



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 18, 2018 – 04:18 PM EST

PDB ID : 6EK0
EMDB ID: : EMD-3883
Title : High-resolution cryo-EM structure of the human 80S ribosome
Authors : Natchiar, S.K.; Myasnikov, A.G.; Kratzat, H.; Hazemann, I.; Klaholz, B.P.
Deposited on : 2017-09-24
Resolution : 2.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

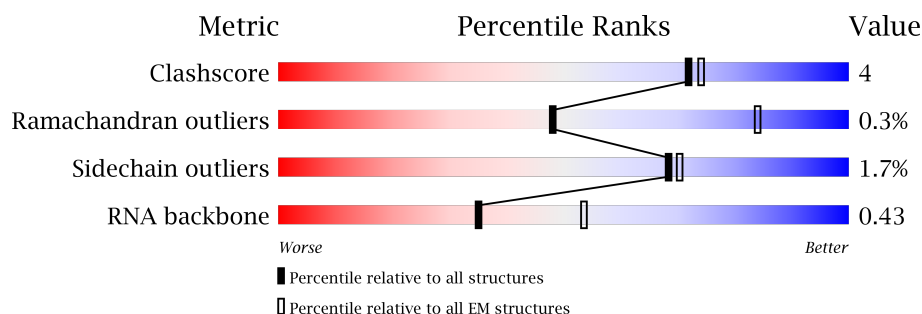
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.























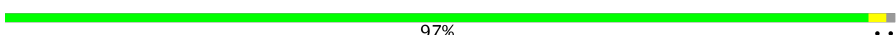




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	L5	5070	45% 24% 5% . 26%
2	L7	120	76% 23% .
3	L8	156	69% 24% 6% .
4	LA	257	81% 13% . .
5	LB	403	79% 20% .
6	LC	427	76% 10% 14%
7	LD	297	81% 18% .
8	LE	288	67% 15% 18%

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Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	


















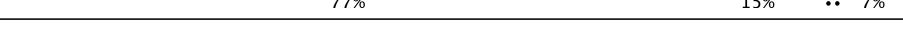


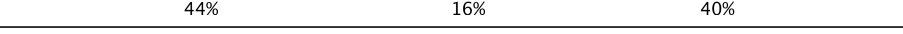
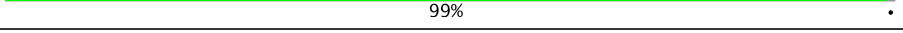
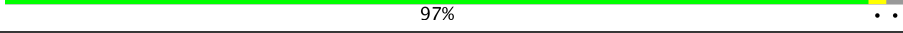
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Mol	Chain	Length	Quality of chain
34	Lf	110	95%
35	Lg	117	97%
36	Lh	123	98%
37	Li	105	95%
38	Lj	97	86%
39	Lk	70	99%
40	Ll	51	94%
41	Lm	128	41%
42	Ln	25	92%
43	Lo	106	99%
44	Lp	92	97%
45	Lr	137	90%
46	Lz	217	96%
47	S2	1869	59%
48	S6	75	47%
49	SA	295	61%
50	SB	264	72%
51	SD	243	78%
52	SE	263	87%
53	SF	204	75%
54	SH	194	77%
55	SI	208	75%
56	SK	165	52%
57	SL	158	84%
58	SP	145	78%

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Mol	Chain	Length	Quality of chain
59	SQ	146	 79% 21% .
60	SR	135	 86% 14%
61	SS	152	 75% 19% . 5%
62	ST	145	 90% 8% ..
63	SU	119	 76% 12% 13%
64	SV	83	 82% 17% .
65	SX	143	 81% 15% ..
66	Sa	115	 85% . 11%
67	Sc	69	 88% . 7%
68	Sd	56	 95% . .
69	Sg	317	 97% ..
70	SC	293	 63% 12% 24%
71	SG	249	 74% 21% 5%
72	SJ	194	 81% 12% . 5%
73	SM	132	 75% 15% . 8%
74	SN	151	 91% 8% ..
75	SO	151	 77% 15% .. 7%
76	SW	130	 86% 12% ..
77	SY	133	 89% 8% ..
78	SZ	125	 44% 16% 40%
79	Sb	84	 99% .
80	Se	59	 97% ..
81	Sf	156	 40% . 57%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	B8Q	L5	1456	X	-	-	-
1	B9H	L5	2786	X	-	-	-
47	B8Q	S2	1219	X	-	-	-
47	E3C	S2	568	X	-	-	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 219596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3773	Total	C	N	O	P	0	0
			80257	35772	14588	26125	3772		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	2113	C	G	conflict	GB 86475748

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2928	1841	583	489	15		

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

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

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- 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 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

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

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	1	0
			870	547	178	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	1740	Total	C	N	O	P	0	0
			36938	16495	6598	12106	1739		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

- Molecule 48 is a RNA chain called Human initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S6	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

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

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

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

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

- Molecule 51 is a protein called 40S ribosomal protein S3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

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

- Molecule 54 is a protein called 40S ribosomal protein S7.

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

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

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

- Molecule 56 is a protein called 40S ribosomal protein S10.

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

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

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

- Molecule 58 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 59 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	146	Total	C	N	O	S	0	0
			1158	736	218	200	4		

- Molecule 60 is a protein called 40S ribosomal protein S17.

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

- Molecule 61 is a protein called 40S ribosomal protein S18.

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

- Molecule 62 is a protein called 40S ribosomal protein S19.

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

- Molecule 63 is a protein called 40S ribosomal protein S20.

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

- Molecule 64 is a protein called 40S ribosomal protein S21.

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

- Molecule 65 is a protein called 40S ribosomal protein S23.

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

- Molecule 66 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sa	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 67 is a protein called 40S ribosomal protein S28.

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

- Molecule 68 is a protein called 40S ribosomal protein S29.

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

- Molecule 69 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SC	222	Total	C	N	O	S	1	0
			1733	1120	301	302	10		

- Molecule 71 is a protein called 40S ribosomal protein S6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SJ	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 73 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SM	122	Total	C	N	O	S	0	0
			942	590	165	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

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

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

- Molecule 75 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 76 is a protein called 40S ribosomal protein S15a.

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

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SY	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

- Molecule 78 is a protein called 40S ribosomal protein S25.

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

- Molecule 79 is a protein called 40S ribosomal protein S27.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

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

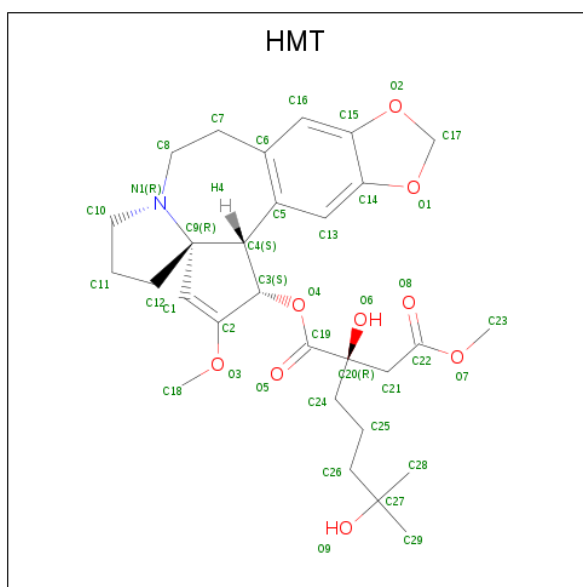
- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	L7	3	Total	Mg	0
			3	3	
82	LV	1	Total	Mg	0
			1	1	
82	Sd	1	Total	Mg	0
			1	1	
82	S2	134	Total	Mg	0
			134	134	
82	L8	6	Total	Mg	0
			6	6	
82	Le	1	Total	Mg	0
			1	1	
82	LN	1	Total	Mg	0
			1	1	
82	SF	1	Total	Mg	0
			1	1	
82	LP	1	Total	Mg	0
			1	1	
82	Lf	1	Total	Mg	0
			1	1	
82	L5	251	Total	Mg	0
			251	251	
82	LT	1	Total	Mg	0
			1	1	

- Molecule 83 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano
yl]cephalotaxine (three-letter code: HMT) (formula: C₂₉H₃₉NO₉).

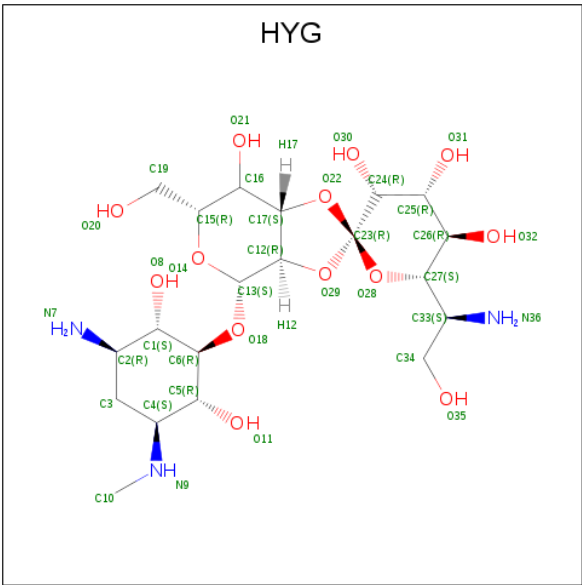


Mol	Chain	Residues	Atoms				AltConf
83	L5	1	Total	C	N	O	0
			39	29	1	9	

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Lm	1	Total	Zn	0
			1	1	
84	Sd	1	Total	Zn	0
			1	1	
84	Lo	1	Total	Zn	0
			1	1	
84	Sf	1	Total	Zn	0
			1	1	
84	Lg	1	Total	Zn	0
			1	1	
84	Lp	1	Total	Zn	0
			1	1	
84	Sa	1	Total	Zn	0
			1	1	
84	Lj	1	Total	Zn	0
			1	1	

- Molecule 85 is HYGROMYCIN B (three-letter code: HYG) (formula: C₂₀H₃₇N₃O₁₃).



Mol	Chain	Residues	Atoms				AltConf
85	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	L5	16	Total	O	0
			16	16	
86	LA	1	Total	O	0
			1	1	
86	LB	1	Total	O	0
			1	1	
86	LC	1	Total	O	0
			1	1	
86	LF	1	Total	O	0
			1	1	
86	LG	1	Total	O	0
			1	1	
86	LH	1	Total	O	0
			1	1	
86	LI	2	Total	O	0
			2	2	
86	LN	1	Total	O	0
			1	1	
86	LS	2	Total	O	0
			2	2	
86	LY	1	Total	O	0
			1	1	

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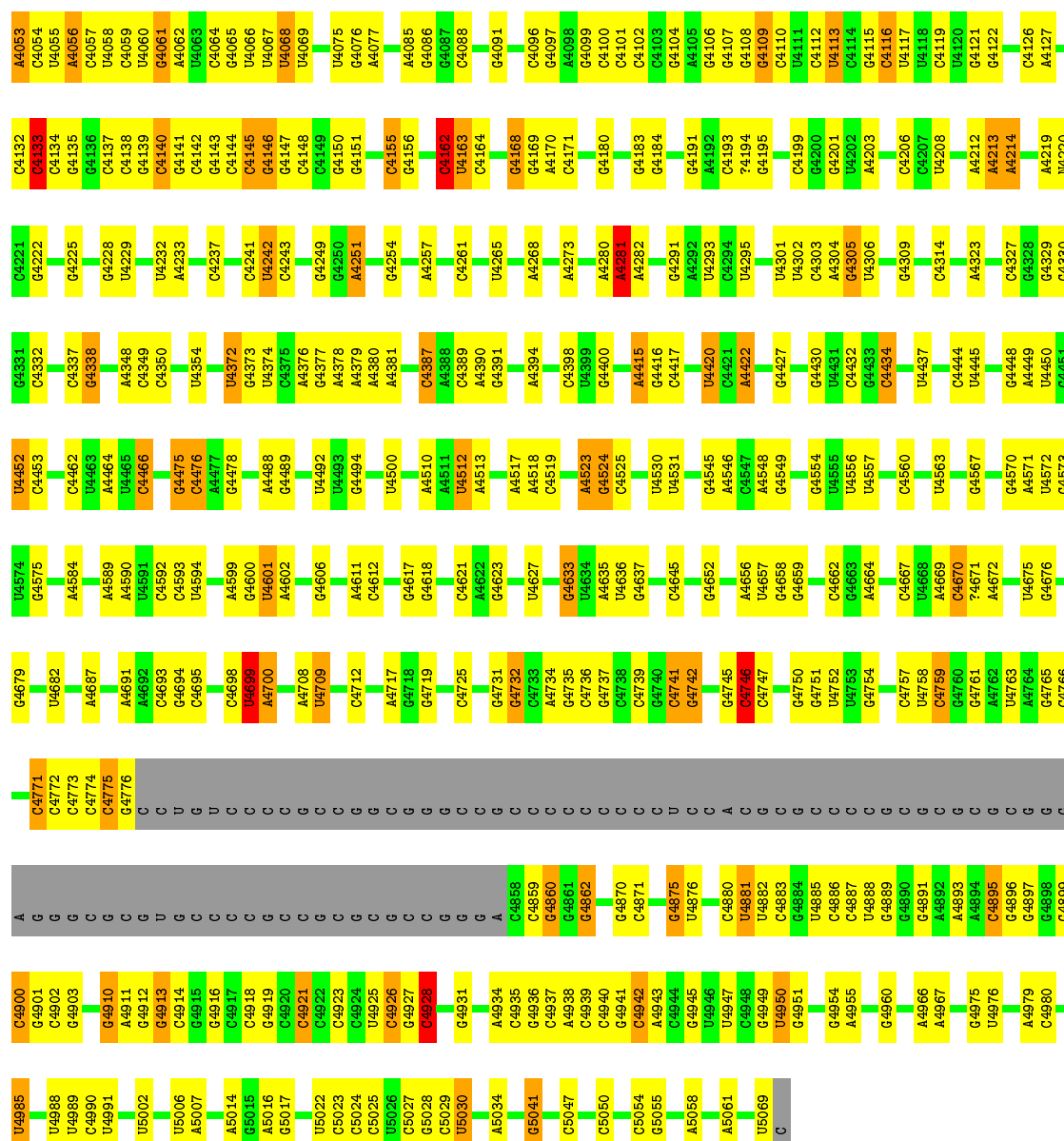
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Mol	Chain	Residues	Atoms		AltConf
86	La	2	Total 2	O 2	0
86	Lb	1	Total 1	O 1	0
86	Lf	1	Total 1	O 1	0
86	Lm	1	Total 1	O 1	0
86	S2	14	Total 14	O 14	0
86	SF	1	Total 1	O 1	0
86	SL	1	Total 1	O 1	0
86	SP	1	Total 1	O 1	0
86	SQ	2	Total 2	O 2	0
86	SR	1	Total 1	O 1	0
86	SS	2	Total 2	O 2	0
86	SV	1	Total 1	O 1	0
86	SC	1	Total 1	O 1	0
86	SG	1	Total 1	O 1	0
86	SJ	1	Total 1	O 1	0
86	SN	1	Total 1	O 1	0
86	Sf	1	Total 1	O 1	0

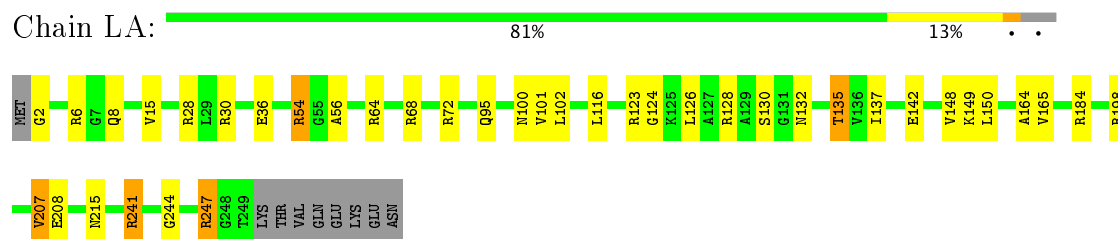




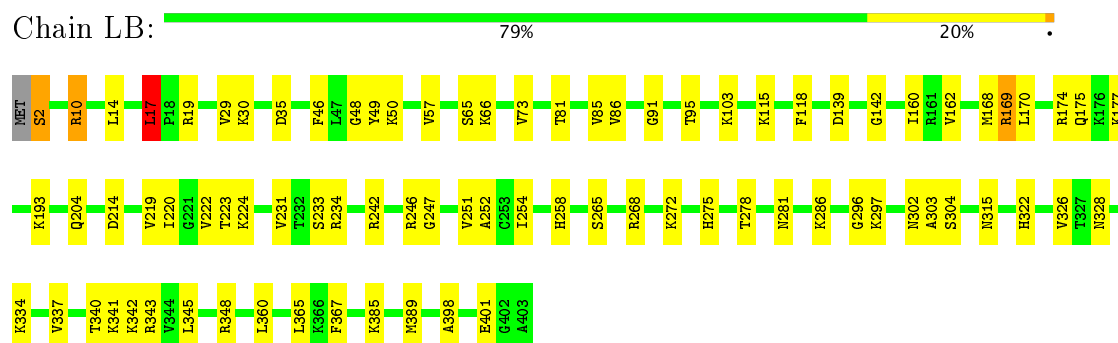




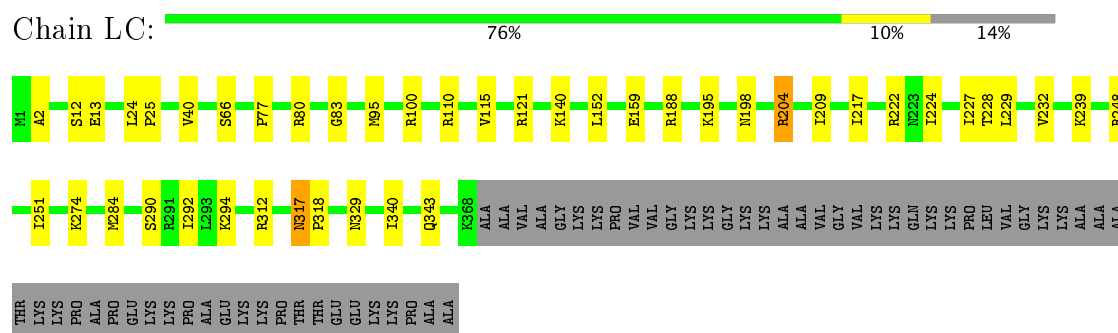
- Molecule 4: 60S ribosomal protein L8




- Molecule 5: 60S ribosomal protein L3



- Molecule 6: 60S ribosomal protein L4



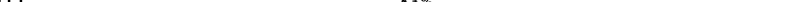
- Molecule 9: 60S ribosomal protein L7

Chain LF:  78% 12% • 9%

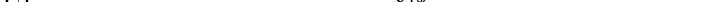
- Molecule 10: 60S ribosomal protein L7a

Chain LG:  74% 16% 9%

- Molecule 11: 60S ribosomal protein L9

Chain LH: 

- Molecule 12: 60S ribosomal protein L10-like

Chain LI:  81% 18%

- Molecule 13: 60S ribosomal protein L11

Chain LJ: 78% 20% .



-
- | Cluster | Number of Genes |
|---------|-----------------|
| MET | 1 |
| A2 | 1 |
| P3 | 1 |
| S4 | 1 |
| R5 | 1 |
| N6 | 1 |
| G7 | 1 |
| K16 | 1 |
| Q19 | 1 |
| V22 | 1 |
| R45 | 1 |
| V69 | 1 |
| T63 | 1 |
| R71 | 1 |
| E80 | 1 |
| A91 | 1 |
| I96 | 1 |
| R102 | 1 |
| R103 | 1 |
| I125 | 1 |
| K130 | 1 |
| P131 | 1 |
| S132 | 1 |
| A133 | 1 |
| P134 | 1 |
| K135 | 1 |
| E142 | 1 |
| E143 | 1 |
| L144 | 1 |
| V154 | 1 |
| V157 | 1 |
| K162 | 1 |
| K163 | 1 |
| R167 | 1 |
| R190 | 1 |
| I194 | 1 |
| R198 | 1 |
| E201 | 1 |
| Q205 | 1 |
| E208 | 1 |
| K211 | 1 |


- [illegible]

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| ME1 | G2 | A3 | Y4 | K14 | R24 | R44 | R67 | R68 | T80 | K83 | P84 | L98 | E104 | L116 | E123 | D124 | T126 | Y127 | K128 | L134 | I135 | T151 | E160 | G177 | I184 | R193 | L200 | Y203 |
|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| Met | ALA | E3 | V4 | L7 | V8 | L9 | D10 | V27 | R31 | R49 | R50 | K51 | Y54 | L55 | L58 | R59 | K60 | F73 | R74 | V84 | M87 | R101 | L102 | D106 | P110 | K116 | R117 | K125 | L129 | K130 | P131 | V145 | G146 | Q173 | K188 | E194 | L198 | V203 |
|-----|-----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|


- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|
| GLU | GLU | GLU | VAL | ALA | GLN | LYS | LYS | LYS | SER | GLN | LYS | LYS | LEU | LYS | LYS | GLN | LYS | MET | ARG | GLU | MET | V2 | R3 | Y4 | S5 | L6 | K16 | R30 | Q34 | R40 | T45 | K49 | Q54 | R62 | R69 | Q80 | G81 | R82 | H83 | P84 | S87 | D108 | V109 | D110 | S111 | L112 | H116 | I117 | Q118 | V119 | A122 | H133 | P143 | I146 | E147 | E154 | GLN | I1E | VAL | PRO | LYS | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|

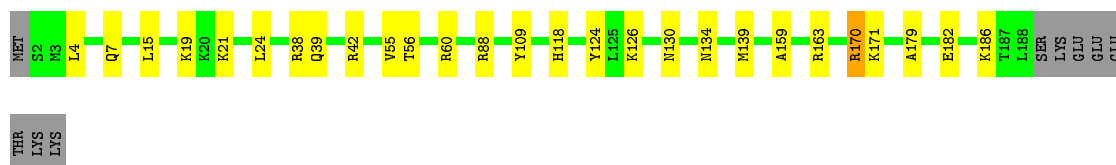
- 


Chain LQ:  89% 10% ..




- Molecule 20: 60S ribosomal protein L19

Chain LR:  82% 13% • 5%




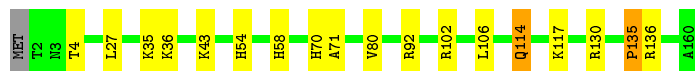
- Molecule 21: 60S ribosomal protein L18a

Chain LS:  84% 15% •



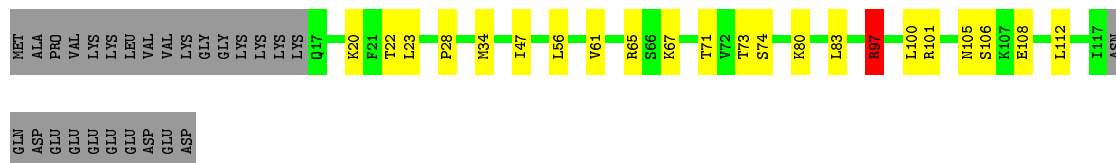
- Molecule 22: 60S ribosomal protein L21

Chain LT:  88% 10% ..




- Molecule 23: 60S ribosomal protein L22

Chain LU:  62% 16% • 21%



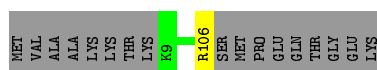
- Molecule 24: 60S ribosomal protein L23

Chain LV:  79% 14% • 6%



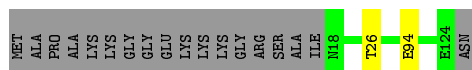
- Molecule 25: 60S ribosomal protein L24

Chain LW:  68% 10% • 21%



- Molecule 32: 60S ribosomal protein L31

Chain Ld: 84% 14%



- Molecule 33: 60S ribosomal protein L32

Chain Le: 93% 5%



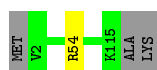
- Molecule 34: 60S ribosomal protein L35a

Chain Lf: 95% ..



- Molecule 35: 60S ribosomal protein L34

Chain Lg: 97% ..



- Molecule 36: 60S ribosomal protein L35

Chain Lh: 98% ..



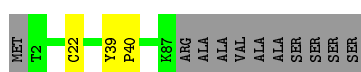
- Molecule 37: 60S ribosomal protein L36

Chain Li: 95% ..



- Molecule 38: 60S ribosomal protein L37

Chain Lj: 86% 11%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  99%



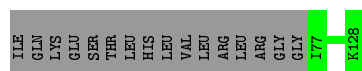
- Molecule 40: 60S ribosomal protein L39

Chain Ll:  94%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:  41%  59%



- Molecule 42: 60S ribosomal protein L41

Chain Ln:  92%



- Molecule 43: 60S ribosomal protein L36a

Chain Lo:  99%



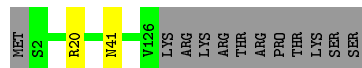
- Molecule 44: 60S ribosomal protein L37a

Chain Lp:  97%

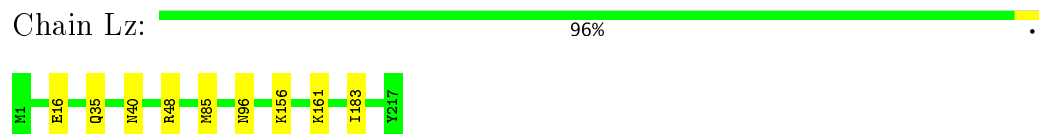


- Molecule 45: 60S ribosomal protein L28

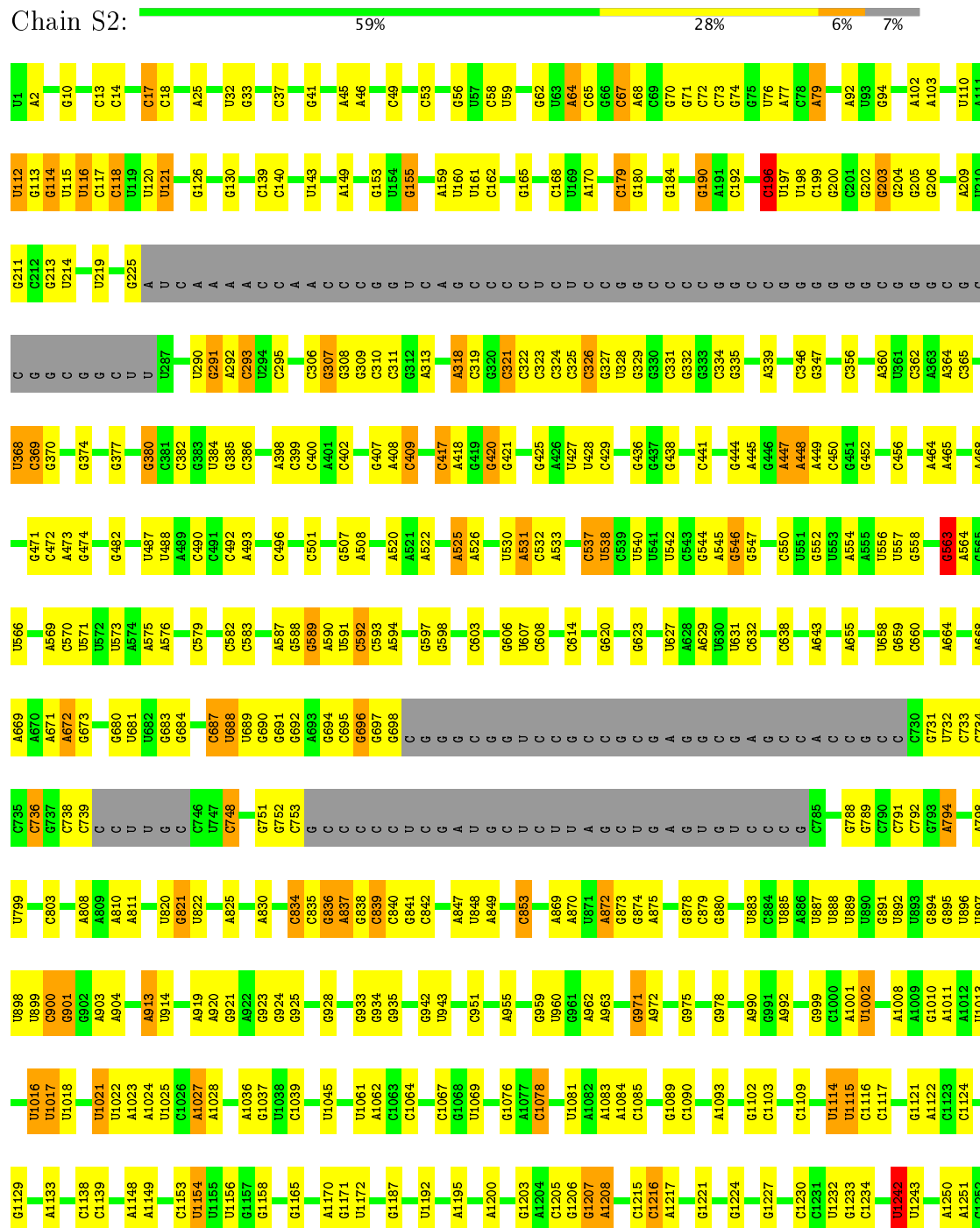
Chain Lr:  90%  9%

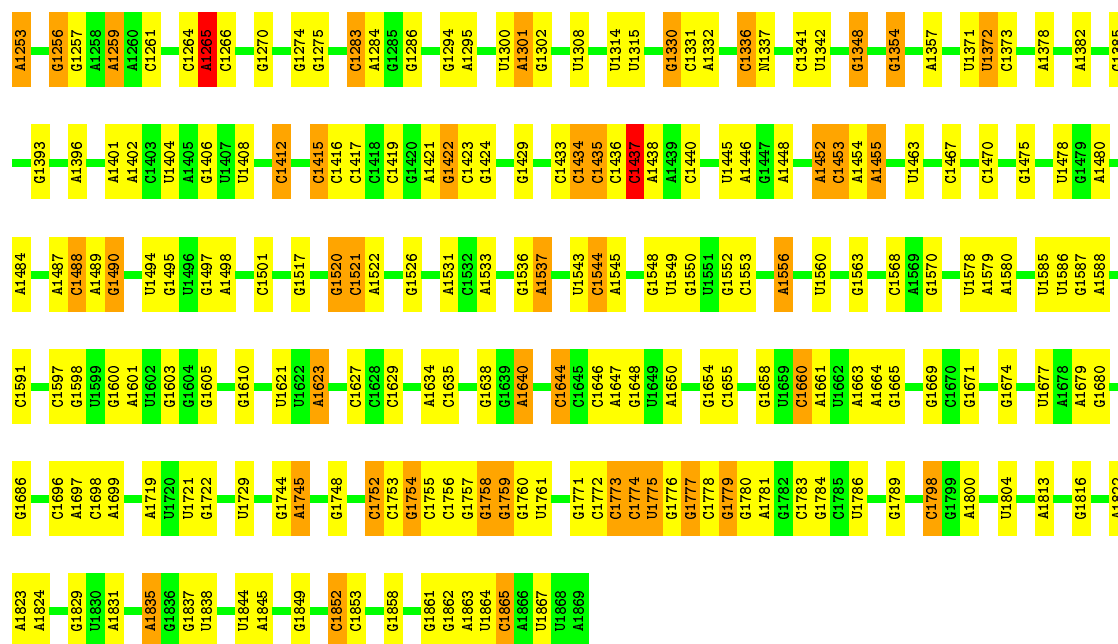


- Molecule 46: 60S ribosomal protein L10a



- Molecule 47: 18S ribosomal RNA





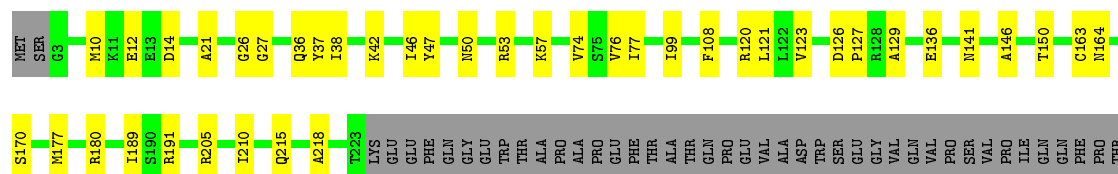
- Molecule 48: Human initiator Met-tRNA-i

