:H3'	19:S2:150:A:H8	1.64	0.62
19:S2:454:U:H2'	19:S2:455:A:H8	1.65	0.62
40:L5:369:G:N2	40:L5:372:A:OP2	2.26	0.62
40:L5:655:C:OP1	45:LC:268:ARG:NH1	2.32	0.62
40:L5:1972:G:C6	40:L5:1973:G:O6	2.52	0.62
40:L5:4525:C:OP1	44:LB:246:ARG:NH1	2.32	0.62
42:L8:62:A:OP1	73:Lh:52:LYS:NZ	2.33	0.62
19:S2:1426:U:OP1	28:SQ:69:ARG:NH1	2.33	0.62
40:L5:312:G:H1	40:L5:325:U:H3	1.47	0.62
19:S2:1289:U:H4'	25:SK:2:LEU:HD21	1.81	0.62
40:L5:1095:A:N1	40:L5:1200:G:C6	2.68	0.62
40:L5:4980:C:N3	57:LP:69:ARG:NH2	2.47	0.62
19:S2:115:U:H2'	19:S2:116:OMU:H6	1.80	0.62
26:SM:52:LEU:HD11	26:SM:62:VAL:HG12	1.82	0.62
38:Pt:23:C:H2'	38:Pt:24:A:H8	1.64	0.62
4:SE:38:LEU:HD22	19:S2:346:C:H5''	1.82	0.62
19:S2:300:U:H2'	19:S2:301:A:H8	1.65	0.62
26:SM:36:ARG:NH1	35:Sf:105:TYR:OH	2.32	0.62
40:L5:3930:U:H3	40:L5:4180:G:H1	1.48	0.62
40:L5:4541:G:N2	40:L5:4544:A:OP2	2.33	0.62
24:SF:39:ILE:HD12	24:SF:68:ILE:HD12	1.82	0.62
28:SQ:43:GLU:OE2	28:SQ:77:HIS:ND1	2.33	0.62
40:L5:1382:G:H2'	40:L5:1383:G:H8	1.64	0.62
19:S2:1183:A:H2'	19:S2:1184:G:H8	1.63	0.61
21:LW:116:LYS:HA	21:LW:119:LYS:HE2	1.81	0.61
28:SQ:32:ILE:HG12	28:SQ:68:ILE:HD12	1.82	0.61
40:L5:1185:G:N2	46:LD:282:GLN:OE1	2.33	0.61
40:L5:3664:G:H2'	40:L5:3665:G:H8	1.64	0.61
40:L5:4084:G:N7	43:LA:72:ARG:NH2	2.45	0.61
66:La:89:ASN:HA	66:La:92:LYS:HE3	1.80	0.61
14:SX:68:LYS:HG3	18:Se:6:LEU:HD23	1.81	0.61
19:S2:1550:G:H3'	19:S2:1579:A:H61	1.65	0.61
36:Sg:99:ARG:NH1	36:Sg:134:THR:O	2.33	0.61
40:L5:3921:U:H1'	40:L5:4543:G:H21	1.65	0.61
43:LA:101:VAL:HG22	43:LA:165:VAL:HG22	1.83	0.61
83:Ls:50:LYS:NZ	83:Ls:91:THR:OG1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Sb:33:MET:HB2	17:Sb:79:PHE:HB2	1.82	0.61
40:L5:1516:G:O2'	53:LL:18:TRP:NE1	2.33	0.61
83:Ls:175:LEU:HD21	83:Ls:182:PRO:HB3	1.81	0.61
9:SL:7:GLU:OE2	9:SL:11:GLN:NE2	2.33	0.61
16:Sa:11:ALA:O	16:Sa:15:ARG:NH2	2.33	0.61
19:S2:104:A:N6	19:S2:356:C:O2	2.33	0.61
19:S2:1528:G:O2'	19:S2:1666:C:OP1	2.17	0.61
40:L5:184:U:O2	40:L5:254:G:O6	2.18	0.61
40:L5:1335:G:H21	45:LC:95:MET:HB2	1.64	0.61
27:SP:56:LEU:HD22	27:SP:80:LEU:HD11	1.81	0.61
40:L5:1850:A:N3	40:L5:2283:G:O2'	2.32	0.61
40:L5:3907:G:N2	90:L5:5294:HMT:O8	2.34	0.61
1:SA:85:ARG:HD3	1:SA:203:PHE:O	2.01	0.61
20:LR:173:ARG:O	20:LR:176:ARG:NH1	2.33	0.61
40:L5:436:C:H2'	40:L5:437:G:H8	1.66	0.61
40:L5:691:C:H2'	40:L5:692:A:H8	1.65	0.61
40:L5:1933:G:H2'	40:L5:1934:A:C8	2.35	0.61
4:SE:42:LEU:HG	4:SE:109:PHE:HD2	1.65	0.61
5:SG:159:ARG:HH12	19:S2:76:U:H2'	1.65	0.61
40:L5:4221:C:OP1	87:L5:5262:SPM:N14	2.34	0.61
40:L5:4322:G:N2	40:L5:4325:A:OP2	2.32	0.61
43:LA:229:ALA:HB3	43:LA:234:LYS:HB3	1.83	0.61
81:Lp:38:THR:HA	81:Lp:45:THR:HA	1.83	0.61
7:SI:168:GLN:OE1	40:L5:5027:C:N4	2.34	0.61
30:ST:102:ARG:HA	30:ST:105:GLN:HB2	1.82	0.61
40:L5:2295:C:H2'	40:L5:2296:G:H8	1.66	0.61
40:L5:1457:G:O2'	58:LQ:75:ARG:NH2	2.34	0.61
17:Sb:11:SER:OG	17:Sb:14:GLU:OE1	2.19	0.60
23:SD:204:LEU:HB2	23:SD:207:HIS:HB3	1.82	0.60
40:L5:511:C:OP2	53:LL:163:LYS:NZ	2.33	0.60
40:L5:1971:C:N4	40:L5:1972:G:O6	2.34	0.60
40:L5:1972:G:N1	40:L5:1995:G:O6	2.34	0.60
40:L5:1354:A:N6	40:L5:1503:A:O4'	2.34	0.60
6:SH:105:THR:HG23	6:SH:107:LYS:H	1.65	0.60
19:S2:1231:C:H42	19:S2:1527:C:H42	1.47	0.60
40:L5:966:A:H5''	40:L5:2092:G:H22	1.66	0.60
40:L5:2033:A:OP1	51:LI:162:ARG:NH2	2.34	0.60
40:L5:2588:C:OP1	40:L5:2768:C:O2'	2.18	0.60
48:LF:105:VAL:HG13	48:LF:136:VAL:HG12	1.84	0.60
61:LU:65:ARG:HG2	61:LU:67:LYS:H	1.64	0.60
19:S2:1222:G:H5''	24:SF:78:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1228:A:H2'	19:S2:1229:G:C8	2.36	0.60
40:L5:62:A:N3	40:L5:77:U:O2'	2.31	0.60
40:L5:3772:U:H3	40:L5:3776:G:H22	1.49	0.60
42:L8:153:C:H2'	42:L8:154:G:H8	1.67	0.60
19:S2:323:C:H2'	19:S2:327:G:H1	1.66	0.60
19:S2:1841:C:H2'	19:S2:1842:4AC:H6	1.83	0.60
34:Sd:22:ARG:NE	34:Sd:36:LEU:O	2.32	0.60
36:Sg:208:ALA:HB2	36:Sg:218:LEU:HD13	1.83	0.60
40:L5:148:C:OP2	49:LG:197:LYS:NZ	2.34	0.60
40:L5:2325:C:O2'	70:Le:124:ASN:ND2	2.34	0.60
4:SE:44:LEU:HD11	4:SE:72:ILE:HD11	1.84	0.60
5:SG:66:GLY:HA2	19:S2:1745:A:H1'	1.81	0.60
10:SN:124:ARG:NH2	19:S2:1024:A:OP2	2.30	0.60
40:L5:644:G:OP1	53:LL:162:LYS:NZ	2.31	0.60
40:L5:1669:A:N3	40:L5:1852:U:O2'	2.33	0.60
40:L5:907:C:H2'	40:L5:908:G:H8	1.66	0.60
46:LD:64:ILE:HD13	46:LD:109:LEU:HD22	1.84	0.60
3:SC:169:TYR:OH	3:SC:175:GLY:O	2.17	0.60
38:Pt:23:C:H2'	38:Pt:24:A:C8	2.36	0.60
2:SB:114:VAL:O	19:S2:1869:A:N6	2.35	0.60
28:SQ:117:ARG:HH21	28:SQ:121:VAL:HG21	1.66	0.60
36:Sg:40:ILE:HB	36:Sg:59:LEU:HB2	1.83	0.60
36:Sg:201:SER:HG	36:Sg:205:SER:H	1.50	0.60
40:L5:940:C:OP1	48:LF:242:ARG:NH2	2.35	0.60
40:L5:3917:A:H2'	40:L5:3918:G:H8	1.67	0.60
40:L5:4347:G:H2'	40:L5:4348:A:C8	2.37	0.60
40:L5:4457:PSU:OP1	62:LV:50:ASN:ND2	2.35	0.60
84:Lt:134:GLY:HA3	84:Lt:152:ILE:HD11	1.83	0.60
16:Sa:38:LYS:HB2	16:Sa:71:LEU:HB2	1.82	0.60
40:L5:1346:C:H2'	40:L5:1347:G:H8	1.66	0.60
40:L5:2623:A:OP1	61:LU:101:ARG:NE	2.35	0.60
40:L5:4742:G:OP1	40:L5:4900:C:N4	2.33	0.60
1:SA:68:ILE:HG22	1:SA:70:ASN:H	1.67	0.59
1:SA:222:VAL:HG13	1:SA:223:THR:HG23	1.83	0.59
36:Sg:10:THR:HG22	36:Sg:308:ARG:HG2	1.82	0.59
40:L5:305:A:OP2	55:LN:15:GLN:NE2	2.32	0.59
40:L5:2579:G:N2	40:L5:2582:A:OP2	2.35	0.59
40:L5:5055:G:N2	69:Ld:118:GLN:OE1	2.31	0.59
43:LA:20:VAL:HA	43:LA:23:ARG:HG3	1.83	0.59
67:Lb:116:LEU:HG	67:Lb:117:ARG:HH21	1.66	0.59
19:S2:1854:U:H2'	19:S2:1855:G:H8	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:SF:101:HIS:HB2	24:SF:108:PRO:HG3	1.83	0.59
24:SF:127:ARG:HG3	24:SF:136:ARG:HB3	1.84	0.59
33:Sc:29:GLN:NE2	33:Sc:66:ARG:O	2.35	0.59
40:L5:654:C:H4'	45:LC:269:LYS:HD3	1.84	0.59
40:L5:3873:G:H2'	40:L5:3874:G:C8	2.37	0.59
40:L5:4910:G:N2	56:LO:106:ASP:O	2.34	0.59
76:Lk:25:ILE:HB	76:Lk:68:GLU:HG2	1.85	0.59
6:SH:31:GLU:HA	6:SH:37:LYS:HG3	1.83	0.59
7:SI:9:HIS:HE1	19:S2:386:C:H4'	1.66	0.59
8:SJ:63:LEU:O	8:SJ:70:ARG:NH1	2.34	0.59
19:S2:1446:A:H5''	31:SU:58:THR:HG23	1.84	0.59
19:S2:1452:A:OP2	22:SR:32:LYS:NZ	2.34	0.59
40:L5:1818:G:OP2	40:L5:1818:G:N2	2.33	0.59
42:L8:14:U:H5''	57:LP:123:PRO:HG3	1.84	0.59
80:Lo:2:VAL:N	80:Lo:90:HIS:O	2.35	0.59
82:Lr:16:PHE:HB3	82:Lr:27:THR:H	1.67	0.59
5:SG:94:ARG:NH2	19:S2:454:U:O2'	2.36	0.59
19:S2:94:G:HO2'	19:S2:508:A:HO2'	1.48	0.59
19:S2:1336:C:O3'	34:Sd:44:ARG:NH2	2.35	0.59
19:S2:1568:C:H2'	19:S2:1569:A:C8	2.38	0.59
40:L5:691:C:H2'	40:L5:692:A:C8	2.37	0.59
40:L5:4861:G:H2'	40:L5:4862:G:H8	1.67	0.59
19:S2:475:C:O2'	19:S2:507:G:N3	2.34	0.59
36:Sg:196:ASN:ND2	36:Sg:236:ILE:O	2.34	0.59
40:L5:2483:G:O6	40:L5:2495:U:O4	2.21	0.59
5:SG:145:PHE:O	21:LW:101:ARG:NH2	2.35	0.59
14:SX:68:LYS:NZ	19:S2:616:A:OP1	2.35	0.59
19:S2:629:A:O2'	19:S2:631:U:OP1	2.21	0.59
19:S2:1130:G:N2	19:S2:1130:G:OP2	2.35	0.59
19:S2:1658:G:OP2	19:S2:1660:C:N4	2.35	0.59
24:SF:126:THR:HA	24:SF:135:ARG:HD2	1.85	0.59
40:L5:97:G:OP1	53:LL:16:LYS:NZ	2.31	0.59
40:L5:1667:G:H21	40:L5:2282:A:H62	1.49	0.59
40:L5:4129:G:O6	40:L5:4156:G:N2	2.36	0.59
17:Sb:72:ARG:HH22	19:S2:1120:U:H5'	1.67	0.59
36:Sg:89:LEU:HB2	36:Sg:101:PHE:HE1	1.65	0.59
46:LD:19:LYS:O	46:LD:24:ARG:NH1	2.34	0.59
3:SC:168:GLY:N	3:SC:179:THR:O	2.30	0.59
28:SQ:58:LEU:HD13	28:SQ:108:ILE:HD11	1.85	0.59
40:L5:709:C:OP1	71:Lf:46:ARG:NH2	2.36	0.59
40:L5:3861:A:H2'	40:L5:3862:A:H8	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:L5:5291:SPD:N6	55:LN:70:GLY:O	2.36	0.59
49:LG:105:GLU:OE2	49:LG:113:ARG:NH2	2.36	0.59
49:LG:200:THR:HG22	49:LG:201:THR:HG23	1.85	0.59
6:SH:53:VAL:HG11	6:SH:172:THR:HA	1.85	0.59
7:SI:81:VAL:HG22	7:SI:102:VAL:HG12	1.85	0.59
15:SY:41:ARG:HG3	15:SY:55:ILE:HB	1.84	0.59
19:S2:1630:A:O2'	29:SS:85:ASN:ND2	2.36	0.59
40:L5:1976:G:H1	40:L5:1990:A:H2	1.50	0.59
40:L5:4246:G:H2'	40:L5:4247:G:H8	1.68	0.59
40:L5:4762:A:OP2	56:LO:12:ARG:NH1	2.36	0.59
19:S2:1563:G:H5''	30:ST:121:ARG:HH21	1.67	0.59
19:S2:1647:A:OP1	28:SQ:138:ARG:NH2	2.36	0.59
19:S2:1858:G:H2'	19:S2:1859:A:H8	1.68	0.59
40:L5:1323:A2M:H2'	40:L5:1324:A:O4'	2.02	0.59
40:L5:2908:U:O2'	40:L5:3586:G:O6	2.19	0.59
40:L5:3726:A:O2'	40:L5:3727:A:O5'	2.21	0.59
40:L5:4238:G:H2'	40:L5:4239:A:H8	1.67	0.59
46:LD:287:PHE:HZ	51:LI:214:SER:HB3	1.68	0.59
2:SB:150:ILE:HG12	19:S2:1124:C:H5''	1.85	0.58
6:SH:12:ASN:ND2	6:SH:14:GLU:OE1	2.36	0.58
40:L5:1207:C:H2'	40:L5:1208:G:H8	1.67	0.58
40:L5:1927:U:OP1	40:L5:1949:U:O2'	2.14	0.58
60:LT:88:ARG:NH1	67:Lb:33:LYS:O	2.36	0.58
8:SJ:162:ARG:NH2	19:S2:583:A:OP1	2.36	0.58
19:S2:1851:MA6:OP1	79:Ln:9:ARG:NH2	2.35	0.58
37:At:68:G:H2'	37:At:69:A:H8	1.69	0.58
40:L5:1188:C:H2'	40:L5:1189:G:C8	2.38	0.58
83:Ls:96:THR:HG22	83:Ls:99:ARG:HH21	1.67	0.58
40:L5:1594:C:HO2'	40:L5:1597:G:HO2'	1.52	0.58
40:L5:2758:G:O2'	40:L5:2765:A:N3	2.34	0.58
40:L5:4761:G:OP2	56:LO:37:ARG:NH2	2.36	0.58
4:SE:45:ILE:HG13	4:SE:61:VAL:HG11	1.85	0.58
19:S2:146:G:H2'	19:S2:147:A:H8	1.68	0.58
19:S2:1069:U:H5''	43:LA:248:GLY:HA2	1.85	0.58
40:L5:1670:G:OP1	67:Lb:12:GLN:NE2	2.33	0.58
40:L5:4077:A:N1	40:L5:4171:C:N4	2.50	0.58
7:SI:31:ARG:NH2	19:S2:381:C:OP1	2.37	0.58
19:S2:1616:U:O2'	19:S2:1661:A:N3	2.32	0.58
19:S2:1644:C:H4'	28:SQ:140:ARG:HB2	1.86	0.58
19:S2:1706:G:O2'	19:S2:1850:MA6:O2'	2.19	0.58
40:L5:4887:C:N4	40:L5:4932:U:H3	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:LI:61:SER:HA	51:LI:126:VAL:HG12	1.84	0.58
5:SG:59:GLN:OE1	5:SG:72:ARG:NH2	2.36	0.58
37:At:6:C:H2'	37:At:7:G:H8	1.69	0.58
40:L5:1906:U:H2'	40:L5:1907:A:H8	1.68	0.58
40:L5:3717:A:OP2	40:L5:3735:G:N2	2.35	0.58
40:L5:5047:C:O2'	40:L5:5050:C:OP2	2.22	0.58
55:LN:155:VAL:O	55:LN:162:ARG:NH2	2.37	0.58
8:SJ:124:HIS:CG	18:Se:35:ARG:HE	2.21	0.58
19:S2:1598:G:N2	19:S2:1599:U:O4	2.36	0.58
19:S2:1598:G:O2'	32:SZ:80:ARG:O	2.20	0.58
40:L5:4637:OMG:OP1	69:Ld:30:HIS:NE2	2.37	0.58
40:L5:4694:G:O2'	50:LH:71:ARG:NH2	2.33	0.58
16:Sa:28:ARG:NH2	19:S2:1839:U:O4	2.29	0.58
19:S2:1673:U:H5''	28:SQ:78:VAL:HG12	1.85	0.58
36:Sg:129:ILE:HB	36:Sg:142:VAL:HB	1.84	0.58
40:L5:172:C:H4'	40:L5:173:C:H5'	1.86	0.58
40:L5:1495:G:H4'	58:LQ:187:LYS:HE3	1.86	0.58
40:L5:2753:G:H2'	40:L5:2754:G:C4	2.39	0.58
64:LY:10:ASP:HB3	64:LY:13:LYS:HB2	1.86	0.58
5:SG:91:GLU:OE1	19:S2:452:G:O2'	2.22	0.58
6:SH:10:LYS:HE3	6:SH:17:ASP:HB3	1.84	0.58
15:SY:107:ARG:NH2	19:S2:492:C:OP2	2.37	0.58
16:Sa:89:ARG:HG3	16:Sa:92:ARG:HH21	1.69	0.58
18:Se:34:ARG:HH21	19:S2:642:U:H5	1.50	0.58
19:S2:645:C:H2'	19:S2:646:G:H8	1.69	0.58
19:S2:696:G:N2	19:S2:730:C:OP2	2.36	0.58
40:L5:2411:C:H2'	40:L5:2412:A:H8	1.68	0.58
40:L5:2884:G:H2'	40:L5:2885:A:H8	1.68	0.58
40:L5:3880:G:H2'	40:L5:3881:G:C8	2.39	0.58
43:LA:107:MET:HB3	43:LA:111:THR:HG21	1.86	0.58
4:SE:94:LYS:NZ	15:SY:19:GLN:OE1	2.36	0.58
5:SG:134:GLY:O	19:S2:65:C:N4	2.35	0.58
13:SW:111:MET:HE3	13:SW:116:ALA:HA	1.84	0.58
19:S2:691:G:N7	19:S2:692:G:N2	2.52	0.58
19:S2:1146:C:O2'	19:S2:1150:A:N1	2.35	0.58
19:S2:1337:4AC:H2'	19:S2:1338:G:C8	2.39	0.58
40:L5:2845:A:N6	40:L5:3843:C:H42	2.02	0.58
47:LE:278:THR:HG22	47:LE:280:GLY:H	1.68	0.58
52:LJ:146:ARG:HG2	52:LJ:147:ARG:HG3	1.86	0.58
19:S2:1562:C:H2'	19:S2:1563:G:C8	2.39	0.57
24:SF:17:ILE:HG21	24:SF:46:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Sg:130:LYS:HG2	36:Sg:141:THR:HG22	1.86	0.57
13:SW:18:GLU:HG3	13:SW:69:LEU:HB3	1.85	0.57
14:SX:95:GLU:OE2	14:SX:140:ARG:NH2	2.35	0.57
16:Sa:5:ARG:HH21	19:S2:1864:U:H3'	1.69	0.57
19:S2:1030:A:H2'	19:S2:1031:A2M:H8	1.86	0.57
19:S2:1606:G:O2'	19:S2:1632:G:N2	2.35	0.57
20:LR:169:ALA:HA	20:LR:172:ARG:HE	1.69	0.57
38:Pt:8:U:O2'	38:Pt:21:A:N1	2.34	0.57
40:L5:416:U:H4'	40:L5:2330:G:H4'	1.86	0.57
40:L5:2088:A:OP2	58:LQ:37:ARG:NH2	2.38	0.57
40:L5:3746:A:H5''	43:LA:244:GLY:HA3	1.86	0.57
40:L5:4604:G:N2	40:L5:4607:A:OP2	2.36	0.57
47:LE:261:ILE:HG23	47:LE:267:LEU:HD23	1.86	0.57
77:Ll:33:ASN:ND2	77:Ll:35:ILE:O	2.37	0.57
10:SN:14:SER:HB3	19:S2:1016:U:H5''	1.86	0.57
19:S2:527:C:H2'	19:S2:528:A:C8	2.38	0.57
19:S2:1010:G:H2'	19:S2:1011:A:H8	1.69	0.57
40:L5:4377:G:O6	66:La:42:ARG:NH1	2.38	0.57
40:L5:4991:U:H2'	40:L5:4992:G:C8	2.39	0.57
43:LA:206:PRO:HG3	43:LA:213:GLY:HA3	1.86	0.57
44:LB:393:LYS:HG3	44:LB:396:ARG:HH21	1.70	0.57
19:S2:1755:C:H2'	19:S2:1756:C:C6	2.39	0.57
26:SM:58:GLU:OE1	26:SM:61:TYR:N	2.37	0.57
40:L5:1390:G:N2	40:L5:1393:G:OP2	2.31	0.57
45:LC:67:TRP:HB3	45:LC:71:ARG:HD3	1.85	0.57
56:LO:126:VAL:HG13	56:LO:127:VAL:HG13	1.85	0.57
4:SE:187:ALA:N	19:S2:809:A:OP1	2.34	0.57
19:S2:1720:U:O2'	40:L5:3796:U:O2'	2.19	0.57
40:L5:424:U:H3	42:L8:10:G:H1	1.51	0.57
40:L5:4194:U:O2'	51:Ll:116:ARG:NH2	2.38	0.57
42:L8:13:G:O2'	57:LP:121:LYS:O	2.19	0.57
50:LH:115:ARG:HD3	50:LH:123:ILE:HD12	1.84	0.57
62:LV:83:ARG:HB2	62:LV:102:ALA:HB3	1.84	0.57
2:SB:149:GLN:NE2	19:S2:1123:C:OP1	2.38	0.57
19:S2:1314:U:H4'	25:SK:8:ARG:HH21	1.69	0.57
40:L5:1358:G:OP1	45:LC:117:THR:N	2.37	0.57
40:L5:3896:C:O2	44:LB:268:ARG:NH2	2.38	0.57
42:L8:19:C:H2'	42:L8:20:A:H8	1.68	0.57
43:LA:172:GLY:HA3	81:Lp:73:THR:HG21	1.87	0.57
1:SA:212:LYS:O	1:SA:215:GLN:NE2	2.37	0.57
5:SG:129:VAL:O	21:LW:80:ARG:NH2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SN:2:GLY:N	19:S2:923:G:OP1	2.38	0.57
10:SN:66:VAL:HG13	10:SN:67:THR:HG23	1.87	0.57
11:SO:143:LYS:HB2	19:S2:1047:C:H5''	1.86	0.57
19:S2:472:C:O2	19:S2:475:C:N4	2.37	0.57
36:Sg:226:HIS:NE2	36:Sg:229:THR:OG1	2.35	0.57
40:L5:4251:A:H5''	52:LJ:108:GLY:HA3	1.86	0.57
11:SO:150:ARG:NH2	19:S2:1854:U:OP1	2.38	0.57
29:SS:22:GLY:HA2	29:SS:56:ALA:HB3	1.87	0.57
40:L5:85:G:O2'	40:L5:97:G:O6	2.21	0.57
40:L5:512:U:O4	40:L5:647:G:O6	2.21	0.57
40:L5:697:G:H2'	40:L5:698:G:H8	1.70	0.57
40:L5:1514:U:H2'	40:L5:1515:A:H8	1.69	0.57
45:LC:39:PHE:O	45:LC:43:ASN:ND2	2.37	0.57
15:SY:55:ILE:HG23	15:SY:75:ILE:HG22	1.87	0.57
19:S2:909:G:OP1	20:LR:172:ARG:NH1	2.38	0.57
19:S2:1228:A:H2'	19:S2:1229:G:H8	1.69	0.57
19:S2:1495:G:N2	34:Sd:42:CYS:SG	2.68	0.57
19:S2:1651:A:H2'	19:S2:1652:G:H8	1.70	0.57
40:L5:1095:A:H2	40:L5:1200:G:C2	2.23	0.57
40:L5:1950:U:H2'	40:L5:1951:G:H8	1.70	0.57
44:LB:50:LYS:HB2	44:LB:345:LEU:HD11	1.87	0.57
40:L5:469:C:N3	47:LE:105:ARG:NH2	2.45	0.57
40:L5:2348:G:OP1	40:L5:2351:OMC:N4	2.38	0.57
40:L5:4670:C:O2'	40:L5:4672:A:OP2	2.23	0.57
42:L8:67:U:H2'	42:L8:68:G:H8	1.70	0.57
4:SE:131:VAL:HA	4:SE:137:PRO:HA	1.87	0.56
10:SN:46:THR:HB	10:SN:86:GLU:HG3	1.86	0.56
16:Sa:11:ALA:H	16:Sa:33:ASP:HB2	1.69	0.56
19:S2:110:U:O2	19:S2:351:G:N2	2.33	0.56
19:S2:1337:4AC:H2'	19:S2:1338:G:H8	1.70	0.56
19:S2:1595:U:H2'	19:S2:1596:U:C6	2.40	0.56
40:L5:13:U:OP2	88:L8:203:SPD:N10	2.37	0.56
40:L5:2317:C:OP1	70:Le:14:LYS:NZ	2.38	0.56
40:L5:3855:C:H2'	40:L5:3856:A:H8	1.70	0.56
40:L5:4094:G:N2	40:L5:4115:G:OP2	2.38	0.56
48:LF:236:ARG:HB2	48:LF:239:GLN:HB2	1.87	0.56
50:LH:95:VAL:HG12	78:Lm:82:LEU:HD13	1.87	0.56
19:S2:556:U:H3'	19:S2:557:U:H4'	1.86	0.56
36:Sg:106:LYS:HE3	36:Sg:126:ASP:HA	1.86	0.56
40:L5:2406:G:N7	77:Ll:2:SER:N	2.53	0.56
1:SA:210:ILE:HG12	22:SR:80:ARG:HE	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:134:HIS:NE2	19:S2:561:A:O2'	2.37	0.56
19:S2:13:C:O2'	19:S2:1356:G:N2	2.38	0.56
19:S2:1455:A:H2'	19:S2:1456:G:H8	1.70	0.56
25:SK:18:GLU:HB2	25:SK:93:THR:HG23	1.86	0.56
38:Pt:50:U:H3	38:Pt:64:G:H1	1.52	0.56
40:L5:20:U:OP2	42:L8:36:G:N2	2.35	0.56
40:L5:22:G:OP1	75:Lj:44:LYS:N	2.39	0.56
40:L5:956:A:H1'	40:L5:2076:G:H5''	1.88	0.56
40:L5:1521:C:OP1	45:LC:100:ARG:NH2	2.32	0.56
40:L5:1730:U:H1'	60:LT:101:SER:HB3	1.88	0.56
40:L5:1795:A:N3	41:L7:79:U:O2'	2.38	0.56
40:L5:1845:U:H2'	40:L5:1846:G:H8	1.71	0.56
40:L5:2544:G:H22	42:L8:124:U:H5'	1.70	0.56
40:L5:3687:A:O2'	43:LA:236:GLY:N	2.38	0.56
40:L5:4177:C:H2'	40:L5:4178:A:H8	1.70	0.56
40:L5:4985:U:O2	44:LB:174:ARG:NH1	2.33	0.56
42:L8:96:C:H5''	73:Lh:66:LYS:HG2	1.88	0.56
43:LA:114:CYS:HB3	43:LA:165:VAL:HB	1.87	0.56
44:LB:36:ASP:OD2	44:LB:38:SER:OG	2.23	0.56
44:LB:222:VAL:O	44:LB:343:ARG:NH1	2.38	0.56
7:SI:4:SER:OG	7:SI:6:ASP:OD2	2.22	0.56
9:SL:135:SER:O	9:SL:139:ARG:NH1	2.38	0.56
19:S2:145:G:H2'	19:S2:146:G:C8	2.40	0.56
19:S2:1737:G:H1	19:S2:1797:U:H3	1.54	0.56
19:S2:1777:G:H2'	19:S2:1778:C:H6	1.70	0.56
40:L5:1541:C:H1'	40:L5:2448:G:H21	1.70	0.56
40:L5:2520:C:H2'	40:L5:2521:G:H8	1.69	0.56
40:L5:4620:OMU:OP2	40:L5:4670:C:N4	2.39	0.56
53:LL:119:GLU:HG2	53:LL:123:LYS:HD2	1.85	0.56
64:LY:33:PRO:HG2	64:LY:105:VAL:HG12	1.88	0.56
34:Sd:22:ARG:HG3	34:Sd:23:VAL:HG23	1.86	0.56
40:L5:1259:G:H2'	40:L5:1260:G:H8	1.70	0.56
40:L5:2275:G:H2'	40:L5:2276:A:C8	2.40	0.56
40:L5:3933:G:H2'	40:L5:3934:G:H8	1.70	0.56
40:L5:4239:A:H2'	40:L5:4240:G:C8	2.41	0.56
59:LS:147:ASP:HB3	59:LS:150:ILE:HB	1.88	0.56
8:SJ:164:PRO:HG2	19:S2:561:A:H5''	1.88	0.56
19:S2:981:A:H2'	19:S2:982:G:C8	2.41	0.56
40:L5:120:A:N1	40:L5:148:C:O2'	2.38	0.56
42:L8:95:A:N3	73:Lh:63:GLN:NE2	2.53	0.56
71:Lf:15:LYS:HB3	71:Lf:25:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SW:52:ILE:HG23	13:SW:61:ILE:HG12	1.86	0.56
18:Se:31:ARG:NH2	19:S2:525:A:O3'	2.39	0.56
19:S2:804:U:H3	19:S2:859:G:H1	1.53	0.56
19:S2:948:C:H2'	19:S2:949:G:H8	1.70	0.56
20:LR:88:ARG:O	40:L5:2725:A:N6	2.38	0.56
40:L5:109:G:OP2	53:LL:74:ARG:NH2	2.37	0.56
40:L5:184:U:O2	40:L5:254:G:C6	2.59	0.56
40:L5:246:G:H2'	40:L5:247:G:H8	1.71	0.56
40:L5:659:G:H2'	40:L5:660:A:H8	1.70	0.56
40:L5:2903:G:H1'	40:L5:2904:U:H5	1.69	0.56
40:L5:4353:PSU:H5'	40:L5:4354:U:H5'	1.86	0.56
40:L5:4532:PSU:OP2	40:L5:4554:G:N1	2.39	0.56
48:LF:127:LYS:HB2	60:LT:133:ALA:HB3	1.86	0.56
49:LG:205:THR:HG22	49:LG:206:GLN:H	1.71	0.56
19:S2:1560:U:O2	19:S2:1575:G:O6	2.22	0.56
23:SD:132:LYS:HB2	23:SD:189:MET:HG2	1.88	0.56
40:L5:4419:U:OP1	40:L5:4421:C:N4	2.39	0.56
40:L5:4740:G:O6	40:L5:4959:U:O2	2.24	0.56
54:LM:11:ARG:NH1	54:LM:58:THR:O	2.39	0.56
59:LS:83:ARG:HG3	59:LS:125:GLN:HB3	1.88	0.56
5:SG:140:ARG:NH1	19:S2:146:G:OP2	2.39	0.56
29:SS:16:LEU:HD13	29:SS:100:ALA:HB2	1.87	0.56
40:L5:1241:C:H1'	67:Lb:119:CYS:HA	1.88	0.56
40:L5:2485:U:H4'	40:L5:2486:G:N2	2.21	0.56
40:L5:4728:U:OP1	44:LB:132:LYS:NZ	2.39	0.56
83:Ls:91:THR:OG1	83:Ls:93:GLU:OE1	2.24	0.56
1:SA:42:LYS:HZ1	1:SA:48:ILE:HD11	1.71	0.56
13:SW:54:ASP:HA	13:SW:59:GLY:HA3	1.88	0.56
13:SW:78:ARG:NH1	19:S2:863:PSU:O2'	2.38	0.56
19:S2:969:U:O2	19:S2:971:G:N1	2.39	0.56
28:SQ:9:SER:HB2	28:SQ:26:LYS:HG3	1.88	0.56
40:L5:1332:C:H2'	40:L5:1333:A:C8	2.40	0.56
40:L5:2568:C:H2'	40:L5:2569:G:H8	1.70	0.56
46:LD:60:ILE:HG13	46:LD:93:THR:HA	1.88	0.56
5:SG:135:PRO:HG2	5:SG:141:ILE:HG22	1.89	0.55
14:SX:67:ARG:NH2	14:SX:114:ASP:OD2	2.39	0.55
23:SD:193:ASP:OD1	23:SD:196:GLY:N	2.36	0.55
40:L5:1866:U:OP1	51:LI:4:ARG:NH1	2.31	0.55
40:L5:4088:C:H2'	40:L5:4089:G:C8	2.41	0.55
58:LQ:15:ARG:NH1	58:LQ:52:PHE:O	2.38	0.55
59:LS:127:MET:HA	60:LT:153:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:LX:64:SER:HB2	73:Lh:69:LEU:HD13	1.87	0.55
11:SO:19:PRO:HG2	11:SO:21:VAL:HG13	1.89	0.55
16:Sa:44:ILE:HG23	16:Sa:45:VAL:HG13	1.88	0.55
19:S2:925:G:N2	19:S2:1017:U:O2	2.29	0.55
24:SF:59:LYS:HB3	24:SF:62:ARG:HD3	1.88	0.55
40:L5:188:G:N2	40:L5:190:G:O6	2.40	0.55
40:L5:714:G:H2'	40:L5:715:G:H8	1.71	0.55
40:L5:736:C:OP1	54:LM:74:ARG:NH2	2.30	0.55
40:L5:1511:U:H2'	40:L5:1512:G:H8	1.70	0.55
40:L5:1872:G:O2'	40:L5:4219:A:N3	2.34	0.55
40:L5:1970:A:N6	40:L5:2015:U:OP2	2.39	0.55
40:L5:4566:U:O2'	44:LB:234:ARG:NH1	2.39	0.55
19:S2:1778:C:H3'	19:S2:1779:G:H8	1.72	0.55
37:At:43:A:H2'	37:At:44:A:H8	1.72	0.55
40:L5:729:G:H5''	48:LF:76:ARG:HD2	1.88	0.55
40:L5:1689:G:OP1	58:LQ:11:ARG:NH2	2.40	0.55
40:L5:2021:G:OP1	83:Ls:58:ASN:N	2.40	0.55
40:L5:2375:A:H2'	40:L5:2376:A:H8	1.71	0.55
76:Lk:14:THR:HA	76:Lk:17:ARG:HD3	1.88	0.55
84:Lt:16:ARG:HE	84:Lt:17:CYS:N	2.03	0.55
6:SH:143:ARG:HB2	6:SH:155:LYS:HB2	1.88	0.55
19:S2:146:G:H2'	19:S2:147:A:C8	2.42	0.55
19:S2:300:U:H2'	19:S2:301:A:C8	2.41	0.55
19:S2:1845:A:H2'	19:S2:1846:G:H8	1.71	0.55
21:LW:72:THR:OG1	21:LW:74:ARG:NH2	2.39	0.55
40:L5:169:G:N2	40:L5:171:U:O4	2.39	0.55
5:SG:162:LEU:O	5:SG:167:LYS:NZ	2.39	0.55
19:S2:1226:G:H21	19:S2:1640:A:N6	2.03	0.55
19:S2:1588:A:H2'	19:S2:1589:A:H8	1.72	0.55
24:SF:49:LEU:HD23	28:SQ:50:LYS:HG2	1.88	0.55
29:SS:121:ARG:HG3	29:SS:131:VAL:HB	1.87	0.55
40:L5:1613:A:H5''	43:LA:183:GLY:HA3	1.89	0.55
40:L5:2609:G:H2'	40:L5:2610:G:H8	1.71	0.55
40:L5:4454:G:H1	40:L5:4526:U:H3	1.54	0.55
45:LC:298:ILE:HD13	58:LQ:131:PRO:HB3	1.88	0.55
46:LD:265:ARG:NH1	46:LD:267:ASN:O	2.38	0.55
51:LI:10:ARG:NH2	51:LI:56:GLU:OE1	2.39	0.55
1:SA:76:VAL:HG12	1:SA:123:VAL:HB	1.88	0.55
2:SB:136:ARG:NH2	19:S2:941:C:OP1	2.40	0.55
8:SJ:136:ARG:N	8:SJ:158:ASP:O	2.39	0.55
20:LR:84:THR:HG22	20:LR:86:ASN:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SP:130:ARG:HD3	27:SP:131:PRO:HD2	1.88	0.55
40:L5:293:G:OP1	87:L5:5263:SPM:N1	2.37	0.55
40:L5:4088:C:OP1	43:LA:37:ARG:NH1	2.39	0.55
40:L5:4472:G:O2'	78:Lm:100:TYR:O	2.24	0.55
19:S2:1402:A:N6	19:S2:1441:U:O2'	2.40	0.55
23:SD:158:ILE:HG23	23:SD:189:MET:HE1	1.89	0.55
40:L5:135:G:H22	73:Lh:94:ARG:HD2	1.71	0.55
40:L5:450:G:O6	40:L5:1297:U:O4	2.24	0.55
40:L5:2049:G:HO2'	40:L5:3884:PSU:HO2'	1.52	0.55
40:L5:4239:A:H2'	40:L5:4240:G:H8	1.71	0.55
40:L5:4693:C:OP1	50:LH:64:ARG:NH1	2.35	0.55
40:L5:4910:G:H4'	44:LB:95:THR:HG22	1.87	0.55
40:L5:5055:G:H2'	40:L5:5056:A:H8	1.71	0.55
52:LJ:29:SER:OG	52:LJ:67:LYS:O	2.19	0.55
83:Ls:103:LEU:HA	83:Ls:106:LYS:HD3	1.89	0.55
4:SE:125:LYS:O	4:SE:142:HIS:N	2.40	0.55
6:SH:160:LYS:HD3	6:SH:189:PHE:HB3	1.88	0.55
19:S2:1144:A:H2'	19:S2:1145:A:C8	2.41	0.55
19:S2:1692:U:H2'	19:S2:1693:G:C8	2.42	0.55
35:Sf:103:LEU:HB2	35:Sf:105:TYR:CE2	2.41	0.55
40:L5:318:A:H2'	40:L5:319:A:H8	1.71	0.55
40:L5:2440:U:H1'	40:L5:2518:G:H2'	1.88	0.55
40:L5:2784:C:H2'	40:L5:2785:C:H6	1.72	0.55
40:L5:4742:G:H2'	40:L5:4743:G:H8	1.71	0.55
45:LC:33:ARG:HD3	45:LC:36:ILE:HD12	1.89	0.55
71:Lf:77:ALA:HA	71:Lf:84:VAL:HA	1.89	0.55
3:SC:70:VAL:HG11	3:SC:93:ILE:HG23	1.89	0.55
19:S2:223:C:H2'	19:S2:224:A:C8	2.42	0.55
19:S2:432:G:H2'	19:S2:433:A:C8	2.42	0.55
24:SF:49:LEU:HD12	24:SF:50:PRO:HD2	1.89	0.55
30:ST:108:GLU:OE2	30:ST:121:ARG:NH1	2.40	0.55
40:L5:280:G:OP2	55:LN:44:ARG:NH1	2.37	0.55
40:L5:2092:G:O2'	40:L5:2262:G:N2	2.40	0.55
40:L5:2458:C:O2'	40:L5:3671:G:N3	2.38	0.55
40:L5:2554:U:O2	40:L5:2764:A:N7	2.40	0.55
46:LD:62:CYS:HB3	46:LD:105:LEU:HD22	1.89	0.55
46:LD:150:LEU:HD12	52:LJ:146:ARG:HG3	1.89	0.55
16:Sa:70:LYS:HD3	19:S2:987:A:H4'	1.89	0.55
19:S2:1588:A:H2'	19:S2:1589:A:C8	2.42	0.55
40:L5:67:C:OP2	40:L5:312:G:N2	2.39	0.55
40:L5:1086:C:H2'	40:L5:1087:A:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1178:G:H5''	40:L5:1180:C:H41	1.72	0.55
40:L5:1591:U:OP2	40:L5:2856:C:O2'	2.25	0.55
40:L5:2041:A:N7	40:L5:4434:C:O2'	2.39	0.55
43:LA:7:GLY:HA2	43:LA:10:LYS:HG3	1.89	0.55
43:LA:107:MET:HE1	43:LA:164:ALA:HB3	1.87	0.55
47:LE:192:LYS:O	71:Lf:108:SER:OG	2.25	0.55
52:LJ:112:HIS:ND1	52:LJ:126:TYR:O	2.27	0.55
84:Lt:65:GLN:NE2	84:Lt:69:ALA:O	2.40	0.55
26:SM:36:ARG:NH2	35:Sf:129:GLY:O	2.40	0.54
40:L5:1939:A:H5'	40:L5:1940:G:H4'	1.89	0.54
40:L5:2577:C:OP1	65:LZ:111:ARG:NH2	2.40	0.54
40:L5:2749:C:H2'	40:L5:2750:G:C8	2.41	0.54
40:L5:4301:U:OP2	40:L5:4303:C:N4	2.40	0.54
40:L5:4667:C:OP1	44:LB:224:LYS:NZ	2.37	0.54
40:L5:4764:A:N6	50:LH:60:TRP:O	2.38	0.54
52:LJ:95:ARG:HG3	52:LJ:175:LEU:HB2	1.90	0.54
65:LZ:12:LEU:HB2	65:LZ:81:MET:HB3	1.88	0.54
19:S2:1059:G:N2	19:S2:1829:G:O3'	2.40	0.54
19:S2:1614:A:OP1	27:SP:42:ARG:NH2	2.40	0.54
19:S2:1623:A:N1	29:SS:132:ARG:NH1	2.56	0.54
19:S2:1628:C:OP1	30:ST:38:LYS:NZ	2.39	0.54
40:L5:52:G:OP1	75:Lj:48:ASN:N	2.36	0.54
40:L5:126:C:H2'	40:L5:127:G:H8	1.72	0.54
40:L5:1732:C:H2'	40:L5:1733:G:C8	2.41	0.54
40:L5:1751:A:H2'	40:L5:1752:G:H8	1.72	0.54
16:Sa:45:VAL:HG22	16:Sa:64:LEU:HD21	1.89	0.54
19:S2:1217:A:H2'	19:S2:1218:C:C6	2.42	0.54
40:L5:1077:C:OP1	40:L5:1215:C:O2'	2.22	0.54
40:L5:1351:G:O6	58:LQ:55:ARG:NH1	2.40	0.54
40:L5:1985:G:N2	40:L5:2004:U:O4	2.41	0.54
40:L5:3661:G:N2	40:L5:3681:G:O2'	2.40	0.54
40:L5:3870:C:H2'	40:L5:3871:A:H8	1.72	0.54
40:L5:4586:G:OP1	56:LO:72:HIS:N	2.33	0.54
1:SA:184:ARG:HB3	1:SA:191:ARG:HE	1.73	0.54
5:SG:135:PRO:HA	19:S2:169:U:H5''	1.90	0.54
9:SL:71:ARG:NE	19:S2:352:U:O2	2.31	0.54
15:SY:55:ILE:HD12	15:SY:75:ILE:HG22	1.88	0.54
19:S2:609:U:H2'	19:S2:610:G:H8	1.72	0.54
19:S2:1438:A:H2'	19:S2:1439:A:H8	1.72	0.54
29:SS:86:ARG:HH21	29:SS:106:LYS:HB3	1.72	0.54
32:SZ:99:LEU:HD11	32:SZ:102:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Pt:38:C:H2'	38:Pt:39:G:H8	1.72	0.54
40:L5:2258:C:N4	47:LE:88:VAL:O	2.35	0.54
40:L5:4188:U:H2'	40:L5:4189:U:C6	2.42	0.54
40:L5:4571:A2M:H2'	40:L5:4572:U:C6	2.43	0.54
40:L5:4594:U:H2'	40:L5:4595:G:H8	1.73	0.54
62:LV:13:LYS:HD3	62:LV:128:LEU:HD22	1.88	0.54
9:SL:111:VAL:HG12	9:SL:140:PHE:HB2	1.89	0.54
19:S2:49:C:H2'	19:S2:472:C:H41	1.72	0.54
19:S2:432:G:H2'	19:S2:433:A:H8	1.73	0.54
19:S2:1620:A:OP1	27:SP:115:TYR:OH	2.22	0.54
40:L5:348:G:OP2	45:LC:198:ASN:ND2	2.39	0.54
40:L5:423:G:OP1	57:LP:62:ARG:NH1	2.40	0.54
40:L5:1346:C:H2'	40:L5:1347:G:C8	2.41	0.54
40:L5:1577:G:O2'	40:L5:1612:G:H4'	2.07	0.54
40:L5:1942:A:H2'	40:L5:1943:A:C8	2.42	0.54
40:L5:2017:A:HO2'	40:L5:2018:C:P	2.30	0.54
47:LE:277:LEU:HB2	71:Lf:4:ARG:HB3	1.90	0.54
51:LI:171:TRP:HB2	51:LI:178:ALA:HA	1.90	0.54
1:SA:77:ILE:HD11	1:SA:124:VAL:HG22	1.90	0.54
19:S2:690:G:OP2	19:S2:690:G:N2	2.34	0.54
19:S2:866:PSU:H2'	19:S2:867:OMG:H8	1.72	0.54
19:S2:1435:C:H42	31:SU:49:LYS:HZ1	1.55	0.54
40:L5:748:G:O6	59:LS:98:ARG:NH2	2.36	0.54
40:L5:2079:G:H2'	40:L5:2080:U:C6	2.43	0.54
84:Lt:57:ARG:HH11	84:Lt:84:ALA:HA	1.71	0.54
2:SB:88:THR:HA	2:SB:98:THR:HA	1.88	0.54
9:SL:81:LYS:HG3	19:S2:394:G:H5'	1.90	0.54
9:SL:120:VAL:HG22	9:SL:145:VAL:HG11	1.88	0.54
19:S2:525:A:H2'	19:S2:526:A:H8	1.72	0.54
19:S2:960:U:O2'	19:S2:962:A:N7	2.35	0.54
40:L5:276:C:H3'	74:Li:29:ARG:HH12	1.73	0.54
40:L5:1175:A:OP1	46:LD:268:ARG:NH1	2.40	0.54
40:L5:1857:C:H2'	40:L5:1858:A:H8	1.71	0.54
40:L5:3846:C:H2'	40:L5:3847:C:H6	1.71	0.54
40:L5:3916:G:H2'	40:L5:3917:A:C8	2.43	0.54
62:LV:85:ARG:NH1	62:LV:99:GLU:O	2.41	0.54
40:L5:114:G:N2	40:L5:276:C:O2'	2.41	0.54
40:L5:444:G:H2'	40:L5:445:U:H6	1.72	0.54
40:L5:1478:C:H2'	40:L5:1479:G:H8	1.73	0.54
40:L5:4448:G:H5''	40:L5:4449:A:H5'	1.90	0.54
45:LC:107:THR:O	45:LC:111:TRP:NE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SG:164:LYS:HB2	5:SG:167:LYS:HG2	1.89	0.54
19:S2:454:U:H2'	19:S2:455:A:C8	2.43	0.54
19:S2:1360:U:O2'	19:S2:1379:A:OP2	2.24	0.54
24:SF:20:PHE:O	24:SF:22:LYS:NZ	2.36	0.54
36:Sg:32:LEU:HA	36:Sg:42:MET:HA	1.90	0.54
38:Pt:51:C:H2'	38:Pt:52:G:H8	1.73	0.54
40:L5:909:A:H2'	40:L5:910:G:H8	1.73	0.54
40:L5:2777:G:H5''	40:L5:2778:G:H5'	1.89	0.54
42:L8:94:G:H21	75:Lj:82:THR:HB	1.73	0.54
43:LA:79:ALA:HA	43:LA:169:VAL:HA	1.89	0.54
9:SL:16:ILE:HD11	9:SL:36:TYR:H	1.73	0.54
9:SL:40:ILE:O	19:S2:291:G:N2	2.40	0.54
28:SQ:42:ILE:HG23	28:SQ:44:PRO:HD2	1.90	0.54
40:L5:38:A:H61	40:L5:41:C:H3'	1.73	0.54
40:L5:217:C:H5	40:L5:219:G:H4'	1.72	0.54
40:L5:2624:G:OP2	61:LU:97:ARG:NH2	2.41	0.54
5:SG:142:ARG:HA	5:SG:147:LEU:HD23	1.90	0.53
7:SI:43:ILE:HG12	7:SI:57:ALA:HA	1.89	0.53
14:SX:17:ARG:NH1	19:S2:658:U:O2	2.41	0.53
14:SX:67:ARG:NH1	19:S2:617:G:N7	2.56	0.53
40:L5:679:C:H2'	40:L5:680:G:C8	2.41	0.53
40:L5:977:C:OP1	45:LC:333:LYS:NZ	2.41	0.53
40:L5:2090:U:OP1	40:L5:2266:C:N4	2.40	0.53
40:L5:3598:C:H2'	40:L5:3599:A:H8	1.73	0.53
40:L5:4127:A:H61	40:L5:4156:G:H2'	1.72	0.53
52:LJ:99:PHE:HA	52:LJ:105:PHE:HB3	1.90	0.53
54:LM:15:VAL:HG22	54:LM:50:MET:HE1	1.90	0.53
56:LO:54:TYR:OH	56:LO:73:PHE:O	2.26	0.53
19:S2:26:U:H2'	19:S2:27:A2M:H8	1.90	0.53
19:S2:342:C:H2'	19:S2:343:A:H8	1.73	0.53
19:S2:1438:A:H2'	19:S2:1439:A:C8	2.42	0.53
23:SD:8:LYS:HG2	31:SU:61:LEU:HD11	1.90	0.53
24:SF:32:ASP:OD2	24:SF:34:SER:OG	2.25	0.53
37:At:29:C:H2'	37:At:30:G:H8	1.73	0.53
40:L5:733:A:N6	40:L5:933:G:O6	2.41	0.53
40:L5:1333:A:H2'	40:L5:1334:A:H8	1.73	0.53
40:L5:3725:G:N7	74:Li:67:LYS:NZ	2.49	0.53
40:L5:4080:C:H2'	40:L5:4081:G:H8	1.74	0.53
7:SI:64:ASN:HA	7:SI:75:LYS:HA	1.90	0.53
14:SX:67:ARG:HG3	14:SX:115:ILE:HG12	1.91	0.53
18:Se:26:LYS:NZ	19:S2:525:A:OP2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1562:C:H2'	19:S2:1563:G:H8	1.73	0.53
19:S2:1845:A:H2'	19:S2:1846:G:C8	2.44	0.53
40:L5:1655:C:O2	40:L5:4390:A:O2'	2.26	0.53
43:LA:51:ASP:HB2	43:LA:58:LEU:HG	1.90	0.53
8:SJ:160:SER:O	8:SJ:163:SER:OG	2.27	0.53
28:SQ:5:GLY:O	28:SQ:27:ARG:NH2	2.41	0.53
37:At:18:G:O6	37:At:55:U:C2	2.62	0.53
40:L5:1175:A:H2	40:L5:1185:G:H22	1.57	0.53
40:L5:2362:U:H2'	40:L5:2363:A2M:H8	1.90	0.53
40:L5:2491:C:H2'	40:L5:2492:C:C6	2.43	0.53
40:L5:2778:G:N2	42:L8:113:C:OP2	2.41	0.53
40:L5:2843:U:O2'	40:L5:4632:U:OP1	2.26	0.53
40:L5:4274:A:H2'	40:L5:4275:G:H8	1.73	0.53
47:LE:164:PHE:HA	47:LE:175:VAL:HG12	1.90	0.53
83:Ls:59:THR:HA	83:Ls:62:ARG:HE	1.73	0.53
9:SL:133:PRO:HG2	19:S2:383:G:H21	1.72	0.53
13:SW:6:VAL:HG13	13:SW:29:PRO:HB2	1.91	0.53
18:Se:58:ASN:HB3	19:S2:608:C:H5'	1.90	0.53
19:S2:28:U:H2'	19:S2:29:G:H8	1.73	0.53
19:S2:90:G:OP1	19:S2:445:A:N6	2.36	0.53
19:S2:1453:C:OP1	22:SR:48:ASN:ND2	2.34	0.53
19:S2:1651:A:O2'	24:SF:83:ASN:OD1	2.27	0.53
40:L5:408:A:O2'	40:L5:411:G:OP2	2.22	0.53
40:L5:441:G:H2'	40:L5:442:G:H8	1.74	0.53
40:L5:1686:C:OP1	67:Lb:19:ASN:ND2	2.36	0.53
40:L5:2835:A:O2'	44:LB:228:TYR:O	2.27	0.53
40:L5:3661:G:H4'	40:L5:3662:A:H5'	1.90	0.53
40:L5:4185:G:OP1	43:LA:2:GLY:N	2.41	0.53
1:SA:207:PRO:HA	1:SA:210:ILE:HG22	1.90	0.53
19:S2:1441:U:O2	19:S2:1443:C:N4	2.39	0.53
21:LW:9:SER:HA	21:LW:52:THR:HG23	1.91	0.53
31:SU:80:PHE:HB3	34:Sd:52:PHE:HB3	1.89	0.53
38:Pt:51:C:H2'	38:Pt:52:G:C8	2.43	0.53
40:L5:209:U:H5	40:L5:233:U:C4	2.27	0.53
40:L5:655:C:H2'	40:L5:656:C:C6	2.44	0.53
40:L5:3717:A:H2'	40:L5:3718:A2M:H8	1.90	0.53
40:L5:4301:U:OP1	60:LT:78:LYS:NZ	2.42	0.53
65:LZ:99:ASP:HB2	65:LZ:102:ARG:HH21	1.72	0.53
1:SA:84:GLN:HG2	1:SA:100:ALA:HB1	1.91	0.53
4:SE:146:THR:HG21	19:S2:122:G:H21	1.74	0.53
5:SG:148:SER:OG	5:SG:151:ASP:OD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:65:PRO:HG2	6:SH:68:GLN:HB2	1.89	0.53
14:SX:107:ARG:HG3	14:SX:110:HIS:HB3	1.91	0.53
40:L5:10:A:H2'	40:L5:11:G:H8	1.74	0.53
40:L5:676:C:H2'	40:L5:677:G:H8	1.74	0.53
40:L5:1241:C:O2'	67:Lb:120:ARG:O	2.21	0.53
40:L5:2756:G:O6	65:LZ:51:ARG:NH2	2.38	0.53
40:L5:4076:G:OP2	40:L5:4163:U:N3	2.38	0.53
41:L7:57:C:H2'	41:L7:58:A:H8	1.72	0.53
49:LG:46:GLN:OE1	49:LG:49:ARG:NH1	2.42	0.53
82:Lr:28:GLU:HG2	82:Lr:31:ASN:HB2	1.90	0.53
4:SE:247:THR:N	4:SE:250:GLU:OE2	2.42	0.53
5:SG:4:ASN:ND2	5:SG:110:ASN:OD1	2.36	0.53
19:S2:159:A2M:O5'	19:S2:159:A2M:H8	2.09	0.53
40:L5:951:G:H2'	40:L5:952:G:H8	1.74	0.53
40:L5:2654:C:H2'	40:L5:2655:C:H6	1.72	0.53
40:L5:4108:G:H2'	40:L5:4109:G:C8	2.44	0.53
41:L7:38:U:N3	41:L7:41:G:OP2	2.41	0.53
55:LN:157:LYS:O	55:LN:162:ARG:NH1	2.42	0.53
12:SV:15:ARG:NH1	12:SV:33:GLN:OE1	2.42	0.53
19:S2:1018:U:H2'	19:S2:1019:C:H6	1.74	0.53
19:S2:1284:A:HO2'	26:SM:106:CYS:HG	1.56	0.53
40:L5:210:C:HO2'	40:L5:234:G:HO2'	1.56	0.53
40:L5:1942:A:N3	40:L5:4432:C:O2'	2.41	0.53
40:L5:2568:C:H2'	40:L5:2569:G:C8	2.43	0.53
40:L5:4522:G:O2'	40:L5:4525:C:OP2	2.26	0.53
49:LG:48:LYS:HD2	63:LX:42:THR:HB	1.91	0.53
56:LO:6:VAL:HG22	56:LO:32:LYS:HB2	1.91	0.53
58:LQ:80:ALA:HB3	58:LQ:100:VAL:HG22	1.91	0.53
5:SG:223:LYS:O	5:SG:227:GLN:NE2	2.42	0.53
14:SX:28:LYS:HD2	14:SX:32:LEU:HD22	1.91	0.53
19:S2:349:A:H2'	19:S2:350:C:C6	2.44	0.53
19:S2:1598:G:N7	32:SZ:85:ARG:NH2	2.57	0.53
28:SQ:72:VAL:HG11	28:SQ:80:GLN:HG3	1.89	0.53
37:At:6:C:H2'	37:At:7:G:C8	2.44	0.53
40:L5:184:U:O2'	40:L5:253:G:N2	2.38	0.53
40:L5:4459:U:H2'	40:L5:4460:U:C6	2.44	0.53
40:L5:4586:G:O6	40:L5:4717:A:N6	2.41	0.53
40:L5:4992:G:H2'	40:L5:4993:G:H8	1.74	0.53
42:L8:38:U:H5'	73:Lh:81:LEU:HD13	1.90	0.53
42:L8:142:U:OP1	55:LN:38:ARG:NH2	2.42	0.53
56:LO:46:ASN:HB3	56:LO:134:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:LU:55:ASN:OD1	61:LU:58:GLY:N	2.38	0.53
5:SG:133:LEU:O	19:S2:168:C:O2'	2.27	0.52
19:S2:500:A:O2'	19:S2:501:C:O4'	2.25	0.52
19:S2:874:G:H2'	19:S2:875:A:C8	2.44	0.52
19:S2:1405:A:H2'	19:S2:1406:G:O4'	2.08	0.52
19:S2:1417:C:N3	19:S2:1422:G:N1	2.48	0.52
40:L5:432:U:OP2	40:L5:3888:G:N2	2.40	0.52
40:L5:1824:G:H2'	40:L5:1825:A:C8	2.44	0.52
40:L5:1996:C:N4	40:L5:2000:G:H22	2.06	0.52
40:L5:4097:G:O6	40:L5:4098:A:N6	2.42	0.52
40:L5:4238:G:H2'	40:L5:4239:A:C8	2.44	0.52
50:LH:92:MET:HE2	50:LH:179:ILE:HG22	1.91	0.52
8:SJ:132:GLN:NE2	19:S2:561:A:N3	2.57	0.52
19:S2:1417:C:N4	19:S2:1422:G:H22	1.97	0.52
36:Sg:207:CYS:HB3	36:Sg:221:LEU:HD21	1.91	0.52
40:L5:67:C:N4	40:L5:325:U:O2'	2.40	0.52
40:L5:1962:A:H5'	40:L5:1963:C:H5	1.74	0.52
40:L5:2260:C:OP1	47:LE:108:LYS:NZ	2.37	0.52
40:L5:2609:G:H2'	40:L5:2610:G:C8	2.45	0.52
40:L5:2809:G:O2'	40:L5:4644:G:OP1	2.26	0.52
40:L5:4485:C:O2'	78:Lm:114:LYS:NZ	2.39	0.52
40:L5:4587:G:OP1	56:LO:61:ARG:NH1	2.35	0.52
45:LC:55:SER:HB3	45:LC:58:ALA:HB2	1.90	0.52
19:S2:17:C:H2'	19:S2:18:C:C6	2.45	0.52
41:L7:119:U:C2	46:LD:261:VAL:HG21	2.44	0.52
1:SA:37:TYR:OH	1:SA:57:LYS:NZ	2.29	0.52
1:SA:145:ILE:HG13	1:SA:159:ILE:HD13	1.91	0.52
4:SE:36:HIS:NE2	4:SE:143:ASP:OD1	2.43	0.52
19:S2:158:A:C2	19:S2:463:C:H1'	2.45	0.52
19:S2:1240:A:N6	27:SP:122:THR:O	2.42	0.52
19:S2:1681:U:O2'	33:Sc:23:SER:O	2.27	0.52
23:SD:136:VAL:HG12	23:SD:186:VAL:HG22	1.91	0.52
23:SD:218:LEU:HD11	36:Sg:189:ILE:HB	1.91	0.52
38:Pt:56:C:C2	80:Lo:104:ILE:HG21	2.44	0.52
40:L5:135:G:N7	73:Lh:97:LYS:HG2	2.25	0.52
40:L5:264:C:H2'	40:L5:265:C:C4	2.44	0.52
40:L5:696:C:H5'	40:L5:697:G:H5'	1.90	0.52
49:LG:103:ARG:NH2	49:LG:192:ARG:O	2.43	0.52
50:LH:24:THR:HA	50:LH:37:ASP:HA	1.91	0.52
52:LJ:15:LEU:HD12	52:LJ:165:TRP:HB2	1.91	0.52
73:Lh:88:THR:HB	73:Lh:91:MET:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Lt:61:LYS:HA	84:Lt:75:PRO:HD2	1.91	0.52
2:SB:52:THR:HG23	2:SB:57:ILE:HA	1.91	0.52
19:S2:1199:A:H2'	19:S2:1200:A:C8	2.45	0.52
25:SK:3:MET:HE1	25:SK:48:ALA:HB2	1.91	0.52
25:SK:15:LEU:HD23	25:SK:79:LEU:HD11	1.90	0.52
40:L5:2279:A:O2'	70:Le:48:ARG:NH2	2.43	0.52
40:L5:2835:A:H2'	40:L5:2836:A:H8	1.75	0.52
40:L5:4758:U:OP2	56:LO:171:LYS:NZ	2.43	0.52
55:LN:120:TRP:HE1	55:LN:123:GLU:HB3	1.73	0.52
17:Sb:54:VAL:HG23	17:Sb:63:LEU:HB2	1.92	0.52
19:S2:53:C:O2'	19:S2:507:G:N7	2.34	0.52
19:S2:1748:G:O6	19:S2:1786:U:O4	2.27	0.52
24:SF:76:MET:O	24:SF:159:ARG:NH2	2.38	0.52
40:L5:2489:C:H4'	40:L5:2491:C:H42	1.74	0.52
43:LA:103:PRO:HA	43:LA:163:ARG:HA	1.92	0.52
65:LZ:46:ILE:HA	65:LZ:70:SER:HA	1.92	0.52
3:SC:81:ILE:HG21	3:SC:88:ILE:HD11	1.92	0.52
4:SE:129:ILE:HD13	4:SE:139:LEU:HD12	1.91	0.52
6:SH:157:HIS:ND1	6:SH:188:GLU:OE2	2.43	0.52
8:SJ:38:ARG:NH1	19:S2:523:A:OP2	2.37	0.52
15:SY:54:VAL:HG22	15:SY:76:TYR:HB2	1.90	0.52
23:SD:137:VAL:HB	23:SD:185:LYS:HB2	1.90	0.52
40:L5:3610:A:H2'	40:L5:3611:A:H8	1.73	0.52
40:L5:5006:U:H4'	40:L5:5007:A:H5'	1.92	0.52
48:LF:29:LYS:HZ3	48:LF:32:ARG:HH12	1.58	0.52
55:LN:164:LEU:O	55:LN:169:ARG:NH2	2.42	0.52
82:Lr:26:SER:OG	82:Lr:28:GLU:OE1	2.23	0.52
83:Ls:18:ILE:HD12	83:Ls:21:LEU:HD21	1.92	0.52
1:SA:3:GLY:N	1:SA:56:GLU:OE1	2.42	0.52
5:SG:116:LYS:HE3	5:SG:125:THR:HG21	1.92	0.52
11:SO:147:ARG:NH2	19:S2:1855:G:OP2	2.43	0.52
12:SV:17:CYS:HB3	12:SV:22:ARG:H	1.75	0.52
26:SM:36:ARG:HD2	35:Sf:103:LEU:HD13	1.92	0.52
40:L5:3658:C:H2'	40:L5:3659:G:H8	1.75	0.52
57:LP:116:HIS:HD2	57:LP:149:ILE:HD12	1.74	0.52
66:La:36:GLY:HA3	66:La:40:HIS:CE1	2.44	0.52
4:SE:73:ASP:OD2	4:SE:145:ARG:NH2	2.43	0.52
5:SG:87:ARG:NH2	19:S2:161:U:O2'	2.43	0.52
7:SI:101:ILE:HD11	7:SI:202:ILE:HD11	1.92	0.52
19:S2:1037:G:H4'	19:S2:1845:A:H4'	1.92	0.52
19:S2:1179:G:N2	19:S2:1182:A:OP2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:261:G:H2'	40:L5:262:G:C8	2.45	0.52
40:L5:262:G:H2'	40:L5:263:G:C8	2.41	0.52
40:L5:1967:A:N6	40:L5:2021:G:O6	2.43	0.52
40:L5:1970:A:H1'	40:L5:2017:A:H61	1.74	0.52
40:L5:2521:G:H2'	40:L5:2522:G:H8	1.75	0.52
40:L5:2539:C:H2'	40:L5:2540:C:C6	2.45	0.52
40:L5:2804:OMC:HM22	40:L5:2805:C:H5'	1.91	0.52
46:LD:106:ALA:HB2	46:LD:166:ALA:HA	1.92	0.52
77:LI:38:ASN:HB3	77:LI:41:ARG:HG2	1.92	0.52
6:SH:138:GLU:N	6:SH:159:ASP:OD2	2.34	0.52
16:Sa:26:CYS:HB3	16:Sa:77:CYS:SG	2.49	0.52
19:S2:328:U:O2'	19:S2:329:G:O5'	2.26	0.52
25:SK:14:LEU:HD22	25:SK:35:LEU:HD13	1.92	0.52
33:Sc:13:ARG:HA	33:Sc:55:VAL:HA	1.90	0.52
34:Sd:21:CYS:HB3	34:Sd:26:ASN:H	1.75	0.52
36:Sg:107:ASP:HB2	36:Sg:125:ARG:HD2	1.92	0.52
40:L5:1514:U:H2'	40:L5:1515:A:C8	2.44	0.52
40:L5:1994:C:H2'	40:L5:1995:G:N7	2.25	0.52
40:L5:2335:C:H2'	40:L5:2336:G:H8	1.74	0.52
40:L5:3754:G:O6	40:L5:3771:C:N4	2.43	0.52
40:L5:4237:C:O3'	40:L5:4326:G:N2	2.43	0.52
44:LB:108:GLU:HG3	44:LB:134:CYS:HB2	1.90	0.52
68:Lc:38:ILE:HG21	68:Lc:63:TYR:HB3	1.92	0.52
74:Li:57:ALA:HA	74:Li:60:LEU:HD12	1.91	0.52
2:SB:117:TRP:HB3	2:SB:153:THR:HA	1.92	0.51
5:SG:131:ARG:HB2	21:LW:82:ILE:HG22	1.92	0.51
19:S2:1277:C:H2'	19:S2:1278:A:C8	2.45	0.51
38:Pt:50:U:H2'	38:Pt:51:C:C6	2.45	0.51
40:L5:231:U:O2	64:LY:103:LYS:NZ	2.30	0.51
40:L5:1177:U:H5''	46:LD:286:SER:HB2	1.91	0.51
40:L5:1352:C:O2'	40:L5:1356:U:OP1	2.28	0.51
40:L5:1449:C:OP1	58:LQ:132:LYS:NZ	2.40	0.51
40:L5:2749:C:H2'	40:L5:2750:G:H8	1.73	0.51
40:L5:4407:G:H1	40:L5:4435:U:H3	1.56	0.51
40:L5:4441:A:H5''	51:LI:114:GLY:HA2	1.91	0.51
40:L5:4967:A:H2'	40:L5:4968:A:H8	1.75	0.51
83:Ls:143:ILE:HG13	83:Ls:158:VAL:HG21	1.92	0.51
11:SO:33:ILE:HG22	11:SO:42:VAL:HA	1.92	0.51
19:S2:149:A:N7	19:S2:169:U:O2	2.44	0.51
19:S2:1348:G:H2'	19:S2:1349:G:H8	1.76	0.51
31:SU:27:ARG:HD3	31:SU:82:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:162:A:H2'	40:L5:163:A:H8	1.74	0.51
40:L5:2815:A2M:HM'2	40:L5:2816:G:H5'	1.92	0.51
69:Ld:22:THR:HG23	69:Ld:122:VAL:HG13	1.92	0.51
84:Lt:10:ILE:HG21	84:Lt:65:GLN:HB3	1.91	0.51
3:SC:210:PRO:HB3	3:SC:240:THR:HG21	1.91	0.51
19:S2:1259:A:H8	19:S2:1264:C:H42	1.58	0.51
40:L5:93:G:H2'	40:L5:94:A:C8	2.46	0.51
40:L5:1604:G:H2'	40:L5:1605:G:C8	2.45	0.51
40:L5:2754:G:OP2	65:LZ:133:LYS:NZ	2.44	0.51
40:L5:3689:G:O2'	40:L5:3818:UY1:OP2	2.29	0.51
40:L5:4075:U:OP1	49:LG:249:ARG:NH2	2.44	0.51
47:LE:177:GLY:HA3	47:LE:182:ASN:HD21	1.74	0.51
19:S2:1113:A:H2'	19:S2:1114:U:C6	2.45	0.51
33:Sc:14:VAL:HA	33:Sc:32:VAL:HG12	1.92	0.51
36:Sg:254:PRO:HA	36:Sg:286:CYS:H	1.75	0.51
40:L5:2630:U:OP1	61:LU:48:LYS:NZ	2.39	0.51
40:L5:4537:C:H2'	40:L5:4538:G:C8	2.43	0.51
42:L8:47:C:H1'	42:L8:61:A:H2'	1.92	0.51
44:LB:119:TYR:OH	44:LB:129:ALA:N	2.43	0.51
46:LD:223:PHE:HB3	46:LD:226:TYR:HB2	1.91	0.51
52:LJ:118:LYS:NZ	52:LJ:119:TYR:O	2.35	0.51
2:SB:224:GLU:HG3	2:SB:227:LYS:H	1.75	0.51
19:S2:1253:A:OP2	19:S2:1526:G:N2	2.39	0.51
24:SF:201:LYS:HA	24:SF:204:ARG:HE	1.75	0.51
35:Sf:132:MET:HG2	35:Sf:141:CYS:SG	2.51	0.51
40:L5:216:C:OP2	40:L5:219:G:O2'	2.28	0.51
40:L5:1751:A:H2'	40:L5:1752:G:C8	2.46	0.51
40:L5:1972:G:H2'	40:L5:1973:G:C8	2.46	0.51
40:L5:3710:G:O2'	40:L5:3712:A:OP2	2.25	0.51
5:SG:84:TYR:OH	5:SG:91:GLU:O	2.29	0.51
19:S2:65:C:O2'	19:S2:67:C:OP1	2.25	0.51
19:S2:980:A:H2'	19:S2:981:A:C8	2.46	0.51
19:S2:1220:A:N3	19:S2:1677:U:O2'	2.36	0.51
20:LR:96:MET:SD	20:LR:100:ARG:NH2	2.84	0.51
40:L5:188:G:N1	40:L5:191:G:O6	2.38	0.51
40:L5:347:A:H2'	40:L5:348:G:C8	2.46	0.51
40:L5:444:G:H2'	40:L5:445:U:C6	2.46	0.51
40:L5:2295:C:H2'	40:L5:2296:G:C8	2.43	0.51
40:L5:3680:U:OP1	43:LA:54:ARG:NH2	2.39	0.51
40:L5:3916:G:H2'	40:L5:3917:A:H8	1.76	0.51
41:L7:87:G:N2	41:L7:90:A:OP2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:291:G:H2'	19:S2:292:A:C8	2.46	0.51
19:S2:604:A:O2'	19:S2:605:A:O4'	2.27	0.51
19:S2:928:G:H1	19:S2:1013:U:H3	1.59	0.51
40:L5:10:A:H2'	40:L5:11:G:C8	2.45	0.51
40:L5:107:G:OP2	53:LL:42:LYS:NZ	2.44	0.51
40:L5:1179:U:H3'	40:L5:1180:C:H5''	1.92	0.51
40:L5:1895:G:O2'	40:L5:1907:A:N3	2.42	0.51
40:L5:3898:G:H5'	44:LB:254:ILE:HG13	1.93	0.51
40:L5:4991:U:H2'	40:L5:4992:G:H8	1.74	0.51
41:L7:7:G:OP1	46:LD:33:ARG:NH1	2.44	0.51
42:L8:8:U:H2'	42:L8:9:A:C8	2.45	0.51
42:L8:75:OMG:OP2	64:LY:74:TYR:OH	2.25	0.51
44:LB:302:ASN:HB2	44:LB:313:SER:HA	1.93	0.51
1:SA:37:TYR:CG	1:SA:162:PRO:HG3	2.46	0.51
2:SB:115:LYS:HG2	19:S2:1869:A:C5	2.45	0.51
8:SJ:18:ARG:HH21	19:S2:4:C:H1'	1.75	0.51
19:S2:339:A:H2	19:S2:340:C:H41	1.58	0.51
19:S2:482:G:N1	19:S2:485:A:OP2	2.41	0.51
19:S2:1103:C:H2'	19:S2:1104:G:C8	2.46	0.51
19:S2:1459:G:OP2	36:Sg:280:LYS:NZ	2.31	0.51
40:L5:325:U:H2'	40:L5:326:C:C6	2.46	0.51
40:L5:1695:U:H2'	40:L5:1696:C:H6	1.75	0.51
40:L5:2490:U:H3'	40:L5:2491:C:C6	2.45	0.51
40:L5:3848:U:H2'	40:L5:3849:A:H8	1.76	0.51
40:L5:4578:G:H2'	40:L5:4579:PSU:H6	1.75	0.51
41:L7:13:A:OP2	41:L7:66:G:N2	2.40	0.51
41:L7:99:G:OP2	59:LS:55:LYS:NZ	2.33	0.51
47:LE:227:HIS:NE2	47:LE:229:GLU:O	2.44	0.51
5:SG:139:SER:OG	19:S2:144:U:OP2	2.27	0.51
19:S2:1004:PSU:H2'	19:S2:1005:G:H8	1.75	0.51
19:S2:1736:G:H2'	19:S2:1737:G:H8	1.75	0.51
40:L5:418:A:H4'	40:L5:2311:C:H5'	1.93	0.51
40:L5:724:C:H1'	45:LC:343:GLN:HG2	1.93	0.51
40:L5:1772:C:H2'	40:L5:1773:U:H6	1.76	0.51
40:L5:1968:G:H4'	83:Ls:112:ARG:HH12	1.76	0.51
40:L5:2897:G:H2'	40:L5:2898:G:C8	2.46	0.51
40:L5:4069:U:H2'	40:L5:4070:U:C6	2.46	0.51
40:L5:4246:G:H2'	40:L5:4247:G:C8	2.46	0.51
40:L5:4262:C:H2'	40:L5:4263:C:H6	1.76	0.51
40:L5:4274:A:H2'	40:L5:4275:G:C8	2.45	0.51
41:L7:55:A:H4'	52:LJ:155:HIS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LF:222:LYS:N	48:LF:232:ASP:OD2	2.41	0.51
3:SC:91:SER:HB3	3:SC:156:ILE:HG23	1.93	0.51
19:S2:287:U:H2'	19:S2:288:G:C8	2.46	0.51
19:S2:919:A:O2'	19:S2:1020:A:N1	2.33	0.51
19:S2:1493:C:N3	19:S2:1500:G:O6	2.44	0.51
40:L5:132:G:C2	40:L5:133:C:H1'	2.46	0.51
40:L5:287:U:H2'	40:L5:288:G:C8	2.46	0.51
40:L5:1732:C:H5''	60:LT:43:LYS:HE2	1.92	0.51
40:L5:2686:G:O2'	40:L5:2688:G:N7	2.37	0.51
40:L5:3938:G:N2	40:L5:4171:C:OP2	2.40	0.51
40:L5:4097:G:N7	40:L5:4099:G:N2	2.58	0.51
59:LS:4:SER:HB3	59:LS:111:ARG:HH22	1.76	0.51
62:LV:62:MET:HE1	62:LV:78:PRO:HG3	1.93	0.51
9:SL:23:VAL:HG23	9:SL:25:LEU:HG	1.93	0.50
19:S2:1039:C:H2'	19:S2:1040:G:H8	1.74	0.50
19:S2:1289:U:C5	35:Sf:97:LYS:HE2	2.46	0.50
23:SD:140:GLY:HA3	23:SD:182:LEU:HD12	1.93	0.50
40:L5:418:A:H2'	40:L5:419:A:C8	2.46	0.50
40:L5:2257:C:O2'	40:L5:2259:G:OP1	2.29	0.50
40:L5:2285:A:H2'	40:L5:2286:G:H8	1.76	0.50
40:L5:2520:C:H2'	40:L5:2521:G:C8	2.46	0.50
40:L5:4173:G:H2'	40:L5:4174:U:C6	2.46	0.50
3:SC:138:GLY:HA3	3:SC:162:ILE:HD13	1.94	0.50
7:SI:44:HIS:ND1	19:S2:1740:C:OP1	2.44	0.50
7:SI:87:ASN:HB3	7:SI:90:LEU:HD23	1.92	0.50
19:S2:170:A:H2'	19:S2:171:A:C8	2.47	0.50
19:S2:1058:A:OP1	38:Pt:38:C:O2'	2.29	0.50
19:S2:1523:C:H2'	19:S2:1524:G:H8	1.75	0.50
19:S2:1585:U:O2'	19:S2:1587:G:OP2	2.26	0.50
36:Sg:167:SER:OG	36:Sg:175:LYS:O	2.27	0.50
37:At:68:G:H2'	37:At:69:A:C8	2.45	0.50
40:L5:137:G:H2'	40:L5:138:G:H8	1.77	0.50
40:L5:359:A:N3	40:L5:363:A:O2'	2.44	0.50
40:L5:2033:A:OP1	59:LS:88:SER:OG	2.27	0.50
40:L5:4622:A:H2'	40:L5:4623:OMG:H8	1.76	0.50
59:LS:71:SER:O	59:LS:76:LYS:NZ	2.39	0.50
71:Lf:54:LYS:O	71:Lf:66:LYS:NZ	2.38	0.50
83:Ls:30:VAL:HG21	83:Ls:187:LEU:HG	1.93	0.50
84:Lt:104:ILE:HG13	84:Lt:106:PHE:HD2	1.76	0.50
9:SL:5:GLN:OE1	9:SL:11:GLN:N	2.42	0.50
19:S2:600:G:H2'	19:S2:601:OMG:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1812:U:H2'	19:S2:1813:A:H8	1.77	0.50
31:SU:26:SER:HB3	31:SU:110:VAL:HG23	1.93	0.50
40:L5:1897:A:O5'	58:LQ:2:GLY:N	2.44	0.50
40:L5:3867:A2M:H8	40:L5:3867:A2M:OP2	2.11	0.50
40:L5:4458:C:H2'	40:L5:4459:U:C6	2.47	0.50
5:SG:167:LYS:HZ3	5:SG:169:PRO:HA	1.76	0.50
19:S2:1689:C:H2'	19:S2:1690:U:H6	1.75	0.50
26:SM:128:PHE:HA	26:SM:131:LYS:HG2	1.92	0.50
29:SS:98:VAL:HG13	29:SS:103:LEU:HD12	1.93	0.50
40:L5:88:A:N7	58:LQ:173:LYS:NZ	2.56	0.50
40:L5:1273:G:C6	47:LE:73:TYR:HB2	2.47	0.50
40:L5:3718:A2M:H2'	40:L5:3719:A:O4'	2.11	0.50
40:L5:4638:U:H3'	40:L5:4639:G:H21	1.76	0.50
6:SH:27:LEU:O	6:SH:37:LYS:NZ	2.44	0.50
19:S2:563:G:N7	19:S2:586:G:N2	2.59	0.50
19:S2:1392:U:H2'	19:S2:1393:G:H8	1.77	0.50
20:LR:74:ARG:NE	40:L5:2891:U:OP2	2.33	0.50
28:SQ:102:GLU:O	28:SQ:106:LYS:N	2.43	0.50
40:L5:964:A:H2'	40:L5:965:G:H4'	1.94	0.50
40:L5:1526:G:H2'	40:L5:1527:A:H8	1.77	0.50
40:L5:2898:G:H2'	40:L5:2899:C:H6	1.77	0.50
40:L5:4220:6MZ:O5'	40:L5:4220:6MZ:H8	2.11	0.50
40:L5:4966:A:H5''	44:LB:128:LYS:HG3	1.94	0.50
42:L8:8:U:H2'	42:L8:9:A:H8	1.76	0.50
43:LA:146:THR:N	43:LA:158:ILE:O	2.42	0.50
44:LB:117:ARG:HA	44:LB:177:LYS:HD2	1.93	0.50
2:SB:123:ALA:HB2	2:SB:165:ARG:HG3	1.93	0.50
5:SG:133:LEU:HD12	19:S2:65:C:C4	2.47	0.50
19:S2:353:C:H2'	19:S2:354:OMU:H6	1.93	0.50
19:S2:898:U:H2'	19:S2:900:C:H1'	1.92	0.50
19:S2:1274:G:H5''	25:SK:47:LYS:HD2	1.94	0.50
23:SD:215:ASP:OD1	23:SD:216:GLU:N	2.41	0.50
40:L5:1207:C:H2'	40:L5:1208:G:C8	2.47	0.50
40:L5:1326:A2M:OP2	40:L5:4445:U:O2'	2.29	0.50
40:L5:1333:A:H2'	40:L5:1334:A:C8	2.45	0.50
40:L5:1914:C:H4'	56:LO:89:PRO:HD3	1.93	0.50
40:L5:3805:U:H2'	40:L5:3806:G:H8	1.76	0.50
40:L5:4503:A:H2'	40:L5:4504:C:C6	2.46	0.50
40:L5:4612:C:C2	50:LH:120:GLU:HB2	2.46	0.50
40:L5:4680:G:H2'	40:L5:4681:A:C8	2.46	0.50
19:S2:558:G:H1'	19:S2:559:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:654:A:OP2	19:S2:655:A:O2'	2.26	0.50
36:Sg:193:GLY:HA3	36:Sg:212:LYS:HB3	1.93	0.50
40:L5:907:C:H2'	40:L5:908:G:C8	2.47	0.50
40:L5:2448:G:OP2	40:L5:2510:G:N1	2.30	0.50
40:L5:4507:A:H2'	40:L5:4508:C:C6	2.47	0.50
40:L5:4704:C:H2'	40:L5:4705:A:H8	1.77	0.50
40:L5:5037:U:H2'	40:L5:5038:A:C8	2.47	0.50
83:Ls:50:LYS:O	83:Ls:92:LYS:NZ	2.44	0.50
84:Lt:119:ARG:HD2	84:Lt:129:ILE:HD11	1.94	0.50
19:S2:880:G:H3'	19:S2:881:G:H8	1.77	0.50
19:S2:1244:PSU:H2'	19:S2:1245:G:H8	1.76	0.50
19:S2:1648:G:N2	19:S2:1675:A:OP2	2.44	0.50
28:SQ:39:LEU:HD11	28:SQ:51:LEU:HB3	1.93	0.50
40:L5:1628:C:H2'	40:L5:1629:G:C8	2.47	0.50
40:L5:3788:C:N4	40:L5:3812:C:O4'	2.45	0.50
40:L5:4273:A:H2'	40:L5:4274:A:C8	2.47	0.50
64:LY:4:ASN:HB3	64:LY:7:VAL:HG12	1.93	0.50
19:S2:656:G:H21	19:S2:663:C:H5''	1.77	0.50
24:SF:28:VAL:HG12	24:SF:110:GLN:HB2	1.94	0.50
40:L5:676:C:H2'	40:L5:677:G:C8	2.47	0.50
40:L5:2284:G:OP1	66:La:7:LYS:NZ	2.34	0.50
40:L5:2361:G:O2'	40:L5:3859:G:O6	2.27	0.50
40:L5:3619:G:H22	40:L5:3624:A:H1'	1.77	0.50
41:L7:6:C:O2'	46:LD:50:ARG:NH2	2.45	0.50
43:LA:143:THR:HG23	43:LA:145:LYS:HG2	1.93	0.50
80:Lo:36:GLN:HB3	80:Lo:39:ARG:HH21	1.76	0.50
5:SG:192:ILE:HD12	5:SG:195:LYS:HD2	1.93	0.49
9:SL:85:THR:HG21	19:S2:373:G:H4'	1.94	0.49
19:S2:1454:A:H2	19:S2:1476:A:H1'	1.76	0.49
19:S2:1512:C:H5''	34:Sd:8:TRP:HZ3	1.76	0.49
31:SU:104:ILE:HG13	31:SU:105:SER:H	1.76	0.49
40:L5:119:G:O4'	49:LG:132:ARG:NH2	2.39	0.49
40:L5:2540:C:H2'	40:L5:2541:G:H8	1.77	0.49
40:L5:2757:A:H2'	40:L5:2758:G:C8	2.47	0.49
40:L5:2835:A:H2'	40:L5:2836:A:C8	2.47	0.49
47:LE:243:THR:HG22	47:LE:245:GLN:H	1.77	0.49
82:Lr:28:GLU:OE2	82:Lr:31:ASN:ND2	2.45	0.49
84:Lt:22:VAL:HA	84:Lt:48:LYS:HE3	1.94	0.49
3:SC:187:ARG:NH1	3:SC:189:GLY:O	2.45	0.49
4:SE:80:ILE:HG23	4:SE:81:THR:HG23	1.94	0.49
6:SH:35:ASP:O	6:SH:39:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SO:44:VAL:HG13	11:SO:53:ILE:HB	1.94	0.49
19:S2:1217:A:H2'	19:S2:1218:C:H6	1.77	0.49
19:S2:1294:G:N1	19:S2:1306:U:O4	2.45	0.49
19:S2:1593:C:H2'	19:S2:1594:A:H8	1.76	0.49
23:SD:64:ARG:HH12	25:SK:73:ASN:HD21	1.60	0.49
40:L5:108:A:O2'	40:L5:334:A:N6	2.41	0.49
40:L5:2324:C:O2'	70:Le:98:GLU:OE2	2.27	0.49
40:L5:2663:G:H2'	40:L5:2664:G:H8	1.76	0.49
40:L5:2882:A:OP1	40:L5:3625:G:N1	2.44	0.49
40:L5:2897:G:H2'	40:L5:2898:G:H8	1.76	0.49
40:L5:3598:C:H2'	40:L5:3599:A:C8	2.47	0.49
40:L5:4524:G:C2	44:LB:252:ALA:HB1	2.47	0.49
40:L5:4774:C:O2'	40:L5:4775:C:O2	2.27	0.49
40:L5:4926:C:H5''	40:L5:4927:G:H21	1.77	0.49
40:L5:4943:A:OP1	47:LE:158:ARG:NH2	2.45	0.49
43:LA:144:LYS:O	43:LA:160:SER:N	2.45	0.49
67:Lb:102:PRO:O	67:Lb:109:ARG:NH2	2.43	0.49
6:SH:57:ARG:HG2	6:SH:172:THR:HG22	1.93	0.49
8:SJ:164:PRO:HB3	8:SJ:170:PRO:HA	1.94	0.49
19:S2:164:A:H2'	19:S2:165:G:C4	2.47	0.49
40:L5:173:C:H5''	53:LL:129:ARG:HH12	1.76	0.49
40:L5:268:G:H2'	40:L5:269:G:H8	1.77	0.49
40:L5:351:C:OP2	45:LC:197:ARG:NH1	2.42	0.49
40:L5:1070:G:O2'	40:L5:1071:C:O5'	2.30	0.49
40:L5:1279:A:O2'	40:L5:1281:G:N7	2.44	0.49
40:L5:1680:G:O6	87:L5:5262:SPM:N1	2.45	0.49
40:L5:3923:A:H2'	40:L5:3924:C:C6	2.47	0.49
40:L5:4584:A:H2'	40:L5:4585:U:O4'	2.11	0.49
41:L7:64:G:H2'	41:L7:65:G:H8	1.78	0.49
42:L8:67:U:H2'	42:L8:68:G:C8	2.47	0.49
50:LH:102:ASN:HB2	50:LH:115:ARG:HB2	1.93	0.49
51:LI:93:PRO:HB2	51:LI:125:THR:HB	1.94	0.49
57:LP:120:ASN:O	57:LP:145:HIS:N	2.41	0.49
71:Lf:78:HIS:N	71:Lf:83:MET:O	2.41	0.49
84:Lt:65:GLN:HG3	84:Lt:67:ARG:H	1.77	0.49
5:SG:11:GLY:HA2	19:S2:166:A2M:HM'1	1.94	0.49
15:SY:20:ARG:NH2	15:SY:22:GLN:OE1	2.43	0.49
19:S2:319:C:H2'	19:S2:320:G:H8	1.77	0.49
19:S2:406:PSU:H2'	19:S2:408:A:H8	1.77	0.49
23:SD:158:ILE:H	23:SD:189:MET:HE1	1.78	0.49
27:SP:20:VAL:HG23	27:SP:24:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Sg:196:ASN:HD22	36:Sg:237:ASN:HA	1.77	0.49
40:L5:57:G:H5''	55:LN:154:PRO:HB2	1.95	0.49
40:L5:1327:C:H2'	40:L5:1328:G:C8	2.48	0.49
40:L5:1334:A:H2'	40:L5:1335:G:H8	1.77	0.49
40:L5:1857:C:H2'	40:L5:1858:A:C8	2.46	0.49
40:L5:2323:C:H2'	40:L5:2324:C:H6	1.76	0.49
40:L5:2683:C:H2'	40:L5:2684:C:H6	1.78	0.49
40:L5:2884:G:H2'	40:L5:2885:A:C8	2.46	0.49
40:L5:4581:G:OP2	44:LB:26:ARG:NH2	2.46	0.49
52:LJ:52:LYS:HB3	52:LJ:65:ASN:HA	1.95	0.49
19:S2:866:PSU:H2'	19:S2:867:OMG:C8	2.46	0.49
19:S2:1259:A:H62	19:S2:1518:C:H3'	1.76	0.49
19:S2:1347:U:H3'	19:S2:1348:G:H21	1.78	0.49
19:S2:1414:A:H2'	19:S2:1415:C:C6	2.47	0.49
36:Sg:68:ASP:HB3	36:Sg:111:VAL:HG12	1.93	0.49
40:L5:29:G:H5''	55:LN:172:ARG:HG2	1.95	0.49
40:L5:662:C:H2'	40:L5:663:G:H8	1.77	0.49
40:L5:1281:G:H5'	45:LC:323:ARG:HB2	1.94	0.49
40:L5:1667:G:N1	40:L5:2281:U:OP2	2.36	0.49
40:L5:1756:U:O2'	40:L5:1758:G:OP2	2.23	0.49
40:L5:1847:C:H2'	40:L5:1848:C:C6	2.48	0.49
40:L5:2671:C:H2'	40:L5:2672:C:C6	2.48	0.49
40:L5:3650:C:OP1	43:LA:217:GLN:NE2	2.39	0.49
40:L5:3944:G:H1	40:L5:4069:U:H3	1.61	0.49
47:LE:270:TYR:OH	54:LM:106:ASP:OD2	2.21	0.49
57:LP:5:SER:OG	57:LP:147:GLU:OE2	2.28	0.49
57:LP:84:PRO:HB2	57:LP:87:SER:HB2	1.94	0.49
59:LS:76:LYS:NZ	59:LS:100:LEU:O	2.42	0.49
69:Ld:92:ARG:HA	69:Ld:102:LEU:HD23	1.94	0.49
83:Ls:65:ILE:HB	83:Ls:69:LEU:HD12	1.93	0.49
9:SL:8:ARG:NH2	19:S2:390:C:O2'	2.42	0.49
11:SO:30:VAL:HG23	11:SO:47:LEU:HD23	1.95	0.49
19:S2:486:A:H1'	19:S2:513:G:H22	1.77	0.49
19:S2:1670:C:H2'	19:S2:1671:G:C8	2.47	0.49
19:S2:1719:A:N6	19:S2:1814:G:O2'	2.45	0.49