Chain S6:



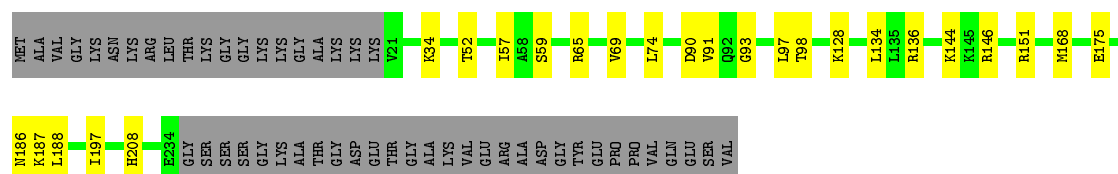
- Molecule 49: 40S ribosomal protein SA

Chain SA:

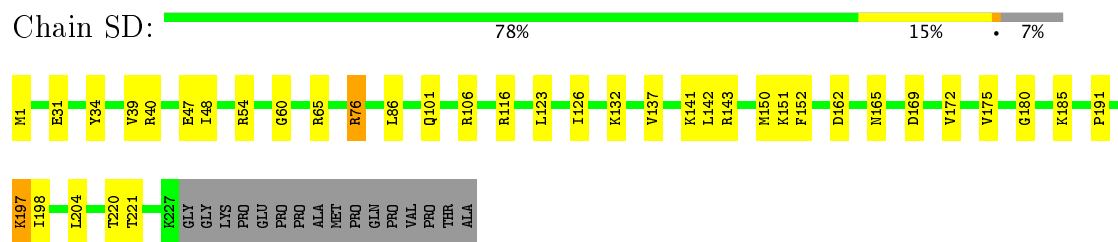


- Molecule 50: 40S ribosomal protein S3a

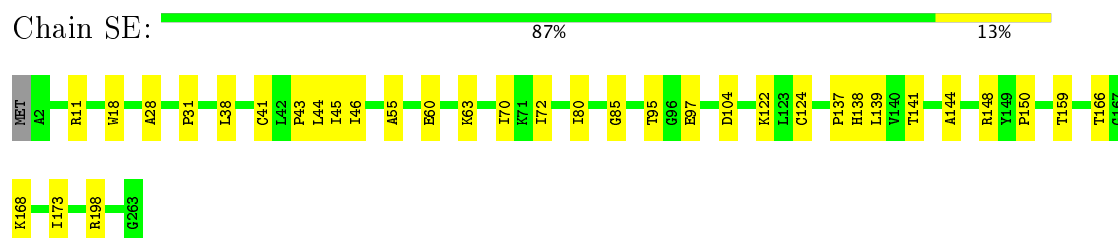
Chain SB:



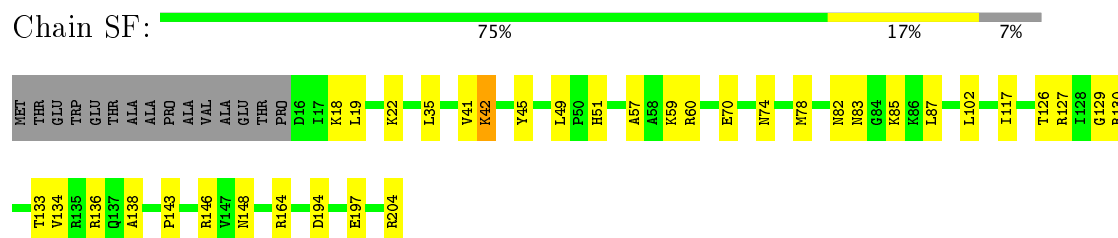
- Molecule 51: 40S ribosomal protein S3



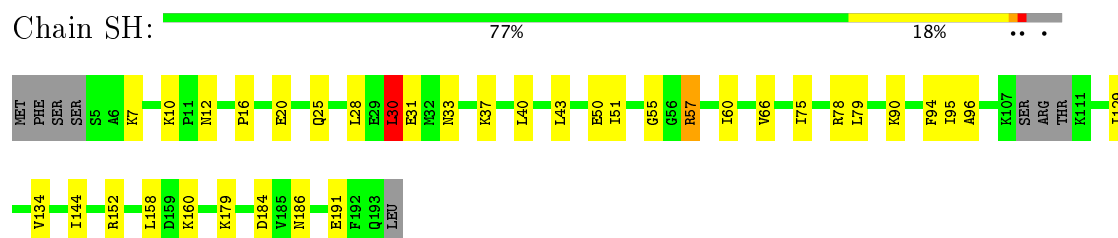
- Molecule 52: 40S ribosomal protein S4, X isoform



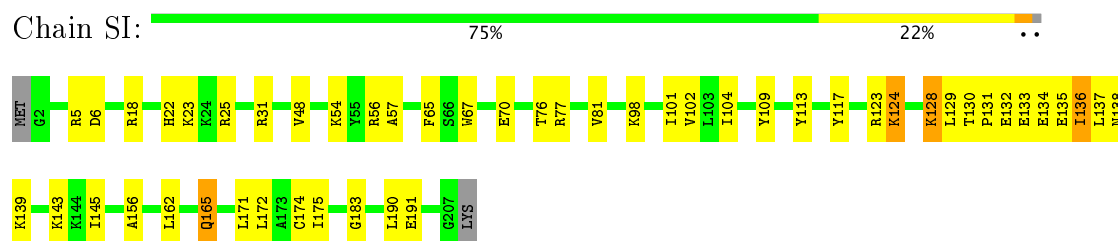
- Molecule 53: 40S ribosomal protein S5



- Molecule 54: 40S ribosomal protein S7

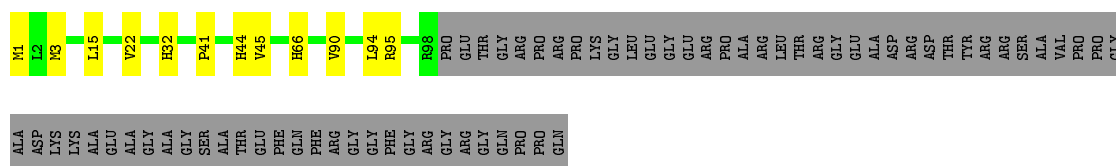


- Molecule 55: 40S ribosomal protein S8



- Molecule 56: 40S ribosomal protein S10





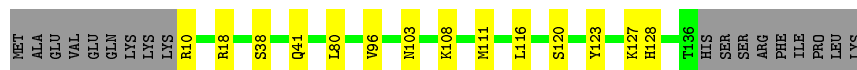
- Molecule 57: 40S ribosomal protein S11

Chain SL: 84% 11% ..



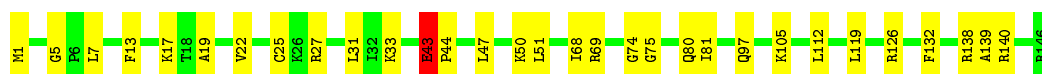
- Molecule 58: 40S ribosomal protein S15

Chain SP: 78% 10% 12%



- Molecule 59: 40S ribosomal protein S16

Chain SQ: 79% 21% .



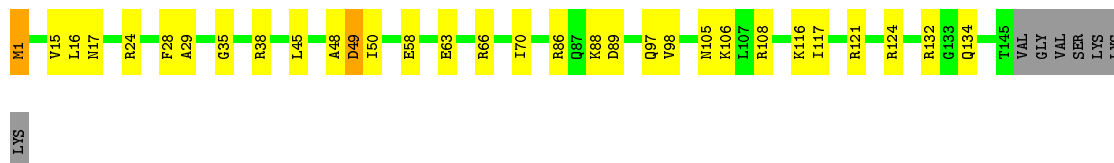
- Molecule 60: 40S ribosomal protein S17

Chain SR: 86% 14%



- Molecule 61: 40S ribosomal protein S18

Chain SS: 75% 19% . 5%

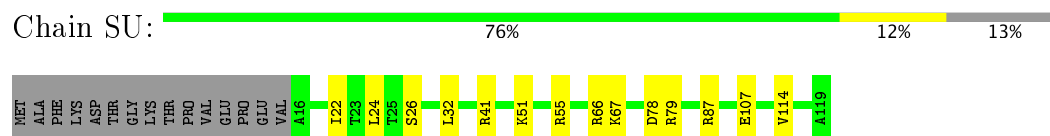


- Molecule 62: 40S ribosomal protein S19

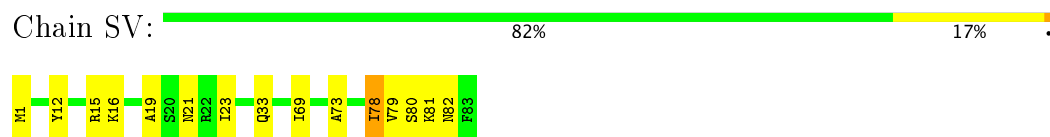
Chain ST: 90% 8% ..



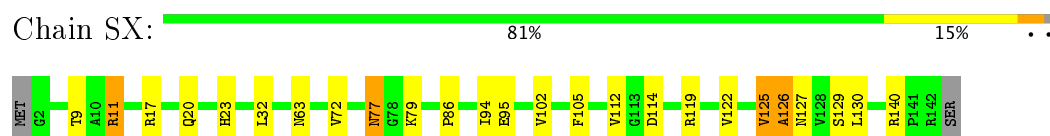
- Molecule 63: 40S ribosomal protein S20



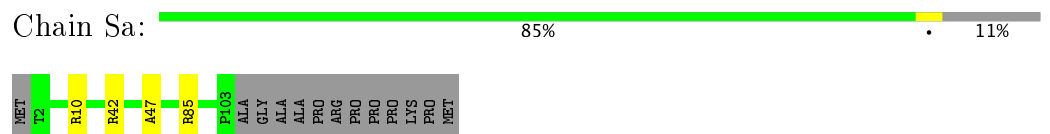
- Molecule 64: 40S ribosomal protein S21



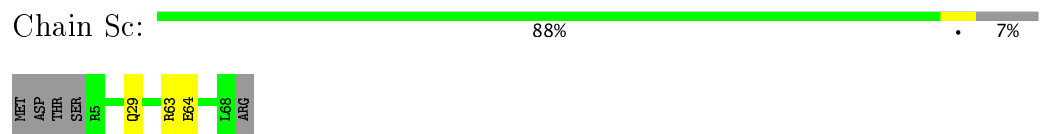
- Molecule 65: 40S ribosomal protein S23



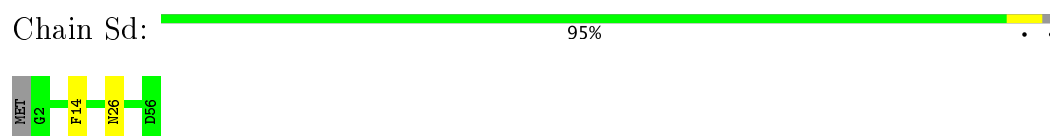
- Molecule 66: 40S ribosomal protein S26



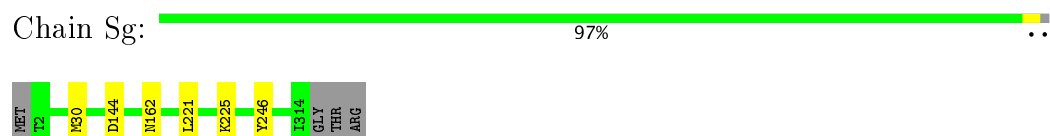
- Molecule 67: 40S ribosomal protein S28



- Molecule 68: 40S ribosomal protein S29

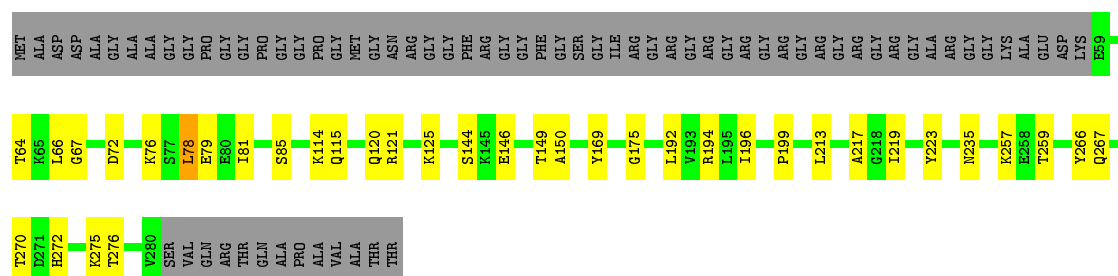


- Molecule 69: Receptor of activated protein C kinase 1

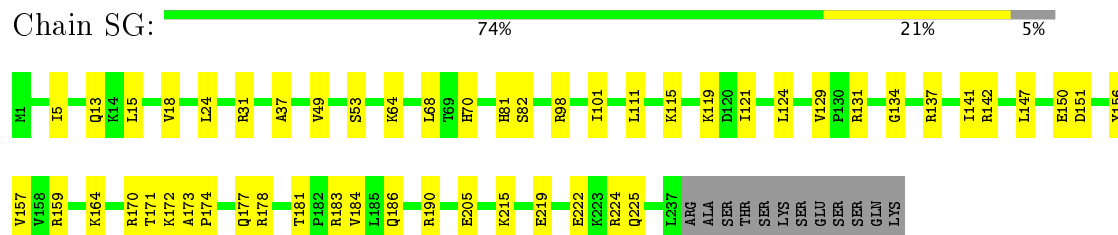


- Molecule 70: 40S ribosomal protein S2

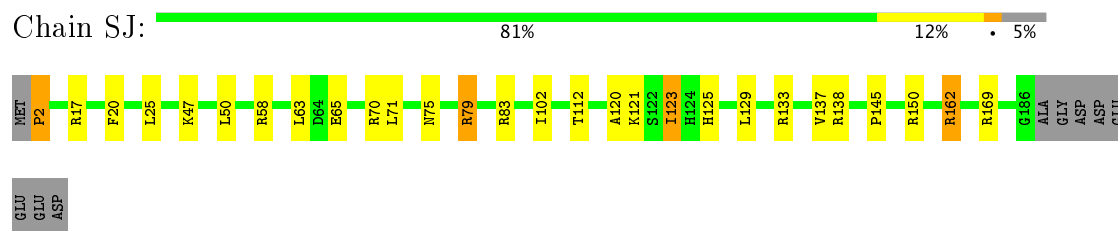




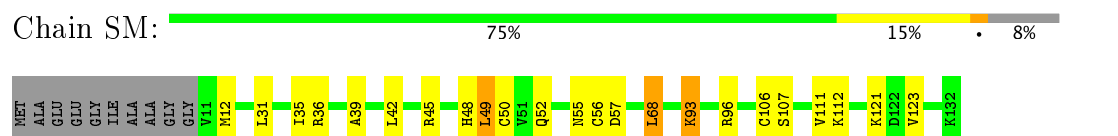
- Molecule 71: 40S ribosomal protein S6



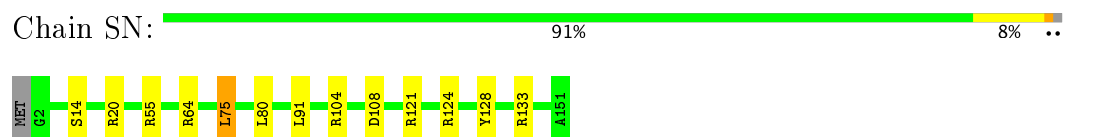
- Molecule 72: 40S ribosomal protein S9



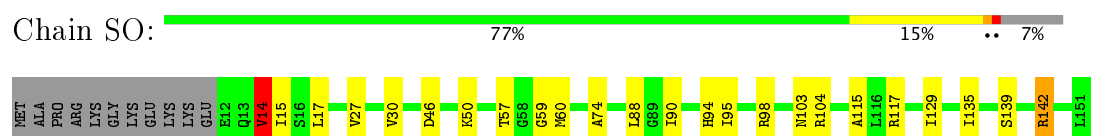
- Molecule 73: 40S ribosomal protein S12




- Molecule 74: 40S ribosomal protein S13



- Molecule 75: 40S ribosomal protein S14



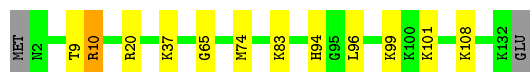
- Molecule 76: 40S ribosomal protein S15a

Chain SW:  86% 12% ..



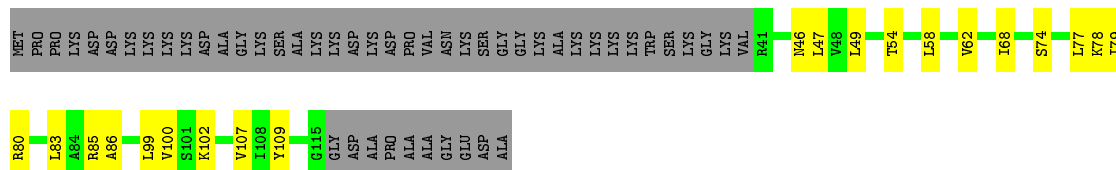
- Molecule 77: 40S ribosomal protein S24

Chain SY:  89% 8% ..



- Molecule 78: 40S ribosomal protein S25

Chain SZ:  44% 16% 40%



- Molecule 79: 40S ribosomal protein S27

Chain Sb:  99% .



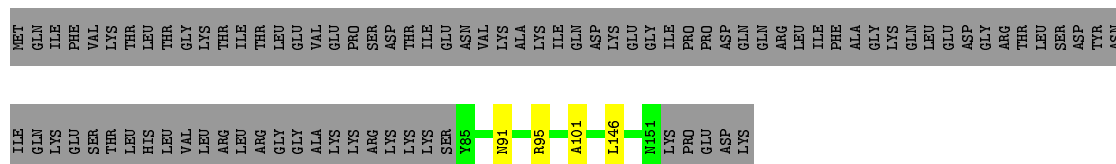
- Molecule 80: 40S ribosomal protein S30

Chain Se:  97% ..



- Molecule 81: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  40% . 57%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	138234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HYG, BGH, 2MG, 4AC, 1MA, P4U, I4U, A2M, B9H, B8Q, MA6, B8T, B8W, E6G, B8H, B8K, UR3, 7MG, OMC, ZN, OMU, MHG, B8N, P7G, 6MZ, MLZ, 5MU, MG, OMG, E7G, HMT, M7A, E3C, 5MC, B9B, PSU

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 >2	RMSZ	# Z >2
1	L5	0.90	1/87128 (0.0%)	1.12	495/135765 (0.4%)
10	LG	0.45	0/1971	0.68	0/2651
11	LH	0.47	0/1537	0.63	1/2066 (0.0%)
12	LI	0.42	0/1751	0.62	1/2340 (0.0%)
13	LJ	0.37	0/1433	0.73	3/1915 (0.2%)
14	LL	0.47	0/1732	0.64	0/2315
15	LM	0.47	0/1161	0.63	0/1554
16	LN	0.57	0/1746	0.64	1/2338 (0.0%)
17	LO	0.51	0/1682	0.61	0/2250
18	LP	0.52	0/1268	0.66	0/1701
19	LQ	0.48	0/1537	0.64	0/2052
2	L7	0.80	0/2858	0.98	4/4455 (0.1%)
20	LR	0.41	0/1582	0.64	1/2091 (0.0%)
21	LS	0.52	0/1493	0.57	0/2003
22	LT	0.49	0/1326	0.64	0/1770
23	LU	0.38	0/839	0.66	0/1126
24	LV	0.49	0/993	0.64	0/1332
25	LW	0.40	0/1030	0.64	0/1364
26	LX	0.44	0/1002	0.62	0/1345
27	LY	0.44	0/1132	0.62	0/1504
28	LZ	0.45	0/1130	0.66	1/1507 (0.1%)
29	La	0.52	0/1191	0.64	0/1591
3	L8	0.91	0/3679	1.08	14/5732 (0.2%)
30	Lb	0.38	0/889	0.64	0/1175
31	Lc	0.44	0/774	0.68	0/1038
32	Ld	0.43	0/903	0.65	0/1216
33	Le	0.52	0/1071	0.61	0/1429
34	Lf	0.56	0/895	0.68	0/1198
35	Lg	0.46	0/916	0.62	0/1220
36	Lh	0.39	0/1023	0.58	0/1351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
37	Li	0.37	0/843	0.57	0/1115
38	Lj	0.52	0/720	0.61	0/952
39	Lk	0.40	0/575	0.60	0/761
4	LA	0.54	0/1936	0.70	1/2596 (0.0%)
40	Ll	0.48	0/454	0.62	0/599
41	Lm	0.46	0/425	0.61	0/561
42	Ln	0.67	0/231	0.66	0/294
43	Lo	0.45	0/887	0.65	0/1170
44	Lp	0.46	0/718	0.60	0/953
45	Lr	0.47	0/1017	0.65	0/1364
46	Lz	0.30	0/1769	0.63	0/2371
47	S2	0.92	4/40440 (0.0%)	1.09	200/62994 (0.3%)
48	S6	0.35	0/1795	0.96	6/2798 (0.2%)
49	SA	0.44	0/1778	0.64	1/2416 (0.0%)
5	LB	0.51	0/3315	0.73	3/4435 (0.1%)
50	SB	0.42	0/1765	0.60	1/2362 (0.0%)
51	SD	0.43	0/1793	0.67	0/2414
52	SE	0.45	0/2118	0.64	2/2849 (0.1%)
53	SF	0.42	0/1516	0.67	1/2037 (0.0%)
54	SH	0.40	0/1519	0.68	1/2033 (0.0%)
55	SI	0.46	0/1715	0.67	1/2287 (0.0%)
56	SK	0.45	0/851	0.67	1/1147 (0.1%)
57	SL	0.56	1/1268 (0.1%)	0.67	0/1696
58	SP	0.42	0/1065	0.68	1/1423 (0.1%)
59	SQ	0.49	0/1176	0.70	1/1572 (0.1%)
6	LC	0.48	0/2971	0.65	1/3988 (0.0%)
60	SR	0.40	0/1105	0.63	0/1484
61	SS	0.41	0/1216	0.64	1/1628 (0.1%)
62	ST	0.43	0/1131	0.59	0/1515
63	SU	0.39	0/831	0.62	0/1115
64	SV	0.41	0/643	0.70	1/860 (0.1%)
65	SX	0.49	0/1116	0.70	0/1490
66	Sa	0.52	0/847	0.64	0/1135
67	Sc	0.45	0/508	0.76	0/680
68	Sd	0.54	0/470	0.71	0/623
69	Sg	0.39	0/2493	0.72	1/3394 (0.0%)
7	LD	0.41	0/2428	0.63	1/3252 (0.0%)
70	SC	0.51	0/1773	0.71	2/2395 (0.1%)
71	SG	0.39	0/1946	0.64	1/2590 (0.0%)
72	SJ	0.49	1/1561 (0.1%)	0.73	1/2083 (0.0%)
73	SM	0.34	0/952	0.60	0/1279
74	SN	0.45	0/1232	0.63	0/1656
75	SO	0.41	0/1062	0.65	1/1425 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
76	SW	0.50	0/1051	0.68	0/1406
77	SY	0.42	0/1094	0.63	0/1452
78	SZ	0.39	0/604	0.71	0/810
79	Sb	0.42	0/665	0.64	0/891
8	LE	0.40	0/1942	0.68	0/2606
80	Se	0.37	0/465	0.60	0/612
81	Sf	0.34	0/560	0.76	1/745 (0.1%)
9	LF	0.50	0/1916	0.69	2/2553 (0.1%)
All	All	0.75	7/231943 (0.0%)	0.96	754/340260 (0.2%)

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	L5	2	0
11	LH	0	2
12	LI	0	1
13	LJ	0	1
14	LL	0	2
15	LM	0	1
16	LN	0	1
17	LO	0	1
22	LT	0	2
23	LU	0	1
25	LW	0	1
27	LY	0	1
32	Ld	0	1
33	Le	0	1
34	Lf	0	3
36	Lh	0	1
38	Lj	0	1
4	LA	0	3
45	Lr	0	1
46	Lz	0	2
47	S2	2	0
5	LB	0	4
51	SD	0	2
53	SF	0	4
54	SH	0	2
55	SI	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	SK	0	1
57	SL	0	2
58	SP	0	1
59	SQ	0	1
62	ST	0	1
63	SU	0	1
64	SV	0	1
65	SX	0	5
66	Sa	0	1
67	Sc	0	2
7	LD	0	1
70	SC	0	1
72	SJ	0	4
73	SM	0	2
75	SO	0	1
77	SY	0	1
78	SZ	0	1
8	LE	0	1
81	Sf	0	1
9	LF	0	2
All	All	4	72

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2465	C	N1-C6	-6.30	1.33	1.37
47	S2	1853	C	N3-C4	-5.44	1.30	1.33
57	SL	128	VAL	CB-CG1	-5.25	1.41	1.52
47	S2	1200	A	N9-C4	-5.21	1.34	1.37
47	S2	1697	A	N9-C4	-5.17	1.34	1.37
47	S2	1203	G	N7-C5	-5.13	1.36	1.39
72	SJ	162	ARG	C-N	-5.10	1.22	1.34

All (754) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	501	C	C2-N1-C1'	14.41	134.65	118.80
1	L5	485	C	N1-C2-O2	13.90	127.24	118.90
47	S2	501	C	N1-C2-O2	13.88	127.23	118.90
1	L5	485	C	C2-N1-C1'	12.47	132.52	118.80
47	S2	293	C	N1-C2-O2	11.94	126.06	118.90
47	S2	356	C	N1-C2-O2	11.79	125.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	485	C	N3-C2-O2	-11.49	113.86	121.90
1	L5	3964	U	C2-N1-C1'	11.28	131.24	117.70
47	S2	501	C	N3-C2-O2	-11.19	114.06	121.90
1	L5	2710	C	N1-C2-O2	11.14	125.58	118.90
1	L5	2710	C	C2-N1-C1'	10.94	130.84	118.80
1	L5	753	C	N1-C2-O2	10.88	125.43	118.90
1	L5	1378	C	N1-C2-O2	10.74	125.34	118.90
1	L5	3964	U	N1-C2-O2	10.64	130.25	122.80
1	L5	3964	U	N3-C2-O2	-10.55	114.82	122.20
47	S2	1453	C	C2-N1-C1'	10.51	130.36	118.80
47	S2	293	C	C2-N1-C1'	10.36	130.19	118.80
1	L5	1214	C	C2-N1-C1'	10.31	130.14	118.80
47	S2	501	C	C6-N1-C1'	-10.28	108.46	120.80
47	S2	356	C	C2-N1-C1'	10.22	130.04	118.80
1	L5	1214	C	N1-C2-O2	9.91	124.85	118.90
1	L5	2814	C	N1-C2-O2	9.84	124.81	118.90
1	L5	753	C	N3-C2-O2	-9.76	115.07	121.90
1	L5	4928	C	C2-N1-C1'	9.74	129.52	118.80
1	L5	969	C	N1-C2-O2	9.71	124.72	118.90
47	S2	537	C	N1-C2-O2	9.63	124.68	118.90
47	S2	427	U	N3-C2-O2	-9.57	115.50	122.20
47	S2	1139	C	C2-N1-C1'	9.45	129.20	118.80
47	S2	1453	C	N1-C2-O2	9.38	124.53	118.90
1	L5	340	C	N1-C2-O2	9.37	124.52	118.90
47	S2	1139	C	N3-C2-O2	-9.34	115.36	121.90
1	L5	4775	C	N1-C2-O2	9.31	124.48	118.90
47	S2	293	C	N3-C2-O2	-9.28	115.40	121.90
1	L5	4557	U	N3-C2-O2	-9.25	115.73	122.20
47	S2	1520	G	C4-N9-C1'	9.23	138.50	126.50
47	S2	118	C	C2-N1-C1'	9.23	128.95	118.80
47	S2	356	C	N3-C2-O2	-9.18	115.47	121.90
1	L5	2501	C	N1-C2-O2	9.05	124.33	118.90
1	L5	1241	C	N1-C2-O2	9.04	124.32	118.90
1	L5	2710	C	N3-C2-O2	-9.04	115.58	121.90
47	S2	1139	C	N1-C2-O2	9.00	124.30	118.90
1	L5	2783	A	C6-N1-C2	8.97	123.98	118.60
1	L5	2255	C	N1-C2-O2	8.91	124.25	118.90
47	S2	1520	G	C8-N9-C1'	-8.84	115.50	127.00
1	L5	233	U	N3-C2-O2	-8.82	116.03	122.20
1	L5	969	C	C2-N1-C1'	8.82	128.50	118.80
47	S2	537	C	C2-N1-C1'	8.74	128.41	118.80
1	L5	2814	C	C2-N1-C1'	8.66	128.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2019	C	N1-C2-O2	8.63	124.08	118.90
1	L5	485	C	C6-N1-C1'	-8.61	110.47	120.80
47	S2	501	C	C6-N1-C2	-8.57	116.87	120.30
1	L5	4557	U	C2-N1-C1'	8.56	127.98	117.70
47	S2	1437	C	C6-N1-C2	-8.47	116.91	120.30
47	S2	1437	C	N1-C2-O2	8.46	123.97	118.90
1	L5	1378	C	N3-C2-O2	-8.40	116.02	121.90
47	S2	1016	U	N3-C2-O2	-8.40	116.32	122.20
1	L5	485	C	C6-N1-C2	-8.36	116.96	120.30
1	L5	753	C	C2-N1-C1'	8.35	127.98	118.80
1	L5	4775	C	N3-C2-O2	-8.35	116.06	121.90
1	L5	1607	C	N1-C2-O2	8.34	123.90	118.90
1	L5	4162	C	N1-C2-O2	8.33	123.90	118.90
47	S2	1853	C	N3-C4-N4	-8.30	112.19	118.00
1	L5	1704	C	C6-N1-C2	-8.29	116.98	120.30
1	L5	1214	C	C6-N1-C2	-8.25	117.00	120.30
1	L5	1821	G	N3-C4-C5	-8.23	124.49	128.60
28	LZ	30	ASP	CB-CG-OD1	8.22	125.70	118.30
1	L5	1241	C	C2-N1-C1'	8.17	127.79	118.80
1	L5	1214	C	N3-C2-O2	-8.15	116.20	121.90
1	L5	1893	C	N1-C2-O2	8.13	123.78	118.90
1	L5	1378	C	C2-N1-C1'	8.12	127.73	118.80
1	L5	340	C	C2-N1-C1'	8.11	127.72	118.80
47	S2	1016	U	N1-C2-O2	8.10	128.47	122.80
1	L5	4709	U	C2-N1-C1'	8.07	127.38	117.70
47	S2	1437	C	C2-N1-C1'	8.05	127.66	118.80
1	L5	992	C	N1-C2-O2	8.05	123.73	118.90
1	L5	233	U	N1-C2-O2	8.04	128.43	122.80
1	L5	4557	U	N1-C2-O2	8.02	128.41	122.80
47	S2	402	C	C5-C6-N1	8.00	125.00	121.00
47	S2	402	C	C6-N1-C2	-8.00	117.10	120.30
1	L5	2096	G	C4-N9-C1'	8.00	136.90	126.50
1	L5	2014	C	N1-C2-O2	7.99	123.70	118.90
1	L5	2814	C	N3-C2-O2	-7.96	116.33	121.90
1	L5	4601	U	C2-N1-C1'	7.95	127.23	117.70
1	L5	1628	C	C6-N1-C2	-7.93	117.13	120.30
3	L8	51	U	N1-C2-O2	7.92	128.34	122.80
1	L5	3964	U	C5-C6-N1	7.90	126.65	122.70
1	L5	4921	C	N1-C2-O2	7.89	123.64	118.90
3	L8	101	C	N1-C2-O2	7.88	123.63	118.90
47	S2	1016	U	C2-N1-C1'	7.87	127.15	117.70
1	L5	2262	G	N3-C4-C5	-7.84	124.68	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	417	G	O4'-C1'-N9	7.83	114.47	108.20
1	L5	2710	C	C6-N1-C2	-7.83	117.17	120.30
1	L5	4667	C	C6-N1-C2	-7.83	117.17	120.30
47	S2	1453	C	C6-N1-C1'	-7.83	111.41	120.80
1	L5	4928	C	N1-C2-O2	7.80	123.58	118.90
1	L5	4601	U	C5-C6-N1	7.80	126.60	122.70
47	S2	118	C	O4'-C1'-N1	7.79	114.43	108.20
47	S2	1283	C	N1-C2-O2	7.79	123.57	118.90
1	L5	1821	G	N3-C4-N9	7.76	130.66	126.00
1	L5	209	U	C2-N1-C1'	7.76	127.01	117.70
48	S6	41	C	N1-C2-O2	7.70	123.52	118.90
69	Sg	144	ASP	CB-CG-OD1	7.70	125.23	118.30
1	L5	100	C	C2-N1-C1'	7.70	127.27	118.80
1	L5	4303	C	C2-N1-C1'	7.70	127.26	118.80
47	S2	1283	C	C6-N1-C2	-7.68	117.23	120.30
1	L5	1821	G	C4-N9-C1'	7.65	136.45	126.50
1	L5	2262	G	C4-N9-C1'	7.64	136.43	126.50
47	S2	1283	C	N3-C2-O2	-7.64	116.55	121.90
47	S2	427	U	C2-N1-C1'	7.63	126.85	117.70
5	LB	360	LEU	CA-CB-CG	7.60	132.77	115.30
1	L5	2410	C	N1-C2-O2	7.59	123.45	118.90
1	L5	4950	U	N1-C2-O2	7.57	128.10	122.80
1	L5	100	C	N1-C2-O2	7.55	123.43	118.90
47	S2	427	U	N1-C2-O2	7.49	128.04	122.80
1	L5	3587	C	N1-C2-O2	7.46	123.37	118.90
1	L5	4709	U	N1-C2-O2	7.45	128.01	122.80
1	L5	4303	C	N3-C2-O2	-7.45	116.69	121.90
1	L5	100	C	N3-C2-O2	-7.44	116.69	121.90
1	L5	2729	C	N1-C2-O2	7.43	123.36	118.90
47	S2	537	C	N3-C2-O2	-7.43	116.70	121.90
1	L5	2262	G	N3-C4-N9	7.43	130.46	126.00
1	L5	2257	C	N1-C2-O2	7.42	123.35	118.90
1	L5	2351	C	N1-C2-O2	7.37	123.32	118.90
1	L5	2710	C	C6-N1-C1'	-7.34	111.99	120.80
1	L5	4162	C	C2-N1-C1'	7.34	126.87	118.80
1	L5	4303	C	C6-N1-C2	-7.32	117.37	120.30
1	L5	1703	C	N1-C2-O2	7.32	123.29	118.90
1	L5	1774	C	N1-C2-O2	7.32	123.29	118.90
1	L5	4928	C	C6-N1-C1'	-7.28	112.06	120.80
1	L5	2255	C	C2-N1-C1'	7.26	126.78	118.80
1	L5	4775	C	C2-N1-C1'	7.24	126.77	118.80
47	S2	331	C	N1-C2-O2	7.23	123.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	LJ	119	TYR	C-N-CA	7.21	139.72	121.70
5	LB	214	ASP	CB-CG-OD1	7.18	124.76	118.30
47	S2	1437	C	N3-C2-O2	-7.17	116.88	121.90
47	S2	356	C	C6-N1-C1'	-7.15	112.22	120.80
1	L5	3605	C	C6-N1-C2	-7.14	117.44	120.30
47	S2	1852	C	N1-C2-O2	7.14	123.19	118.90
47	S2	1265	A	C2-N3-C4	7.14	114.17	110.60
1	L5	3964	U	C6-N1-C2	-7.13	116.72	121.00
1	L5	4621	C	C6-N1-C2	-7.12	117.45	120.30
1	L5	4887	C	N1-C2-O2	7.12	123.17	118.90
3	L8	51	U	N3-C2-O2	-7.11	117.22	122.20
1	L5	41	C	C6-N1-C2	-7.10	117.46	120.30
1	L5	992	C	C6-N1-C2	-7.09	117.47	120.30
47	S2	293	C	C6-N1-C1'	-7.07	112.32	120.80
1	L5	1214	C	C5-C6-N1	7.05	124.53	121.00
47	S2	1022	U	N1-C2-O2	7.04	127.73	122.80
1	L5	2096	G	N3-C4-N9	7.04	130.22	126.00
1	L5	2096	G	C8-N9-C1'	-7.04	117.85	127.00
47	S2	659	G	C4-N9-C1'	7.03	135.64	126.50
1	L5	4162	C	N3-C2-O2	-7.03	116.98	121.90
47	S2	293	C	C6-N1-C2	-7.02	117.49	120.30
1	L5	1241	C	N3-C2-O2	-7.01	116.99	121.90
1	L5	3968	U	N1-C2-O2	7.01	127.70	122.80
1	L5	4281	A	O4'-C1'-N9	7.01	113.81	108.20
47	S2	456	C	C6-N1-C2	-7.01	117.50	120.30
1	L5	4950	U	N3-C2-O2	-7.00	117.30	122.20
1	L5	1439	C	C6-N1-C2	-6.99	117.50	120.30
1	L5	4398	C	N1-C2-O2	6.98	123.09	118.90
1	L5	340	C	N3-C2-O2	-6.98	117.01	121.90
1	L5	3920	U	N3-C2-O2	-6.97	117.32	122.20
5	LB	17	LEU	CA-CB-CG	6.97	131.32	115.30
47	S2	1283	C	C2-N1-C1'	6.96	126.46	118.80
1	L5	914	U	P-O3'-C3'	6.96	128.05	119.70
1	L5	1178	G	N3-C4-N9	6.95	130.17	126.00
1	L5	906	C	N1-C2-O2	6.93	123.06	118.90
3	L8	101	C	N3-C2-O2	-6.93	117.05	121.90
1	L5	209	U	N1-C2-O2	6.92	127.65	122.80
1	L5	2255	C	N3-C2-O2	-6.92	117.06	121.90
1	L5	981	C	P-O3'-C3'	6.92	128.00	119.70
1	L5	2905	C	N1-C2-O2	6.91	123.05	118.90
1	L5	2096	G	N3-C4-C5	-6.90	125.15	128.60
1	L5	3926	C	N1-C2-O2	6.88	123.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1139	C	C6-N1-C2	-6.87	117.55	120.30
1	L5	1607	C	N3-C2-O2	-6.87	117.09	121.90
47	S2	1852	C	C2-N1-C1'	6.86	126.35	118.80
48	S6	41	C	N3-C2-O2	-6.86	117.10	121.90
1	L5	2501	C	N3-C2-O2	-6.86	117.10	121.90
47	S2	118	C	C6-N1-C1'	-6.84	112.59	120.80
1	L5	2760	G	P-O3'-C3'	6.83	127.90	119.70
1	L5	112	C	N1-C2-O2	6.82	122.99	118.90
47	S2	592	C	C2-N1-C1'	6.82	126.30	118.80
1	L5	1082	C	OP1-P-O3'	6.80	120.17	105.20
1	L5	1214	C	C6-N1-C1'	-6.80	112.64	120.80
47	S2	1078	C	N1-C2-O2	6.79	122.98	118.90
1	L5	2019	C	N3-C2-O2	-6.79	117.15	121.90
1	L5	971	U	N1-C2-O2	6.78	127.55	122.80
1	L5	1083	U	O5'-P-OP1	-6.78	99.59	105.70
1	L5	504	G	C4-N9-C1'	6.77	135.30	126.50
47	S2	501	C	C5-C6-N1	6.75	124.38	121.00
1	L5	2867	C	N1-C2-O2	6.75	122.95	118.90
12	LI	111	LEU	CA-CB-CG	6.74	130.80	115.30
47	S2	1437	C	C5-C6-N1	6.74	124.37	121.00
1	L5	2014	C	C2-N1-C1'	6.74	126.21	118.80
1	L5	255	C	C6-N1-C2	-6.72	117.61	120.30
1	L5	131	C	N1-C2-O2	6.72	122.93	118.90
47	S2	118	C	N1-C2-O2	6.71	122.93	118.90
1	L5	971	U	C2-N1-C1'	6.70	125.74	117.70
1	L5	992	C	N3-C2-O2	-6.69	117.22	121.90
1	L5	4206	C	N1-C2-O2	6.69	122.91	118.90
47	S2	593	C	N1-C2-O2	6.68	122.91	118.90
1	L5	2351	C	C5-C6-N1	6.68	124.34	121.00
1	L5	511	C	N3-C2-O2	-6.67	117.23	121.90
1	L5	1439	C	N1-C2-O2	6.67	122.91	118.90
1	L5	4880	C	N1-C2-O2	6.66	122.90	118.90
1	L5	115	C	C2-N1-C1'	6.66	126.13	118.80
59	SQ	7	LEU	CA-CB-CG	6.65	130.60	115.30
1	L5	753	C	C6-N1-C2	-6.65	117.64	120.30
47	S2	1853	C	C5-C4-N4	6.62	124.84	120.20
47	S2	1696	C	C6-N1-C2	-6.62	117.65	120.30
1	L5	1505	C	C6-N1-C2	-6.62	117.65	120.30
1	L5	3772	U	C2-N1-C1'	6.61	125.63	117.70
1	L5	1809	C	N1-C2-O2	6.61	122.86	118.90
1	L5	2528	G	C4-N9-C1'	6.61	135.09	126.50
1	L5	2394	G	O4'-C1'-N9	6.60	113.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4950	U	C2-N1-C1'	6.59	125.61	117.70
1	L5	3964	U	C6-N1-C1'	-6.58	111.99	121.20
1	L5	4303	C	N1-C2-O2	6.58	122.85	118.90
1	L5	2257	C	C2-N1-C1'	6.57	126.03	118.80
47	S2	1578	U	N3-C2-O2	-6.56	117.61	122.20
1	L5	1082	C	P-O3'-C3'	6.56	127.57	119.70
1	L5	969	C	N3-C2-O2	-6.55	117.31	121.90
53	SF	19	LEU	CA-CB-CG	6.54	130.33	115.30
47	S2	331	C	N3-C2-O2	-6.53	117.33	121.90
49	SA	14	ASP	CB-CG-OD1	6.51	124.16	118.30
1	L5	1821	G	C2-N3-C4	6.49	115.14	111.90
3	L8	101	C	C2-N1-C1'	6.48	125.93	118.80
1	L5	483	G	N3-C4-C5	-6.47	125.37	128.60
1	L5	1633	G	OP1-P-O3'	6.46	119.41	105.20
47	S2	1314	U	C2-N1-C1'	6.45	125.44	117.70
52	SE	139	LEU	CA-CB-CG	6.44	130.11	115.30
47	S2	356	C	C6-N1-C2	-6.44	117.72	120.30
1	L5	1620	U	N1-C2-O2	6.43	127.30	122.80
47	S2	1207	G	C4-N9-C1'	-6.42	118.15	126.50
1	L5	2262	G	C8-N9-C1'	-6.42	118.65	127.00
1	L5	4928	C	N3-C2-O2	-6.42	117.41	121.90
71	SG	68	LEU	CA-CB-CG	6.42	130.06	115.30
47	S2	1578	U	N1-C2-O2	6.40	127.28	122.80
1	L5	969	C	C6-N1-C1'	-6.40	113.12	120.80
1	L5	4709	U	N3-C2-O2	-6.39	117.73	122.20
1	L5	274	C	N1-C2-O2	6.38	122.73	118.90
47	S2	325	C	C2-N1-C1'	6.37	125.81	118.80
47	S2	659	G	C8-N9-C1'	-6.37	118.72	127.00
50	SB	188	LEU	CA-CB-CG	6.36	129.93	115.30
47	S2	1453	C	N3-C2-O2	-6.35	117.46	121.90
1	L5	489	C	N1-C2-O2	6.35	122.71	118.90
1	L5	1439	C	C5-C6-N1	6.34	124.17	121.00
1	L5	2033	A	P-O3'-C3'	6.34	127.31	119.70
1	L5	2014	C	N3-C2-O2	-6.33	117.47	121.90
1	L5	4913	G	P-O3'-C3'	6.31	127.27	119.70
1	L5	1703	C	N3-C2-O2	-6.31	117.48	121.90
47	S2	130	G	C4-N9-C1'	6.30	134.70	126.50
47	S2	1139	C	C6-N1-C1'	-6.30	113.24	120.80
1	L5	1178	G	C4-N9-C1'	6.30	134.69	126.50
1	L5	2814	C	C6-N1-C1'	-6.29	113.25	120.80
47	S2	1315	U	N3-C2-O2	-6.29	117.80	122.20
47	S2	1453	C	C5-C6-N1	6.29	124.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1620	U	N3-C2-O2	-6.28	117.80	122.20
48	S6	54	A	P-O3'-C3'	6.28	127.24	119.70
1	L5	4387	C	C6-N1-C2	-6.27	117.79	120.30
1	L5	3968	U	N3-C2-O2	-6.26	117.81	122.20
1	L5	1853	G	C4-N9-C1'	6.26	134.63	126.50
1	L5	53	C	C6-N1-C2	-6.25	117.80	120.30
1	L5	2607	C	C6-N1-C2	-6.24	117.80	120.30
47	S2	409	C	N1-C2-O2	6.24	122.64	118.90
47	S2	1022	U	N3-C2-O2	-6.24	117.84	122.20
1	L5	2019	C	C2-N1-C1'	6.23	125.65	118.80
1	L5	124	C	C6-N1-C2	-6.23	117.81	120.30
1	L5	4432	C	C6-N1-C2	-6.22	117.81	120.30
1	L5	133	C	N1-C2-O2	6.22	122.63	118.90
1	L5	1191	C	N1-C2-O2	6.22	122.63	118.90
1	L5	485	C	C5-C6-N1	6.21	124.10	121.00
1	L5	4241	C	N1-C2-O2	6.20	122.62	118.90
47	S2	688	U	P-O3'-C3'	6.19	127.13	119.70
47	S2	1022	U	C2-N1-C1'	6.19	125.13	117.70
1	L5	2729	C	N3-C2-O2	-6.18	117.57	121.90
1	L5	1821	G	C8-N9-C1'	-6.18	118.96	127.00
1	L5	2409	U	C4-C5-C6	6.18	123.41	119.70
1	L5	1241	C	C6-N1-C1'	-6.18	113.38	120.80
1	L5	511	C	C6-N1-C2	-6.17	117.83	120.30
1	L5	2410	C	C5-C6-N1	6.17	124.08	121.00
1	L5	1704	C	C2-N1-C1'	6.16	125.58	118.80
47	S2	1660	C	C2-N1-C1'	6.16	125.57	118.80
1	L5	483	G	C2-N3-C4	6.15	114.98	111.90
1	L5	1404	G	C4-N9-C1'	6.15	134.50	126.50
1	L5	4667	C	C5-C6-N1	6.15	124.07	121.00
1	L5	1178	G	N3-C4-C5	-6.14	125.53	128.60
47	S2	1774	C	N1-C2-O2	6.14	122.59	118.90
1	L5	1535	C	C5-C6-N1	6.13	124.06	121.00
1	L5	4237	C	N1-C2-O2	6.13	122.58	118.90
47	S2	112	U	P-O3'-C3'	6.13	127.06	119.70
47	S2	592	C	N1-C2-O2	6.13	122.58	118.90
47	S2	1261	C	C6-N1-C2	-6.13	117.85	120.30
1	L5	511	C	N1-C2-O2	6.12	122.58	118.90
1	L5	2501	C	C2-N1-C1'	6.12	125.54	118.80
47	S2	872	A	O4'-C1'-N9	6.12	113.10	108.20
1	L5	2792	C	C6-N1-C2	-6.12	117.85	120.30
47	S2	1103	C	C6-N1-C2	-6.10	117.86	120.30
47	S2	1415	C	C6-N1-C2	-6.09	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	504	G	N3-C4-N9	6.08	129.65	126.00
1	L5	41	C	C5-C6-N1	6.08	124.04	121.00
1	L5	2710	C	C5-C6-N1	6.06	124.03	121.00
47	S2	1315	U	N1-C2-O2	6.06	127.04	122.80
1	L5	4926	C	C2-N1-C1'	6.06	125.46	118.80
1	L5	367	C	C6-N1-C2	-6.04	117.89	120.30
1	L5	3866	C	C6-N1-C2	-6.04	117.89	120.30
47	S2	537	C	C6-N1-C2	-6.04	117.89	120.30
47	S2	1865	C	C6-N1-C2	-6.03	117.89	120.30
1	L5	1216	C	C2-N1-C1'	6.03	125.43	118.80
47	S2	537	C	C6-N1-C1'	-6.03	113.57	120.80
1	L5	1182	C	C2-N1-C1'	6.01	125.42	118.80
1	L5	988	C	N1-C2-O2	6.01	122.51	118.90
1	L5	2528	G	N3-C4-N9	6.01	129.60	126.00
70	SC	192	LEU	CA-CB-CG	6.00	129.10	115.30
1	L5	1535	C	C6-N1-C2	-6.00	117.90	120.30
1	L5	2675	G	P-O3'-C3'	6.00	126.90	119.70
47	S2	325	C	N1-C2-O2	6.00	122.50	118.90
1	L5	4662	C	C6-N1-C2	-6.00	117.90	120.30
1	L5	969	C	C5-C6-N1	5.99	124.00	121.00
1	L5	3926	C	C6-N1-C2	-5.99	117.90	120.30
47	S2	130	G	N3-C4-N9	5.99	129.59	126.00
3	L8	28	C	C6-N1-C2	-5.98	117.91	120.30
1	L5	1632	A	C2-N3-C4	5.98	113.59	110.60
47	S2	531	A	OP1-P-O3'	5.98	118.35	105.20
47	S2	687	C	C2-N1-C1'	5.98	125.38	118.80
1	L5	1893	C	C2-N1-C1'	5.97	125.37	118.80
1	L5	1707	C	C6-N1-C2	-5.97	117.91	120.30
1	L5	504	G	C8-N9-C1'	-5.97	119.24	127.00
1	L5	4476	C	C2-N1-C1'	5.97	125.37	118.80
1	L5	971	U	N3-C2-O2	-5.97	118.02	122.20
1	L5	1243	C	C6-N1-C2	-5.96	117.92	120.30
47	S2	291	G	P-O3'-C3'	5.96	126.86	119.70
1	L5	1367	C	C2-N1-C1'	5.96	125.36	118.80
1	L5	4350	C	N1-C2-O2	5.96	122.47	118.90
47	S2	1434	C	P-O3'-C3'	5.96	126.85	119.70
47	S2	1261	C	N3-C2-O2	-5.95	117.73	121.90
1	L5	4398	C	N3-C2-O2	-5.95	117.74	121.90
1	L5	2416	G	P-O3'-C3'	5.95	126.84	119.70
1	L5	3587	C	N3-C2-O2	-5.95	117.74	121.90
1	L5	4594	U	N1-C2-O2	5.95	126.96	122.80
1	L5	1853	G	C8-N9-C1'	-5.94	119.28	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	593	C	N3-C2-O2	-5.93	117.75	121.90
1	L5	1704	C	N3-C2-O2	-5.93	117.75	121.90
1	L5	2783	A	C5-C6-N1	-5.92	114.74	117.70
1	L5	1378	C	C6-N1-C1'	-5.92	113.69	120.80
1	L5	1687	U	N3-C2-O2	-5.92	118.05	122.20
47	S2	1422	G	C4-N9-C1'	5.92	134.20	126.50
1	L5	2729	C	C6-N1-C2	-5.92	117.93	120.30
1	L5	115	C	N1-C2-O2	5.91	122.45	118.90
1	L5	963	G	C4-N9-C1'	5.91	134.19	126.50
1	L5	1384	C	C6-N1-C2	-5.91	117.94	120.30
1	L5	67	C	C6-N1-C2	-5.91	117.94	120.30
9	LF	179	LEU	CA-CB-CG	5.90	128.88	115.30
1	L5	3926	C	N3-C2-O2	-5.90	117.77	121.90
1	L5	992	C	C5-C6-N1	5.90	123.95	121.00
1	L5	4594	U	N3-C2-O2	-5.89	118.07	122.20
1	L5	2337	C	N1-C2-O2	5.89	122.44	118.90
3	L8	51	U	C2-N1-C1'	5.89	124.77	117.70
1	L5	1663	C	C5-C6-N1	5.88	123.94	121.00
1	L5	4709	U	C5-C6-N1	5.88	125.64	122.70
47	S2	293	C	C5-C6-N1	5.88	123.94	121.00
47	S2	632	C	C6-N1-C2	-5.88	117.95	120.30
47	S2	1520	G	N3-C4-N9	5.88	129.53	126.00
47	S2	1078	C	N3-C2-O2	-5.88	117.79	121.90
1	L5	112	C	N3-C2-O2	-5.87	117.79	121.90
1	L5	3605	C	C5-C6-N1	5.87	123.94	121.00
1	L5	96	U	N1-C2-O2	5.87	126.91	122.80
1	L5	4918	C	N1-C2-O2	5.87	122.42	118.90
47	S2	1124	C	C6-N1-C2	-5.86	117.95	120.30
1	L5	2014	C	C6-N1-C2	-5.86	117.96	120.30
1	L5	3673	C	P-O3'-C3'	5.86	126.73	119.70
1	L5	4243	C	N1-C2-O2	5.84	122.41	118.90
1	L5	4557	U	C6-N1-C1'	-5.84	113.02	121.20
1	L5	3772	U	N1-C2-O2	5.84	126.89	122.80
1	L5	3968	U	C2-N1-C1'	5.84	124.70	117.70
1	L5	4068	U	N1-C2-O2	5.83	126.88	122.80
1	L5	4887	C	C2-N1-C1'	5.82	125.21	118.80
47	S2	563	G	P-O3'-C3'	5.82	126.68	119.70
1	L5	2019	C	C6-N1-C2	-5.82	117.97	120.30
1	L5	1915	C	N3-C2-O2	-5.81	117.83	121.90
47	S2	1853	C	N1-C2-O2	5.81	122.39	118.90
1	L5	4206	C	N3-C2-O2	-5.81	117.83	121.90
1	L5	738	C	C6-N1-C2	-5.81	117.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1809	C	C2-N1-C1'	5.80	125.18	118.80
47	S2	1865	C	N3-C2-O2	-5.80	117.84	121.90
47	S2	853	C	N1-C2-O2	5.79	122.38	118.90
1	L5	233	U	N1-C1'-C2'	5.79	121.52	114.00
1	L5	3668	C	N1-C2-O2	5.79	122.37	118.90
2	L7	14	C	N1-C2-O2	5.78	122.37	118.90
47	S2	1207	G	C8-N9-C1'	5.78	134.52	127.00
1	L5	233	U	C2-N1-C1'	5.78	124.63	117.70
1	L5	3587	C	C2-N1-C1'	5.77	125.15	118.80
1	L5	2528	G	N3-C4-C5	-5.77	125.72	128.60
2	L7	78	C	C6-N1-C2	-5.77	117.99	120.30
1	L5	1243	C	N1-C2-O2	5.77	122.36	118.90
1	L5	3975	C	C6-N1-C2	-5.77	117.99	120.30
47	S2	1261	C	N1-C2-O2	5.76	122.36	118.90
1	L5	1884	C	N1-C2-O2	5.76	122.36	118.90
1	L5	3841	C	N1-C2-O2	5.76	122.36	118.90
1	L5	2783	A	N1-C2-N3	-5.76	126.42	129.30
1	L5	4921	C	N3-C2-O2	-5.75	117.87	121.90
47	S2	17	C	C5-C6-N1	5.75	123.88	121.00
1	L5	2528	G	C8-N9-C1'	-5.75	119.53	127.00
2	L7	78	C	N1-C2-O2	5.75	122.35	118.90
1	L5	3685	C	C6-N1-C2	-5.75	118.00	120.30
47	S2	1314	U	N1-C2-O2	5.74	126.82	122.80
1	L5	209	U	N3-C2-O2	-5.74	118.18	122.20
1	L5	274	C	C6-N1-C2	-5.74	118.00	120.30
47	S2	53	C	N1-C2-O2	5.74	122.34	118.90
1	L5	1404	G	N3-C4-N9	5.74	129.44	126.00
1	L5	2583	C	N1-C2-O2	5.74	122.34	118.90
1	L5	4068	U	N3-C2-O2	-5.74	118.19	122.20
11	LH	146	LEU	CA-CB-CG	5.74	128.49	115.30
1	L5	1340	C	C6-N1-C2	-5.73	118.01	120.30
1	L5	2257	C	N3-C2-O2	-5.73	117.89	121.90
47	S2	409	C	C5-C6-N1	5.73	123.86	121.00
1	L5	367	C	C5-C6-N1	5.72	123.86	121.00
1	L5	4880	C	N3-C2-O2	-5.72	117.89	121.90
1	L5	28	C	C6-N1-C2	-5.72	118.01	120.30
1	L5	4766	C	N1-C2-O2	5.72	122.33	118.90
47	S2	687	C	N1-C2-O2	5.71	122.33	118.90
1	L5	1505	C	C5-C6-N1	5.71	123.85	121.00
1	L5	1914	C	C6-N1-C2	-5.71	118.02	120.30
1	L5	3711	A	N1-C6-N6	-5.71	115.18	118.60
47	S2	417	C	O4'-C1'-N1	5.70	112.76	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1774	C	N3-C2-O2	-5.70	117.91	121.90
47	S2	356	C	C5-C6-N1	5.69	123.84	121.00
1	L5	2577	C	N1-C2-O2	5.69	122.31	118.90
1	L5	1772	C	C5-C6-N1	5.68	123.84	121.00
54	SH	30	LEU	CA-CB-CG	5.68	128.38	115.30
47	S2	490	C	C5-C6-N1	5.68	123.84	121.00
1	L5	4758	U	N1-C2-O2	5.68	126.78	122.80
1	L5	449	C	N1-C2-O2	5.67	122.31	118.90
1	L5	2084	C	P-O3'-C3'	5.67	126.51	119.70
1	L5	4682	U	N1-C2-O2	5.67	126.77	122.80
1	L5	209	U	C6-N1-C1'	-5.67	113.26	121.20
1	L5	1182	C	N1-C2-O2	5.67	122.30	118.90
1	L5	1252	C	N1-C2-O2	5.67	122.30	118.90
1	L5	3734	U	C2-N1-C1'	5.67	124.50	117.70
47	S2	37	C	N1-C2-O2	5.67	122.30	118.90
47	S2	1696	C	N1-C2-O2	5.67	122.30	118.90
1	L5	290	U	N3-C2-O2	-5.66	118.23	122.20
1	L5	4758	U	N3-C2-O2	-5.66	118.24	122.20
1	L5	925	C	C6-N1-C2	-5.66	118.04	120.30
47	S2	1348	G	C4-N9-C1'	5.63	133.82	126.50
47	S2	1660	C	N3-C2-O2	-5.63	117.96	121.90
47	S2	496	C	C6-N1-C2	-5.62	118.05	120.30
1	L5	131	C	N3-C2-O2	-5.62	117.97	121.90
1	L5	1178	G	C8-N9-C1'	-5.62	119.70	127.00
1	L5	4133	C	C6-N1-C2	-5.62	118.05	120.30
47	S2	1415	C	N1-C2-O2	5.62	122.27	118.90
1	L5	4109	G	N3-C4-C5	-5.62	125.79	128.60
16	LN	134	LEU	CA-CB-CG	5.62	128.22	115.30
1	L5	1663	C	C6-N1-C2	-5.61	118.06	120.30
47	S2	537	C	C5-C6-N1	5.61	123.81	121.00
47	S2	1064	C	N1-C2-O2	5.61	122.27	118.90
47	S2	420	G	P-O3'-C3'	5.61	126.43	119.70
1	L5	1414	C	N1-C2-O2	5.61	122.27	118.90
1	L5	4900	C	N1-C2-O2	5.61	122.26	118.90
1	L5	1633	G	P-O3'-C3'	5.61	126.43	119.70
61	SS	49	ASP	CB-CG-OD1	5.61	123.34	118.30
1	L5	1772	C	C6-N1-C2	-5.60	118.06	120.30
47	S2	1207	G	N3-C4-N9	-5.60	122.64	126.00
1	L5	220	C	C6-N1-C2	-5.60	118.06	120.30
1	L5	2410	C	C2-N1-C1'	5.60	124.96	118.80
47	S2	1315	U	C2-N1-C1'	5.60	124.42	117.70
1	L5	340	C	C6-N1-C1'	-5.59	114.09	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2820	C	N1-C2-O2	5.59	122.25	118.90
47	S2	1154	U	C2-N1-C1'	5.59	124.41	117.70
47	S2	1422	G	N3-C4-N9	5.59	129.35	126.00
1	L5	2351	C	C6-N1-C2	-5.58	118.07	120.30
1	L5	1304	C	N1-C2-O2	5.58	122.25	118.90
47	S2	1064	C	C6-N1-C2	-5.58	118.07	120.30
1	L5	2077	C	C6-N1-C2	-5.57	118.07	120.30
1	L5	4758	U	C2-N1-C1'	5.57	124.38	117.70
47	S2	803	C	C6-N1-C2	-5.57	118.07	120.30
47	S2	1729	U	N3-C2-O2	-5.56	118.31	122.20
47	S2	1852	C	N3-C2-O2	-5.55	118.01	121.90
47	S2	331	C	C2-N1-C1'	5.55	124.91	118.80
75	SO	14	VAL	C-N-CA	5.55	135.58	121.70
1	L5	2593	C	C6-N1-C2	-5.55	118.08	120.30
1	L5	1893	C	C5-C6-N1	5.54	123.77	121.00
47	S2	456	C	C5-C6-N1	5.54	123.77	121.00
1	L5	940	C	C6-N1-C2	-5.54	118.08	120.30
47	S2	1798	C	N1-C2-O2	5.54	122.22	118.90
47	S2	196	C	N1-C2-O2	5.54	122.22	118.90
64	SV	78	ILE	CG1-CB-CG2	-5.54	99.22	111.40
1	L5	115	C	N3-C2-O2	-5.53	118.03	121.90
1	L5	1687	U	N1-C2-O2	5.53	126.67	122.80
47	S2	1853	C	N3-C2-O2	-5.53	118.03	121.90
3	L8	83	C	P-O3'-C3'	5.53	126.33	119.70
47	S2	441	C	N3-C2-O2	-5.52	118.03	121.90
1	L5	1661	C	N1-C2-O2	5.52	122.21	118.90
1	L5	694	C	N1-C2-O2	5.51	122.20	118.90
1	L5	2000	G	C4-N9-C1'	5.51	133.66	126.50
47	S2	1696	C	N3-C2-O2	-5.51	118.04	121.90
47	S2	402	C	C2-N3-C4	5.50	122.65	119.90
47	S2	14	C	C6-N1-C2	-5.50	118.10	120.30
47	S2	17	C	C6-N1-C2	-5.50	118.10	120.30
47	S2	1149	A	C2-N3-C4	5.50	113.35	110.60
1	L5	988	C	C2-N1-C1'	5.50	124.85	118.80
47	S2	49	C	N1-C2-O2	5.50	122.20	118.90
1	L5	4337	C	C6-N1-C2	-5.50	118.10	120.30
1	L5	483	G	N3-C4-N9	5.49	129.29	126.00
1	L5	1894	C	C6-N1-C2	-5.49	118.11	120.30
2	L7	78	C	N3-C2-O2	-5.48	118.06	121.90
48	S6	30	G	C4-N9-C1'	5.48	133.62	126.50
1	L5	1431	C	N1-C2-O2	5.48	122.19	118.90
1	L5	2817	C	C6-N1-C2	-5.47	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	904	C	C6-N1-C2	-5.47	118.11	120.30
1	L5	282	C	N3-C2-O2	-5.47	118.07	121.90
1	L5	406	C	P-O3'-C3'	5.47	126.26	119.70
1	L5	282	C	N1-C2-O2	5.47	122.18	118.90
47	S2	1852	C	C5-C6-N1	5.46	123.73	121.00
1	L5	3713	U	N1-C2-O2	5.45	126.62	122.80
1	L5	4739	C	N1-C2-O2	5.45	122.17	118.90
47	S2	130	G	C8-N9-C1'	-5.45	119.92	127.00
1	L5	332	C	C6-N1-C2	-5.45	118.12	120.30
1	L5	4155	C	N1-C2-O2	5.45	122.17	118.90
1	L5	4712	C	C6-N1-C2	-5.44	118.12	120.30
1	L5	340	C	C6-N1-C2	-5.44	118.12	120.30
1	L5	992	C	C2-N1-C1'	5.43	124.78	118.80
1	L5	1243	C	C5-C6-N1	5.43	123.72	121.00
1	L5	112	C	C2-N1-C1'	5.43	124.77	118.80
1	L5	1579	C	C5-C6-N1	5.43	123.72	121.00
1	L5	1096	C	C6-N1-C2	-5.43	118.13	120.30
1	L5	1344	C	C6-N1-C2	-5.43	118.13	120.30
1	L5	3789	C	C5-C6-N1	5.42	123.71	121.00
47	S2	1314	U	N3-C2-O2	-5.42	118.40	122.20
1	L5	4645	C	C6-N1-C2	-5.42	118.13	120.30
47	S2	118	C	C6-N1-C2	-5.42	118.13	120.30
47	S2	1115	U	N1-C2-O2	5.42	126.59	122.80
1	L5	1971	C	C6-N1-C2	-5.42	118.13	120.30
1	L5	3772	U	O4'-C1'-N1	5.41	112.53	108.20
1	L5	1597	G	O4'-C1'-N9	5.41	112.53	108.20
1	L5	294	G	C4-N9-C1'	5.41	133.53	126.50
52	SE	104	ASP	CB-CG-OD1	5.41	123.17	118.30
1	L5	2337	C	C6-N1-C2	-5.40	118.14	120.30
1	L5	3866	C	C5-C6-N1	5.40	123.70	121.00
47	S2	1336	C	C6-N1-C2	-5.40	118.14	120.30
1	L5	1521	C	C6-N1-C2	-5.40	118.14	120.30
1	L5	436	C	N1-C2-O2	5.39	122.14	118.90
1	L5	4068	U	C2-N1-C1'	5.39	124.17	117.70
1	L5	988	C	C6-N1-C2	-5.39	118.14	120.30
47	S2	25	A	O4'-C1'-N9	5.39	112.51	108.20
47	S2	490	C	C6-N1-C2	-5.39	118.15	120.30
1	L5	1439	C	N3-C2-O2	-5.38	118.13	121.90
3	L8	11	C	C6-N1-C2	-5.38	118.15	120.30
47	S2	1230	C	C6-N1-C2	-5.38	118.15	120.30
47	S2	1265	A	N3-C4-N9	5.38	131.71	127.40
1	L5	716	C	C6-N1-C2	-5.38	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3920	U	N1-C2-O2	5.38	126.57	122.80
47	S2	118	C	N3-C2-O2	-5.38	118.13	121.90
1	L5	4243	C	N3-C2-O2	-5.38	118.14	121.90
1	L5	100	C	C6-N1-C1'	-5.38	114.35	120.80
1	L5	753	C	C6-N1-C1'	-5.37	114.35	120.80
1	L5	2410	C	C6-N1-C2	-5.37	118.15	120.30
1	L5	343	C	C6-N1-C2	-5.36	118.15	120.30
1	L5	1439	C	C2-N1-C1'	5.36	124.70	118.80
1	L5	290	U	N1-C2-O2	5.36	126.55	122.80
1	L5	53	C	N3-C2-O2	-5.35	118.16	121.90
1	L5	1577	G	C2-N3-C4	5.35	114.57	111.90
1	L5	1552	G	O4'-C1'-N9	5.34	112.47	108.20
1	L5	5030	U	C5-C6-N1	5.34	125.37	122.70
47	S2	1422	G	N3-C4-C5	-5.34	125.93	128.60
47	S2	130	G	N3-C4-C5	-5.34	125.93	128.60
72	SJ	50	LEU	CA-CB-CG	5.34	127.58	115.30
1	L5	4682	U	N3-C2-O2	-5.33	118.47	122.20
1	L5	308	G	C4-N9-C1'	5.33	133.43	126.50
1	L5	4106	G	C4-N9-C1'	5.33	133.43	126.50
1	L5	906	C	N3-C2-O2	-5.33	118.17	121.90
47	S2	1798	C	N3-C2-O2	-5.33	118.17	121.90
47	S2	112	U	C2'-C3'-O3'	5.33	122.22	113.70
1	L5	1661	C	C6-N1-C2	-5.32	118.17	120.30
47	S2	853	C	N3-C2-O2	-5.31	118.18	121.90
1	L5	1702	C	C2-N1-C1'	5.30	124.63	118.80
1	L5	340	C	C5-C6-N1	5.30	123.65	121.00
1	L5	1540	C	N1-C2-O2	5.30	122.08	118.90
47	S2	836	G	C4-N9-C1'	5.30	133.38	126.50
1	L5	1404	G	C8-N9-C1'	-5.29	120.12	127.00
47	S2	427	U	C6-N1-C2	-5.29	117.83	121.00
47	S2	1655	C	C6-N1-C2	-5.29	118.18	120.30
47	S2	1039	C	C6-N1-C2	-5.29	118.18	120.30
47	S2	1556	A	C2-N3-C4	5.28	113.24	110.60
1	L5	2334	C	N1-C2-O2	5.28	122.07	118.90
1	L5	1404	G	N3-C4-C5	-5.27	125.96	128.60
1	L5	4900	C	C2-N1-C1'	5.27	124.60	118.80
47	S2	307	G	N3-C4-C5	-5.27	125.97	128.60
1	L5	1216	C	C6-N1-C2	-5.27	118.19	120.30
47	S2	592	C	N3-C2-O2	-5.27	118.21	121.90
1	L5	3950	U	C2-N1-C1'	5.26	124.02	117.70
1	L5	3968	U	C5-C6-N1	5.26	125.33	122.70
1	L5	1050	C	N1-C2-O2	5.26	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L8	111	U	C2-N1-C1'	5.26	124.01	117.70
4	LA	102	LEU	CA-CB-CG	5.26	127.40	115.30
7	LD	36	LEU	CA-CB-CG	5.25	127.38	115.30
47	S2	118	C	C5-C6-N1	5.25	123.63	121.00
1	L5	504	G	N3-C4-C5	-5.25	125.97	128.60
1	L5	4766	C	C6-N1-C2	-5.25	118.20	120.30
1	L5	4945	G	N3-C4-N9	5.24	129.15	126.00
58	SP	80	LEU	CA-CB-CG	5.24	127.36	115.30
1	L5	2905	C	N3-C2-O2	-5.24	118.23	121.90
1	L5	1915	C	C2-N1-C1'	5.24	124.56	118.80
1	L5	3752	C	N1-C2-O2	5.24	122.04	118.90
1	L5	4116	C	OP2-P-O3'	5.24	116.72	105.20
1	L5	464	G	C4-N9-C1'	5.24	133.31	126.50
1	L5	2255	C	C6-N1-C1'	-5.24	114.52	120.80
1	L5	2304	U	N3-C2-O2	-5.24	118.54	122.20
1	L5	1252	C	C6-N1-C2	-5.23	118.21	120.30
1	L5	1884	C	N3-C2-O2	-5.23	118.24	121.90
56	SK	15	LEU	CA-CB-CG	5.23	127.33	115.30
1	L5	1929	A	C2-N3-C4	5.23	113.22	110.60
1	L5	3734	U	N1-C2-O2	5.23	126.46	122.80
55	SI	172	LEU	CA-CB-CG	5.23	127.32	115.30
1	L5	2048	U	N1-C2-O2	5.23	126.46	122.80
1	L5	3841	C	C6-N1-C2	-5.22	118.21	120.30
1	L5	1929	A	C4-N9-C1'	5.22	135.70	126.30
1	L5	963	G	N3-C4-C5	-5.22	125.99	128.60
47	S2	1865	C	C2-N1-C1'	5.22	124.54	118.80
1	L5	3636	C	C6-N1-C2	-5.22	118.21	120.30
47	S2	140	C	C6-N1-C2	-5.21	118.21	120.30
47	S2	1205	C	C6-N1-C2	-5.21	118.22	120.30
1	L5	3931	C	C6-N1-C2	-5.21	118.22	120.30
1	L5	1632	A	C4-N9-C1'	5.21	135.68	126.30
1	L5	3882	C	N1-C2-O2	5.21	122.03	118.90
6	LC	2	ALA	C-N-CA	5.21	134.71	121.70
1	L5	3588	C	C6-N1-C2	-5.20	118.22	120.30
1	L5	4775	C	C6-N1-C2	-5.20	118.22	120.30
47	S2	1852	C	C6-N1-C2	-5.20	118.22	120.30
1	L5	4350	C	C6-N1-C2	-5.20	118.22	120.30
1	L5	4241	C	C2-N1-C1'	5.20	124.52	118.80
1	L5	2820	C	N3-C2-O2	-5.19	118.26	121.90
48	S6	65	C	N1-C2-O2	5.19	122.02	118.90
1	L5	4771	C	C5-C6-N1	5.19	123.60	121.00
47	S2	1259	A	C2-N3-C4	5.19	113.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1078	A	O4'-C1'-N9	5.19	112.35	108.20
47	S2	18	C	C6-N1-C2	-5.19	118.22	120.30
47	S2	1453	C	C6-N1-C2	-5.19	118.23	120.30
1	L5	4928	C	O4'-C1'-N1	5.18	112.35	108.20
1	L5	504	G	P-O3'-C3'	5.18	125.91	119.70
1	L5	2337	C	C5-C6-N1	5.18	123.59	121.00
1	L5	2492	C	C6-N1-C2	-5.17	118.23	120.30
1	L5	672	C	N1-C2-O2	5.17	122.00	118.90
1	L5	4918	C	N3-C2-O2	-5.17	118.28	121.90
1	L5	1906	U	N3-C2-O2	-5.17	118.58	122.20
1	L5	2033	A	OP1-P-O3'	5.17	116.57	105.20
48	S6	54	A	OP1-P-O3'	5.17	116.57	105.20
3	L8	101	C	C6-N1-C2	-5.17	118.23	120.30
1	L5	1203	G	N3-C4-N9	5.16	129.10	126.00
1	L5	1449	C	N1-C2-O2	5.16	122.00	118.90
47	S2	579	C	N1-C2-O2	5.16	122.00	118.90
1	L5	1520	C	C6-N1-C2	-5.16	118.24	120.30
1	L5	274	C	C5-C6-N1	5.15	123.58	121.00
1	L5	9	C	C6-N1-C2	-5.15	118.24	120.30
1	L5	4886	C	N1-C2-O2	5.15	121.99	118.90
1	L5	2867	C	N3-C2-O2	-5.15	118.30	121.90
1	L5	3841	C	N3-C2-O2	-5.15	118.30	121.90
1	L5	4563	U	C5-C6-N1	5.15	125.27	122.70
47	S2	1078	C	C2-N1-C1'	5.15	124.46	118.80
1	L5	3772	U	N3-C2-O2	-5.14	118.60	122.20
47	S2	1002	U	C2-N1-C1'	5.14	123.87	117.70
1	L5	1540	C	C6-N1-C2	-5.14	118.24	120.30
70	SC	213	LEU	CA-CB-CG	5.14	127.11	115.30
1	L5	274	C	N3-C2-O2	-5.13	118.31	121.90
47	S2	1396	A	C2-N3-C4	5.13	113.16	110.60
1	L5	1762	C	C2-N1-C1'	5.12	124.44	118.80
1	L5	3604	A	C2-N3-C4	5.12	113.16	110.60
1	L5	1809	C	N3-C2-O2	-5.12	118.31	121.90
1	L5	3950	U	N1-C2-O2	5.12	126.39	122.80
47	S2	441	C	N1-C2-O2	5.12	121.97	118.90
47	S2	1501	C	C5-C6-N1	5.12	123.56	121.00
1	L5	1264	C	N1-C2-O2	5.12	121.97	118.90
1	L5	4887	C	N3-C2-O2	-5.12	118.32	121.90
47	S2	632	C	C5-C6-N1	5.12	123.56	121.00
1	L5	2036	C	C6-N1-C2	-5.11	118.25	120.30
1	L5	2892	C	N1-C2-O2	5.11	121.97	118.90
1	L5	4712	C	N3-C2-O2	-5.11	118.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	417	C	P-O3'-C3'	5.11	125.83	119.70
47	S2	1115	U	C2-N1-C1'	5.11	123.83	117.70
1	L5	216	C	C6-N1-C2	-5.11	118.26	120.30
1	L5	1077	C	C6-N1-C2	-5.11	118.26	120.30
1	L5	1661	C	N3-C2-O2	-5.11	118.33	121.90
1	L5	4698	C	N1-C2-O2	5.11	121.97	118.90
1	L5	4594	U	C2-N1-C1'	5.10	123.82	117.70
1	L5	53	C	N1-C2-O2	5.10	121.96	118.90
1	L5	4699	U	OP1-P-O3'	5.10	116.42	105.20
1	L5	4162	C	C6-N1-C1'	-5.10	114.68	120.80
1	L5	4350	C	N3-C2-O2	-5.09	118.33	121.90
1	L5	2905	C	C2-N1-C1'	5.09	124.40	118.80
1	L5	4241	C	N3-C2-O2	-5.09	118.33	121.90
1	L5	4926	C	N1-C2-O2	5.09	121.95	118.90
1	L5	3588	C	C5-C6-N1	5.08	123.54	121.00
1	L5	963	G	C8-N9-C1'	-5.08	120.39	127.00
1	L5	3713	U	N3-C2-O2	-5.08	118.64	122.20
47	S2	168	C	C6-N1-C2	-5.08	118.27	120.30
1	L5	2892	C	C6-N1-C2	-5.08	118.27	120.30
1	L5	4337	C	C5-C6-N1	5.08	123.54	121.00
47	S2	1348	G	C8-N9-C1'	-5.07	120.40	127.00
1	L5	1431	C	N3-C2-O2	-5.07	118.35	121.90
1	L5	1346	C	C6-N1-C2	-5.07	118.27	120.30
47	S2	531	A	P-O3'-C3'	5.07	125.78	119.70
1	L5	706	C	N1-C2-O2	5.07	121.94	118.90
3	L8	84	A	O5'-P-OP2	-5.07	101.14	105.70
1	L5	981	C	C6-N1-C2	-5.06	118.28	120.30
1	L5	1340	C	C5-C6-N1	5.06	123.53	121.00
1	L5	654	C	N1-C2-O2	5.06	121.94	118.90
1	L5	4601	U	N1-C2-O2	5.06	126.34	122.80
47	S2	53	C	N3-C2-O2	-5.06	118.36	121.90
81	Sf	146	LEU	CA-CB-CG	5.06	126.94	115.30
1	L5	4895	C	N1-C2-O2	5.06	121.94	118.90
1	L5	4199	C	C6-N1-C2	-5.06	118.28	120.30
1	L5	220	C	N1-C2-O2	5.06	121.93	118.90
20	LR	15	LEU	CA-CB-CG	5.06	126.93	115.30
1	L5	141	C	N1-C2-O2	5.05	121.93	118.90
1	L5	1579	C	C6-N1-C2	-5.05	118.28	120.30
1	L5	1762	C	N1-C2-O2	5.05	121.93	118.90
3	L8	150	C	N1-C2-O2	5.05	121.93	118.90
1	L5	1509	C	C6-N1-C2	-5.05	118.28	120.30
1	L5	2410	C	N3-C2-O2	-5.04	118.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1367	C	N1-C2-O2	5.04	121.92	118.90
47	S2	1655	C	C5-C6-N1	5.04	123.52	121.00
1	L5	1666	C	C6-N1-C2	-5.04	118.28	120.30
1	L5	3870	C	N1-C2-O2	5.04	121.92	118.90
1	L5	3789	C	C6-N1-C2	-5.04	118.28	120.30
13	LJ	15	LEU	CA-CB-CG	5.04	126.89	115.30
1	L5	345	C	C5-C6-N1	5.04	123.52	121.00
1	L5	3632	C	C6-N1-C2	-5.04	118.29	120.30
1	L5	1704	C	N1-C2-O2	5.03	121.92	118.90
47	S2	687	C	N3-C2-O2	-5.03	118.38	121.90
47	S2	179	C	N1-C2-O2	5.03	121.92	118.90
47	S2	632	C	N1-C2-O2	5.03	121.92	118.90
1	L5	79	C	C6-N1-C2	-5.03	118.29	120.30
1	L5	4466	C	N1-C2-O2	5.03	121.92	118.90
47	S2	1415	C	C5-C6-N1	5.03	123.51	121.00
47	S2	1114	U	O4'-C1'-N1	5.02	112.22	108.20
1	L5	1176	C	C6-N1-C2	-5.02	118.29	120.30
47	S2	1018	U	C5-C6-N1	5.02	125.21	122.70
1	L5	302	C	C6-N1-C2	-5.02	118.29	120.30
1	L5	2533	C	C6-N1-C2	-5.01	118.29	120.30
3	L8	99	U	N1-C2-O2	5.01	126.31	122.80
1	L5	3668	C	N3-C2-O2	-5.01	118.39	121.90
13	LJ	95	ARG	CA-CB-CG	5.01	124.42	113.40
47	S2	1242	U	C5-C6-N1	-5.01	120.20	122.70
47	S2	638	C	N1-C2-O2	5.01	121.90	118.90
1	L5	4434	C	N1-C2-O2	5.00	121.90	118.90
1	L5	4593	C	C6-N1-C2	-5.00	118.30	120.30
1	L5	4709	U	C6-N1-C1'	-5.00	114.19	121.20
9	LF	221	LYS	C-N-CA	5.00	134.21	121.70
1	L5	294	G	N3-C4-N9	5.00	129.00	126.00
1	L5	1674	C	C5-C6-N1	5.00	123.50	121.00
1	L5	2509	C	C6-N1-C2	-5.00	118.30	120.30
1	L5	3844	U	N3-C2-O2	-5.00	118.70	122.20
1	L5	4746	C	N1-C2-O2	5.00	121.90	118.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L5	1456	B8Q	C4
1	L5	2786	B9H	C4
47	S2	568	E3C	C4
47	S2	1219	B8Q	C4