27:SP:81:ARG:HB2	27:SP:117:GLY:HA3	1.95	0.49
46:LD:52:ILE:HB	46:LD:63:GLN:HB2	1.94	0.49
4:SE:45:ILE:HA	4:SE:61:VAL:HG21	1.95	0.49
16:Sa:43:ASN:OD1	16:Sa:66:LYS:NZ	2.45	0.49
19:S2:388:U:H2'	19:S2:389:A:H8	1.78	0.49
19:S2:952:G:H2'	19:S2:953:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1653:U:H3	19:S2:1671:G:H1	1.58	0.49
36:Sg:21:ILE:N	36:Sg:288:SER:OG	2.43	0.49
39:CI:71:ARG:NH1	40:L5:2624:G:OP1	2.35	0.49
40:L5:194:C:H1'	64:LY:121:ARG:HH12	1.78	0.49
40:L5:1523:A:N3	40:L5:4389:C:O2'	2.44	0.49
40:L5:1681:G:OP2	40:L5:1853:G:N1	2.32	0.49
40:L5:1837:A:OP2	60:LT:108:ARG:NH1	2.45	0.49
40:L5:2351:OMC:HM22	45:LC:95:MET:HG3	1.94	0.49
40:L5:2353:U:H2'	40:L5:2354:G:H8	1.77	0.49
40:L5:4111:U:H2'	40:L5:4112:C:H5	1.77	0.49
40:L5:4531:U:H4'	40:L5:4532:PSU:H5''	1.93	0.49
41:L7:60:G:H2'	41:L7:61:G:H8	1.76	0.49
49:LG:246:SER:HA	49:LG:249:ARG:HE	1.77	0.49
66:La:75:LEU:HG	66:La:113:GLY:HA2	1.94	0.49
2:SB:168:MET:HA	2:SB:171:ILE:HG12	1.94	0.49
5:SG:15:LEU:HD22	19:S2:155:G:H4'	1.95	0.49
5:SG:183:ARG:NH1	19:S2:317:C:OP2	2.46	0.49
19:S2:1392:U:H2'	19:S2:1393:G:C8	2.48	0.49
35:Sf:107:LYS:NZ	35:Sf:108:VAL:O	2.46	0.49
36:Sg:35:SER:OG	36:Sg:36:ARG:N	2.46	0.49
40:L5:150:U:O4	49:LG:187:LYS:NZ	2.41	0.49
40:L5:425:U:H2'	40:L5:426:A:H8	1.78	0.49
40:L5:1292:C:H3'	40:L5:1293:G:H21	1.76	0.49
40:L5:2075:G:H2'	40:L5:2076:G:H8	1.77	0.49
40:L5:4356:G:H2'	40:L5:4357:G:H8	1.78	0.49
41:L7:110:G:H2'	41:L7:111:C:C6	2.48	0.49
42:L8:19:C:H2'	42:L8:20:A:C8	2.46	0.49
59:LS:34:ALA:HB1	59:LS:39:VAL:HB	1.93	0.49
71:Lf:14:TYR:HA	71:Lf:26:ALA:HA	1.95	0.49
80:Lo:33:LEU:HA	80:Lo:38:LYS:HG2	1.95	0.49
83:Ls:47:LEU:HG	83:Ls:51:ALA:HB3	1.95	0.49
11:SO:96:LYS:HD3	11:SO:132:VAL:HG11	1.94	0.49
13:SW:26:LEU:HB2	17:Sb:7:LEU:HD23	1.95	0.49
15:SY:34:THR:O	19:S2:570:C:O2'	2.31	0.49
19:S2:737:G:H8	19:S2:738:C:H4'	1.77	0.49
19:S2:993:G:OP1	19:S2:1131:G:N2	2.38	0.49
19:S2:1317:C:H2'	19:S2:1318:G:H8	1.77	0.49
34:Sd:17:GLY:HA2	34:Sd:27:ARG:HD3	1.94	0.49
37:At:43:A:H2'	37:At:44:A:C8	2.48	0.49
40:L5:1258:G:H2'	40:L5:1259:G:C8	2.48	0.49
40:L5:1516:G:H2'	40:L5:1518:A:H62	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1555:G:O6	81:Lp:4:ARG:NH1	2.40	0.49
40:L5:2285:A:H2'	40:L5:2286:G:C8	2.48	0.49
40:L5:4759:C:H2'	40:L5:4760:G:C8	2.48	0.49
52:LJ:78:LYS:HE3	52:LJ:82:ILE:HD11	1.95	0.49
5:SG:183:ARG:HH22	19:S2:316:G:H5''	1.78	0.49
19:S2:1401:A:H2'	19:S2:1402:A:C8	2.47	0.49
19:S2:1501:C:H2'	19:S2:1502:C:H6	1.78	0.49
19:S2:1797:U:H2'	19:S2:1798:C:C6	2.48	0.49
37:At:63:G:H2'	37:At:64:G:H8	1.77	0.49
40:L5:133:C:H2'	40:L5:134:G:H4'	1.94	0.49
40:L5:162:A:H2'	40:L5:163:A:C8	2.48	0.49
40:L5:424:U:H2'	40:L5:425:U:C6	2.48	0.49
40:L5:717:U:H2'	40:L5:718:C:C6	2.47	0.49
40:L5:1097:C:H2'	40:L5:1098:G:C8	2.48	0.49
40:L5:2407:G:O6	77:Ll:2:SER:OG	2.27	0.49
40:L5:2622:G:H2'	40:L5:2623:A:C8	2.47	0.49
40:L5:2784:C:H2'	40:L5:2785:C:C6	2.48	0.49
40:L5:2811:G:N1	40:L5:2814:C:OP2	2.46	0.49
40:L5:3607:U:H2'	40:L5:3608:A:C8	2.48	0.49
40:L5:3658:C:H2'	40:L5:3659:G:C8	2.48	0.49
40:L5:4510:A:C2	40:L5:4592:C:H4'	2.47	0.49
40:L5:5055:G:H2'	40:L5:5056:A:C8	2.47	0.49
41:L7:28:C:O2'	41:L7:54:A:N1	2.43	0.49
68:Lc:22:MET:O	68:Lc:23:LYS:HG3	2.12	0.49
80:Lo:6:LYS:HG3	80:Lo:94:GLY:HA3	1.93	0.49
3:SC:165:VAL:HG21	3:SC:217:ALA:HB1	1.94	0.48
6:SH:126:HIS:HA	6:SH:129:ILE:HG12	1.95	0.48
10:SN:99:ARG:HH12	10:SN:143:SER:HB3	1.78	0.48
19:S2:5:U:H2'	19:S2:6:G:H8	1.78	0.48
19:S2:24:C:O2'	19:S2:25:A:O5'	2.31	0.48
19:S2:1240:A:C2	27:SP:100:LYS:HB2	2.48	0.48
40:L5:136:C:N4	73:Lh:77:LYS:O	2.46	0.48
40:L5:921:C:H2'	40:L5:922:C:C6	2.48	0.48
40:L5:1479:G:H2'	40:L5:1480:C:C6	2.48	0.48
40:L5:1950:U:H2'	40:L5:1951:G:C8	2.48	0.48
40:L5:2503:G:H1'	40:L5:2505:C:H5	1.77	0.48
40:L5:2848:G:O2'	40:L5:3838:U:O4	2.31	0.48
43:LA:116:LEU:HB3	43:LA:126:LEU:HB2	1.94	0.48
67:Lb:90:SER:HB2	67:Lb:95:ARG:HH12	1.78	0.48
5:SG:4:ASN:HB3	5:SG:110:ASN:HA	1.95	0.48
21:LW:61:LYS:NZ	40:L5:5038:A:OP1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SU:93:SER:H	31:SU:97:ILE:HD11	1.79	0.48
38:Pt:6:C:H2'	38:Pt:7:G:C8	2.48	0.48
40:L5:1327:C:H2'	40:L5:1328:G:H8	1.78	0.48
40:L5:1876:U:H2'	40:L5:1877:G:C8	2.48	0.48
40:L5:2640:G:H2'	40:L5:2641:A:C8	2.47	0.48
40:L5:3819:G:H2'	40:L5:3820:G:H8	1.77	0.48
40:L5:3877:A:O2'	40:L5:4400:G:N2	2.42	0.48
40:L5:4459:U:H2'	40:L5:4460:U:H6	1.77	0.48
40:L5:4643:G:H2'	40:L5:4644:G:H8	1.78	0.48
40:L5:4685:U:H2'	40:L5:4686:G:C8	2.48	0.48
40:L5:4699:U:H1'	40:L5:4700:A:H5''	1.94	0.48
41:L7:61:G:O2'	46:LD:279:ARG:NH1	2.45	0.48
42:L8:6:C:H2'	42:L8:7:U:C6	2.48	0.48
46:LD:111:ASN:ND2	46:LD:116:ASP:OD2	2.44	0.48
55:LN:4:TYR:HA	55:LN:7:ILE:HD12	1.96	0.48
63:LX:140:LEU:HD23	63:LX:144:TYR:HB3	1.95	0.48
67:Lb:41:ARG:HH21	67:Lb:45:PHE:HE2	1.61	0.48
3:SC:107:LEU:HB3	3:SC:233:LEU:HD21	1.94	0.48
19:S2:27:A2M:H2'	19:S2:28:U:O4'	2.14	0.48
19:S2:1243:U:OP2	19:S2:1518:C:O2'	2.29	0.48
21:LW:7:SER:HB2	21:LW:13:ILE:HD11	1.94	0.48
23:SD:74:GLN:NE2	23:SD:81:GLU:OE2	2.46	0.48
31:SU:21:ARG:N	31:SU:115:THR:O	2.41	0.48
40:L5:1480:C:O2'	40:L5:1482:G:OP2	2.32	0.48
40:L5:3785:A2M:HM'1	40:L5:4537:C:H1'	1.95	0.48
40:L5:4314:C:OP1	60:LT:70:HIS:ND1	2.46	0.48
44:LB:45:ALA:HB3	44:LB:183:ILE:HG23	1.95	0.48
2:SB:36:PRO:HB2	2:SB:38:MET:HG2	1.94	0.48
2:SB:132:GLY:O	2:SB:219:LYS:NZ	2.39	0.48
4:SE:75:LYS:NZ	19:S2:122:G:OP1	2.37	0.48
4:SE:121:TYR:HA	4:SE:163:ASP:HA	1.96	0.48
19:S2:484:A2M:H8	19:S2:484:A2M:O5'	2.13	0.48
19:S2:640:A:H2'	19:S2:641:A:C8	2.47	0.48
19:S2:925:G:O6	19:S2:1017:U:O4	2.32	0.48
19:S2:1542:C:H4'	30:ST:11:GLN:HB2	1.94	0.48
19:S2:1692:U:H2'	19:S2:1693:G:H8	1.77	0.48
23:SD:47:GLU:HG2	23:SD:85:GLU:HB2	1.94	0.48
40:L5:422:C:H2'	40:L5:423:G:H8	1.79	0.48
40:L5:1541:C:H5''	43:LA:21:LYS:HG2	1.95	0.48
40:L5:1683:PSU:H2'	40:L5:1684:A:C8	2.48	0.48
63:LX:141:ALA:HB3	63:LX:144:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SE:179:ASN:HA	4:SE:231:GLY:HA2	1.96	0.48
5:SG:22:ARG:NH2	44:LB:306:ASP:O	2.44	0.48
9:SL:105:ARG:NH1	19:S2:355:G:OP1	2.44	0.48
10:SN:7:PRO:HG3	19:S2:996:A:H5''	1.94	0.48
19:S2:1716:C:H2'	19:S2:1717:C:H6	1.78	0.48
36:Sg:119:GLN:HB3	36:Sg:131:LEU:HD11	1.95	0.48
40:L5:56:A:H4'	55:LN:157:LYS:HD2	1.94	0.48
40:L5:197:A:N6	40:L5:242:U:H3	2.12	0.48
40:L5:1180:C:H1'	40:L5:1183:C:C2	2.49	0.48
40:L5:1824:G:H2'	40:L5:1825:A:H8	1.79	0.48
40:L5:2327:G:H2'	40:L5:2328:G:H8	1.77	0.48
40:L5:2663:G:H2'	40:L5:2664:G:C8	2.48	0.48
40:L5:2764:A:H2'	40:L5:2765:A:H8	1.78	0.48
40:L5:3927:U:H2'	40:L5:3928:A:H8	1.79	0.48
40:L5:5002:U:O2	40:L5:5045:G:N2	2.34	0.48
42:L8:22:U:OP2	45:LC:196:MET:HG2	2.13	0.48
54:LM:7:VAL:N	59:LS:152:PHE:O	2.43	0.48
57:LP:13:LYS:HB3	57:LP:152:GLU:HB2	1.94	0.48
84:Lt:59:THR:H	84:Lt:80:LEU:HD11	1.77	0.48
5:SG:13:GLN:HE21	19:S2:153:G:H21	1.60	0.48
17:Sb:67:THR:OG1	17:Sb:70:LYS:O	2.26	0.48
17:Sb:68:GLY:HA2	19:S2:928:G:H21	1.78	0.48
19:S2:1143:A:O3'	19:S2:1355:C:N4	2.47	0.48
19:S2:1457:U:H2'	19:S2:1458:G:H8	1.79	0.48
40:L5:62:A:OP1	55:LN:172:ARG:NH1	2.47	0.48
40:L5:685:C:H4'	40:L5:686:A:C4	2.48	0.48
40:L5:950:G:H2'	40:L5:951:G:H8	1.79	0.48
40:L5:1472:C:N4	40:L5:1493:G:O6	2.47	0.48
40:L5:1554:A:OP2	81:Lp:4:ARG:NE	2.36	0.48
40:L5:2535:G:H2'	40:L5:2536:A:C8	2.49	0.48
40:L5:2902:G:N2	40:L5:3597:G:O6	2.46	0.48
40:L5:4069:U:H2'	40:L5:4070:U:H6	1.78	0.48
40:L5:4503:A:H2'	40:L5:4504:C:H6	1.77	0.48
40:L5:4676:G:OP1	44:LB:281:ASN:ND2	2.45	0.48
40:L5:4920:C:H2'	40:L5:4921:C:H6	1.77	0.48
46:LD:120:GLU:O	46:LD:248:ARG:NH1	2.46	0.48
64:LY:73:VAL:HA	64:LY:80:ILE:HG22	1.96	0.48
1:SA:183:LEU:O	1:SA:188:THR:OG1	2.32	0.48
8:SJ:176:LYS:HA	8:SJ:179:LYS:HG2	1.94	0.48
9:SL:39:ASN:O	19:S2:292:A:O2'	2.26	0.48
19:S2:527:C:H2'	19:S2:528:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1348:G:N2	19:S2:1348:G:OP2	2.45	0.48
19:S2:1447:G:H2'	19:S2:1448:A:C8	2.49	0.48
19:S2:1490:OMG:N2	31:SU:72:GLU:OE1	2.47	0.48
19:S2:1524:G:O2'	38:Pt:30:G:OP1	2.32	0.48
19:S2:1532:C:H3'	19:S2:1637:A:H62	1.77	0.48
40:L5:505:G:N2	40:L5:653:U:O2	2.36	0.48
40:L5:1645:C:H2'	40:L5:1646:A:C8	2.49	0.48
40:L5:1733:G:N3	40:L5:4214:A:H2'	2.29	0.48
40:L5:2297:G:H4'	45:LC:242:PRO:HB2	1.96	0.48
40:L5:4657:U:O2'	40:L5:4659:G:OP2	2.31	0.48
41:L7:63:C:H5'	41:L7:64:G:H5''	1.94	0.48
47:LE:91:THR:HG22	47:LE:108:LYS:HB3	1.96	0.48
49:LG:209:SER:HA	49:LG:212:LYS:HG3	1.95	0.48
70:Le:88:LEU:HD12	70:Le:97:ALA:HB2	1.96	0.48
83:Ls:29:ILE:HG13	83:Ls:190:GLN:HB2	1.94	0.48
83:Ls:50:LYS:NZ	83:Ls:93:GLU:OE1	2.46	0.48
1:SA:77:ILE:HG22	1:SA:99:ILE:HB	1.95	0.48
4:SE:112:HIS:NE2	4:SE:237:SER:O	2.47	0.48
4:SE:247:THR:OG1	4:SE:250:GLU:OE1	2.25	0.48
5:SG:146:ASN:HB2	21:LW:101:ARG:HH22	1.78	0.48
5:SG:174:PRO:HB3	19:S2:65:C:C6	2.48	0.48
7:SI:184:ARG:HD2	19:S2:219:U:H1'	1.96	0.48
19:S2:1203:G:H2'	19:S2:1204:A:C8	2.49	0.48
40:L5:417:G:OP1	40:L5:2329:U:O2'	2.32	0.48
40:L5:436:C:H2'	40:L5:437:G:C8	2.46	0.48
40:L5:1172:C:O2'	40:L5:1173:G:H8	1.97	0.48
40:L5:2309:G:O2'	42:L8:18:U:O2	2.32	0.48
40:L5:2745:A:H2'	40:L5:2746:A:H8	1.79	0.48
40:L5:4881:U:O4	54:LM:116:LYS:NZ	2.42	0.48
40:L5:4884:G:N7	47:LE:272:ARG:NH2	2.61	0.48
64:LY:2:LYS:HD2	64:LY:7:VAL:HG13	1.95	0.48
75:Lj:28:HIS:CE1	75:Lj:30:GLN:HB3	2.49	0.48
5:SG:2:LYS:HB2	5:SG:108:VAL:HG12	1.95	0.48
5:SG:156:TYR:OH	21:LW:96:GLN:OE1	2.31	0.48
19:S2:388:U:H2'	19:S2:389:A:C8	2.48	0.48
19:S2:1457:U:H2'	19:S2:1458:G:C8	2.49	0.48
24:SF:28:VAL:HG11	24:SF:109:LEU:HB2	1.96	0.48
40:L5:94:A:H5''	66:La:34:ASN:HB2	1.96	0.48
40:L5:159:C:OP2	74:Li:27:SER:N	2.46	0.48
40:L5:433:A:N3	40:L5:3867:A2M:H4'	2.28	0.48
40:L5:945:U:OP1	45:LC:342:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1269:G:HO2'	40:L5:1440:U:HO2'	1.58	0.48
40:L5:2079:G:H2'	40:L5:2080:U:H6	1.79	0.48
40:L5:3688:U:OP2	43:LA:198:ARG:NH2	2.47	0.48
40:L5:3722:G:H2'	40:L5:3723:A:C8	2.47	0.48
40:L5:4910:G:H1	56:LO:108:ILE:H	1.62	0.48
47:LE:225:PRO:HG2	47:LE:226:ARG:HH11	1.78	0.48
53:LL:48:PRO:HG3	73:Lh:118:LYS:HE2	1.94	0.48
65:LZ:27:LYS:O	65:LZ:42:LEU:N	2.42	0.48
74:Li:45:ARG:NH2	74:Li:49:GLY:O	2.39	0.48
76:Lk:26:LYS:HD3	76:Lk:69:LEU:HD22	1.96	0.48
78:Lm:99:CYS:HB3	78:Lm:115:CYS:HB3	1.96	0.48
2:SB:138:PHE:O	2:SB:213:ARG:N	2.47	0.48
4:SE:17:HIS:NE2	4:SE:39:ARG:O	2.45	0.48
7:SI:116:HIS:CG	7:SI:152:ARG:HH21	2.31	0.48
8:SJ:136:ARG:HD3	8:SJ:160:SER:HA	1.96	0.48
11:SO:98:ARG:HG3	11:SO:134:PRO:HD3	1.96	0.48
14:SX:137:LYS:NZ	19:S2:30:C:O3'	2.47	0.48
15:SY:11:LYS:HB2	15:SY:24:VAL:HG12	1.95	0.48
19:S2:329:G:H2'	19:S2:330:G:H8	1.79	0.48
19:S2:1221:G:H2'	19:S2:1222:G:H8	1.79	0.48
19:S2:1581:C:H5'	19:S2:1582:C:H5	1.78	0.48
20:LR:168:GLU:HA	20:LR:171:LYS:HG2	1.96	0.48
40:L5:1779:U:H2'	40:L5:1780:A:C8	2.48	0.48
40:L5:1973:G:H4'	84:Lt:78:SER:H	1.79	0.48
40:L5:2633:U:H2'	40:L5:2634:C:C6	2.49	0.48
48:LF:90:ALA:HB2	48:LF:125:LEU:HD11	1.96	0.48
71:Lf:7:SER:HB2	71:Lf:103:VAL:HB	1.96	0.48
2:SB:70:SER:OG	2:SB:71:LEU:N	2.47	0.47
5:SG:132:ARG:NE	19:S2:151:C:O2'	2.47	0.47
8:SJ:79:ARG:NH2	19:S2:820:U:OP2	2.39	0.47
19:S2:1113:A:N6	19:S2:1121:G:O6	2.47	0.47
19:S2:1566:G:O6	30:ST:101:ARG:NH1	2.45	0.47
21:LW:46:PRO:HB2	21:LW:52:THR:HG21	1.95	0.47
40:L5:1394:G:OP1	53:LL:186:ARG:NH1	2.47	0.47
40:L5:1697:G:H22	40:L5:2084:C:P	2.36	0.47
40:L5:2018:C:H2'	40:L5:2019:C:C6	2.49	0.47
40:L5:3809:G:OP2	40:L5:3809:G:N2	2.30	0.47
45:LC:110:ARG:O	45:LC:113:ARG:NH1	2.46	0.47
48:LF:162:ILE:HD12	48:LF:167:ILE:HB	1.96	0.47
51:LI:91:LEU:HD12	51:LI:135:ILE:HG23	1.95	0.47
58:LQ:63:LEU:N	58:LQ:87:THR:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LQ:157:GLY:O	58:LQ:188:ASN:ND2	2.46	0.47
1:SA:110:ASN:ND2	19:S2:1350:U:O2	2.46	0.47
3:SC:187:ARG:HD3	3:SC:192:LEU:HD12	1.97	0.47
4:SE:36:HIS:CE1	4:SE:85:GLY:HA3	2.49	0.47
5:SG:50:VAL:HG21	5:SG:111:LEU:HB3	1.94	0.47
7:SI:133:GLU:HA	7:SI:136:ILE:HG12	1.96	0.47
19:S2:371:A:N3	19:S2:394:G:N2	2.62	0.47
19:S2:429:C:H2'	19:S2:430:C:H6	1.79	0.47
19:S2:822:U:O4	19:S2:826:A:N7	2.47	0.47
19:S2:1174:PSU:H2'	19:S2:1175:G:H8	1.79	0.47
19:S2:1414:A:H2'	19:S2:1415:C:H6	1.79	0.47
36:Sg:176:VAL:HG23	36:Sg:185:LYS:HB2	1.96	0.47
40:L5:401:G:OP1	57:LP:16:LYS:NZ	2.37	0.47
40:L5:1511:U:H2'	40:L5:1512:G:C8	2.48	0.47
40:L5:4578:G:H2'	40:L5:4579:PSU:C6	2.49	0.47
44:LB:46:PHE:HE2	44:LB:81:THR:HB	1.79	0.47
44:LB:300:LYS:HG3	44:LB:311:ASP:HA	1.96	0.47
64:LY:55:VAL:HG12	64:LY:106:ILE:HA	1.96	0.47
1:SA:32:PHE:HA	1:SA:35:GLU:HB2	1.95	0.47
1:SA:74:VAL:HG23	1:SA:121:LEU:HB3	1.95	0.47
5:SG:136:LYS:HB2	19:S2:65:C:H41	1.78	0.47
5:SG:227:GLN:HB3	5:SG:231:ARG:HH21	1.80	0.47
19:S2:113:G:H22	19:S2:292:A:H2'	1.78	0.47
19:S2:656:G:N2	19:S2:663:C:H5''	2.28	0.47
19:S2:1166:G:N2	19:S2:1193:U:O2	2.34	0.47
19:S2:1623:A:C6	29:SS:132:ARG:HD3	2.50	0.47
20:LR:110:ARG:NH1	40:L5:2665:U:OP2	2.42	0.47
22:SR:58:MET:HA	22:SR:61:ILE:HG22	1.94	0.47
24:SF:102:LEU:HD21	32:SZ:110:THR:HB	1.95	0.47
26:SM:83:LYS:HE2	26:SM:103:VAL:HG13	1.95	0.47
29:SS:106:LYS:HA	29:SS:106:LYS:HD2	1.70	0.47
40:L5:509:A:N6	66:La:106:SER:OG	2.47	0.47
40:L5:1336:G:H2'	40:L5:2346:C:H42	1.78	0.47
40:L5:1692:C:H4'	58:LQ:143:ARG:HH12	1.80	0.47
40:L5:1996:C:H42	40:L5:2000:G:N2	2.12	0.47
40:L5:2476:G:H2'	40:L5:2477:A:H8	1.80	0.47
40:L5:2690:C:H2'	40:L5:2691:U:C6	2.50	0.47
40:L5:3610:A:H2'	40:L5:3611:A:C8	2.50	0.47
40:L5:3664:G:H2'	40:L5:3665:G:C8	2.46	0.47
40:L5:4742:G:H2'	40:L5:4743:G:C8	2.50	0.47
40:L5:4906:C:H2'	40:L5:4907:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:LD:183:TYR:HA	46:LD:190:PHE:HA	1.95	0.47
54:LM:30:VAL:HG23	54:LM:52:PHE:HZ	1.79	0.47
62:LV:111:GLU:HG3	62:LV:131:ARG:HD3	1.96	0.47
15:SY:9:THR:H	19:S2:837:A:N6	2.12	0.47
19:S2:404:G:H2'	19:S2:405:G:C8	2.49	0.47
19:S2:1252:C:N4	28:SQ:146:ARG:O	2.48	0.47
40:L5:665:C:H1'	40:L5:668:C:H41	1.80	0.47
40:L5:1895:G:OP1	48:LF:96:ARG:NH2	2.47	0.47
40:L5:2898:G:H2'	40:L5:2899:C:C6	2.50	0.47
40:L5:3928:A:OP1	55:LN:90:ASN:ND2	2.47	0.47
40:L5:4683:U:OP2	40:L5:4706:G:N1	2.38	0.47
40:L5:4913:G:H4'	40:L5:4914:C:O5'	2.15	0.47
42:L8:130:C:H2'	42:L8:131:G:H8	1.79	0.47
43:LA:30:ARG:HB3	43:LA:74:GLU:HG3	1.96	0.47
49:LG:251:ALA:HA	49:LG:254:GLU:HB2	1.96	0.47
60:LT:27:LEU:HB3	60:LT:31:MET:HE3	1.95	0.47
4:SE:247:THR:HG1	4:SE:250:GLU:CD	2.19	0.47
6:SH:7:LYS:HE2	6:SH:10:LYS:HB3	1.96	0.47
7:SI:72:CYS:HG	7:SI:112:TRP:CG	2.32	0.47
15:SY:13:MET:HE1	15:SY:15:ASN:HB3	1.96	0.47
17:Sb:36:LYS:HB3	17:Sb:78:SER:HB2	1.96	0.47
19:S2:329:G:H2'	19:S2:330:G:C8	2.49	0.47
19:S2:588:G:H4'	19:S2:589:G:H5'	1.96	0.47
21:LW:44:ARG:HD3	40:L5:3615:G:H1'	1.97	0.47
40:L5:1637:A:OP1	40:L5:1640:C:N4	2.45	0.47
41:L7:23:A:H2'	41:L7:24:C:C6	2.49	0.47
42:L8:148:A:H2'	42:L8:149:G:C8	2.50	0.47
52:LJ:92:TYR:HB3	52:LJ:172:GLY:HA2	1.97	0.47
3:SC:253:PRO:HA	3:SC:256:TRP:CE2	2.49	0.47
9:SL:13:GLN:HB2	9:SL:16:ILE:HD12	1.96	0.47
19:S2:414:A:H2'	19:S2:415:A:H8	1.80	0.47
19:S2:484:A2M:HM'3	19:S2:484:A2M:H1'	1.58	0.47
19:S2:1144:A:OP1	19:S2:1355:C:N4	2.48	0.47
19:S2:1253:A:H4'	19:S2:1254:C:H5''	1.96	0.47
19:S2:1521:C:H5'	29:SS:129:LEU:HD22	1.97	0.47
19:S2:1822:A:H2'	19:S2:1823:A:C8	2.49	0.47
40:L5:287:U:H2'	40:L5:288:G:H8	1.78	0.47
40:L5:1086:C:H2'	40:L5:1087:A:C8	2.48	0.47
40:L5:2266:C:O2	82:Lr:39:ARG:NH2	2.42	0.47
40:L5:2401:A2M:H1'	40:L5:2401:A2M:HM'3	1.56	0.47
40:L5:3830:A2M:H1'	40:L5:3830:A2M:HM'3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4860:G:H2'	40:L5:4861:G:C8	2.49	0.47
40:L5:4967:A:H2'	40:L5:4968:A:C8	2.49	0.47
45:LC:141:GLY:O	45:LC:182:LYS:NZ	2.48	0.47
54:LM:113:MET:HE3	54:LM:113:MET:HB3	1.85	0.47
3:SC:104:ASP:HA	3:SC:130:ILE:HG22	1.95	0.47
10:SN:109:LYS:HD2	19:S2:1032:C:H5''	1.97	0.47
19:S2:379:C:H2'	19:S2:380:G:C8	2.49	0.47
19:S2:1049:A:OP2	19:S2:1068:G:N1	2.32	0.47
19:S2:1281:G:H3'	19:S2:1282:A:H8	1.80	0.47
19:S2:1593:C:H2'	19:S2:1594:A:C8	2.49	0.47
19:S2:1713:C:H2'	19:S2:1714:U:C6	2.50	0.47
24:SF:30:ILE:HG23	24:SF:117:ILE:HD11	1.95	0.47
26:SM:79:VAL:HG11	26:SM:85:LEU:HB2	1.97	0.47
28:SQ:9:SER:N	28:SQ:99:TYR:OH	2.47	0.47
31:SU:20:ILE:HA	31:SU:116:ILE:HA	1.96	0.47
32:SZ:63:PRO:HG3	32:SZ:97:ILE:HD11	1.97	0.47
34:Sd:3:HIS:CE1	34:Sd:5:GLN:HB2	2.50	0.47
35:Sf:141:CYS:H	35:Sf:145:CYS:HB3	1.80	0.47
37:At:1:G:H2'	37:At:2:U:C6	2.50	0.47
40:L5:318:A:H2'	40:L5:319:A:C8	2.48	0.47
40:L5:714:G:H2'	40:L5:715:G:C8	2.49	0.47
40:L5:951:G:H2'	40:L5:952:G:C8	2.50	0.47
40:L5:2374:A:H2'	40:L5:2375:A:C8	2.50	0.47
40:L5:2611:A:H2'	40:L5:2612:G:C8	2.50	0.47
40:L5:2765:A:H2'	40:L5:2766:A:C8	2.49	0.47
40:L5:2901:G:H2'	40:L5:2902:G:H5''	1.97	0.47
40:L5:3688:U:H2'	40:L5:3689:G:C8	2.49	0.47
40:L5:3867:A2M:HM'3	40:L5:3867:A2M:H1'	1.53	0.47
40:L5:3917:A:H2'	40:L5:3918:G:C8	2.49	0.47
42:L8:90:C:H2'	42:L8:91:A:C8	2.50	0.47
42:L8:141:C:H2'	42:L8:142:U:C6	2.49	0.47
44:LB:29:VAL:HA	44:LB:220:ILE:HD13	1.97	0.47
51:LI:36:LEU:HD11	51:LI:69:ARG:HD2	1.96	0.47
52:LJ:63:ARG:HH12	80:Lo:103:VAL:HB	1.80	0.47
80:Lo:69:ARG:HG3	80:Lo:82:MET:HE1	1.97	0.47
1:SA:106:GLY:N	1:SA:136:GLU:OE2	2.47	0.47
3:SC:144:SER:HB3	3:SC:150:ALA:HB2	1.97	0.47
19:S2:1347:U:H2'	19:S2:1348:G:N3	2.30	0.47
19:S2:1842:4AC:H2'	19:S2:1843:G:H8	1.80	0.47
24:SF:22:LYS:HG3	24:SF:23:TRP:CD2	2.50	0.47
24:SF:68:ILE:HD11	24:SF:116:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1669:A:OP1	67:Lb:18:ARG:NH2	2.46	0.47
40:L5:2049:G:H2'	40:L5:2050:G:C8	2.49	0.47
40:L5:2375:A:H2'	40:L5:2376:A:C8	2.50	0.47
40:L5:2651:C:O2'	40:L5:2653:C:OP1	2.30	0.47
40:L5:2694:G:H5'	40:L5:2695:A:C2	2.50	0.47
40:L5:2720:C:H2'	40:L5:2721:G:O4'	2.15	0.47
40:L5:4076:G:OP1	49:LG:73:ARG:NE	2.48	0.47
40:L5:4260:U:H2'	40:L5:4261:C:C6	2.50	0.47
40:L5:4305:G:O5'	60:LT:83:LYS:NZ	2.46	0.47
40:L5:4594:U:H2'	40:L5:4595:G:C8	2.50	0.47
46:LD:146:LEU:HB2	46:LD:163:LEU:HD12	1.96	0.47
65:LZ:11:VAL:HG12	65:LZ:82:PRO:HA	1.97	0.47
79:Ln:2:ARG:HB3	79:Ln:5:TRP:CD1	2.50	0.47
1:SA:159:ILE:HG12	12:SV:34:MET:HE1	1.97	0.47
9:SL:57:ASP:HB3	9:SL:60:CYS:HB2	1.95	0.47
19:S2:27:A2M:HM'3	19:S2:27:A2M:H1'	1.65	0.47
19:S2:795:A:H2'	19:S2:796:G:C8	2.49	0.47
19:S2:878:G:C6	19:S2:908:A:N1	2.83	0.47
19:S2:929:G:H2'	19:S2:930:C:O4'	2.15	0.47
20:LR:12:SER:OG	20:LR:17:CYS:O	2.27	0.47
31:SU:28:ASN:HD21	31:SU:31:SER:HB3	1.79	0.47
36:Sg:260:ASP:OD2	36:Sg:263:GLY:N	2.41	0.47
40:L5:1278:C:H2'	40:L5:1279:A:O4'	2.15	0.47
40:L5:1323:A2M:HM'3	40:L5:1323:A2M:H1'	1.47	0.47
40:L5:1389:U:OP1	40:L5:1497:A:O2'	2.28	0.47
40:L5:1932:A:OP1	56:LO:49:ARG:NH2	2.39	0.47
40:L5:2098:G:H2'	40:L5:2099:G:C8	2.49	0.47
40:L5:2869:U:O2'	40:L5:2881:A:N7	2.46	0.47
40:L5:3861:A:H2'	40:L5:3862:A:C8	2.50	0.47
40:L5:5004:C:H2'	40:L5:5005:G:O4'	2.14	0.47
43:LA:180:LEU:HD21	81:Lp:22:LEU:HB3	1.96	0.47
44:LB:17:LEU:O	44:LB:19:ARG:N	2.46	0.47
78:Lm:79:GLU:CD	78:Lm:81:SER:HG	2.23	0.47
4:SE:57:THR:OG1	4:SE:59:ASP:OD1	2.30	0.47
6:SH:17:ASP:HB2	6:SH:20:GLU:HB2	1.96	0.47
8:SJ:3:VAL:HB	8:SJ:5:ARG:HD3	1.95	0.47
10:SN:20:ARG:HH21	13:SW:56:HIS:HB3	1.80	0.47
13:SW:105:THR:HB	13:SW:126:LEU:HD11	1.97	0.47
14:SX:71:ARG:NH1	14:SX:82:THR:OG1	2.40	0.47
19:S2:85:A:H2'	19:S2:86:C:H6	1.80	0.47
19:S2:409:C:H2'	19:S2:410:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:534:G:H2'	19:S2:535:G:C8	2.50	0.47
19:S2:1566:G:N7	30:ST:101:ARG:NH2	2.63	0.47
35:Sf:124:ASP:OD1	35:Sf:124:ASP:N	2.47	0.47
36:Sg:173:LEU:HD11	36:Sg:187:ASN:HB3	1.97	0.47
36:Sg:191:HIS:ND1	36:Sg:213:ASP:OD2	2.31	0.47
36:Sg:259:TRP:CD1	36:Sg:266:ILE:HG12	2.49	0.47
36:Sg:259:TRP:HD1	36:Sg:266:ILE:HG12	1.79	0.47
40:L5:1468:C:OP1	66:La:132:ARG:NH2	2.47	0.47
40:L5:1973:G:H2'	40:L5:1974:U:C5	2.50	0.47
40:L5:4091:G:H2'	40:L5:4092:G:C8	2.50	0.47
1:SA:25:LEU:O	1:SA:164:ASN:ND2	2.48	0.46
2:SB:224:GLU:HB3	2:SB:227:LYS:HE3	1.97	0.46
11:SO:39:ASP:OD1	11:SO:40:THR:N	2.47	0.46
19:S2:28:U:H2'	19:S2:29:G:C8	2.49	0.46
19:S2:996:A:H2'	19:S2:997:A:C8	2.50	0.46
19:S2:1226:G:O6	19:S2:1641:A:N6	2.48	0.46
19:S2:1524:G:N7	29:SS:141:ARG:NH1	2.63	0.46
19:S2:1569:A:H5'	30:ST:41:LYS:HD3	1.96	0.46
19:S2:1657:G:H2'	19:S2:1658:G:H8	1.80	0.46
20:LR:105:LEU:HD23	20:LR:138:LEU:HD23	1.97	0.46
27:SP:28:MET:HG2	27:SP:32:GLN:HG3	1.97	0.46
40:L5:1677:PSU:H4'	40:L5:1680:G:C2	2.51	0.46
40:L5:1881:C:H5'	40:L5:2281:U:H1'	1.98	0.46
40:L5:2415:U:H2'	40:L5:2416:G:C8	2.49	0.46
40:L5:2535:G:H2'	40:L5:2536:A:H8	1.81	0.46
40:L5:3667:C:H4'	43:LA:8:GLN:HA	1.96	0.46
40:L5:3688:U:H2'	40:L5:3689:G:H8	1.78	0.46
40:L5:3798:U:O2'	40:L5:3800:A:N7	2.32	0.46
40:L5:3825:A2M:H2'	40:L5:3826:C:C6	2.49	0.46
40:L5:4896:G:H2'	40:L5:4897:G:H8	1.80	0.46
68:Lc:26:LYS:HB2	68:Lc:97:ILE:HB	1.97	0.46
8:SJ:145:PRO:HD2	19:S2:522:A:H5''	1.97	0.46
19:S2:21:U:H2'	19:S2:22:A:C8	2.50	0.46
19:S2:159:A2M:H2'	19:S2:160:U:H6	1.79	0.46
19:S2:1473:G:N1	19:S2:1476:A:OP2	2.37	0.46
40:L5:126:C:H2'	40:L5:127:G:C8	2.50	0.46
40:L5:1377:G:H4'	40:L5:1378:C:H3'	1.97	0.46
40:L5:1996:C:N4	40:L5:2000:G:N2	2.62	0.46
40:L5:3952:A:O2'	40:L5:3953:G:O4'	2.30	0.46
40:L5:4570:G:H2'	40:L5:4571:A2M:H8	1.96	0.46
2:SB:117:TRP:CD1	2:SB:153:THR:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:204:ILE:O	19:S2:1121:G:O2'	2.33	0.46
5:SG:7:PHE:HE1	5:SG:9:ALA:HB3	1.80	0.46
10:SN:12:SER:OG	19:S2:1015:U:O4	2.31	0.46
19:S2:51:U:H2'	19:S2:52:G:C8	2.50	0.46
19:S2:218:U:H2'	19:S2:219:U:C6	2.51	0.46
19:S2:433:A:H2'	19:S2:434:G:C8	2.50	0.46
19:S2:602:G:H3'	19:S2:603:C:H2'	1.96	0.46
27:SP:32:GLN:HA	27:SP:35:GLN:HG2	1.98	0.46
40:L5:1461:C:H2'	40:L5:1462:A:H8	1.81	0.46
40:L5:4101:C:O2	40:L5:4107:G:N2	2.49	0.46
40:L5:4415:A:OP1	51:LI:154:ARG:NH2	2.48	0.46
40:L5:4508:C:H5''	62:LV:43:LYS:HD3	1.97	0.46
40:L5:4883:C:H2'	40:L5:4884:G:C8	2.51	0.46
44:LB:217:ILE:HD13	44:LB:284:ILE:HD11	1.97	0.46
46:LD:234:ASP:OD1	46:LD:235:MET:N	2.48	0.46
52:LJ:100:SER:OG	52:LJ:104:ASN:O	2.34	0.46
80:Lo:74:GLU:OE1	80:Lo:77:CYS:N	2.46	0.46
13:SW:86:LEU:HB3	13:SW:117:ARG:HH21	1.81	0.46
16:Sa:12:LYS:HG3	16:Sa:15:ARG:HB2	1.96	0.46
19:S2:649:PSU:H2'	19:S2:650:A:H8	1.80	0.46
19:S2:812:A:H2'	19:S2:813:A:H8	1.80	0.46
19:S2:1739:C:H2'	19:S2:1740:C:H6	1.80	0.46
19:S2:1752:C:N4	19:S2:1754:G:N7	2.63	0.46
23:SD:45:ARG:HB2	23:SD:83:SER:HA	1.96	0.46
40:L5:271:C:H2'	40:L5:272:U:H6	1.80	0.46
40:L5:2063:G:H2'	40:L5:2064:G:H8	1.80	0.46
40:L5:2497:C:H2'	40:L5:2498:C:H6	1.80	0.46
40:L5:3825:A2M:H1'	40:L5:3825:A2M:HM'3	1.52	0.46
40:L5:4643:G:H2'	40:L5:4644:G:C8	2.51	0.46
46:LD:103:LEU:HG	46:LD:247:ILE:HG21	1.97	0.46
52:LJ:90:ARG:NH2	52:LJ:108:GLY:O	2.43	0.46
66:La:71:PRO:HG2	66:La:108:TYR:HA	1.98	0.46
76:Lk:12:LEU:HB3	76:Lk:16:ARG:HH21	1.81	0.46
19:S2:96:C:H2'	19:S2:97:U:C6	2.51	0.46
19:S2:159:A2M:H2'	19:S2:160:U:C6	2.50	0.46
19:S2:436:OMG:OP2	19:S2:471:G:O2'	2.28	0.46
19:S2:1334:G:OP1	23:SD:139:SER:OG	2.34	0.46
19:S2:1454:A:C2	19:S2:1476:A:H1'	2.51	0.46
40:L5:2007:G:H21	40:L5:2012:A:H62	1.63	0.46
40:L5:2353:U:H2'	40:L5:2354:G:C8	2.51	0.46
40:L5:2722:G:H2'	40:L5:2723:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:2751:G:H2'	40:L5:2752:G:H8	1.81	0.46
40:L5:2832:A:H2'	40:L5:2833:A:H8	1.81	0.46
40:L5:3683:C:O2'	43:LA:174:ARG:NH2	2.48	0.46
40:L5:4622:A:H4'	44:LB:13:SER:HB2	1.98	0.46
40:L5:4769:G:H5'	40:L5:4873:G:H1	1.80	0.46
41:L7:64:G:H2'	41:L7:65:G:C8	2.51	0.46
41:L7:107:G:H2'	41:L7:108:G:H8	1.81	0.46
42:L8:22:U:OP1	64:LY:11:ARG:NE	2.45	0.46
51:LI:73:ASN:HB2	51:LI:87:MET:HE1	1.97	0.46
53:LL:140:SER:HA	53:LL:143:GLU:HG2	1.96	0.46
83:LS:30:VAL:HG23	83:LS:189:ILE:HA	1.97	0.46
2:SB:30:TRP:CE2	11:SO:19:PRO:HD3	2.51	0.46
6:SH:137:SER:HB3	6:SH:162:GLN:HE21	1.79	0.46
8:SJ:113:GLN:HG3	8:SJ:149:VAL:HG21	1.97	0.46
11:SO:32:HIS:CE1	11:SO:96:LYS:HD2	2.50	0.46
19:S2:940:U:H3	19:S2:1002:U:H3	1.63	0.46
19:S2:1010:G:H2'	19:S2:1011:A:C8	2.50	0.46
19:S2:1570:G:N7	30:ST:97:LYS:NZ	2.58	0.46
19:S2:1650:A:OP1	28:SQ:137:ALA:N	2.48	0.46
21:LW:86:SER:OG	21:LW:89:ASP:OD2	2.28	0.46
23:SD:106:ARG:HG2	23:SD:175:VAL:HG22	1.97	0.46
30:ST:18:LEU:HD22	30:ST:58:ALA:HA	1.98	0.46
37:At:52:G:H2'	37:At:53:G:C8	2.51	0.46
40:L5:139:G:H2'	40:L5:140:G:H8	1.80	0.46
40:L5:965:G:N2	40:L5:2092:G:H1'	2.30	0.46
40:L5:1199:G:H2'	40:L5:1200:G:C8	2.49	0.46
40:L5:1636:U:H5''	40:L5:1637:A:H5'	1.98	0.46
40:L5:3727:A:O3'	74:Li:74:LYS:NZ	2.49	0.46
40:L5:4277:G:O2'	40:L5:4282:A:N1	2.43	0.46
40:L5:4637:OMG:H2'	40:L5:4638:U:C6	2.51	0.46
40:L5:4736:C:H2'	40:L5:4737:G:H8	1.79	0.46
40:L5:4906:C:H2'	40:L5:4907:G:C8	2.51	0.46
40:L5:4967:A:OP1	44:LB:125:SER:OG	2.28	0.46
45:LC:298:ILE:HD12	58:LQ:35:LEU:HD21	1.97	0.46
50:LH:93:ARG:HD2	50:LH:143:GLU:HG2	1.97	0.46
60:LT:18:PRO:HB2	60:LT:21:LYS:HG3	1.97	0.46
3:SC:256:TRP:CE2	13:SW:68:ARG:HD3	2.51	0.46
5:SG:161:PRO:HA	5:SG:171:THR:HA	1.98	0.46
19:S2:943:U:H2'	19:S2:944:A:H8	1.81	0.46
21:LW:72:THR:O	21:LW:74:ARG:NH1	2.49	0.46
23:SD:175:VAL:HB	23:SD:182:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:At:18:G:C6	37:At:55:U:O2	2.68	0.46
40:L5:217:C:OP2	40:L5:219:G:O2'	2.23	0.46
40:L5:2640:G:H2'	40:L5:2641:A:H8	1.81	0.46
40:L5:3774:A:H2'	40:L5:3775:A:C8	2.50	0.46
40:L5:4344:U:H3	40:L5:4368:G:H1	1.63	0.46
40:L5:4458:C:H2'	40:L5:4459:U:H6	1.81	0.46
45:LC:269:LYS:HA	45:LC:269:LYS:HD2	1.66	0.46
75:Lj:20:ARG:HD2	75:Lj:39:TYR:CZ	2.49	0.46
19:S2:528:A:H2'	19:S2:529:A:C8	2.51	0.46
19:S2:1311:C:H2'	19:S2:1312:G:C8	2.51	0.46
22:SR:17:ILE:HD11	22:SR:54:VAL:HA	1.98	0.46
23:SD:80:PRO:HG2	23:SD:83:SER:HB3	1.96	0.46
24:SF:187:SER:HB3	24:SF:190:ILE:HG12	1.98	0.46
36:Sg:4:GLN:H	36:Sg:313:THR:HB	1.80	0.46
37:At:3:C:H2'	37:At:4:U:H6	1.81	0.46
40:L5:1091:C:H2'	40:L5:1092:G:C8	2.51	0.46
40:L5:1270:A:H8	40:L5:2106:G:H21	1.61	0.46
40:L5:1972:G:O2'	84:Lt:117:ARG:NH2	2.49	0.46
40:L5:2647:A:H3'	40:L5:2648:G:H8	1.80	0.46
40:L5:2683:C:H2'	40:L5:2684:C:C6	2.51	0.46
40:L5:2756:G:H2'	40:L5:2757:A:C8	2.51	0.46
40:L5:3697:U:O2'	40:L5:3817:A:OP2	2.33	0.46
40:L5:3898:G:N2	44:LB:260:ALA:O	2.35	0.46
40:L5:4476:C:O2'	40:L5:4478:G:OP2	2.32	0.46
40:L5:4563:U:H2'	40:L5:4564:A:H8	1.81	0.46
40:L5:4743:G:H2'	40:L5:4744:A:C8	2.50	0.46
41:L7:57:C:H2'	41:L7:58:A:C8	2.51	0.46
44:LB:57:VAL:HG22	44:LB:73:VAL:HG12	1.97	0.46
44:LB:220:ILE:HG23	44:LB:278:THR:HG22	1.97	0.46
46:LD:37:VAL:HG12	46:LD:50:ARG:HD3	1.97	0.46
46:LD:233:PRO:HA	46:LD:236:MET:HG3	1.97	0.46
61:LU:44:GLN:HB2	61:LU:56:LEU:HD21	1.97	0.46
4:SE:134:LYS:N	19:S2:298:G:OP1	2.42	0.46
5:SG:56:ASN:HB2	5:SG:108:VAL:HG22	1.97	0.46
6:SH:165:ASN:HA	6:SH:168:HIS:HE1	1.81	0.46
7:SI:117:TYR:HB3	7:SI:119:LEU:HD13	1.96	0.46
19:S2:1174:PSU:H2'	19:S2:1175:G:C8	2.51	0.46
19:S2:1499:U:H2'	19:S2:1500:G:H8	1.81	0.46
36:Sg:168:CYS:HB2	36:Sg:195:LEU:HB3	1.97	0.46
38:Pt:6:C:H2'	38:Pt:7:G:H8	1.81	0.46
40:L5:34:A:H2'	40:L5:35:U:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:935:A:O2'	54:LM:44:GLN:O	2.31	0.46
40:L5:1339:U:H2'	40:L5:1340:OMC:C6	2.51	0.46
40:L5:1439:C:H4'	48:LF:34:ARG:HH12	1.81	0.46
40:L5:1461:C:H2'	40:L5:1462:A:C8	2.51	0.46
40:L5:1913:C:H2'	40:L5:1914:C:C6	2.51	0.46
40:L5:2787:A2M:HM'2	40:L5:2787:A2M:HI1'	1.61	0.46
40:L5:5053:U:H3'	40:L5:5054:C:C6	2.50	0.46
42:L8:71:A:N6	42:L8:83:C:O4'	2.48	0.46
42:L8:78:G:H2'	42:L8:79:G:C8	2.50	0.46
47:LE:166:LYS:HD2	47:LE:208:ILE:HG21	1.98	0.46
54:LM:93:LYS:HA	54:LM:96:GLU:HB3	1.97	0.46
17:Sb:35:VAL:HG11	17:Sb:63:LEU:HD13	1.98	0.46
19:S2:929:G:H21	19:S2:1104:G:H4'	1.81	0.46
19:S2:1277:C:H2'	19:S2:1278:A:H8	1.80	0.46
19:S2:1303:C:H2'	19:S2:1304:U:C6	2.50	0.46
19:S2:1345:G:OP1	19:S2:1688:C:O2'	2.34	0.46
19:S2:1568:C:OP1	30:ST:98:SER:N	2.42	0.46
19:S2:1736:G:H2'	19:S2:1737:G:C8	2.50	0.46
24:SF:40:ALA:HB3	24:SF:67:PRO:HA	1.98	0.46
27:SP:81:ARG:NH2	27:SP:117:GLY:O	2.49	0.46
40:L5:7:C:H2'	40:L5:8:U:C6	2.51	0.46
40:L5:349:A:OP1	45:LC:50:GLN:N	2.46	0.46
40:L5:393:U:H2'	40:L5:394:G:C8	2.51	0.46
40:L5:415:G:O6	42:L8:20:A:N6	2.49	0.46
40:L5:442:G:H2'	40:L5:443:G:H8	1.81	0.46
40:L5:662:C:H2'	40:L5:663:G:C8	2.51	0.46
40:L5:1241:C:H42	67:Lb:114:LYS:HE3	1.80	0.46
40:L5:1328:G:H2'	40:L5:1329:G:C8	2.50	0.46
40:L5:2523:G:H2'	40:L5:2524:U:C6	2.51	0.46
40:L5:4255:A:H2'	40:L5:4256:A:C4	2.51	0.46
40:L5:4581:G:HO2'	44:LB:92:TYR:HH	1.58	0.46
41:L7:32:A:O2'	41:L7:41:G:N7	2.36	0.46
41:L7:77:A:H62	41:L7:99:G:H21	1.64	0.46
41:L7:82:G:H2'	41:L7:83:A:C8	2.51	0.46
44:LB:231:VAL:HG21	44:LB:251:VAL:HG23	1.98	0.46
55:LN:116:LEU:HD22	55:LN:135:ILE:HD11	1.97	0.46
69:Ld:36:VAL:HG21	69:Ld:44:ARG:HG2	1.97	0.46
70:Le:43:ASN:OD1	70:Le:46:ARG:N	2.40	0.46
84:Lt:130:LYS:HD2	84:Lt:155:ILE:HD13	1.97	0.46
3:SC:180:VAL:HG23	3:SC:197:PRO:HG3	1.98	0.45
4:SE:48:LEU:HD12	4:SE:61:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SO:136:PRO:HB3	19:S2:944:A:H1'	1.97	0.45
19:S2:644:OMG:H2'	19:S2:645:C:C6	2.51	0.45
19:S2:838:G:H1'	19:S2:839:C:H3'	1.98	0.45
19:S2:1098:C:H2'	19:S2:1099:G:C8	2.51	0.45
19:S2:1221:G:H2'	19:S2:1222:G:C8	2.51	0.45
19:S2:1382:A:H2'	19:S2:1383:A2M:H8	1.98	0.45
19:S2:1433:C:O2	31:SU:19:ARG:NH2	2.49	0.45
20:LR:80:LYS:HA	20:LR:80:LYS:HD2	1.77	0.45
40:L5:497:G:H1	40:L5:658:C:N4	2.14	0.45
40:L5:730:G:C4	48:LF:73:ARG:HD3	2.51	0.45
40:L5:1305:C:OP1	88:L5:5286:SPD:N1	2.49	0.45
40:L5:1471:U:H2'	40:L5:1472:C:C6	2.51	0.45
40:L5:1472:C:H2'	40:L5:1473:U:H6	1.81	0.45
40:L5:1669:A:H5''	67:Lb:15:LYS:HD2	1.98	0.45
40:L5:2468:U:H2'	40:L5:2506:G:H22	1.81	0.45
40:L5:2486:G:O6	40:L5:2493:G:O6	2.33	0.45
40:L5:2538:U:H2'	40:L5:2539:C:C6	2.52	0.45
40:L5:3736:A:H2'	40:L5:3737:A:C8	2.51	0.45
42:L8:7:U:H2'	42:L8:8:U:C6	2.51	0.45
3:SC:232:THR:HG22	3:SC:235:ASN:H	1.80	0.45
4:SE:124:CYS:HB3	4:SE:141:THR:OG1	2.16	0.45
14:SX:104:GLY:O	19:S2:648:A:H4'	2.15	0.45
15:SY:10:ARG:HA	19:S2:839:C:H41	1.80	0.45
31:SU:31:SER:HB2	31:SU:107:GLU:HG3	1.98	0.45
40:L5:959:G:O2'	40:L5:2263:A:N6	2.49	0.45
40:L5:2080:U:H2'	40:L5:2081:C:C6	2.50	0.45
40:L5:2743:A:H2'	40:L5:2744:A:C8	2.51	0.45
40:L5:3681:G:OP2	43:LA:128:ARG:NE	2.38	0.45
40:L5:4080:C:H2'	40:L5:4081:G:C8	2.51	0.45
40:L5:4389:C:H2'	40:L5:4390:A:C8	2.52	0.45
40:L5:4523:A2M:H1'	40:L5:4558:U:C4	2.50	0.45
40:L5:4563:U:C2	40:L5:4564:A:C8	3.04	0.45
42:L8:144:U:H2'	42:L8:145:C:C6	2.51	0.45
45:LC:13:GLU:OE1	45:LC:161:TYR:OH	2.30	0.45
52:LJ:93:GLU:HB3	52:LJ:175:LEU:HD11	1.98	0.45
58:LQ:155:ALA:HB3	58:LQ:158:THR:HG23	1.98	0.45
73:Lh:9:LEU:HB3	73:Lh:60:VAL:HG11	1.97	0.45
80:Lo:36:GLN:HA	80:Lo:39:ARG:HE	1.81	0.45
5:SG:103:ASP:H	5:SG:106:LEU:HD13	1.81	0.45
19:S2:1256:G:H1	34:Sd:31:ILE:HG12	1.81	0.45
19:S2:1261:C:O2	34:Sd:10:HIS:NE2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SP:108:LYS:HD2	29:SS:117:ILE:HG22	1.98	0.45
30:ST:134:ILE:HA	30:ST:137:GLN:HG2	1.96	0.45
31:SU:66:ARG:NH1	31:SU:75:LYS:HD3	2.29	0.45
35:Sf:93:HIS:CE1	35:Sf:96:LYS:HD3	2.51	0.45
36:Sg:109:LEU:HD12	36:Sg:152:SER:HA	1.98	0.45
40:L5:12:A:OP1	88:L8:203:SPD:N10	2.49	0.45
40:L5:1195:G:H2'	40:L5:1196:G:C8	2.51	0.45
40:L5:2283:G:H2'	40:L5:2284:G:H8	1.80	0.45
40:L5:2624:G:O6	61:LU:88:LYS:NZ	2.47	0.45
40:L5:2844:A:N6	40:L5:3839:G:O2'	2.50	0.45
40:L5:3870:C:H2'	40:L5:3871:A:C8	2.50	0.45
40:L5:3911:C:H2'	40:L5:3912:U:H6	1.81	0.45
40:L5:3927:U:H2'	40:L5:3928:A:C8	2.52	0.45
40:L5:4095:G:N2	40:L5:4099:G:H22	2.14	0.45
40:L5:4460:U:H2'	40:L5:4461:C:H6	1.81	0.45
40:L5:4704:C:H2'	40:L5:4705:A:C8	2.52	0.45
40:L5:4870:G:OP2	54:LM:5:ARG:NH1	2.38	0.45
42:L8:15:G:O2'	42:L8:16:G:O4'	2.20	0.45
56:LO:3:GLU:OE1	56:LO:5:GLN:NE2	2.37	0.45
84:Lt:106:PHE:HB2	84:Lt:109:ILE:HG12	1.99	0.45
1:SA:18:PHE:HD1	1:SA:173:LEU:HD21	1.82	0.45
13:SW:30:CYS:SG	13:SW:31:SER:N	2.89	0.45
15:SY:35:VAL:HG13	15:SY:40:ILE:HD11	1.97	0.45
19:S2:325:C:N3	19:S2:326:C:O2'	2.49	0.45
19:S2:1688:C:H2'	19:S2:1689:C:C6	2.51	0.45
32:SZ:72:VAL:HG13	32:SZ:76:ARG:HH21	1.80	0.45
40:L5:151:G:OP2	55:LN:4:TYR:OH	2.24	0.45
40:L5:1392:A:H2'	40:L5:1393:G:C8	2.50	0.45
40:L5:2318:G:N2	40:L5:2321:G:OP2	2.27	0.45
40:L5:2744:A:H2'	40:L5:2745:A:C8	2.52	0.45
40:L5:3718:A2M:H2	40:L5:3934:G:O4'	2.16	0.45
40:L5:3787:G:H1'	40:L5:3789:C:H41	1.81	0.45
40:L5:4098:A:H2'	40:L5:4099:G:H4'	1.98	0.45
40:L5:4575:G:H2'	40:L5:4576:PSU:H6	1.81	0.45
40:L5:4981:G:H3'	40:L5:4982:A:H8	1.82	0.45
41:L7:46:C:H2'	41:L7:47:G:H8	1.81	0.45
42:L8:130:C:H2'	42:L8:131:G:C8	2.52	0.45
43:LA:47:ASP:OD1	43:LA:48:ILE:N	2.49	0.45
44:LB:168:MET:HE2	44:LB:175:GLN:HG2	1.97	0.45
45:LC:11:TYR:CZ	45:LC:148:PRO:HB2	2.52	0.45
68:Lc:65:MET:HE3	68:Lc:65:MET:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:121:LEU:HD12	1:SA:121:LEU:HA	1.86	0.45
2:SB:146:ARG:HH22	19:S2:1112:U:H1'	1.80	0.45
14:SX:37:LYS:NZ	19:S2:1810:U:O3'	2.49	0.45
19:S2:57:U:O2'	19:S2:499:G:N3	2.44	0.45
19:S2:587:A:H5'	19:S2:592:C:H41	1.82	0.45
19:S2:1031:A2M:HM'3	19:S2:1031:A2M:H1'	1.66	0.45
19:S2:1107:G:C6	19:S2:1126:G:C6	3.05	0.45
19:S2:1225:U:H2'	19:S2:1226:G:H8	1.82	0.45
30:ST:98:SER:OG	30:ST:101:ARG:NH2	2.49	0.45
40:L5:418:A:C2	42:L8:17:A:H1'	2.51	0.45
40:L5:1569:U:H2'	40:L5:1570:G:C8	2.51	0.45
40:L5:2376:A:H2'	40:L5:2377:C:C6	2.51	0.45
40:L5:3841:OMC:HM23	40:L5:3841:OMC:H1'	1.80	0.45
43:LA:145:LYS:HD3	43:LA:145:LYS:HA	1.76	0.45
48:LF:80:ASN:HB3	60:LT:142:ARG:HA	1.99	0.45
61:LU:60:VAL:HG13	61:LU:61:VAL:HG23	1.99	0.45
65:LZ:42:LEU:HD21	65:LZ:96:VAL:HG12	1.97	0.45
1:SA:5:LEU:HB2	1:SA:8:LEU:HB2	1.99	0.45
10:SN:69:ASN:ND2	19:S2:916:A:N7	2.64	0.45
19:S2:102:A:H4'	19:S2:104:A:C8	2.51	0.45
19:S2:1039:C:H2'	19:S2:1040:G:C8	2.52	0.45
19:S2:1545:A:N3	19:S2:1671:G:O2'	2.36	0.45
20:LR:160:GLU:OE1	20:LR:163:ARG:NH1	2.48	0.45
30:ST:77:LYS:HA	30:ST:94:ARG:HG2	1.99	0.45
33:Sc:20:ARG:HD3	33:Sc:28:THR:HG22	1.98	0.45
40:L5:951:G:H5'	71:Lf:109:ARG:HD3	1.98	0.45
40:L5:1345:A:H2'	40:L5:1346:C:C6	2.52	0.45
40:L5:3606:U:H2'	40:L5:3607:U:C6	2.52	0.45
40:L5:3700:C:H2'	40:L5:3746:A:H61	1.82	0.45
40:L5:3825:A2M:H2'	40:L5:3826:C:H6	1.82	0.45
40:L5:3848:U:H2'	40:L5:3849:A:C8	2.51	0.45
40:L5:4122:G:O2'	65:LZ:136:PHE:OXT	2.32	0.45
40:L5:4147:G:H2'	40:L5:4148:C:C6	2.52	0.45
40:L5:4475:G:P	50:LH:173:ARG:HH12	2.40	0.45
40:L5:4637:OMG:HM23	40:L5:4637:OMG:H1'	1.66	0.45
49:LG:90:GLN:OE1	49:LG:94:GLN:NE2	2.49	0.45
3:SC:191:VAL:HG11	3:SC:236:PHE:HA	1.98	0.45
11:SO:29:GLY:O	11:SO:94:HIS:N	2.49	0.45
16:Sa:2:THR:HG22	19:S2:1199:A:H5''	1.98	0.45
19:S2:194:C:H2'	19:S2:195:C:H6	1.81	0.45
19:S2:1192:U:H2'	19:S2:1193:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1490:OMG:HM23	19:S2:1490:OMG:H1'	1.79	0.45
36:Sg:126:ASP:OD2	36:Sg:130:LYS:NZ	2.50	0.45
40:L5:138:G:H2'	40:L5:139:G:H8	1.81	0.45
40:L5:502:C:H3'	40:L5:503:C:H3'	1.98	0.45
40:L5:1284:G:H21	47:LE:130:LYS:HG3	1.82	0.45
40:L5:2422:OMC:HM23	40:L5:2422:OMC:H1'	1.70	0.45
40:L5:2895:A:H2'	40:L5:2896:G:C8	2.52	0.45
40:L5:4493:PSU:H2'	40:L5:4494:OMG:H8	1.81	0.45
47:LE:178:PRO:HB2	47:LE:181:LEU:HG	1.98	0.45
53:LL:150:LEU:HD23	53:LL:154:VAL:HG22	1.98	0.45
68:Lc:47:ILE:HG12	68:Lc:72:HIS:HB3	1.99	0.45
5:SG:172:LYS:HD3	19:S2:65:C:H4'	1.99	0.45
8:SJ:25:LEU:HD13	19:S2:640:A:H5''	1.98	0.45
19:S2:689:U:H2'	19:S2:690:G:O4'	2.17	0.45
19:S2:825:A:H2'	19:S2:826:A:C8	2.52	0.45
19:S2:1630:A:OP1	29:SS:40:TYR:N	2.39	0.45
19:S2:1667:U:H2'	19:S2:1668:U:C6	2.51	0.45
19:S2:1679:A:H2'	24:SF:60:ARG:HD2	1.98	0.45
21:LW:5:LEU:HD12	21:LW:30:GLN:NE2	2.32	0.45
23:SD:126:ILE:O	23:SD:129:SER:OG	2.33	0.45
36:Sg:68:ASP:OD2	36:Sg:155:ARG:NH2	2.50	0.45
40:L5:303:C:OP2	55:LN:68:ARG:NH2	2.34	0.45
40:L5:423:G:H2'	40:L5:424:U:C6	2.52	0.45
40:L5:455:C:O2'	40:L5:456:C:H5'	2.17	0.45
40:L5:742:G:H2'	40:L5:743:G:H8	1.82	0.45
40:L5:1338:G:H4'	40:L5:1339:U:H6	1.81	0.45
40:L5:1800:U:H2'	40:L5:1801:A:C8	2.52	0.45
40:L5:2351:OMC:HM23	40:L5:2351:OMC:H1'	1.75	0.45
40:L5:2610:G:H2'	40:L5:2611:A:C8	2.52	0.45
40:L5:3816:A:OP1	40:L5:3818:UY1:N1	2.50	0.45
40:L5:3839:G:N2	40:L5:3843:C:O2'	2.50	0.45
40:L5:3910:C:H2'	40:L5:3911:C:H6	1.82	0.45
42:L8:9:A:H2'	42:L8:10:G:H8	1.81	0.45
46:LD:211:LEU:HB3	46:LD:219:TYR:HB2	1.98	0.45
2:SB:65:ARG:HB3	11:SO:48:SER:HB2	1.98	0.45
9:SL:7:GLU:HG2	9:SL:9:ALA:H	1.81	0.45
13:SW:11:LEU:HA	13:SW:11:LEU:HD23	1.76	0.45
19:S2:511:U:H2'	19:S2:512:A:H8	1.82	0.45
19:S2:809:A:H2'	19:S2:810:A:O4'	2.16	0.45
19:S2:974:C:H2'	19:S2:975:G:C8	2.52	0.45
19:S2:1092:G:H2'	19:S2:1093:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1373:C:H2'	19:S2:1374:C:H6	1.82	0.45
24:SF:67:PRO:HG2	24:SF:70:GLU:HB3	1.98	0.45
29:SS:80:PRO:HG2	30:ST:36:THR:HG21	1.98	0.45
37:At:1:G:H2'	37:At:2:U:H6	1.82	0.45
40:L5:432:U:H1'	87:L5:5292:SPM:H61	1.98	0.45
40:L5:462:G:H2'	40:L5:463:A:C8	2.52	0.45
40:L5:716:C:OP1	45:LC:317:ASN:HB2	2.17	0.45
40:L5:1335:G:N2	45:LC:95:MET:HB2	2.32	0.45
40:L5:1536:PSU:O4	40:L5:1635:C:O2'	2.31	0.45
40:L5:1972:G:C6	40:L5:1973:G:C6	3.04	0.45
40:L5:2764:A:H2'	40:L5:2765:A:C8	2.52	0.45
40:L5:3736:A:H2'	40:L5:3737:A:H8	1.82	0.45
40:L5:3834:C:H2'	40:L5:3835:C:H6	1.82	0.45
40:L5:4113:U:H4'	40:L5:4115:G:C4	2.52	0.45
40:L5:4389:C:H2'	40:L5:4390:A:H8	1.82	0.45
40:L5:4601:U:C2	40:L5:4610:A:N6	2.84	0.45
42:L8:36:G:C5	73:Lh:89:ARG:HD3	2.52	0.45
73:Lh:89:ARG:O	73:Lh:93:ARG:HG2	2.17	0.45
1:SA:120:ARG:HD2	3:SC:266:TYR:HB3	1.99	0.45
4:SE:144:ALA:HB3	19:S2:121:OMU:HM23	1.99	0.45
11:SO:32:HIS:CG	19:S2:975:G:H4'	2.52	0.45
11:SO:62:VAL:HG22	11:SO:64:ALA:H	1.82	0.45
19:S2:194:C:H2'	19:S2:195:C:C6	2.52	0.45
19:S2:564:A:H2'	19:S2:565:G:O4'	2.17	0.45
19:S2:1109:C:O2	22:SR:125:GLY:N	2.44	0.45
19:S2:1610:G:O2'	29:SS:86:ARG:NH1	2.50	0.45
19:S2:1828:C:H2'	19:S2:1829:G:H8	1.81	0.45
31:SU:20:ILE:HG13	31:SU:116:ILE:HG22	1.99	0.45
40:L5:123:C:H2'	40:L5:124:C:H6	1.82	0.45
40:L5:230:G:OP1	64:LY:15:ARG:NH1	2.46	0.45
40:L5:307:A:N3	40:L5:310:G:O2'	2.49	0.45
40:L5:4571:A2M:HM'3	40:L5:4571:A2M:H1'	1.68	0.45
40:L5:4727:A:H2'	40:L5:4728:U:O4'	2.16	0.45
52:LJ:97:ASN:ND2	52:LJ:177:GLY:O	2.50	0.45
56:LO:34:VAL:HG22	56:LO:103:LYS:HB2	1.99	0.45
6:SH:73:GLN:HA	6:SH:76:GLN:HB2	1.99	0.44
19:S2:130:G:O2'	19:S2:131:C:O3'	2.35	0.44
19:S2:517:OMC:HM23	19:S2:517:OMC:H1'	1.81	0.44
19:S2:1620:A:H1'	19:S2:1624:U:OP2	2.17	0.44
19:S2:1713:C:H2'	19:S2:1714:U:H6	1.81	0.44
29:SS:51:ASP:HB3	29:SS:54:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Sg:31:ILE:HG12	36:Sg:45:LEU:HD21	1.98	0.44
40:L5:267:G:H2'	40:L5:268:G:C8	2.52	0.44
40:L5:2112:G:O2'	40:L5:2250:C:N4	2.50	0.44
40:L5:2424:OMG:HM23	40:L5:2424:OMG:H1'	1.79	0.44
40:L5:4138:C:H3'	40:L5:4139:G:H8	1.82	0.44
40:L5:4569:U:OP1	44:LB:21:ARG:NH1	2.50	0.44
40:L5:4743:G:H2'	40:L5:4744:A:H8	1.82	0.44
40:L5:4770:U:H2'	40:L5:4771:C:C6	2.51	0.44
40:L5:4935:C:H2'	40:L5:4936:G:C8	2.52	0.44
44:LB:217:ILE:HD11	44:LB:333:LEU:HD21	1.98	0.44
50:LH:41:ILE:HG22	50:LH:43:VAL:HG13	1.98	0.44
53:LL:182:LEU:HD11	66:La:146:LEU:HD21	1.98	0.44
57:LP:95:LEU:HD23	57:LP:95:LEU:HA	1.85	0.44
71:Lf:40:GLU:O	71:Lf:109:ARG:NH2	2.43	0.44
72:Lg:33:LEU:HD23	72:Lg:33:LEU:HA	1.84	0.44
84:Lt:83:LYS:HD2	84:Lt:86:LYS:HE2	1.99	0.44
3:SC:74:LYS:HD3	3:SC:74:LYS:HA	1.71	0.44
4:SE:139:LEU:HB2	4:SE:150:PRO:HG3	2.00	0.44
19:S2:804:U:H2'	19:S2:805:U:C6	2.51	0.44
19:S2:867:OMG:H3'	19:S2:868:G:H21	1.81	0.44
19:S2:924:G:H1	19:S2:1018:U:H3	1.64	0.44
19:S2:1064:C:H2'	19:S2:1065:G:H8	1.83	0.44
19:S2:1093:A:H2'	19:S2:1094:C:H6	1.82	0.44
19:S2:1388:A:H61	23:SD:161:GLY:HA3	1.82	0.44
19:S2:1673:U:O2'	24:SF:84:GLY:O	2.28	0.44
23:SD:131:ALA:HA	23:SD:191:PRO:HD3	1.99	0.44
30:ST:64:LEU:HD12	30:ST:122:LYS:HA	1.99	0.44
37:At:9:A:O2'	37:At:10:G:N7	2.46	0.44
37:At:56:C:H2'	37:At:57:G:C8	2.52	0.44
40:L5:106:A:H1'	40:L5:336:A:N3	2.33	0.44
40:L5:713:C:H2'	40:L5:714:G:C8	2.52	0.44
40:L5:1270:A:H2'	40:L5:2107:C:O2	2.18	0.44
40:L5:1367:C:O2'	40:L5:1369:C:OP2	2.36	0.44
40:L5:1424:G:O6	40:L5:1462:A:N6	2.50	0.44
40:L5:1431:C:H2'	40:L5:1432:G:O4'	2.17	0.44
40:L5:1656:U:OP2	66:La:26:ARG:NH2	2.37	0.44
40:L5:1777:C:H2'	40:L5:1778:C:C6	2.52	0.44
40:L5:1800:U:H2'	40:L5:1801:A:H8	1.82	0.44
40:L5:1876:U:H2'	40:L5:1877:G:H8	1.82	0.44
40:L5:2406:G:H4'	77:Ll:48:LYS:HE3	1.99	0.44
40:L5:2508:U:H2'	40:L5:2509:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4071:U:H2'	40:L5:4072:C:C6	2.53	0.44
40:L5:4178:A:H2'	40:L5:4179:G:C8	2.52	0.44
40:L5:4336:A:H5''	40:L5:4337:C:H5'	1.99	0.44
40:L5:4715:C:OP2	44:LB:31:SER:OG	2.35	0.44
40:L5:4754:G:N1	40:L5:4880:C:N3	2.65	0.44
40:L5:4767:C:H2'	40:L5:4768:G:H8	1.82	0.44
40:L5:4980:C:H3'	40:L5:4981:G:H21	1.82	0.44
70:Le:66:THR:HA	70:Le:69:MET:HE3	1.99	0.44
84:Lt:61:LYS:HB3	84:Lt:74:VAL:HG13	1.99	0.44
4:SE:106:LYS:HD2	4:SE:108:ARG:NH2	2.33	0.44
9:SL:80:MET:HA	9:SL:86:ILE:HG22	1.99	0.44
19:S2:224:A:H2'	19:S2:225:G:C8	2.52	0.44
19:S2:382:C:H2'	19:S2:383:G:C8	2.53	0.44
19:S2:494:C:N4	19:S2:509:OMG:HN22	2.15	0.44
19:S2:516:A:N1	19:S2:643:A:O2'	2.42	0.44
19:S2:835:C:H5'	19:S2:836:G:C8	2.52	0.44
19:S2:909:G:H2'	19:S2:910:G:C8	2.52	0.44
19:S2:1109:C:C4	22:SR:126:MET:HE2	2.52	0.44
19:S2:1227:G:C2	19:S2:1228:A:C8	3.06	0.44
19:S2:1585:U:O2	28:SQ:73:LYS:NZ	2.39	0.44
19:S2:1801:A:H2'	19:S2:1802:C:C6	2.52	0.44
19:S2:1828:C:H2'	19:S2:1829:G:C8	2.51	0.44
35:Sf:132:MET:HE2	35:Sf:139:HIS:HB3	1.99	0.44
37:At:51:C:H2'	37:At:52:G:H8	1.82	0.44
40:L5:395:A:H2'	40:L5:396:A:C8	2.53	0.44
40:L5:928:C:H2'	40:L5:929:A:C8	2.52	0.44
40:L5:1355:G:P	58:LQ:108:ARG:HH22	2.41	0.44
40:L5:1553:A:O2'	81:Lp:9:GLY:O	2.32	0.44
40:L5:1830:G:H2'	40:L5:1831:G:C8	2.53	0.44
40:L5:2108:G:H2'	40:L5:2109:G:C8	2.53	0.44
40:L5:2610:G:H2'	40:L5:2611:A:H8	1.83	0.44
40:L5:3951:G:O2'	40:L5:3952:A:OP1	2.36	0.44
40:L5:4196:OMG:HM23	40:L5:4196:OMG:H1'	1.84	0.44
40:L5:4600:G:H4'	40:L5:4601:U:O5'	2.16	0.44
40:L5:4870:G:H2'	54:LM:91:TRP:CZ2	2.53	0.44
57:LP:107:LEU:HB2	57:LP:152:GLU:OE2	2.17	0.44
59:LS:30:MET:HB3	59:LS:30:MET:HE2	1.85	0.44
73:Lh:80:PRO:HD2	73:Lh:83:LEU:HD12	1.98	0.44
19:S2:60:A:N3	19:S2:316:G:O2'	2.39	0.44
19:S2:927:C:H2'	19:S2:928:G:H8	1.82	0.44
19:S2:929:G:N2	19:S2:1104:G:H4'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:986:G:OP2	19:S2:988:C:N4	2.50	0.44
19:S2:1096:G:N2	19:S2:1136:U:O2	2.36	0.44
19:S2:1201:U:H2'	19:S2:1202:U:C6	2.52	0.44
19:S2:1393:G:H2'	19:S2:1394:G:C8	2.52	0.44
19:S2:1597:C:OP2	32:SZ:85:ARG:NH1	2.35	0.44
19:S2:1801:A:H2'	19:S2:1802:C:H6	1.82	0.44
36:Sg:205:SER:C	36:Sg:221:LEU:HD23	2.43	0.44
40:L5:35:U:H4'	40:L5:1525:A:C2	2.52	0.44
40:L5:321:U:H2'	40:L5:322:C:C6	2.52	0.44
40:L5:1700:G:H5'	40:L5:1702:C:OP2	2.18	0.44
40:L5:1878:G:H2'	40:L5:1879:C:C6	2.52	0.44
40:L5:2693:G:H2'	40:L5:2694:G:C2	2.52	0.44
40:L5:2857:A:H2'	40:L5:2858:A:O4'	2.16	0.44
40:L5:3607:U:H2'	40:L5:3608:A:H8	1.81	0.44
40:L5:3729:U:H2'	40:L5:3730:U:C6	2.52	0.44
40:L5:3731:C:OP1	80:Lo:30:LYS:NZ	2.50	0.44
40:L5:3947:A:C6	40:L5:4068:U:H1'	2.52	0.44
40:L5:4723:A:H2'	40:L5:4724:A:C8	2.51	0.44
42:L8:25:G:H2'	42:L8:26:C:C6	2.53	0.44
43:LA:131:GLY:H	43:LA:169:VAL:HG13	1.83	0.44
51:LI:96:VAL:HG22	51:LI:125:THR:HG22	1.99	0.44
57:LP:39:MET:HG2	57:LP:43:LYS:HD3	2.00	0.44
19:S2:106:C:H2'	19:S2:107:A:C8	2.41	0.44
19:S2:525:A:H2'	19:S2:526:A:C8	2.51	0.44
19:S2:1093:A:H2'	19:S2:1094:C:C6	2.52	0.44
19:S2:1236:G:H2'	19:S2:1237:C:C6	2.53	0.44
19:S2:1271:C:O2	34:Sd:2:GLY:N	2.50	0.44
19:S2:1522:A:OP2	29:SS:144:ARG:NE	2.51	0.44
27:SP:20:VAL:HG11	27:SP:36:LEU:HD21	1.98	0.44
36:Sg:16:GLY:HA3	36:Sg:36:ARG:HB2	1.98	0.44
40:L5:251:C:H2'	40:L5:252:C:C6	2.53	0.44
40:L5:456:C:N4	40:L5:701:G:O6	2.50	0.44
40:L5:1700:G:H5''	40:L5:1704:C:N4	2.31	0.44
40:L5:1730:U:H2'	40:L5:1731:C:C6	2.53	0.44
40:L5:3667:C:H2'	40:L5:3668:C:H6	1.83	0.44
45:LC:340:ILE:HD13	47:LE:51:VAL:HG21	1.99	0.44
50:LH:103:VAL:HG11	50:LH:144:LEU:HD21	2.00	0.44
1:SA:67:ALA:HB1	12:SV:35:ASN:HB2	1.99	0.44
2:SB:117:TRP:HD1	2:SB:153:THR:HG22	1.83	0.44
11:SO:129:ILE:HG13	16:Sa:65:PRO:HG2	2.00	0.44
19:S2:89:C:H2'	19:S2:90:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:429:C:H2'	19:S2:430:C:C6	2.53	0.44
20:LR:10:LEU:HD22	20:LR:38:ARG:HG2	1.99	0.44
23:SD:60:GLY:HA3	23:SD:65:ARG:H	1.83	0.44
29:SS:66:ARG:O	29:SS:70:ILE:HG12	2.18	0.44
36:Sg:272:GLN:OE1	36:Sg:308:ARG:NH1	2.51	0.44
38:Pt:58:A:O2'	38:Pt:61:C:N4	2.50	0.44
40:L5:153:G:H2'	40:L5:154:G:H8	1.82	0.44
40:L5:286:U:H2'	40:L5:287:U:C6	2.53	0.44
40:L5:492:U:H2'	40:L5:493:G:O4'	2.17	0.44
40:L5:1350:C:H2'	40:L5:1351:G:C8	2.52	0.44
40:L5:1503:A:H4'	40:L5:1504:G:H5'	2.00	0.44
40:L5:1996:C:N3	40:L5:2000:G:N1	2.62	0.44
42:L8:90:C:H2'	42:L8:91:A:H8	1.81	0.44
44:LB:288:GLY:HA3	44:LB:330:PHE:CE1	2.52	0.44
60:LT:75:VAL:HG22	60:LT:88:ARG:HG2	1.99	0.44
82:Lr:73:PRO:HA	82:Lr:76:SER:HB2	1.98	0.44
1:SA:149:ASN:N	1:SA:152:SER:OG	2.48	0.44
5:SG:67:VAL:HG12	5:SG:69:THR:HG22	2.00	0.44
7:SI:61:ASP:O	7:SI:78:ILE:N	2.32	0.44
19:S2:160:U:O4	19:S2:468:A2M:H4'	2.17	0.44
19:S2:368:U:H3'	19:S2:369:C:H2'	1.98	0.44
19:S2:409:C:H2'	19:S2:410:G:C8	2.52	0.44
19:S2:1482:C:O2'	23:SD:161:GLY:N	2.48	0.44
19:S2:1488:C:H3'	19:S2:1489:A:H4'	1.99	0.44
19:S2:1566:G:N2	19:S2:1569:A:OP2	2.40	0.44
19:S2:1657:G:H2'	19:S2:1658:G:C8	2.52	0.44
36:Sg:191:HIS:NE2	36:Sg:209:SER:OG	2.51	0.44
36:Sg:256:ILE:HB	36:Sg:270:LEU:HB2	1.99	0.44
40:L5:978:G:H2'	40:L5:979:C:C6	2.52	0.44
40:L5:1249:C:H2'	40:L5:1250:C:H6	1.83	0.44
40:L5:1666:C:H2'	40:L5:1667:G:O4'	2.18	0.44
40:L5:2476:G:H2'	40:L5:2477:A:C8	2.53	0.44
40:L5:4460:U:H2'	40:L5:4461:C:C6	2.53	0.44
43:LA:137:ILE:HD11	43:LA:149:LYS:HB2	2.00	0.44
55:LN:113:LEU:HB2	55:LN:134:LEU:HD12	1.99	0.44
63:LX:73:HIS:HD2	63:LX:115:LYS:HE2	1.82	0.44
80:Lo:70:LEU:HD12	80:Lo:81:ARG:HB3	2.00	0.44
7:SI:116:HIS:CD2	7:SI:152:ARG:HH21	2.36	0.44
8:SJ:84:ILE:O	8:SJ:108:ARG:NE	2.51	0.44
10:SN:47:PRO:HA	10:SN:50:ILE:HD12	1.99	0.44
11:SO:35:ALA:O	11:SO:109:GLY:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Se:45:VAL:HG12	18:Se:47:PRO:HD3	2.00	0.44
19:S2:549:C:N3	19:S2:550:C:N4	2.64	0.44
19:S2:634:A:H2'	19:S2:635:G:H8	1.83	0.44
19:S2:878:G:N1	19:S2:908:A:C2	2.68	0.44
19:S2:1004:PSU:H2'	19:S2:1005:G:C8	2.51	0.44
19:S2:1337:4AC:O5'	19:S2:1337:4AC:H6	2.18	0.44
19:S2:1689:C:H2'	19:S2:1690:U:C6	2.51	0.44
26:SM:91:LEU:HD12	26:SM:106:CYS:HB2	1.99	0.44
36:Sg:153:CYS:SG	36:Sg:198:VAL:HG12	2.58	0.44
36:Sg:156:PHE:HA	36:Sg:165:ILE:HD12	2.00	0.44
38:Pt:52:G:H2'	38:Pt:53:G:H8	1.83	0.44
40:L5:1238:A:H5''	47:LE:60:SER:HB3	2.00	0.44
40:L5:1375:C:OP1	45:LC:121:ARG:NE	2.40	0.44
40:L5:1517:G:H1	45:LC:104:PRO:HD2	1.83	0.44
40:L5:1840:G:H2'	40:L5:1841:C:C6	2.53	0.44
40:L5:1942:A:H4'	41:L7:88:A:C6	2.52	0.44
40:L5:2063:G:H2'	40:L5:2064:G:C8	2.53	0.44
40:L5:2274:C:H5''	45:LC:312:ARG:HB3	1.99	0.44
40:L5:2333:G:H5''	45:LC:195:LYS:HE3	2.00	0.44
40:L5:2372:U:H2'	40:L5:2373:C:C6	2.53	0.44
40:L5:2787:A2M:C8	40:L5:2801:U:H3	2.31	0.44
40:L5:5014:A:H2'	40:L5:5015:G:O4'	2.17	0.44
44:LB:240:LEU:HB2	44:LB:248:LEU:HA	1.98	0.44
47:LE:131:LYS:O	47:LE:136:HIS:NE2	2.50	0.44
5:SG:46:LYS:HD3	5:SG:46:LYS:HA	1.86	0.44
8:SJ:2:PRO:O	19:S2:509:OMG:H5''	2.18	0.44
11:SO:94:HIS:CE1	11:SO:128:ARG:H	2.35	0.44
14:SX:52:LEU:HD11	14:SX:73:GLN:HB2	1.99	0.44
19:S2:595:U:H2'	19:S2:596:U:C6	2.53	0.44
19:S2:888:U:H4'	19:S2:889:U:H5'	1.98	0.44
23:SD:23:GLU:HG2	25:SK:64:TRP:HE1	1.82	0.44
32:SZ:102:LYS:HA	32:SZ:102:LYS:HD3	1.85	0.44
40:L5:267:G:H2'	40:L5:268:G:H8	1.82	0.44
40:L5:376:A:H3'	40:L5:377:A:H8	1.82	0.44
40:L5:1198:G:H2'	40:L5:1199:G:C8	2.53	0.44
40:L5:2295:C:O2'	45:LC:45:ARG:NH2	2.50	0.44
40:L5:2801:U:O2'	75:Lj:12:ARG:NH1	2.50	0.44
40:L5:3777:G:H22	40:L5:3816:A:P	2.41	0.44
40:L5:4392:OMG:HM23	40:L5:4392:OMG:H1'	1.84	0.44
40:L5:4688:C:H2'	40:L5:4689:PSU:C6	2.53	0.44
51:LI:91:LEU:HD23	51:LI:91:LEU:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:LJ:96:LYS:HB2	52:LJ:163:MET:HE2	2.00	0.44
57:LP:118:GLN:HE21	57:LP:120:ASN:ND2	2.13	0.44
62:LV:106:VAL:HG12	62:LV:112:MET:HA	1.99	0.44
13:SW:36:ARG:HA	13:SW:36:ARG:HD2	1.77	0.43
19:S2:1795:G:H2'	19:S2:1796:G:H8	1.83	0.43
23:SD:71:ALA:HB3	25:SK:20:VAL:HG11	2.00	0.43
28:SQ:53:GLU:OE2	28:SQ:85:ARG:NH2	2.51	0.43
36:Sg:39:THR:HG23	36:Sg:60:ARG:HG2	1.99	0.43
40:L5:19:G:P	73:Lh:93:ARG:HE	2.41	0.43
40:L5:288:G:H2'	40:L5:289:C:C6	2.53	0.43
40:L5:1317:U:H2'	40:L5:1318:C:C6	2.53	0.43
41:L7:4:U:H2'	41:L7:5:A:H8	1.83	0.43
43:LA:95:GLN:O	43:LA:100:ASN:ND2	2.35	0.43
62:LV:70:PRO:HA	62:LV:73:ARG:HG3	1.99	0.43
63:LX:129:ARG:NH2	63:LX:131:ASP:OD2	2.51	0.43
64:LY:67:ILE:HD12	64:LY:107:THR:HG21	1.99	0.43
82:Lr:47:LYS:HB2	82:Lr:102:TYR:CZ	2.53	0.43
5:SG:5:ILE:HG13	5:SG:111:LEU:HD12	1.99	0.43
8:SJ:30:LYS:HG2	18:Se:42:PHE:CE2	2.53	0.43
8:SJ:137:VAL:HG12	8:SJ:138:ARG:HG2	2.00	0.43
19:S2:1275:G:N2	19:S2:1506:A:OP2	2.38	0.43
19:S2:1329:U:O2'	19:S2:1332:A:OP2	2.30	0.43
19:S2:1739:C:H2'	19:S2:1740:C:C6	2.53	0.43
35:Sf:93:HIS:HE1	35:Sf:96:LYS:HD3	1.83	0.43
40:L5:76:A:H5'	53:LL:101:ARG:NH1	2.33	0.43
40:L5:161:G:H2'	40:L5:162:A:H8	1.82	0.43
40:L5:441:G:H2'	40:L5:442:G:C8	2.51	0.43
40:L5:1778:C:O2'	46:LD:2:GLY:O	2.34	0.43
40:L5:2022:C:H2'	40:L5:2023:C:O4'	2.18	0.43
40:L5:4092:G:C6	40:L5:4093:G:C6	3.07	0.43
41:L7:114:U:H2'	41:L7:115:A:C8	2.53	0.43
42:L8:9:A:H2'	42:L8:10:G:C8	2.53	0.43
42:L8:70:G:O2'	42:L8:87:G:N2	2.51	0.43
44:LB:161:ARG:HG2	44:LB:184:GLN:HA	2.00	0.43
56:LO:37:ARG:HD2	56:LO:108:ILE:HD11	1.99	0.43
63:LX:81:LEU:HG	63:LX:83:THR:HG23	2.00	0.43
5:SG:131:ARG:HD3	19:S2:168:C:H4'	2.01	0.43
7:SI:47:ARG:HH22	19:S2:446:G:P	2.42	0.43
8:SJ:104:ASP:OD1	8:SJ:105:PHE:N	2.51	0.43
19:S2:142:C:H42	19:S2:329:G:H5''	1.82	0.43
19:S2:576:A2M:HM'3	19:S2:576:A2M:HI'	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1513:C:H2'	19:S2:1514:G:C8	2.50	0.43
19:S2:1593:C:P	32:SZ:103:HIS:HE2	2.41	0.43
19:S2:1670:C:H2'	19:S2:1671:G:H8	1.82	0.43
22:SR:114:LEU:HB2	22:SR:117:LEU:HG	2.00	0.43
40:L5:400:A2M:HM'3	40:L5:400:A2M:H1'	1.76	0.43
40:L5:491:G:H2'	40:L5:492:U:C6	2.53	0.43
40:L5:518:G:H1	40:L5:643:C:H2'	1.83	0.43
40:L5:1645:C:H2'	40:L5:1646:A:H8	1.84	0.43
40:L5:1884:C:H2'	40:L5:1885:G:H8	1.83	0.43
40:L5:2521:G:H2'	40:L5:2522:G:C8	2.52	0.43
40:L5:2890:C:H42	40:L5:3611:A:H61	1.66	0.43
40:L5:4174:U:H2'	40:L5:4175:G:C8	2.47	0.43
40:L5:4524:G:H2'	40:L5:4525:C:H6	1.83	0.43
40:L5:4996:C:OP1	69:Ld:32:ARG:NH1	2.39	0.43
43:LA:51:ASP:HB3	43:LA:54:ARG:HB3	2.00	0.43
5:SG:38:ALA:HB1	5:SG:41:LEU:HD13	2.01	0.43
10:SN:72:LEU:HD22	19:S2:1019:C:H5''	1.99	0.43
13:SW:76:SER:OG	19:S2:1158:G:O3'	2.35	0.43
14:SX:90:CYS:HB3	14:SX:130:LEU:HD11	1.99	0.43
19:S2:601:OMG:H2'	19:S2:602:G:C8	2.53	0.43
19:S2:1171:G:O2'	19:S2:1187:G:O6	2.32	0.43
19:S2:1491:G:H2'	19:S2:1492:U:C6	2.54	0.43
27:SP:59:ARG:O	27:SP:63:ALA:N	2.44	0.43