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	142	GLU	Peptide
4	LA	241	ARG	Sidechain
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	2	SER	Peptide
5	LB	258	HIS	Peptide
5	LB	296	GLY	Peptide
7	LD	86	TYR	Peptide
8	LE	129	GLY	Peptide
9	LF	221	LYS	Peptide
9	LF	86	GLU	Peptide
11	LH	106	GLN	Peptide
11	LH	173	ARG	Peptide
12	LI	14	ASN	Peptide
13	LJ	94	LEU	Peptide
14	LL	144	LEU	Peptide
14	LL	154	VAL	Peptide
15	LM	87	ALA	Peptide
16	LN	124	ASP	Peptide
17	LO	110	PRO	Peptide
22	LT	135	PRO	Peptide
22	LT	136	ARG	Peptide
23	LU	97	ARG	Peptide
25	LW	79	GLN	Peptide
27	LY	71	VAL	Peptide
32	Ld	94	GLU	Peptide
33	Le	91	CYS	Peptide
34	Lf	103	VAL	Peptide
34	Lf	106	TYR	Peptide
34	Lf	79	GLY	Peptide
36	Lh	86	LYS	Peptide
38	Lj	39	TYR	Peptide
45	Lr	20	ARG	Peptide
46	Lz	16	GLU	Peptide
46	Lz	183	ILE	Peptide
70	SC	76	LYS	Peptide
51	SD	142	LEU	Peptide
51	SD	204	LEU	Peptide
53	SF	126	THR	Peptide
53	SF	127	ARG	Peptide
53	SF	42	LYS	Peptide
53	SF	78	MET	Peptide

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Mol	Chain	Res	Type	Group
54	SH	134	VAL	Peptide
54	SH	158	LEU	Peptide
55	SI	165	GLN	Peptide
55	SI	18	ARG	Sidechain
72	SJ	137	VAL	Peptide
72	SJ	2	PRO	Peptide
72	SJ	65	GLU	Peptide
56	SK	66	HIS	Peptide
57	SL	20	LYS	Peptide
57	SL	28	THR	Peptide
73	SM	36	ARG	Peptide
73	SM	93	LYS	Peptide
75	SO	139	SER	Peptide
58	SP	127	LYS	Peptide
59	SQ	43	GLU	Peptide
62	ST	46	ALA	Peptide
63	SU	107	GLU	Peptide
64	SV	78	ILE	Peptide
65	SX	11	ARG	Sidechain
65	SX	125	VAL	Peptide
65	SX	126	ALA	Peptide
65	SX	77	ASN	Peptide
65	SX	86	PRO	Peptide
77	SY	94	HIS	Peptide
78	SZ	46	ASN	Peptide
66	Sa	10	ARG	Sidechain
67	Sc	29	GLN	Peptide
67	Sc	63	ARG	Peptide
81	Sf	101	ALA	Peptide