40:L5:697:G:H2'	40:L5:698:G:C8	2.53	0.43
40:L5:2326:G:H5''	70:Le:127:ALA:HB1	2.01	0.43
40:L5:3867:A2M:H2'	40:L5:3868:G:O4'	2.18	0.43
40:L5:4089:G:H2'	40:L5:4090:G:H8	1.83	0.43
40:L5:4090:G:H2'	40:L5:4091:G:H8	1.84	0.43
40:L5:4619:U:H2'	40:L5:4620:OMU:H6	1.99	0.43
40:L5:4859:C:H2'	40:L5:4860:G:C8	2.53	0.43
40:L5:4883:C:N4	47:LE:181:LEU:O	2.43	0.43
47:LE:141:ARG:NH1	71:Lf:108:SER:O	2.50	0.43
49:LG:162:ASP:HB3	49:LG:163:PRO:HD3	1.99	0.43
60:LT:43:LYS:N	60:LT:95:HIS:O	2.48	0.43
71:Lf:45:LYS:HD2	71:Lf:105:LEU:HA	2.00	0.43
2:SB:127:VAL:HG21	2:SB:176:VAL:HB	2.01	0.43
4:SE:101:LEU:HD11	4:SE:109:PHE:HB3	2.00	0.43
19:S2:441:C:H2'	19:S2:442:C:C6	2.54	0.43
36:Sg:239:LEU:HD11	36:Sg:248:LEU:HD21	2.01	0.43
40:L5:1095:A:H2'	40:L5:1096:C:C6	2.53	0.43
40:L5:1100:U:H3	40:L5:1194:G:H1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1274:A:O2'	40:L5:1275:G:H8	2.00	0.43
40:L5:1307:A:H2'	40:L5:1308:C:C6	2.53	0.43
40:L5:1727:U:H2'	40:L5:1728:U:C6	2.53	0.43
40:L5:1978:C:H2'	40:L5:1979:A:H8	1.82	0.43
40:L5:3871:A:H2'	40:L5:3872:A:C8	2.54	0.43
40:L5:4081:G:H2'	40:L5:4082:G:C8	2.54	0.43
40:L5:4319:C:H2'	40:L5:4320:G:H8	1.83	0.43
40:L5:4527:G:OP2	40:L5:4527:G:N2	2.49	0.43
40:L5:4920:C:H2'	40:L5:4921:C:C6	2.53	0.43
43:LA:112:ILE:HD11	81:Lp:79:VAL:HG13	2.00	0.43
47:LE:157:HIS:CD2	47:LE:187:ARG:HH11	2.37	0.43
49:LG:218:LEU:O	49:LG:222:ILE:HG12	2.19	0.43
62:LV:64:THR:HG22	62:LV:76:VAL:HA	2.00	0.43
65:LZ:38:TYR:HE1	65:LZ:40:HIS:HB3	1.84	0.43
68:Lc:60:ILE:HD13	68:Lc:93:THR:HG21	1.99	0.43
1:SA:220:LYS:HD3	1:SA:220:LYS:HA	1.84	0.43
3:SC:178:HIS:HB3	3:SC:200:ARG:HE	1.81	0.43
8:SJ:59:GLU:O	8:SJ:62:THR:OG1	2.27	0.43
19:S2:350:C:O2'	19:S2:383:G:N1	2.37	0.43
19:S2:568:C:H2'	19:S2:569:A:C8	2.54	0.43
19:S2:1313:A:H5''	25:SK:5:LYS:HE3	2.00	0.43
19:S2:1317:C:H2'	19:S2:1318:G:C8	2.54	0.43
19:S2:1487:A:H2'	19:S2:1488:C:C6	2.54	0.43
20:LR:134:ASN:OD1	20:LR:135:LYS:N	2.51	0.43
28:SQ:8:GLN:HG3	28:SQ:99:TYR:CE1	2.53	0.43
28:SQ:110:ASP:HA	28:SQ:113:ILE:HG22	2.01	0.43
40:L5:283:G:H2'	40:L5:284:G:H8	1.84	0.43
40:L5:500:G:O2'	40:L5:504:G:H3'	2.19	0.43
40:L5:920:C:H2'	40:L5:921:C:C6	2.53	0.43
40:L5:1662:C:H2'	40:L5:1663:C:C6	2.53	0.43
40:L5:2095:A:H1'	40:L5:2096:G:N2	2.34	0.43
40:L5:2249:C:H2'	40:L5:2250:C:C5	2.53	0.43
40:L5:2364:OMG:H1'	40:L5:2364:OMG:HM23	1.66	0.43
40:L5:2634:C:H2'	40:L5:2635:U:H6	1.84	0.43
40:L5:2870:A:H2'	40:L5:2871:A:H8	1.84	0.43
40:L5:3796:U:H2'	40:L5:3797:C:C6	2.53	0.43
40:L5:3920:PSU:H2'	40:L5:3921:U:C6	2.54	0.43
40:L5:4139:G:H1'	40:L5:4146:G:N1	2.33	0.43
40:L5:4159:C:H2'	40:L5:4160:C:C6	2.54	0.43
40:L5:4401:G:H2'	40:L5:4402:C:C6	2.54	0.43
40:L5:4776:G:H22	40:L5:4859:C:H1'	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:L8:44:A:H2'	42:L8:45:C:C6	2.53	0.43
43:LA:36:GLU:HG3	43:LA:91:GLY:HA2	1.99	0.43
43:LA:242:ARG:NH1	43:LA:243:THR:O	2.52	0.43
48:LF:226:HIS:CD2	48:LF:234:GLY:HA3	2.54	0.43
69:Ld:37:GLY:O	69:Ld:41:ARG:HG3	2.19	0.43
78:Lm:80:PRO:HA	78:Lm:83:ARG:HB3	1.99	0.43
82:Lr:32:LEU:HD21	82:Lr:50:GLY:HA2	2.01	0.43
4:SE:103:TYR:HB2	4:SE:182:MET:HE2	1.99	0.43
15:SY:119:GLY:O	19:S2:84:A:O2'	2.31	0.43
19:S2:354:OMU:HM23	19:S2:354:OMU:H1'	1.73	0.43
19:S2:534:G:H2'	19:S2:535:G:H8	1.82	0.43
19:S2:1616:U:H2'	19:S2:1617:G:C8	2.53	0.43
19:S2:1677:U:OP2	24:SF:63:LYS:NZ	2.35	0.43
22:SR:41:ILE:HD13	22:SR:50:ILE:HD12	1.99	0.43
23:SD:134:CYS:SG	23:SD:135:GLU:N	2.91	0.43
36:Sg:101:PHE:CE2	36:Sg:136:GLY:HA2	2.53	0.43
36:Sg:258:ILE:HG23	36:Sg:267:VAL:HB	2.00	0.43
37:At:40:C:H2'	37:At:41:G:H8	1.84	0.43
37:At:67:G:H2'	37:At:68:G:C8	2.54	0.43
40:L5:6:C:H2'	40:L5:7:C:C6	2.54	0.43
40:L5:132:G:H2'	40:L5:133:C:H4'	2.00	0.43
40:L5:958:G:C2	47:LE:124:LYS:HD2	2.53	0.43
40:L5:2421:G:H1'	57:LP:139:TYR:CE2	2.54	0.43
40:L5:4094:G:H1	40:L5:4114:C:H2'	1.84	0.43
40:L5:4364:G:H2'	40:L5:4365:C:C6	2.54	0.43
41:L7:37:G:H2'	41:L7:38:U:O4'	2.18	0.43
42:L8:153:C:H2'	42:L8:154:G:C8	2.51	0.43
47:LE:190:HIS:HB3	47:LE:193:PHE:HD1	1.83	0.43
52:LJ:35:ARG:NH2	52:LJ:126:TYR:OH	2.51	0.43
68:Lc:51:ASN:HB2	68:Lc:77:ASN:HB2	2.01	0.43
19:S2:159:A2M:H1'	19:S2:159:A2M:HM'3	1.55	0.43
19:S2:201:C:H3'	19:S2:202:G:H21	1.83	0.43
19:S2:656:G:H5'	19:S2:662:G:N2	2.34	0.43
19:S2:671:A:H4'	19:S2:672:A:H5''	2.00	0.43
19:S2:1023:A:H2'	19:S2:1024:A:C8	2.53	0.43
29:SS:84:LEU:HD22	29:SS:97:GLN:HB2	2.00	0.43
30:ST:104:LEU:HD22	30:ST:121:ARG:HD2	2.00	0.43
36:Sg:45:LEU:HB3	36:Sg:47:ARG:HE	1.83	0.43
40:L5:271:C:H2'	40:L5:272:U:C6	2.54	0.43
40:L5:318:A:O2'	40:L5:3727:A:H1'	2.19	0.43
40:L5:948:C:H2'	40:L5:949:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1247:U:H2'	40:L5:1248:C:C6	2.54	0.43
40:L5:1749:A:H2'	40:L5:1750:G:H8	1.84	0.43
40:L5:3911:C:H2'	40:L5:3912:U:C6	2.54	0.43
40:L5:4561:C:H2'	40:L5:4562:C:H6	1.84	0.43
40:L5:4630:G:H2'	40:L5:4631:G:H8	1.82	0.43
40:L5:4745:G:N2	40:L5:4955:A:N1	2.60	0.43
41:L7:4:U:H2'	41:L7:5:A:C8	2.53	0.43
47:LE:207:LYS:HA	47:LE:207:LYS:HD3	1.71	0.43
57:LP:24:VAL:HG12	57:LP:86:LYS:HG2	2.00	0.43
61:LU:80:LYS:HE2	61:LU:110:TYR:CZ	2.54	0.43
70:Le:124:ASN:HB2	70:Le:127:ALA:HB2	2.00	0.43
75:Lj:28:HIS:HE1	75:Lj:30:GLN:HB3	1.84	0.43
1:SA:177:MET:HE1	1:SA:180:ARG:HH21	1.84	0.43
4:SE:123:LEU:HD22	4:SE:159:THR:HG22	2.00	0.43
5:SG:232:ARG:HD3	5:SG:232:ARG:HA	1.86	0.43
7:SI:13:LYS:NZ	9:SL:108:ASN:O	2.51	0.43
14:SX:9:THR:HG22	19:S2:681:PSU:H4'	2.01	0.43
15:SY:29:HIS:NE2	15:SY:69:THR:OG1	2.37	0.43
19:S2:158:A:N1	19:S2:463:C:H1'	2.34	0.43
19:S2:669:A:O2'	19:S2:670:A:O4'	2.27	0.43
19:S2:808:A:H2	19:S2:855:G:H22	1.67	0.43
19:S2:812:A:H2'	19:S2:813:A:C8	2.54	0.43
19:S2:1406:G:H2'	19:S2:1407:U:C6	2.54	0.43
19:S2:1410:C:H2'	19:S2:1411:G:C8	2.53	0.43
19:S2:1421:A:H3'	19:S2:1422:G:C8	2.54	0.43
19:S2:1513:C:OP1	34:Sd:12:ARG:NH2	2.36	0.43
21:LW:102:LYS:HA	21:LW:105:ARG:HG2	2.01	0.43
36:Sg:178:ASN:HB3	36:Sg:181:ASN:OD1	2.18	0.43
37:At:22:U:H2'	37:At:23:C:C6	2.53	0.43
37:At:49:C:H2'	37:At:50:U:C6	2.54	0.43
39:CI:55:LEU:HD22	61:LU:99:TRP:CG	2.53	0.43
40:L5:1352:C:H2'	40:L5:1353:G:O4'	2.19	0.43
40:L5:1464:C:H2'	40:L5:1465:G:O4'	2.19	0.43
40:L5:1569:U:H2'	40:L5:1570:G:H8	1.83	0.43
40:L5:1684:A:H4'	40:L5:4304:A:H4'	2.01	0.43
40:L5:2081:C:H2'	40:L5:2082:G:C8	2.53	0.43
40:L5:2654:C:H2'	40:L5:2655:C:C6	2.52	0.43
40:L5:3942:A:H3'	40:L5:3943:A:H8	1.84	0.43
40:L5:3950:U:C4	40:L5:3951:G:H1'	2.54	0.43
40:L5:4620:OMU:H1'	40:L5:4620:OMU:HM23	1.77	0.43
40:L5:4736:C:H2'	40:L5:4737:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4892:A:H2'	40:L5:4893:A:O4'	2.18	0.43
42:L8:75:OMG:H1'	42:L8:75:OMG:HM23	1.73	0.43
46:LD:41:LYS:NZ	60:LT:30:TYR:O	2.38	0.43
51:LI:152:LEU:HB3	51:LI:165:ILE:HD12	2.00	0.43
65:LZ:135:ARG:HD2	65:LZ:135:ARG:HA	1.83	0.43
84:Lt:16:ARG:NE	84:Lt:17:CYS:H	2.09	0.43
1:SA:43:SER:HB2	22:SR:126:MET:HG2	2.01	0.43
2:SB:85:LYS:HB2	2:SB:101:HIS:HB3	2.00	0.43
10:SN:43:LYS:HE2	10:SN:43:LYS:HB2	1.92	0.43
19:S2:520:A:O2'	19:S2:825:A:N3	2.51	0.43
19:S2:1198:G:H2'	19:S2:1199:A:H8	1.83	0.43
19:S2:1538:C:H2'	19:S2:1539:U:C6	2.53	0.43
19:S2:1545:A:H4'	28:SQ:75:GLY:H	1.84	0.43
28:SQ:20:THR:HG23	28:SQ:73:LYS:H	1.84	0.43
37:At:3:C:H2'	37:At:4:U:C6	2.54	0.43
38:Pt:73:A:O2'	51:LI:109:ASP:O	2.30	0.43
40:L5:169:G:O6	40:L5:170:C:N4	2.52	0.43
40:L5:396:A:H2'	40:L5:397:G:C8	2.54	0.43
40:L5:1320:U:O2'	40:L5:1891:A:N1	2.47	0.43
40:L5:1478:C:H2'	40:L5:1479:G:C8	2.52	0.43
40:L5:1669:A:H4'	40:L5:1685:G:H21	1.83	0.43
40:L5:1685:G:H2'	40:L5:1686:C:H6	1.83	0.43
40:L5:2437:C:H5'	63:LX:127:LEU:HB3	2.01	0.43
40:L5:4377:G:N7	66:La:42:ARG:NH2	2.67	0.43
51:LI:190:LEU:HD23	51:LI:199:TYR:HA	2.00	0.43
54:LM:37:LEU:HD12	54:LM:37:LEU:HA	1.84	0.43
2:SB:145:LYS:HE3	2:SB:145:LYS:HB2	1.90	0.42
2:SB:175:GLU:HB3	2:SB:187:LYS:NZ	2.32	0.42
4:SE:21:ASP:HB2	19:S2:829:C:H5''	2.01	0.42
4:SE:61:VAL:HA	4:SE:64:ILE:HG22	2.01	0.42
8:SJ:22:LYS:NZ	19:S2:604:A:O3'	2.42	0.42
19:S2:386:C:H2'	19:S2:387:C:C6	2.54	0.42
19:S2:495:U:H2'	19:S2:496:C:O4'	2.19	0.42
19:S2:1236:G:H2'	19:S2:1237:C:H6	1.83	0.42
33:Sc:58:LEU:HD23	33:Sc:58:LEU:HA	1.88	0.42
37:At:18:G:O2'	37:At:57:G:N2	2.47	0.42
38:Pt:27:U:H2'	38:Pt:28:U:H6	1.83	0.42
40:L5:66:A:O2'	40:L5:326:C:O2	2.31	0.42
40:L5:260:C:H2'	40:L5:261:G:C8	2.54	0.42
40:L5:727:C:H2'	40:L5:728:U:C6	2.54	0.42
40:L5:947:C:OP1	45:LC:336:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1259:G:H2'	40:L5:1260:G:C8	2.53	0.42
40:L5:2543:A:H2	40:L5:2773:G:H22	1.66	0.42
40:L5:2648:G:H2'	40:L5:2649:G:H8	1.83	0.42
40:L5:3893:C:H2'	40:L5:3894:A:H8	1.84	0.42
40:L5:4582:C:N4	40:L5:4722:G:O6	2.51	0.42
40:L5:4878:C:H2'	40:L5:4879:C:C6	2.54	0.42
40:L5:5002:U:OP2	44:LB:385:LYS:NZ	2.41	0.42
42:L8:69:PSU:H2'	42:L8:70:G:O4'	2.19	0.42
42:L8:138:C:H2'	42:L8:139:G:C8	2.54	0.42
43:LA:80:GLU:HB2	43:LA:170:ALA:HA	2.01	0.42
49:LG:94:GLN:HG3	49:LG:218:LEU:HD21	2.00	0.42
58:LQ:178:ARG:N	66:La:51:GLY:HA2	2.34	0.42
1:SA:32:PHE:CD1	19:S2:1097:G:H4'	2.54	0.42
1:SA:41:ARG:NH1	1:SA:47:TYR:OH	2.52	0.42
6:SH:118:ARG:HD3	6:SH:118:ARG:HA	1.77	0.42
8:SJ:2:PRO:HD2	19:S2:428:OMU:H4'	2.00	0.42
8:SJ:32:ILE:HD11	8:SJ:40:LYS:HG2	2.00	0.42
19:S2:61:A:H1'	19:S2:316:G:H1'	2.01	0.42
19:S2:1102:G:C6	19:S2:1131:G:C6	3.07	0.42
19:S2:1230:C:H2'	19:S2:1231:C:H6	1.84	0.42
19:S2:1705:C:H2'	19:S2:1706:G:C8	2.54	0.42
19:S2:1850:MA6:H8	19:S2:1850:MA6:O5'	2.19	0.42
22:SR:99:ASP:HB3	22:SR:102:THR:HG23	2.01	0.42
23:SD:173:ARG:HA	23:SD:173:ARG:HD3	1.89	0.42
25:SK:18:GLU:HA	25:SK:91:PRO:HB3	2.01	0.42
26:SM:95:ASP:HB3	26:SM:99:LYS:HB3	2.01	0.42
40:L5:388:A:H5'	40:L5:389:A:H5'	2.01	0.42
40:L5:728:U:OP1	48:LF:73:ARG:NH1	2.52	0.42
40:L5:1415:G:H2'	40:L5:1416:G:C8	2.54	0.42
40:L5:2732:G:H2'	40:L5:2733:C:C6	2.54	0.42
40:L5:4765:G:H2'	40:L5:4766:C:O4'	2.19	0.42
40:L5:4873:G:C8	56:LO:179:LYS:HE3	2.54	0.42
44:LB:48:GLY:O	44:LB:345:LEU:N	2.44	0.42
44:LB:103:LYS:HB3	44:LB:153:MET:HE2	2.01	0.42
56:LO:15:LEU:HB2	56:LO:18:ARG:HB2	2.01	0.42
64:LY:54:GLU:HB2	64:LY:67:ILE:HG22	2.01	0.42
84:Lt:10:ILE:HG12	84:Lt:65:GLN:HG2	2.01	0.42
7:SI:116:HIS:CE1	7:SI:152:ARG:HH21	2.38	0.42
7:SI:157:LYS:NZ	7:SI:158:ILE:O	2.48	0.42
16:Sa:13:LYS:HD3	16:Sa:13:LYS:HA	1.74	0.42
19:S2:526:A:H2'	19:S2:527:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:974:C:H2'	19:S2:975:G:H8	1.83	0.42
19:S2:1765:C:H5''	19:S2:1771:G:N7	2.34	0.42
23:SD:39:VAL:HG22	23:SD:48:ILE:HG12	2.01	0.42
36:Sg:228:TYR:CE2	36:Sg:230:LEU:HB2	2.55	0.42
38:Pt:56:C:H2'	38:Pt:57:G:C8	2.54	0.42
40:L5:745:G:H2'	40:L5:746:A:C8	2.54	0.42
40:L5:1812:C:H5''	67:Lb:56:LYS:HE3	2.00	0.42
40:L5:2019:C:H2'	40:L5:2020:U:C6	2.54	0.42
40:L5:2465:C:H2'	40:L5:2466:G:O4'	2.19	0.42
40:L5:2580:U:O2'	65:LZ:79:HIS:ND1	2.52	0.42
40:L5:3608:A:H2'	40:L5:3609:G:H8	1.84	0.42
40:L5:4122:G:H1'	72:Lg:94:ALA:HB2	2.01	0.42
40:L5:4471:PSU:OP1	50:LH:168:LYS:NZ	2.48	0.42
40:L5:4590:A2M:HM'3	40:L5:4590:A2M:H1'	1.50	0.42
41:L7:108:G:OP1	46:LD:273:LEU:HB2	2.20	0.42
44:LB:66:LYS:HG2	62:LV:11:GLY:HA3	2.01	0.42
46:LD:164:LYS:HD2	46:LD:164:LYS:HA	1.84	0.42
51:LI:80:CYS:SG	51:LI:147:HIS:ND1	2.91	0.42
52:LJ:44:THR:HA	52:LJ:78:LYS:HE2	2.02	0.42
56:LO:121:PRO:HA	56:LO:124:LEU:HD12	2.01	0.42
58:LQ:50:ARG:HA	58:LQ:53:MET:HE3	2.00	0.42
61:LU:80:LYS:HZ1	61:LU:109:SER:H	1.66	0.42
67:Lb:69:ALA:HA	67:Lb:72:ILE:HD12	2.00	0.42
69:Ld:33:ILE:HD11	69:Ld:45:ALA:HA	2.01	0.42
72:Lg:64:LEU:HD23	72:Lg:67:LEU:HD12	2.01	0.42
83:Ls:58:ASN:ND2	83:Ls:84:GLY:O	2.52	0.42
1:SA:70:ASN:HB3	1:SA:73:ASP:HB2	2.01	0.42
4:SE:124:CYS:HB2	4:SE:160:ILE:HG13	2.01	0.42
12:SV:30:ALA:O	12:SV:60:ARG:HD3	2.19	0.42
19:S2:373:G:H2'	19:S2:374:G:H8	1.84	0.42
19:S2:455:A:H2'	19:S2:456:C:C6	2.54	0.42
19:S2:601:OMG:H1'	19:S2:601:OMG:HM23	1.62	0.42
19:S2:1113:A:N6	19:S2:1121:G:C6	2.88	0.42
19:S2:1279:C:H2'	19:S2:1280:G:C8	2.55	0.42
19:S2:1601:A:O4'	19:S2:1636:G:N2	2.53	0.42
20:LR:148:ASP:OD1	20:LR:149:LYS:N	2.52	0.42
40:L5:909:A:H2'	40:L5:910:G:C8	2.54	0.42
40:L5:1338:G:H4'	40:L5:1339:U:C6	2.55	0.42
40:L5:2670:C:H2'	40:L5:2671:C:C6	2.55	0.42
40:L5:2789:A:H1'	77:LI:45:ARG:HH22	1.85	0.42
40:L5:4088:C:O2	49:LG:53:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4091:G:H3'	40:L5:4114:C:H42	1.84	0.42
40:L5:4208:U:OP2	60:LT:4:THR:OG1	2.29	0.42
44:LB:206:PRO:HG2	44:LB:209:GLN:HG3	2.00	0.42
50:LH:84:VAL:HG23	50:LH:85:THR:HG23	2.02	0.42
2:SB:122:GLU:HG2	2:SB:140:VAL:HG12	2.00	0.42
2:SB:144:LYS:HD3	2:SB:208:HIS:CG	2.55	0.42
4:SE:122:LYS:HE2	4:SE:124:CYS:SG	2.59	0.42
7:SI:10:LYS:HB3	7:SI:10:LYS:HE3	1.87	0.42
7:SI:78:ILE:HG13	7:SI:104:ILE:HG22	2.00	0.42
9:SL:133:PRO:HG2	19:S2:383:G:N2	2.33	0.42
13:SW:88:LYS:NZ	19:S2:420:G:OP1	2.52	0.42
19:S2:1129:G:H2'	19:S2:1130:G:C4	2.53	0.42
19:S2:1791:A:H2'	19:S2:1792:G:O4'	2.20	0.42
19:S2:1817:G:H2'	19:S2:1818:A:C8	2.55	0.42
20:LR:46:LYS:HE2	40:L5:2710:C:N4	2.34	0.42
30:ST:42:HIS:HB3	30:ST:93:SER:HB3	2.02	0.42
36:Sg:296:GLN:O	36:Sg:312:VAL:HG12	2.20	0.42
40:L5:158:A:H5''	40:L5:159:C:H2'	2.01	0.42
40:L5:409:G:N3	57:LP:3:ARG:NH1	2.68	0.42
40:L5:1253:G:HO2'	40:L5:1257:A:H62	1.56	0.42
40:L5:1366:G:N2	53:LL:33:ILE:HD13	2.34	0.42
40:L5:1985:G:H1'	40:L5:2003:G:H2'	2.02	0.42
40:L5:2395:A:N6	40:L5:2820:C:O2	2.53	0.42
40:L5:2430:C:H2'	40:L5:2431:A:H8	1.83	0.42
40:L5:2483:G:N2	40:L5:2495:U:O2	2.43	0.42
40:L5:4403:PSU:HN3	40:L5:4440:G:H1	1.68	0.42
40:L5:4769:G:H2'	40:L5:4770:U:H6	1.84	0.42
40:L5:4885:U:O4	47:LE:272:ARG:NH2	2.52	0.42
45:LC:171:LEU:HD13	45:LC:180:ILE:HG13	2.01	0.42
48:LF:116:GLN:HB2	58:LQ:3:VAL:HG12	2.02	0.42
59:LS:94:TYR:OH	59:LS:96:GLU:OE2	2.28	0.42
67:Lb:91:ARG:HB3	67:Lb:94:ASP:HB2	2.01	0.42
1:SA:124:VAL:HG12	1:SA:125:THR:O	2.19	0.42
10:SN:73:ARG:HD2	19:S2:916:A:C6	2.54	0.42
19:S2:14:C:O2	19:S2:668:A2M:H2	2.20	0.42
19:S2:29:G:H2'	19:S2:30:C:C6	2.54	0.42
19:S2:696:G:H21	19:S2:737:G:N2	2.18	0.42
19:S2:834:C:H42	19:S2:839:C:H42	1.68	0.42
19:S2:947:G:H2'	19:S2:948:C:C6	2.55	0.42
19:S2:1218:C:H2'	19:S2:1219:C:C6	2.55	0.42
19:S2:1545:A:H2'	19:S2:1546:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1643:U:H2'	19:S2:1644:C:C6	2.54	0.42
19:S2:1716:C:H2'	19:S2:1717:C:C6	2.54	0.42
19:S2:1842:4AC:H2'	19:S2:1843:G:C8	2.54	0.42
26:SM:113:ASP:OD1	26:SM:114:TYR:N	2.51	0.42
30:ST:80:GLY:HA3	30:ST:94:ARG:HA	2.02	0.42
32:SZ:103:HIS:CE1	32:SZ:104:ARG:HG2	2.54	0.42
37:At:52:G:H2'	37:At:53:G:H8	1.83	0.42
40:L5:121:A:H62	40:L5:152:U:H3	1.66	0.42
40:L5:295:A:C8	80:Lo:39:ARG:NH1	2.88	0.42
40:L5:701:G:H2'	40:L5:702:U:C6	2.54	0.42
40:L5:702:U:H2'	40:L5:703:G:O4'	2.20	0.42
40:L5:1211:G:H2'	40:L5:1212:G:H8	1.84	0.42
40:L5:1315:C:H2'	40:L5:1316:OMG:H8	1.84	0.42
40:L5:1351:G:H2'	40:L5:1352:C:C6	2.54	0.42
40:L5:1789:C:H2'	40:L5:1790:U:C6	2.54	0.42
40:L5:1933:G:H8	40:L5:1933:G:O5'	2.01	0.42
40:L5:2028:C:H2'	40:L5:2029:A:H8	1.85	0.42
40:L5:2264:C:H2'	40:L5:2265:G:O4'	2.19	0.42
40:L5:2411:C:H2'	40:L5:2412:A:C8	2.52	0.42
40:L5:3910:C:H2'	40:L5:3911:C:C6	2.55	0.42
40:L5:4184:G:H5'	43:LA:233:ARG:HB2	2.01	0.42
40:L5:4716:C:H2'	40:L5:4717:A:H8	1.85	0.42
87:L5:5292:SPM:H62	87:L5:5292:SPM:H31	1.81	0.42
50:LH:151:ILE:O	50:LH:155:SER:OG	2.31	0.42
76:Lk:57:LYS:HA	76:Lk:60:LEU:HG	2.02	0.42
8:SJ:87:LEU:HD13	8:SJ:100:LEU:HD21	2.02	0.42
8:SJ:173:VAL:HG23	19:S2:560:A:H3'	2.01	0.42
19:S2:959:G:H1'	19:S2:964:A:H61	1.85	0.42
19:S2:991:G:C6	19:S2:1134:G:H4'	2.54	0.42
19:S2:1373:C:H2'	19:S2:1374:C:C6	2.55	0.42
19:S2:1568:C:OP1	30:ST:96:SER:OG	2.33	0.42
19:S2:1862:G:H1'	19:S2:1863:A:H2'	2.02	0.42
26:SM:60:MET:HE3	26:SM:64:LEU:HB2	2.01	0.42
27:SP:45:LEU:HD23	27:SP:45:LEU:HA	1.84	0.42
38:Pt:35:A:H2'	38:Pt:36:C:H6	1.85	0.42
40:L5:138:G:H2'	40:L5:139:G:C8	2.55	0.42
40:L5:670:G:H2'	40:L5:671:G:H8	1.84	0.42
40:L5:1626:G:OP2	55:LN:77:LYS:NZ	2.52	0.42
40:L5:1744:PSU:C4	40:L5:1745:G:C8	3.07	0.42
40:L5:2832:A:H2'	40:L5:2833:A:C8	2.54	0.42
40:L5:3732:A:H2'	40:L5:3733:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:3919:C:H2'	40:L5:3920:PSU:H6	1.84	0.42
40:L5:4070:U:H2'	40:L5:4071:U:C6	2.54	0.42
40:L5:4141:G:H5'	40:L5:4142:C:H5	1.84	0.42
40:L5:4262:C:H2'	40:L5:4263:C:C6	2.54	0.42
40:L5:4278:C:OP2	60:LT:22:HIS:ND1	2.46	0.42
40:L5:4977:A:H2'	40:L5:4978:G:C8	2.55	0.42
54:LM:104:MET:HG3	54:LM:108:ASP:HB2	2.01	0.42
62:LV:127:ASP:OD1	62:LV:128:LEU:N	2.52	0.42
69:Ld:18:ASN:OD1	69:Ld:19:GLU:N	2.53	0.42
5:SG:59:GLN:NE2	19:S2:466:G:H1'	2.34	0.42
7:SI:49:ARG:HE	19:S2:446:G:H5''	1.84	0.42
8:SJ:114:VAL:HG11	8:SJ:135:ILE:HG12	2.02	0.42
9:SL:42:LEU:HG	19:S2:291:G:C2	2.54	0.42
14:SX:46:HIS:HB3	14:SX:101:LEU:HD11	2.01	0.42
17:Sb:17:ARG:HD2	19:S2:1127:C:H4'	2.01	0.42
18:Se:12:VAL:HG23	19:S2:616:A:H1'	2.02	0.42
19:S2:90:G:H2'	19:S2:91:A:O4'	2.20	0.42
19:S2:959:G:H1'	19:S2:964:A:N6	2.35	0.42
19:S2:1285:G:N1	26:SM:57:ASP:OD1	2.53	0.42
25:SK:12:TYR:HE1	25:SK:52:LEU:HD11	1.84	0.42
40:L5:304:C:H2'	40:L5:305:A:O4'	2.20	0.42
40:L5:730:G:OP2	48:LF:76:ARG:NE	2.46	0.42
40:L5:742:G:H2'	40:L5:743:G:C8	2.54	0.42
40:L5:750:U:C2	40:L5:751:G:C8	3.07	0.42
40:L5:1414:C:O2'	40:L5:1415:G:H5'	2.20	0.42
40:L5:1517:G:H2'	40:L5:1518:A:C5	2.55	0.42
40:L5:2059:C:H2'	40:L5:2060:G:H8	1.84	0.42
40:L5:4190:U:O2'	40:L5:4382:G:OP2	2.33	0.42
40:L5:4411:G:H2'	40:L5:4412:C:C6	2.54	0.42
40:L5:4859:C:N4	40:L5:4860:G:O6	2.53	0.42
40:L5:5051:C:H4'	44:LB:324:GLY:HA2	2.02	0.42
41:L7:33:U:H2'	41:L7:34:C:C6	2.55	0.42
42:L8:45:C:H2'	42:L8:46:G:H8	1.84	0.42
53:LL:130:LYS:HZ2	53:LL:131:PRO:HG2	1.85	0.42
54:LM:122:ILE:HB	56:LO:189:ILE:HD11	2.02	0.42
55:LN:146:PRO:C	55:LN:148:THR:H	2.28	0.42
59:LS:27:LEU:HB3	60:LT:148:PRO:HB3	2.01	0.42
6:SH:145:ARG:NH1	13:SW:51:GLU:OE1	2.52	0.42
8:SJ:29:LEU:HD23	18:Se:41:ARG:HD2	2.01	0.42
19:S2:5:U:H2'	19:S2:6:G:C8	2.54	0.42
19:S2:120:U:H2'	19:S2:121:OMU:H6	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:319:C:H2'	19:S2:320:G:C8	2.53	0.42
19:S2:462:OMC:H1'	19:S2:462:OMC:HM23	1.80	0.42
19:S2:468:A2M:H1'	19:S2:468:A2M:HM'3	1.62	0.42
19:S2:512:A:H4'	19:S2:576:A2M:H2	2.02	0.42
19:S2:634:A:H2'	19:S2:635:G:C8	2.54	0.42
19:S2:644:OMG:H1'	19:S2:644:OMG:HM23	1.72	0.42
19:S2:1057:C:O2'	19:S2:1059:G:N7	2.39	0.42
19:S2:1355:C:H2'	19:S2:1356:G:O4'	2.19	0.42
19:S2:1391:OMC:HM23	19:S2:1391:OMC:H1'	1.89	0.42
25:SK:16:PHE:HB2	25:SK:79:LEU:HD13	2.02	0.42
31:SU:66:ARG:HH12	31:SU:75:LYS:HA	1.85	0.42
37:At:5:C:H2'	37:At:6:C:H6	1.85	0.42
40:L5:398:A2M:H1'	40:L5:398:A2M:HM'3	1.81	0.42
40:L5:683:C:H2'	40:L5:684:G:O4'	2.19	0.42
40:L5:1244:G:H2'	40:L5:1245:C:H6	1.85	0.42
40:L5:1510:G:H2'	40:L5:1511:U:C6	2.54	0.42
40:L5:1660:U:N3	40:L5:2345:G:OP1	2.44	0.42
40:L5:1973:G:O2'	84:Lt:78:SER:HB2	2.19	0.42
40:L5:2045:G:O2'	40:L5:2046:G:H5''	2.19	0.42
40:L5:2053:C:H41	56:LO:53:LYS:NZ	2.18	0.42
40:L5:2400:G:H21	72:Lg:6:THR:HG22	1.84	0.42
40:L5:3731:C:H2'	40:L5:3732:A:H8	1.85	0.42
40:L5:4411:G:H2'	40:L5:4412:C:H6	1.85	0.42
40:L5:4493:PSU:H2'	40:L5:4494:OMG:C8	2.55	0.42
40:L5:4597:U:H2'	40:L5:4598:C:O4'	2.20	0.42
40:L5:4945:G:C2	71:Lf:5:LEU:HD12	2.54	0.42
43:LA:46:LYS:HD3	43:LA:46:LYS:HA	1.90	0.42
43:LA:196:TRP:HB3	43:LA:197:PRO:HD3	2.02	0.42
45:LC:334:THR:HG21	48:LF:51:TYR:OH	2.20	0.42
57:LP:131:ARG:HG3	57:LP:137:ASN:OD1	2.19	0.42
59:LS:81:TRP:HB3	59:LS:127:MET:HE3	2.02	0.42
1:SA:8:LEU:HD23	1:SA:191:ARG:HH12	1.84	0.42
2:SB:174:ARG:NE	2:SB:175:GLU:OE2	2.46	0.42
3:SC:114:LYS:HD3	3:SC:121:ARG:CZ	2.50	0.42
4:SE:95:THR:HG22	15:SY:16:ARG:HH11	1.84	0.42
4:SE:139:LEU:HD22	4:SE:147:ILE:HD11	2.01	0.42
15:SY:12:PHE:HD1	15:SY:23:MET:HB3	1.84	0.42
18:Se:39:ASN:HA	18:Se:43:VAL:HG22	2.01	0.42
19:S2:109:PSU:H2'	19:S2:110:U:C6	2.55	0.42
19:S2:118:C:H2'	19:S2:119:U:O4'	2.19	0.42
19:S2:452:G:H2'	19:S2:453:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1409:A:H2'	19:S2:1410:C:C6	2.55	0.42
19:S2:1447:G:H2'	19:S2:1448:A:H8	1.85	0.42
19:S2:1792:G:H2'	19:S2:1793:A:H8	1.84	0.42
19:S2:1849:G:H2'	19:S2:1850:MA6:C8	2.50	0.42
20:LR:54:PRO:HG3	39:CI:70:ALA:HB2	2.02	0.42
27:SP:108:LYS:HG2	27:SP:111:MET:HG3	2.02	0.42
40:L5:281:U:H2'	40:L5:282:C:H6	1.85	0.42
40:L5:358:C:H2'	40:L5:359:A:C8	2.55	0.42
40:L5:506:C:H2'	40:L5:507:G:H8	1.85	0.42
40:L5:513:U:H3'	40:L5:514:U:H4'	2.02	0.42
40:L5:678:C:H2'	40:L5:679:C:C6	2.54	0.42
40:L5:1555:G:N7	81:Lp:4:ARG:NH2	2.62	0.42
40:L5:1702:C:H2'	40:L5:1703:C:O4'	2.20	0.42
40:L5:1846:G:H2'	40:L5:1847:C:C6	2.54	0.42
40:L5:1890:G:OP2	40:L5:1890:G:N2	2.32	0.42
40:L5:2102:G:H1'	40:L5:2103:G:N7	2.34	0.42
40:L5:3633:C:H2'	40:L5:3634:G:C8	2.54	0.42
40:L5:4261:C:H2'	40:L5:4262:C:C6	2.55	0.42
40:L5:4601:U:H2'	40:L5:4602:A:H8	1.85	0.42
40:L5:4859:C:H2'	40:L5:4860:G:H8	1.85	0.42
40:L5:4954:G:H2'	40:L5:4955:A:C8	2.54	0.42
40:L5:4961:G:H2'	40:L5:4962:C:C6	2.55	0.42
40:L5:4970:C:C2	40:L5:4971:A:C8	3.08	0.42
40:L5:4971:A:O3'	57:LP:55:LYS:NZ	2.42	0.42
42:L8:52:A:H5'	77:Ll:21:ARG:HD3	2.02	0.42
45:LC:361:LEU:HA	45:LC:364:LYS:HG2	2.02	0.42
47:LE:138:ARG:HH21	47:LE:170:SER:HA	1.85	0.42
73:Lh:21:LEU:HD11	73:Lh:25:LYS:HE2	2.01	0.42
84:Lt:15:LEU:HD13	84:Lt:60:VAL:HG13	2.02	0.42
4:SE:108:ARG:NH2	19:S2:846:G:OP2	2.52	0.41
19:S2:96:C:H2'	19:S2:97:U:H6	1.85	0.41
19:S2:107:A:H61	19:S2:354:OMU:C4	2.30	0.41
19:S2:668:A2M:H1'	19:S2:668:A2M:HM'3	1.70	0.41
19:S2:1344:A:N1	19:S2:1385:G:O2'	2.53	0.41
26:SM:53:ALA:HA	26:SM:79:VAL:HG12	2.01	0.41
36:Sg:63:SER:HB3	36:Sg:84:ASP:HB3	2.02	0.41
38:Pt:27:U:H2'	38:Pt:28:U:C6	2.55	0.41
40:L5:500:G:H1'	40:L5:504:G:H2'	2.02	0.41
40:L5:667:A:H5''	40:L5:668:C:H5''	2.01	0.41
40:L5:1253:G:H2'	40:L5:1256:G:H5'	2.01	0.41
40:L5:1767:A:N7	40:L5:1769:G:H4'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1998:A:N6	83:Ls:40:MET:HG2	2.35	0.41
40:L5:2638:G:N1	40:L5:2718:U:H2'	2.35	0.41
40:L5:3821:A:H2'	40:L5:3822:PSU:C6	2.55	0.41
40:L5:3832:U:H2'	40:L5:3833:C:C6	2.55	0.41
40:L5:3953:G:N2	40:L5:4059:C:O2'	2.53	0.41
40:L5:4475:G:OP1	50:LH:173:ARG:NH1	2.49	0.41
40:L5:4540:C:H2'	40:L5:4541:G:C8	2.55	0.41
40:L5:4622:A:H2'	40:L5:4623:OMG:C8	2.55	0.41
41:L7:92:C:H2'	41:L7:93:G:C8	2.47	0.41
41:L7:112:U:H2'	41:L7:113:G:H8	1.85	0.41
46:LD:164:LYS:HG2	46:LD:195:HIS:CE1	2.55	0.41
58:LQ:27:LEU:HD23	58:LQ:27:LEU:HA	1.93	0.41
77:Ll:48:LYS:HD2	77:Ll:48:LYS:HA	1.84	0.41
3:SC:82:TYR:CZ	3:SC:164:PRO:HD3	2.55	0.41
4:SE:29:PRO:HA	19:S2:496:C:H5'	2.02	0.41
9:SL:28:THR:HA	9:SL:29:GLY:HA2	1.80	0.41
15:SY:124:ASN:HD22	19:S2:84:A:H5''	1.86	0.41
19:S2:15:U:H2'	19:S2:16:G:O4'	2.20	0.41
19:S2:62:G:O2'	19:S2:172:OMU:OP1	2.37	0.41
19:S2:573:U:H1'	19:S2:576:A2M:N7	2.36	0.41
19:S2:604:A:H1'	19:S2:639:C:O2'	2.20	0.41
19:S2:956:G:H2'	19:S2:957:A:H8	1.84	0.41
19:S2:1101:U:H2'	19:S2:1102:G:H8	1.85	0.41
19:S2:1203:G:H2'	19:S2:1204:A:H8	1.85	0.41
19:S2:1464:C:H4'	22:SR:60:ARG:NH1	2.34	0.41
19:S2:1608:U:H3	19:S2:1631:U:H3	1.68	0.41
22:SR:35:CYS:HA	22:SR:38:ILE:HG12	2.03	0.41
34:Sd:3:HIS:HD1	34:Sd:5:GLN:H	1.68	0.41
36:Sg:206:LEU:HD12	36:Sg:218:LEU:HB3	2.01	0.41
40:L5:6:C:H2'	40:L5:7:C:H6	1.84	0.41
40:L5:480:C:H2'	40:L5:481:G:C8	2.55	0.41
40:L5:718:C:H2'	40:L5:719:C:O4'	2.19	0.41
40:L5:1194:G:H2'	40:L5:1195:G:C8	2.55	0.41
40:L5:1251:C:H2'	40:L5:1252:C:C6	2.54	0.41
40:L5:1874:A:H2'	40:L5:1875:C:C6	2.55	0.41
40:L5:2770:C:H2'	40:L5:2771:G:C8	2.55	0.41
40:L5:4070:U:H2'	40:L5:4071:U:H6	1.85	0.41
40:L5:4192:A:H2'	40:L5:4193:C:H6	1.85	0.41
40:L5:4941:G:H2'	40:L5:4942:C:C6	2.54	0.41
44:LB:80:GLU:OE1	44:LB:323:TYR:OH	2.31	0.41
45:LC:368:LYS:HA	45:LC:368:LYS:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:LD:37:VAL:HB	46:LD:67:ALA:HB2	2.02	0.41
47:LE:222:LEU:N	47:LE:237:LYS:HE2	2.35	0.41
49:LG:167:VAL:HG12	49:LG:170:LEU:HD12	2.02	0.41
53:LL:103:ARG:H	53:LL:103:ARG:HD3	1.84	0.41
80:Lo:24:THR:HA	80:Lo:93:LEU:HD21	2.02	0.41
83:Ls:82:ILE:HG23	83:Ls:86:VAL:HG23	2.02	0.41
15:SY:68:LYS:HE2	15:SY:68:LYS:HB3	1.91	0.41
16:Sa:34:LYS:NZ	19:S2:1862:G:O6	2.52	0.41
19:S2:12:U:H2'	19:S2:13:C:H6	1.86	0.41
19:S2:939:U:H2'	19:S2:940:U:C6	2.55	0.41
19:S2:1328:OMG:HM23	19:S2:1328:OMG:H1'	1.71	0.41
19:S2:1383:A2M:HM'3	19:S2:1383:A2M:H1'	1.61	0.41
19:S2:1415:C:H2'	19:S2:1416:C:H6	1.85	0.41
19:S2:1628:C:H2'	19:S2:1629:C:C6	2.55	0.41
29:SS:26:ILE:HD13	29:SS:56:ALA:HA	2.02	0.41
36:Sg:215:GLN:HA	36:Sg:231:ASP:HA	2.02	0.41
38:Pt:4:U:H2'	38:Pt:5:C:C6	2.55	0.41
40:L5:68:U:OP1	55:LN:178:HIS:ND1	2.46	0.41
40:L5:92:C:C2	66:La:55:LYS:HE2	2.55	0.41
40:L5:425:U:H2'	40:L5:426:A:C8	2.55	0.41
40:L5:1472:C:H2'	40:L5:1473:U:C6	2.55	0.41
40:L5:1494:U:H2'	40:L5:1495:G:H8	1.84	0.41
40:L5:1727:U:H2'	40:L5:1728:U:H6	1.85	0.41
40:L5:2050:G:H2'	40:L5:2051:C:C6	2.56	0.41
40:L5:2419:C:H2'	40:L5:2420:A:H8	1.85	0.41
40:L5:2458:C:H5''	55:LN:67:ARG:HD2	2.01	0.41
40:L5:2691:U:H2'	40:L5:2692:U:H6	1.85	0.41
40:L5:3588:C:H2'	40:L5:3589:G:O4'	2.20	0.41
40:L5:3891:A:O2'	57:LP:64:ASN:ND2	2.53	0.41
40:L5:4127:A:H62	40:L5:4157:A:H62	1.68	0.41
40:L5:4281:A:H2'	40:L5:4282:A:H2'	2.01	0.41
40:L5:4457:PSU:O4	44:LB:252:ALA:HB3	2.20	0.41
65:LZ:38:TYR:CE1	65:LZ:40:HIS:HB3	2.55	0.41
1:SA:52:LYS:HB2	22:SR:109:LEU:HD13	2.03	0.41
1:SA:184:ARG:HB3	1:SA:191:ARG:NE	2.33	0.41
8:SJ:18:ARG:NH2	19:S2:4:C:H1'	2.35	0.41
19:S2:1255:G:OP1	19:S2:1256:G:O2'	2.30	0.41
19:S2:1495:G:H2'	19:S2:1496:U:C6	2.55	0.41
20:LR:60:ARG:NH1	40:L5:2808:G:O3'	2.53	0.41
21:LW:81:ALA:HB2	21:LW:87:LEU:HB2	2.01	0.41
21:LW:102:LYS:HA	21:LW:105:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SD:193:ASP:OD2	23:SD:198:ILE:HG12	2.21	0.41
28:SQ:17:LYS:HE2	28:SQ:17:LYS:HB3	1.95	0.41
31:SU:19:ARG:O	31:SU:117:ALA:N	2.49	0.41
32:SZ:65:TYR:C	32:SZ:111:ARG:HD3	2.44	0.41
40:L5:44:A:N3	40:L5:94:A:H2	2.18	0.41
40:L5:399:G:N2	57:LP:101:ASN:OD1	2.51	0.41
40:L5:434:A:H3'	40:L5:435:A:H8	1.85	0.41
40:L5:665:C:H4'	40:L5:666:G:H5'	2.02	0.41
40:L5:1100:U:O4	40:L5:1194:G:O6	2.39	0.41
40:L5:1408:G:O2'	40:L5:1411:C:N4	2.54	0.41
40:L5:1503:A:H1'	40:L5:1504:G:C8	2.55	0.41
40:L5:1669:A:C2	40:L5:1852:U:H4'	2.56	0.41
40:L5:2078:C:H2'	40:L5:2079:G:C8	2.55	0.41
40:L5:2358:G:H2'	40:L5:2359:U:O4'	2.19	0.41
40:L5:2421:G:H8	57:LP:139:TYR:CZ	2.38	0.41
40:L5:3718:A2M:HM'3	40:L5:3718:A2M:H1'	1.70	0.41
40:L5:3744:OMG:HM23	40:L5:3744:OMG:H1'	1.74	0.41
40:L5:3871:A:H2'	40:L5:3872:A:H8	1.85	0.41
40:L5:3952:A:H2'	40:L5:3953:G:C8	2.56	0.41
40:L5:4383:U:H2'	40:L5:4384:U:C6	2.55	0.41
40:L5:4617:G:OP1	44:LB:62:ARG:NH1	2.54	0.41
40:L5:4965:U:H4'	40:L5:4966:A:H5'	2.03	0.41
41:L7:5:A:O2'	46:LD:63:GLN:OE1	2.29	0.41
41:L7:35:U:O2	41:L7:45:U:O2'	2.38	0.41
55:LN:35:ALA:HA	55:LN:65:ARG:HB3	2.01	0.41
62:LV:69:LYS:HB2	62:LV:72:LEU:HD12	2.01	0.41
1:SA:210:ILE:HD11	22:SR:80:ARG:HB3	2.02	0.41
2:SB:128:LYS:HE2	2:SB:219:LYS:HD3	2.02	0.41
2:SB:175:GLU:HB3	2:SB:187:LYS:HZ1	1.84	0.41
2:SB:228:LEU:HD12	2:SB:231:LEU:HD11	2.02	0.41
3:SC:60:TRP:CE2	3:SC:92:GLU:HB2	2.55	0.41
6:SH:46:THR:OG1	6:SH:97:GLN:NE2	2.52	0.41
16:Sa:60:ASP:OD1	16:Sa:61:ALA:N	2.52	0.41
19:S2:352:U:H2'	19:S2:353:C:C6	2.55	0.41
19:S2:482:G:N2	19:S2:484:A2M:H3'	2.36	0.41
19:S2:1726:G:H1	19:S2:1808:U:H3	1.67	0.41
19:S2:1816:G:O2'	40:L5:3807:A:O2'	2.15	0.41
40:L5:5:A:H1'	49:LG:192:ARG:HH21	1.85	0.41
40:L5:302:C:H2'	40:L5:303:C:C6	2.55	0.41
40:L5:443:G:H2'	40:L5:444:G:C8	2.55	0.41
40:L5:751:G:H2'	40:L5:752:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1443:A:H2'	40:L5:1444:G:C8	2.56	0.41
40:L5:1486:C:H2'	40:L5:1487:G:H8	1.86	0.41
40:L5:2000:G:H4'	40:L5:2001:G:C8	2.55	0.41
40:L5:2648:G:H2'	40:L5:2649:G:C8	2.56	0.41
40:L5:2723:U:H2'	40:L5:2724:G:C8	2.56	0.41
40:L5:2888:G:H2'	40:L5:2889:G:H8	1.85	0.41
40:L5:4478:G:N2	40:L5:4608:G:O2'	2.52	0.41
40:L5:4524:G:H2'	40:L5:4525:C:C6	2.56	0.41
40:L5:4947:U:H2'	40:L5:4948:C:C6	2.55	0.41
41:L7:15:C:H2'	41:L7:16:A:H8	1.86	0.41
41:L7:16:A:H2'	41:L7:17:C:C6	2.56	0.41
42:L8:15:G:H2'	42:L8:16:G:C4	2.56	0.41
45:LC:5:ARG:HB3	45:LC:24:LEU:HB3	2.02	0.41
48:LF:50:ILE:HD12	48:LF:186:CYS:HB3	2.03	0.41
59:LS:70:LYS:HD3	59:LS:70:LYS:HA	1.85	0.41
4:SE:55:ALA:HB1	4:SE:60:GLU:HB2	2.03	0.41
7:SI:25:ARG:HH22	19:S2:434:G:P	2.44	0.41
19:S2:16:G:H5'	19:S2:669:A:N6	2.35	0.41
19:S2:155:G:H2'	19:S2:156:G:H8	1.85	0.41
19:S2:788:G:O2'	19:S2:789:G:H5''	2.21	0.41
19:S2:806:U:H2'	19:S2:807:G:C8	2.54	0.41
19:S2:1422:G:H4'	19:S2:1423:C:H3'	2.02	0.41
19:S2:1501:C:H2'	19:S2:1502:C:C6	2.56	0.41
19:S2:1528:G:H2'	19:S2:1529:C:C6	2.56	0.41
23:SD:8:LYS:HB3	31:SU:61:LEU:HD21	2.02	0.41
23:SD:135:GLU:HB2	23:SD:153:VAL:HG23	2.01	0.41
25:SK:97:SER:C	25:SK:98:ARG:HD2	2.46	0.41
28:SQ:73:LYS:HD2	28:SQ:73:LYS:HA	1.78	0.41
36:Sg:185:LYS:HA	36:Sg:185:LYS:HD2	1.83	0.41
37:At:51:C:H2'	37:At:52:G:C8	2.56	0.41
37:At:53:G:N1	37:At:62:C:N3	2.69	0.41
38:Pt:72:C:H2'	38:Pt:73:A:C8	2.56	0.41
40:L5:494:U:H2'	40:L5:495:C:C6	2.55	0.41
40:L5:1688:G:H2'	40:L5:1689:G:C8	2.55	0.41
40:L5:2384:U:H2'	40:L5:2385:U:C6	2.55	0.41
40:L5:2402:G:H2'	40:L5:2403:A:H8	1.85	0.41
40:L5:3616:U:H4'	40:L5:3617:G:H5'	2.02	0.41
40:L5:4097:G:N7	40:L5:4098:A:N6	2.69	0.41
40:L5:4573:G:H2'	40:L5:4574:U:C6	2.55	0.41
40:L5:5002:U:H2'	40:L5:5003:U:C6	2.56	0.41
46:LD:41:LYS:HB2	60:LT:68:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LF:240:ILE:HD12	48:LF:240:ILE:HA	1.92	0.41
58:LQ:86:ILE:HD12	58:LQ:105:VAL:HG22	2.03	0.41
60:LT:108:ARG:NH2	60:LT:130:ARG:HH21	2.18	0.41
82:Lr:46:ARG:CZ	82:Lr:70:GLN:HG3	2.50	0.41
4:SE:187:ALA:H	19:S2:809:A:P	2.43	0.41
10:SN:84:LEU:HD23	10:SN:84:LEU:HA	1.92	0.41
16:Sa:23:CYS:HB3	16:Sa:28:ARG:H	1.86	0.41
16:Sa:33:ASP:OD1	16:Sa:34:LYS:N	2.53	0.41
19:S2:29:G:H2'	19:S2:30:C:H6	1.86	0.41
19:S2:85:A:H2'	19:S2:86:C:C6	2.55	0.41
19:S2:94:G:O2'	19:S2:508:A:O2'	2.25	0.41
19:S2:118:C:H1'	19:S2:445:A:C5	2.56	0.41
19:S2:456:C:H2'	19:S2:457:C:C6	2.56	0.41
19:S2:946:U:H2'	19:S2:947:G:C8	2.55	0.41
23:SD:202:LYS:HE3	23:SD:202:LYS:HB2	1.86	0.41
24:SF:122:ARG:HG3	33:Sc:57:THR:HG21	2.03	0.41
40:L5:1426:G:N1	40:L5:1458:C:OP2	2.38	0.41
40:L5:1427:A:OP2	40:L5:1457:G:N1	2.49	0.41
40:L5:1617:G:H1'	40:L5:2513:A:N6	2.36	0.41
40:L5:1646:A:H2'	40:L5:1647:U:C6	2.55	0.41
40:L5:1703:C:H41	48:LF:39:GLN:NE2	2.19	0.41
40:L5:1848:C:H2'	40:L5:1849:U:O4'	2.20	0.41
40:L5:2029:A:H2'	40:L5:2030:A:C8	2.55	0.41
40:L5:2081:C:H2'	40:L5:2082:G:H8	1.85	0.41
40:L5:2374:A:H2'	40:L5:2375:A:H8	1.86	0.41
40:L5:2519:U:H1'	40:L5:2520:C:C6	2.56	0.41
40:L5:2735:G:H2'	40:L5:2736:G:H8	1.85	0.41
40:L5:3813:A:N3	40:L5:4538:G:O2'	2.46	0.41
40:L5:3920:PSU:H2'	40:L5:3921:U:H6	1.85	0.41
40:L5:4177:C:H2'	40:L5:4178:A:C8	2.52	0.41
40:L5:4210:U:H3	40:L5:4222:G:H1	1.68	0.41
40:L5:4318:C:H4'	80:Lo:17:LYS:HA	2.02	0.41
40:L5:4592:C:H2'	40:L5:4593:C:C6	2.56	0.41
40:L5:4759:C:OP1	56:LO:116:LYS:NZ	2.40	0.41
40:L5:4767:C:H2'	40:L5:4768:G:C8	2.56	0.41
49:LG:230:TYR:HA	49:LG:233:ILE:HD12	2.02	0.41
58:LQ:88:ASP:HB2	58:LQ:109:ALA:HB2	2.02	0.41
58:LQ:154:LYS:HB3	58:LQ:154:LYS:HE2	1.89	0.41
1:SA:42:LYS:HG3	1:SA:44:ASP:H	1.85	0.41
1:SA:155:ARG:HH22	19:S2:1137:U:H4'	1.85	0.41
6:SH:33:ASN:ND2	6:SH:37:LYS:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:77:LEU:HA	8:SJ:80:ARG:HE	1.85	0.41
11:SO:65:ASP:HB3	19:S2:963:A:OP1	2.21	0.41
19:S2:323:C:H5'	19:S2:324:C:OP1	2.21	0.41
19:S2:1269:G:H2'	19:S2:1270:G:C8	2.56	0.41
19:S2:1661:A:OP2	34:Sd:32:ARG:NH2	2.46	0.41
20:LR:82:LYS:HA	20:LR:82:LYS:HD2	1.95	0.41
35:Sf:103:LEU:HB2	35:Sf:105:TYR:CD2	2.55	0.41
36:Sg:88:ARG:HG2	36:Sg:97:THR:HG21	2.02	0.41
36:Sg:159:ASN:ND2	36:Sg:162:ASN:OD1	2.54	0.41
40:L5:123:C:H2'	40:L5:124:C:C6	2.55	0.41
40:L5:139:G:H2'	40:L5:140:G:C8	2.54	0.41
40:L5:1198:G:H2'	40:L5:1199:G:H8	1.86	0.41
40:L5:1366:G:H4'	40:L5:1367:C:OP1	2.20	0.41
40:L5:2386:U:H2'	40:L5:2387:G:H8	1.85	0.41
40:L5:2817:C:H2'	40:L5:2818:C:H6	1.85	0.41
40:L5:2856:C:H2'	40:L5:2857:A:O4'	2.21	0.41
40:L5:3608:A:H2'	40:L5:3609:G:C8	2.56	0.41
40:L5:3819:G:H2'	40:L5:3820:G:C8	2.55	0.41
40:L5:3856:A:H5''	57:LP:83:TRP:O	2.21	0.41
40:L5:4348:A:C6	40:L5:4350:C:C4	3.08	0.41
40:L5:4642:U:H2'	40:L5:4643:G:H8	1.84	0.41
40:L5:4761:G:H5''	56:LO:12:ARG:CZ	2.50	0.41
40:L5:4927:G:H5''	40:L5:4928:C:H5	1.85	0.41
41:L7:75:G:N2	41:L7:100:A:OP2	2.52	0.41
44:LB:103:LYS:HD3	44:LB:103:LYS:HA	1.92	0.41
45:LC:138:MET:HE3	45:LC:138:MET:HB3	1.97	0.41
47:LE:222:LEU:H	47:LE:237:LYS:HE2	1.85	0.41
47:LE:239:LYS:HA	47:LE:239:LYS:HD2	1.90	0.41
50:LH:51:LYS:HE2	50:LH:54:ARG:HH12	1.85	0.41
67:Lb:43:MET:HE2	67:Lb:43:MET:HB3	1.87	0.41
2:SB:38:MET:HG2	2:SB:38:MET:H	1.68	0.41
3:SC:131:GLY:HA3	3:SC:137:VAL:HA	2.02	0.41
3:SC:184:VAL:HG23	3:SC:243:ALA:HB1	2.03	0.41
5:SG:218:LYS:HD2	5:SG:218:LYS:HA	1.84	0.41
7:SI:10:LYS:HD3	19:S2:387:C:P	2.60	0.41
7:SI:130:THR:N	7:SI:131:PRO:HD2	2.36	0.41
8:SJ:104:ASP:O	8:SJ:108:ARG:HG2	2.20	0.41
8:SJ:152:ASP:OD1	8:SJ:153:SER:N	2.53	0.41
11:SO:124:MET:HE3	11:SO:124:MET:HB2	1.99	0.41
13:SW:6:VAL:HG21	19:S2:685:A:H5'	2.03	0.41
15:SY:93:ARG:HH21	19:S2:575:A:P	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:63:U:O2'	19:S2:170:A:N3	2.46	0.41
19:S2:602:G:OP2	19:S2:603:C:O2'	2.33	0.41
19:S2:666:U:H2'	19:S2:667:U:C6	2.56	0.41
19:S2:1134:G:H2'	19:S2:1135:C:H6	1.86	0.41
19:S2:1172:U:H2'	19:S2:1173:A:H8	1.85	0.41
19:S2:1198:G:H2'	19:S2:1199:A:C8	2.55	0.41
19:S2:1232:PSU:H2'	19:S2:1233:G:H8	1.86	0.41
19:S2:1731:A:H2'	19:S2:1732:G:C8	2.56	0.41
19:S2:1733:U:H2'	19:S2:1734:G:O4'	2.21	0.41
19:S2:1858:G:H2'	19:S2:1859:A:C8	2.52	0.41
20:LR:135:LYS:HG3	20:LR:136:ARG:N	2.32	0.41
20:LR:148:ASP:HA	20:LR:151:ARG:HB3	2.02	0.41
21:LW:87:LEU:HD12	21:LW:90:ILE:HD11	2.03	0.41
22:SR:41:ILE:HA	23:SD:208:VAL:HG12	2.03	0.41
24:SF:42:LYS:HD3	24:SF:42:LYS:HA	1.62	0.41
24:SF:91:ARG:O	24:SF:95:HIS:ND1	2.54	0.41
30:ST:40:ALA:HB3	30:ST:43:LYS:HG3	2.02	0.41
36:Sg:31:ILE:HG13	36:Sg:43:TRP:HB2	2.02	0.41
37:At:22:U:H2'	37:At:23:C:H6	1.86	0.41
40:L5:25:A:C8	40:L5:341:G:C8	3.09	0.41
40:L5:288:G:H2'	40:L5:289:C:H6	1.85	0.41
40:L5:364:G:O2'	40:L5:375:G:O6	2.36	0.41
40:L5:393:U:O2	57:LP:97:ASN:ND2	2.53	0.41
40:L5:426:A:H2'	40:L5:427:A:H8	1.86	0.41
40:L5:711:A:H2'	40:L5:712:C:C6	2.56	0.41
40:L5:958:G:N2	47:LE:124:LYS:HB3	2.35	0.41
40:L5:1084:C:H2'	40:L5:1085:C:H6	1.85	0.41
40:L5:1825:A:H2'	40:L5:1826:G:C8	2.56	0.41
40:L5:1921:C:C4	59:LS:161:ARG:HD2	2.56	0.41
40:L5:1942:A:H4'	41:L7:88:A:N1	2.36	0.41
40:L5:2045:G:O6	40:L5:3870:C:O2'	2.39	0.41
40:L5:2107:C:N4	40:L5:2108:G:O6	2.54	0.41
40:L5:2533:C:H2'	40:L5:2534:C:C6	2.55	0.41
40:L5:2599:G:N2	40:L5:2747:U:O4	2.54	0.41
40:L5:3833:C:H2'	40:L5:3834:C:C6	2.56	0.41
40:L5:4364:G:H2'	40:L5:4365:C:H6	1.85	0.41
40:L5:4716:C:H5''	44:LB:276:HIS:O	2.21	0.41
40:L5:4896:G:H2'	40:L5:4897:G:C8	2.55	0.41
40:L5:4911:A:OP1	44:LB:97:ARG:NH2	2.46	0.41
40:L5:5002:U:H2'	40:L5:5003:U:H6	1.85	0.41
40:L5:5058:A:H4'	69:Ld:23:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:L7:3:C:H2'	41:L7:4:U:C6	2.56	0.41
41:L7:3:C:H2'	41:L7:4:U:H6	1.86	0.41
43:LA:117:GLU:HB2	43:LA:162:ASN:HB3	2.02	0.41
46:LD:42:ASN:HD21	60:LT:69:GLN:NE2	2.18	0.41
47:LE:96:VAL:HG11	47:LE:105:ARG:NH1	2.34	0.41
47:LE:144:ILE:HG12	47:LE:196:ALA:HB2	2.03	0.41
54:LM:123:ILE:HD13	56:LO:182:GLU:HG2	2.02	0.41
56:LO:124:LEU:HD23	56:LO:124:LEU:HA	1.96	0.41
65:LZ:60:LYS:HE2	65:LZ:60:LYS:HB2	1.97	0.41
68:Lc:52:CYS:HB3	68:Lc:57:LYS:HE2	2.02	0.41
69:Ld:114:PHE:HA	69:Ld:117:LEU:HD12	2.02	0.41
6:SH:91:HIS:ND1	6:SH:172:THR:HG21	2.35	0.41
6:SH:158:LEU:HD23	6:SH:158:LEU:HA	1.94	0.41
7:SI:139:LYS:HE2	7:SI:139:LYS:HB2	1.86	0.41
8:SJ:115:PHE:HA	8:SJ:120:ALA:HB3	2.03	0.41
19:S2:323:C:H2'	19:S2:327:G:H22	1.86	0.41
19:S2:1362:U:H5''	19:S2:1363:C:H5	1.86	0.41
19:S2:1567:G:H2'	19:S2:1568:C:C6	2.55	0.41
19:S2:1803:U:H2'	19:S2:1804:U:H6	1.85	0.41
19:S2:1803:U:H2'	19:S2:1804:U:C6	2.55	0.41
20:LR:59:SER:HA	40:L5:2634:C:H5'	2.03	0.41
24:SF:31:ASN:OD1	24:SF:32:ASP:N	2.54	0.41
25:SK:63:ALA:HB2	25:SK:68:TYR:CE2	2.56	0.41
32:SZ:99:LEU:HD21	32:SZ:102:LYS:HB2	2.03	0.41
36:Sg:30:MET:HE3	36:Sg:30:MET:HB3	1.90	0.41
36:Sg:270:LEU:HD13	36:Sg:310:TRP:CD2	2.56	0.41
38:Pt:5:C:H2'	38:Pt:6:C:C6	2.57	0.41
40:L5:229:G:H2'	40:L5:230:G:C8	2.56	0.41
40:L5:480:C:H2'	40:L5:481:G:H8	1.86	0.41
40:L5:708:G:OP1	71:Lf:89:ARG:NH1	2.54	0.41
40:L5:1464:C:H5''	67:Lb:32:LEU:HD12	2.02	0.41
40:L5:1513:U:H2'	40:L5:1514:U:H6	1.86	0.41
40:L5:1577:G:H5'	40:L5:1578:U:H5''	2.03	0.41
40:L5:1667:G:N2	40:L5:2282:A:H62	2.18	0.41
40:L5:2422:OMC:O5'	40:L5:2422:OMC:H6	2.04	0.41
40:L5:2539:C:H2'	40:L5:2540:C:H6	1.84	0.41
40:L5:2605:G:H2'	40:L5:2606:G:H8	1.84	0.41
40:L5:2876:OMG:HM22	40:L5:2877:G:H5'	2.02	0.41
40:L5:4456:OMC:HM23	40:L5:4456:OMC:H1'	1.86	0.41
41:L7:75:G:H1'	41:L7:76:U:H5	1.85	0.41
43:LA:183:GLY:HA2	43:LA:186:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LF:226:HIS:HB3	48:LF:229:GLU:HG2	2.03	0.41
53:LL:65:ARG:HG3	66:La:69:PHE:CD2	2.56	0.41
57:LP:37:LYS:HE2	57:LP:37:LYS:HB3	1.83	0.41
1:SA:189:ILE:HG22	1:SA:191:ARG:H	1.86	0.40
5:SG:7:PHE:CD1	5:SG:10:THR:HG22	2.56	0.40
7:SI:99:ASN:HB2	19:S2:377:G:O5'	2.22	0.40
8:SJ:63:LEU:HD12	8:SJ:63:LEU:HA	1.88	0.40
8:SJ:163:SER:HA	8:SJ:164:PRO:HD3	1.92	0.40
13:SW:57:ARG:HD2	19:S2:919:A:H4'	2.03	0.40
19:S2:21:U:H2'	19:S2:22:A:H8	1.85	0.40
19:S2:615:C:H2'	19:S2:616:A:O4'	2.22	0.40
19:S2:1088:U:H4'	19:S2:1089:G:OP2	2.21	0.40
19:S2:1359:U:H2'	19:S2:1360:U:H6	1.86	0.40
19:S2:1410:C:H2'	19:S2:1411:G:H8	1.85	0.40
21:LW:2:LYS:HE2	44:LB:71:GLU:HB3	2.03	0.40
21:LW:52:THR:HG22	21:LW:54:LEU:H	1.85	0.40
23:SD:109:LEU:HD22	23:SD:115:VAL:HG12	2.03	0.40
38:Pt:5:C:H2'	38:Pt:6:C:H6	1.86	0.40
40:L5:303:C:H2'	40:L5:304:C:C6	2.56	0.40
40:L5:1211:G:H2'	40:L5:1212:G:C8	2.56	0.40
40:L5:1473:U:H2'	40:L5:1474:C:C6	2.55	0.40
40:L5:1494:U:H2'	40:L5:1495:G:C8	2.56	0.40
40:L5:1517:G:H22	45:LC:103:ALA:HA	1.87	0.40
40:L5:1779:U:H2'	40:L5:1780:A:H8	1.86	0.40
40:L5:1819:G:H1'	46:LD:115:MET:HE1	2.03	0.40
40:L5:1978:C:H2'	40:L5:1979:A:C8	2.56	0.40
40:L5:2274:C:H2'	40:L5:2275:G:C8	2.56	0.40
40:L5:2344:U:O4	66:La:3:SER:OG	2.34	0.40
40:L5:2517:A:H5'	72:Lg:62:LYS:HD3	2.03	0.40
40:L5:2780:C:H2'	40:L5:2781:G:C8	2.46	0.40
40:L5:3702:A:C6	40:L5:3774:A:C6	3.09	0.40
40:L5:3723:A:H2'	40:L5:3724:A:H8	1.85	0.40
40:L5:4392:OMG:HM21	40:L5:4394:A:H2'	2.03	0.40
40:L5:4685:U:H2'	40:L5:4686:G:H8	1.86	0.40
40:L5:4724:A:H2'	40:L5:4725:C:C6	2.56	0.40
40:L5:4883:C:H2'	40:L5:4884:G:H8	1.86	0.40
44:LB:136:LYS:HE2	44:LB:136:LYS:HB3	1.88	0.40
44:LB:317:LEU:HB3	44:LB:372:SER:HB2	2.03	0.40
46:LD:50:ARG:NH1	46:LD:147:ASP:OD2	2.54	0.40
47:LE:277:LEU:HD23	47:LE:277:LEU:HA	1.90	0.40
53:LL:111:GLN:O	53:LL:115:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:LX:74:TYR:CD2	73:Lh:25:LYS:HD3	2.56	0.40
75:Lj:60:GLY:HA2	75:Lj:64:MET:SD	2.61	0.40
83:Ls:133:GLU:HG2	83:Ls:134:LYS:HG2	2.02	0.40
3:SC:246:LYS:HB2	3:SC:249:SER:HB2	2.03	0.40
9:SL:35:ARG:NH2	9:SL:55:TYR:O	2.55	0.40
14:SX:101:LEU:HB3	14:SX:124:LYS:HB2	2.02	0.40
14:SX:106:GLY:HA2	19:S2:648:A:H5''	2.03	0.40
14:SX:129:SER:HB2	19:S2:29:G:H4'	2.04	0.40
17:Sb:36:LYS:NZ	17:Sb:40:CYS:O	2.50	0.40
19:S2:1242:U:O2	19:S2:1517:G:O2'	2.29	0.40
19:S2:1452:A:H5''	22:SR:48:ASN:HD22	1.86	0.40
22:SR:16:ILE:HG22	23:SD:210:ILE:HG12	2.03	0.40
22:SR:30:THR:O	22:SR:34:VAL:HG23	2.21	0.40
40:L5:18:C:H2'	40:L5:19:G:C8	2.56	0.40
40:L5:919:C:H2'	40:L5:920:C:H6	1.85	0.40
40:L5:1238:A:O2'	48:LF:52:GLU:OE2	2.37	0.40
40:L5:1340:OMC:H1'	40:L5:1340:OMC:HM23	1.74	0.40
40:L5:1734:G:N2	40:L5:1735:U:O4	2.37	0.40
40:L5:1896:A:OP1	48:LF:97:GLY:N	2.54	0.40
40:L5:2293:U:H2'	40:L5:2294:G:C8	2.56	0.40
40:L5:2622:G:H2'	40:L5:2623:A:H8	1.87	0.40
40:L5:2803:U:H2'	40:L5:2804:OMC:C6	2.56	0.40
40:L5:4277:G:H5''	60:LT:17:ARG:HG2	2.03	0.40
40:L5:4642:U:H2'	40:L5:4643:G:C8	2.57	0.40
42:L8:140:C:H2'	42:L8:141:C:C6	2.57	0.40
49:LG:70:LEU:HD23	49:LG:70:LEU:HA	1.88	0.40
49:LG:87:LEU:HD23	49:LG:87:LEU:HA	1.79	0.40
57:LP:141:SER:OG	57:LP:142:SER:N	2.55	0.40
63:LX:65:ALA:HB2	73:Lh:69:LEU:HD11	2.03	0.40
65:LZ:13:VAL:HA	65:LZ:80:LEU:HD23	2.03	0.40
73:Lh:95:LEU:HB3	73:Lh:99:GLU:HG3	2.03	0.40
77:Ll:44:TRP:O	77:Ll:48:LYS:NZ	2.47	0.40
6:SH:111:LYS:HD2	19:S2:796:G:H21	1.85	0.40
7:SI:12:ARG:HH21	7:SI:18:ARG:HA	1.86	0.40
10:SN:102:LEU:HD12	10:SN:102:LEU:HA	1.93	0.40
13:SW:44:HIS:NE2	13:SW:112:ASP:OD2	2.54	0.40
14:SX:56:GLY:HA3	18:Se:3:HIS:CE1	2.56	0.40
19:S2:448:A:H4'	19:S2:449:A:H5''	2.03	0.40
19:S2:884:C:H2'	19:S2:885:U:O4'	2.21	0.40
19:S2:942:G:H2'	19:S2:943:U:C6	2.56	0.40
19:S2:1103:C:H2'	19:S2:1104:G:H8	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1260:A:C2	19:S2:1620:A:C4	3.09	0.40
19:S2:1523:C:H2'	19:S2:1524:G:C8	2.55	0.40
19:S2:1531:A:P	30:ST:84:ARG:HH21	2.45	0.40
19:S2:1651:A:H2'	19:S2:1652:G:C8	2.54	0.40
19:S2:1770:G:O3'	19:S2:1771:G:N2	2.47	0.40
20:LR:23:TRP:HB2	20:LR:53:LYS:HG3	2.03	0.40
20:LR:173:ARG:HG2	20:LR:176:ARG:NH2	2.36	0.40
23:SD:51:LEU:HD12	23:SD:91:VAL:HB	2.03	0.40
25:SK:18:GLU:HG2	25:SK:20:VAL:HG22	2.03	0.40
26:SM:71:GLU:CD	35:Sf:114:ILE:HB	2.46	0.40
31:SU:69:PRO:O	34:Sd:40:ARG:NH2	2.54	0.40
36:Sg:71:ILE:HG22	36:Sg:72:SER:O	2.21	0.40
40:L5:124:C:H2'	40:L5:125:C:H6	1.86	0.40
40:L5:302:C:H2'	40:L5:303:C:H6	1.87	0.40
40:L5:1177:U:O2'	40:L5:1178:G:H3'	2.20	0.40
40:L5:1458:C:C2	40:L5:1459:A:C8	3.09	0.40
40:L5:1595:G:H1'	40:L5:1597:G:H21	1.86	0.40
40:L5:2004:U:H3	40:L5:2016:C:H1'	1.87	0.40
40:L5:2108:G:H2'	40:L5:2109:G:H8	1.86	0.40
40:L5:2460:A:OP2	88:L5:5291:SPD:N10	2.54	0.40
40:L5:2634:C:H2'	40:L5:2635:U:C6	2.57	0.40
40:L5:2836:A:C2	40:L5:3895:G:H4'	2.56	0.40
40:L5:3653:A:H4'	43:LA:179:ILE:HB	2.03	0.40
40:L5:4091:G:H3'	40:L5:4114:C:N4	2.36	0.40
40:L5:4147:G:H2'	40:L5:4148:C:H6	1.86	0.40
40:L5:4188:U:H2'	40:L5:4189:U:H6	1.86	0.40
40:L5:4593:C:H2'	40:L5:4594:U:H6	1.86	0.40
40:L5:4629:U:C2	40:L5:4630:G:C8	3.09	0.40
40:L5:5010:PSU:H2'	40:L5:5011:A:C8	2.56	0.40
40:L5:5010:PSU:H2'	40:L5:5011:A:H8	1.87	0.40
41:L7:12:U:OP2	41:L7:67:C:O2'	2.40	0.40
44:LB:196:TRP:O	44:LB:199:GLU:HG2	2.21	0.40
44:LB:217:ILE:HD12	44:LB:347:LEU:HB3	2.03	0.40
48:LF:136:VAL:HG23	48:LF:140:ILE:HD13	2.04	0.40
52:LJ:114:ASP:OD1	52:LJ:115:LEU:N	2.54	0.40
55:LN:5:LYS:HG3	74:Li:40:VAL:HG11	2.03	0.40
59:LS:82:LEU:HA	59:LS:127:MET:HG2	2.02	0.40
75:Lj:28:HIS:HB3	75:Lj:31:LYS:HB2	2.02	0.40
3:SC:205:VAL:HG12	19:S2:1:U:H1'	2.02	0.40
4:SE:75:LYS:HD2	4:SE:77:ARG:HH22	1.85	0.40
6:SH:19:PHE:CZ	6:SH:50:GLU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:49:LYS:HB3	6:SH:61:ILE:HB	2.03	0.40
7:SI:172:LEU:HD12	7:SI:190:LEU:HD13	2.03	0.40
8:SJ:52:LYS:HB3	8:SJ:52:LYS:HE2	1.71	0.40
10:SN:26:LEU:HD11	10:SN:60:VAL:HG12	2.03	0.40
16:Sa:38:LYS:HE2	16:Sa:38:LYS:HB3	1.91	0.40
17:Sb:32:PHE:HB3	17:Sb:82:LYS:HE3	2.03	0.40
17:Sb:45:THR:OG1	17:Sb:82:LYS:NZ	2.54	0.40
19:S2:888:U:O2'	19:S2:898:U:N3	2.52	0.40
19:S2:1425:G:H2'	19:S2:1426:U:C6	2.57	0.40
19:S2:1467:C:H2'	19:S2:1468:C:C6	2.56	0.40
19:S2:1491:G:HO2'	31:SU:70:CYS:HG	1.66	0.40
19:S2:1717:C:H2'	19:S2:1718:G:O4'	2.22	0.40
19:S2:1740:C:H2'	19:S2:1741:U:C6	2.56	0.40
20:LR:135:LYS:O	20:LR:136:ARG:C	2.64	0.40
20:LR:169:ALA:O	20:LR:173:ARG:HB2	2.21	0.40
20:LR:175:GLU:O	20:LR:178:GLN:HG3	2.20	0.40
22:SR:79:GLU:O	22:SR:83:ASN:HB2	2.22	0.40
24:SF:31:ASN:HD21	24:SF:117:ILE:HG21	1.86	0.40
24:SF:167:LYS:HG2	24:SF:171:GLU:HB2	2.02	0.40
31:SU:79:ARG:NH2	34:Sd:56:ASP:OXT	2.48	0.40
39:CI:63:ARG:HA	39:CI:63:ARG:HD2	1.93	0.40
40:L5:432:U:C2	87:L5:5292:SPM:H91	2.57	0.40
40:L5:937:U:H2'	40:L5:938:C:C6	2.57	0.40
40:L5:1360:G:P	53:LL:28:GLN:HE22	2.44	0.40
40:L5:1691:G:H5'	58:LQ:15:ARG:HG2	2.03	0.40
40:L5:1929:A:C8	40:L5:1932:A:H1'	2.57	0.40
40:L5:2414:G:H2'	40:L5:2415:U:C6	2.57	0.40
40:L5:2508:U:H2'	40:L5:2509:C:C6	2.57	0.40
40:L5:2522:G:H2'	40:L5:2523:G:C8	2.57	0.40
40:L5:2715:G:H2'	40:L5:2716:C:C6	2.57	0.40
40:L5:3650:C:C2	40:L5:3651:A:C8	3.10	0.40
40:L5:3729:U:H2'	40:L5:3730:U:H6	1.86	0.40
40:L5:3888:G:O6	56:LO:96:GLN:NE2	2.55	0.40
40:L5:4195:G:O2'	40:L5:4442:PSU:OP1	2.27	0.40
40:L5:4258:C:H2'	40:L5:4259:C:C6	2.56	0.40
40:L5:4477:A:H2'	40:L5:4478:G:H8	1.86	0.40
40:L5:4638:U:H2'	40:L5:4639:G:N3	2.37	0.40
40:L5:4773:C:H2'	40:L5:4774:C:C6	2.57	0.40
41:L7:7:G:H5''	46:LD:22:ARG:HD3	2.03	0.40
42:L8:52:A:H4'	77:LI:19:GLN:HA	2.04	0.40
43:LA:245:ARG:HA	43:LA:245:ARG:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:LE:223:ARG:HB3	47:LE:224:LYS:HB2	2.04	0.40
48:LF:36:LYS:HD3	48:LF:36:LYS:HA	1.76	0.40
76:Lk:5:ILE:HG21	76:Lk:11:PHE:HB2	2.04	0.40
76:Lk:55:LYS:HE2	76:Lk:55:LYS:HB3	1.87	0.40
83:Ls:120:GLU:OE2	83:Ls:122:THR:OG1	2.39	0.40
5:SG:151:ASP:OD1	21:LW:105:ARG:NH1	2.55	0.40
19:S2:375:U:H2'	19:S2:376:A:C8	2.55	0.40
19:S2:468:A2M:H2'	19:S2:469:A:O4'	2.21	0.40
19:S2:980:A:H2'	19:S2:981:A:H8	1.84	0.40
19:S2:1141:G:H2'	19:S2:1142:G:C8	2.57	0.40
19:S2:1424:G:N2	30:ST:3:GLY:HA3	2.36	0.40
19:S2:1443:C:H1'	28:SQ:22:VAL:HG21	2.04	0.40
19:S2:1558:C:H2'	19:S2:1559:C:C6	2.56	0.40
24:SF:88:MET:HA	24:SF:91:ARG:HG2	2.04	0.40
28:SQ:25:CYS:HB2	28:SQ:91:ALA:HB1	2.02	0.40
31:SU:99:LYS:HD3	31:SU:99:LYS:HA	1.84	0.40
38:Pt:71:A:H2'	38:Pt:72:C:C6	2.57	0.40
40:L5:214:G:H2'	40:L5:215:C:C6	2.56	0.40
40:L5:654:C:H3'	40:L5:655:C:H6	1.85	0.40
40:L5:1614:C:H2'	40:L5:1615:C:H6	1.87	0.40
40:L5:1951:G:H4'	59:LS:95:ARG:HH22	1.85	0.40
40:L5:2333:G:OP1	42:L8:20:A:O2'	2.40	0.40
40:L5:2540:C:H2'	40:L5:2541:G:C8	2.54	0.40
40:L5:2727:C:H2'	40:L5:2728:U:C6	2.56	0.40
40:L5:3723:A:H2'	40:L5:3724:A:C8	2.57	0.40
40:L5:4195:G:N2	51:LI:116:ARG:HA	2.37	0.40
40:L5:4667:C:H2'	40:L5:4668:U:O4'	2.22	0.40
42:L8:141:C:H2'	42:L8:142:U:H6	1.85	0.40
45:LC:180:ILE:HD11	45:LC:227:ILE:HD11	2.04	0.40
45:LC:349:LEU:HD23	45:LC:349:LEU:HA	1.96	0.40
46:LD:89:LYS:HE2	46:LD:229:ASN:HB2	2.04	0.40
47:LE:224:LYS:HB2	47:LE:224:LYS:HE2	1.95	0.40
54:LM:24:LEU:HD11	54:LM:86:TRP:CD2	2.57	0.40
62:LV:75:LYS:HE3	62:LV:77:HIS:CE1	2.57	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	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
2	SB	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
3	SC	218/222 (98%)	205 (94%)	13 (6%)	0	100	100
4	SE	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
5	SG	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
6	SH	182/189 (96%)	166 (91%)	16 (9%)	0	100	100
7	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
8	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
9	SL	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
10	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
11	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
12	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
13	SW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
14	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
15	SY	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
16	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
17	Sb	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
18	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
20	LR	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
21	LW	112/124 (90%)	110 (98%)	2 (2%)	0	100	100
22	SR	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	49
23	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
24	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
25	SK	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
26	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
28	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
29	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
30	ST	141/143 (99%)	140 (99%)	1 (1%)	0	100	100
31	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
32	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
33	Sc	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
34	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
35	Sf	65/67 (97%)	53 (82%)	12 (18%)	0	100	100
36	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
39	CI	29/31 (94%)	29 (100%)	0	0	100	100
43	LA	246/248 (99%)	235 (96%)	11 (4%)	0	100	100
44	LB	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
45	LC	366/368 (100%)	345 (94%)	21 (6%)	0	100	100
46	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
47	LE	236/250 (94%)	216 (92%)	20 (8%)	0	100	100
48	LF	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
49	LG	239/241 (99%)	228 (95%)	11 (5%)	0	100	100
50	LH	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
51	LI	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
52	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
53	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
54	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
55	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
56	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
57	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
58	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
59	LS	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
60	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
61	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
62	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
64	LY	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
65	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
66	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
67	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
68	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
69	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
70	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
71	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
72	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
73	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
74	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
75	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
76	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
77	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
78	Lm	50/52 (96%)	50 (100%)	0	0	100	100
79	Ln	22/24 (92%)	22 (100%)	0	0	100	100
80	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
81	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
82	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
83	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
84	Lt	128/157 (82%)	104 (81%)	24 (19%)	0	100	100
All	All	11672/11907 (98%)	11110 (95%)	561 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	SR	129	LYS