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	L5	80257	0	40195	341	0
2	L7	2558	0	1296	12	0
3	L8	3315	0	1685	14	0
4	LA	1898	0	1992	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	LB	3244	0	3389	53	0
6	LC	2928	0	3105	26	0
7	LD	2382	0	2410	31	0
8	LE	1904	0	2055	28	0
9	LF	1878	0	2009	18	0
10	LG	1935	0	2087	23	0
11	LH	1518	0	1601	18	0
12	LI	1711	0	1748	22	0
13	LJ	1410	0	1440	24	0
14	LL	1701	0	1818	19	0
15	LM	1138	0	1204	11	0
16	LN	1701	0	1749	19	0
17	LO	1650	0	1794	18	0
18	LP	1242	0	1269	18	0
19	LQ	1513	0	1628	13	0
20	LR	1566	0	1728	17	0
21	LS	1453	0	1490	17	0
22	LT	1298	0	1366	13	0
23	LU	825	0	850	12	0
24	LV	979	0	1039	12	0
25	LW	1015	0	1079	15	0
26	LX	985	0	1066	9	0
27	LY	1115	0	1205	15	0
28	LZ	1107	0	1182	12	0
29	La	1162	0	1213	0	0
30	Lb	876	0	948	0	0
31	Lc	764	0	804	0	0
32	Ld	888	0	930	0	0
33	Le	1053	0	1147	0	0
34	Lf	876	0	912	0	0
35	Lg	906	0	1002	0	0
36	Lh	1015	0	1148	0	0
37	Li	832	0	917	0	0
38	Lj	705	0	737	0	0
39	Lk	569	0	637	0	0
40	Ll	444	0	483	0	0
41	Lm	430	0	466	0	0
42	Ln	230	0	276	0	0
43	Lo	870	0	945	0	0
44	Lp	708	0	756	0	0
45	Lr	1002	0	1068	0	0
46	Lz	1741	0	1854	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	S2	36938	0	18612	158	0
48	S6	1604	0	816	9	0
49	SA	1741	0	1746	21	0
50	SB	1738	0	1809	14	0
51	SD	1765	0	1865	20	0
52	SE	2076	0	2177	21	0
53	SF	1495	0	1549	19	0
54	SH	1497	0	1590	21	0
55	SI	1686	0	1772	53	0
56	SK	827	0	854	6	0
57	SL	1247	0	1323	9	0
58	SP	1045	0	1095	8	0
59	SQ	1158	0	1231	19	0
60	SR	1090	0	1149	13	0
61	SS	1198	0	1261	22	0
62	ST	1112	0	1146	8	0
63	SU	821	0	883	9	0
64	SV	636	0	637	9	0
65	SX	1098	0	1167	13	0
66	Sa	829	0	883	0	0
67	Sc	506	0	536	0	0
68	Sd	459	0	448	0	0
69	Sg	2436	0	2393	0	0
70	SC	1733	0	1826	23	0
71	SG	1923	0	2089	35	0
72	SJ	1533	0	1653	17	0
73	SM	942	0	961	11	0
74	SN	1208	0	1294	9	0
75	SO	1049	0	1073	14	0
76	SW	1034	0	1080	14	0
77	SY	1073	0	1155	8	0
78	SZ	598	0	656	12	0
79	Sb	651	0	672	0	0
80	Se	459	0	503	0	0
81	Sf	548	0	551	0	0
82	L5	251	0	0	0	0
82	L7	3	0	0	0	0
82	L8	6	0	0	0	0
82	LN	1	0	0	0	0
82	LP	1	0	0	0	0
82	LT	1	0	0	0	0
82	LV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	Le	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	134	0	0	0	0
82	SF	1	0	0	0	0
82	Sd	1	0	0	0	0
83	L5	39	0	39	3	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lo	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Sa	1	0	0	0	0
84	Sd	1	0	0	0	0
84	Sf	1	0	0	0	0
85	S2	36	0	37	0	0
86	L5	16	0	0	0	0
86	LA	1	0	0	1	0
86	LB	1	0	0	0	0
86	LC	1	0	0	0	0
86	LF	1	0	0	0	0
86	LG	1	0	0	0	0
86	LH	1	0	0	0	0
86	LI	2	0	0	0	0
86	LN	1	0	0	0	0
86	LS	2	0	0	0	0
86	LY	1	0	0	0	0
86	La	2	0	0	0	0
86	Lb	1	0	0	0	0
86	Lf	1	0	0	0	0
86	Lm	1	0	0	0	0
86	S2	14	0	0	0	0
86	SC	1	0	0	0	0
86	SF	1	0	0	0	0
86	SG	1	0	0	0	0
86	SJ	1	0	0	0	0
86	SL	1	0	0	0	0
86	SN	1	0	0	0	0
86	SP	1	0	0	0	0
86	SQ	2	0	0	0	0
86	SR	1	0	0	0	0
86	SS	2	0	0	0	0
86	SV	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Sf	1	0	0	0	0
All	All	219596	0	162253	1167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1167) 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)
55:SI:130:THR:OG1	55:SI:134:GLU:CB	1.69	1.40
55:SI:130:THR:CA	55:SI:134:GLU:HB3	1.49	1.33
55:SI:130:THR:CB	55:SI:134:GLU:HB3	1.67	1.24
55:SI:123:ARG:HD3	55:SI:129:LEU:CD1	1.69	1.22
55:SI:123:ARG:HD3	55:SI:129:LEU:HD12	1.31	1.08
55:SI:130:THR:OG1	55:SI:134:GLU:HB2	1.38	1.08
55:SI:123:ARG:NE	55:SI:129:LEU:HD13	1.74	1.01
55:SI:123:ARG:CD	55:SI:129:LEU:CD1	2.41	0.97
55:SI:130:THR:CA	55:SI:134:GLU:CB	2.44	0.96
55:SI:130:THR:O	55:SI:134:GLU:N	1.92	0.91
55:SI:130:THR:OG1	55:SI:134:GLU:HB3	1.48	0.90
55:SI:123:ARG:CD	55:SI:129:LEU:HD13	2.03	0.88
55:SI:123:ARG:CZ	55:SI:129:LEU:HD13	2.08	0.83
55:SI:130:THR:HA	55:SI:134:GLU:HB3	1.58	0.82
55:SI:124:LYS:HD2	55:SI:124:LYS:H	1.49	0.78
1:L5:4517:A:N7	5:LB:2:SER:N	2.35	0.74
55:SI:130:THR:OG1	55:SI:134:GLU:CG	2.36	0.74
5:LB:315:ASN:HD21	5:LB:326:VAL:H	1.37	0.73
55:SI:124:LYS:N	55:SI:124:LYS:HD2	2.03	0.73
47:S2:533:A:H61	47:S2:550:C:H42	1.37	0.73
11:LH:7:ASN:HD22	11:LH:56:ARG:HH21	1.36	0.71
47:S2:925:G:H1	47:S2:1017:U:H3	1.39	0.69
18:LP:109:VAL:HA	18:LP:112:LEU:HD13	1.74	0.69
25:LW:96:GLN:HB2	25:LW:101:ARG:HH21	1.57	0.69
27:LY:8:THR:HG22	27:LY:10:ASP:H	1.56	0.69
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.75	0.69
1:L5:4162:C:H5	10:LG:73:ARG:HH12	1.41	0.69
77:SY:99:LYS:HD3	77:SY:101:LYS:HE2	1.76	0.68
11:LH:113:GLU:HG2	11:LH:125:ARG:HG2	1.76	0.68
1:L5:4523:A2M:H5''	1:L5:4524:G:H5'	1.76	0.67
73:SM:49:LEU:HD22	73:SM:123:VAL:HG21	1.76	0.66
54:SH:12:ASN:ND2	54:SH:16:PRO:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SA:38:ILE:HD11	49:SA:47:TYR:HB3	1.76	0.66
1:L5:5027:C:H5	55:SI:77:ARG:HH21	1.43	0.66
70:SC:275:LYS:HG3	70:SC:276:THR:HG23	1.77	0.66
1:L5:375:G:OP2	13:LJ:52:LYS:NZ	105.81	0.65
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.76	0.65
1:L5:2362:U:H2'	1:L5:2363:A2M:H8	1.77	0.65
1:L5:4452:U:H5'	83:L5:5348:HMT:H16	1.78	0.65
22:LT:43:LYS:O	22:LT:58:HIS:ND1	2.30	0.65
1:L5:1521:C:OP1	6:LC:100:ARG:NH2	2.30	0.65
47:S2:65:C:H4'	71:SG:172:LYS:HE2	1.78	0.65
14:LL:198:ARG:HA	14:LL:201:GLU:HG2	1.78	0.65
14:LL:133:ALA:HB1	14:LL:135:LYS:HE3	1.79	0.64
4:LA:247:ARG:NH1	47:S2:1069:U:O2'	2.30	0.64
55:SI:31:ARG:HH12	55:SI:48:VAL:HG12	1.63	0.64
13:LJ:43:LEU:HD12	13:LJ:44:THR:HG23	1.78	0.64
49:SA:42:LYS:HD3	49:SA:46:ILE:HB	1.80	0.63
55:SI:130:THR:HG1	55:SI:134:GLU:HB2	1.59	0.63
47:S2:563:G:H1	47:S2:592:C:H5	1.45	0.63
72:SJ:47:LYS:HB3	72:SJ:102:ILE:HD12	1.79	0.63
1:L5:2469:C:H5	1:L5:2471:G:H1	1.46	0.63
1:L5:1940:G:N2	1:L5:4434:C:OP1	2.32	0.63
47:S2:834:C:H42	47:S2:839:C:H42	1.46	0.63
1:L5:2738:C:H5''	4:LA:184:ARG:HH12	1.64	0.63
1:L5:4942:C:H5''	8:LE:155:GLY:HA2	1.80	0.63
47:S2:928:G:H1	47:S2:1013:U:H3	1.47	0.63
3:L8:122:G:H1	3:L8:128:C:H41	1.46	0.62
8:LE:256:GLN:O	8:LE:260:LYS:NZ	2.32	0.62
11:LH:120:GLU:OE2	11:LH:124:ARG:NH2	2.31	0.62
1:L5:2474:G:N2	1:L5:2502:G:O2'	2.33	0.62
47:S2:1192:U:OP2	65:SX:119:ARG:NH2	2.32	0.62
4:LA:101:VAL:HG22	4:LA:165:VAL:HG22	1.82	0.62
1:L5:2812:A:H5'	20:LR:88:ARG:HB3	1.80	0.62
47:S2:1640:A:OP1	48:S6:33:C:N4	2.32	0.62
1:L5:3663:A:N6	1:L5:4168:G:O2'	2.33	0.62
47:S2:1488:C:O2'	47:S2:1490:G:OP2	2.17	0.62
61:SS:45:LEU:HD22	61:SS:50:ILE:HD11	1.82	0.62
20:LR:109:TYR:OH	20:LR:139:MET:SD	2.58	0.62
47:S2:919:A:OP2	74:SN:64:ARG:NH2	2.33	0.62
1:L5:1726:U:H5'	9:LF:135:ILE:HD11	1.82	0.61
1:L5:4731:G:N2	1:L5:4732:G:N3	2.48	0.61
71:SG:64:LYS:HZ3	71:SG:81:HIS:HB3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:129:GLY:H	53:SF:136:ARG:HH11	1.47	0.61
1:L5:27:C:OP1	16:LN:193:ARG:NH1	2.33	0.61
47:S2:65:C:N4	71:SG:134:GLY:O	2.33	0.61
54:SH:160:LYS:NZ	54:SH:191:GLU:OE1	2.33	0.61
11:LH:31:ARG:NH1	11:LH:149:ASN:OD1	2.32	0.61
1:L5:1767:A:N7	58:SP:10:ARG:NH1	2.48	0.61
1:L5:1797:E7G:OP1	9:LF:104:LYS:NZ	2.33	0.61
1:L5:4746:C:H42	1:L5:4954:G:H1	1.48	0.61
23:LU:20:LYS:H	23:LU:73:THR:HA	1.66	0.61
47:S2:582:C:OP1	72:SJ:162:ARG:NH1	2.34	0.61
1:L5:2298:U:OP1	6:LC:204:ARG:NH2	2.33	0.61
23:LU:61:VAL:HG23	23:LU:74:SER:HB3	1.82	0.61
47:S2:380:G:OP1	55:SI:56:ARG:NH2	2.33	0.61
76:SW:3:ARG:HH22	76:SW:28:ARG:HH21	1.49	0.60
1:L5:3968:U:O4	1:L5:3969:G:N2	2.34	0.60
55:SI:124:LYS:CD	55:SI:124:LYS:H	2.12	0.60
1:L5:3951:G:N2	1:L5:4061:G:O6	2.35	0.60
6:LC:140:LYS:O	6:LC:204:ARG:NH1	2.35	0.60
1:L5:4717:A:OP2	5:LB:30:LYS:NZ	2.32	0.60
54:SH:51:ILE:HG21	54:SH:179:LYS:HE3	1.83	0.60
47:S2:1156:U:OP1	76:SW:71:LYS:NZ	2.35	0.60
47:S2:526:A:HO2'	72:SJ:125:HIS:HD1	1.50	0.59
47:S2:526:A:O2'	72:SJ:125:HIS:ND1	2.32	0.59
19:LQ:39:THR:HG22	19:LQ:41:SER:H	1.66	0.59
28:LZ:12:LEU:HB2	28:LZ:81:MET:HB3	1.84	0.59
47:S2:507:G:OP1	77:SY:108:LYS:NZ	2.33	0.59
55:SI:132:GLU:HA	55:SI:132:GLU:OE1	2.00	0.59
1:L5:1952:G:H4'	21:LS:93:MET:HG3	1.83	0.59
1:L5:4046:A:OP1	1:L5:4048:A:N6	2.36	0.59
1:L5:968:C:H5'	8:LE:110:ARG:HD3	1.84	0.59
1:L5:3969:G:N2	1:L5:4053:A:O2'	2.36	0.59
11:LH:37:ASP:OD1	11:LH:39:ASN:ND2	2.36	0.59
48:S6:50:A:H61	48:S6:62:C:H42	1.51	0.59
25:LW:105:ARG:NH2	71:SG:150:GLU:O	2.36	0.59
7:LD:240:TYR:O	7:LD:244:HIS:ND1	2.34	0.58
54:SH:55:GLY:H	54:SH:57:ARG:HE	1.50	0.58
55:SI:130:THR:HG23	55:SI:131:PRO:HD3	1.85	0.58
9:LF:101:VAL:O	9:LF:106:ARG:NH1	2.35	0.58
12:LI:30:LYS:HD3	12:LI:63:GLU:HG3	1.84	0.58
47:S2:1122:A:N3	50:SB:146:ARG:NH1	2.50	0.58
47:S2:326:C:O2	47:S2:327:G:N2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:10:ARG:HH22	5:LB:265:SER:HB2	1.68	0.58
7:LD:206:ASP:OD1	7:LD:209:ARG:NH1	2.36	0.58
10:LG:261:LEU:HD13	10:LG:264:LYS:HD3	1.86	0.58
1:L5:2846:G:O2'	24:LV:19:GLY:O	2.20	0.58
1:L5:1654:G:N2	1:L5:1678:C:OP1	2.37	0.58
1:L5:4985:U:O2	5:LB:174:ARG:NH1	2.36	0.58
1:L5:1755:C:N4	1:L5:1776:A:N1	2.52	0.58
1:L5:3896:C:O2'	5:LB:268:ARG:NH2	2.33	0.58
1:L5:2856:C:O2	5:LB:242:ARG:NH2	2.36	0.58
1:L5:977:C:OP2	8:LE:59:ARG:NH2	2.36	0.58
1:L5:3807:A:HO2'	47:S2:1816:G:HO2'	1.51	0.58
51:SD:132:LYS:HE3	51:SD:191:PRO:HA	1.85	0.58
54:SH:10:LYS:NZ	54:SH:20:GLU:OE1	2.37	0.58
61:SS:15:VAL:HG12	61:SS:16:LEU:HD12	1.86	0.58
1:L5:4489:G:N2	1:L5:4592:C:OP1	2.37	0.58
9:LF:96:ARG:HH12	9:LF:224:THR:HG22	1.68	0.58
75:SO:57:THR:HB	75:SO:60:MET:HG3	1.86	0.58
70:SC:199:PRO:HG3	72:SJ:58:ARG:HE	1.67	0.58
1:L5:4910:G:N2	17:LO:106:ASP:O	2.36	0.57
73:SM:50:CYS:SG	73:SM:52:GLN:NE2	2.75	0.57
1:L5:2544:G:N2	3:L8:126:C:OP1	2.37	0.57
1:L5:4075:U:OP1	10:LG:249:ARG:NH2	2.37	0.57
3:L8:123:U:O2'	3:L8:126:C:N4	2.34	0.57
10:LG:57:TRP:O	10:LG:62:ARG:NH2	2.38	0.57
73:SM:106:CYS:SG	73:SM:107:SER:N	2.76	0.57
10:LG:200:THR:HG22	10:LG:201:THR:HG23	1.85	0.57
24:LV:87:SER:OG	25:LW:19:ARG:NH1	2.36	0.57
47:S2:1758:G:N1	47:S2:1772:C:OP2	2.36	0.57
48:S6:29:G:O2'	48:S6:30:G:N7	2.36	0.57
23:LU:23:LEU:HD22	23:LU:83:LEU:HD21	1.86	0.57
51:SD:141:LYS:O	51:SD:143:ARG:NH2	2.37	0.57
1:L5:2626:U:O4	23:LU:97:ARG:NH1	2.38	0.57
5:LB:35:ASP:OD2	5:LB:193:LYS:NZ	2.38	0.57
8:LE:185:PRO:HA	8:LE:250:GLN:HE22	1.70	0.57
4:LA:135:THR:HG23	4:LA:149:LYS:HB3	1.87	0.57
16:LN:104:GLU:HA	16:LN:160:GLU:HG3	1.87	0.57
2:L7:47:G:H21	7:LD:222:GLN:HE22	1.53	0.57
5:LB:222:VAL:O	5:LB:343:ARG:NH1	2.38	0.57
64:SV:19:ALA:O	76:SW:23:ARG:NH2	2.38	0.57
1:L5:2601:A:N6	1:L5:2744:A:OP2	2.34	0.57
1:L5:4942:C:OP1	8:LE:187:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LL:80:GLU:OE2	14:LL:102:ARG:NH1	2.38	0.57
62:ST:6:VAL:O	62:ST:11:GLN:NE2	2.36	0.57
1:L5:4980:C:N3	18:LP:69:ARG:NH2	2.53	0.56
8:LE:161:ARG:NH2	8:LE:273:SER:OG	2.38	0.56
47:S2:121:OMU:HM23	52:SE:144:ALA:HB3	1.86	0.56
1:L5:138:G:H2'	1:L5:139:G:H8	1.70	0.56
1:L5:1968:G:OP2	1:L5:1970:A:N6	2.38	0.56
1:L5:2003:G:H1	1:L5:2016:C:H42	1.50	0.56
4:LA:116:LEU:HD11	4:LA:148:VAL:HG21	1.87	0.56
7:LD:223:PHE:HB3	7:LD:226:TYR:HB2	1.88	0.56
47:S2:955:A:N6	47:S2:971:G:O2'	2.38	0.56
64:SV:80:SER:OG	64:SV:82:ASN:OD1	2.21	0.56
26:LX:88:LYS:NZ	26:LX:92:ASP:OD2	2.37	0.56
51:SD:31:GLU:O	51:SD:54:ARG:NH2	2.36	0.56
71:SG:70:HIS:HB3	71:SG:101:ILE:HB	1.87	0.56
1:L5:3688:U:OP2	4:LA:198:ARG:NH1	2.38	0.56
1:L5:4774:C:O2	1:L5:4860:G:N2	2.38	0.56
47:S2:538:U:O2	47:S2:546:G:N2	2.38	0.56
47:S2:334:C:OP2	71:SG:190:ARG:NH2	2.38	0.56
61:SS:63:GLU:OE1	61:SS:66:ARG:NH2	2.38	0.56
1:L5:3689:G:O2'	1:L5:3818:U:OP2	2.24	0.56
1:L5:4893:A:OP1	17:LO:188:LYS:NZ	2.39	0.56
60:SR:59:LYS:O	60:SR:63:ARG:NH1	2.39	0.56
1:L5:4725:C:OP1	5:LB:103:LYS:NZ	2.33	0.56
10:LG:103:ARG:HE	10:LG:193:LEU:HA	1.71	0.56
25:LW:101:ARG:HH12	71:SG:156:TYR:HE2	1.53	0.56
26:LX:71:LEU:HD22	26:LX:103:LYS:HD2	1.88	0.56
3:L8:71:A:OP1	27:LY:27:ARG:NH2	2.36	0.56
1:L5:699:C:O2'	1:L5:968:C:O2	2.21	0.56
1:L5:97:G:OP1	14:LL:16:LYS:NZ	2.38	0.56
47:S2:1021:U:OP1	74:SN:128:TYR:OH	2.22	0.56
1:L5:1370:G:O6	6:LC:239:LYS:NZ	2.38	0.56
1:L5:2042:A:N3	1:L5:4462:C:O2'	2.37	0.56
1:L5:182:G:N2	1:L5:256:G:OP2	2.38	0.56
11:LH:113:GLU:OE1	11:LH:115:ARG:NH2	2.39	0.56
15:LM:41:PRO:HG3	15:LM:73:VAL:HG23	1.88	0.56
51:SD:106:ARG:HG3	51:SD:175:VAL:HG22	1.86	0.56
64:SV:1:MET:N	86:SV:101:HOH:O	2.38	0.56
1:L5:489:C:H42	1:L5:664:G:H1	1.51	0.56
1:L5:4194:I4U:O2'	12:LI:116:ARG:NH1	2.38	0.56
12:LI:35:ASP:OD1	12:LI:86:HIS:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SH:66:VAL:HG22	54:SH:96:ALA:HB1	1.86	0.56
76:SW:27:ILE:HB	76:SW:61:ILE:HB	1.86	0.56
1:L5:3965:A:N6	1:L5:4040:C:OP1	2.39	0.55
4:LA:137:ILE:HD11	4:LA:149:LYS:HB2	1.89	0.55
12:LI:150:GLU:OE2	12:LI:153:ARG:NH1	2.38	0.55
1:L5:1824:G:H5'	22:LT:35:LYS:HE3	1.87	0.55
1:L5:2575:U:OP1	28:LZ:48:ARG:NH2	2.39	0.55
7:LD:33:ARG:HH21	22:LT:27:LEU:HD23	1.70	0.55
16:LN:124:ASP:HB3	16:LN:127:TYR:H	1.70	0.55
28:LZ:66:SER:HB2	28:LZ:122:TYR:HE2	1.71	0.55
47:S2:821:G:N7	72:SJ:138[B]:ARG:NH2	2.54	0.55
75:SO:30:VAL:HG12	75:SO:94:HIS:HB2	1.87	0.55
1:L5:1695:U:O2'	1:L5:1719:A:N1	2.39	0.55
1:L5:3937:C:H1'	16:LN:125:SER:HB3	1.88	0.55
7:LD:86:TYR:HH	7:LD:100:CYS:HG	1.54	0.55
49:SA:76:VAL:HG12	49:SA:123:VAL:HB	1.89	0.55
53:SF:49:LEU:HD12	59:SQ:50:LYS:HG2	1.89	0.55
1:L5:2487:G:H22	1:L5:2492:C:H1'	1.70	0.55
9:LF:157:ARG:NH2	9:LF:212:LYS:O	2.40	0.55
1:L5:2269:C:N4	19:LQ:21:GLN:OE1	2.39	0.55
52:SE:55:ALA:HB1	52:SE:60:GLU:HG3	1.88	0.55
71:SG:159:ARG:HG2	71:SG:173:ALA:HB2	1.88	0.55
57:SL:88:ILE:HD13	57:SL:128:VAL:HG21	1.88	0.55
5:LB:10:ARG:NH1	5:LB:265:SER:O	2.38	0.55
20:LR:39:GLN:OE1	20:LR:42:ARG:NH2	2.39	0.55
47:S2:1372:U:OP1	47:S2:1385:G:N2	2.35	0.55
61:SS:105:ASN:OD1	61:SS:108:ARG:NH2	2.40	0.55
4:LA:126:LEU:HD13	4:LA:150:LEU:HD11	1.89	0.55
12:LI:31:ILE:HD11	12:LI:89:VAL:HG21	1.89	0.55
18:LP:45:THR:HG22	18:LP:49:LYS:HE2	1.87	0.55
24:LV:39:ILE:HG12	24:LV:61:VAL:HG11	1.88	0.55
47:S2:153:G:H21	71:SG:13:GLN:HE22	1.55	0.55
73:SM:35:ILE:O	73:SM:39:ALA:N	2.34	0.55
78:SZ:99:LEU:HD11	78:SZ:102:LYS:HB2	1.87	0.55
1:L5:2562:G:O2'	1:L5:2565:A:N6	2.40	0.55
1:L5:4910:G:H4'	5:LB:95:THR:HG22	1.88	0.55
1:L5:1193:C:H2'	1:L5:1194:G:H8	1.72	0.55
1:L5:1179:U:O5'	7:LD:289:ARG:NH2	2.40	0.55
6:LC:317:ASN:ND2	6:LC:318:PRO:O	2.40	0.55
70:SC:72:ASP:OD2	70:SC:272:HIS:NE2	2.33	0.55
54:SH:31:GLU:HA	54:SH:37:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SJ:71:LEU:O	72:SJ:75:ASN:ND2	2.40	0.55
47:S2:951:C:O2'	75:SO:50:LYS:NZ	2.39	0.55
47:S2:1563:G:OP1	62:ST:121:ARG:NH2	2.40	0.55
1:L5:1503:A:H4'	1:L5:1504:G:H5'	1.89	0.54
15:LM:90:ARG:HA	15:LM:93:LYS:HG2	1.87	0.54
21:LS:28:TYR:OH	21:LS:52:LYS:NZ	2.40	0.54
27:LY:109:LEU:HD12	27:LY:115:ARG:HH21	1.71	0.54
52:SE:44:LEU:HD21	52:SE:70:ILE:HG21	1.89	0.54
11:LH:8:GLN:HE22	11:LH:71:ARG:HG3	1.72	0.54
63:SU:67:LYS:HB2	63:SU:78:ASP:HB2	1.89	0.54
1:L5:1889:U:OP2	1:L5:1890:G:N2	2.39	0.54
1:L5:3960:A:N6	1:L5:4043:G:N7	2.55	0.54
9:LF:171:ASP:HB3	9:LF:174:LEU:HD13	1.89	0.54
1:L5:510:U:OP1	14:LL:163:LYS:NZ	2.40	0.54
47:S2:696:G:O2'	47:S2:736:C:N3	2.40	0.54
55:SI:133:GLU:O	55:SI:137:LEU:HD22	2.08	0.54
47:S2:1650:A:H5''	59:SQ:139:ALA:HB2	1.87	0.54
4:LA:241:ARG:HG3	4:LA:241:ARG:HH11	1.73	0.54
2:L7:6:C:H4'	7:LD:52:ILE:HD13	1.89	0.54
21:LS:15:ARG:HB3	21:LS:27:LEU:HD23	1.89	0.54
47:S2:1521:C:OP2	61:SS:124:ARG:NH2	2.35	0.54
49:SA:163:CYS:SG	49:SA:164:ASN:N	2.75	0.54
58:SP:103:ASN:ND2	58:SP:120:SER:OG	2.38	0.54
59:SQ:25:CYS:HB3	59:SQ:68:ILE:HG12	1.89	0.54
77:SY:20:ARG:NH2	77:SY:74:MET:SD	2.81	0.54
77:SY:83:LYS:NZ	77:SY:96:LEU:O	2.41	0.54
1:L5:1741:G:O6	2:L7:103:A:O2'	2.24	0.54
1:L5:942:G:OP1	9:LF:245:ARG:NH1	2.39	0.54
11:LH:91:LYS:HD3	11:LH:145:ILE:HD13	1.89	0.54
1:L5:2033:A:OP1	12:LI:162:ARG:NH1	2.40	0.54
47:S2:1658:G:OP2	47:S2:1660:C:N4	2.41	0.54
1:L5:2532:C:O2'	26:LX:93:ASN:ND2	2.34	0.54
25:LW:77:LYS:HD2	25:LW:79:GLN:HE22	1.73	0.54
61:SS:98:VAL:HG11	61:SS:106:LYS:HD2	1.90	0.54
54:SH:79:LEU:HD22	54:SH:94:PHE:HZ	1.72	0.54
58:SP:96:VAL:HG11	58:SP:116:LEU:HB3	1.89	0.54
4:LA:95:GLN:O	4:LA:100:ASN:ND2	2.37	0.54
28:LZ:5:MET:O	28:LZ:28:ASN:ND2	2.40	0.54
70:SC:196:ILE:HB	70:SC:223:TYR:HB2	1.90	0.54
64:SV:12:TYR:HB3	70:SC:79:GLU:HB2	1.90	0.54
55:SI:191:GLU:O	57:SL:19:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1559:G:OP1	20:LR:126:LYS:NZ	2.41	0.53
1:L5:4133:C:H42	1:L5:4151:G:H1	1.56	0.53
12:LI:47:PRO:HG2	12:LI:142:LEU:HG	1.89	0.53
60:SR:61:ILE:HG22	60:SR:66:VAL:HB	1.89	0.53
47:S2:1156:U:O4	70:SC:194:ARG:NH1	2.40	0.53
73:SM:31:LEU:HD22	73:SM:112:LYS:H	1.74	0.53
1:L5:2673:G:H5''	1:L5:2674:A:H3'	1.90	0.53
1:L5:4939:C:OP1	8:LE:187:ARG:NH1	2.40	0.53
1:L5:3955:G:O2'	1:L5:3966:A:N7	2.39	0.53
47:S2:1610:G:OP1	61:SS:121:ARG:NH2	2.40	0.53
52:SE:31:PRO:HG2	52:SE:38:LEU:HB2	1.90	0.53
52:SE:148:ARG:NH1	71:SG:205:GLU:OE2	2.41	0.53
25:LW:80:ARG:NH2	71:SG:129:VAL:O	2.34	0.53
71:SG:181:THR:HG22	71:SG:183:ARG:H	1.73	0.53
1:L5:1763:C:H41	1:L5:1764:G:H21	1.55	0.53
1:L5:4112:C:H5''	1:L5:4113:U:H5	1.74	0.53
10:LG:257:LYS:HE2	10:LG:261:LEU:HG	1.90	0.53
11:LH:47:LEU:HD12	11:LH:53:LYS:HE3	1.89	0.53
21:LS:95:ARG:NH2	21:LS:112:ASP:OD2	2.42	0.53
47:S2:1336:C:N4	47:S2:1337:4AC:O7	2.42	0.53
47:S2:70:G:H21	47:S2:79:A:H62	1.55	0.53
55:SI:133:GLU:HG2	55:SI:133:GLU:O	2.08	0.53
1:L5:1436:C:H42	1:L5:1448:G:H1	1.57	0.53
1:L5:759:G:H22	1:L5:904:C:H2'	1.73	0.53
5:LB:286:LYS:HE2	5:LB:365:LEU:HD12	1.89	0.53
20:LR:4:LEU:HD13	20:LR:24:LEU:HD23	1.91	0.53
47:S2:1354:G:N1	47:S2:1357:A:OP2	2.41	0.53
47:S2:1568:C:OP1	62:ST:96:SER:OG	2.27	0.53
51:SD:116:ARG:NH2	51:SD:150:MET:SD	2.82	0.53
55:SI:22:HIS:ND1	55:SI:23:LYS:O	2.40	0.53
65:SX:72:VAL:HG11	65:SX:102:VAL:HG11	1.91	0.53
1:L5:2337:C:H4'	20:LR:19:LYS:HB2	95.10	0.53
3:L8:75:G:OP2	27:LY:74:TYR:OH	2.26	0.53
10:LG:223:ARG:HB2	10:LG:227:ASN:HB2	1.90	0.53
47:S2:1284:A:HO2'	73:SM:106:CYS:HG	1.52	0.53
55:SI:48:VAL:HG11	55:SI:54:LYS:HE3	1.90	0.53
1:L5:1962:A:OP2	1:L5:2024:G:N1	2.35	0.53
1:L5:3788:C:N4	1:L5:3812:C:OP2	2.42	0.53
54:SH:144:ILE:HG23	76:SW:52:ILE:HB	1.89	0.53
58:SP:123:TYR:OH	61:SS:124:ARG:NH1	2.42	0.53
59:SQ:17:LYS:HA	59:SQ:126:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:88:A:N7	19:LQ:173:LYS:NZ	2.57	0.53
27:LY:54:GLU:HA	27:LY:69:LYS:HA	1.90	0.53
1:L5:2533:C:OP1	26:LX:139:ARG:NH2	2.42	0.52
7:LD:166:ALA:HB1	7:LD:171:LEU:HD12	1.90	0.52
55:SI:113:TYR:OH	55:SI:156:ALA:O	2.28	0.52
1:L5:461:G:H2'	1:L5:462:G:H8	1.73	0.52
1:L5:4675:U:OP1	5:LB:334:LYS:NZ	2.42	0.52
1:L5:4525:C:OP1	5:LB:246:ARG:NH1	2.41	0.52
13:LJ:153:ALA:HA	13:LJ:156:ARG:HE	1.74	0.52
17:LO:54:TYR:OH	17:LO:73:PHE:O	2.28	0.52
49:SA:108:PHE:HB2	49:SA:136:GLU:HG2	1.91	0.52
5:LB:219:VAL:HG11	5:LB:337:VAL:HG13	1.91	0.52
6:LC:198:ASN:ND2	27:LY:10:ASP:OD1	2.42	0.52
24:LV:65:VAL:HG22	24:LV:73:ARG:HA	1.89	0.52
59:SQ:13:PHE:HA	59:SQ:22:VAL:HA	1.91	0.52
47:S2:1597:C:OP2	78:SZ:85:ARG:NH2	2.38	0.52
71:SG:141:ILE:HD11	71:SG:157:VAL:HA	1.91	0.52
57:SL:120:VAL:HG22	57:SL:145:VAL:HG11	1.91	0.52
58:SP:38:SER:OG	58:SP:41:GLN:NE2	2.43	0.52
1:L5:141:C:N4	1:L5:142:G:O6	2.42	0.52
8:LE:245:GLN:HA	8:LE:248:ILE:HG12	1.90	0.52
9:LF:131:ASN:OD1	9:LF:134:ARG:NH2	2.42	0.52
18:LP:30:ARG:HA	18:LP:119:VAL:HG21	1.90	0.52
51:SD:39:VAL:HG13	51:SD:48:ILE:HG12	1.92	0.52
52:SE:43:PRO:HG2	52:SE:46:ILE:HG12	1.91	0.52
52:SE:60:GLU:HA	52:SE:63:LYS:HG2	1.92	0.52
47:S2:1598:G:O2'	78:SZ:80:ARG:O	2.27	0.52
1:L5:1977:C:N4	1:L5:2002:A:O2'	2.42	0.52
4:LA:56:ALA:HB2	4:LA:130:SER:HB3	1.91	0.52
12:LI:47:PRO:HD2	12:LI:141:LYS:HA	1.91	0.52
12:LI:179:ASP:OD1	12:LI:179:ASP:N	2.35	0.52
70:SC:115:GLN:HE22	70:SC:120:GLN:HE21	1.57	0.52
63:SU:55:ARG:HG2	63:SU:87:ARG:HG2	1.92	0.52
1:L5:4140:C:O2	1:L5:4145:C:O2'	2.28	0.52
1:L5:1872:G:O2'	1:L5:4219:A:N3	2.38	0.52
27:LY:131:GLU:HA	27:LY:134:LYS:HE3	1.91	0.52
53:SF:18:LYS:HE3	53:SF:22:LYS:HA	1.91	0.52
73:SM:42:LEU:HD22	73:SM:68:LEU:HD12	1.92	0.52
1:L5:1447:C:O2	1:L5:2099:G:N2	2.43	0.52
1:L5:4935:C:H2'	1:L5:4936:G:H8	1.74	0.52
5:LB:175:GLN:NE2	5:LB:177:LYS:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:224:LYS:HG3	5:LB:340:THR:HG22	1.92	0.52
6:LC:290:SER:OG	6:LC:294:LYS:NZ	2.43	0.52
9:LF:213:LEU:HB3	9:LF:247:MET:HG2	1.92	0.52
12:LI:207:ASP:OD1	12:LI:210:ARG:NH2	2.43	0.52
47:S2:1013:U:OP1	47:S2:1129:G:O2'	2.26	0.52
47:S2:190:G:O2'	47:S2:209:A:N6	2.43	0.52
72:SJ:83:ARG:HE	72:SJ:150:ARG:HD3	1.74	0.52
5:LB:48:GLY:HA3	5:LB:81:THR:HG22	1.91	0.51
23:LU:22:THR:HG22	23:LU:71:THR:HG22	1.92	0.51
47:S2:1677:U:OP1	53:SF:148:ASN:ND2	2.36	0.51
52:SE:11:ARG:HA	52:SE:28:ALA:HB2	1.93	0.51
55:SI:131:PRO:O	55:SI:135:GLU:OE1	2.28	0.51
1:L5:4478:G:O2'	1:L5:4602:A:N1	2.42	0.51
1:L5:1755:C:H1'	7:LD:3:PHE:HE1	1.73	0.51
24:LV:58:GLY:HA2	24:LV:125:CYS:HB3	1.92	0.51
1:L5:3961:G:N2	1:L5:4043:G:O6	2.43	0.51
1:L5:4618:G:H5''	24:LV:15:ARG:HB3	1.93	0.51
1:L5:3680:U:OP1	4:LA:54:ARG:NH1	2.44	0.51
15:LM:93:LYS:HA	15:LM:96:GLU:HG2	1.91	0.51
70:SC:64:THR:HG23	70:SC:66:LEU:H	1.75	0.51
55:SI:133:GLU:HG3	55:SI:136:ILE:HG22	1.92	0.51
1:L5:1447:C:N3	1:L5:2099:G:N1	2.58	0.51
6:LC:152:LEU:HD23	6:LC:251:ILE:HG12	1.93	0.51
1:L5:746:A:N6	1:L5:913:U:O2	2.44	0.51
23:LU:100:LEU:HD23	23:LU:112:LEU:HD23	1.93	0.51
52:SE:95:THR:HG23	52:SE:97:GLU:HG2	1.93	0.51
47:S2:1455:A:OP1	60:SR:5:ARG:NH1	2.43	0.51
1:L5:151:G:OP2	16:LN:4:TYR:OH	2.23	0.51
1:L5:3977:C:O2'	1:L5:4035:G:N7	2.43	0.51
1:L5:4213:A:H5''	1:L5:4214:A:H5'	1.92	0.51
1:L5:736:C:OP1	15:LM:74:ARG:NH1	2.44	0.51
16:LN:68:ARG:HA	16:LN:98:LEU:HD21	1.93	0.51
51:SD:172:VAL:HG22	51:SD:185:LYS:HG2	1.93	0.51
1:L5:62:A:N3	1:L5:77:U:O2'	2.38	0.51
9:LF:115:ARG:NH1	19:LQ:4:ASP:O	2.40	0.51
47:S2:1208:A:OP2	47:S2:1835:A:O2'	2.29	0.51
7:LD:194:VAL:HA	7:LD:197:LYS:HD3	1.93	0.51
1:L5:3967:G:N2	1:L5:4056:A:O2'	2.44	0.51
8:LE:264:ILE:HD11	8:LE:267:LEU:HD22	1.92	0.51
11:LH:42:ASN:HD21	17:LO:131:PRO:HB2	1.75	0.51
1:L5:4415:1MA:OP1	12:LI:154:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:963:G:N7	1:L5:964:A:N6	2.59	0.50
7:LD:50:ARG:NH2	7:LD:72:ASP:OD2	2.39	0.50
51:SD:40:ARG:NH1	51:SD:47:GLU:OE2	2.42	0.50
47:S2:1470:C:OP2	53:SF:59:LYS:NZ	2.44	0.50
54:SH:95:ILE:HD11	54:SH:129:ILE:HG12	1.92	0.50
47:S2:935:G:O2'	74:SN:108:ASP:OD1	2.26	0.50
59:SQ:97:GLN:HB3	59:SQ:105:LYS:HD3	1.93	0.50
65:SX:63:ASN:ND2	65:SX:114:ASP:OD2	2.44	0.50
1:L5:2811:G:N1	1:L5:2814:C:OP2	2.35	0.50
1:L5:989:U:O2'	1:L5:990:C:O4'	2.27	0.50
20:LR:4:LEU:HD23	20:LR:7:GLN:HE21	1.75	0.50
25:LW:34:ALA:HA	25:LW:37:GLU:HG3	1.93	0.50
27:LY:4:ASN:HB3	27:LY:7:VAL:HG22	1.92	0.50
51:SD:48:ILE:HB	51:SD:86:LEU:HD23	1.92	0.50
52:SE:122:LYS:NZ	52:SE:124:CYS:SG	2.84	0.50
1:L5:4208:U:OP2	22:LT:4:THR:OG1	2.29	0.50
1:L5:4492:U:O2'	1:L5:4512:U:O2	2.27	0.50
5:LB:220:ILE:HD11	5:LB:348:ARG:HE	1.76	0.50
24:LV:22:VAL:O	24:LV:24:ALA:N	2.44	0.50
25:LW:71:ARG:HH12	47:S2:1781:A:H2'	1.77	0.50
28:LZ:64:LYS:HA	28:LZ:67:LYS:HE3	1.93	0.50
28:LZ:99:ASP:HB2	28:LZ:102:ARG:HE	1.76	0.50
53:SF:102:LEU:HD11	78:SZ:100:VAL:HG21	1.92	0.50
54:SH:60:ILE:HG23	54:SH:90:LYS:HD2	1.93	0.50
75:SO:57:THR:HG22	75:SO:59:GLY:H	1.75	0.50
1:L5:1969:G:O6	1:L5:2019:C:N4	2.44	0.50
1:L5:2896:G:H5''	20:LR:134:ASN:HD22	1.76	0.50
6:LC:66:SER:HA	6:LC:77:PRO:HA	1.93	0.50
18:LP:119:VAL:HG12	18:LP:146:ILE:HG12	1.93	0.50
47:S2:975:G:OP1	75:SO:98:ARG:NH1	2.40	0.50
76:SW:80:ASP:N	76:SW:80:ASP:OD1	2.43	0.50
1:L5:2848:G:O2'	1:L5:3838:U:O4	2.22	0.50
4:LA:207:VAL:HG23	4:LA:208:GLU:HG3	1.92	0.50
5:LB:14:LEU:HD23	5:LB:17:LEU:HD21	1.94	0.50
5:LB:19:ARG:HB2	5:LB:234:ARG:HH21	1.77	0.50
49:SA:177:MET:SD	49:SA:180:ARG:NH2	2.69	0.50
72:SJ:63:LEU:O	72:SJ:70:ARG:NH1	2.45	0.50
11:LH:103:VAL:HG22	11:LH:114:ILE:HG12	1.93	0.50
13:LJ:40:LEU:HD23	13:LJ:43:LEU:HD21	1.93	0.50
16:LN:123:GLU:HG2	16:LN:128:LYS:HG3	1.93	0.50
27:LY:56:GLN:HB3	27:LY:67:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1115:U:O2'	47:S2:1117:C:OP2	2.27	0.50
47:S2:681:U:H4'	65:SX:9:THR:HG22	1.93	0.50
1:L5:2658:G:N2	1:L5:2676:A:OP2	2.34	0.50
1:L5:2714:G:H2'	1:L5:2715:G:H8	1.77	0.50
1:L5:3653:A:N6	1:L5:3691:G:O2'	2.41	0.50
5:LB:46:PHE:HE2	5:LB:81:THR:HB	1.77	0.50
47:S2:959:G:OP1	75:SO:104:ARG:NH1	2.36	0.50
75:SO:103:ASN:HD21	75:SO:142:ARG:HA	1.77	0.50
1:L5:3654:G:O2'	1:L5:3693:U:OP1	2.26	0.50
1:L5:99:A:H5''	16:LN:184:ILE:HD13	1.94	0.50
7:LD:256:LYS:HD2	7:LD:257:PRO:HD2	1.93	0.50
25:LW:105:ARG:HH12	71:SG:151:ASP:HA	1.76	0.50
1:L5:1940:G:H1	1:L5:4434:C:H5''	1.77	0.50
8:LE:101:ASN:OD1	8:LE:105:ARG:NH2	2.45	0.50
18:LP:118:GLN:NE2	18:LP:147:GLU:OE2	2.45	0.50
27:LY:4:ASN:HD22	27:LY:5:PRO:HD2	1.76	0.50
47:S2:1024:A:OP2	74:SN:124:ARG:NH2	2.36	0.50
47:S2:672:A:N6	47:S2:1027:A:OP1	2.41	0.50
47:S2:913:A:H1'	54:SH:66:VAL:HB	1.94	0.50
1:L5:992:C:N4	1:L5:994:G:N7	2.46	0.49
47:S2:1669:G:OP1	63:SU:79:ARG:NH1	2.44	0.49
6:LC:159:GLU:HA	6:LC:217:ILE:HB	1.92	0.49
9:LF:86:GLU:HG3	22:LT:135:PRO:HB3	1.93	0.49
47:S2:197:U:H5'	47:S2:203:G:H22	1.77	0.49
50:SB:90:ASP:HB3	50:SB:97:LEU:HD12	1.94	0.49
52:SE:18:TRP:HH2	52:SE:31:PRO:HD3	1.76	0.49
1:L5:1907:A:H4'	9:LF:223:LYS:HE3	1.94	0.49
12:LI:66:GLU:HG3	12:LI:69:ARG:HH11	1.76	0.49
22:LT:102:ARG:HG2	22:LT:106:LEU:HG	1.94	0.49
47:S2:588:G:H4'	47:S2:589:G:H5'	1.93	0.49
49:SA:189:ILE:HG22	49:SA:191:ARG:H	1.77	0.49
49:SA:77:ILE:HG13	49:SA:99:ILE:HB	1.95	0.49
64:SV:16:LYS:H	70:SC:259:THR:HG21	1.77	0.49
54:SH:184:ASP:OD1	54:SH:184:ASP:N	2.42	0.49
55:SI:101:ILE:HD12	55:SI:190:LEU:HD11	1.93	0.49
1:L5:4041:C:H5'	1:L5:4042:G:H5''	1.95	0.49
1:L5:4476:C:O2'	1:L5:4478:G:OP2	2.27	0.49
1:L5:4546:A:N7	4:LA:215:ASN:ND2	2.60	0.49
55:SI:6:ASP:N	55:SI:6:ASP:OD1	2.43	0.49
72:SJ:20:PHE:HA	72:SJ:25:LEU:HD11	1.94	0.49
1:L5:2062:C:O2'	21:LS:111:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2112:G:H4'	1:L5:2251:G:H1	1.77	0.49
1:L5:3811:G:O2'	1:L5:3814:U:OP2	2.30	0.49
1:L5:4623:OMG:OP1	5:LB:19:ARG:NH2	2.46	0.49
5:LB:29:VAL:HG13	5:LB:348:ARG:HD3	1.94	0.49
70:SC:144:SER:HB3	70:SC:150:ALA:HB2	1.95	0.49
55:SI:174:CYS:SG	55:SI:175:ILE:N	2.86	0.49
1:L5:1870:C:H2'	1:L5:1871:A2M:H8	1.94	0.49
1:L5:3597:G:O2'	1:L5:3598:C:O4'	2.31	0.49
1:L5:4242:U:H3	1:L5:4281:A:H2	1.59	0.49
3:L8:150:C:N4	10:LG:52:THR:O	2.45	0.49
5:LB:223:THR:HB	5:LB:275:HIS:H	1.77	0.49
73:SM:48:HIS:HB2	73:SM:111:VAL:HG23	1.93	0.49
65:SX:102:VAL:HG12	65:SX:122:VAL:HG22	1.95	0.49
1:L5:1802:A:N3	22:LT:130:ARG:NH1	2.61	0.49
5:LB:85:VAL:HG22	5:LB:204:GLN:HG2	1.93	0.49
47:S2:1036:A:N3	47:S2:1844:U:O2'	2.43	0.49
55:SI:65:PHE:O	55:SI:109:TYR:OH	2.29	0.49
59:SQ:74:GLY:O	59:SQ:80:GLN:NE2	2.35	0.49
1:L5:2702:C:OP1	23:LU:101:ARG:NH2	2.45	0.49
56:SK:90:VAL:HB	56:SK:94:LEU:HD12	1.94	0.49
1:L5:1966:C:H42	1:L5:2021:G:H1	1.59	0.49
1:L5:4452:U:H5'	83:L5:5348:HMT:H7	1.94	0.49
47:S2:1158:G:H5''	76:SW:76:SER:HB3	1.94	0.49
47:S2:64:A:OP1	71:SG:177:GLN:NE2	2.46	0.49
1:L5:1508:A:OP1	6:LC:110:ARG:NH1	2.46	0.48
1:L5:2838:G:H5'	5:LB:247:GLY:HA2	1.94	0.48
1:L5:4163:U:H5'	1:L5:4164:C:H5''	1.95	0.48
11:LH:89:ARG:HG3	11:LH:145:ILE:HD11	1.94	0.48
15:LM:104:MET:O	15:LM:109:ARG:NH1	2.46	0.48
1:L5:228:C:O2'	27:LY:14:ASN:ND2	2.44	0.48
70:SC:169:TYR:OH	70:SC:175:GLY:O	2.23	0.48
54:SH:40:LEU:HD12	54:SH:43:LEU:HD11	1.95	0.48
13:LJ:90:ARG:NH2	13:LJ:110:GLN:OE1	2.45	0.48
13:LJ:35:ARG:NH2	13:LJ:122:SER:O	2.40	0.48
20:LR:159:ALA:O	20:LR:163:ARG:N	2.42	0.48
49:SA:37:TYR:OH	49:SA:57:LYS:NZ	2.46	0.48
73:SM:56:CYS:SG	73:SM:57:ASP:N	2.86	0.48
64:SV:16:LYS:HG2	64:SV:23:ILE:HD13	1.94	0.48
17:LO:10:ASP:OD2	21:LS:171:ARG:NH2	2.46	0.48
1:L5:4046:A:O2'	48:S6:56:C:O2	2.28	0.48
49:SA:36:GLN:O	49:SA:53:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:52:THR:HG23	50:SB:57:ILE:HA	1.95	0.48
52:SE:159:THR:HB	52:SE:173:ILE:HG23	1.96	0.48
52:SE:45:ILE:HG23	52:SE:46:ILE:HG23	1.95	0.48
53:SF:70:GLU:OE2	53:SF:74:ASN:ND2	2.46	0.48
47:S2:190:G:H5''	55:SI:145:ILE:HG12	1.94	0.48
58:SP:18:ARG:HD2	61:SS:88:LYS:HG2	1.95	0.48
5:LB:170:LEU:O	5:LB:328:ASN:ND2	2.45	0.48
15:LM:81:ASP:OD1	15:LM:81:ASP:N	2.46	0.48
19:LQ:15:ARG:NH1	19:LQ:52:PHE:O	2.47	0.48
20:LR:179:ALA:HA	20:LR:182:GLU:HB2	1.95	0.48
1:L5:2112:G:O2'	1:L5:2250:C:N4	2.47	0.48
1:L5:390:C:H42	1:L5:401:G:H1	1.61	0.48
13:LJ:113:ILE:HD13	13:LJ:119:TYR:HB2	1.96	0.48
47:S2:94:G:O2'	47:S2:508:A:O2'	2.25	0.48
47:S2:943:U:O2'	75:SO:135:ILE:O	2.30	0.48
2:L7:60:G:O2'	7:LD:268:ARG:NH1	2.46	0.48
61:SS:86:ARG:NH1	61:SS:89:ASP:OD1	2.40	0.48
63:SU:22:ILE:HG12	63:SU:114:VAL:HG22	1.94	0.48
1:L5:3596:A:N6	57:SL:3:ASP:OD1	2.47	0.48
1:L5:5041:G:N2	5:LB:389:MET:O	2.44	0.48
1:L5:1932:A:OP2	17:LO:49:ARG:NH2	2.46	0.48
1:L5:369:G:N2	1:L5:372:A:OP2	2.39	0.48
10:LG:218:LEU:O	10:LG:222:ILE:N	2.45	0.48
19:LQ:130:SER:OG	19:LQ:134:CYS:N	2.47	0.48
47:S2:399:C:H5	47:S2:680:G:H5''	1.79	0.48
51:SD:76:ARG:HB2	56:SK:22:VAL:HG11	1.94	0.48
54:SH:30:LEU:O	54:SH:33:ASN:ND2	2.47	0.48
1:L5:500:G:O5'	1:L5:504:G:N2	2.47	0.48
4:LA:30:ARG:NH2	4:LA:36:GLU:OE1	2.46	0.48
11:LH:103:VAL:HG11	11:LH:144:LEU:HD21	1.96	0.48
17:LO:125:LYS:HG2	17:LO:129:LEU:HD12	1.96	0.48
51:SD:220:THR:OG1	51:SD:221:THR:N	2.47	0.48
73:SM:31:LEU:HD13	73:SM:111:VAL:HG12	1.95	0.48
1:L5:455:C:N3	1:L5:456:C:N4	2.62	0.47
8:LE:178:PRO:HB2	8:LE:181:LEU:HD12	1.97	0.47
2:L7:89:G:N2	12:LI:56:GLU:OE2	2.38	0.47
47:S2:1253:A:OP2	47:S2:1526:G:N2	2.37	0.47
47:S2:1644:C:H4'	59:SQ:140:ARG:HB2	1.95	0.47
59:SQ:31:LEU:HD23	59:SQ:69:ARG:HH21	1.79	0.47
1:L5:1270:A:O2'	1:L5:1439:C:O2	2.32	0.47
1:L5:75:G:O6	14:LL:103:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LP:6:LEU:HD12	18:LP:116:HIS:CD2	2.48	0.47
19:LQ:159:PRO:HA	19:LQ:160:HIS:HA	1.63	0.47
49:SA:120:ARG:HD2	70:SC:266:TYR:HB3	1.97	0.47
1:L5:2611:A:H5'	1:L5:2688:G:H4'	1.95	0.47
1:L5:301:G:H5''	16:LN:98:LEU:HD13	1.96	0.47
1:L5:2901:G:H1	1:L5:3598:C:H42	1.63	0.47
18:LP:122:ALA:HB3	18:LP:143:PRO:HG2	1.96	0.47
47:S2:196:C:H42	47:S2:203:G:H2'	1.78	0.47
1:L5:1238:A:O3'	9:LF:48:LYS:NZ	2.48	0.47
1:L5:4146:G:H2'	1:L5:4147:G:H8	1.78	0.47
1:L5:4430:G:OP1	12:LI:30:LYS:NZ	2.45	0.47
26:LX:148:ASP:HA	26:LX:151:ASN:HD22	1.79	0.47
47:S2:1467:C:H5''	60:SR:1:MET:HG3	1.96	0.47
60:SR:60:ARG:HE	60:SR:66:VAL:HG11	1.80	0.47
78:SZ:68:ILE:HB	78:SZ:109:TYR:HB2	1.96	0.47
1:L5:1174:G:H22	1:L5:1186:U:H3	1.61	0.47
1:L5:1962:A:N6	1:L5:2026:A:O2'	2.48	0.47
6:LC:40:VAL:HG22	6:LC:115:VAL:HG11	1.97	0.47
7:LD:184:ASP:HB3	7:LD:189:GLU:HB3	1.97	0.47
47:S2:1543:U:H4'	59:SQ:43:GLU:HG3	1.95	0.47
71:SG:219:GLU:HA	71:SG:222:GLU:HB2	1.96	0.47
55:SI:133:GLU:O	55:SI:137:LEU:CD2	2.63	0.47
75:SO:74:ALA:HB1	75:SO:115:ALA:HB2	1.96	0.47
8:LE:177:GLY:HA3	8:LE:184:VAL:HB	1.97	0.47
13:LJ:51:SER:HB3	13:LJ:71:HIS:CD2	2.49	0.47
26:LX:129:ARG:NH2	26:LX:133:GLU:OE2	2.44	0.47
61:SS:1:MET:HB3	78:SZ:86:ALA:HB1	1.95	0.47
1:L5:120:A:N1	1:L5:148:C:O2'	2.38	0.47
1:L5:4077:A:N1	1:L5:4171:C:N4	2.61	0.47
1:L5:467:U:H5	1:L5:686:A:H61	1.63	0.47
10:LG:134:PRO:HB3	10:LG:206:GLN:HG2	1.96	0.47
17:LO:8:VAL:HG12	17:LO:117:ARG:HG3	1.96	0.47
50:SB:57:ILE:HG22	50:SB:59:SER:H	1.79	0.47
60:SR:67:ARG:HA	60:SR:68:GLY:HA3	1.57	0.47
76:SW:46:TYR:HD2	76:SW:69:LEU:HD13	1.78	0.47
1:L5:3965:A:O2'	1:L5:4038:C:O2	2.32	0.47
1:L5:5006:U:H4'	1:L5:5007:A:H5'	1.97	0.47
2:L7:5:A:OP1	13:LJ:147:ARG:NH2	2.35	0.47
9:LF:94:ARG:HB2	9:LF:114:LEU:HD23	1.97	0.47
12:LI:109:ASP:HA	12:LI:110:ARG:HA	1.67	0.47
22:LT:71:ALA:HA	22:LT:92:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2663:G:OP1	20:LR:118:HIS:ND1	2.42	0.47
1:L5:346:G:OP1	27:LY:8:THR:OG1	2.32	0.47
49:SA:21:ALA:O	49:SA:170:SER:OG	2.32	0.47
71:SG:215:LYS:NZ	71:SG:219:GLU:OE2	2.47	0.47
72:SJ:112:THR:HG22	72:SJ:123:ILE:HD11	1.96	0.47
1:L5:2092:G:N2	1:L5:2262:G:O6	2.48	0.47
1:L5:3955:G:H1'	1:L5:3966:A:H62	1.79	0.47
1:L5:4752:U:H4'	17:LO:4:VAL:HG11	1.97	0.47
1:L5:482:G:N2	1:L5:673:C:O2	2.48	0.47
7:LD:65:ALA:HB2	7:LD:74:ILE:HD13	1.97	0.47
8:LE:153:LEU:HD11	8:LE:195:ILE:HG13	1.96	0.47
13:LJ:26:VAL:HG23	13:LJ:28:GLU:H	1.80	0.47
47:S2:10:G:H21	70:SC:114:LYS:HA	1.78	0.47
47:S2:522:A:H5''	72:SJ:145:PRO:HD2	1.96	0.47
63:SU:26:SER:HB3	63:SU:32:LEU:HD22	1.96	0.47
1:L5:2111:G:O6	1:L5:2251:G:O2'	2.33	0.47
10:LG:26:LYS:HG3	10:LG:28:VAL:HG13	1.97	0.47
47:S2:1330:G:H4'	47:S2:1331:C:H3'	1.97	0.47
47:S2:1402:A:H5'	63:SU:51:LYS:HE3	1.97	0.47
47:S2:384:U:O4	55:SI:5:ARG:NH2	2.46	0.47
60:SR:36:GLU:OE1	60:SR:47:ARG:NH1	2.48	0.47
61:SS:132:ARG:HB2	61:SS:134:GLN:HE22	1.79	0.47
1:L5:1513:U:H4'	14:LL:4:SER:HB2	1.97	0.46
1:L5:2528:G:H4'	1:L5:2783:A:H4'	1.97	0.46
7:LD:111:ASN:HB3	7:LD:116:ASP:HB3	1.97	0.46
12:LI:38:ARG:HD3	12:LI:83:ASP:HB2	1.97	0.46
19:LQ:151:HIS:ND1	19:LQ:164:LYS:O	2.48	0.46
23:LU:28:PRO:HB2	23:LU:34:MET:HG2	1.97	0.46
47:S2:1752:C:N3	47:S2:1779:G:N1	2.57	0.46
1:L5:408:A:O2'	1:L5:411:G:OP2	2.27	0.46
5:LB:220:ILE:HG12	5:LB:278:THR:HG23	1.97	0.46
16:LN:116:LEU:HD22	16:LN:135:ILE:HD11	1.97	0.46
75:SO:17:LEU:HD13	75:SO:88:LEU:HD12	1.98	0.46
1:L5:2910:G:O6	1:L5:3585:G:N1	2.48	0.46
1:L5:4759:C:OP1	17:LO:116:LYS:NZ	2.49	0.46
1:L5:5002:U:OP2	5:LB:385:LYS:NZ	2.42	0.46
1:L5:757:G:H1	1:L5:906:C:H42	1.62	0.46
1:L5:4763:U:HO2'	21:LS:174:THR:HG1	1.62	0.46
23:LU:105:ASN:OD1	23:LU:106:SER:N	2.49	0.46
47:S2:748:C:H42	47:S2:794:A:H61	1.62	0.46
51:SD:60:GLY:HA3	51:SD:65:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LW:80:ARG:HB2	71:SG:131:ARG:HH11	1.80	0.46
72:SJ:133:ARG:HH22	77:SY:65:GLY:HA2	1.79	0.46
1:L5:4261:C:OP1	13:LJ:19:LYS:NZ	2.42	0.46
1:L5:4389:C:H2'	1:L5:4390:A:C8	2.49	0.46
1:L5:740:G:H1	1:L5:925:C:H42	1.64	0.46
7:LD:178:LYS:HE2	7:LD:179:ARG:HH22	1.80	0.46
13:LJ:15:LEU:HG	13:LJ:165:TRP:HB2	1.98	0.46
28:LZ:96:VAL:HG12	28:LZ:110:ALA:HB1	1.98	0.46
50:SB:91:VAL:HG12	50:SB:93:GLY:H	1.80	0.46
58:SP:108:LYS:NZ	61:SS:116:LYS:O	2.48	0.46
1:L5:74:G:H5'	14:LL:59:VAL:HG13	1.96	0.46
1:L5:980:U:H3	1:L5:1274:A:H61	1.62	0.46
5:LB:65:SER:OG	5:LB:66:LYS:N	2.47	0.46
1:L5:1280:C:N4	8:LE:52:ARG:O	2.46	0.46
1:L5:1864:G:OP2	12:LI:14:ASN:ND2	2.49	0.46
47:S2:94:G:HO2'	47:S2:508:A:HO2'	1.53	0.46
70:SC:146:GLU:OE1	70:SC:149:THR:N	2.47	0.46
60:SR:28:PHE:HA	60:SR:55:THR:HG21	1.97	0.46
76:SW:69:LEU:HD21	76:SW:72:CYS:HB3	1.97	0.46
1:L5:1244:G:N2	1:L5:1267:C:O2	2.46	0.46
1:L5:961:G:O2'	1:L5:964:A:N6	2.45	0.46
5:LB:49:TYR:OH	5:LB:168:MET:SD	2.66	0.46
8:LE:223:ARG:HA	8:LE:224:LYS:HA	1.71	0.46
1:L5:4126:C:OP1	10:LG:37:LYS:NZ	2.49	0.46
20:LR:21:LYS:HE3	20:LR:55:VAL:HA	1.98	0.46
71:SG:137:ARG:HD2	71:SG:178:ARG:HD3	1.97	0.46
75:SO:27:VAL:HG13	75:SO:90:ILE:HA	1.97	0.46
83:L5:5348:HMT:O8	83:L5:5348:HMT:O6	2.34	0.46
7:LD:80:ALA:HA	7:LD:83:LEU:HD13	1.97	0.46
13:LJ:10:ASN:N	13:LJ:10:ASN:OD1	2.49	0.46
13:LJ:56:THR:OG1	13:LJ:62:ILE:O	2.30	0.46
22:LT:114:GLN:HA	22:LT:117:LYS:HZ3	1.81	0.46
47:S2:1549:U:OP1	51:SD:34:TYR:OH	29.79	0.46
3:L8:14:OMU:HM23	3:L8:14:OMU:H1'	1.75	0.46
1:L5:73:A:N7	14:LL:103:ARG:NH2	2.64	0.46
49:SA:127:PRO:HG3	49:SA:146:ALA:HB1	1.98	0.46
51:SD:197:LYS:HG2	51:SD:198:ILE:HG23	1.97	0.46
1:L5:251:C:OP1	13:LJ:85:LYS:NZ	175.12	0.46
5:LB:91:GLY:HA2	5:LB:160:ILE:HA	1.97	0.46
47:S2:1453:C:H4'	60:SR:49:LYS:HA	1.98	0.46
47:S2:1756:C:H42	47:S2:1775:U:H3	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:155:G:H4'	71:SG:15:LEU:HD13	1.98	0.46
1:L5:2568:C:N4	1:L5:2569:G:O6	2.49	0.46
1:L5:3672:G:H4'	16:LN:67:ARG:HH12	1.81	0.46
1:L5:3946:G:H21	1:L5:3947:A:H62	1.64	0.46
1:L5:4327:C:OP1	22:LT:70:HIS:NE2	2.47	0.46
1:L5:4338:G:O2'	1:L5:4372:U:O4	2.29	0.46
5:LB:322:HIS:O	5:LB:342:LYS:NZ	2.43	0.46
14:LL:6:ASN:HD22	14:LL:7:GLY:H	1.63	0.46
47:S2:1435:C:O2'	47:S2:1437:C:N4	2.49	0.46
50:SB:144:LYS:HD2	50:SB:208:HIS:HB3	1.97	0.46
52:SE:137:PRO:HG2	52:SE:150:PRO:HD2	1.98	0.46
47:S2:1544:C:O2'	59:SQ:80:GLN:NE2	2.49	0.46
47:S2:1256:G:H8	63:SU:66:ARG:HB2	1.81	0.46
1:L5:1886:G:O2'	1:L5:1909:P7G:O2'	2.33	0.45
21:LS:115:ALA:O	21:LS:118:ARG:NH2	2.49	0.45
23:LU:80:LYS:HE3	23:LU:108:GLU:HA	1.97	0.45
70:SC:267:GLN:HA	70:SC:270:THR:HG23	1.98	0.45
51:SD:123:LEU:HD22	51:SD:152:PHE:HB3	1.98	0.45
53:SF:35:LEU:HD22	53:SF:117:ILE:HD13	1.98	0.45
1:L5:1273:G:O6	1:L5:1274:A:N6	2.50	0.45
1:L5:3710:G:H4'	1:L5:3711:A:H5'	1.98	0.45
18:LP:40:HIS:NE2	18:LP:110:ASP:O	2.49	0.45
47:S2:1647:A:OP1	59:SQ:138:ARG:NH2	2.44	0.45
47:S2:900:C:H5'	47:S2:901:G:C8	2.51	0.45
57:SL:29:GLY:HA3	57:SL:30:LYS:HA	1.64	0.45
1:L5:1850:A:N3	1:L5:2283:G:O2'	2.50	0.45
1:L5:190:G:H2'	1:L5:191:G:H8	1.80	0.45
1:L5:727:C:OP1	9:LF:73:ARG:NH2	2.45	0.45
27:LY:31:SER:HA	27:LY:48:PRO:HA	1.98	0.45
47:S2:368:U:OP1	47:S2:369:C:O2'	2.30	0.45
1:L5:2084:C:H42	19:LQ:14:ARG:HG3	1.81	0.45
1:L5:230:G:OP1	27:LY:15:ARG:NH1	2.48	0.45
10:LG:180:PRO:HG3	10:LG:219:VAL:HG13	1.99	0.45
28:LZ:99:ASP:O	28:LZ:102:ARG:NE	2.49	0.45
47:S2:1531:A:H4'	47:S2:1605:G:H4'	1.99	0.45
47:S2:448:A:H5''	55:SI:25:ARG:HA	1.98	0.45
47:S2:960:U:O2'	47:S2:962:A:N7	2.39	0.45
50:SB:34:LYS:O	50:SB:98:THR:OG1	2.28	0.45
47:S2:114:G:N7	57:SL:69:ARG:NH2	2.63	0.45
60:SR:28:PHE:HZ	60:SR:48:ASN:HB2	1.80	0.45
9:LF:29:LYS:O	9:LF:33:LEU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LI:10:ARG:HE	12:LI:160:PRO:HB2	1.81	0.45
49:SA:27:GLY:H	49:SA:46:ILE:HG23	1.82	0.45
55:SI:134:GLU:O	55:SI:138:ASN:ND2	2.50	0.45
1:L5:26:C:O2'	1:L5:338:A:N3	2.46	0.45
11:LH:47:LEU:HD22	11:LH:55:LEU:HD13	1.98	0.45
47:S2:1010:G:H2'	47:S2:1011:A:C8	2.52	0.45
52:SE:124:CYS:HB3	52:SE:141:THR:HB	1.98	0.45
53:SF:133:THR:HG22	53:SF:134:VAL:HG23	1.98	0.45
1:L5:2555:G:H1	1:L5:2572:C:H42	1.63	0.45
15:LM:95:ILE:HD11	15:LM:124:LYS:HD2	33.52	0.45
23:LU:65:ARG:NH2	23:LU:67:LYS:O	2.50	0.45
47:S2:1270:G:O2'	47:S2:1301:A:N7	2.47	0.45
50:SB:65:ARG:NH2	75:SO:46:ASP:OD2	2.49	0.45
53:SF:194:ASP:HA	53:SF:197:GLU:HG2	1.98	0.45
1:L5:2705:G:H22	1:L5:2710:C:H5	1.64	0.45
1:L5:4612:C:C2	11:LH:120:GLU:HB2	2.52	0.45
24:LV:61:VAL:N	24:LV:79:ALA:O	2.46	0.45
47:S2:1025:U:OP1	47:S2:1090:C:O2'	2.28	0.45
48:S6:9:U:H4'	48:S6:48:C:H4'	1.99	0.45
49:SA:74:VAL:HG12	49:SA:121:LEU:HB3	1.99	0.45
1:L5:2362:U:OP1	18:LP:82:ARG:NH2	2.47	0.45
1:L5:4417:C:N4	1:L5:4422:A:O2'	2.50	0.45
15:LM:11:ARG:HE	15:LM:61:ILE:HG12	1.82	0.45
47:S2:1445:U:O4	47:S2:1446:A:N6	2.50	0.45
76:SW:57:ARG:HD2	76:SW:57:ARG:H	1.80	0.45
1:L5:1326:A2M:OP2	1:L5:4445:U:O2'	2.31	0.45
1:L5:3957:U:H5'	1:L5:3959:U:H5	1.82	0.45
1:L5:4902:C:H42	1:L5:4919:G:H1	1.64	0.45
6:LC:290:SER:O	6:LC:294:LYS:NZ	2.41	0.45
1:L5:1280:C:H5'	8:LE:52:ARG:HH21	1.82	0.45
8:LE:98:GLY:HA3	8:LE:99:ASP:HA	1.80	0.45
13:LJ:31:ASP:HB2	13:LJ:35:ARG:HE	1.81	0.45
14:LL:91:ALA:HB1	14:LL:96:ILE:HB	1.99	0.45
24:LV:85:ARG:NH1	24:LV:99:GLU:O	2.50	0.45
49:SA:26:GLY:O	49:SA:150:THR:OG1	2.31	0.45
50:SB:128:LYS:HA	50:SB:134:LEU:HA	1.98	0.45
47:S2:1017:U:H5'	74:SN:55:ARG:HD3	1.99	0.45
47:S2:921:G:C5	76:SW:28:ARG:HD2	2.51	0.45
1:L5:168:C:O2	1:L5:267:G:N2	2.38	0.44
1:L5:3973:G:N2	1:L5:3974:G:O6	2.50	0.44
1:L5:3954:A:N6	1:L5:4056:A:N1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:67:C:O3'	16:LN:177:GLY:HA2	2.17	0.44
26:LX:104:ALA:O	26:LX:134:LYS:NZ	2.47	0.44
47:S2:1084:A:OP1	47:S2:1858:G:O2'	2.29	0.44
47:S2:1093:A:H4'	76:SW:3:ARG:HH21	1.82	0.44
60:SR:90:ALA:O	60:SR:93:GLN:NE2	2.50	0.44
61:SS:35:GLY:O	61:SS:97:GLN:NE2	2.50	0.44
1:L5:4323:A:C8	7:LD:153:THR:HG21	2.52	0.44
12:LI:43:VAL:O	12:LI:171:TRP:NE1	2.43	0.44
28:LZ:41:ALA:HB2	28:LZ:77:TYR:HE1	1.81	0.44
72:SJ:120:ALA:HB2	72:SJ:129:LEU:HD12	1.98	0.44
61:SS:28:PHE:HE1	61:SS:38:ARG:HE	1.64	0.44
78:SZ:102:LYS:HA	78:SZ:107:VAL:HG12	1.99	0.44
1:L5:2318:G:N2	1:L5:2321:G:OP2	2.42	0.44
1:L5:2:G:OP2	26:LX:39:LYS:NZ	2.46	0.44
2:L7:13:A:O2'	7:LD:24:ARG:NH1	2.50	0.44
1:L5:1175:A:H5''	7:LD:268:ARG:HH21	1.82	0.44
8:LE:91:THR:HG22	8:LE:108:LYS:HB3	1.99	0.44
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.52	0.44
53:SF:143:PRO:HA	53:SF:146:ARG:HG2	2.00	0.44
59:SQ:5:GLY:O	59:SQ:27:ARG:NH2	2.51	0.44
1:L5:133:C:H3'	1:L5:134:G:H8	1.81	0.44
1:L5:197:A:N3	1:L5:222:C:O2'	2.46	0.44
1:L5:2482:C:H2'	1:L5:2483:G:H4'	1.99	0.44
3:L8:106:G:H4'	3:L8:137:A:H5'	1.99	0.44
7:LD:282:GLN:HA	7:LD:285:ALA:HB3	1.99	0.44
20:LR:170:ARG:HD3	20:LR:171:LYS:HD2	2.00	0.44
47:S2:1102:G:OP2	50:SB:151:ARG:NH1	2.51	0.44
54:SH:50:GLU:HB3	54:SH:60:ILE:HG22	2.00	0.44
2:L7:73:U:O2'	2:L7:102:U:O4	2.31	0.44
47:S2:1216:C:O2'	47:S2:1644:C:OP1	2.34	0.44
55:SI:130:THR:N	55:SI:131:PRO:HD2	2.32	0.44
55:SI:70:GLU:OE2	55:SI:117:TYR:OH	2.25	0.44
57:SL:23:VAL:HG23	57:SL:26:GLY:H	1.83	0.44
47:S2:837:A:H61	77:SY:9:THR:H	1.65	0.44
1:L5:374:G:O2'	6:LC:80:ARG:O	2.35	0.44
2:L7:74:A:N3	21:LS:53:LYS:NZ	2.53	0.44
4:LA:116:LEU:HB2	4:LA:126:LEU:HB2	2.00	0.44
17:LO:84:VAL:HG21	17:LO:102:LEU:HD22	2.00	0.44
1:L5:1456:B8Q:O2'	19:LQ:73:PRO:O	2.35	0.44
59:SQ:19:ALA:HB2	59:SQ:75:GLY:HA3	2.00	0.44
1:L5:3589:G:N2	1:L5:3590:G:N7	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LJ:85:LYS:HD2	13:LJ:115:LEU:HB3	1.99	0.44
47:S2:1550:G:H3'	47:S2:1579:A:H61	1.83	0.44
50:SB:175:GLU:OE1	50:SB:187:LYS:NZ	2.51	0.44
71:SG:159:ARG:HH21	71:SG:171:THR:HG23	1.82	0.44
55:SI:165:GLN:HG3	55:SI:171:LEU:HD23	1.99	0.44
62:ST:129:ARG:HG2	62:ST:133:ARG:HH12	1.82	0.44
1:L5:4741:C:H4'	1:L5:4742:G:H5'	1.99	0.44
6:LC:121:ARG:HE	6:LC:274:LYS:HD3	1.83	0.44
14:LL:194:ILE:H	14:LL:194:ILE:HG13	1.59	0.44
2:L7:94:C:H4'	21:LS:122:HIS:HB2	1.99	0.44
21:LS:77:ASN:HD21	21:LS:98:ARG:HH11	1.65	0.44
47:S2:1536:G:H2'	47:S2:1537:A:C8	2.52	0.44
54:SH:144:ILE:HD11	54:SH:152:ARG:HB3	1.99	0.44
1:L5:3898:G:H5'	5:LB:254:ILE:HG13	2.00	0.44
5:LB:398:ALA:HA	5:LB:401:GLU:HB2	1.99	0.44
10:LG:175:ARG:HH11	10:LG:230:TYR:HD2	1.66	0.44
75:SO:14:VAL:HG23	75:SO:15:ILE:HA	2.00	0.44
1:L5:4220:6MZ:H8	1:L5:4220:6MZ:O2P	2.17	0.43
1:L5:423:G:OP1	18:LP:62:ARG:NH2	2.50	0.43
1:L5:755:C:H2'	1:L5:756:G:H8	1.82	0.43
3:L8:21:C:OP1	6:LC:195:LYS:NZ	2.48	0.43
5:LB:139:ASP:OD2	5:LB:142:GLY:N	2.51	0.43
7:LD:272:SER:OG	7:LD:273:LEU:N	2.50	0.43
71:SG:18:VAL:HG11	71:SG:24:LEU:HD21	2.00	0.43
65:SX:129:SER:OG	65:SX:130:LEU:N	2.51	0.43
1:L5:2666:U:OP2	20:LR:124:TYR:OH	2.35	0.43
1:L5:4699:U:H1'	1:L5:4700:A:H5"	1.99	0.43
1:L5:4771:C:N4	1:L5:4862:G:O6	2.50	0.43
14:LL:205:GLN:HA	14:LL:208:GLU:HB2	1.99	0.43
47:S2:1623:A:N1	61:SS:132:ARG:NH1	2.65	0.43
49:SA:141:ASN:ND2	70:SC:85:SER:O	2.51	0.43
57:SL:35:ARG:NH1	57:SL:53:GLY:O	2.51	0.43
47:S2:1627:C:H5"	62:ST:41:LYS:HD3	2.00	0.43
1:L5:1600:A:H5'	18:LP:133:HIS:HA	2.00	0.43
1:L5:1707:C:H2'	5:LB:103:LYS:HD3	122.55	0.43
4:LA:124:GLY:O	4:LA:128:ARG:NH2	2.47	0.43
6:LC:66:SER:OG	6:LC:66:SER:O	2.32	0.43
15:LM:24:LEU:HD11	15:LM:86:TRP:CG	2.53	0.43
47:S2:1284:A:O2'	73:SM:106:CYS:SG	2.68	0.43
1:L5:1267:C:H2'	1:L5:1268:G:H8	1.84	0.43
1:L5:131:C:O2	1:L5:138:G:N2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2418:A:N1	1:L5:2429:A:O2'	2.48	0.43
1:L5:2422:OMC:H1'	1:L5:2422:OMC:HM23	1.83	0.43
1:L5:2521:G:H2'	1:L5:2522:7MG:H82	2.00	0.43
1:L5:1556:C:O2'	1:L5:2669:C:OP1	2.28	0.43
1:L5:3970:G:O2'	1:L5:4052:C:N4	2.49	0.43
1:L5:753:C:H41	1:L5:910:G:H1	1.67	0.43
3:L8:60:G:O6	3:L8:96:C:O2'	2.31	0.43
10:LG:244:PRO:HA	10:LG:247:VAL:HG12	1.99	0.43
12:LI:54:SER:HB3	12:LI:135:ILE:HD11	2.00	0.43
22:LT:114:GLN:HG2	22:LT:117:LYS:HZ3	1.83	0.43
48:S6:50:A:H2	48:S6:64:U:H3	1.66	0.43
74:SN:75:LEU:HD12	74:SN:80:LEU:HG	1.99	0.43
1:L5:4043:G:H3'	1:L5:4045:G:H1'	1.99	0.43
21:LS:88:SER:OG	21:LS:89:GLY:N	2.51	0.43
47:S2:118:C:H1'	47:S2:445:A:C5	2.54	0.43
60:SR:92:ASP:N	60:SR:92:ASP:OD1	2.52	0.43
1:L5:67:C:OP2	1:L5:312:G:N2	2.50	0.43
1:L5:4633:G:N2	1:L5:4664:A:N7	2.67	0.43
3:L8:102:G:OP2	3:L8:104:A:O2'	2.32	0.43
8:LE:43:HIS:CD2	8:LE:44:CYS:H	2.37	0.43
12:LI:36:LEU:HD22	12:LI:69:ARG:HH21	1.83	0.43
1:L5:2820:C:H5''	20:LR:56:THR:HG23	1.99	0.43
47:S2:1357:A:OP1	70:SC:125:LYS:NZ	2.50	0.43
47:S2:690:G:OP2	47:S2:690:G:N2	2.48	0.43
47:S2:428:U:H4'	72:SJ:2:PRO:HD2	2.00	0.43
57:SL:77:VAL:O	57:SL:123:GLY:N	2.47	0.43
78:SZ:54:THR:O	78:SZ:58:LEU:N	2.51	0.43
1:L5:4736:C:H2'	1:L5:4737:G:C8	2.54	0.43
1:L5:4881:U:C4	15:LM:113:MET:HG2	2.54	0.43
1:L5:490:C:H1'	1:L5:666:G:H1	1.82	0.43
16:LN:80:THR:OG1	16:LN:80:THR:O	2.36	0.43
47:S2:1452:A:O2'	47:S2:1475:G:N2	2.52	0.43
48:S6:8:G:H1	48:S6:66:C:H42	1.66	0.43
51:SD:141:LYS:HD3	51:SD:180:GLY:HA3	2.01	0.43
1:L5:1305:C:OP1	3:L8:7:U:O2'	2.37	0.43
1:L5:2017:A:H5''	1:L5:2018:C:H5	1.84	0.43
1:L5:4700:A:N1	11:LH:72:THR:HG21	2.34	0.43
2:L7:52:C:H4'	13:LJ:11:PRO:HG3	2.01	0.43
3:L8:114:G:H1	3:L8:136:U:H3	1.65	0.43
5:LB:57:VAL:HB	5:LB:367:PHE:HB3	2.00	0.43
8:LE:277:LEU:HA	8:LE:281:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LJ:92:TYR:HB3	13:LJ:172:GLY:HA2	2.00	0.43
24:LV:94:VAL:HG21	25:LW:20:ARG:HE	1.83	0.43
47:S2:1679:A:H2'	53:SF:60:ARG:HD2	2.00	0.43
47:S2:77:A:O2'	71:SG:174:PRO:O	2.31	0.43
1:L5:2561:C:N4	1:L5:2562:G:O6	2.52	0.43
1:L5:4676:G:OP1	5:LB:281:ASN:ND2	2.52	0.43
3:L8:105:C:H4'	3:L8:106:G:H5''	2.01	0.43
14:LL:125:ILE:HD12	14:LL:142:GLU:HB3	2.00	0.43
47:S2:1591:C:H5'	53:SF:85:LYS:HE3	1.99	0.43
47:S2:1759:G:N2	47:S2:1773:C:OP1	2.51	0.43
53:SF:41:VAL:HG23	53:SF:42:LYS:HG3	1.99	0.43
71:SG:5:ILE:HG13	71:SG:111:LEU:HB2	2.00	0.43
47:S2:377:G:H5'	55:SI:98:LYS:HB3	2.01	0.43
1:L5:3667:C:H4'	4:LA:8:GLN:HA	2.01	0.43
7:LD:191:ASN:HB3	7:LD:194:VAL:HG12	2.00	0.43
10:LG:231:ASP:O	10:LG:235:ARG:NE	2.52	0.43
1:L5:4301:U:H4'	22:LT:54:HIS:CD2	2.54	0.43
47:S2:67:C:H2'	71:SG:164:LYS:HD3	1.99	0.43
1:L5:3892:U:H4'	18:LP:80:GLN:HE22	1.84	0.42
2:L7:55:A:O2'	13:LJ:151:ILE:O	2.28	0.42
17:LO:194:GLU:O	17:LO:198:THR:OG1	2.27	0.42
61:SS:48:ALA:HB2	61:SS:70:ILE:HD12	2.00	0.42
65:SX:94:ILE:HG12	65:SX:125:VAL:HG21	2.00	0.42
6:LC:340:ILE:HG21	8:LE:50:LEU:HD13	2.00	0.42
13:LJ:108:GLY:HA2	13:LJ:129:ASP:HA	2.02	0.42
1:L5:2072:C:OP1	19:LQ:2:GLY:N	2.52	0.42
71:SG:181:THR:HB	71:SG:184:VAL:HG23	2.01	0.42
47:S2:165:G:H4'	71:SG:53:SER:HB3	2.02	0.42
61:SS:49:ASP:OD1	61:SS:66:ARG:NH2	2.52	0.42
76:SW:30:CYS:N	76:SW:59:GLY:O	2.51	0.42
1:L5:1590:C:H4'	1:L5:2857:A:H5'	2.01	0.42
1:L5:4891:G:H1	1:L5:4928:C:H5	1.67	0.42
16:LN:135:ILE:HD12	16:LN:151:ILE:HD13	2.00	0.42
23:LU:47:ILE:HG21	23:LU:56:LEU:HD23	2.01	0.42
58:SP:111:MET:HB3	61:SS:117:ILE:HG21	2.01	0.42
61:SS:24:ARG:HB2	61:SS:29:ALA:HB2	2.01	0.42
1:L5:1408:G:O2'	1:L5:1411:C:O2	2.35	0.42
1:L5:3707:U:H2'	1:L5:3708:C:C6	2.54	0.42
9:LF:129:SER:HA	9:LF:132:MET:HG2	2.02	0.42
10:LG:107:LYS:HA	10:LG:110:LYS:HB3	2.00	0.42
17:LO:74:ARG:HD3	17:LO:146:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:424:U:OP1	18:LP:34:GLN:NE2	2.52	0.42
47:S2:1754:G:C5	47:S2:1755:C:H1'	2.54	0.42
13:LJ:129:ASP:OD1	13:LJ:129:ASP:N	2.52	0.42
51:SD:137:VAL:HG22	51:SD:151:LYS:HB2	2.01	0.42
47:S2:1679:A:N6	53:SF:57:ALA:O	2.49	0.42
59:SQ:112:LEU:HD22	59:SQ:119:LEU:HD13	2.02	0.42
61:SS:58:GLU:N	61:SS:58:GLU:OE1	2.51	0.42
65:SX:95:GLU:OE2	65:SX:140:ARG:NH1	2.52	0.42
78:SZ:79:ILE:HG23	78:SZ:83:LEU:HB2	2.00	0.42
1:L5:4693:C:OP1	11:LH:64:ARG:NH2	2.52	0.42
5:LB:231:VAL:HG21	5:LB:251:VAL:HG23	2.01	0.42
1:L5:959:G:C8	8:LE:123:ARG:HG2	2.55	0.42
59:SQ:51:LEU:HB2	59:SQ:81:ILE:HG23	2.01	0.42
59:SQ:132:PHE:HD2	63:SU:79:ARG:HH12	1.67	0.42
1:L5:1359:G:H4'	16:LN:203:TYR:HB2	2.02	0.42
1:L5:2520:C:H2'	1:L5:2521:G:C8	2.54	0.42
5:LB:86:VAL:HG13	5:LB:162:VAL:HG13	2.02	0.42
47:S2:1752:C:N4	47:S2:1777:G:O6	2.52	0.42
47:S2:346:C:H5''	52:SE:38:LEU:HD22	2.00	0.42
53:SF:138:ALA:HB2	53:SF:204:ARG:HA	2.01	0.42
71:SG:37:ALA:HA	71:SG:49:VAL:HG12	2.02	0.42
71:SG:64:LYS:NZ	71:SG:82:SER:OG	2.42	0.42
55:SI:76:THR:HG21	55:SI:104:ILE:HD12	2.01	0.42
75:SO:95:ILE:HB	75:SO:129:ILE:HA	2.00	0.42
47:S2:571:U:H5''	77:SY:37:LYS:HG3	2.01	0.42
1:L5:280:G:H5''	16:LN:14:LYS:HE2	2.02	0.42
4:LA:54:ARG:HH22	4:LA:128:ARG:HH11	1.67	0.42
8:LE:179:LEU:HB2	8:LE:250:GLN:NE2	2.35	0.42
56:SK:1:MET:HG3	56:SK:3:MET:HG3	2.02	0.42
1:L5:2378:G:N2	1:L5:2381:A:OP2	2.50	0.42
1:L5:280:G:OP2	16:LN:44:ARG:NH2	2.49	0.42
5:LB:115:LYS:HA	5:LB:118:PHE:HD2	1.84	0.42
6:LC:228:THR:OG1	6:LC:248:ARG:NH2	2.49	0.42
1:L5:945:U:O2	6:LC:343:GLN:NE2	2.49	0.42
7:LD:240:TYR:HB3	7:LD:244:HIS:CE1	2.55	0.42
10:LG:156:VAL:HG13	10:LG:184:ILE:HG13	2.02	0.42
28:LZ:29:ILE:HG22	28:LZ:32:GLY:H	1.84	0.42
47:S2:894:G:H8	47:S2:895:G:C8	2.37	0.42
71:SG:121:ILE:HD12	71:SG:124:LEU:HD22	2.00	0.42
1:L5:387:G:HO2'	1:L5:412:G:H1	1.66	0.42
1:L5:4251:A:H5''	13:LJ:108:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4571:A2M:H2'	1:L5:4572:U:H6	1.85	0.42
1:L5:4669:A:N3	1:L5:4671:B8T:O2'	2.53	0.42
6:LC:284:MET:HB2	19:LQ:28:LEU:HD23	2.02	0.42
1:L5:4691:A:O2'	11:LH:68:ALA:O	2.38	0.42
1:L5:4875:G:H2'	21:LS:169:THR:HG22	2.01	0.42
47:S2:1242:U:O2	47:S2:1517:G:O2'	2.28	0.42
47:S2:848:U:H2'	47:S2:849:A:H8	1.85	0.42
49:SA:205:ARG:NE	49:SA:210:ILE:HG12	2.35	0.42
55:SI:81:VAL:HG22	55:SI:102:VAL:HG12	2.01	0.42
47:S2:1016:U:H5'	74:SN:14:SER:HB3	2.01	0.42
65:SX:77:ASN:O	65:SX:79:LYS:N	2.51	0.42
1:L5:2405:G:O2'	1:L5:2791:C:O2'	2.32	0.41
1:L5:3938:G:OP2	16:LN:24:ARG:NE	2.53	0.41
1:L5:4097:G:N2	1:L5:4113:U:O4'	2.53	0.41
1:L5:4169:G:H4'	1:L5:4171:C:C2	2.54	0.41
1:L5:4670:C:O2'	1:L5:4672:A:OP2	2.34	0.41
4:LA:28:ARG:HD2	4:LA:123:ARG:HD2	2.02	0.41
5:LB:50:LYS:HB2	5:LB:345:LEU:HD11	2.02	0.41
7:LD:103:LEU:HD22	7:LD:244:HIS:HD2	1.85	0.41
1:L5:2796:G:H5'	14:LL:45:ARG:HH11	78.28	0.41
25:LW:46:PRO:HG2	25:LW:54:LEU:HD23	2.01	0.41
47:S2:520:A:O2'	47:S2:825:A:N3	2.44	0.41
51:SD:169:ASP:OD1	51:SD:169:ASP:N	2.53	0.41
55:SI:57:ALA:HB2	55:SI:183:GLY:HA2	2.01	0.41
1:L5:510:U:H3	1:L5:649:A:H61	1.68	0.41
1:L5:495:C:O2	1:L5:659:G:N1	2.53	0.41
4:LA:2:GLY:HA2	4:LA:207:VAL:HG12	2.03	0.41
25:LW:20:ARG:HG2	25:LW:30:GLN:HG3	2.02	0.41
47:S2:179:C:H3'	47:S2:180:G:H8	1.84	0.41
49:SA:126:ASP:HB3	49:SA:129:ALA:HB3	2.01	0.41
71:SG:222:GLU:OE1	71:SG:225:GLN:NE2	2.53	0.41
64:SV:69:ILE:O	64:SV:73:ALA:N	2.51	0.41
65:SX:20:GLN:HA	65:SX:23:HIS:HD2	1.85	0.41
1:L5:1096:C:O2	1:L5:1200:G:N2	2.53	0.41
1:L5:1281:G:N1	8:LE:128:HIS:HB2	2.35	0.41
1:L5:2906:G:H2'	1:L5:2908:U:H1'	2.03	0.41
1:L5:1625:OMG:N1	1:L5:3918:G:OP1	2.46	0.41
1:L5:4935:C:H2'	1:L5:4936:G:C8	2.55	0.41
1:L5:729:2MG:N2	21:LS:66:GLN:O	2.53	0.41
5:LB:302:ASN:O	5:LB:304:SER:N	2.50	0.41
10:LG:68:ALA:O	10:LG:72:LYS:NZ	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1171:G:O2'	47:S2:1187:G:O6	2.30	0.41
47:S2:1674:G:OP1	53:SF:51:HIS:NE2	2.41	0.41
47:S2:573:U:O2'	47:S2:575:A:N7	2.40	0.41
52:SE:41:CYS:HA	52:SE:85:GLY:HA2	2.03	0.41
65:SX:105:PHE:HB3	65:SX:112:VAL:HG21	2.02	0.41
1:L5:1072:C:H2'	1:L5:1073:G:C8	2.55	0.41
1:L5:167:C:H1'	1:L5:269:G:H22	1.85	0.41
5:LB:169:ARG:HD3	5:LB:170:LEU:HG	2.02	0.41
1:L5:4085:A:H5''	10:LG:56:LYS:HB2	2.02	0.41
18:LP:108:ASP:N	18:LP:108:ASP:OD1	2.52	0.41
24:LV:69:LYS:HA	24:LV:70:PRO:HD3	1.81	0.41
27:LY:23:SER:HA	27:LY:26:ARG:HB2	2.01	0.41
52:SE:138:HIS:CD2	52:SE:148:ARG:HG2	2.56	0.41
72:SJ:138[A]:ARG:H	72:SJ:138[A]:ARG:HG3	1.62	0.41
1:L5:1522:OMG:H2'	1:L5:1653:A:H61	1.85	0.41
1:L5:4524:G:C2	5:LB:252:ALA:HB1	2.55	0.41
5:LB:170:LEU:HB3	5:LB:328:ASN:HD21	1.85	0.41
6:LC:209:ILE:HB	6:LC:229:LEU:HD13	2.01	0.41
17:LO:55:LEU:HD23	17:LO:58:LEU:HD12	2.02	0.41
47:S2:399:C:O4'	65:SX:11:ARG:CZ	2.68	0.41
54:SH:7:LYS:NZ	54:SH:20:GLU:O	2.40	0.41
55:SI:130:THR:C	55:SI:134:GLU:H	2.13	0.41
55:SI:133:GLU:HA	55:SI:136:ILE:HB	2.02	0.41
56:SK:41:PRO:HD2	56:SK:44:HIS:HD2	1.86	0.41
62:ST:38:LYS:NZ	62:ST:43:LYS:O	2.40	0.41
78:SZ:74:SER:HA	78:SZ:79:ILE:HB	2.02	0.41
1:L5:206:U:O2'	1:L5:208:A:N7	2.44	0.41
1:L5:2749:C:H2'	1:L5:2750:G:C8	2.55	0.41
1:L5:3723:A2M:HM'3	1:L5:3723:A2M:H1'	1.89	0.41
1:L5:4309:G:H5'	1:L5:4338:G:H5''	2.02	0.41
4:LA:72:ARG:NH1	86:LA:401:HOH:O	2.41	0.41
6:LC:224:ILE:HB	6:LC:227:ILE:HD12	2.01	0.41
24:LV:111:GLU:HG3	24:LV:131:ARG:HD3	2.01	0.41
25:LW:123:LYS:NZ	47:S2:321:C:OP2	2.35	0.41
54:SH:37:LYS:HD3	54:SH:37:LYS:HA	1.92	0.41
1:L5:2394:G:O2'	1:L5:2819:U:O4	2.36	0.41
1:L5:3848:U:H2'	1:L5:3849:A:C8	2.55	0.41
1:L5:506:C:H42	1:L5:652:G:H1	1.68	0.41
1:L5:759:G:N2	1:L5:904:C:H2'	2.36	0.41
5:LB:233:SER:OG	5:LB:272:LYS:NZ	2.40	0.41
7:LD:279:ARG:HG2	7:LD:283:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LP:4:TYR:CZ	18:LP:16:LYS:HD3	2.55	0.41
26:LX:73:HIS:HB3	26:LX:116:LEU:HD23	2.02	0.41
47:S2:1232:U:H2'	47:S2:1233:G:C8	2.55	0.41
70:SC:272:HIS:HA	70:SC:275:LYS:HE3	2.01	0.41
54:SH:75:ILE:HG22	54:SH:78:ARG:HH11	1.85	0.41
78:SZ:49:LEU:H	78:SZ:83:LEU:HD11	1.86	0.41
17:LO:51:LYS:HE2	17:LO:55:LEU:HD11	2.03	0.41
17:LO:7:LEU:HB2	17:LO:31:ARG:HH21	1.86	0.41
28:LZ:47:ASP:OD2	28:LZ:69:LYS:NZ	2.39	0.41
48:S6:6:G:H2'	48:S6:7:A:H8	1.84	0.41
51:SD:162:ASP:OD1	51:SD:165:ASN:ND2	2.48	0.41
1:L5:1601:A:OP2	1:L5:3643:A:N6	2.53	0.41
1:L5:3861:A:H2'	1:L5:3862:A:C8	2.56	0.41
47:S2:1265:A:H2	47:S2:1517:G:H22	1.69	0.41
47:S2:1779:G:H2'	47:S2:1780:G:H8	1.86	0.41
47:S2:444:G:N1	47:S2:447:A:OP2	2.51	0.41
52:SE:166:THR:HG22	52:SE:168:LYS:HD3	2.03	0.41
53:SF:82:ASN:OD1	53:SF:82:ASN:N	2.53	0.41
71:SG:142:ARG:HB2	71:SG:147:LEU:HB2	2.03	0.41
55:SI:162:LEU:HD12	55:SI:165:GLN:HE21	1.86	0.41
56:SK:32:HIS:HD2	56:SK:45:VAL:HG11	1.85	0.41
56:SK:94:LEU:HA	56:SK:94:LEU:HD23	1.93	0.41
74:SN:20:ARG:HH21	76:SW:56:HIS:HB3	1.85	0.41
65:SX:17:ARG:HA	65:SX:17:ARG:HD3	1.84	0.41
1:L5:4420:U:O4	1:L5:4475:G:N2	2.54	0.41
1:L5:679:C:H2'	1:L5:680:G:C8	2.56	0.41
1:L5:3682:A:H5''	4:LA:132:ASN:ND2	2.36	0.41
1:L5:3746:A:H5''	4:LA:244:GLY:HA3	2.03	0.41
1:L5:4305:G:C6	22:LT:80:VAL:HG11	2.56	0.41
47:S2:159:A2M:H2	47:S2:468:A:O4'	2.21	0.41
47:S2:1759:G:O2'	47:S2:1773:C:O2'	2.33	0.41
70:SC:78:LEU:HD23	70:SC:81:ILE:HD12	2.03	0.41
54:SH:25:GLN:HA	54:SH:28:LEU:HB3	2.02	0.41
55:SI:130:THR:HG23	55:SI:131:PRO:CD	2.50	0.41
1:L5:2871:A:H62	1:L5:2878:G:H21	1.68	0.41
1:L5:512:U:H2'	1:L5:513:U:H4'	2.03	0.41
7:LD:60:ILE:H	7:LD:80:ALA:HB3	1.85	0.41
13:LJ:57:VAL:HG22	13:LJ:62:ILE:HG12	2.03	0.41
14:LL:16:LYS:HG2	14:LL:19:GLN:HE21	12.19	0.41
1:L5:4148:C:P	28:LZ:59:LYS:HZ1	2.44	0.41
49:SA:215:GLN:HA	49:SA:218:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SC:217:ALA:HB3	70:SC:219:ILE:HG12	2.03	0.41
64:SV:16:LYS:NZ	70:SC:257:LYS:O	2.33	0.41
1:L5:367:C:O2'	6:LC:83:GLY:O	2.32	0.40
8:LE:149:ILE:HD12	8:LE:199:THR:HB	2.03	0.40
8:LE:264:ILE:HA	8:LE:265:PRO:HD3	1.93	0.40
1:L5:2808:G:O3'	20:LR:60:ARG:NH1	2.53	0.40
21:LS:45:TRP:HA	21:LS:48:VAL:HG12	2.02	0.40
47:S2:1037:G:H4'	47:S2:1845:A:H4'	2.02	0.40
47:S2:116:OMU:HM22	47:S2:117:C:H5'	2.02	0.40
47:S2:525:A:H2'	47:S2:526:A:C8	2.56	0.40
47:S2:71:G:O6	71:SG:170:ARG:NH1	2.54	0.40
47:S2:839:C:H41	77:SY:10:ARG:HA	1.87	0.40
47:S2:923:G:H2'	47:S2:924:G:C8	2.56	0.40
48:S6:8:G:N2	48:S6:67:U:O2	2.54	0.40
51:SD:101:GLN:HG3	51:SD:126:ILE:HD11	2.03	0.40
71:SG:49:VAL:HG22	71:SG:115:LYS:HB3	2.03	0.40
59:SQ:31:LEU:HD11	59:SQ:33:LYS:HE3	2.03	0.40
63:SU:24:LEU:HB3	63:SU:32:LEU:HD11	2.03	0.40
1:L5:1794:A:H5''	1:L5:4214:A:H61	1.86	0.40
4:LA:116:LEU:HD23	4:LA:164:ALA:HB2	2.03	0.40
6:LC:24:LEU:HD12	6:LC:25:PRO:HD2	2.02	0.40
18:LP:84:PRO:HB2	18:LP:87:SER:HB2	2.03	0.40
47:S2:1745:A:N6	47:S2:1789:G:O2'	2.55	0.40
70:SC:64:THR:HG23	70:SC:67:GLY:H	1.85	0.40
47:S2:318:A:N6	71:SG:186:GLN:HE22	2.19	0.40
61:SS:38:ARG:HB3	62:ST:45:LEU:HD21	2.02	0.40
1:L5:3610:A:H2'	1:L5:3611:A:C8	2.57	0.40
1:L5:4044:U:OP1	1:L5:4045:G:O2'	2.37	0.40
1:L5:4281:A:H2'	1:L5:4282:A:H2'	2.03	0.40
5:LB:57:VAL:HG22	5:LB:73:VAL:HG22	2.04	0.40
10:LG:86:ALA:HA	10:LG:183:ILE:HB	2.03	0.40
14:LL:130:LYS:HD2	14:LL:131:PRO:HD2	2.03	0.40
14:LL:71:ARG:HA	14:LL:157:VAL:HG11	2.03	0.40
16:LN:200:LEU:HD22	16:LN:204:ARG:NH1	2.37	0.40
21:LS:17:LEU:HA	21:LS:18:PRO:HD3	1.88	0.40
50:SB:168:MET:HG2	50:SB:197:ILE:HG21	2.02	0.40
52:SE:45:ILE:HD12	52:SE:80:ILE:HD12	2.02	0.40
74:SN:91:LEU:HD11	74:SN:121:ARG:HE	1.85	0.40
62:ST:2:PRO:HA	62:ST:3:GLY:HA3	1.84	0.40
78:SZ:77:LEU:HB2	78:SZ:79:ILE:HD12	2.03	0.40
1:L5:1322:1MA:O2'	1:L5:1324:A:OP2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1999:A:O2'	1:L5:2018:C:O2'	2.37	0.40
6:LC:12:SER:OG	6:LC:13:GLU:N	2.54	0.40
7:LD:76:CYS:SG	7:LD:77:ALA:N	2.94	0.40
10:LG:160:ASP:OD1	10:LG:160:ASP:N	2.53	0.40
12:LI:68:ALA:HB2	12:LI:158:LYS:HB2	2.03	0.40
14:LL:19:GLN:HA	14:LL:22:VAL:HG23	2.04	0.40
15:LM:134:ALA:O	15:LM:137:LYS:NZ	2.52	0.40
19:LQ:72:LEU:HA	19:LQ:73:PRO:HD3	1.97	0.40
21:LS:81:TRP:HZ3	21:LS:130:GLU:HG2	1.87	0.40
47:S2:942:G:OP1	50:SB:136:ARG:NH2	2.52	0.40
50:SB:69:VAL:HG13	50:SB:74:LEU:HD22	2.04	0.40
47:S2:13:C:H5'	70:SC:235:ASN:HD21	1.85	0.40
72:SJ:79:ARG:HH12	72:SJ:83:ARG:HH21	1.70	0.40
1:L5:223:G:H4'	1:L5:225:G:N7	2.37	0.40
1:L5:2708:U:H4'	1:L5:2709:C:H5"	2.04	0.40
1:L5:3736:A:H2'	1:L5:3737:A:C8	2.55	0.40
5:LB:315:ASN:ND2	5:LB:326:VAL:H	2.13	0.40
8:LE:258:LEU:HD23	8:LE:262:LYS:HE2	2.03	0.40
17:LO:54:TYR:HD2	17:LO:145:VAL:HG21	1.87	0.40
1:L5:1913:C:O2'	17:LO:87:MET:O	2.33	0.40
1:L5:2527:A:P	20:LR:38:ARG:HH22	2.45	0.40
25:LW:77:LYS:HB3	25:LW:79:GLN:HE22	1.86	0.40
47:S2:1412:C:H42	47:S2:1429:G:H1	1.69	0.40
52:SE:44:LEU:HD13	52:SE:72:ILE:HD11	2.03	0.40
55:SI:128:LYS:HB3	55:SI:128:LYS:HE2	1.79	0.40
53:SF:87:LEU:HD11	59:SQ:47:LEU:HD11	2.04	0.40
49:SA:205:ARG:NH1	60:SR:84:TYR:HB3	2.37	0.40
64:SV:15:ARG:HH12	64:SV:33:GLN:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	221 (90%)	25 (10%)	0	100	100
5	LB	401/403 (100%)	377 (94%)	23 (6%)	1 (0%)	51	82
6	LC	365/427 (86%)	335 (92%)	29 (8%)	1 (0%)	44	77
7	LD	291/297 (98%)	269 (92%)	22 (8%)	0	100	100
8	LE	232/288 (81%)	204 (88%)	28 (12%)	0	100	100
9	LF	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
10	LG	240/266 (90%)	215 (90%)	24 (10%)	1 (0%)	38	72
11	LH	188/192 (98%)	171 (91%)	17 (9%)	0	100	100
12	LI	211/214 (99%)	186 (88%)	24 (11%)	1 (0%)	32	68
13	LJ	174/178 (98%)	154 (88%)	20 (12%)	0	100	100
14	LL	208/211 (99%)	182 (88%)	26 (12%)	0	100	100
15	LM	137/215 (64%)	123 (90%)	13 (10%)	1 (1%)	25	60
16	LN	201/204 (98%)	185 (92%)	13 (6%)	3 (2%)	12	39
17	LO	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
18	LP	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
19	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
20	LR	185/196 (94%)	175 (95%)	10 (5%)	0	100	100
21	LS	173/176 (98%)	161 (93%)	12 (7%)	0	100	100
22	LT	157/160 (98%)	144 (92%)	13 (8%)	0	100	100
23	LU	99/128 (77%)	85 (86%)	14 (14%)	0	100	100
24	LV	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
25	LW	122/157 (78%)	107 (88%)	15 (12%)	0	100	100
26	LX	118/156 (76%)	108 (92%)	10 (8%)	0	100	100
27	LY	132/145 (91%)	125 (95%)	6 (4%)	1 (1%)	22	57
28	LZ	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
29	La	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
30	Lb	105/159 (66%)	91 (87%)	14 (13%)	0	100	100
31	Lc	96/115 (84%)	82 (85%)	14 (15%)	0	100	100
32	Ld	105/125 (84%)	96 (91%)	9 (9%)	0	100	100
33	Le	126/135 (93%)	116 (92%)	9 (7%)	1 (1%)	22	57
34	Lf	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	9	33
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
38	Lj	84/97 (87%)	75 (89%)	8 (10%)	1 (1%)	15	46
39	Lk	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
40	Ll	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
44	Lp	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
46	Lz	215/217 (99%)	154 (72%)	61 (28%)	0	100	100
49	SA	219/295 (74%)	192 (88%)	26 (12%)	1 (0%)	32	68
50	SB	212/264 (80%)	198 (93%)	14 (7%)	0	100	100
51	SD	225/243 (93%)	198 (88%)	27 (12%)	0	100	100
52	SE	260/263 (99%)	241 (93%)	19 (7%)	0	100	100
53	SF	187/204 (92%)	167 (89%)	20 (11%)	0	100	100
54	SH	182/194 (94%)	159 (87%)	23 (13%)	0	100	100
55	SI	204/208 (98%)	189 (93%)	14 (7%)	1 (0%)	32	68
56	SK	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
57	SL	151/158 (96%)	134 (89%)	17 (11%)	0	100	100
58	SP	125/145 (86%)	112 (90%)	12 (10%)	1 (1%)	22	57
59	SQ	142/146 (97%)	124 (87%)	16 (11%)	2 (1%)	13	41
60	SR	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
61	SS	143/152 (94%)	127 (89%)	16 (11%)	0	100	100
62	ST	141/145 (97%)	128 (91%)	12 (8%)	1 (1%)	25	60
63	SU	102/119 (86%)	90 (88%)	12 (12%)	0	100	100
64	SV	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	6	25
65	SX	139/143 (97%)	125 (90%)	12 (9%)	2 (1%)	13	41
66	Sa	101/115 (88%)	89 (88%)	11 (11%)	1 (1%)	18	51
67	Sc	62/69 (90%)	45 (73%)	16 (26%)	1 (2%)	11	37
68	Sd	53/56 (95%)	50 (94%)	2 (4%)	1 (2%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Sg	311/317 (98%)	264 (85%)	46 (15%)	1 (0%)	44	77
70	SC	221/293 (75%)	198 (90%)	22 (10%)	1 (0%)	32	68
71	SG	235/249 (94%)	219 (93%)	16 (7%)	0	100	100
72	SJ	184/194 (95%)	165 (90%)	18 (10%)	1 (0%)	32	68
73	SM	120/132 (91%)	108 (90%)	12 (10%)	0	100	100
74	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
75	SO	138/151 (91%)	122 (88%)	16 (12%)	0	100	100
76	SW	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
77	SY	130/133 (98%)	121 (93%)	9 (7%)	0	100	100
78	SZ	73/125 (58%)	61 (84%)	11 (15%)	1 (1%)	13	41
79	Sb	81/84 (96%)	69 (85%)	12 (15%)	0	100	100
80	Se	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
81	Sf	65/156 (42%)	47 (72%)	18 (28%)	0	100	100
All	All	11565/12905 (90%)	10453 (90%)	1082 (9%)	30 (0%)	48	77