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	SA	183/183 (100%)	183 (100%)	0	100	100
2	SB	195/195 (100%)	195 (100%)	0	100	100
3	SC	186/188 (99%)	186 (100%)	0	100	100
4	SE	224/224 (100%)	224 (100%)	0	100	100
5	SG	207/207 (100%)	207 (100%)	0	100	100
6	SH	166/169 (98%)	166 (100%)	0	100	100
7	SI	178/178 (100%)	178 (100%)	0	100	100
8	SJ	161/161 (100%)	161 (100%)	0	100	100
9	SL	137/137 (100%)	137 (100%)	0	100	100
10	SN	130/130 (100%)	130 (100%)	0	100	100
11	SO	107/110 (97%)	107 (100%)	0	100	100
12	SV	67/67 (100%)	67 (100%)	0	100	100
13	SW	112/112 (100%)	112 (100%)	0	100	100
14	SX	113/113 (100%)	113 (100%)	0	100	100
15	SY	113/113 (100%)	113 (100%)	0	100	100
16	Sa	89/89 (100%)	89 (100%)	0	100	100
17	Sb	75/75 (100%)	75 (100%)	0	100	100
18	Se	47/47 (100%)	47 (100%)	0	100	100
20	LR	166/166 (100%)	164 (99%)	2 (1%)	63	73
21	LW	95/103 (92%)	95 (100%)	0	100	100
22	SR	122/122 (100%)	120 (98%)	2 (2%)	55	69
23	SD	190/190 (100%)	190 (100%)	0	100	100
24	SF	159/159 (100%)	159 (100%)	0	100	100
25	SK	89/89 (100%)	89 (100%)	0	100	100
26	SM	102/104 (98%)	102 (100%)	0	100	100
27	SP	107/107 (100%)	107 (100%)	0	100	100
28	SQ	119/119 (100%)	119 (100%)	0	100	100
29	SS	126/126 (100%)	126 (100%)	0	100	100
30	ST	113/113 (100%)	113 (100%)	0	100	100
31	SU	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	SZ	66/66 (100%)	66 (100%)	0	100	100
33	Sc	57/57 (100%)	57 (100%)	0	100	100
34	Sd	48/48 (100%)	48 (100%)	0	100	100
35	Sf	60/60 (100%)	60 (100%)	0	100	100
36	Sg	272/272 (100%)	272 (100%)	0	100	100
39	CI	25/25 (100%)	25 (100%)	0	100	100
43	LA	190/190 (100%)	190 (100%)	0	100	100
44	LB	348/348 (100%)	348 (100%)	0	100	100
45	LC	306/306 (100%)	306 (100%)	0	100	100
46	LD	246/247 (100%)	246 (100%)	0	100	100
47	LE	212/222 (96%)	212 (100%)	0	100	100
48	LF	194/194 (100%)	194 (100%)	0	100	100
49	LG	203/205 (99%)	203 (100%)	0	100	100
50	LH	169/169 (100%)	169 (100%)	0	100	100
51	LI	180/180 (100%)	180 (100%)	0	100	100
52	LJ	143/148 (97%)	143 (100%)	0	100	100
53	LL	176/176 (100%)	176 (100%)	0	100	100
54	LM	118/118 (100%)	118 (100%)	0	100	100
55	LN	171/171 (100%)	171 (100%)	0	100	100
56	LO	173/173 (100%)	173 (100%)	0	100	100
57	LP	134/134 (100%)	134 (100%)	0	100	100
58	LQ	164/164 (100%)	164 (100%)	0	100	100
59	LS	156/156 (100%)	156 (100%)	0	100	100
60	LT	139/139 (100%)	139 (100%)	0	100	100
61	LU	91/91 (100%)	91 (100%)	0	100	100
62	LV	101/101 (100%)	101 (100%)	0	100	100
63	LX	108/108 (100%)	108 (100%)	0	100	100
64	LY	124/124 (100%)	124 (100%)	0	100	100
65	LZ	117/117 (100%)	117 (100%)	0	100	100
66	La	120/120 (100%)	120 (100%)	0	100	100
67	Lb	88/101 (87%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Lc	83/83 (100%)	83 (100%)	0	100	100
69	Ld	98/98 (100%)	98 (100%)	0	100	100
70	Le	114/114 (100%)	114 (100%)	0	100	100
71	Lf	88/88 (100%)	88 (100%)	0	100	100
72	Lg	98/98 (100%)	98 (100%)	0	100	100
73	Lh	109/109 (100%)	109 (100%)	0	100	100
74	Li	86/86 (100%)	86 (100%)	0	100	100
75	Lj	73/73 (100%)	73 (100%)	0	100	100
76	Lk	64/64 (100%)	64 (100%)	0	100	100
77	Ll	47/47 (100%)	47 (100%)	0	100	100
78	Lm	48/48 (100%)	48 (100%)	0	100	100
79	Ln	23/23 (100%)	23 (100%)	0	100	100
80	Lo	93/93 (100%)	93 (100%)	0	100	100
81	Lp	74/74 (100%)	74 (100%)	0	100	100
82	Lr	109/109 (100%)	109 (100%)	0	100	100
83	Ls	162/164 (99%)	162 (100%)	0	100	100
84	Lt	107/130 (82%)	107 (100%)	0	100	100
All	All	10147/10221 (99%)	10143 (100%)	4 (0%)	100	100