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
65	SX	127	ASN
15	LM	88	ALA
59	SQ	44	PRO
62	ST	41	LYS
64	SV	81	LYS
67	Sc	64	GLU
68	Sd	14	PHE
70	SC	78	LEU
5	LB	303	ALA
34	Lf	107	PRO
59	SQ	43	GLU
65	SX	126	ALA
66	Sa	47	ALA
49	SA	12	GLU
55	SI	139	LYS
58	SP	128	HIS
72	SJ	123	ILE
78	SZ	47	LEU

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Mol	Chain	Res	Type
10	LG	130	THR
34	Lf	80	ASN
27	LY	72	GLN
64	SV	79	VAL
69	Sg	246	TYR
16	LN	83	LYS
16	LN	84	PRO
12	LI	15	LYS
33	Le	73	GLY
6	LC	232	VAL
38	Lj	40	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	183 (96%)	7 (4%)	39	74
5	LB	349/349 (100%)	344 (99%)	5 (1%)	71	91
6	LC	305/347 (88%)	297 (97%)	8 (3%)	51	83
7	LD	246/250 (98%)	241 (98%)	5 (2%)	60	87
8	LE	209/252 (83%)	207 (99%)	2 (1%)	80	95
9	LF	195/215 (91%)	192 (98%)	3 (2%)	70	91
10	LG	204/223 (92%)	195 (96%)	9 (4%)	33	67
11	LH	169/171 (99%)	167 (99%)	2 (1%)	75	93
12	LI	180/181 (99%)	177 (98%)	3 (2%)	66	89
13	LJ	148/149 (99%)	144 (97%)	4 (3%)	50	82
14	LL	176/177 (99%)	171 (97%)	5 (3%)	49	82
15	LM	118/161 (73%)	117 (99%)	1 (1%)	85	96
16	LN	171/172 (99%)	169 (99%)	2 (1%)	75	93
17	LO	173/174 (99%)	168 (97%)	5 (3%)	48	81
18	LP	134/163 (82%)	133 (99%)	1 (1%)	87	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LQ	164/165 (99%)	161 (98%)	3 (2%)	64	89
20	LR	166/175 (95%)	163 (98%)	3 (2%)	64	89
21	LS	156/157 (99%)	155 (99%)	1 (1%)	89	97
22	LT	139/140 (99%)	137 (99%)	2 (1%)	71	91
23	LU	91/115 (79%)	90 (99%)	1 (1%)	78	94
24	LV	101/107 (94%)	99 (98%)	2 (2%)	60	87
25	LW	103/126 (82%)	101 (98%)	2 (2%)	62	88
26	LX	108/133 (81%)	108 (100%)	0	100	100
27	LY	124/135 (92%)	120 (97%)	4 (3%)	44	78
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	117 (98%)	3 (2%)	53	83
30	Lb	88/126 (70%)	85 (97%)	3 (3%)	42	76
31	Lc	83/97 (86%)	82 (99%)	1 (1%)	75	93
32	Ld	98/110 (89%)	97 (99%)	1 (1%)	80	95
33	Le	114/121 (94%)	113 (99%)	1 (1%)	82	95
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	78	94
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	80	95
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	82	95
37	Li	86/89 (97%)	84 (98%)	2 (2%)	56	85
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	71	91
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	45 (96%)	2 (4%)	33	68
41	Lm	47/115 (41%)	47 (100%)	0	100	100
42	Ln	23/24 (96%)	22 (96%)	1 (4%)	33	68
43	Lo	94/94 (100%)	94 (100%)	0	100	100
44	Lp	74/75 (99%)	72 (97%)	2 (3%)	50	82
45	Lr	109/121 (90%)	108 (99%)	1 (1%)	82	95
46	Lz	195/196 (100%)	188 (96%)	7 (4%)	40	75
49	SA	183/243 (75%)	181 (99%)	2 (1%)	78	94
50	SB	195/231 (84%)	194 (100%)	1 (0%)	91	97
51	SD	190/202 (94%)	187 (98%)	3 (2%)	68	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	SE	224/225 (100%)	223 (100%)	1 (0%)	93	98
53	SF	159/170 (94%)	155 (98%)	4 (2%)	53	83
54	SH	166/174 (95%)	163 (98%)	3 (2%)	64	89
55	SI	178/180 (99%)	173 (97%)	5 (3%)	49	82
56	SK	89/136 (65%)	88 (99%)	1 (1%)	78	94
57	SL	137/142 (96%)	133 (97%)	4 (3%)	48	81
58	SP	113/130 (87%)	113 (100%)	0	100	100
59	SQ	121/121 (100%)	120 (99%)	1 (1%)	85	96
60	SR	122/122 (100%)	122 (100%)	0	100	100
61	SS	126/132 (96%)	124 (98%)	2 (2%)	68	90
62	ST	113/115 (98%)	112 (99%)	1 (1%)	82	95
63	SU	94/107 (88%)	93 (99%)	1 (1%)	78	94
64	SV	67/67 (100%)	66 (98%)	1 (2%)	70	91
65	SX	113/115 (98%)	112 (99%)	1 (1%)	82	95
66	Sa	90/98 (92%)	87 (97%)	3 (3%)	43	77
67	Sc	57/62 (92%)	57 (100%)	0	100	100
68	Sd	48/49 (98%)	47 (98%)	1 (2%)	59	86
69	Sg	272/275 (99%)	268 (98%)	4 (2%)	70	91
70	SC	189/225 (84%)	188 (100%)	1 (0%)	91	97
71	SG	207/218 (95%)	203 (98%)	4 (2%)	62	88
72	SJ	162/168 (96%)	158 (98%)	4 (2%)	53	83
73	SM	102/108 (94%)	94 (92%)	8 (8%)	15	39
74	SN	130/131 (99%)	127 (98%)	3 (2%)	56	85
75	SO	110/119 (92%)	107 (97%)	3 (3%)	50	82
76	SW	112/113 (99%)	110 (98%)	2 (2%)	64	89
77	SY	114/115 (99%)	113 (99%)	1 (1%)	82	95
78	SZ	66/103 (64%)	64 (97%)	2 (3%)	46	80
79	Sb	75/76 (99%)	75 (100%)	0	100	100
80	Se	47/48 (98%)	46 (98%)	1 (2%)	59	86
81	Sf	60/140 (43%)	58 (97%)	2 (3%)	43	77
All	All	10077/10995 (92%)	9899 (98%)	178 (2%)	68	89