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

Mol	Chain	Res	Type
20	LR	135	LYS
20	LR	137	ILE
22	SR	79	GLU
22	SR	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	SA	50	ASN
2	SB	75	GLN
2	SB	101	HIS
3	SC	115	GLN
4	SE	161	GLN

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Mol	Chain	Res	Type
6	SH	126	HIS
6	SH	162	GLN
7	SI	9	HIS
7	SI	52	ASN
8	SJ	177	ASN
13	SW	15	ASN
13	SW	98	GLN
14	SX	16	HIS
15	SY	124	ASN
16	Sa	17	HIS
18	Se	15	GLN
20	LR	39	GLN
20	LR	143	HIS
21	LW	48	GLN
24	SF	79	HIS
25	SK	7	ASN
26	SM	48	HIS
28	SQ	48	GLN
28	SQ	142	GLN
29	SS	72	GLN
29	SS	85	ASN
29	SS	97	GLN
30	ST	105	GLN
31	SU	85	HIS
32	SZ	46	ASN
32	SZ	112	ASN
34	Sd	37	ASN
36	Sg	285	GLN
43	LA	194	ASN
44	LB	184	GLN
45	LC	38	ASN
45	LC	119	GLN
45	LC	317	ASN
45	LC	347	HIS
45	LC	362	GLN
46	LD	267	ASN
46	LD	275	GLN
48	LF	205	ASN
48	LF	239	GLN
49	LG	82	GLN
49	LG	90	GLN
49	LG	94	GLN

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Mol	Chain	Res	Type
49	LG	112	GLN
50	LH	98	HIS
50	LH	102	ASN
50	LH	140	GLN
50	LH	188	GLN
50	LH	189	GLN
52	LJ	46	GLN
52	LJ	167	GLN
54	LM	34	ASN
54	LM	48	GLN
54	LM	66	HIS
55	LN	32	GLN
56	LO	14	HIS
56	LO	143	HIS
56	LO	199	HIS
57	LP	64	ASN
57	LP	75	GLN
57	LP	80	GLN
57	LP	120	ASN
58	LQ	21	GLN
60	LT	69	GLN
60	LT	127	GLN
60	LT	144	ASN
63	LX	57	GLN
63	LX	111	GLN
64	LY	14	ASN
65	LZ	76	ASN
65	LZ	78	ASN
66	La	19	HIS
66	La	34	ASN
66	La	40	HIS
68	Lc	51	ASN
70	Le	107	ASN
70	Le	124	ASN
71	Lf	21	GLN
72	Lg	114	GLN
73	Lh	20	GLN
75	Lj	13	ASN
75	Lj	28	HIS
75	Lj	66	HIS
82	Lr	30	ASN
83	Ls	58	ASN

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Mol	Chain	Res	Type
84	Lt	118	HIS
84	Lt	137	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S2	1715/1740 (98%)	408 (23%)	4 (0%)
37	At	69/71 (97%)	16 (23%)	0
38	Pt	72/74 (97%)	15 (20%)	0
40	L5	3643/3655 (99%)	816 (22%)	18 (0%)
41	L7	119/120 (99%)	16 (13%)	0
42	L8	155/156 (99%)	27 (17%)	0
All	All	5773/5816 (99%)	1298 (22%)	22 (0%)

All (1298) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S2	2	A
19	S2	3	C
19	S2	14	C
19	S2	25	A
19	S2	33	G
19	S2	37	C
19	S2	41	G
19	S2	42	A
19	S2	44	U
19	S2	45	A
19	S2	46	A
19	S2	49	C
19	S2	56	G
19	S2	62	G
19	S2	67	C
19	S2	68	A
19	S2	72	C
19	S2	73	C
19	S2	74	G
19	S2	76	U
19	S2	92	A
19	S2	99	A2M
19	S2	103	A
19	S2	113	G

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Mol	Chain	Res	Type
19	S2	114	G
19	S2	115	U
19	S2	126	G
19	S2	130	G
19	S2	142	C
19	S2	143	U
19	S2	149	A
19	S2	158	A
19	S2	160	U
19	S2	162	C
19	S2	168	C
19	S2	170	A
19	S2	175	A
19	S2	179	C
19	S2	188	C
19	S2	190	G
19	S2	196	C
19	S2	198	U
19	S2	200	G
19	S2	203	G
19	S2	207	G
19	S2	208	G
19	S2	214	U
19	S2	220	U
19	S2	288	G
19	S2	291	G
19	S2	292	A
19	S2	295	C
19	S2	302	A
19	S2	303	C
19	S2	306	C
19	S2	307	G
19	S2	308	G
19	S2	309	G
19	S2	311	C
19	S2	312	G
19	S2	318	A
19	S2	319	C
19	S2	323	C
19	S2	324	C
19	S2	325	C
19	S2	326	C

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Mol	Chain	Res	Type
19	S2	328	U
19	S2	329	G
19	S2	332	G
19	S2	335	G
19	S2	339	A
19	S2	340	C
19	S2	349	A
19	S2	351	G
19	S2	360	A
19	S2	361	U
19	S2	362	C
19	S2	364	A
19	S2	368	U
19	S2	369	C
19	S2	370	G
19	S2	381	C
19	S2	383	G
19	S2	385	G
19	S2	398	A
19	S2	407	G
19	S2	408	A
19	S2	409	C
19	S2	426	A
19	S2	448	A
19	S2	449	A
19	S2	450	C
19	S2	452	G
19	S2	464	A
19	S2	465	A
19	S2	471	G
19	S2	472	C
19	S2	473	A
19	S2	474	G
19	S2	476	A
19	S2	482	G
19	S2	487	U
19	S2	488	U
19	S2	492	C
19	S2	493	A
19	S2	502	C
19	S2	517	OMC
19	S2	531	A

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Mol	Chain	Res	Type
19	S2	532	C
19	S2	536	A
19	S2	537	C
19	S2	540	U
19	S2	542	U
19	S2	544	G
19	S2	546	G
19	S2	547	G
19	S2	551	U
19	S2	557	U
19	S2	558	G
19	S2	563	G
19	S2	564	A
19	S2	576	A2M
19	S2	583	A
19	S2	587	A
19	S2	589	G
19	S2	590	A
19	S2	591	U
19	S2	592	C
19	S2	604	A
19	S2	606	G
19	S2	607	U
19	S2	614	C
19	S2	617	G
19	S2	623	G
19	S2	628	A
19	S2	631	U
19	S2	638	C
19	S2	643	A
19	S2	644	OMG
19	S2	655	A
19	S2	660	C
19	S2	663	C
19	S2	664	A
19	S2	668	A2M
19	S2	669	A
19	S2	671	A
19	S2	672	A
19	S2	673	G
19	S2	683	OMG
19	S2	688	U

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Mol	Chain	Res	Type
19	S2	689	U
19	S2	692	G
19	S2	695	C
19	S2	696	G
19	S2	697	G
19	S2	732	U
19	S2	733	C
19	S2	738	C
19	S2	749	U
19	S2	750	C
19	S2	751	G
19	S2	752	G
19	S2	753	C
19	S2	788	G
19	S2	789	G
19	S2	791	C
19	S2	792	C
19	S2	797	C
19	S2	798	G
19	S2	799	OMU
19	S2	801	PSU
19	S2	809	A
19	S2	821	G
19	S2	822	U
19	S2	823	U
19	S2	824	C
19	S2	827	A
19	S2	830	A
19	S2	834	C
19	S2	835	C
19	S2	836	G
19	S2	837	A
19	S2	838	G
19	S2	839	C
19	S2	840	C
19	S2	842	C
19	S2	844	U
19	S2	847	A
19	S2	863	PSU
19	S2	867	OMG
19	S2	870	A
19	S2	874	G

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Mol	Chain	Res	Type
19	S2	877	C
19	S2	878	G
19	S2	880	G
19	S2	888	U
19	S2	889	U
19	S2	891	G
19	S2	894	G
19	S2	896	U
19	S2	897	U
19	S2	898	U
19	S2	899	U
19	S2	900	C
19	S2	901	G
19	S2	903	A
19	S2	912	C
19	S2	913	A
19	S2	917	U
19	S2	919	A
19	S2	920	A
19	S2	933	G
19	S2	950	C
19	S2	954	U
19	S2	963	A
19	S2	970	G
19	S2	971	G
19	S2	972	A
19	S2	982	G
19	S2	990	A
19	S2	992	A
19	S2	999	G
19	S2	1001	A
19	S2	1002	U
19	S2	1008	A
19	S2	1017	U
19	S2	1023	A
19	S2	1027	A
19	S2	1045	PSU
19	S2	1060	A
19	S2	1061	U
19	S2	1062	A
19	S2	1067	C
19	S2	1078	C

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Mol	Chain	Res	Type
19	S2	1083	A
19	S2	1085	C
19	S2	1108	G
19	S2	1109	C
19	S2	1113	A
19	S2	1116	C
19	S2	1118	C
19	S2	1119	A
19	S2	1121	G
19	S2	1123	C
19	S2	1133	A
19	S2	1138	C
19	S2	1149	A
19	S2	1150	A
19	S2	1153	C
19	S2	1154	U
19	S2	1161	U
19	S2	1195	A
19	S2	1200	A
19	S2	1207	G
19	S2	1208	A
19	S2	1215	C
19	S2	1216	C
19	S2	1217	A
19	S2	1220	A
19	S2	1224	G
19	S2	1227	G
19	S2	1240	A
19	S2	1242	U
19	S2	1243	U
19	S2	1248	B8N
19	S2	1251	A
19	S2	1253	A
19	S2	1256	G
19	S2	1257	G
19	S2	1264	C
19	S2	1271	C
19	S2	1272	OMC
19	S2	1274	G
19	S2	1275	G
19	S2	1281	G
19	S2	1282	A

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Mol	Chain	Res	Type
19	S2	1283	C
19	S2	1285	G
19	S2	1286	G
19	S2	1288	OMU
19	S2	1290	G
19	S2	1294	G
19	S2	1295	A
19	S2	1298	G
19	S2	1301	A
19	S2	1302	G
19	S2	1303	C
19	S2	1304	U
19	S2	1308	U
19	S2	1320	G
19	S2	1333	U
19	S2	1342	U
19	S2	1354	G
19	S2	1357	A
19	S2	1358	U
19	S2	1371	U
19	S2	1372	U
19	S2	1375	G
19	S2	1376	A
19	S2	1378	A
19	S2	1382	A
19	S2	1401	A
19	S2	1402	A
19	S2	1406	G
19	S2	1408	U
19	S2	1413	G
19	S2	1414	A
19	S2	1418	C
19	S2	1419	C
19	S2	1420	G
19	S2	1421	A
19	S2	1422	G
19	S2	1423	C
19	S2	1428	G
19	S2	1432	U
19	S2	1433	C
19	S2	1435	C
19	S2	1436	C

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Mol	Chain	Res	Type
19	S2	1437	C
19	S2	1438	A
19	S2	1442	OMU
19	S2	1449	G
19	S2	1454	A
19	S2	1455	A
19	S2	1462	U
19	S2	1463	U
19	S2	1464	C
19	S2	1480	A
19	S2	1489	A
19	S2	1490	OMG
19	S2	1492	U
19	S2	1494	U
19	S2	1497	G
19	S2	1498	A
19	S2	1507	G
19	S2	1509	U
19	S2	1520	G
19	S2	1521	C
19	S2	1531	A
19	S2	1533	A
19	S2	1534	C
19	S2	1544	C
19	S2	1547	C
19	S2	1552	G
19	S2	1555	U
19	S2	1556	A
19	S2	1558	C
19	S2	1560	U
19	S2	1573	G
19	S2	1574	C
19	S2	1580	A
19	S2	1581	C
19	S2	1585	U
19	S2	1587	G
19	S2	1588	A
19	S2	1598	G
19	S2	1600	G
19	S2	1604	G
19	S2	1606	G
19	S2	1621	U

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Mol	Chain	Res	Type
19	S2	1623	A
19	S2	1633	A
19	S2	1634	A
19	S2	1637	A
19	S2	1639	G7M
19	S2	1648	G
19	S2	1654	G
19	S2	1656	G
19	S2	1663	A
19	S2	1664	A
19	S2	1665	G
19	S2	1683	C
19	S2	1695	A
19	S2	1699	A
19	S2	1715	A
19	S2	1721	U
19	S2	1722	G
19	S2	1744	G
19	S2	1745	A
19	S2	1752	C
19	S2	1753	C
19	S2	1754	G
19	S2	1755	C
19	S2	1757	G
19	S2	1758	G
19	S2	1759	G
19	S2	1761	U
19	S2	1772	C
19	S2	1773	C
19	S2	1774	C
19	S2	1777	G
19	S2	1783	C
19	S2	1784	G
19	S2	1786	U
19	S2	1798	C
19	S2	1810	U
19	S2	1819	A
19	S2	1824	A
19	S2	1825	A
19	S2	1835	A
19	S2	1838	U
19	S2	1849	G

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Mol	Chain	Res	Type
19	S2	1851	MA6
19	S2	1861	G
19	S2	1862	G
19	S2	1863	A
19	S2	1864	U
19	S2	1865	C
37	At	8	U
37	At	9	A
37	At	10	G
37	At	14	A
37	At	21	A
37	At	22	U
37	At	26	G
37	At	36	C
37	At	47	U
37	At	48	C
37	At	49	C
37	At	58	A
37	At	60	A
37	At	61	C
37	At	63	G
37	At	67	G
38	Pt	8	U
38	Pt	9	A
38	Pt	13	U
38	Pt	21	A
38	Pt	31	C
38	Pt	46	G
38	Pt	47	U
38	Pt	48	C
38	Pt	49	C
38	Pt	58	A
38	Pt	67	G
38	Pt	71	A
38	Pt	72	C
38	Pt	74	C
38	Pt	76	A
40	L5	25	A
40	L5	30	C
40	L5	39	A
40	L5	42	A
40	L5	48	G

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Mol	Chain	Res	Type
40	L5	56	A
40	L5	59	A
40	L5	64	A
40	L5	65	A
40	L5	73	A
40	L5	91	G
40	L5	104	G
40	L5	109	G
40	L5	110	C
40	L5	116	G
40	L5	119	G
40	L5	120	A
40	L5	122	U
40	L5	127	G
40	L5	132	G
40	L5	133	C
40	L5	134	G
40	L5	135	G
40	L5	136	C
40	L5	144	G
40	L5	159	C
40	L5	164	G
40	L5	165	A
40	L5	171	U
40	L5	172	C
40	L5	176	G
40	L5	182	G
40	L5	183	C
40	L5	184	U
40	L5	185	C
40	L5	186	G
40	L5	188	G
40	L5	197	A
40	L5	200	U
40	L5	209	U
40	L5	213	G
40	L5	216	C
40	L5	218	A
40	L5	220	C
40	L5	233	U
40	L5	234	G
40	L5	235	A

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Mol	Chain	Res	Type
40	L5	255	C
40	L5	256	G
40	L5	261	G
40	L5	264	C
40	L5	265	C
40	L5	266	C
40	L5	267	G
40	L5	275	C
40	L5	280	G
40	L5	297	U
40	L5	306	A
40	L5	310	G
40	L5	315	G
40	L5	316	U
40	L5	340	C
40	L5	357	U
40	L5	373	G
40	L5	387	G
40	L5	388	A
40	L5	396	A
40	L5	399	G
40	L5	407	A
40	L5	409	G
40	L5	410	A
40	L5	412	G
40	L5	413	G
40	L5	431	G
40	L5	432	U
40	L5	440	U
40	L5	446	C
40	L5	449	C
40	L5	450	G
40	L5	452	A
40	L5	453	G
40	L5	454	U
40	L5	456	C
40	L5	457	G
40	L5	465	G
40	L5	467	U
40	L5	479	G
40	L5	484	U
40	L5	485	C

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Mol	Chain	Res	Type
40	L5	486	C
40	L5	489	C
40	L5	494	U
40	L5	495	C
40	L5	496	G
40	L5	497	G
40	L5	498	C
40	L5	502	C
40	L5	503	C
40	L5	504	G
40	L5	505	G
40	L5	509	A
40	L5	510	U
40	L5	512	U
40	L5	513	U
40	L5	514	U
40	L5	516	C
40	L5	517	C
40	L5	518	G
40	L5	519	C
40	L5	643	C
40	L5	654	C
40	L5	655	C
40	L5	656	C
40	L5	657	C
40	L5	658	C
40	L5	659	G
40	L5	666	G
40	L5	667	A
40	L5	668	C
40	L5	672	C
40	L5	673	C
40	L5	682	G
40	L5	686	A
40	L5	687	U
40	L5	696	C
40	L5	704	C
40	L5	708	G
40	L5	719	C
40	L5	731	G
40	L5	738	C
40	L5	739	G

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Mol	Chain	Res	Type
40	L5	742	G
40	L5	758	G
40	L5	759	G
40	L5	904	C
40	L5	905	C
40	L5	911	U
40	L5	912	G
40	L5	913	U
40	L5	914	U
40	L5	915	A
40	L5	917	A
40	L5	923	C
40	L5	924	C
40	L5	926	G
40	L5	927	G
40	L5	932	A
40	L5	933	G
40	L5	935	A
40	L5	936	C
40	L5	941	C
40	L5	943	A
40	L5	945	U
40	L5	956	A
40	L5	959	G
40	L5	960	A
40	L5	961	G
40	L5	962	C
40	L5	965	G
40	L5	966	A
40	L5	967	C
40	L5	968	C
40	L5	969	C
40	L5	970	G
40	L5	982	U
40	L5	985	C
40	L5	986	C
40	L5	989	U
40	L5	1070	G
40	L5	1071	C
40	L5	1072	C
40	L5	1075	G
40	L5	1076	C

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Mol	Chain	Res	Type
40	L5	1082	C
40	L5	1083	U
40	L5	1095	A
40	L5	1168	G
40	L5	1169	G
40	L5	1171	G
40	L5	1172	C
40	L5	1173	G
40	L5	1175	A
40	L5	1177	U
40	L5	1179	U
40	L5	1180	C
40	L5	1181	C
40	L5	1182	C
40	L5	1183	C
40	L5	1184	A
40	L5	1187	G
40	L5	1189	G
40	L5	1200	G
40	L5	1202	C
40	L5	1203	G
40	L5	1205	G
40	L5	1210	C
40	L5	1211	G
40	L5	1215	C
40	L5	1218	G
40	L5	1219	G
40	L5	1222	A
40	L5	1242	G
40	L5	1246	G
40	L5	1247	U
40	L5	1253	G
40	L5	1254	A
40	L5	1256	G
40	L5	1257	A
40	L5	1258	G
40	L5	1263	A
40	L5	1266	G
40	L5	1267	C
40	L5	1269	G
40	L5	1270	A
40	L5	1271	G

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Mol	Chain	Res	Type
40	L5	1272	C
40	L5	1273	G
40	L5	1275	G
40	L5	1280	C
40	L5	1284	G
40	L5	1287	G
40	L5	1294	A
40	L5	1295	C
40	L5	1296	G
40	L5	1301	C
40	L5	1314	C
40	L5	1326	A2M
40	L5	1344	C
40	L5	1354	A
40	L5	1359	G
40	L5	1364	U
40	L5	1365	C
40	L5	1366	G
40	L5	1367	C
40	L5	1370	G
40	L5	1379	C
40	L5	1381	U
40	L5	1387	A
40	L5	1394	G
40	L5	1398	A
40	L5	1399	G
40	L5	1404	G
40	L5	1407	C
40	L5	1408	G
40	L5	1409	C
40	L5	1410	U
40	L5	1415	G
40	L5	1417	C
40	L5	1420	A
40	L5	1433	A
40	L5	1437	C
40	L5	1438	U
40	L5	1439	C
40	L5	1442	C
40	L5	1443	A
40	L5	1444	G
40	L5	1445	U

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Mol	Chain	Res	Type
40	L5	1446	C
40	L5	1447	C
40	L5	1457	G
40	L5	1465	G
40	L5	1472	C
40	L5	1482	G
40	L5	1483	C
40	L5	1497	A
40	L5	1498	G
40	L5	1502	G
40	L5	1517	G
40	L5	1523	A
40	L5	1524	A2M
40	L5	1534	A2M
40	L5	1536	PSU
40	L5	1537	A
40	L5	1547	A
40	L5	1562	G
40	L5	1566	C
40	L5	1574	G
40	L5	1578	U
40	L5	1591	U
40	L5	1596	U
40	L5	1597	G
40	L5	1624	G
40	L5	1625	OMG
40	L5	1631	A
40	L5	1633	G
40	L5	1634	A
40	L5	1641	G
40	L5	1654	G
40	L5	1660	U
40	L5	1661	C
40	L5	1676	C
40	L5	1677	PSU
40	L5	1680	G
40	L5	1697	G
40	L5	1699	A
40	L5	1700	G
40	L5	1701	A
40	L5	1702	C
40	L5	1703	C

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Mol	Chain	Res	Type
40	L5	1704	C
40	L5	1705	G
40	L5	1718	C
40	L5	1719	A
40	L5	1721	G
40	L5	1729	A
40	L5	1731	C
40	L5	1742	A
40	L5	1757	U
40	L5	1758	G
40	L5	1760	G
40	L5	1761	G
40	L5	1763	C
40	L5	1764	G
40	L5	1765	A
40	L5	1766	A
40	L5	1767	A
40	L5	1768	C
40	L5	1770	A
40	L5	1787	A
40	L5	1803	G
40	L5	1804	A
40	L5	1806	G
40	L5	1810	G
40	L5	1815	G
40	L5	1820	C
40	L5	1821	G
40	L5	1822	U
40	L5	1833	G
40	L5	1836	G
40	L5	1837	A
40	L5	1842	G
40	L5	1855	G
40	L5	1869	G
40	L5	1888	A
40	L5	1893	C
40	L5	1897	A
40	L5	1916	G
40	L5	1917	A
40	L5	1918	U
40	L5	1919	G
40	L5	1920	C

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Mol	Chain	Res	Type
40	L5	1921	C
40	L5	1922	G
40	L5	1925	G
40	L5	1931	C
40	L5	1932	A
40	L5	1936	C
40	L5	1938	C
40	L5	1948	G
40	L5	1961	G
40	L5	1962	A
40	L5	1965	G
40	L5	1967	A
40	L5	1971	C
40	L5	1972	G
40	L5	1974	U
40	L5	1975	G
40	L5	1978	C
40	L5	1980	U
40	L5	1982	G
40	L5	1983	A
40	L5	1984	A
40	L5	1985	G
40	L5	1986	U
40	L5	1987	C
40	L5	1989	G
40	L5	1991	A
40	L5	1992	U
40	L5	1995	G
40	L5	1997	U
40	L5	1998	A
40	L5	1999	A
40	L5	2001	G
40	L5	2002	A
40	L5	2003	G
40	L5	2011	C
40	L5	2014	C
40	L5	2017	A
40	L5	2018	C
40	L5	2024	G
40	L5	2025	A
40	L5	2026	A
40	L5	2046	G

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Mol	Chain	Res	Type
40	L5	2048	U
40	L5	2052	G
40	L5	2055	G
40	L5	2056	G
40	L5	2069	A
40	L5	2084	C
40	L5	2085	G
40	L5	2092	G
40	L5	2093	A
40	L5	2094	G
40	L5	2095	A
40	L5	2097	U
40	L5	2098	G
40	L5	2100	A
40	L5	2102	G
40	L5	2103	G
40	L5	2105	A
40	L5	2107	C
40	L5	2110	C
40	L5	2112	G
40	L5	2250	C
40	L5	2252	G
40	L5	2253	A
40	L5	2256	C
40	L5	2258	C
40	L5	2259	G
40	L5	2261	G
40	L5	2262	G
40	L5	2289	C
40	L5	2300	A
40	L5	2301	G
40	L5	2313	A
40	L5	2316	G
40	L5	2322	G
40	L5	2331	G
40	L5	2333	G
40	L5	2348	G
40	L5	2351	OMC
40	L5	2360	A
40	L5	2389	A
40	L5	2395	A
40	L5	2397	G

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Mol	Chain	Res	Type
40	L5	2398	U
40	L5	2402	G
40	L5	2410	C
40	L5	2417	A
40	L5	2425	U
40	L5	2453	A
40	L5	2464	C
40	L5	2465	C
40	L5	2469	C
40	L5	2470	C
40	L5	2471	G
40	L5	2474	G
40	L5	2475	G
40	L5	2478	C
40	L5	2479	G
40	L5	2483	G
40	L5	2484	A
40	L5	2485	U
40	L5	2487	G
40	L5	2488	C
40	L5	2489	C
40	L5	2490	U
40	L5	2504	C
40	L5	2505	C
40	L5	2506	G
40	L5	2507	A
40	L5	2513	A
40	L5	2519	U
40	L5	2537	A
40	L5	2544	G
40	L5	2546	G
40	L5	2547	G
40	L5	2554	U
40	L5	2555	G
40	L5	2559	G
40	L5	2560	C
40	L5	2565	A
40	L5	2581	A
40	L5	2583	C
40	L5	2586	G
40	L5	2587	A
40	L5	2589	C

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Mol	Chain	Res	Type
40	L5	2601	A
40	L5	2607	C
40	L5	2618	G
40	L5	2627	C
40	L5	2643	G
40	L5	2653	C
40	L5	2658	G
40	L5	2662	G
40	L5	2669	C
40	L5	2673	G
40	L5	2675	G
40	L5	2676	A
40	L5	2686	G
40	L5	2687	U
40	L5	2694	G
40	L5	2695	A
40	L5	2696	A
40	L5	2702	C
40	L5	2703	G
40	L5	2706	G
40	L5	2708	U
40	L5	2709	C
40	L5	2711	G
40	L5	2719	C
40	L5	2721	G
40	L5	2724	G
40	L5	2726	G
40	L5	2739	C
40	L5	2742	G
40	L5	2743	A
40	L5	2754	G
40	L5	2759	G
40	L5	2761	U
40	L5	2763	U
40	L5	2769	U
40	L5	2770	C
40	L5	2788	U
40	L5	2790	U
40	L5	2794	C
40	L5	2799	G
40	L5	2806	A
40	L5	2812	A

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Mol	Chain	Res	Type
40	L5	2814	C
40	L5	2826	U
40	L5	2827	G
40	L5	2828	U
40	L5	2829	U
40	L5	2833	A
40	L5	2835	A
40	L5	2855	G
40	L5	2877	G
40	L5	2895	A
40	L5	2900	U
40	L5	2902	G
40	L5	2903	G
40	L5	2904	U
40	L5	2905	C
40	L5	2906	G
40	L5	2907	G
40	L5	2908	U
40	L5	3588	C
40	L5	3590	G
40	L5	3591	C
40	L5	3592	G
40	L5	3594	C
40	L5	3595	U
40	L5	3596	A
40	L5	3597	G
40	L5	3599	A
40	L5	3604	A
40	L5	3605	C
40	L5	3615	G
40	L5	3616	U
40	L5	3617	G
40	L5	3626	G
40	L5	3630	A
40	L5	3635	A
40	L5	3643	A
40	L5	3644	U
40	L5	3646	A
40	L5	3652	A
40	L5	3662	A
40	L5	3664	G
40	L5	3673	C

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Mol	Chain	Res	Type
40	L5	3674	G
40	L5	3680	U
40	L5	3698	G
40	L5	3701	OMC
40	L5	3710	G
40	L5	3711	A
40	L5	3726	A
40	L5	3727	A
40	L5	3746	A
40	L5	3748	A
40	L5	3753	G
40	L5	3760	A
40	L5	3764	U
40	L5	3770	U
40	L5	3771	C
40	L5	3774	A
40	L5	3775	A
40	L5	3776	G
40	L5	3777	G
40	L5	3778	U
40	L5	3785	A2M
40	L5	3786	U
40	L5	3792	OMG
40	L5	3811	G
40	L5	3812	C
40	L5	3817	A
40	L5	3819	G
40	L5	3822	PSU
40	L5	3824	A
40	L5	3838	U
40	L5	3840	U
40	L5	3876	A
40	L5	3877	A
40	L5	3878	C
40	L5	3879	G
40	L5	3890	A
40	L5	3892	U
40	L5	3897	G
40	L5	3898	G
40	L5	3901	A
40	L5	3906	A
40	L5	3907	G

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Mol	Chain	Res	Type
40	L5	3908	A
40	L5	3915	U
40	L5	3938	G
40	L5	3939	G
40	L5	3942	A
40	L5	3943	A
40	L5	3944	G
40	L5	3946	G
40	L5	3947	A
40	L5	3948	C
40	L5	3949	A
40	L5	3950	U
40	L5	3952	A
40	L5	4057	C
40	L5	4058	U
40	L5	4059	C
40	L5	4060	U
40	L5	4062	A
40	L5	4064	C
40	L5	4065	G
40	L5	4068	U
40	L5	4069	U
40	L5	4076	G
40	L5	4093	G
40	L5	4095	G
40	L5	4096	C
40	L5	4097	G
40	L5	4098	A
40	L5	4099	G
40	L5	4104	G
40	L5	4105	A
40	L5	4107	G
40	L5	4108	G
40	L5	4111	U
40	L5	4112	C
40	L5	4114	C
40	L5	4115	G
40	L5	4116	C
40	L5	4121	G
40	L5	4122	G
40	L5	4125	C
40	L5	4127	A

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Mol	Chain	Res	Type
40	L5	4133	C
40	L5	4140	C
40	L5	4141	G
40	L5	4142	C
40	L5	4143	G
40	L5	4144	C
40	L5	4145	C
40	L5	4146	G
40	L5	4156	G
40	L5	4162	C
40	L5	4163	U
40	L5	4170	A
40	L5	4183	G
40	L5	4184	G
40	L5	4191	G
40	L5	4203	A
40	L5	4212	A
40	L5	4219	A
40	L5	4220	6MZ
40	L5	4222	G
40	L5	4229	U
40	L5	4232	U
40	L5	4233	A
40	L5	4234	A
40	L5	4241	C
40	L5	4243	C
40	L5	4249	G
40	L5	4251	A
40	L5	4254	G
40	L5	4257	A
40	L5	4258	C
40	L5	4265	U
40	L5	4268	A
40	L5	4273	A
40	L5	4279	A
40	L5	4280	A
40	L5	4287	G
40	L5	4291	G
40	L5	4295	U
40	L5	4304	A
40	L5	4305	G
40	L5	4306	OMU

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Mol	Chain	Res	Type
40	L5	4314	C
40	L5	4319	C
40	L5	4326	G
40	L5	4329	G
40	L5	4330	G
40	L5	4332	C
40	L5	4349	C
40	L5	4350	C
40	L5	4354	U
40	L5	4373	G
40	L5	4377	G
40	L5	4378	A
40	L5	4379	A
40	L5	4381	A
40	L5	4387	C
40	L5	4394	A
40	L5	4422	A
40	L5	4438	U
40	L5	4444	C
40	L5	4447	5MC
40	L5	4448	G
40	L5	4449	A
40	L5	4464	A
40	L5	4466	C
40	L5	4475	G
40	L5	4488	A
40	L5	4500	PSU
40	L5	4512	U
40	L5	4513	A
40	L5	4519	C
40	L5	4523	A2M
40	L5	4524	G
40	L5	4528	G
40	L5	4545	G
40	L5	4548	A
40	L5	4549	G
40	L5	4560	C
40	L5	4569	U
40	L5	4575	G
40	L5	4581	G
40	L5	4584	A
40	L5	4590	A2M

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Mol	Chain	Res	Type
40	L5	4599	A
40	L5	4601	U
40	L5	4610	A
40	L5	4618	OMG
40	L5	4635	A
40	L5	4636	PSU
40	L5	4637	OMG
40	L5	4652	G
40	L5	4656	A
40	L5	4670	C
40	L5	4671	C
40	L5	4672	A
40	L5	4693	C
40	L5	4694	G
40	L5	4695	C
40	L5	4700	A
40	L5	4707	A
40	L5	4708	A
40	L5	4709	U
40	L5	4719	G
40	L5	4734	A
40	L5	4740	G
40	L5	4741	C
40	L5	4742	G
40	L5	4745	G
40	L5	4750	G
40	L5	4754	G
40	L5	4757	C
40	L5	4759	C
40	L5	4761	G
40	L5	4765	G
40	L5	4771	C
40	L5	4772	C
40	L5	4775	C
40	L5	4776	G
40	L5	4859	C
40	L5	4860	G
40	L5	4862	G
40	L5	4864	U
40	L5	4867	G
40	L5	4870	G
40	L5	4871	C

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Mol	Chain	Res	Type
40	L5	4875	G
40	L5	4876	U
40	L5	4877	G
40	L5	4881	U
40	L5	4882	U
40	L5	4883	C
40	L5	4889	G
40	L5	4895	C
40	L5	4896	G
40	L5	4898	G
40	L5	4899	G
40	L5	4900	C
40	L5	4901	G
40	L5	4910	G
40	L5	4912	G
40	L5	4914	C
40	L5	4923	C
40	L5	4925	U
40	L5	4927	G
40	L5	4928	C
40	L5	4934	A
40	L5	4937	C
40	L5	4940	C
40	L5	4941	G
40	L5	4943	A
40	L5	4944	C
40	L5	4951	G
40	L5	4960	G
40	L5	4963	G
40	L5	4976	U
40	L5	4985	U
40	L5	4988	U
40	L5	4989	U
40	L5	4990	C
40	L5	4991	U
40	L5	4995	U
40	L5	5006	U
40	L5	5013	C
40	L5	5014	A
40	L5	5017	G
40	L5	5020	G
40	L5	5023	C

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Mol	Chain	Res	Type
40	L5	5024	C
40	L5	5027	C
40	L5	5028	G
40	L5	5030	U
40	L5	5034	A
40	L5	5041	G
40	L5	5050	C
40	L5	5054	C
40	L5	5055	G
40	L5	5058	A
40	L5	5061	A
40	L5	5062	G
40	L5	5069	U
41	L7	7	G
41	L7	11	A
41	L7	22	A
41	L7	24	C
41	L7	37	G
41	L7	38	U
41	L7	53	U
41	L7	63	C
41	L7	64	G
41	L7	89	G
41	L7	91	C
41	L7	97	G
41	L7	100	A
41	L7	102	U
41	L7	110	G
41	L7	111	C
42	L8	34	U
42	L8	35	C
42	L8	38	U
42	L8	52	A
42	L8	59	A
42	L8	62	A
42	L8	63	U
42	L8	80	A
42	L8	82	A
42	L8	83	C
42	L8	84	A
42	L8	85	U
42	L8	86	U

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Mol	Chain	Res	Type
42	L8	87	G
42	L8	94	G
42	L8	103	A
42	L8	105	C
42	L8	111	U
42	L8	114	G
42	L8	123	U
42	L8	124	U
42	L8	125	C
42	L8	126	C
42	L8	127	U
42	L8	147	G
42	L8	150	C
42	L8	151	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	S2	291	G
19	S2	531	A
19	S2	563	G
19	S2	688	U
40	L5	183	C
40	L5	406	C
40	L5	914	U
40	L5	1082	C
40	L5	1176	C
40	L5	1366	G
40	L5	1633	G
40	L5	1977	C
40	L5	2416	G
40	L5	2675	G
40	L5	2760	G
40	L5	3673	C
40	L5	3726	A
40	L5	3951	G
40	L5	4447	5MC
40	L5	4600	G
40	L5	4699	U
40	L5	4913	G

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$
19	OMC	S2	517	19	19,22,23	0.53	0	25,31,34	0.73	0
40	A2M	L5	1871	40,86	22,25,26	1.25	1 (4%)	30,36,39	1.59	6 (20%)
19	PSU	S2	406	19	18,21,22	1.15	1 (5%)	21,30,33	1.94	5 (23%)
19	MA6	S2	1851	19	23,26,27	1.26	2 (8%)	33,38,41	3.36	12 (36%)
40	PSU	L5	4471	40	18,21,22	1.08	1 (5%)	21,30,33	1.78	4 (19%)
19	OMU	S2	354	19	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
19	OMG	S2	1328	19	23,26,27	0.46	0	32,38,41	0.42	0
19	PSU	S2	801	19	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
19	OMG	S2	509	19	23,26,27	0.48	0	32,38,41	0.48	0
42	PSU	L8	55	42	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
40	PSU	L5	4973	40	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
40	A2M	L5	1524	40	22,25,26	1.28	2 (9%)	30,36,39	1.51	8 (26%)
40	5MC	L5	3782	40,86	19,22,23	0.53	0	26,32,35	0.75	0
42	PSU	L8	69	42	18,21,22	1.09	1 (5%)	21,30,33	1.82	5 (23%)
40	PSU	L5	1683	40	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
19	PSU	S2	93	19	18,21,22	1.09	1 (5%)	21,30,33	1.82	4 (19%)
40	OMU	L5	3925	40	19,22,23	3.36	7 (36%)	25,31,34	1.84	5 (20%)
19	PSU	S2	651	19	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	OMC	L5	4456	40	19,22,23	0.56	0	25,31,34	0.81	1 (4%)
19	OMC	S2	462	19	19,22,23	0.52	0	25,31,34	0.72	0
40	OMC	L5	3869	40	19,22,23	0.54	0	25,31,34	0.60	0
19	PSU	S2	1045	19	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
40	PSU	L5	4636	40	18,21,22	1.14	1 (5%)	21,30,33	1.95	6 (28%)
40	PSU	L5	4628	40	18,21,22	1.06	1 (5%)	21,30,33	1.89	5 (23%)
19	OMU	S2	172	19	19,22,23	3.37	7 (36%)	25,31,34	1.83	4 (16%)
19	PSU	S2	686	19	18,21,22	1.16	1 (5%)	21,30,33	1.89	4 (19%)
19	OMU	S2	1442	19	19,22,23	3.41	7 (36%)	25,31,34	1.81	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	A2M	S2	1031	19	22,25,26	1.23	1 (4%)	30,36,39	1.50	8 (26%)
40	A2M	L5	2363	40,86	22,25,26	1.21	1 (4%)	30,36,39	1.52	8 (26%)
40	OMC	L5	2351	40,86	19,22,23	0.52	0	25,31,34	0.72	1 (4%)
19	OMU	S2	428	19	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
40	OMG	L5	4228	40	23,26,27	0.49	0	32,38,41	0.57	0
19	OMC	S2	1703	19	19,22,23	0.51	0	25,31,34	0.70	0
40	PSU	L5	4296	40	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
40	PSU	L5	4532	40	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
40	OMG	L5	3627	40	23,26,27	0.48	0	32,38,41	0.65	0
40	OMG	L5	4392	40	23,26,27	0.46	0	32,38,41	0.48	0
19	4AC	S2	1337	19	21,24,25	0.37	0	28,34,37	0.72	1 (3%)
40	PSU	L5	3851	40	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
19	PSU	S2	1177	19	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
40	OMC	L5	1340	40	19,22,23	0.55	0	25,31,34	0.68	0
40	OMG	L5	2876	40	23,26,27	0.50	0	32,38,41	0.47	0
19	PSU	S2	863	19	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
19	6MZ	S2	1832	19,86	22,25,26	3.99	11 (50%)	29,36,39	2.37	12 (41%)
40	PSU	L5	4576	40	18,21,22	1.11	1 (5%)	21,30,33	1.85	5 (23%)
40	PSU	L5	5001	40	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
40	OMC	L5	3841	40	19,22,23	0.51	0	25,31,34	0.58	0
40	OMC	L5	2422	40,86	19,22,23	0.58	0	25,31,34	0.83	0
40	A2M	L5	3867	40	22,25,26	1.25	1 (4%)	30,36,39	1.52	8 (26%)
40	PSU	L5	3639	40	18,21,22	1.13	1 (5%)	21,30,33	1.92	5 (23%)
40	OMG	L5	3899	40	23,26,27	0.49	0	32,38,41	0.51	0
40	A2M	L5	400	40	22,25,26	1.25	1 (4%)	30,36,39	1.54	6 (20%)
40	PSU	L5	4500	40	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
19	A2M	S2	99	19,86	22,25,26	1.23	1 (4%)	30,36,39	1.54	7 (23%)
40	OMU	L5	4306	40	19,22,23	3.36	7 (36%)	25,31,34	1.80	4 (16%)
40	PSU	L5	3637	40	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
40	PSU	L5	1744	40,86	18,21,22	1.11	1 (5%)	21,30,33	1.86	5 (23%)
40	PSU	L5	4457	40	18,21,22	1.09	1 (5%)	21,30,33	1.86	5 (23%)
40	PSU	L5	1677	40	18,21,22	1.11	1 (5%)	21,30,33	2.08	6 (28%)
19	OMC	S2	1272	19	19,22,23	0.53	0	25,31,34	0.73	0
40	PSU	L5	2839	40	18,21,22	1.13	1 (5%)	21,30,33	1.83	4 (19%)
40	OMC	L5	3808	40,86	19,22,23	0.56	0	25,31,34	0.89	2 (8%)
19	A2M	S2	1383	19	22,25,26	1.23	1 (4%)	30,36,39	1.61	6 (20%)
40	PSU	L5	4361	40	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	OMU	L5	4620	40	19,22,23	3.33	7 (36%)	25,31,34	1.74	4 (16%)
40	PSU	L5	3920	40,86	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
40	PSU	L5	5010	40	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	3884	40	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
40	1MA	L5	1322	40	21,25,26	0.51	0	30,37,40	0.77	1 (3%)
19	OMU	S2	121	19	19,22,23	3.36	7 (36%)	25,31,34	1.76	5 (20%)
40	A2M	L5	1323	40	22,25,26	1.22	1 (4%)	30,36,39	1.55	9 (30%)
40	PSU	L5	4431	40	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
40	OMG	L5	3744	40	23,26,27	0.47	0	32,38,41	0.46	0
19	PSU	S2	1232	19	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
40	PSU	L5	1862	40	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	4293	40	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
40	OMG	L5	2364	40,86	23,26,27	0.47	0	32,38,41	0.46	0
19	B8N	S2	1248	19	25,29,30	3.28	6 (24%)	28,42,45	1.96	8 (28%)
40	PSU	L5	1860	40	18,21,22	1.13	1 (5%)	21,30,33	1.89	4 (19%)
40	A2M	L5	3830	40	22,25,26	1.23	1 (4%)	30,36,39	1.55	7 (23%)
40	OMG	L5	4618	40	23,26,27	0.50	0	32,38,41	0.46	0
40	PSU	L5	1582	40	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
40	PSU	L5	4552	40	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
40	A2M	L5	3718	40	22,25,26	1.22	1 (4%)	30,36,39	1.57	7 (23%)
19	PSU	S2	1244	19	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	OMG	L5	4499	40	23,26,27	0.46	0	32,38,41	0.53	0
19	PSU	S2	105	19	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
40	A2M	L5	1326	40	22,25,26	1.19	1 (4%)	30,36,39	1.54	9 (30%)
19	PSU	S2	649	19	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
19	PSU	S2	1046	19	18,21,22	1.11	1 (5%)	21,30,33	1.83	4 (19%)
40	OMC	L5	2824	40	19,22,23	0.54	0	25,31,34	0.73	1 (4%)
40	OMG	L5	4637	40	23,26,27	0.46	0	32,38,41	0.46	0
42	OMG	L8	75	42	23,26,27	0.46	0	32,38,41	0.52	0
40	PSU	L5	3844	40	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
19	G7M	S2	1639	19	23,26,27	2.69	8 (34%)	34,39,42	2.47	11 (32%)
40	OMU	L5	2837	40	19,22,23	3.37	7 (36%)	25,31,34	1.86	5 (20%)
40	PSU	L5	3822	40	18,21,22	1.11	1 (5%)	21,30,33	2.01	6 (28%)
19	PSU	S2	1004	19	18,21,22	1.08	1 (5%)	21,30,33	1.86	4 (19%)
40	PSU	L5	4521	40,86	18,21,22	1.15	1 (5%)	21,30,33	1.96	5 (23%)
19	A2M	S2	468	19	22,25,26	1.26	1 (4%)	30,36,39	1.53	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	OMG	S2	644	19	23,26,27	0.45	0	32,38,41	0.45	0
40	OMG	L5	4494	40	23,26,27	0.48	0	32,38,41	0.53	0
40	OMC	L5	2365	40,86	19,22,23	0.53	0	25,31,34	0.61	0
19	PSU	S2	814	19	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
19	PSU	S2	109	19	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
19	4AC	S2	1842	19	21,24,25	0.37	0	28,34,37	0.48	0
19	PSU	S2	866	19	18,21,22	1.09	1 (5%)	21,30,33	1.87	5 (23%)
40	OMU	L5	4227	40	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
19	OMU	S2	627	19	19,22,23	3.37	7 (36%)	25,31,34	1.82	5 (20%)
40	OMG	L5	1625	40	23,26,27	0.48	0	32,38,41	0.48	0
40	OMG	L5	1316	40	23,26,27	0.49	0	32,38,41	0.51	0
19	OMG	S2	683	19	23,26,27	0.52	0	32,38,41	0.45	0
19	OMC	S2	174	19	19,22,23	0.51	0	25,31,34	0.69	0
19	PSU	S2	1056	19	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
40	OMG	L5	2424	40	23,26,27	0.48	0	32,38,41	0.54	0
19	A2M	S2	668	19,86	22,25,26	1.30	1 (4%)	30,36,39	1.53	7 (23%)
40	A2M	L5	3785	40,86	22,25,26	1.16	1 (4%)	30,36,39	1.67	9 (30%)
19	A2M	S2	484	19	22,25,26	1.23	2 (9%)	30,36,39	1.47	8 (26%)
19	PSU	S2	1174	19	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
19	PSU	S2	681	19	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
19	OMU	S2	1326	19	19,22,23	3.35	7 (36%)	25,31,34	1.83	5 (20%)
40	5MC	L5	4447	40	19,22,23	0.60	0	26,32,35	0.63	0
40	OMC	L5	3701	40	19,22,23	0.54	0	25,31,34	0.81	1 (4%)
40	A2M	L5	3825	40	22,25,26	1.24	2 (9%)	30,36,39	1.51	9 (30%)
40	6MZ	L5	4220	40	22,25,26	3.01	5 (22%)	29,36,39	2.37	10 (34%)
40	PSU	L5	4579	40	18,21,22	1.06	1 (5%)	21,30,33	1.89	4 (19%)
19	OMC	S2	1391	19	19,22,23	0.52	0	25,31,34	0.91	1 (4%)
19	OMU	S2	1288	19	19,22,23	3.46	7 (36%)	25,31,34	1.79	5 (20%)
19	OMG	S2	436	19	23,26,27	0.47	0	32,38,41	0.49	0
40	PSU	L5	4299	40	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	OMC	L5	3887	40	19,22,23	0.52	0	25,31,34	0.65	0
40	A2M	L5	2815	40	22,25,26	1.24	2 (9%)	30,36,39	1.48	8 (26%)
19	OMG	S2	1490	19	23,26,27	0.48	0	32,38,41	0.45	0
40	OMG	L5	4623	40	23,26,27	0.47	0	32,38,41	0.47	0
40	UR3	L5	4530	40	19,22,23	2.80	7 (36%)	26,32,35	1.58	4 (15%)
19	OMU	S2	116	19	19,22,23	3.35	7 (36%)	25,31,34	1.72	4 (16%)
40	A2M	L5	1534	40,86	22,25,26	1.22	1 (4%)	30,36,39	1.62	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	A2M	L5	4523	40,86	22,25,26	1.27	1 (4%)	30,36,39	1.61	8 (26%)
40	PSU	L5	4673	40	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
40	PSU	L5	3695	40	18,21,22	1.10	1 (5%)	21,30,33	1.91	6 (28%)
40	PSU	L5	2632	40	18,21,22	1.08	1 (5%)	21,30,33	2.03	6 (28%)
40	PSU	L5	1792	40	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
40	OMG	L5	1522	40	23,26,27	0.48	0	32,38,41	0.61	0
19	A2M	S2	166	19	22,25,26	1.25	1 (4%)	30,36,39	1.57	7 (23%)
40	A2M	L5	2787	40	22,25,26	1.22	1 (4%)	30,36,39	1.46	7 (23%)
40	OMC	L5	2861	40	19,22,23	0.54	0	25,31,34	1.03	2 (8%)
19	MA6	S2	1850	19	23,26,27	2.65	8 (34%)	33,38,41	3.40	14 (42%)
19	PSU	S2	1367	19	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
40	A2M	L5	2401	40	22,25,26	1.20	1 (4%)	30,36,39	1.52	7 (23%)
19	A2M	S2	159	19	22,25,26	1.23	2 (9%)	30,36,39	1.51	8 (26%)
40	PSU	L5	4493	40	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
40	PSU	L5	4353	40	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
40	UY1	L5	3818	40	19,22,23	4.95	9 (47%)	21,31,34	2.01	5 (23%)
40	A2M	L5	398	40	22,25,26	1.24	1 (4%)	30,36,39	1.55	8 (26%)
40	OMC	L5	4536	40	19,22,23	0.54	0	25,31,34	0.60	0
40	PSU	L5	3853	40,86	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
40	OMU	L5	4498	40	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
40	OMG	L5	4370	40	23,26,27	0.46	0	32,38,41	0.47	0
19	PSU	S2	966	19,86	18,21,22	1.13	1 (5%)	21,30,33	1.87	5 (23%)
40	PSU	L5	4312	40	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
40	A2M	L5	4571	40	22,25,26	1.22	1 (4%)	30,36,39	1.51	8 (26%)
19	A2M	S2	576	19	22,25,26	1.23	1 (4%)	30,36,39	1.53	5 (16%)
40	PSU	L5	4442	40	18,21,22	1.10	1 (5%)	21,30,33	1.94	6 (28%)
40	PSU	L5	1781	40	18,21,22	1.09	1 (5%)	21,30,33	1.79	4 (19%)
40	PSU	L5	1782	40	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
40	PSU	L5	1536	40	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
40	OMC	L5	2804	40	19,22,23	0.52	0	25,31,34	0.60	0
40	OMG	L5	4196	40,38	23,26,27	0.47	0	32,38,41	0.50	0
19	PSU	S2	1081	19	18,21,22	1.09	1 (5%)	21,30,33	1.98	6 (28%)
19	OMG	S2	601	19	23,26,27	0.52	0	32,38,41	0.67	0
19	OMG	S2	867	19	23,26,27	0.44	0	32,38,41	0.55	0
19	OMU	S2	799	19	19,22,23	3.42	7 (36%)	25,31,34	1.82	4 (16%)
40	PSU	L5	4403	40	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PSU	L5	4972	40	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)
40	A2M	L5	4590	40	22,25,26	1.22	1 (4%)	30,36,39	1.53	6 (20%)
19	A2M	S2	27	19	22,25,26	1.23	1 (4%)	30,36,39	1.52	8 (26%)
40	OMG	L5	3792	40	23,26,27	0.47	0	32,38,41	0.51	0
40	PSU	L5	4689	40	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)

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
19	OMC	S2	517	19	-	1/9/27/28	0/2/2/2
40	A2M	L5	1871	40,86	-	0/9/27/28	0/3/3/3
19	PSU	S2	406	19	-	1/7/25/26	0/2/2/2
19	MA6	S2	1851	19	-	1/11/29/30	0/3/3/3
40	PSU	L5	4471	40	-	0/7/25/26	0/2/2/2
19	OMU	S2	354	19	-	1/9/27/28	0/2/2/2
19	OMG	S2	1328	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	801	19	-	3/7/25/26	0/2/2/2
19	OMG	S2	509	19	-	0/9/27/28	0/3/3/3
42	PSU	L8	55	42	-	0/7/25/26	0/2/2/2
40	PSU	L5	4973	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	1524	40	-	3/9/27/28	0/3/3/3
40	5MC	L5	3782	40,86	-	1/7/25/26	0/2/2/2
42	PSU	L8	69	42	-	0/7/25/26	0/2/2/2
40	PSU	L5	1683	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	93	19	-	0/7/25/26	0/2/2/2
40	OMU	L5	3925	40	-	1/9/27/28	0/2/2/2
19	PSU	S2	651	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	4456	40	-	0/9/27/28	0/2/2/2
19	OMC	S2	462	19	-	1/9/27/28	0/2/2/2
40	OMC	L5	3869	40	-	0/9/27/28	0/2/2/2
19	PSU	S2	1045	19	-	2/7/25/26	0/2/2/2
40	PSU	L5	4636	40	-	2/7/25/26	0/2/2/2
40	PSU	L5	4628	40	-	0/7/25/26	0/2/2/2
19	OMU	S2	172	19	-	2/9/27/28	0/2/2/2
19	PSU	S2	686	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	1442	19	-	3/9/27/28	0/2/2/2
19	A2M	S2	1031	19	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	A2M	L5	2363	40,86	-	0/9/27/28	0/3/3/3
40	OMC	L5	2351	40,86	-	1/9/27/28	0/2/2/2
19	OMU	S2	428	19	-	3/9/27/28	0/2/2/2
40	OMG	L5	4228	40	-	0/9/27/28	0/3/3/3
19	OMC	S2	1703	19	-	1/9/27/28	0/2/2/2
40	PSU	L5	4296	40	-	2/7/25/26	0/2/2/2
40	PSU	L5	4532	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3627	40	-	0/9/27/28	0/3/3/3
40	OMG	L5	4392	40	-	0/9/27/28	0/3/3/3
19	4AC	S2	1337	19	-	1/11/29/30	0/2/2/2
40	PSU	L5	3851	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1177	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	1340	40	-	1/9/27/28	0/2/2/2
40	OMG	L5	2876	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	863	19	-	2/7/25/26	0/2/2/2
19	6MZ	S2	1832	19,86	-	2/9/27/28	0/3/3/3
40	PSU	L5	4576	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	5001	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3841	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	2422	40,86	-	3/9/27/28	0/2/2/2
40	A2M	L5	3867	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	3639	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3899	40	-	3/9/27/28	0/3/3/3
40	A2M	L5	400	40	-	0/9/27/28	0/3/3/3
40	PSU	L5	4500	40	-	3/7/25/26	0/2/2/2
19	A2M	S2	99	19,86	-	2/9/27/28	0/3/3/3
40	OMU	L5	4306	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3637	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1744	40,86	-	0/7/25/26	0/2/2/2
40	PSU	L5	4457	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1677	40	-	1/7/25/26	0/2/2/2
19	OMC	S2	1272	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	2839	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3808	40,86	-	0/9/27/28	0/2/2/2
19	A2M	S2	1383	19	-	3/9/27/28	0/3/3/3
40	PSU	L5	4361	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	4620	40	-	1/9/27/28	0/2/2/2
40	PSU	L5	3920	40,86	-	0/7/25/26	0/2/2/2
40	PSU	L5	5010	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3884	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	1MA	L5	1322	40	-	0/7/25/26	0/3/3/3
19	OMU	S2	121	19	-	0/9/27/28	0/2/2/2
40	A2M	L5	1323	40	-	3/9/27/28	0/3/3/3
40	PSU	L5	4431	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3744	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	1232	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1862	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4293	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	2364	40,86	-	2/9/27/28	0/3/3/3
19	B8N	S2	1248	19	-	7/16/34/35	0/2/2/2
40	PSU	L5	1860	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	3830	40	-	1/9/27/28	0/3/3/3
40	OMG	L5	4618	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	1582	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4552	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	3718	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	1244	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	4499	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	105	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1326	40	-	3/9/27/28	0/3/3/3
19	PSU	S2	649	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	1046	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	2824	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4637	40	-	3/9/27/28	0/3/3/3
42	OMG	L8	75	42	-	1/9/27/28	0/3/3/3
40	PSU	L5	3844	40	-	1/7/25/26	0/2/2/2
19	G7M	S2	1639	19	-	2/7/25/26	0/3/3/3
40	OMU	L5	2837	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3822	40	-	4/7/25/26	0/2/2/2
19	PSU	S2	1004	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	4521	40,86	-	1/7/25/26	0/2/2/2
19	A2M	S2	468	19	-	1/9/27/28	0/3/3/3
19	OMG	S2	644	19	-	4/9/27/28	0/3/3/3
40	OMG	L5	4494	40	-	0/9/27/28	0/3/3/3
40	OMC	L5	2365	40,86	-	0/9/27/28	0/2/2/2
19	PSU	S2	814	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	109	19	-	0/7/25/26	0/2/2/2
19	4AC	S2	1842	19	-	0/11/29/30	0/2/2/2
19	PSU	S2	866	19	-	0/7/25/26	0/2/2/2
40	OMU	L5	4227	40	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OMU	S2	627	19	-	2/9/27/28	0/2/2/2
40	OMG	L5	1625	40	-	3/9/27/28	0/3/3/3
40	OMG	L5	1316	40	-	1/9/27/28	0/3/3/3
19	OMG	S2	683	19	-	2/9/27/28	0/3/3/3
19	OMC	S2	174	19	-	0/9/27/28	0/2/2/2
19	PSU	S2	1056	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	2424	40	-	1/9/27/28	0/3/3/3
19	A2M	S2	668	19,86	-	3/9/27/28	0/3/3/3
40	A2M	L5	3785	40,86	-	1/9/27/28	0/3/3/3
19	A2M	S2	484	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	1174	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	681	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	1326	19	-	0/9/27/28	0/2/2/2
40	5MC	L5	4447	40	-	4/7/25/26	0/2/2/2
40	OMC	L5	3701	40	-	4/9/27/28	0/2/2/2
40	A2M	L5	3825	40	-	1/9/27/28	0/3/3/3
40	6MZ	L5	4220	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	4579	40	-	0/7/25/26	0/2/2/2
19	OMC	S2	1391	19	-	0/9/27/28	0/2/2/2
19	OMU	S2	1288	19	-	3/9/27/28	0/2/2/2
19	OMG	S2	436	19	-	0/9/27/28	0/3/3/3
40	PSU	L5	4299	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3887	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	2815	40	-	0/9/27/28	0/3/3/3
19	OMG	S2	1490	19	-	2/9/27/28	0/3/3/3
40	OMG	L5	4623	40	-	0/9/27/28	0/3/3/3
40	UR3	L5	4530	40	-	0/7/25/26	0/2/2/2
19	OMU	S2	116	19	-	0/9/27/28	0/2/2/2
40	A2M	L5	1534	40,86	-	1/9/27/28	0/3/3/3
40	A2M	L5	4523	40,86	-	2/9/27/28	0/3/3/3
40	PSU	L5	4673	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3695	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	2632	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1792	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	1522	40	-	0/9/27/28	0/3/3/3
19	A2M	S2	166	19	-	0/9/27/28	0/3/3/3
40	A2M	L5	2787	40	-	5/9/27/28	0/3/3/3
40	OMC	L5	2861	40	-	3/9/27/28	0/2/2/2
19	MA6	S2	1850	19	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PSU	S2	1367	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	2401	40	-	3/9/27/28	0/3/3/3
19	A2M	S2	159	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	4493	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4353	40	-	0/7/25/26	0/2/2/2
40	UY1	L5	3818	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	398	40	-	1/9/27/28	0/3/3/3
40	OMC	L5	4536	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3853	40,86	-	0/7/25/26	0/2/2/2
40	OMU	L5	4498	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4370	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	966	19,86	-	0/7/25/26	0/2/2/2
40	PSU	L5	4312	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	4571	40	-	0/9/27/28	0/3/3/3
19	A2M	S2	576	19	-	4/9/27/28	0/3/3/3
40	PSU	L5	4442	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1781	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1782	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1536	40	-	2/7/25/26	0/2/2/2
40	OMC	L5	2804	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4196	40,38	-	0/9/27/28	0/3/3/3
19	PSU	S2	1081	19	-	1/7/25/26	0/2/2/2
19	OMG	S2	601	19	-	1/9/27/28	0/3/3/3
19	OMG	S2	867	19	-	3/9/27/28	0/3/3/3
19	OMU	S2	799	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	4403	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4972	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	4590	40	-	4/9/27/28	0/3/3/3
19	A2M	S2	27	19	-	1/9/27/28	0/3/3/3
40	OMG	L5	3792	40	-	3/9/27/28	0/3/3/3
40	PSU	L5	4689	40	-	0/7/25/26	0/2/2/2

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	3818	UY1	C6-C5	12.93	1.49	1.35
19	S2	1832	6MZ	C6-N6	12.62	1.48	1.34
40	L5	4220	6MZ	C6-N6	12.51	1.48	1.34
40	L5	3818	UY1	C2-N1	11.92	1.52	1.36
19	S2	1288	OMU	C2-N1	8.80	1.52	1.38
19	S2	799	OMU	C2-N1	8.62	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1442	OMU	C2-N1	8.59	1.51	1.38
19	S2	1832	6MZ	C3'-C2'	-8.37	1.30	1.53
40	L5	3925	OMU	C2-N1	8.30	1.51	1.38
19	S2	172	OMU	C2-N1	8.29	1.51	1.38
40	L5	2837	OMU	C2-N1	8.25	1.51	1.38
40	L5	4306	OMU	C2-N1	8.24	1.51	1.38
40	L5	4227	OMU	C2-N1	8.24	1.51	1.38
19	S2	354	OMU	C2-N1	8.23	1.51	1.38
19	S2	121	OMU	C2-N1	8.22	1.51	1.38
40	L5	4620	OMU	C2-N1	8.21	1.51	1.38
19	S2	627	OMU	C2-N1	8.18	1.51	1.38
40	L5	4498	OMU	C2-N1	8.16	1.51	1.38
19	S2	116	OMU	C2-N1	8.15	1.51	1.38
19	S2	428	OMU	C2-N1	8.12	1.51	1.38
19	S2	1326	OMU	C2-N1	8.11	1.51	1.38
19	S2	1248	B8N	C6-N1	7.95	1.55	1.36
40	L5	3818	UY1	C2-N3	7.90	1.50	1.37
19	S2	1850	MA6	C3'-C2'	-7.82	1.32	1.53
19	S2	1248	B8N	C4-N3	-7.77	1.26	1.40
19	S2	1248	B8N	C4-C5	7.10	1.63	1.47
19	S2	1288	OMU	C2-N3	7.02	1.50	1.38
19	S2	116	OMU	C2-N3	6.97	1.50	1.38
19	S2	799	OMU	C2-N3	6.96	1.50	1.38
19	S2	1442	OMU	C2-N3	6.95	1.50	1.38
40	L5	4498	OMU	C2-N3	6.94	1.50	1.38
19	S2	121	OMU	C2-N3	6.94	1.50	1.38
40	L5	4227	OMU	C2-N3	6.93	1.50	1.38
40	L5	4306	OMU	C2-N3	6.92	1.50	1.38
19	S2	354	OMU	C2-N3	6.92	1.50	1.38
19	S2	627	OMU	C2-N3	6.91	1.50	1.38
19	S2	428	OMU	C2-N3	6.89	1.50	1.38
19	S2	172	OMU	C2-N3	6.87	1.49	1.38
40	L5	3925	OMU	C2-N3	6.86	1.49	1.38
19	S2	1326	OMU	C2-N3	6.86	1.49	1.38
40	L5	4620	OMU	C2-N3	6.85	1.49	1.38
40	L5	2837	OMU	C2-N3	6.84	1.49	1.38
40	L5	4530	UR3	C2-N1	6.79	1.47	1.38
19	S2	1639	G7M	C4-N3	6.76	1.49	1.34
40	L5	4530	UR3	C6-C5	6.31	1.49	1.35
19	S2	1288	OMU	C6-C5	5.96	1.48	1.35
19	S2	627	OMU	C6-C5	5.91	1.48	1.35
40	L5	4227	OMU	C6-C5	5.90	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	4498	OMU	C6-C5	5.90	1.48	1.35
40	L5	4530	UR3	C2-N3	5.90	1.50	1.39
19	S2	799	OMU	C6-C5	5.90	1.48	1.35
19	S2	121	OMU	C6-C5	5.90	1.48	1.35
19	S2	428	OMU	C6-C5	5.90	1.48	1.35
19	S2	1248	B8N	C2-N1	5.90	1.56	1.39
19	S2	354	OMU	C6-C5	5.87	1.48	1.35
19	S2	1442	OMU	C6-C5	5.85	1.48	1.35
19	S2	1326	OMU	C6-C5	5.85	1.48	1.35
19	S2	172	OMU	C6-C5	5.85	1.48	1.35
40	L5	4306	OMU	C6-C5	5.84	1.48	1.35
40	L5	2837	OMU	C6-C5	5.82	1.48	1.35
19	S2	116	OMU	C6-C5	5.82	1.48	1.35
40	L5	3925	OMU	C6-C5	5.81	1.48	1.35
40	L5	4620	OMU	C6-C5	5.77	1.48	1.35
19	S2	1639	G7M	C2-N3	5.59	1.46	1.33
40	L5	2837	OMU	O4-C4	-5.54	1.13	1.24
40	L5	3818	UY1	C6-N1	5.49	1.45	1.36
40	L5	3925	OMU	O4-C4	-5.48	1.13	1.24
19	S2	1326	OMU	O4-C4	-5.47	1.13	1.24
40	L5	4227	OMU	O4-C4	-5.47	1.13	1.24
19	S2	627	OMU	O4-C4	-5.44	1.13	1.24
19	S2	172	OMU	O4-C4	-5.42	1.13	1.24
40	L5	4620	OMU	O4-C4	-5.42	1.13	1.24
19	S2	116	OMU	O4-C4	-5.41	1.14	1.24
19	S2	354	OMU	O4-C4	-5.41	1.14	1.24
40	L5	4306	OMU	O4-C4	-5.41	1.14	1.24
19	S2	1248	B8N	C6-C5	5.41	1.42	1.35
19	S2	428	OMU	O4-C4	-5.40	1.14	1.24
19	S2	799	OMU	O4-C4	-5.40	1.14	1.24
19	S2	1288	OMU	O4-C4	-5.39	1.14	1.24
40	L5	4498	OMU	O4-C4	-5.38	1.14	1.24
19	S2	1442	OMU	O4-C4	-5.38	1.14	1.24
19	S2	121	OMU	O4-C4	-5.36	1.14	1.24
19	S2	1639	G7M	C2-N2	5.00	1.45	1.34
19	S2	1832	6MZ	O4'-C4'	4.74	1.55	1.45
19	S2	1832	6MZ	O4'-C1'	-4.69	1.31	1.42
19	S2	1639	G7M	C5-N7	-4.63	1.33	1.39
40	L5	3818	UY1	C4-N3	4.54	1.47	1.38
19	S2	627	OMU	C4-N3	4.46	1.46	1.38
40	L5	4498	OMU	C4-N3	4.42	1.46	1.38
19	S2	428	OMU	C4-N3	4.42	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1832	6MZ	C5'-C4'	-4.39	1.38	1.51
40	L5	4306	OMU	C4-N3	4.39	1.46	1.38
19	S2	172	OMU	C4-N3	4.39	1.46	1.38
19	S2	354	OMU	C4-N3	4.39	1.46	1.38
19	S2	116	OMU	C4-N3	4.38	1.46	1.38
19	S2	1288	OMU	C4-N3	4.37	1.46	1.38
19	S2	1326	OMU	C4-N3	4.37	1.46	1.38
19	S2	1442	OMU	C4-N3	4.35	1.46	1.38
40	L5	2837	OMU	C4-N3	4.34	1.46	1.38
19	S2	121	OMU	C4-N3	4.33	1.46	1.38
40	L5	3925	OMU	C4-N3	4.31	1.46	1.38
40	L5	4227	OMU	C4-N3	4.30	1.46	1.38
40	L5	4620	OMU	C4-N3	4.29	1.46	1.38
19	S2	799	OMU	C4-N3	4.27	1.45	1.38
19	S2	1850	MA6	O4'-C4'	4.20	1.54	1.45
19	S2	1850	MA6	C5'-C4'	-4.12	1.39	1.51
19	S2	1639	G7M	C5-C6	3.91	1.54	1.43
19	S2	686	PSU	C6-C5	3.82	1.39	1.35
19	S2	801	PSU	C6-C5	3.78	1.39	1.35
19	S2	1248	B8N	C1'-C5	3.78	1.58	1.50
19	S2	1046	PSU	C6-C5	3.76	1.39	1.35
19	S2	966	PSU	C6-C5	3.76	1.39	1.35
40	L5	4361	PSU	C6-C5	3.74	1.39	1.35
19	S2	1174	PSU	C6-C5	3.73	1.39	1.35
19	S2	1177	PSU	C6-C5	3.73	1.39	1.35
19	S2	1367	PSU	C6-C5	3.72	1.39	1.35
19	S2	406	PSU	C6-C5	3.72	1.39	1.35
40	L5	1860	PSU	C6-C5	3.71	1.39	1.35
40	L5	4293	PSU	C6-C5	3.71	1.39	1.35
40	L5	4312	PSU	C6-C5	3.71	1.39	1.35
19	S2	109	PSU	C6-C5	3.71	1.39	1.35
40	L5	1683	PSU	C6-C5	3.71	1.39	1.35
40	L5	4636	PSU	C6-C5	3.71	1.39	1.35
40	L5	1582	PSU	C6-C5	3.70	1.39	1.35
19	S2	1244	PSU	C6-C5	3.70	1.39	1.35
40	L5	4500	PSU	C6-C5	3.70	1.39	1.35
40	L5	4521	PSU	C6-C5	3.69	1.39	1.35
40	L5	3851	PSU	C6-C5	3.69	1.39	1.35
19	S2	651	PSU	C6-C5	3.68	1.39	1.35
40	L5	1781	PSU	C6-C5	3.68	1.39	1.35
40	L5	2839	PSU	C6-C5	3.68	1.39	1.35
19	S2	814	PSU	C6-C5	3.68	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1045	PSU	C6-C5	3.67	1.39	1.35
42	L8	55	PSU	C6-C5	3.67	1.39	1.35
19	S2	1850	MA6	O4'-C1'	-3.66	1.33	1.42
40	L5	5001	PSU	C6-C5	3.66	1.39	1.35
19	S2	93	PSU	C6-C5	3.66	1.39	1.35
40	L5	1792	PSU	C6-C5	3.65	1.39	1.35
40	L5	4403	PSU	C6-C5	3.65	1.39	1.35
19	S2	863	PSU	C6-C5	3.64	1.39	1.35
40	L5	4299	PSU	C6-C5	3.64	1.39	1.35
19	S2	1232	PSU	C6-C5	3.63	1.39	1.35
40	L5	4973	PSU	C6-C5	3.62	1.39	1.35
19	S2	649	PSU	C6-C5	3.62	1.39	1.35
40	L5	5010	PSU	C6-C5	3.62	1.39	1.35
40	L5	3639	PSU	C6-C5	3.61	1.39	1.35
40	L5	4471	PSU	C6-C5	3.61	1.39	1.35
40	L5	3844	PSU	C6-C5	3.61	1.39	1.35
40	L5	1782	PSU	C6-C5	3.60	1.39	1.35
40	L5	4532	PSU	C6-C5	3.60	1.39	1.35
40	L5	4296	PSU	C6-C5	3.59	1.39	1.35
40	L5	4552	PSU	C6-C5	3.59	1.39	1.35
40	L5	1862	PSU	C6-C5	3.57	1.39	1.35
40	L5	4431	PSU	C6-C5	3.57	1.39	1.35
40	L5	3637	PSU	C6-C5	3.57	1.39	1.35
19	S2	1004	PSU	C6-C5	3.57	1.39	1.35
40	L5	4353	PSU	C6-C5	3.56	1.39	1.35
40	L5	1744	PSU	C6-C5	3.56	1.39	1.35
40	L5	4576	PSU	C6-C5	3.55	1.39	1.35
40	L5	3853	PSU	C6-C5	3.55	1.39	1.35
19	S2	105	PSU	C6-C5	3.55	1.39	1.35
40	L5	4493	PSU	C6-C5	3.54	1.39	1.35
19	S2	1081	PSU	C6-C5	3.54	1.39	1.35
42	L8	69	PSU	C6-C5	3.54	1.39	1.35
40	L5	3695	PSU	C6-C5	3.54	1.39	1.35
40	L5	3818	UY1	O4-C4	-3.53	1.16	1.23
19	S2	866	PSU	C6-C5	3.53	1.39	1.35
40	L5	4972	PSU	C6-C5	3.53	1.39	1.35
40	L5	3884	PSU	C6-C5	3.53	1.39	1.35
19	S2	681	PSU	C6-C5	3.51	1.39	1.35
40	L5	4673	PSU	C6-C5	3.50	1.39	1.35
40	L5	3920	PSU	C6-C5	3.49	1.39	1.35
40	L5	4442	PSU	C6-C5	3.49	1.39	1.35
40	L5	4457	PSU	C6-C5	3.48	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	668	A2M	O5'-C5'	-3.46	1.34	1.44
19	S2	576	A2M	O5'-C5'	-3.44	1.34	1.44
40	L5	4689	PSU	C6-C5	3.43	1.39	1.35
40	L5	2632	PSU	C6-C5	3.42	1.39	1.35
19	S2	1056	PSU	C6-C5	3.41	1.39	1.35
40	L5	4579	PSU	C6-C5	3.40	1.39	1.35
19	S2	1383	A2M	O5'-C5'	-3.39	1.34	1.44
40	L5	1323	A2M	O5'-C5'	-3.39	1.34	1.44
40	L5	3822	PSU	C6-C5	3.39	1.39	1.35
40	L5	400	A2M	O5'-C5'	-3.38	1.34	1.44
19	S2	99	A2M	O5'-C5'	-3.38	1.34	1.44
40	L5	1677	PSU	C6-C5	3.35	1.39	1.35
40	L5	1536	PSU	C6-C5	3.35	1.39	1.35
40	L5	4628	PSU	C6-C5	3.35	1.39	1.35
40	L5	4523	A2M	O5'-C5'	-3.34	1.34	1.44
19	S2	27	A2M	O5'-C5'	-3.33	1.34	1.44
40	L5	1534	A2M	O5'-C5'	-3.33	1.34	1.44
19	S2	468	A2M	O5'-C5'	-3.32	1.34	1.44
40	L5	3825	A2M	O5'-C5'	-3.32	1.34	1.44
19	S2	1031	A2M	O5'-C5'	-3.31	1.34	1.44
40	L5	3830	A2M	O5'-C5'	-3.31	1.34	1.44
40	L5	4571	A2M	O5'-C5'	-3.30	1.34	1.44
40	L5	2787	A2M	O5'-C5'	-3.29	1.34	1.44
19	S2	166	A2M	O5'-C5'	-3.29	1.34	1.44
40	L5	3718	A2M	O5'-C5'	-3.29	1.34	1.44
40	L5	2815	A2M	O5'-C5'	-3.28	1.34	1.44
40	L5	3867	A2M	O5'-C5'	-3.28	1.34	1.44
40	L5	1871	A2M	O5'-C5'	-3.28	1.34	1.44
40	L5	2363	A2M	O5'-C5'	-3.27	1.34	1.44
40	L5	398	A2M	O5'-C5'	-3.27	1.34	1.44
40	L5	3785	A2M	O5'-C5'	-3.25	1.34	1.44
40	L5	3818	UY1	O2-C2	-3.24	1.16	1.23
19	S2	484	A2M	O5'-C5'	-3.24	1.34	1.44
40	L5	2401	A2M	O5'-C5'	-3.23	1.34	1.44
40	L5	3818	UY1	C1'-C5	3.23	1.57	1.50
40	L5	1524	A2M	O5'-C5'	-3.20	1.34	1.44
40	L5	4220	6MZ	C5-N7	-3.17	1.33	1.39
19	S2	1850	MA6	C6-N6	3.17	1.45	1.36
19	S2	1851	MA6	C6-N6	3.17	1.45	1.36
40	L5	4590	A2M	O5'-C5'	-3.14	1.35	1.44
40	L5	1326	A2M	O5'-C5'	-3.14	1.35	1.44
19	S2	1832	6MZ	C2'-C1'	3.08	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	159	A2M	O5'-C5'	-3.08	1.35	1.44
19	S2	1832	6MZ	C5-N7	-3.06	1.33	1.39
19	S2	1832	6MZ	C5-C4	-2.99	1.33	1.39
40	L5	4220	6MZ	C5-C4	-2.98	1.33	1.39
19	S2	428	OMU	C5-C4	2.93	1.50	1.43
19	S2	1850	MA6	O3'-C3'	2.92	1.50	1.43
40	L5	4220	6MZ	C8-N9	-2.91	1.32	1.37
19	S2	172	OMU	C5-C4	2.90	1.50	1.43
19	S2	799	OMU	C5-C4	2.89	1.50	1.43
19	S2	627	OMU	C5-C4	2.89	1.50	1.43
19	S2	1288	OMU	C5-C4	2.88	1.49	1.43
40	L5	4227	OMU	C5-C4	2.87	1.49	1.43
19	S2	1639	G7M	C2-N1	2.87	1.44	1.37
40	L5	3925	OMU	C5-C4	2.87	1.49	1.43
40	L5	4498	OMU	C5-C4	2.86	1.49	1.43
19	S2	1326	OMU	C5-C4	2.86	1.49	1.43
19	S2	1442	OMU	C5-C4	2.83	1.49	1.43
19	S2	121	OMU	C5-C4	2.81	1.49	1.43
19	S2	1288	OMU	C6-N1	2.79	1.44	1.38
19	S2	354	OMU	C5-C4	2.78	1.49	1.43
19	S2	116	OMU	C5-C4	2.77	1.49	1.43
40	L5	2837	OMU	C5-C4	2.76	1.49	1.43
40	L5	2837	OMU	C6-N1	2.75	1.44	1.38
19	S2	799	OMU	C6-N1	2.75	1.44	1.38
40	L5	4620	OMU	C5-C4	2.75	1.49	1.43
40	L5	4306	OMU	C5-C4	2.74	1.49	1.43
19	S2	1832	6MZ	C8-N9	-2.73	1.32	1.37
19	S2	1442	OMU	C6-N1	2.71	1.44	1.38
40	L5	4498	OMU	C6-N1	2.67	1.44	1.38
40	L5	4306	OMU	C6-N1	2.67	1.44	1.38
40	L5	4227	OMU	C6-N1	2.66	1.44	1.38
19	S2	121	OMU	C6-N1	2.66	1.44	1.38
19	S2	627	OMU	C6-N1	2.66	1.44	1.38
19	S2	116	OMU	C6-N1	2.66	1.44	1.38
19	S2	1832	6MZ	O3'-C3'	2.65	1.49	1.43
19	S2	1326	OMU	C6-N1	2.65	1.44	1.38
19	S2	428	OMU	C6-N1	2.64	1.44	1.38
19	S2	354	OMU	C6-N1	2.63	1.44	1.38
40	L5	4530	UR3	C6-N1	2.62	1.44	1.38
40	L5	3925	OMU	C6-N1	2.62	1.44	1.38
19	S2	172	OMU	C6-N1	2.59	1.44	1.38
40	L5	4620	OMU	C6-N1	2.56	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1639	G7M	C6-N1	2.55	1.43	1.38
19	S2	1639	G7M	O6-C6	-2.51	1.18	1.23
40	L5	4530	UR3	O2-C2	-2.49	1.17	1.22
19	S2	1850	MA6	C2'-C1'	2.39	1.61	1.53
40	L5	4530	UR3	C5-C4	2.33	1.49	1.43
40	L5	4530	UR3	C3U-N3	2.26	1.51	1.47
19	S2	1850	MA6	C5-C4	-2.23	1.35	1.39
19	S2	1851	MA6	C5-C4	-2.21	1.35	1.39
40	L5	1524	A2M	O4'-C4'	-2.17	1.40	1.45
40	L5	3818	UY1	C4-C5	2.14	1.50	1.44
19	S2	1832	6MZ	C6-N1	-2.13	1.31	1.35
40	L5	4220	6MZ	C6-N1	-2.05	1.31	1.35
40	L5	2815	A2M	C5-C4	2.04	1.42	1.39
19	S2	159	A2M	C5-C4	2.01	1.42	1.39
40	L5	3825	A2M	C5-C4	2.01	1.42	1.39
19	S2	484	A2M	C5-C4	2.01	1.42	1.39

All (710) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	N1-C6-N6	-11.85	102.41	116.86
19	S2	1850	MA6	N1-C6-N6	-11.17	103.24	116.86
19	S2	1851	MA6	C5-C6-N6	7.85	137.76	125.33
19	S2	1850	MA6	C5-C6-N6	7.34	136.94	125.33
19	S2	1639	G7M	C1'-N9-C4	6.79	146.55	126.49
19	S2	1639	G7M	C1'-N9-C8	-6.66	104.26	126.74
19	S2	172	OMU	C4-N3-C2	-5.77	119.45	126.61
40	L5	3925	OMU	C4-N3-C2	-5.77	119.45	126.61
19	S2	1326	OMU	C4-N3-C2	-5.74	119.48	126.61
19	S2	627	OMU	C4-N3-C2	-5.72	119.51	126.61
19	S2	428	OMU	C4-N3-C2	-5.69	119.55	126.61
19	S2	1832	6MZ	N1-C2-N3	-5.66	120.02	128.58
40	L5	4227	OMU	C4-N3-C2	-5.65	119.60	126.61
40	L5	2837	OMU	C4-N3-C2	-5.64	119.61	126.61
19	S2	799	OMU	C4-N3-C2	-5.60	119.67	126.61
40	L5	4306	OMU	C4-N3-C2	-5.60	119.67	126.61
19	S2	1851	MA6	N1-C2-N3	-5.59	120.13	128.58
40	L5	4498	OMU	C4-N3-C2	-5.58	119.69	126.61
19	S2	354	OMU	C4-N3-C2	-5.55	119.72	126.61
19	S2	1442	OMU	C4-N3-C2	-5.49	119.79	126.61
40	L5	4220	6MZ	N1-C2-N3	-5.44	120.35	128.58
40	L5	4530	UR3	C4-N3-C2	-5.43	120.21	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1850	MA6	N1-C2-N3	-5.38	120.44	128.58
40	L5	4620	OMU	C4-N3-C2	-5.32	120.01	126.61
19	S2	1248	B8N	C5-C4-N3	5.31	125.78	116.15
19	S2	121	OMU	C4-N3-C2	-5.29	120.05	126.61
19	S2	1288	OMU	C4-N3-C2	-5.26	120.08	126.61
19	S2	116	OMU	C4-N3-C2	-5.24	120.10	126.61
19	S2	1851	MA6	N9-C8-N7	-5.22	106.53	113.94
40	L5	1677	PSU	C4-N3-C2	-5.14	119.29	126.37
19	S2	1850	MA6	N9-C8-N7	-5.11	106.68	113.94
40	L5	2632	PSU	N1-C2-N3	4.99	120.43	115.17
40	L5	1677	PSU	N1-C2-N3	4.98	120.42	115.17
40	L5	2632	PSU	C4-N3-C2	-4.98	119.51	126.37
40	L5	4220	6MZ	C5-C4-N3	-4.96	119.89	126.72
40	L5	4293	PSU	C4-N3-C2	-4.96	119.54	126.37
40	L5	4636	PSU	C4-N3-C2	-4.93	119.58	126.37
19	S2	1081	PSU	N1-C2-N3	4.93	120.37	115.17
19	S2	1081	PSU	C4-N3-C2	-4.93	119.58	126.37
40	L5	4521	PSU	C4-N3-C2	-4.90	119.62	126.37
40	L5	4500	PSU	C4-N3-C2	-4.90	119.62	126.37
40	L5	4493	PSU	C4-N3-C2	-4.90	119.62	126.37
40	L5	3884	PSU	C4-N3-C2	-4.89	119.63	126.37
40	L5	4431	PSU	C4-N3-C2	-4.89	119.64	126.37
19	S2	406	PSU	C4-N3-C2	-4.89	119.64	126.37
40	L5	4552	PSU	C4-N3-C2	-4.88	119.64	126.37
40	L5	4296	PSU	C4-N3-C2	-4.88	119.65	126.37
19	S2	1232	PSU	N1-C2-N3	4.87	120.30	115.17
19	S2	1832	6MZ	N9-C8-N7	-4.87	107.03	113.94
40	L5	1536	PSU	C4-N3-C2	-4.86	119.67	126.37
40	L5	1782	PSU	N1-C2-N3	4.86	120.30	115.17
40	L5	3853	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	3637	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	4353	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	3822	PSU	C4-N3-C2	-4.85	119.68	126.37
19	S2	649	PSU	C4-N3-C2	-4.85	119.69	126.37
19	S2	686	PSU	C4-N3-C2	-4.85	119.69	126.37
40	L5	3637	PSU	N1-C2-N3	4.84	120.27	115.17
40	L5	4972	PSU	N1-C2-N3	4.84	120.27	115.17
19	S2	1244	PSU	N1-C2-N3	4.83	120.27	115.17
40	L5	4521	PSU	N1-C2-N3	4.83	120.26	115.17
40	L5	4293	PSU	N1-C2-N3	4.83	120.26	115.17
40	L5	4431	PSU	N1-C2-N3	4.83	120.26	115.17
42	L8	55	PSU	C4-N3-C2	-4.83	119.72	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4493	PSU	N1-C2-N3	4.83	120.26	115.17
19	S2	105	PSU	N1-C2-N3	4.82	120.26	115.17
19	S2	863	PSU	N1-C2-N3	4.82	120.25	115.17
40	L5	4552	PSU	N1-C2-N3	4.82	120.25	115.17
40	L5	1782	PSU	C4-N3-C2	-4.82	119.73	126.37
40	L5	5010	PSU	C4-N3-C2	-4.81	119.74	126.37
40	L5	3695	PSU	N1-C2-N3	4.81	120.25	115.17
40	L5	3920	PSU	C4-N3-C2	-4.81	119.75	126.37
40	L5	3639	PSU	N1-C2-N3	4.81	120.24	115.17
19	S2	649	PSU	N1-C2-N3	4.81	120.24	115.17
40	L5	4299	PSU	C4-N3-C2	-4.81	119.75	126.37
40	L5	3920	PSU	N1-C2-N3	4.80	120.24	115.17
40	L5	4579	PSU	N1-C2-N3	4.80	120.23	115.17
42	L8	55	PSU	N1-C2-N3	4.80	120.23	115.17
40	L5	4442	PSU	N1-C2-N3	4.80	120.23	115.17
19	S2	1850	MA6	C5-C4-N3	-4.80	120.11	126.72
40	L5	3818	UY1	C4-N3-C2	-4.80	119.76	126.37
40	L5	3844	PSU	C4-N3-C2	-4.80	119.77	126.37
40	L5	1582	PSU	N1-C2-N3	4.80	120.23	115.17
19	S2	406	PSU	N1-C2-N3	4.79	120.22	115.17
40	L5	3853	PSU	N1-C2-N3	4.79	120.22	115.17
40	L5	4299	PSU	N1-C2-N3	4.79	120.22	115.17
19	S2	1232	PSU	C4-N3-C2	-4.79	119.78	126.37
40	L5	4689	PSU	N1-C2-N3	4.78	120.21	115.17
40	L5	4500	PSU	N1-C2-N3	4.78	120.20	115.17
40	L5	4628	PSU	N1-C2-N3	4.78	120.20	115.17
40	L5	1862	PSU	C4-N3-C2	-4.78	119.79	126.37
40	L5	1536	PSU	N1-C2-N3	4.77	120.20	115.17
19	S2	866	PSU	C4-N3-C2	-4.77	119.80	126.37
19	S2	863	PSU	C4-N3-C2	-4.77	119.80	126.37
40	L5	4673	PSU	C4-N3-C2	-4.77	119.80	126.37
40	L5	4973	PSU	C4-N3-C2	-4.77	119.80	126.37
40	L5	3639	PSU	C4-N3-C2	-4.77	119.80	126.37
40	L5	1862	PSU	N1-C2-N3	4.77	120.19	115.17
40	L5	1860	PSU	C4-N3-C2	-4.76	119.81	126.37
19	S2	1004	PSU	N1-C2-N3	4.76	120.19	115.17
19	S2	651	PSU	N1-C2-N3	4.76	120.18	115.17
40	L5	3822	PSU	N1-C2-N3	4.76	120.18	115.17
40	L5	4361	PSU	N1-C2-N3	4.76	120.18	115.17
40	L5	4579	PSU	C4-N3-C2	-4.76	119.82	126.37
19	S2	651	PSU	C4-N3-C2	-4.75	119.82	126.37
40	L5	4353	PSU	N1-C2-N3	4.75	120.18	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1367	PSU	C4-N3-C2	-4.75	119.83	126.37
40	L5	3851	PSU	C4-N3-C2	-4.74	119.84	126.37
40	L5	4972	PSU	C4-N3-C2	-4.74	119.84	126.37
40	L5	4636	PSU	N1-C2-N3	4.74	120.17	115.17
19	S2	801	PSU	N1-C2-N3	4.74	120.16	115.17
40	L5	4973	PSU	N1-C2-N3	4.73	120.16	115.17
40	L5	1683	PSU	N1-C2-N3	4.73	120.16	115.17
19	S2	814	PSU	C4-N3-C2	-4.73	119.85	126.37
19	S2	681	PSU	N1-C2-N3	4.73	120.16	115.17
40	L5	1582	PSU	C4-N3-C2	-4.73	119.86	126.37
19	S2	681	PSU	C4-N3-C2	-4.72	119.86	126.37
19	S2	1174	PSU	C4-N3-C2	-4.72	119.86	126.37
19	S2	1832	6MZ	C5-C4-N3	-4.72	120.22	126.72
40	L5	4296	PSU	N1-C2-N3	4.72	120.15	115.17
19	S2	1367	PSU	N1-C2-N3	4.71	120.14	115.17
19	S2	109	PSU	C4-N3-C2	-4.71	119.88	126.37
19	S2	1177	PSU	C4-N3-C2	-4.71	119.88	126.37
40	L5	1792	PSU	N1-C2-N3	4.71	120.13	115.17
40	L5	3851	PSU	N1-C2-N3	4.71	120.13	115.17
40	L5	3695	PSU	C4-N3-C2	-4.70	119.89	126.37
40	L5	3884	PSU	N1-C2-N3	4.70	120.13	115.17
19	S2	1056	PSU	N1-C2-N3	4.70	120.13	115.17
19	S2	1045	PSU	N1-C2-N3	4.70	120.13	115.17
40	L5	5010	PSU	N1-C2-N3	4.70	120.13	115.17
42	L8	69	PSU	C4-N3-C2	-4.70	119.90	126.37
19	S2	966	PSU	C4-N3-C2	-4.70	119.90	126.37
40	L5	4403	PSU	C4-N3-C2	-4.70	119.90	126.37
19	S2	1046	PSU	N1-C2-N3	4.69	120.12	115.17
40	L5	4673	PSU	N1-C2-N3	4.69	120.12	115.17
40	L5	1860	PSU	N1-C2-N3	4.69	120.11	115.17
19	S2	93	PSU	N1-C2-N3	4.69	120.11	115.17
40	L5	4312	PSU	N1-C2-N3	4.69	120.11	115.17
40	L5	1683	PSU	C4-N3-C2	-4.68	119.92	126.37
40	L5	5001	PSU	C4-N3-C2	-4.68	119.93	126.37
40	L5	4312	PSU	C4-N3-C2	-4.68	119.93	126.37
40	L5	3844	PSU	N1-C2-N3	4.68	120.10	115.17
40	L5	4628	PSU	C4-N3-C2	-4.67	119.93	126.37
40	L5	4532	PSU	N1-C2-N3	4.67	120.10	115.17
19	S2	1174	PSU	N1-C2-N3	4.67	120.09	115.17
19	S2	966	PSU	N1-C2-N3	4.67	120.09	115.17
40	L5	4442	PSU	C4-N3-C2	-4.67	119.94	126.37
19	S2	1244	PSU	C4-N3-C2	-4.67	119.94	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	C5-C4-N3	-4.67	120.29	126.72
19	S2	1045	PSU	C4-N3-C2	-4.66	119.95	126.37
19	S2	1177	PSU	N1-C2-N3	4.66	120.08	115.17
19	S2	686	PSU	N1-C2-N3	4.66	120.08	115.17
19	S2	93	PSU	C4-N3-C2	-4.64	119.98	126.37
19	S2	801	PSU	C4-N3-C2	-4.63	119.99	126.37
19	S2	1056	PSU	C4-N3-C2	-4.63	120.00	126.37
19	S2	109	PSU	N1-C2-N3	4.63	120.05	115.17
19	S2	866	PSU	N1-C2-N3	4.62	120.05	115.17
40	L5	4576	PSU	C4-N3-C2	-4.62	120.01	126.37
40	L5	1744	PSU	C4-N3-C2	-4.61	120.02	126.37
40	L5	4457	PSU	C4-N3-C2	-4.61	120.02	126.37
19	S2	1004	PSU	C4-N3-C2	-4.61	120.02	126.37
40	L5	4220	6MZ	N9-C8-N7	-4.60	107.41	113.94
40	L5	1792	PSU	C4-N3-C2	-4.60	120.03	126.37
19	S2	814	PSU	N1-C2-N3	4.60	120.02	115.17
19	S2	105	PSU	C4-N3-C2	-4.59	120.04	126.37
40	L5	4361	PSU	C4-N3-C2	-4.59	120.05	126.37
19	S2	1046	PSU	C4-N3-C2	-4.59	120.05	126.37
40	L5	1781	PSU	N1-C2-N3	4.59	120.01	115.17
40	L5	4471	PSU	N1-C2-N3	4.58	120.00	115.17
40	L5	4457	PSU	N1-C2-N3	4.58	120.00	115.17
40	L5	4576	PSU	N1-C2-N3	4.57	119.99	115.17
40	L5	4403	PSU	N1-C2-N3	4.57	119.98	115.17
42	L8	69	PSU	N1-C2-N3	4.57	119.98	115.17
40	L5	5001	PSU	N1-C2-N3	4.56	119.97	115.17
40	L5	2839	PSU	N1-C2-N3	4.54	119.96	115.17
40	L5	2839	PSU	C4-N3-C2	-4.54	120.12	126.37
40	L5	4689	PSU	C4-N3-C2	-4.54	120.12	126.37
40	L5	4532	PSU	C4-N3-C2	-4.53	120.13	126.37
40	L5	1744	PSU	N1-C2-N3	4.52	119.94	115.17
19	S2	1639	G7M	C2-N3-C4	4.51	120.07	112.30
19	S2	1248	B8N	C4-N3-C2	-4.50	120.09	125.62
40	L5	1781	PSU	C4-N3-C2	-4.49	120.18	126.37
40	L5	4471	PSU	C4-N3-C2	-4.46	120.23	126.37
40	L5	3818	UY1	N1-C2-N3	4.44	119.85	115.17
19	S2	1850	MA6	C3'-C2'-C1'	4.08	109.17	101.46
19	S2	1850	MA6	C4-C5-C6	4.07	120.12	115.91
19	S2	1850	MA6	C4-N9-C8	4.04	109.98	105.74
19	S2	1383	A2M	C3'-C2'-C1'	-4.03	95.08	102.81
19	S2	1639	G7M	C5-C4-N3	-3.99	120.61	128.15
19	S2	1639	G7M	C5-C6-N1	3.99	120.08	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	121	OMU	N3-C2-N1	3.98	120.07	114.89
19	S2	1851	MA6	C4-N9-C8	3.94	109.88	105.74
19	S2	1288	OMU	N3-C2-N1	3.94	120.02	114.89
40	L5	2837	OMU	N3-C2-N1	3.93	120.01	114.89
40	L5	3925	OMU	N3-C2-N1	3.93	120.00	114.89
40	L5	4220	6MZ	C9-N6-C6	-3.92	119.21	122.85
40	L5	4227	OMU	N3-C2-N1	3.92	120.00	114.89
19	S2	799	OMU	N3-C2-N1	3.90	119.97	114.89
19	S2	354	OMU	N3-C2-N1	3.85	119.90	114.89
19	S2	1326	OMU	N3-C2-N1	3.84	119.89	114.89
40	L5	4498	OMU	N3-C2-N1	3.83	119.88	114.89
19	S2	172	OMU	C5-C4-N3	3.82	120.15	114.80
19	S2	428	OMU	N3-C2-N1	3.80	119.83	114.89
19	S2	1442	OMU	N3-C2-N1	3.80	119.83	114.89
40	L5	4306	OMU	N3-C2-N1	3.79	119.83	114.89
19	S2	627	OMU	N3-C2-N1	3.76	119.78	114.89
19	S2	1850	MA6	N3-C4-N9	3.75	133.54	127.17
40	L5	2837	OMU	C5-C4-N3	3.73	120.03	114.80
40	L5	3718	A2M	C3'-C2'-C1'	-3.72	95.67	102.81
19	S2	116	OMU	N3-C2-N1	3.70	119.71	114.89
19	S2	1851	MA6	C4-C5-C6	3.70	119.73	115.91
19	S2	1326	OMU	C5-C4-N3	3.70	119.98	114.80
40	L5	3925	OMU	C5-C4-N3	3.70	119.98	114.80
19	S2	627	OMU	C5-C4-N3	3.69	119.97	114.80
40	L5	4620	OMU	N3-C2-N1	3.65	119.64	114.89
19	S2	1248	B8N	C1'-C5-C4	3.64	123.14	117.61
19	S2	799	OMU	C5-C4-N3	3.64	119.90	114.80
19	S2	172	OMU	N3-C2-N1	3.64	119.62	114.89
19	S2	428	OMU	C5-C4-N3	3.61	119.86	114.80
40	L5	4530	UR3	C5-C4-N3	3.58	119.76	115.04
40	L5	4227	OMU	C5-C4-N3	3.58	119.81	114.80
40	L5	4306	OMU	C5-C4-N3	3.56	119.79	114.80
40	L5	4620	OMU	C5-C4-N3	3.56	119.78	114.80
19	S2	354	OMU	C5-C4-N3	3.56	119.78	114.80
19	S2	1442	OMU	C5-C4-N3	3.54	119.76	114.80
40	L5	1871	A2M	C3'-C2'-C1'	-3.54	96.02	102.81
40	L5	4523	A2M	C3'-C2'-C1'	-3.53	96.04	102.81
40	L5	4498	OMU	C5-C4-N3	3.51	119.72	114.80
40	L5	3718	A2M	O3'-C3'-C2'	3.50	120.97	111.19
19	S2	1851	MA6	C2-N1-C6	3.49	120.36	111.83
19	S2	576	A2M	O3'-C3'-C2'	3.48	120.92	111.19
40	L5	3818	UY1	C6-C5-C4	3.46	120.51	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	N3-C4-N9	3.45	133.03	127.17
19	S2	116	OMU	C5-C4-N3	3.44	119.62	114.80
40	L5	4220	6MZ	N3-C4-N9	3.43	133.00	127.17
40	L5	4220	6MZ	C4-C5-C6	3.41	119.62	116.78
19	S2	1832	6MZ	C2-N3-C4	3.40	120.13	111.83
40	L5	4220	6MZ	C2-N3-C4	3.39	120.10	111.83
19	S2	1383	A2M	O3'-C3'-C2'	3.37	120.61	111.19
19	S2	99	A2M	C3'-C2'-C1'	-3.37	96.36	102.81
40	L5	3830	A2M	C3'-C2'-C1'	-3.36	96.37	102.81
19	S2	1850	MA6	C2-N1-C6	3.36	120.03	111.83
19	S2	1639	G7M	O6-C6-C5	-3.35	120.54	128.01
19	S2	1639	G7M	CN7-N7-C5	3.34	130.97	126.80
19	S2	121	OMU	C5-C4-N3	3.32	119.44	114.80
40	L5	1534	A2M	C3'-C2'-C1'	-3.31	96.46	102.81
19	S2	1288	OMU	C5-C4-N3	3.30	119.43	114.80
19	S2	99	A2M	O3'-C3'-C2'	3.28	120.36	111.19
19	S2	1832	6MZ	C4-N9-C8	3.28	109.18	105.74
40	L5	3785	A2M	C4'-O4'-C1'	-3.27	102.25	109.47
19	S2	1248	B8N	N3-C2-N1	3.26	120.70	116.72
40	L5	398	A2M	O3'-C3'-C2'	3.25	120.30	111.19
19	S2	1851	MA6	C2-N3-C4	3.21	119.67	111.83
19	S2	1832	6MZ	N3-C4-N9	3.20	132.61	127.17
40	L5	398	A2M	C3'-C2'-C1'	-3.20	96.69	102.81
19	S2	1851	MA6	C5-N7-C8	3.19	108.47	103.45
40	L5	2363	A2M	C3'-C2'-C1'	-3.19	96.69	102.81
19	S2	1832	6MZ	C5-N7-C8	3.19	108.46	103.45
40	L5	3785	A2M	O3'-C3'-C2'	3.17	120.05	111.19
40	L5	3818	UY1	C6-N1-C2	-3.16	119.76	122.69
40	L5	400	A2M	O3'-C3'-C2'	3.16	120.02	111.19
40	L5	4523	A2M	C4-N9-C1'	-3.14	119.28	126.63
40	L5	1871	A2M	O3'-C3'-C2'	3.14	119.98	111.19
19	S2	1850	MA6	C2-N3-C4	3.13	119.48	111.83
19	S2	576	A2M	C3'-C2'-C1'	-3.13	96.81	102.81
40	L5	2837	OMU	O4-C4-C5	-3.11	119.81	125.16
19	S2	159	A2M	O3'-C3'-C2'	3.10	119.86	111.19
40	L5	4523	A2M	O3'-C3'-C2'	3.08	119.82	111.19
19	S2	27	A2M	O3'-C3'-C2'	3.08	119.80	111.19
40	L5	1871	A2M	C4-N9-C1'	-3.08	119.44	126.63
19	S2	166	A2M	O3'-C3'-C2'	3.07	119.79	111.19
19	S2	1850	MA6	C5-N7-C8	3.07	108.28	103.45
40	L5	3830	A2M	O3'-C3'-C2'	3.07	119.79	111.19
40	L5	4220	6MZ	C4-N9-C8	3.06	108.95	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	2861	OMC	C1'-N1-C2	3.06	125.19	118.44
40	L5	1677	PSU	C6-C5-C4	3.06	120.24	118.17
19	S2	166	A2M	C3'-C2'-C1'	-3.05	96.96	102.81
40	L5	2787	A2M	O3'-C3'-C2'	3.03	119.67	111.19
40	L5	1683	PSU	O2-C2-N1	-3.03	119.67	122.79
40	L5	4220	6MZ	C5-N7-C8	3.02	108.20	103.45
19	S2	1031	A2M	O3'-C3'-C2'	3.02	119.63	111.19
40	L5	4689	PSU	O2-C2-N1	-3.02	119.68	122.79
19	S2	668	A2M	O3'-C3'-C2'	3.01	119.62	111.19
19	S2	1639	G7M	N9-C4-N3	3.00	131.96	125.95
19	S2	172	OMU	O4-C4-C5	-2.99	120.00	125.16
40	L5	1524	A2M	O3'-C3'-C2'	2.99	119.55	111.19
40	L5	3925	OMU	O4-C4-C5	-2.99	120.01	125.16
19	S2	1442	OMU	O4-C4-C5	-2.97	120.03	125.16
19	S2	468	A2M	O3'-C3'-C2'	2.97	119.50	111.19
19	S2	27	A2M	C3'-C2'-C1'	-2.97	97.12	102.81
19	S2	166	A2M	C4-N9-C1'	-2.97	119.69	126.63
19	S2	1832	6MZ	C4-C5-C6	2.96	119.24	116.78
19	S2	1383	A2M	C4-N9-C1'	-2.96	119.70	126.63
40	L5	4571	A2M	O3'-C3'-C2'	2.96	119.48	111.19
40	L5	3825	A2M	O3'-C3'-C2'	2.96	119.46	111.19
40	L5	2787	A2M	O4'-C1'-C2'	2.96	111.68	106.59
40	L5	4306	OMU	O4-C4-C5	-2.95	120.07	125.16
40	L5	2401	A2M	O3'-C3'-C2'	2.95	119.43	111.19
19	S2	428	OMU	O4-C4-C5	-2.94	120.10	125.16
40	L5	3785	A2M	C4-N9-C1'	-2.93	119.77	126.63
40	L5	1323	A2M	C2'-C1'-N9	2.93	118.57	113.75
40	L5	4628	PSU	O2-C2-N1	-2.93	119.77	122.79
40	L5	4689	PSU	C6-N1-C2	-2.92	119.98	122.69
40	L5	2363	A2M	O3'-C3'-C2'	2.92	119.37	111.19
19	S2	799	OMU	O4-C4-C5	-2.92	120.12	125.16
19	S2	1850	MA6	C1'-N9-C8	-2.92	120.61	127.09
19	S2	468	A2M	C3'-C2'-C1'	-2.91	97.24	102.81
19	S2	354	OMU	O4-C4-C5	-2.91	120.15	125.16
19	S2	627	OMU	O4-C4-C5	-2.90	120.16	125.16
40	L5	4227	OMU	O4-C4-C5	-2.90	120.16	125.16
40	L5	4620	OMU	O4-C4-C5	-2.89	120.17	125.16
40	L5	4498	OMU	O4-C4-C5	-2.89	120.18	125.16
40	L5	4590	A2M	C4-N9-C1'	-2.88	119.89	126.63
40	L5	1534	A2M	O3'-C3'-C2'	2.88	119.26	111.19
40	L5	4590	A2M	O3'-C3'-C2'	2.88	119.25	111.19
19	S2	1232	PSU	O2-C2-N1	-2.88	119.82	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1639	G7M	C2-N1-C6	-2.88	119.89	125.11
40	L5	4521	PSU	O2-C2-N1	-2.88	119.82	122.79
40	L5	4500	PSU	O2-C2-N1	-2.86	119.83	122.79
40	L5	2632	PSU	O2-C2-N1	-2.86	119.84	122.79
40	L5	4457	PSU	O2-C2-N1	-2.86	119.84	122.79
19	S2	116	OMU	O4-C4-C5	-2.85	120.24	125.16
19	S2	105	PSU	O2-C2-N1	-2.85	119.84	122.79
40	L5	4442	PSU	O2-C2-N1	-2.85	119.85	122.79
40	L5	3830	A2M	C4-N9-C1'	-2.85	119.96	126.63
40	L5	1326	A2M	O3'-C3'-C2'	2.85	119.17	111.19
19	S2	1244	PSU	O2-C2-N1	-2.85	119.85	122.79
40	L5	2815	A2M	C2'-C1'-N9	2.85	118.44	113.75
19	S2	1326	OMU	O4-C4-C5	-2.85	120.25	125.16
19	S2	468	A2M	C4-N9-C1'	-2.85	119.98	126.63
40	L5	4523	A2M	C1'-N9-C8	2.84	133.40	127.09
19	S2	1248	B8N	O4-C4-N3	-2.84	115.38	119.99
40	L5	1871	A2M	C1'-N9-C8	2.84	133.39	127.09
40	L5	1534	A2M	C4-N9-C1'	-2.84	120.00	126.63
40	L5	3867	A2M	C4-N9-C1'	-2.83	120.00	126.63
40	L5	4973	PSU	O2-C2-N1	-2.83	119.87	122.79
19	S2	681	PSU	O2-C2-N1	-2.83	119.87	122.79
40	L5	4636	PSU	O2-C2-N1	-2.82	119.88	122.79
40	L5	1782	PSU	O2-C2-N1	-2.81	119.89	122.79
19	S2	668	A2M	C4-N9-C1'	-2.81	120.06	126.63
40	L5	1326	A2M	C2'-C1'-N9	2.81	118.38	113.75
40	L5	2401	A2M	C4-N9-C1'	-2.81	120.07	126.63
19	S2	99	A2M	C4-N9-C1'	-2.80	120.08	126.63
40	L5	2401	A2M	C3'-C2'-C1'	-2.79	97.46	102.81
19	S2	121	OMU	O4-C4-C5	-2.79	120.35	125.16
40	L5	398	A2M	C4-N9-C1'	-2.79	120.11	126.63
19	S2	1081	PSU	O2-C2-N1	-2.78	119.92	122.79
40	L5	2632	PSU	C6-C5-C4	2.78	120.05	118.17
19	S2	1056	PSU	O2-C2-N1	-2.78	119.92	122.79
19	S2	649	PSU	O2-C2-N1	-2.78	119.92	122.79
40	L5	4312	PSU	O2-C2-N1	-2.77	119.93	122.79
40	L5	3822	PSU	O2-C2-N1	-2.77	119.93	122.79
19	S2	1174	PSU	O2-C2-N1	-2.77	119.93	122.79
40	L5	1860	PSU	O2-C2-N1	-2.77	119.94	122.79
19	S2	484	A2M	O3'-C3'-C2'	2.77	118.93	111.19
19	S2	801	PSU	O2-C2-N1	-2.76	119.94	122.79
19	S2	27	A2M	C4-N9-C1'	-2.76	120.17	126.63
40	L5	3808	OMC	C1'-N1-C2	2.75	124.52	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3853	PSU	O2-C2-N1	-2.75	119.95	122.79
40	L5	3637	PSU	O2-C2-N1	-2.74	119.96	122.79
19	S2	863	PSU	O2-C2-N1	-2.74	119.96	122.79
19	S2	1177	PSU	O2-C2-N1	-2.74	119.96	122.79
40	L5	4590	A2M	C3'-C2'-C1'	-2.74	97.57	102.81
19	S2	651	PSU	O2-C2-N1	-2.73	119.97	122.79
19	S2	1367	PSU	O2-C2-N1	-2.73	119.97	122.79
40	L5	2815	A2M	O3'-C3'-C2'	2.72	118.81	111.19
19	S2	1046	PSU	O2-C2-N1	-2.72	119.98	122.79
19	S2	668	A2M	O4'-C1'-C2'	2.72	111.27	106.59
40	L5	4972	PSU	O2-C2-N1	-2.72	119.98	122.79
40	L5	400	A2M	C4-N9-C1'	-2.72	120.28	126.63
19	S2	1004	PSU	O2-C2-N1	-2.71	119.99	122.79
19	S2	1383	A2M	C1'-N9-C8	2.71	133.11	127.09
40	L5	3867	A2M	O3'-C3'-C2'	2.71	118.77	111.19
40	L5	4576	PSU	O2-C2-N1	-2.71	120.00	122.79
19	S2	1288	OMU	O4-C4-C5	-2.70	120.50	125.16
19	S2	406	PSU	O2-C2-N1	-2.70	120.00	122.79
19	S2	1004	PSU	C6-N1-C2	-2.70	120.19	122.69
40	L5	4590	A2M	C1'-N9-C8	2.70	133.09	127.09
40	L5	4579	PSU	O2-C2-N1	-2.70	120.00	122.79
19	S2	105	PSU	C6-N1-C2	-2.70	120.19	122.69
19	S2	866	PSU	O2-C2-N1	-2.70	120.01	122.79
19	S2	1639	G7M	CN7-N7-C8	-2.69	120.71	124.79
40	L5	3920	PSU	O2-C2-N1	-2.69	120.01	122.79
40	L5	1862	PSU	O2-C2-N1	-2.69	120.02	122.79
40	L5	1536	PSU	O2-C2-N1	-2.69	120.02	122.79
40	L5	3639	PSU	O2-C2-N1	-2.69	120.02	122.79
19	S2	668	A2M	C1'-N9-C8	2.68	133.04	127.09
40	L5	3718	A2M	C4-N9-C1'	-2.68	120.36	126.63
42	L8	55	PSU	O2-C2-N1	-2.68	120.03	122.79
19	S2	166	A2M	C1'-N9-C8	2.68	133.04	127.09
40	L5	1792	PSU	O2-C2-N1	-2.67	120.03	122.79
40	L5	1323	A2M	O3'-C3'-C2'	2.67	118.67	111.19
40	L5	1744	PSU	O2-C2-N1	-2.67	120.03	122.79
40	L5	1323	A2M	C4-N9-C1'	-2.67	120.39	126.63
40	L5	4293	PSU	O2-C2-N1	-2.67	120.04	122.79
40	L5	1582	PSU	O2-C2-N1	-2.67	120.04	122.79
40	L5	2839	PSU	O2-C2-N1	-2.66	120.04	122.79
40	L5	4493	PSU	O2-C2-N1	-2.66	120.05	122.79
40	L5	398	A2M	C1'-N9-C8	2.66	132.99	127.09
40	L5	1677	PSU	O2-C2-N1	-2.65	120.05	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1031	A2M	C4-N9-C1'	-2.65	120.43	126.63
40	L5	3830	A2M	C1'-N9-C8	2.65	132.98	127.09
19	S2	27	A2M	C1'-N9-C8	2.65	132.97	127.09
40	L5	3884	PSU	O2-C2-N1	-2.65	120.06	122.79
40	L5	3867	A2M	C1'-N9-C8	2.65	132.97	127.09
40	L5	1534	A2M	C1'-N9-C8	2.64	132.96	127.09
19	S2	99	A2M	C1'-N9-C8	2.64	132.96	127.09
40	L5	1524	A2M	O4'-C1'-C2'	2.64	111.14	106.59
19	S2	159	A2M	C1'-N9-C8	2.64	132.96	127.09
40	L5	4628	PSU	C6-N1-C2	-2.64	120.24	122.69
19	S2	109	PSU	O2-C2-N1	-2.63	120.07	122.79
19	S2	484	A2M	C4-N9-C1'	-2.63	120.48	126.63
40	L5	3785	A2M	C1'-N9-C8	2.63	132.93	127.09
40	L5	3718	A2M	C1'-N9-C8	2.63	132.92	127.09
19	S2	966	PSU	O2-C2-N1	-2.62	120.08	122.79
40	L5	3851	PSU	O2-C2-N1	-2.62	120.08	122.79
19	S2	576	A2M	C4-N9-C1'	-2.62	120.50	126.63
40	L5	1781	PSU	O2-C2-N1	-2.62	120.08	122.79
40	L5	4353	PSU	O2-C2-N1	-2.62	120.08	122.79
40	L5	1326	A2M	C4-N9-C1'	-2.62	120.51	126.63
40	L5	1683	PSU	C6-N1-C2	-2.62	120.26	122.69
19	S2	686	PSU	O2-C2-N1	-2.61	120.09	122.79
40	L5	2363	A2M	C4-N9-C1'	-2.61	120.53	126.63
40	L5	3695	PSU	C6-N1-C2	-2.61	120.27	122.69
19	S2	1244	PSU	C6-N1-C2	-2.61	120.27	122.69
40	L5	4532	PSU	O2-C2-N1	-2.61	120.10	122.79
19	S2	1045	PSU	O2-C2-N1	-2.60	120.10	122.79
40	L5	4673	PSU	O2-C2-N1	-2.60	120.11	122.79
19	S2	1056	PSU	C6-N1-C2	-2.60	120.28	122.69
40	L5	4532	PSU	C6-N1-C2	-2.60	120.28	122.69
40	L5	4471	PSU	O2-C2-N1	-2.60	120.11	122.79
40	L5	4299	PSU	O2-C2-N1	-2.59	120.11	122.79
40	L5	2401	A2M	C1'-N9-C8	2.59	132.85	127.09
40	L5	4442	PSU	C6-N1-C2	-2.59	120.29	122.69
40	L5	400	A2M	C3'-C2'-C1'	-2.59	97.85	102.81
40	L5	5010	PSU	O2-C2-N1	-2.59	120.12	122.79
40	L5	1323	A2M	O4'-C1'-C2'	2.59	111.04	106.59
40	L5	4471	PSU	C6-N1-C2	-2.59	120.29	122.69
19	S2	1337	4AC	N4-C4-N3	2.58	118.06	113.87
40	L5	4296	PSU	O2-C2-N1	-2.58	120.13	122.79
19	S2	468	A2M	C1'-N9-C8	2.58	132.82	127.09
40	L5	4361	PSU	O2-C2-N1	-2.57	120.14	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	484	A2M	C1'-N9-C8	2.57	132.80	127.09
40	L5	3867	A2M	C3'-C2'-C1'	-2.57	97.89	102.81
19	S2	814	PSU	O2-C2-N1	-2.56	120.14	122.79
40	L5	4579	PSU	C6-N1-C2	-2.56	120.32	122.69
40	L5	3818	UY1	O2-C2-N1	-2.55	120.15	122.79
19	S2	681	PSU	C6-N1-C2	-2.55	120.32	122.69
19	S2	1031	A2M	C3'-C2'-C1'	-2.55	97.92	102.81
19	S2	1391	OMC	C1'-N1-C2	2.55	124.06	118.44
40	L5	400	A2M	C1'-N9-C8	2.53	132.72	127.09
19	S2	1031	A2M	C1'-N9-C8	2.53	132.72	127.09
40	L5	1534	A2M	C2'-C1'-N9	2.53	117.92	113.75
40	L5	1782	PSU	C6-N1-C2	-2.53	120.34	122.69
19	S2	159	A2M	C4-N9-C1'	-2.53	120.72	126.63
19	S2	93	PSU	O2-C2-N1	-2.53	120.18	122.79
40	L5	2363	A2M	C1'-N9-C8	2.53	132.70	127.09
19	S2	1288	OMU	C1'-N1-C2	2.52	122.12	117.59
40	L5	4431	PSU	O2-C2-N1	-2.52	120.19	122.79
40	L5	4571	A2M	C4-N9-C1'	-2.51	120.76	126.63
40	L5	3825	A2M	C4-N9-C1'	-2.51	120.76	126.63
40	L5	2839	PSU	C6-N1-C2	-2.51	120.36	122.69
42	L8	69	PSU	O2-C2-N1	-2.50	120.20	122.79
40	L5	1582	PSU	C6-N1-C2	-2.50	120.37	122.69
40	L5	4972	PSU	C6-N1-C2	-2.50	120.37	122.69
40	L5	3639	PSU	C6-N1-C2	-2.50	120.37	122.69
19	S2	801	PSU	C6-N1-C2	-2.50	120.37	122.69
40	L5	1323	A2M	C1'-N9-C8	2.50	132.63	127.09
40	L5	4571	A2M	C3'-C2'-C1'	-2.49	98.04	102.81
40	L5	4576	PSU	C6-N1-C2	-2.49	120.38	122.69
19	S2	1046	PSU	C6-N1-C2	-2.49	120.38	122.69
40	L5	4361	PSU	C6-N1-C2	-2.48	120.39	122.69
40	L5	3822	PSU	O4'-C1'-C2'	2.48	108.58	105.15
40	L5	4552	PSU	O2-C2-N1	-2.48	120.23	122.79
40	L5	4590	A2M	O4'-C1'-C2'	2.47	110.85	106.59
40	L5	3844	PSU	O2-C2-N1	-2.47	120.24	122.79
40	L5	5001	PSU	O2-C2-N1	-2.47	120.24	122.79
40	L5	4457	PSU	C6-N1-C2	-2.47	120.40	122.69
19	S2	1232	PSU	C6-N1-C2	-2.46	120.41	122.69
40	L5	3825	A2M	C3'-C2'-C1'	-2.46	98.10	102.81
19	S2	1851	MA6	C1'-N9-C8	-2.46	121.64	127.09
40	L5	4312	PSU	C6-N1-C2	-2.46	120.41	122.69
19	S2	1177	PSU	C6-N1-C2	-2.46	120.41	122.69
40	L5	1744	PSU	C6-N1-C2	-2.45	120.41	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	2861	OMC	C1'-N1-C6	-2.45	115.54	120.78
40	L5	2632	PSU	C6-N1-C2	-2.45	120.42	122.69
40	L5	3822	PSU	C6-N1-C2	-2.45	120.42	122.69
40	L5	4403	PSU	O2-C2-N1	-2.44	120.27	122.79
40	L5	1781	PSU	C6-N1-C2	-2.44	120.42	122.69
40	L5	2787	A2M	C4-N9-C1'	-2.44	120.92	126.63
40	L5	3920	PSU	C6-N1-C2	-2.44	120.43	122.69
19	S2	1174	PSU	C6-N1-C2	-2.43	120.43	122.69
19	S2	576	A2M	C1'-N9-C8	2.43	132.49	127.09
40	L5	3825	A2M	C1'-N9-C8	2.42	132.47	127.09
40	L5	4571	A2M	C1'-N9-C8	2.42	132.47	127.09
19	S2	863	PSU	C6-N1-C2	-2.42	120.45	122.69
19	S2	649	PSU	C6-N1-C2	-2.41	120.45	122.69
40	L5	4521	PSU	C6-N1-C2	-2.41	120.45	122.69
40	L5	4493	PSU	C6-C5-C4	2.41	119.80	118.17
40	L5	1326	A2M	O4'-C1'-C2'	2.40	110.72	106.59
40	L5	1792	PSU	C6-N1-C2	-2.40	120.46	122.69
40	L5	1326	A2M	C1'-N9-C8	2.39	132.41	127.09
40	L5	3884	PSU	C6-N1-C2	-2.39	120.47	122.69
42	L8	55	PSU	C6-N1-C2	-2.39	120.47	122.69
40	L5	4973	PSU	C6-N1-C2	-2.39	120.48	122.69
19	S2	651	PSU	C6-N1-C2	-2.38	120.48	122.69
40	L5	1862	PSU	C6-N1-C2	-2.37	120.49	122.69
40	L5	4220	6MZ	C5-C6-N1	2.37	120.69	118.15
40	L5	1860	PSU	C6-N1-C2	-2.36	120.50	122.69
40	L5	3637	PSU	C6-N1-C2	-2.36	120.50	122.69
40	L5	1536	PSU	C6-N1-C2	-2.36	120.50	122.69
19	S2	166	A2M	O4'-C1'-C2'	2.36	110.65	106.59
19	S2	1045	PSU	C6-N1-C2	-2.36	120.50	122.69
19	S2	93	PSU	C6-N1-C2	-2.36	120.50	122.69
40	L5	3785	A2M	O4'-C1'-N9	2.36	112.62	108.09
40	L5	4299	PSU	C6-N1-C2	-2.35	120.51	122.69
40	L5	1524	A2M	C4'-O4'-C1'	-2.35	104.27	109.47
19	S2	109	PSU	C6-N1-C2	-2.35	120.51	122.69
19	S2	966	PSU	C6-N1-C2	-2.34	120.52	122.69
19	S2	1081	PSU	C6-N1-C2	-2.34	120.52	122.69
40	L5	4552	PSU	C6-N1-C2	-2.34	120.52	122.69
40	L5	4293	PSU	C6-N1-C2	-2.33	120.53	122.69
40	L5	4431	PSU	C6-N1-C2	-2.33	120.53	122.69
40	L5	4552	PSU	C6-C5-C4	2.33	119.75	118.17
19	S2	406	PSU	C6-N1-C2	-2.33	120.53	122.69
19	S2	1367	PSU	C6-N1-C2	-2.33	120.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	5010	PSU	C6-N1-C2	-2.33	120.53	122.69
40	L5	1323	A2M	C3'-C2'-C1'	-2.31	98.38	102.81
40	L5	1524	A2M	C4-N9-C1'	-2.31	121.23	126.63
40	L5	1744	PSU	O4'-C1'-C2'	2.31	108.35	105.15
40	L5	4500	PSU	C6-N1-C2	-2.31	120.55	122.69
40	L5	1326	A2M	C3'-C2'-C1'	-2.30	98.40	102.81
40	L5	4442	PSU	O4'-C1'-C2'	2.30	108.33	105.15
42	L8	69	PSU	C6-N1-C2	-2.30	120.56	122.69
40	L5	4456	OMC	C1'-N1-C2	2.30	123.51	118.44
40	L5	1524	A2M	C1'-N9-C8	2.29	132.19	127.09
40	L5	4673	PSU	C6-N1-C2	-2.29	120.56	122.69
19	S2	1031	A2M	O4'-C1'-C2'	2.29	110.53	106.59
40	L5	4403	PSU	O4'-C1'-C2'	2.29	108.32	105.15
40	L5	4590	A2M	C6-C5-C4	-2.29	114.05	117.18
19	S2	866	PSU	C6-N1-C2	-2.29	120.57	122.69
19	S2	1232	PSU	C6-C5-C4	2.29	119.72	118.17
19	S2	686	PSU	C6-N1-C2	-2.28	120.57	122.69
40	L5	3853	PSU	C6-N1-C2	-2.28	120.57	122.69
40	L5	3825	A2M	O4'-C1'-C2'	2.28	110.52	106.59
19	S2	428	OMU	O2-C2-N1	-2.28	119.83	122.80
40	L5	3695	PSU	C6-C5-C4	2.28	119.71	118.17
19	S2	627	OMU	O2-C2-N1	-2.28	119.83	122.80
40	L5	4523	A2M	O4'-C1'-C2'	2.28	110.51	106.59
40	L5	4296	PSU	C6-N1-C2	-2.27	120.58	122.69
40	L5	4353	PSU	C6-N1-C2	-2.27	120.58	122.69
19	S2	484	A2M	O4'-C1'-C2'	2.27	110.50	106.59
40	L5	4530	UR3	C6-N1-C2	-2.27	119.94	121.80
19	S2	159	A2M	C2'-C1'-N9	2.27	117.48	113.75
40	L5	1677	PSU	O4'-C1'-C2'	2.26	108.28	105.15
19	S2	1326	OMU	O2-C2-N1	-2.26	119.85	122.80
19	S2	814	PSU	C6-N1-C2	-2.26	120.59	122.69
40	L5	4500	PSU	C6-C5-C4	2.26	119.70	118.17
40	L5	4523	A2M	C6-C5-C4	-2.26	114.09	117.18
40	L5	3851	PSU	C6-N1-C2	-2.26	120.59	122.69
19	S2	1442	OMU	C1'-N1-C2	2.26	121.65	117.59
40	L5	400	A2M	O4'-C1'-C2'	2.26	110.48	106.59
40	L5	4636	PSU	C6-N1-C2	-2.26	120.60	122.69
19	S2	484	A2M	O4'-C4'-C3'	2.25	109.63	105.15
40	L5	2787	A2M	C1'-N9-C8	2.25	132.09	127.09
40	L5	1322	1MA	N1-C6-N6	2.25	125.35	119.71
40	L5	3844	PSU	C6-N1-C2	-2.24	120.61	122.69
19	S2	468	A2M	O4'-C1'-C2'	2.24	110.45	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1081	PSU	C6-C5-C4	2.24	119.69	118.17
40	L5	4498	OMU	O2-C2-N1	-2.24	119.89	122.80
19	S2	1832	6MZ	C5-C6-N1	2.23	120.54	118.15
40	L5	3695	PSU	O2-C2-N1	-2.23	120.49	122.79
40	L5	5001	PSU	C6-N1-C2	-2.22	120.63	122.69
40	L5	4493	PSU	C6-N1-C2	-2.22	120.63	122.69
19	S2	1248	B8N	C31-N3-C4	2.22	120.32	117.18
19	S2	166	A2M	C6-C5-C4	-2.22	114.15	117.18
19	S2	354	OMU	O2-C2-N1	-2.22	119.91	122.80
40	L5	1871	A2M	C6-C5-C4	-2.22	114.15	117.18
40	L5	3785	A2M	C3'-C2'-C1'	-2.21	98.58	102.81
40	L5	3853	PSU	C6-C5-C4	2.21	119.66	118.17
19	S2	1832	6MZ	C3'-C2'-C1'	2.21	105.64	101.46
40	L5	4457	PSU	O4'-C1'-C2'	2.21	108.20	105.15
19	S2	1248	B8N	O4'-C1'-C2'	2.20	108.19	105.15
19	S2	468	A2M	C6-C5-C4	-2.20	114.18	117.18
19	S2	866	PSU	O4'-C1'-C2'	2.19	108.19	105.15
40	L5	4530	UR3	C1'-N1-C2	2.19	120.63	117.04
40	L5	3822	PSU	C6-C5-C4	2.19	119.65	118.17
40	L5	4972	PSU	C6-C5-C4	2.19	119.65	118.17
40	L5	3785	A2M	C6-C5-C4	-2.19	114.19	117.18
19	S2	1383	A2M	C6-C5-C4	-2.18	114.20	117.18
40	L5	3825	A2M	C2'-C1'-N9	2.18	117.34	113.75
40	L5	4403	PSU	C6-N1-C2	-2.18	120.67	122.69
40	L5	1782	PSU	C6-C5-C4	2.18	119.64	118.17
40	L5	4571	A2M	O4'-C1'-C2'	2.17	110.33	106.59
19	S2	406	PSU	O4'-C1'-C2'	2.17	108.15	105.15
40	L5	3639	PSU	C6-C5-C4	2.17	119.64	118.17
19	S2	668	A2M	O4'-C4'-C3'	2.17	109.45	105.15
19	S2	1248	B8N	O4-C4-C5	-2.16	118.83	122.58
19	S2	159	A2M	O3'-C3'-C4'	-2.16	104.87	111.08
40	L5	3867	A2M	C6-C5-C4	-2.16	114.23	117.18
19	S2	1031	A2M	C6-C5-C4	-2.16	114.23	117.18
40	L5	1677	PSU	C6-N1-C2	-2.16	120.69	122.69
40	L5	4442	PSU	C6-C5-C4	2.16	119.63	118.17
19	S2	649	PSU	C6-C5-C4	2.16	119.63	118.17
40	L5	2815	A2M	O4'-C4'-C3'	2.16	109.43	105.15
40	L5	1871	A2M	O4'-C1'-C2'	2.15	110.30	106.59
19	S2	27	A2M	C6-C5-C4	-2.14	114.25	117.18
40	L5	4227	OMU	O2-C2-N1	-2.14	120.01	122.80
40	L5	1534	A2M	C6-C5-C4	-2.14	114.26	117.18
40	L5	3701	OMC	C1'-N1-C2	2.13	123.15	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3785	A2M	C5-C6-N1	2.13	122.92	117.51
40	L5	398	A2M	C6-C5-C4	-2.13	114.27	117.18
19	S2	121	OMU	O2-C2-N1	-2.13	120.03	122.80
40	L5	3830	A2M	C6-C5-C4	-2.13	114.28	117.18
19	S2	1832	6MZ	C4-C5-N7	-2.12	108.15	110.58
40	L5	2787	A2M	O4'-C4'-C3'	2.12	109.37	105.15
40	L5	4431	PSU	C6-C5-C4	2.12	119.61	118.17
19	S2	27	A2M	O4'-C1'-C2'	2.12	110.24	106.59
40	L5	400	A2M	C6-C5-C4	-2.12	114.28	117.18
40	L5	3825	A2M	C6-C5-C4	-2.12	114.29	117.18
40	L5	4636	PSU	C6-C5-C4	2.11	119.60	118.17
40	L5	4353	PSU	C6-C5-C4	2.11	119.60	118.17
19	S2	1639	G7M	N9-C8-N7	-2.11	107.36	112.48
40	L5	3637	PSU	C6-C5-C4	2.11	119.60	118.17
40	L5	3925	OMU	O2-C2-N1	-2.10	120.07	122.80
40	L5	4576	PSU	O4'-C1'-C2'	2.10	108.05	105.15
19	S2	966	PSU	O4'-C1'-C2'	2.09	108.05	105.15
40	L5	3785	A2M	C2-N1-C6	-2.09	115.29	118.73
40	L5	2401	A2M	C6-C5-C4	-2.09	114.32	117.18
40	L5	2363	A2M	C2-N1-C6	-2.09	115.29	118.73
40	L5	1582	PSU	C6-C5-C4	2.09	119.58	118.17
40	L5	2363	A2M	O4'-C1'-C2'	2.09	110.19	106.59
40	L5	1534	A2M	C2-N1-C6	-2.09	115.30	118.73
40	L5	4296	PSU	C6-C5-C4	2.09	119.58	118.17
19	S2	668	A2M	C6-C5-C4	-2.09	114.33	117.18
40	L5	1524	A2M	C2-N1-C6	-2.08	115.31	118.73
40	L5	4571	A2M	C2-N1-C6	-2.08	115.31	118.73
40	L5	1323	A2M	C6-C5-C4	-2.08	114.34	117.18
40	L5	3867	A2M	O4'-C1'-C2'	2.08	110.17	106.59
19	S2	99	A2M	C6-C5-C4	-2.08	114.34	117.18
40	L5	4636	PSU	O4'-C1'-C2'	2.08	108.02	105.15
19	S2	1031	A2M	C5-C6-N1	2.07	122.78	117.51
40	L5	3808	OMC	C1'-N1-C6	-2.07	116.35	120.78
19	S2	1081	PSU	O4'-C1'-C2'	2.07	108.02	105.15
40	L5	4521	PSU	C6-C5-C4	2.07	119.57	118.17
40	L5	2837	OMU	O2-C2-N1	-2.07	120.10	122.80
40	L5	2815	A2M	C5-C6-N1	2.07	122.77	117.51
40	L5	4523	A2M	C4'-O4'-C1'	-2.07	104.90	109.47
40	L5	3695	PSU	O4'-C1'-C2'	2.07	108.01	105.15
19	S2	159	A2M	C2-N1-C6	-2.07	115.33	118.73
40	L5	2815	A2M	C2-N1-C6	-2.07	115.34	118.73
40	L5	1534	A2M	C5-C6-N1	2.06	122.75	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	L8	69	PSU	O4'-C1'-C2'	2.06	108.00	105.15
40	L5	1524	A2M	C2'-C1'-N9	2.06	117.14	113.75
40	L5	398	A2M	C5-C6-N1	2.06	122.73	117.51
40	L5	3718	A2M	C6-C5-C4	-2.06	114.37	117.18
19	S2	27	A2M	C5-C6-N1	2.05	122.72	117.51
40	L5	2815	A2M	O4'-C1'-C2'	2.05	110.12	106.59
40	L5	2401	A2M	C2-N1-C6	-2.05	115.36	118.73
40	L5	3867	A2M	C2-N1-C6	-2.05	115.36	118.73
40	L5	3830	A2M	O4'-C1'-C2'	2.04	110.11	106.59
40	L5	2401	A2M	C5-C6-N1	2.04	122.70	117.51
40	L5	398	A2M	C2-N1-C6	-2.04	115.37	118.73
40	L5	1326	A2M	C2-N1-C6	-2.04	115.38	118.73
40	L5	3718	A2M	C2-N1-C6	-2.04	115.38	118.73
40	L5	4293	PSU	C6-C5-C4	2.04	119.55	118.17
19	S2	576	A2M	C6-C5-C4	-2.04	114.39	117.18
19	S2	468	A2M	C5-C6-N1	2.04	122.69	117.51
40	L5	2351	OMC	C1'-N1-C2	2.04	122.94	118.44
40	L5	3825	A2M	C5-C6-N1	2.04	122.68	117.51
40	L5	1323	A2M	C5-C6-N1	2.04	122.68	117.51
40	L5	2824	OMC	C1'-N1-C2	2.03	122.93	118.44
40	L5	3920	PSU	O4'-C1'-C2'	2.03	107.97	105.15
19	S2	159	A2M	O4'-C1'-C2'	2.03	110.09	106.59
40	L5	1323	A2M	C2-N1-C6	-2.03	115.39	118.73
19	S2	484	A2M	C6-C5-C4	-2.03	114.40	117.18
19	S2	484	A2M	C2-N1-C6	-2.03	115.39	118.73
40	L5	2363	A2M	C6-C5-C4	-2.03	114.41	117.18
19	S2	1832	6MZ	C9-N6-C6	-2.03	120.97	122.85
19	S2	159	A2M	C5-C6-N1	2.03	122.66	117.51
19	S2	1383	A2M	C5-C6-N1	2.03	122.66	117.51
19	S2	166	A2M	C5-C6-N1	2.02	122.65	117.51
40	L5	2815	A2M	C4-N9-C1'	-2.02	121.90	126.63
19	S2	484	A2M	C5-C6-N1	2.02	122.65	117.51
40	L5	2363	A2M	C5-C6-N1	2.02	122.64	117.51
40	L5	1524	A2M	C5-C6-N1	2.02	122.64	117.51
40	L5	3718	A2M	C5-C6-N1	2.02	122.64	117.51
40	L5	3867	A2M	C5-C6-N1	2.02	122.63	117.51
40	L5	2815	A2M	C1'-N9-C8	2.02	131.57	127.09
40	L5	398	A2M	O4'-C1'-C2'	2.02	110.06	106.59
40	L5	4571	A2M	C5-C6-N1	2.02	122.63	117.51
40	L5	2787	A2M	C2-N1-C6	-2.02	115.42	118.73
19	S2	99	A2M	C5-C6-N1	2.02	122.63	117.51
40	L5	1534	A2M	O3'-C3'-C4'	-2.01	105.30	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4628	PSU	O4'-C1'-C2'	2.01	107.94	105.15
19	S2	27	A2M	C2-N1-C6	-2.01	115.42	118.73
40	L5	3920	PSU	C6-C5-C4	2.01	119.53	118.17
19	S2	1031	A2M	C2-N1-C6	-2.01	115.43	118.73
40	L5	1326	A2M	O4'-C4'-C3'	2.01	109.14	105.15
40	L5	4571	A2M	C2'-C1'-N9	2.01	117.06	113.75
40	L5	3830	A2M	C5-C6-N1	2.01	122.61	117.51
40	L5	4523	A2M	C5-C6-N1	2.01	122.61	117.51
40	L5	2632	PSU	O4'-C1'-C2'	2.01	107.93	105.15
40	L5	3825	A2M	C2-N1-C6	-2.01	115.43	118.73
19	S2	99	A2M	C2-N1-C6	-2.01	115.43	118.73
40	L5	2787	A2M	C5-C6-N1	2.01	122.60	117.51
40	L5	1326	A2M	C5-C6-N1	2.00	122.60	117.51
19	S2	668	A2M	C2-N1-C6	-2.00	115.44	118.73
19	S2	1367	PSU	C6-C5-C4	2.00	119.53	118.17
19	S2	1850	MA6	C2'-C3'-C4'	2.00	106.48	102.61

There are no chirality outliers.

All (163) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	L8	75	OMG	C1'-C2'-O2'-CM2
19	S2	27	A2M	C1'-C2'-O2'-CM'
19	S2	159	A2M	C1'-C2'-O2'-CM'
19	S2	354	OMU	C1'-C2'-O2'-CM2
19	S2	468	A2M	C1'-C2'-O2'-CM'
19	S2	484	A2M	C1'-C2'-O2'-CM'
19	S2	576	A2M	C1'-C2'-O2'-CM'
19	S2	601	OMG	C1'-C2'-O2'-CM2
19	S2	644	OMG	O4'-C4'-C5'-O5'
19	S2	644	OMG	C1'-C2'-O2'-CM2
19	S2	668	A2M	C1'-C2'-O2'-CM'
19	S2	683	OMG	O4'-C4'-C5'-O5'
19	S2	683	OMG	C3'-C4'-C5'-O5'
19	S2	863	PSU	O4'-C4'-C5'-O5'
19	S2	1031	A2M	C1'-C2'-O2'-CM'
19	S2	1272	OMC	C3'-C4'-C5'-O5'
19	S2	1272	OMC	O4'-C4'-C5'-O5'
19	S2	1288	OMU	C3'-C4'-C5'-O5'
19	S2	1288	OMU	O4'-C4'-C5'-O5'
19	S2	1328	OMG	C1'-C2'-O2'-CM2
19	S2	1337	4AC	N3-C4-N4-C7

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Mol	Chain	Res	Type	Atoms
19	S2	1383	A2M	C1'-C2'-O2'-CM'
19	S2	1442	OMU	C1'-C2'-O2'-CM2
19	S2	1442	OMU	O4'-C4'-C5'-O5'
19	S2	1832	6MZ	C5-C6-N6-C9
19	S2	1832	6MZ	N1-C6-N6-C9
40	L5	1316	OMG	C1'-C2'-O2'-CM2
40	L5	1323	A2M	C1'-C2'-O2'-CM'
40	L5	1326	A2M	O4'-C4'-C5'-O5'
40	L5	1326	A2M	C3'-C4'-C5'-O5'
40	L5	1326	A2M	C1'-C2'-O2'-CM'
40	L5	1340	OMC	C1'-C2'-O2'-CM2
40	L5	1524	A2M	O4'-C4'-C5'-O5'
40	L5	1524	A2M	C1'-C2'-O2'-CM'
40	L5	1536	PSU	C3'-C4'-C5'-O5'
40	L5	1536	PSU	O4'-C4'-C5'-O5'
40	L5	1625	OMG	O4'-C4'-C5'-O5'
40	L5	2351	OMC	C1'-C2'-O2'-CM2
40	L5	2364	OMG	C1'-C2'-O2'-CM2
40	L5	2401	A2M	C1'-C2'-O2'-CM'
40	L5	2422	OMC	C1'-C2'-O2'-CM2
40	L5	2787	A2M	C1'-C2'-O2'-CM'
40	L5	2861	OMC	C1'-C2'-O2'-CM2
40	L5	3701	OMC	O4'-C4'-C5'-O5'
40	L5	3718	A2M	C1'-C2'-O2'-CM'
40	L5	3744	OMG	C1'-C2'-O2'-CM2
40	L5	3792	OMG	O4'-C4'-C5'-O5'
40	L5	3822	PSU	O4'-C4'-C5'-O5'
40	L5	3825	A2M	C1'-C2'-O2'-CM'
40	L5	3830	A2M	C1'-C2'-O2'-CM'
40	L5	3867	A2M	C1'-C2'-O2'-CM'
40	L5	4220	6MZ	O4'-C4'-C5'-O5'
40	L5	4447	5MC	C2'-C1'-N1-C2
40	L5	4447	5MC	C2'-C1'-N1-C6
40	L5	4500	PSU	O4'-C4'-C5'-O5'
40	L5	4590	A2M	O4'-C4'-C5'-O5'
40	L5	4590	A2M	C1'-C2'-O2'-CM'
40	L5	4620	OMU	C1'-C2'-O2'-CM2
40	L5	4636	PSU	C2'-C1'-C5-C4
40	L5	4637	OMG	C1'-C2'-O2'-CM2
19	S2	99	A2M	O4'-C4'-C5'-O5'
19	S2	576	A2M	O4'-C4'-C5'-O5'
19	S2	576	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
19	S2	799	OMU	C3'-C4'-C5'-O5'
19	S2	799	OMU	O4'-C4'-C5'-O5'
19	S2	801	PSU	C3'-C4'-C5'-O5'
19	S2	863	PSU	C3'-C4'-C5'-O5'
40	L5	1524	A2M	C3'-C4'-C5'-O5'
40	L5	3822	PSU	C3'-C4'-C5'-O5'
40	L5	4500	PSU	C3'-C4'-C5'-O5'
40	L5	4590	A2M	C3'-C4'-C5'-O5'
40	L5	4618	OMG	C3'-C4'-C5'-O5'
19	S2	172	OMU	O4'-C4'-C5'-O5'
19	S2	1045	PSU	C3'-C4'-C5'-O5'
19	S2	1045	PSU	O4'-C4'-C5'-O5'
19	S2	1248	B8N	O4'-C4'-C5'-O5'
19	S2	1442	OMU	C3'-C4'-C5'-O5'
19	S2	1639	G7M	O4'-C4'-C5'-O5'
19	S2	1639	G7M	C3'-C4'-C5'-O5'
40	L5	2401	A2M	O4'-C4'-C5'-O5'
40	L5	2787	A2M	C3'-C4'-C5'-O5'
40	L5	3701	OMC	C3'-C4'-C5'-O5'
40	L5	4523	A2M	O4'-C4'-C5'-O5'
40	L5	4618	OMG	O4'-C4'-C5'-O5'
40	L5	4637	OMG	O4'-C4'-C5'-O5'
40	L5	4637	OMG	C3'-C4'-C5'-O5'
40	L5	2787	A2M	C2'-C1'-N9-C8
19	S2	644	OMG	C3'-C4'-C5'-O5'
40	L5	1323	A2M	O4'-C4'-C5'-O5'
40	L5	1625	OMG	C3'-C4'-C5'-O5'
40	L5	3792	OMG	C3'-C4'-C5'-O5'
40	L5	4220	6MZ	C3'-C4'-C5'-O5'
19	S2	99	A2M	C3'-C4'-C5'-O5'
19	S2	668	A2M	O4'-C4'-C5'-O5'
19	S2	668	A2M	C3'-C4'-C5'-O5'
40	L5	2401	A2M	C3'-C4'-C5'-O5'
19	S2	1248	B8N	N34-C33-C34-O36
40	L5	2787	A2M	C2'-C1'-N9-C4
19	S2	801	PSU	O4'-C4'-C5'-O5'
19	S2	867	OMG	C3'-C4'-C5'-O5'
19	S2	1383	A2M	O4'-C4'-C5'-O5'
40	L5	2422	OMC	O4'-C4'-C5'-O5'
19	S2	1851	MA6	C3'-C4'-C5'-O5'
40	L5	3899	OMG	C3'-C4'-C5'-O5'
40	L5	4523	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	L5	3701	OMC	O4'-C1'-N1-C2
40	L5	4590	A2M	C4'-C5'-O5'-P
19	S2	172	OMU	C3'-C4'-C5'-O5'
19	S2	1248	B8N	C3'-C4'-C5'-O5'
40	L5	1323	A2M	C3'-C4'-C5'-O5'
40	L5	3701	OMC	O4'-C1'-N1-C6
19	S2	1490	OMG	C1'-C2'-O2'-CM2
40	L5	2424	OMG	C1'-C2'-O2'-CM2
19	S2	1383	A2M	C3'-C4'-C5'-O5'
40	L5	2422	OMC	C3'-C4'-C5'-O5'
40	L5	4447	5MC	O4'-C1'-N1-C6
19	S2	1703	OMC	O4'-C4'-C5'-O5'
19	S2	428	OMU	C2'-C1'-N1-C6
19	S2	644	OMG	C4'-C5'-O5'-P
40	L5	1534	A2M	C4'-C5'-O5'-P
40	L5	3818	UY1	C4'-C5'-O5'-P
40	L5	3887	OMC	C4'-C5'-O5'-P
40	L5	4500	PSU	C4'-C5'-O5'-P
19	S2	406	PSU	O4'-C1'-C5-C4
19	S2	1248	B8N	O4'-C1'-C5-C4
40	L5	1677	PSU	O4'-C1'-C5-C4
40	L5	3822	PSU	O4'-C1'-C5-C4
40	L5	4521	PSU	O4'-C1'-C5-C4
40	L5	4636	PSU	O4'-C1'-C5-C4
40	L5	3792	OMG	C4'-C5'-O5'-P
19	S2	867	OMG	O4'-C4'-C5'-O5'
40	L5	2787	A2M	O4'-C4'-C5'-O5'
40	L5	4447	5MC	O4'-C1'-N1-C2
19	S2	801	PSU	C4'-C5'-O5'-P
19	S2	867	OMG	C4'-C5'-O5'-P
40	L5	3844	PSU	C4'-C5'-O5'-P
40	L5	2876	OMG	C3'-C2'-O2'-CM2
40	L5	3782	5MC	O4'-C4'-C5'-O5'
40	L5	3899	OMG	O4'-C4'-C5'-O5'
19	S2	1490	OMG	C4'-C5'-O5'-P
19	S2	428	OMU	O4'-C1'-N1-C6
19	S2	462	OMC	C1'-C2'-O2'-CM2
40	L5	3925	OMU	C1'-C2'-O2'-CM2
40	L5	398	A2M	O4'-C4'-C5'-O5'
40	L5	4296	PSU	C3'-C4'-C5'-O5'
19	S2	1248	B8N	O4'-C1'-C5-C6
40	L5	3822	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
19	S2	627	OMU	O4'-C1'-N1-C6
19	S2	627	OMU	C2'-C1'-N1-C6
19	S2	576	A2M	C4'-C5'-O5'-P
40	L5	2364	OMG	O4'-C4'-C5'-O5'
19	S2	428	OMU	O4'-C1'-N1-C2
40	L5	2861	OMC	C2'-C1'-N1-C2
19	S2	1248	B8N	N3-C31-C32-C33
19	S2	517	OMC	C3'-C4'-C5'-O5'
19	S2	1081	PSU	C4'-C5'-O5'-P
40	L5	1625	OMG	C4'-C5'-O5'-P
40	L5	3899	OMG	C4'-C5'-O5'-P
19	S2	1288	OMU	C2'-C1'-N1-C2
19	S2	1248	B8N	N34-C33-C34-O35
40	L5	2861	OMC	O4'-C4'-C5'-O5'
40	L5	3785	A2M	O4'-C4'-C5'-O5'
40	L5	4296	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

94 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	517	OMC	1	0
40	L5	1871	A2M	1	0
19	S2	406	PSU	1	0
19	S2	1851	MA6	2	0
40	L5	4471	PSU	1	0
19	S2	354	OMU	3	0
19	S2	1328	OMG	1	0
19	S2	509	OMG	3	0
42	L8	69	PSU	1	0
40	L5	1683	PSU	2	0
40	L5	4456	OMC	1	0
19	S2	462	OMC	1	0
19	S2	172	OMU	1	0
19	S2	1031	A2M	2	0
40	L5	2363	A2M	1	0
40	L5	2351	OMC	3	0
19	S2	428	OMU	1	0
40	L5	4532	PSU	2	0
40	L5	4392	OMG	2	0
19	S2	1337	4AC	3	0
40	L5	1340	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	2876	OMG	1	0
19	S2	863	PSU	1	0
40	L5	4576	PSU	1	0
40	L5	3841	OMC	1	0
40	L5	2422	OMC	2	0
40	L5	3867	A2M	4	0
40	L5	400	A2M	1	0
40	L5	1744	PSU	1	0
40	L5	4457	PSU	2	0
40	L5	1677	PSU	1	0
19	S2	1383	A2M	2	0
40	L5	4620	OMU	3	0
40	L5	3920	PSU	3	0
40	L5	5010	PSU	2	0
40	L5	3884	PSU	1	0
19	S2	121	OMU	2	0
40	L5	1323	A2M	2	0
40	L5	3744	OMG	1	0
19	S2	1232	PSU	1	0
40	L5	2364	OMG	1	0
40	L5	3830	A2M	1	0
40	L5	3718	A2M	4	0
19	S2	1244	PSU	1	0
40	L5	1326	A2M	2	0
19	S2	649	PSU	1	0
40	L5	4637	OMG	3	0
42	L8	75	OMG	2	0
40	L5	3822	PSU	1	0
19	S2	1004	PSU	2	0
19	S2	468	A2M	3	0
19	S2	644	OMG	2	0
40	L5	4494	OMG	2	0
19	S2	109	PSU	1	0
19	S2	1842	4AC	3	0
19	S2	866	PSU	2	0
40	L5	1316	OMG	1	0
40	L5	2424	OMG	1	0
19	S2	668	A2M	3	0
40	L5	3785	A2M	1	0
19	S2	484	A2M	3	0
19	S2	1174	PSU	2	0
19	S2	681	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	3825	A2M	4	0
40	L5	4220	6MZ	1	0
40	L5	4579	PSU	2	0
19	S2	1391	OMC	1	0
19	S2	436	OMG	1	0
40	L5	2815	A2M	1	0
19	S2	1490	OMG	2	0
40	L5	4623	OMG	2	0
19	S2	116	OMU	1	0
40	L5	4523	A2M	2	0
19	S2	166	A2M	1	0
40	L5	2787	A2M	2	0
19	S2	1850	MA6	4	0
40	L5	2401	A2M	1	0
19	S2	159	A2M	5	0
40	L5	4493	PSU	2	0
40	L5	4353	PSU	1	0
40	L5	3818	UY1	2	0
40	L5	398	A2M	1	0
40	L5	4571	A2M	3	0
19	S2	576	A2M	3	0
40	L5	4442	PSU	1	0
40	L5	1536	PSU	1	0
40	L5	2804	OMC	2	0
40	L5	4196	OMG	1	0
19	S2	601	OMG	3	0
19	S2	867	OMG	3	0
40	L5	4403	PSU	1	0
40	L5	4590	A2M	1	0
19	S2	27	A2M	3	0
40	L5	4689	PSU	1	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
88	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.83	0
88	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPM	L5	5266	-	13,13,13	0.35	0	12,12,12	0.92	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	1.02	0
88	SPD	L5	5282	-	9,9,9	0.33	0	8,8,8	0.82	0
88	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.89	0
88	SPD	L5	5291	-	9,9,9	0.32	0	8,8,8	0.81	0
87	SPM	L5	5290	-	13,13,13	0.35	0	12,12,12	0.82	0
88	SPD	L8	203	-	9,9,9	0.33	0	8,8,8	0.84	0
89	3HE	L5	5293	40	21,21,21	0.49	0	23,30,30	1.10	2 (8%)
88	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.83	0
88	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.80	0
87	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.95	0
90	HMT	L5	5294	-	41,43,43	0.73	1 (2%)	43,66,66	0.64	0
87	SPM	L5	5287	-	13,13,13	0.35	0	12,12,12	0.95	0
87	SPM	L5	5262	-	13,13,13	0.35	0	12,12,12	1.01	0
88	SPD	L5	5260	-	9,9,9	0.32	0	8,8,8	0.90	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.89	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
88	SPD	L5	5289	-	-	2/7/7/7	-
88	SPD	L5	5286	-	-	2/7/7/7	-
87	SPM	L5	5266	-	-	3/11/11/11	-
87	SPM	L5	5258	-	-	2/11/11/11	-
88	SPD	L5	5282	-	-	1/7/7/7	-
88	SPD	L5	5283	-	-	1/7/7/7	-
88	SPD	L5	5288	-	-	1/7/7/7	-
88	SPD	L5	5291	-	-	2/7/7/7	-
87	SPM	L5	5290	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L8	203	-	-	1/7/7/7	-
89	3HE	L5	5293	40	-	6/8/36/36	0/2/2/2
88	SPD	L5	5284	-	-	2/7/7/7	-
88	SPD	L5	5285	-	-	2/7/7/7	-
87	SPM	L5	5263	-	-	2/11/11/11	-
90	HMT	L5	5294	-	-	0/27/74/74	0/5/5/5
87	SPM	L5	5287	-	-	2/11/11/11	-
87	SPM	L5	5262	-	-	2/11/11/11	-
88	SPD	L5	5260	-	-	1/7/7/7	-
87	SPM	L5	5292	-	-	2/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5294	HMT	C20-C19	-3.18	1.49	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	L5	5293	3HE	C2-C3-C4	2.33	114.30	109.66
89	L5	5293	3HE	C6-C5-C4	2.24	111.99	108.29

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5293	3HE	C4-C5-C7-C8
89	L5	5293	3HE	C6-C5-C7-C8
87	L5	5266	SPM	C2-C3-C4-N5
87	L5	5290	SPM	N10-C11-C12-C13
87	L5	5287	SPM	C12-C11-N10-C9
88	L8	203	SPD	C4-C5-N6-C7
88	L5	5284	SPD	C2-C3-C4-C5
88	L5	5289	SPD	C4-C5-N6-C7
89	L5	5293	3HE	C4-C5-C7-O3
88	L5	5285	SPD	C2-C3-C4-C5
87	L5	5292	SPM	C6-C7-C8-C9
88	L5	5286	SPD	C8-C7-N6-C5
87	L5	5263	SPM	C2-C3-C4-N5
87	L5	5287	SPM	N1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
88	L5	5286	SPD	C4-C5-N6-C7
89	L5	5293	3HE	C7-C8-C9-C10
87	L5	5266	SPM	C6-C7-C8-C9
87	L5	5258	SPM	C6-C7-C8-C9
87	L5	5290	SPM	C8-C9-N10-C11
88	L5	5282	SPD	C2-C3-C4-C5
88	L5	5285	SPD	C3-C4-C5-N6
88	L5	5289	SPD	C3-C4-C5-N6
87	L5	5262	SPM	C7-C6-N5-C4
89	L5	5293	3HE	C7-C8-C9-C13
87	L5	5263	SPM	N1-C2-C3-C4
88	L5	5291	SPD	C8-C7-N6-C5
87	L5	5258	SPM	C3-C4-N5-C6
88	L5	5288	SPD	C2-C3-C4-C5
88	L5	5283	SPD	C3-C4-C5-N6
87	L5	5266	SPM	C3-C4-N5-C6
88	L5	5260	SPD	N6-C7-C8-C9
87	L5	5292	SPM	C7-C6-N5-C4
88	L5	5284	SPD	N1-C2-C3-C4
89	L5	5293	3HE	C6-C5-C7-O3
87	L5	5262	SPM	C2-C3-C4-N5
88	L5	5291	SPD	C4-C5-N6-C7
87	L5	5290	SPM	C6-C7-C8-C9

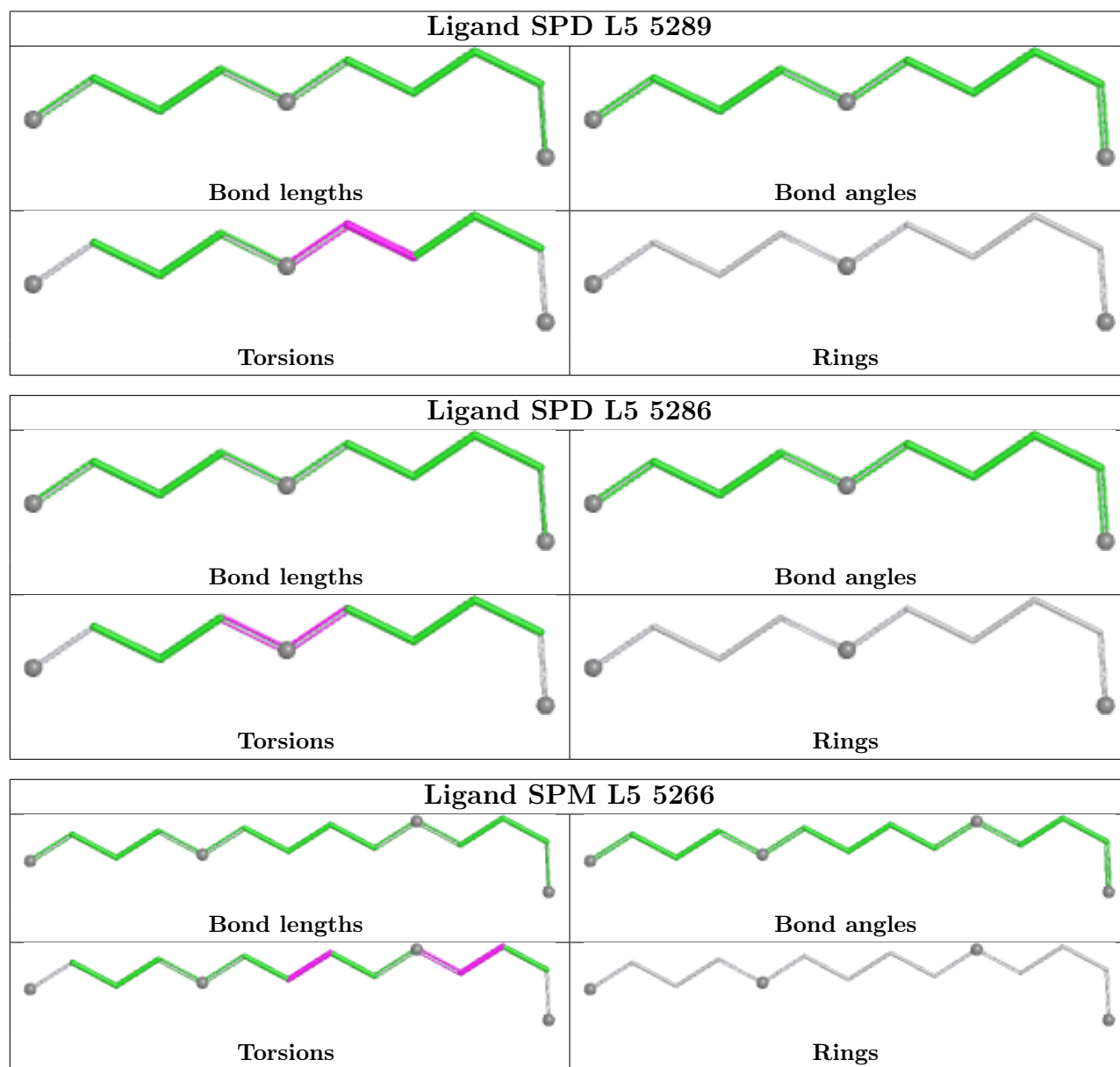
There are no ring outliers.

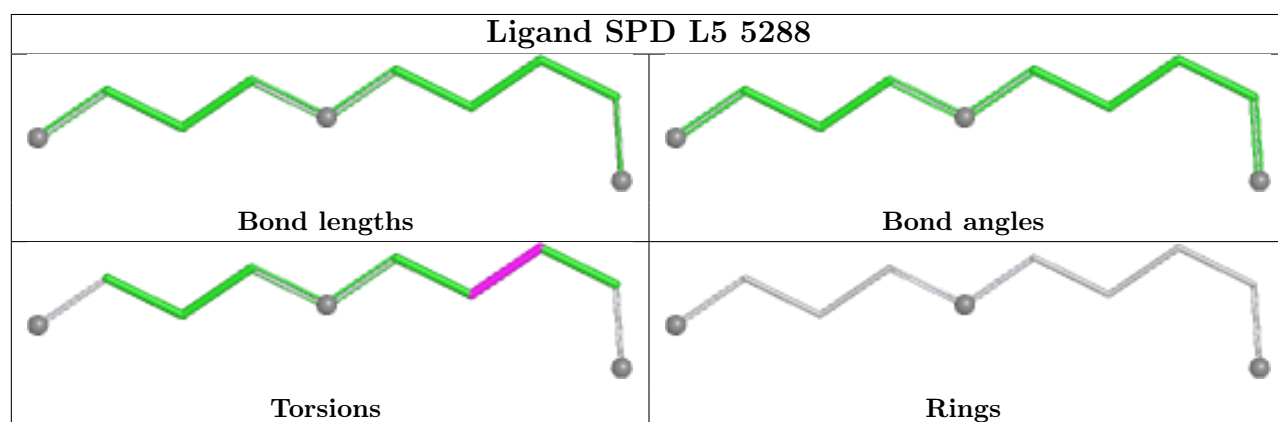
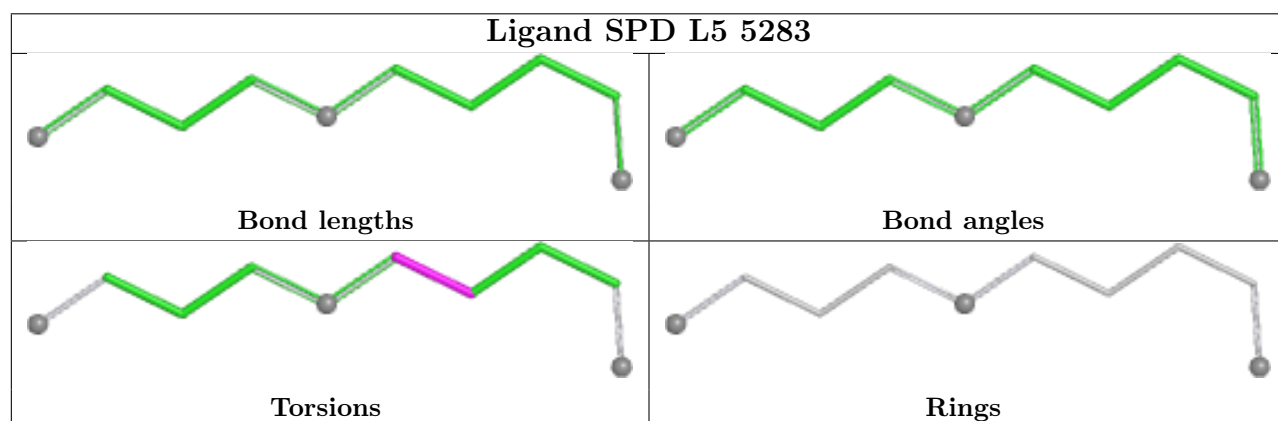
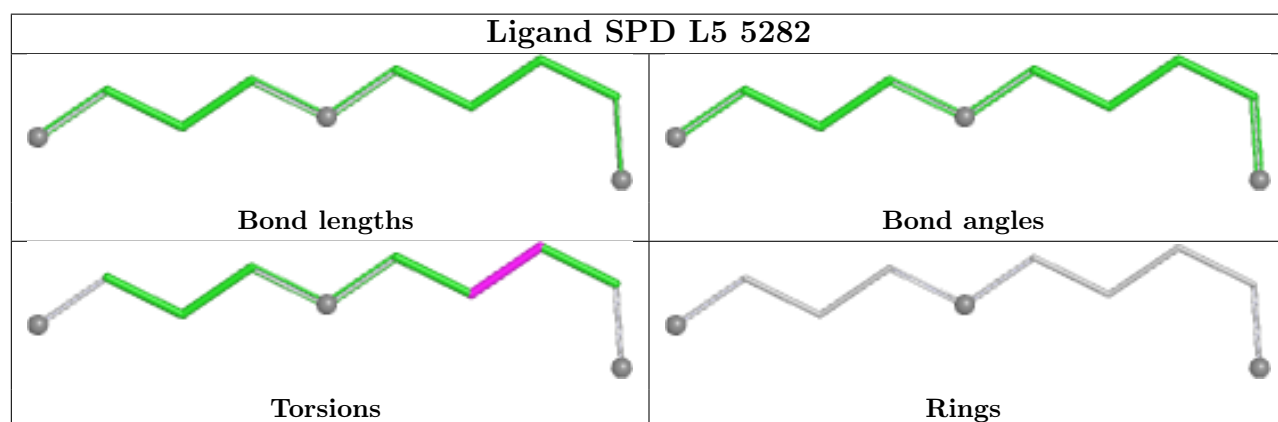
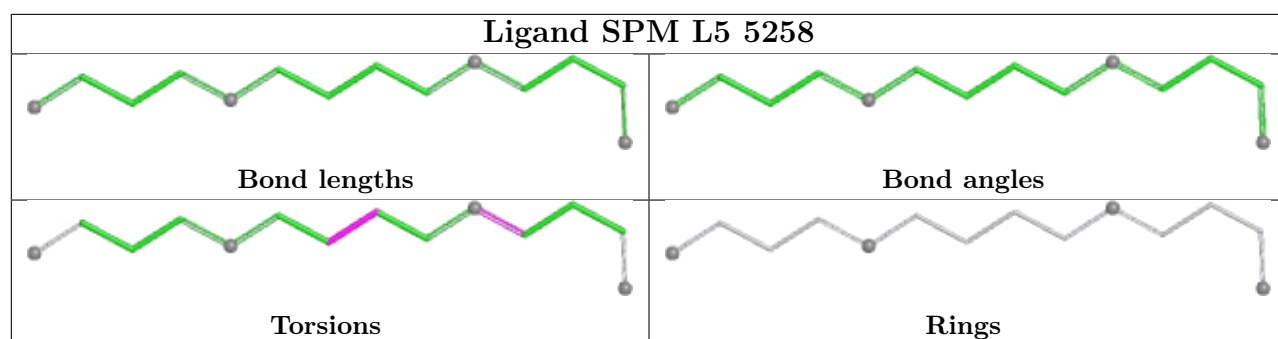
7 monomers are involved in 13 short contacts:

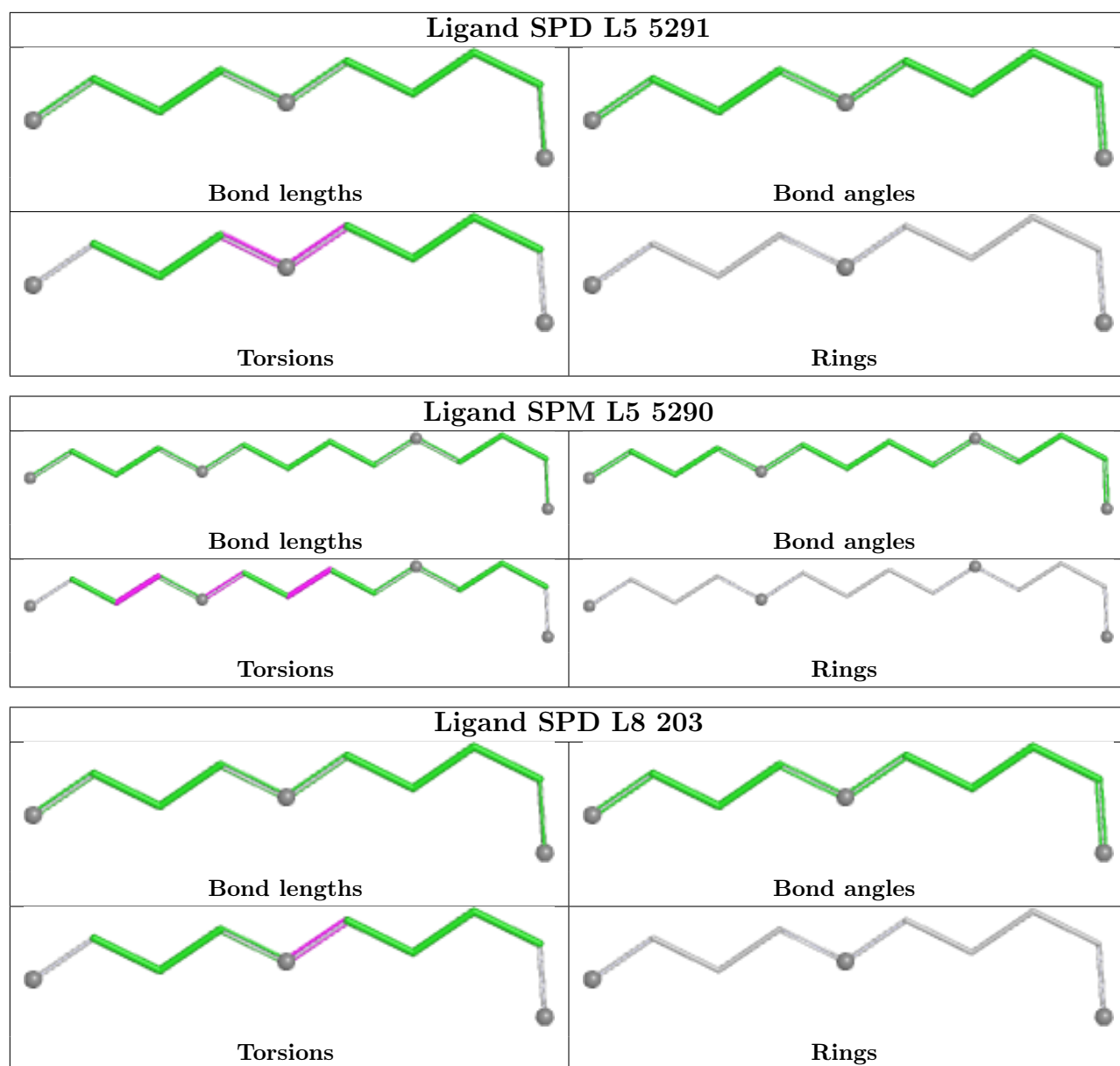
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5286	SPD	1	0
88	L5	5291	SPD	2	0
88	L8	203	SPD	2	0
87	L5	5263	SPM	1	0
90	L5	5294	HMT	1	0
87	L5	5262	SPM	2	0
87	L5	5292	SPM	4	0

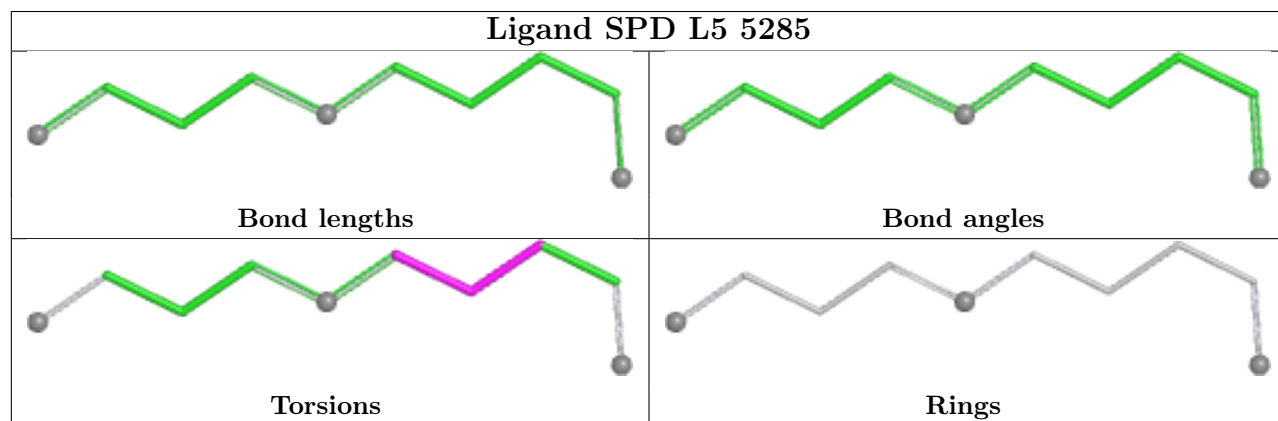
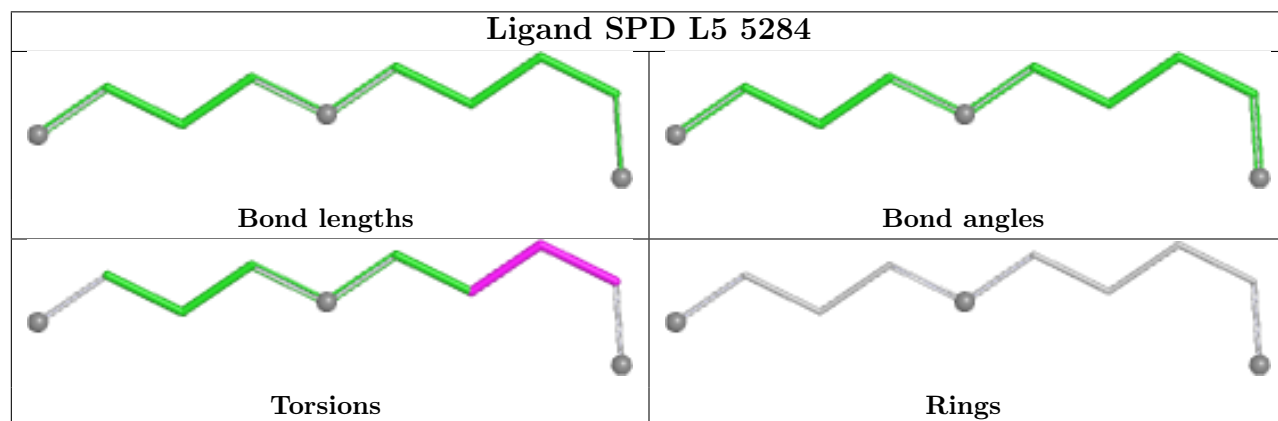
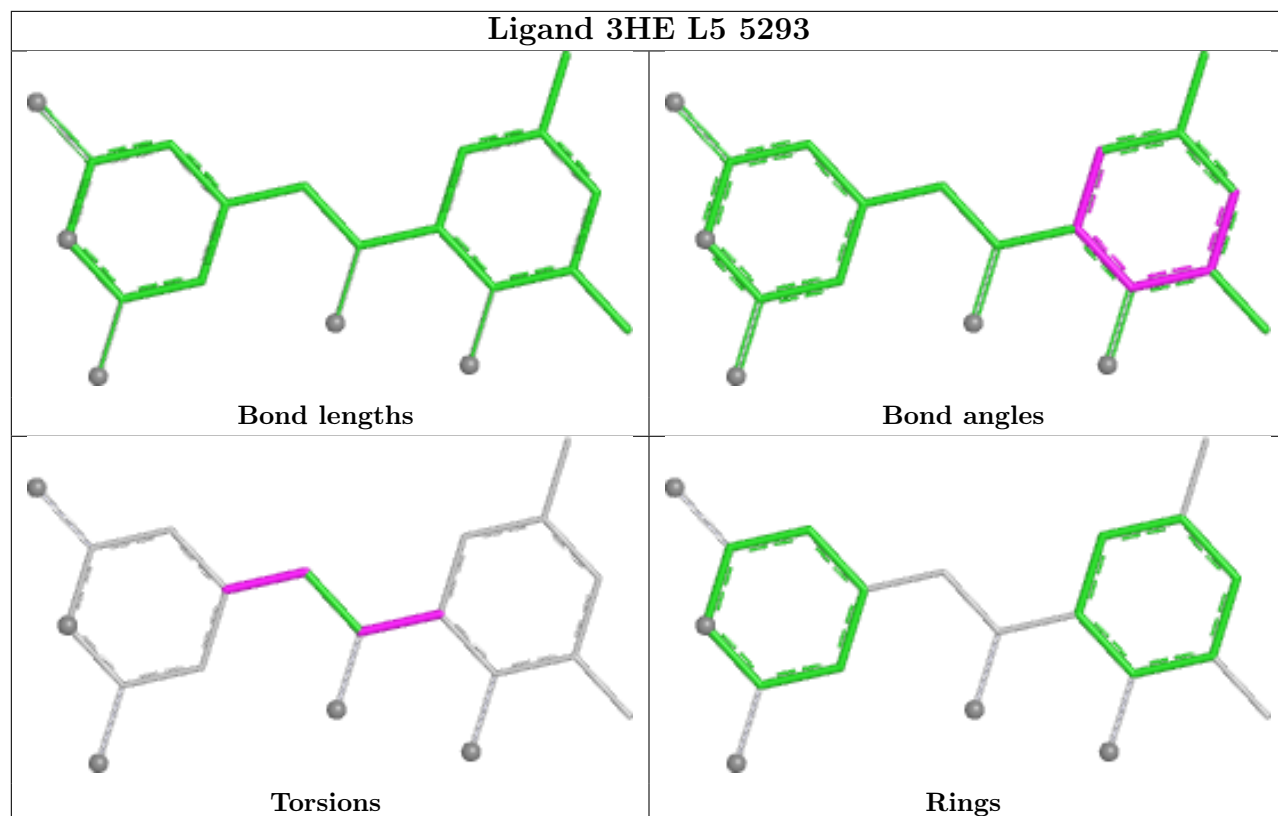
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

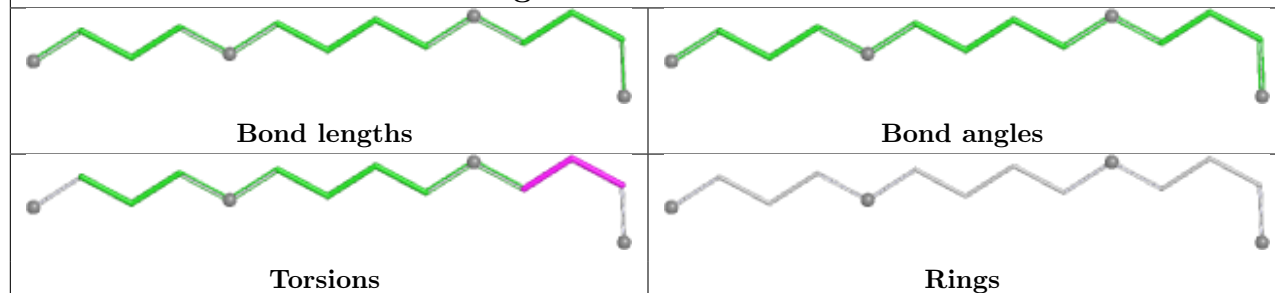




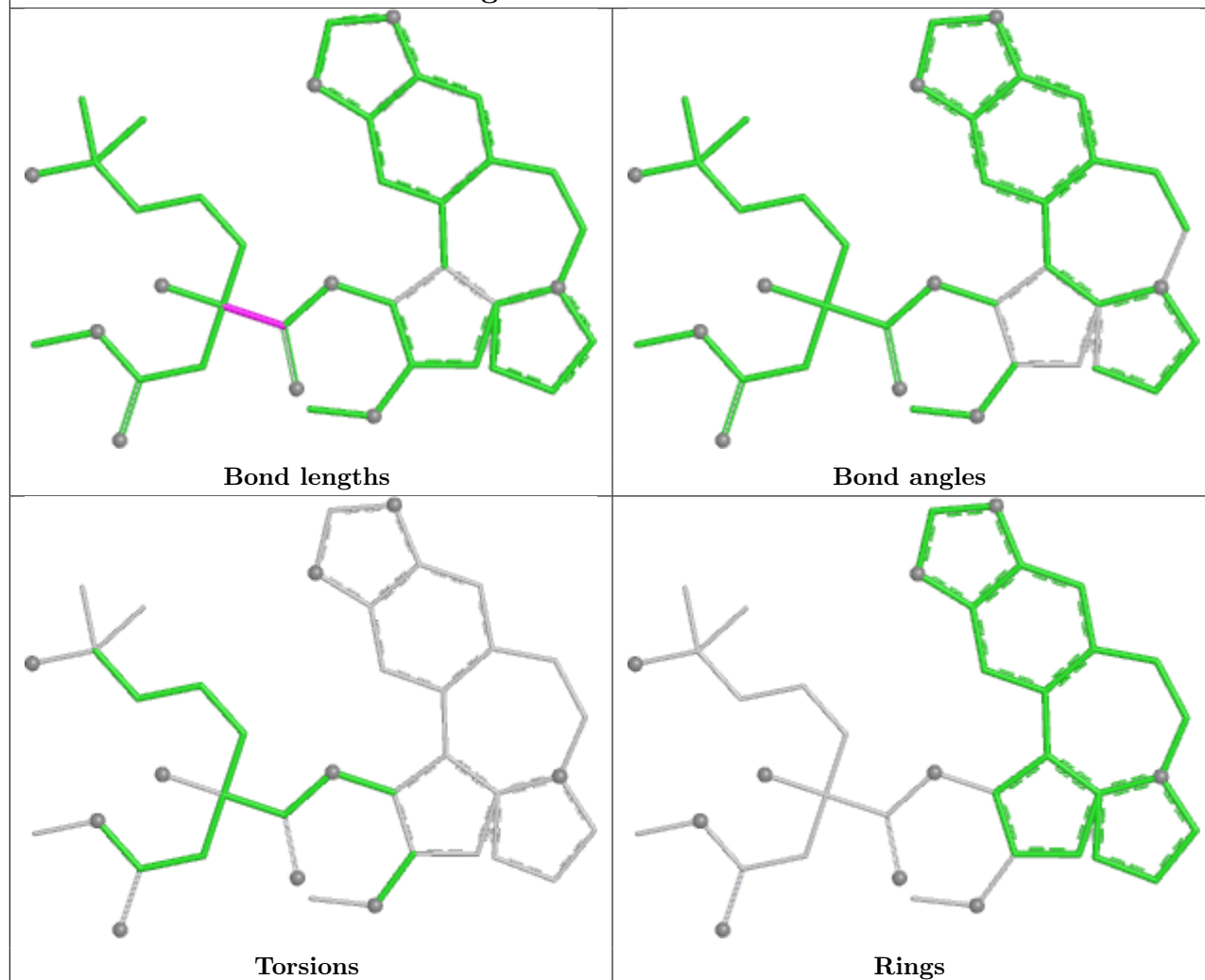




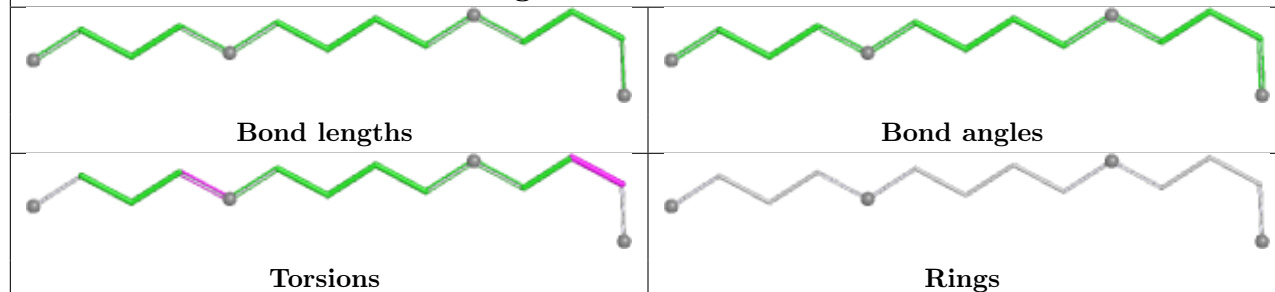
Ligand SPM L5 5263

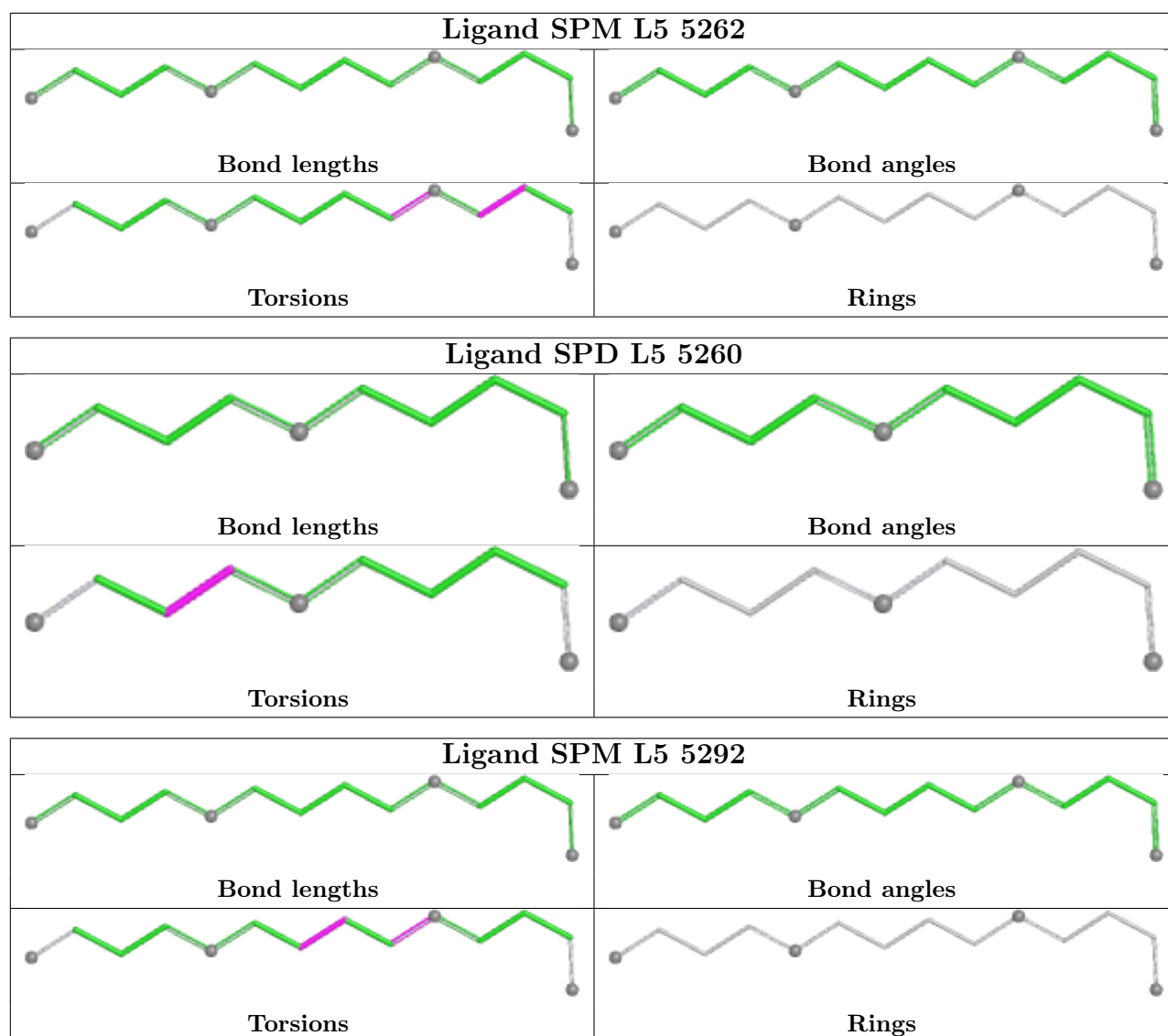


Ligand HMT L5 5294



Ligand SPM L5 5287





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	L5	10
19	S2	4
37	At	1
38	Pt	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	26.68
1	L5	1706:A	O3'	1716:G	P	21.17
1	L5	2910:G	O3'	3584:C	P	20.68
1	L5	3954:A	O3'	4056:A	P	17.41
1	L5	760:G	O3'	903:C	P	16.91
1	L5	4776:G	O3'	4858:C	P	14.21
1	L5	519:C	O3'	642:G	P	13.93
1	L5	2112:G	O3'	2249:C	P	13.81
1	S2	698:G	O3'	730:C	P	13.52
1	S2	739:C	O3'	746:C	P	13.16
1	At	15:G	O3'	18:G	P	12.47
1	L5	990:C	O3'	1064:G	P	12.03
1	L5	1222:A	O3'	1234:G	P	11.96
1	L5	1100:U	O3'	1167:C	P	11.90
1	Pt	15:G	O3'	18:G	P	9.35
1	S2	225:G	O3'	287:U	P	8.63

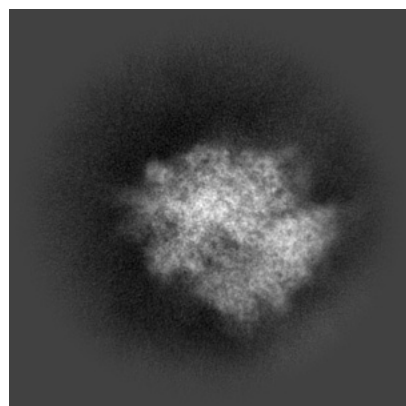
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71340. These allow visual inspection of the internal detail of the map and identification of artifacts.

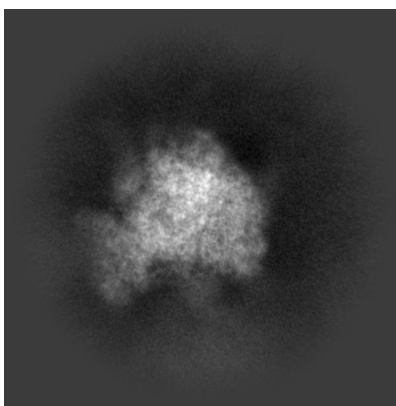
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

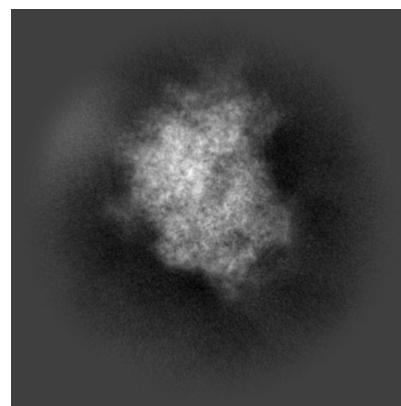
6.1.1 Primary map



X

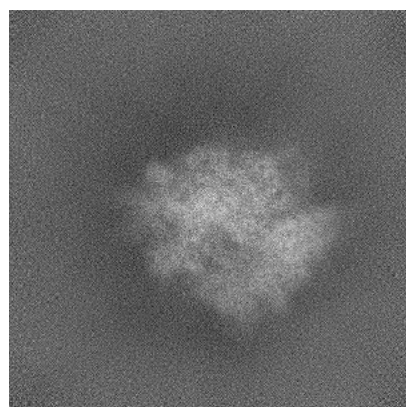


Y

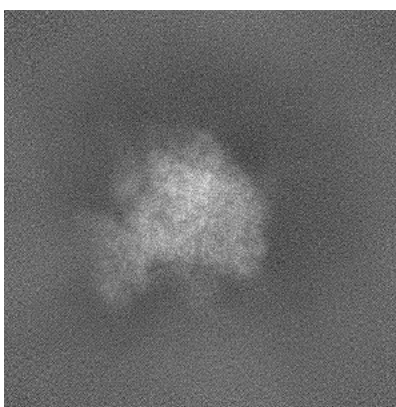


Z

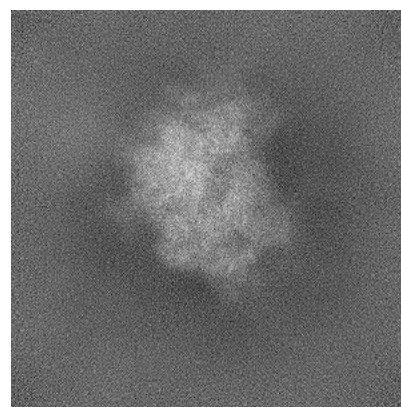
6.1.2 Raw map



X



Y

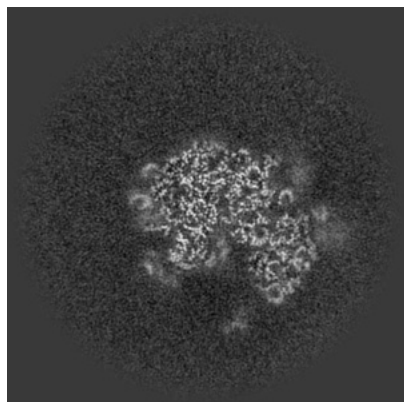


Z

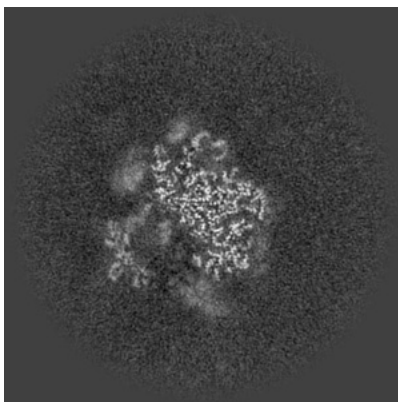
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

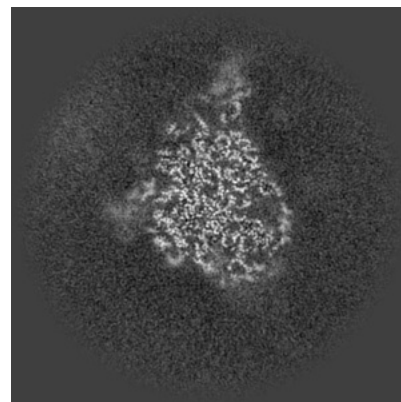
6.2.1 Primary map



X Index: 256

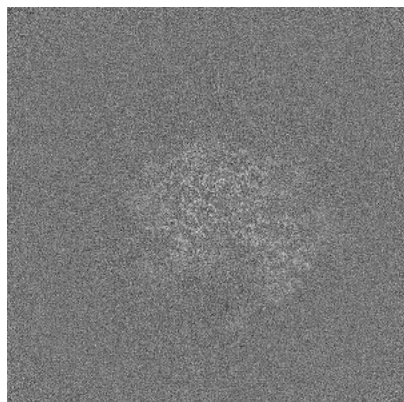


Y Index: 256

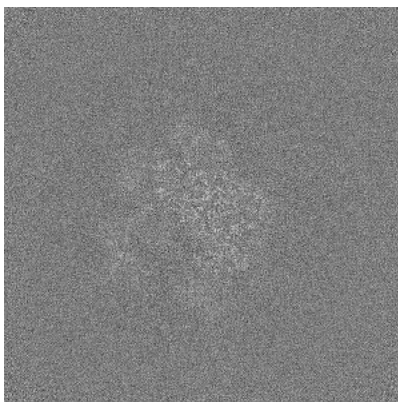


Z Index: 256

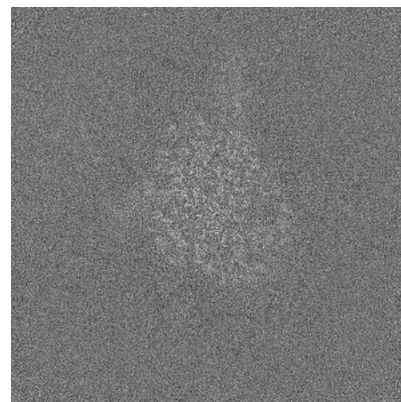
6.2.2 Raw map



X Index: 256



Y Index: 256

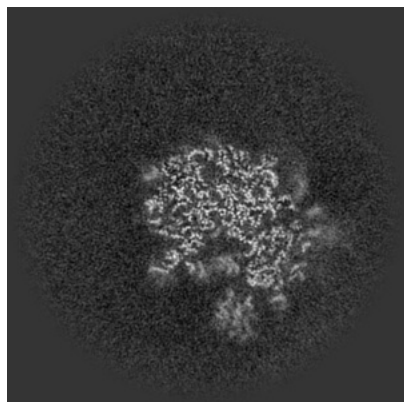


Z Index: 256

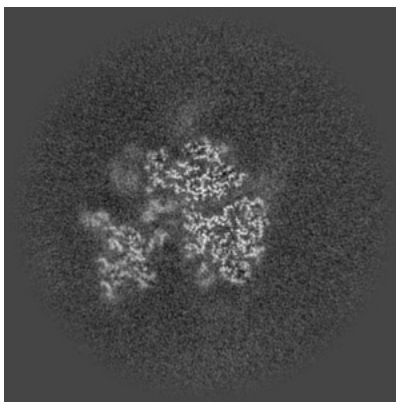
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

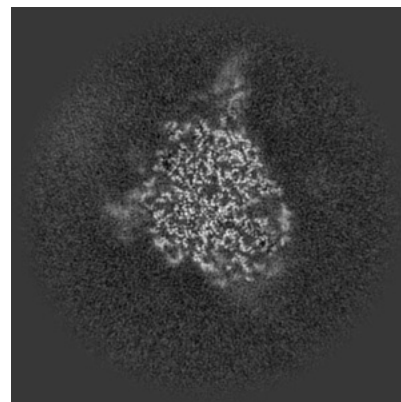
6.3.1 Primary map



X Index: 243

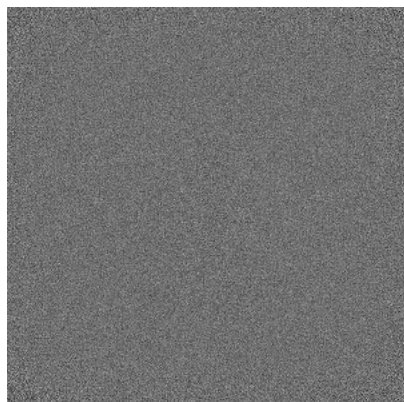


Y Index: 276

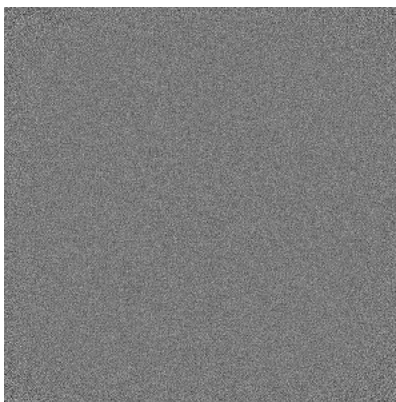


Z Index: 258

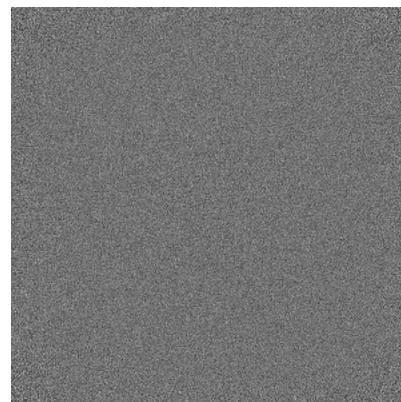
6.3.2 Raw map



X Index: 0



Y Index: 0

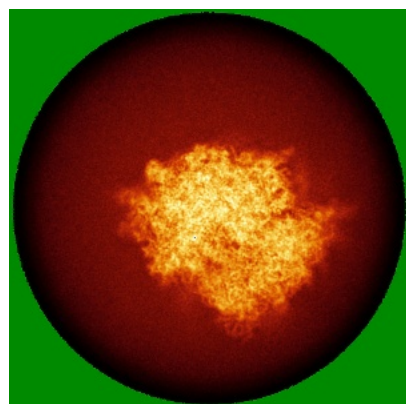


Z Index: 0

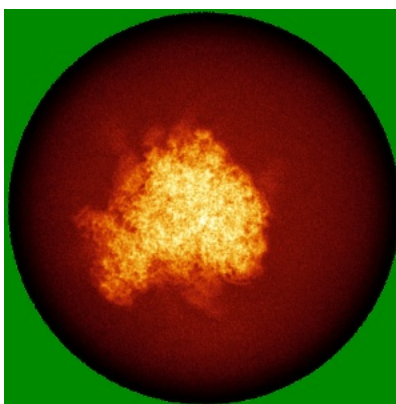
The images above show the largest variance slices of the map in three orthogonal directions.

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

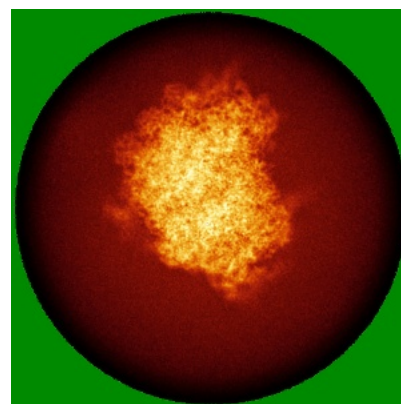
6.4.1 Primary map



X

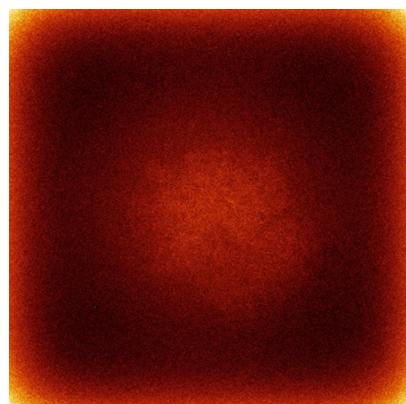


Y

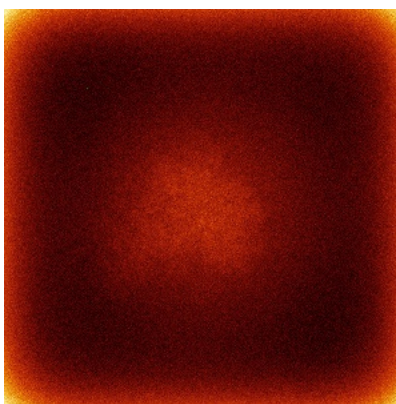


Z

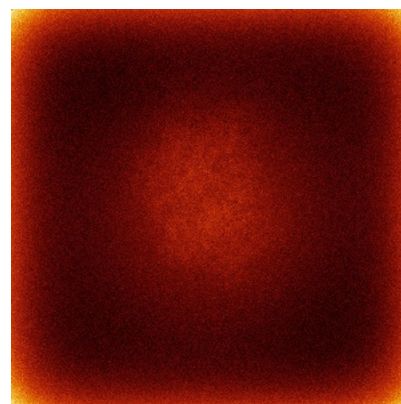
6.4.2 Raw map



X



Y

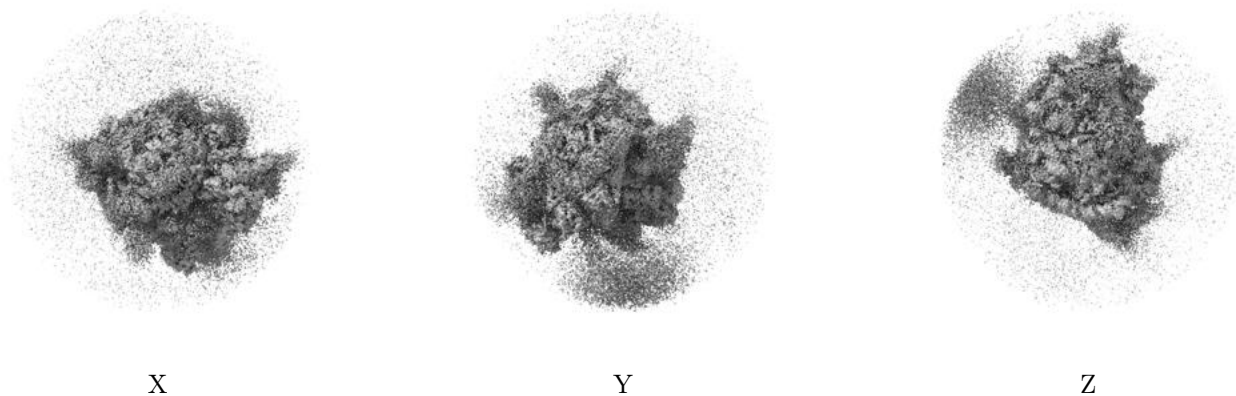


Z

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

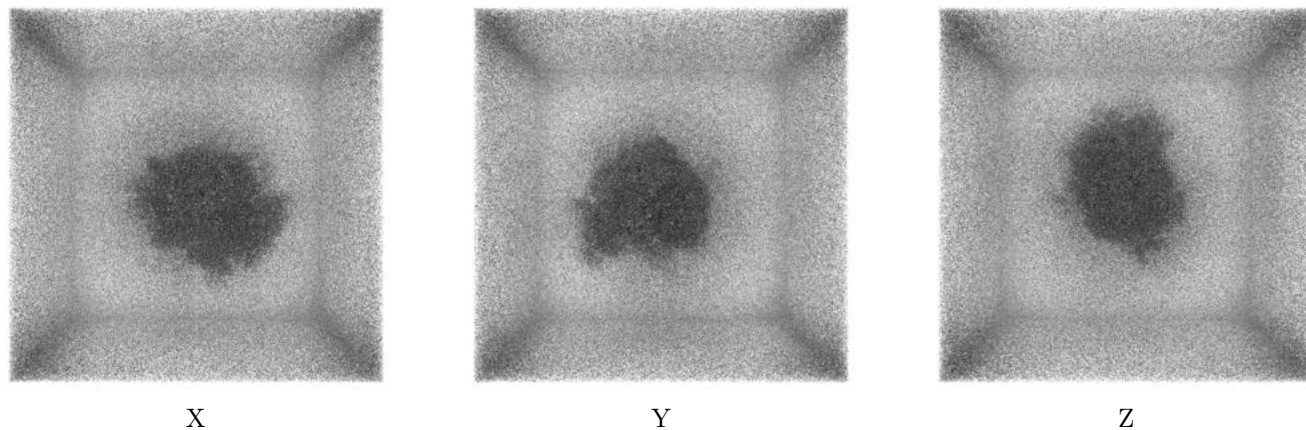
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0758. 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.

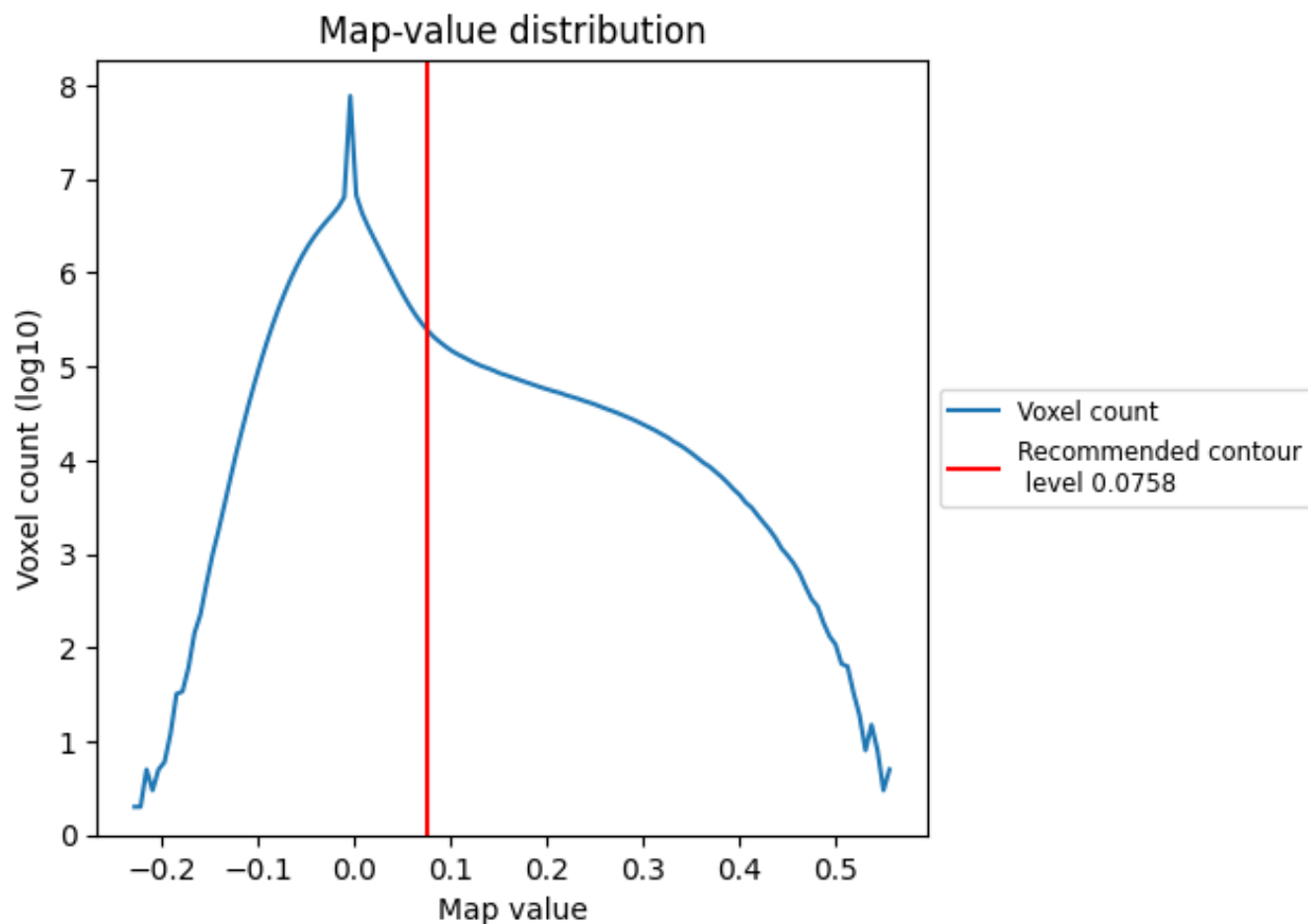
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

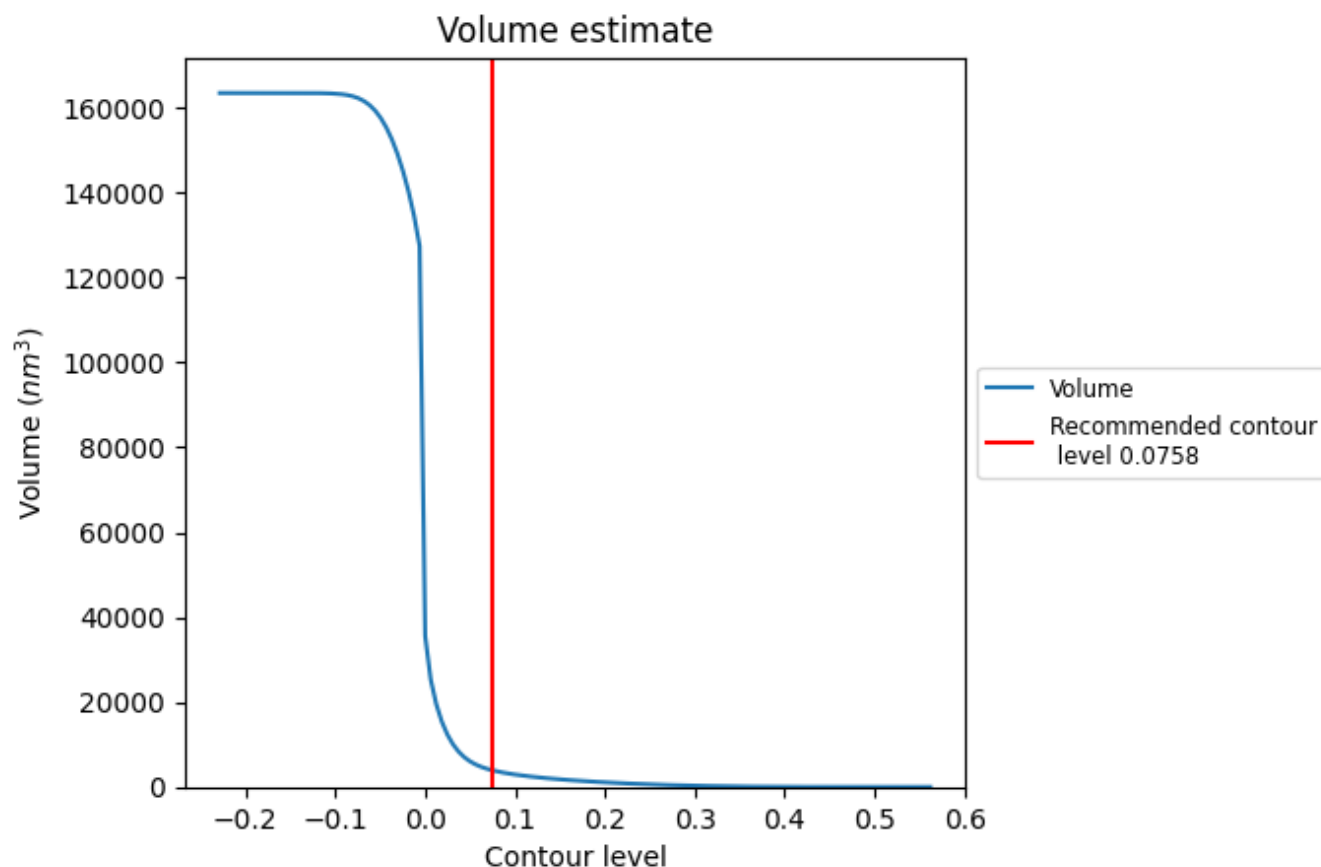
This section contains the results of statistical analysis of the map.

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.

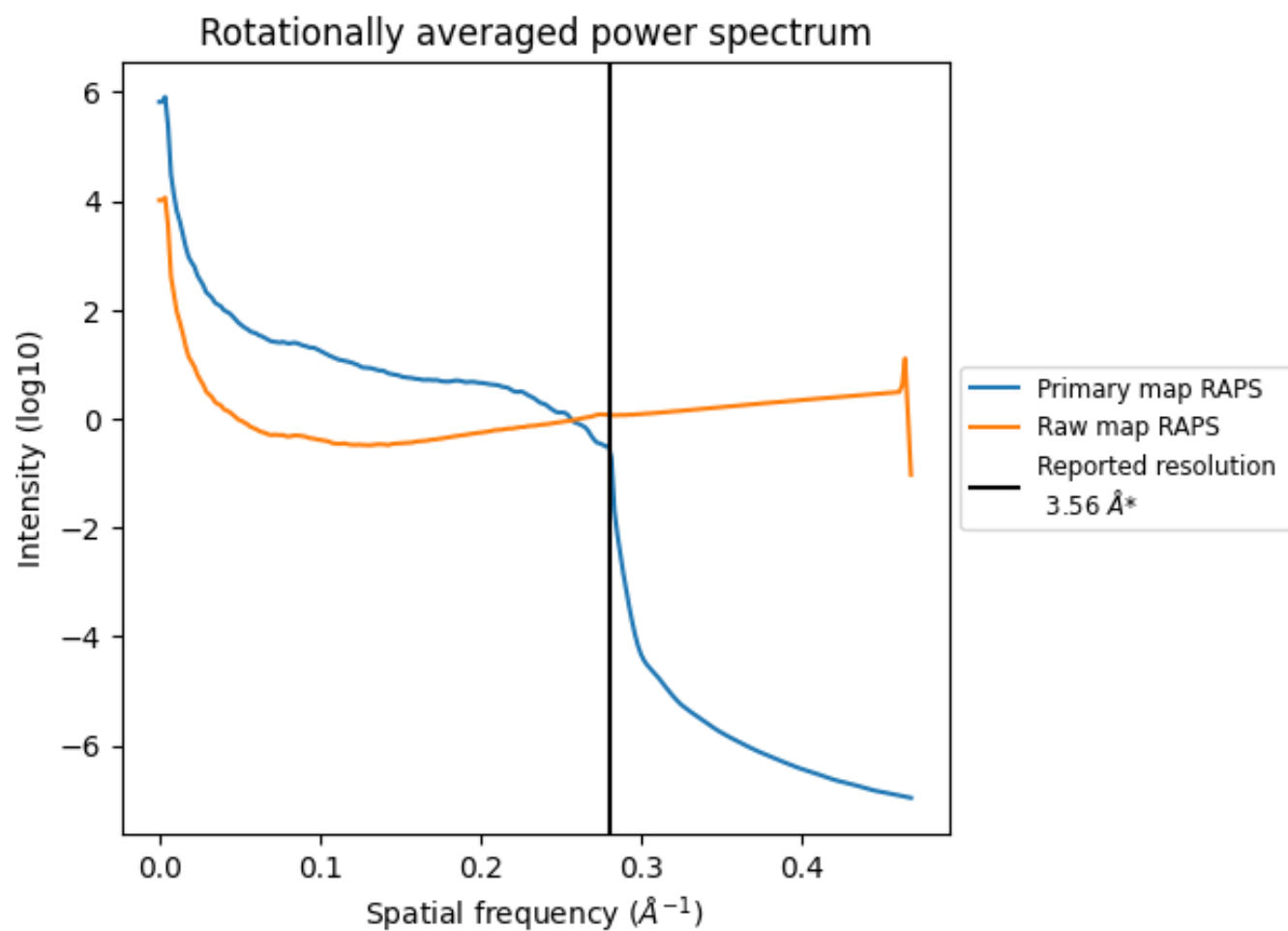
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3880 nm^3 ; this corresponds to an approximate mass of 3505 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

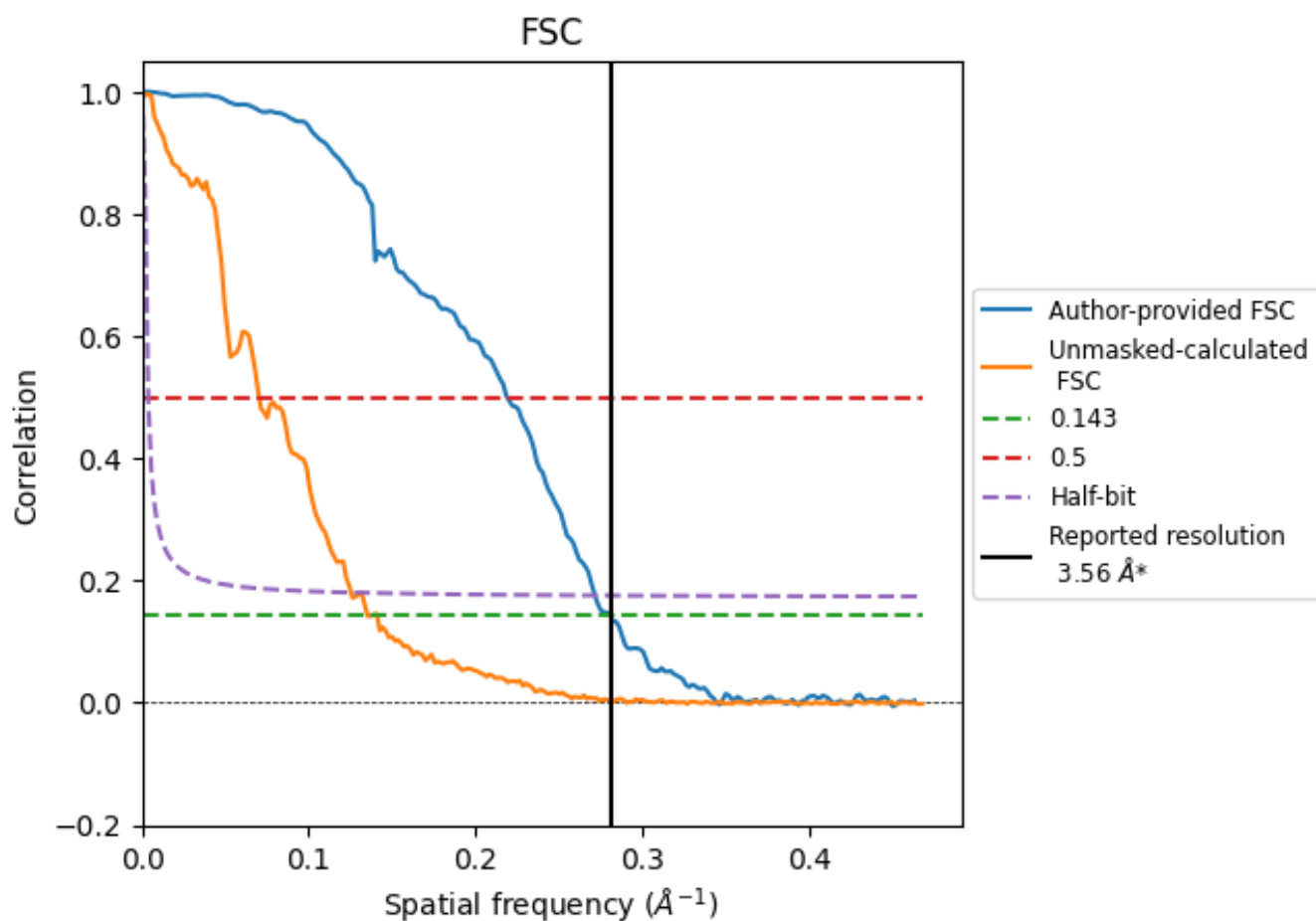


*Reported resolution corresponds to spatial frequency of 0.281 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.281 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

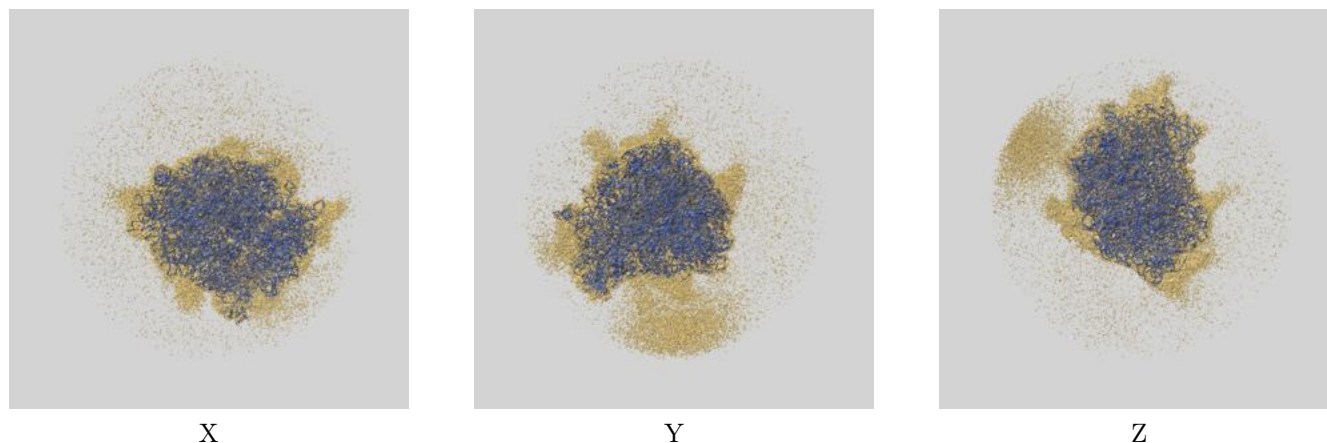
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	4.56	3.68
Unmasked-calculated*	7.40	14.25	7.98

*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 7.40 differs from the reported value 3.56 by more than 10 %

9 Map-model fit [i](#)

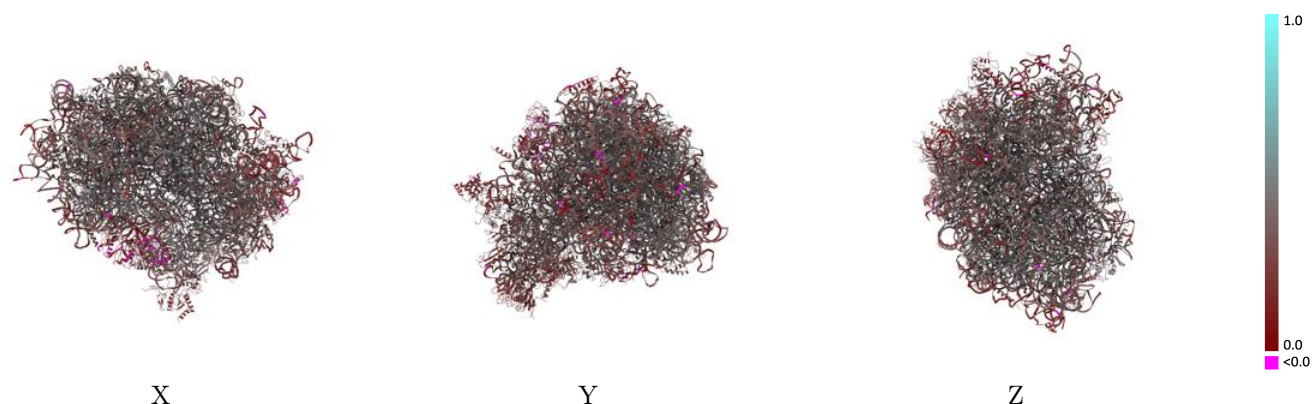
This section contains information regarding the fit between EMDB map EMD-71340 and PDB model 9P7F. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



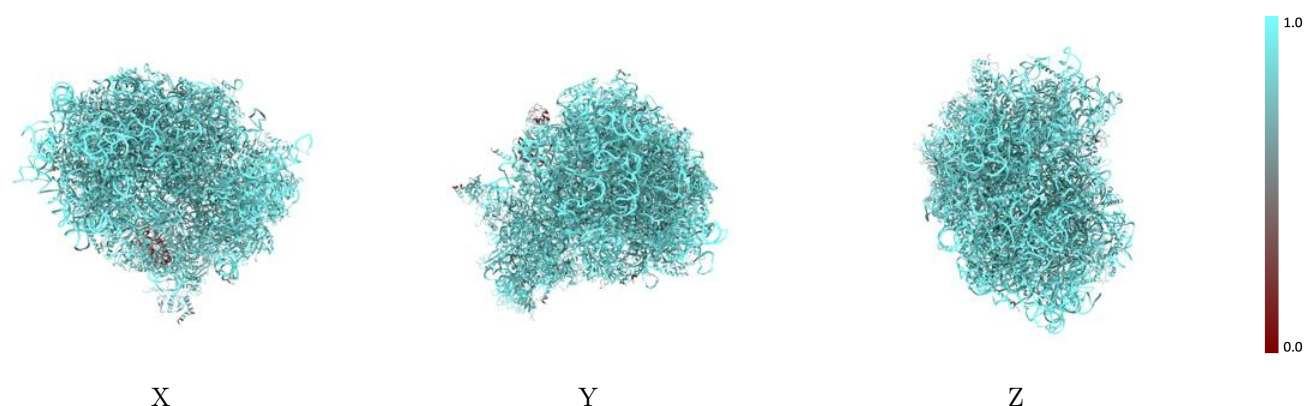
The images above show the 3D surface view of the map at the recommended contour level 0.0758 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



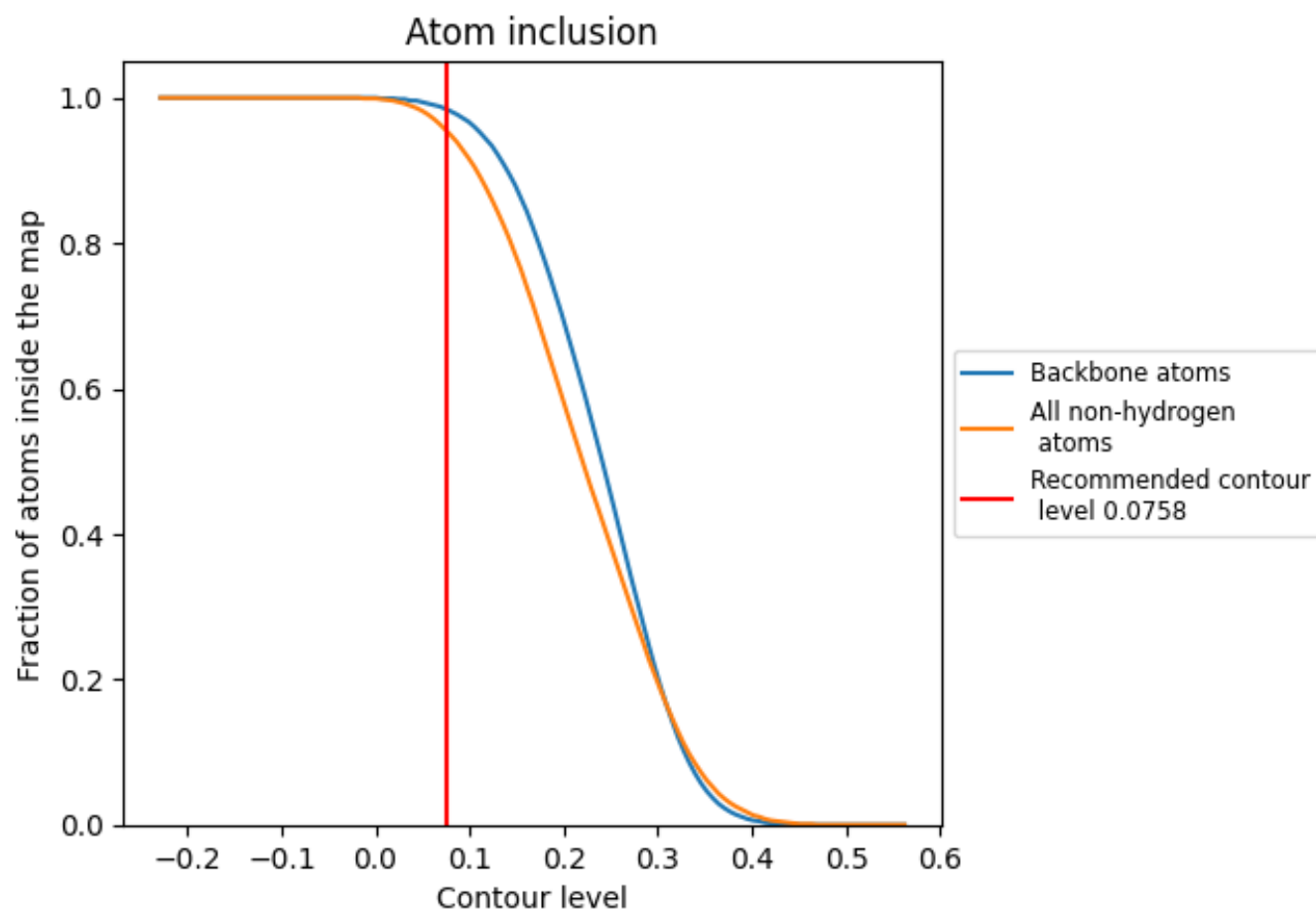
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0758).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.0758) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9540	 0.3750
At	 0.9600	 0.2810
CI	 0.7570	 0.3430
L5	 0.9890	 0.3840
L7	 1.0000	 0.4110
L8	 0.9960	 0.3950
LA	 0.9470	 0.4420
LB	 0.9220	 0.4300
LC	 0.9340	 0.4280
LD	 0.9320	 0.3830
LE	 0.9280	 0.3730
LF	 0.9350	 0.4200
LG	 0.8890	 0.3720
LH	 0.9180	 0.4170
LI	 0.9360	 0.4220
LJ	 0.9000	 0.3480
LL	 0.9230	 0.4140
LM	 0.9320	 0.3970
LN	 0.9530	 0.4380
LO	 0.9170	 0.4090
LP	 0.9270	 0.4310
LQ	 0.9450	 0.4370
LR	 0.9190	 0.3840
LS	 0.9340	 0.4360
LT	 0.9330	 0.4270
LU	 0.9050	 0.3490
LV	 0.9470	 0.4470
LW	 0.8980	 0.3390
LX	 0.9310	 0.4130
LY	 0.9450	 0.4060
LZ	 0.9490	 0.4060
La	 0.9540	 0.4450
Lb	 0.9030	 0.3650
Lc	 0.8980	 0.3800
Ld	 0.9290	 0.4320



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Chain	Atom inclusion	Q-score
Le	 0.9370	 0.4540
Lf	 0.9510	 0.4490
Lg	 0.9370	 0.4240
Lh	 0.9150	 0.3990
Li	 0.9320	 0.4070
Lj	 0.9600	 0.4340
Lk	 0.9010	 0.3650
Ll	 0.9430	 0.4180
Lm	 0.9420	 0.4220
Ln	 0.9520	 0.4250
Lo	 0.9430	 0.4310
Lp	 0.9230	 0.4190
Lr	 0.9370	 0.4300
Ls	 0.6420	 0.1560
Lt	 0.6030	 0.1120
Pt	 0.9700	 0.3110
S2	 0.9930	 0.3670
SA	 0.8760	 0.3250
SB	 0.8680	 0.3280
SC	 0.9350	 0.3790
SD	 0.9100	 0.3440
SE	 0.9270	 0.3580
SF	 0.8490	 0.3120
SG	 0.9050	 0.3200
SH	 0.8860	 0.3010
SI	 0.9200	 0.3650
SJ	 0.9040	 0.3430
SK	 0.8970	 0.3110
SL	 0.9050	 0.3860
SM	 0.7500	 0.2240
SN	 0.8920	 0.3540
SO	 0.8810	 0.3460
SP	 0.9140	 0.3320
SQ	 0.9100	 0.3210
SR	 0.8720	 0.3060
SS	 0.8770	 0.3170
ST	 0.9120	 0.3160
SU	 0.9020	 0.3060
SV	 0.9260	 0.3600
SW	 0.9390	 0.3840
SX	 0.9270	 0.4100
SY	 0.8860	 0.3430

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Chain	Atom inclusion	Q-score
SZ	 0.8080	 0.2790
Sa	 0.9460	 0.3880
Sb	 0.9120	 0.3490
Sc	 0.8700	 0.3370
Sd	 0.9570	 0.3600
Se	 0.8630	 0.3320
Sf	 0.8420	 0.2530
Sg	 0.9020	 0.2570