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	6	ARG
4	LA	15	VAL
4	LA	64	ARG
4	LA	68	ARG
4	LA	135	THR
4	LA	207	VAL
4	LA	247	ARG
5	LB	10	ARG
5	LB	169	ARG
5	LB	297	LYS
5	LB	341[A]	LYS
5	LB	341[B]	LYS
6	LC	95	MET
6	LC	188	ARG
6	LC	204	ARG
6	LC	222	ARG
6	LC	292	ILE
6	LC	312	ARG
6	LC	317	ASN
6	LC	329	ASN
7	LD	58	ARG
7	LD	85	LYS
7	LD	212	MET
7	LD	248	ARG
7	LD	250	ASN
8	LE	52	ARG
8	LE	56	ARG
9	LF	29	LYS
9	LF	119	ASN
9	LF	236	ARG
10	LG	35	ARG
10	LG	59	ARG
10	LG	62	ARG
10	LG	111	LYS
10	LG	137[A]	ARG
10	LG	137[B]	ARG
10	LG	175	ARG
10	LG	235	ARG
10	LG	259	LYS
11	LH	116	ASN
11	LH	156	ASN
12	LI	87	MET

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Mol	Chain	Res	Type
12	LI	101	LYS
12	LI	121	LYS
13	LJ	63	ARG
13	LJ	64	ARG
13	LJ	95	ARG
13	LJ	146	ARG
14	LL	6	ASN
14	LL	63	THR
14	LL	162	LYS
14	LL	167	ARG
14	LL	190	ARG
15	LM	63	LYS
16	LN	193	ARG
16	LN	204	ARG
17	LO	27	VAL
17	LO	60	LYS
17	LO	101	ARG
17	LO	145	VAL
17	LO	173	GLN
18	LP	4	TYR
19	LQ	14	ARG
19	LQ	104	ARG
19	LQ	178	ARG
20	LR	130	ASN
20	LR	170	ARG
20	LR	186	LYS
21	LS	83	ARG
22	LT	36	LYS
22	LT	114	GLN
23	LU	97	ARG
24	LV	15	ARG
24	LV	46	LYS
25	LW	43	LYS
25	LW	110	ARG
27	LY	4	ASN
27	LY	27	ARG
27	LY	79	VAL
27	LY	84	ARG
29	La	92	LYS
29	La	93	ASN
29	La	132	ARG
30	Lb	41	ARG

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Mol	Chain	Res	Type
30	Lb	60	ASN
30	Lb	68	ARG
31	Lc	106	ARG
32	Ld	26	THR
33	Le	43	ASN
34	Lf	80	ASN
35	Lg	54	ARG
36	Lh	7	ARG
37	Li	29	ARG
37	Li	56	ARG
38	Lj	22	CYS
40	Ll	36	ARG
40	Ll	46	ARG
42	Ln	22	GLN
44	Lp	49	ARG
44	Lp	84	ARG
45	Lr	41	ASN
46	Lz	35	GLN
46	Lz	40	ASN
46	Lz	48	ARG
46	Lz	85	MET
46	Lz	96	ASN
46	Lz	156	LYS
46	Lz	161	LYS
49	SA	10	MET
49	SA	50	ASN
50	SB	186	ASN
51	SD	1	MET
51	SD	76	ARG
51	SD	197	LYS
52	SE	198	ARG
53	SF	45	TYR
53	SF	83	ASN
53	SF	130	ARG
53	SF	164	ARG
54	SH	30	LEU
54	SH	57	ARG
54	SH	186	ASN
55	SI	67	TRP
55	SI	124	LYS
55	SI	128	LYS
55	SI	136	ILE

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Mol	Chain	Res	Type
55	SI	143	LYS
56	SK	95	ARG
57	SL	56	ILE
57	SL	65	ASN
57	SL	69	ARG
57	SL	89	ARG
59	SQ	1	MET
61	SS	1	MET
61	SS	17	ASN
62	ST	41	LYS
63	SU	41	ARG
64	SV	21	ASN
65	SX	32	LEU
66	Sa	42	ARG
66	Sa	85[A]	ARG
66	Sa	85[B]	ARG
68	Sd	26	ASN
69	Sg	30	MET
69	Sg	162	ASN
69	Sg	221	LEU
69	Sg	225	LYS
70	SC	121	ARG
71	SG	31	ARG
71	SG	98	ARG
71	SG	119	LYS
71	SG	224	ARG
72	SJ	17	ARG
72	SJ	79	ARG
72	SJ	121	LYS
72	SJ	169	ARG
73	SM	12	MET
73	SM	45	ARG
73	SM	49	LEU
73	SM	55	ASN
73	SM	68	LEU
73	SM	93	LYS
73	SM	96	ARG
73	SM	121	LYS
74	SN	75	LEU
74	SN	104	ARG
74	SN	133	ARG
75	SO	14	VAL

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Mol	Chain	Res	Type
75	SO	117	ARG
75	SO	142	ARG
76	SW	57	ARG
76	SW	103	VAL
77	SY	10	ARG
78	SZ	62	VAL
78	SZ	78	LYS
80	Se	8	ARG
81	Sf	91	ASN
81	Sf	95	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	132	ASN
5	LB	184	GLN
5	LB	186	ASN
6	LC	38	ASN
6	LC	317	ASN
6	LC	329	ASN
7	LD	195	HIS
7	LD	250	ASN
7	LD	282	GLN
8	LE	250	GLN
11	LH	7	ASN
11	LH	8	GLN
11	LH	42	ASN
11	LH	116	ASN
11	LH	156	ASN
14	LL	6	ASN
16	LN	182	HIS
16	LN	196	ASN
18	LP	21	ASN
18	LP	56	GLN
18	LP	80	GLN
18	LP	116	HIS
19	LQ	188	ASN
20	LR	7	GLN
20	LR	130	ASN
21	LS	77	ASN
25	LW	17	HIS
25	LW	48	GLN

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Mol	Chain	Res	Type
25	LW	79	GLN
26	LX	93	ASN
26	LX	125	ASN
27	LY	4	ASN
27	LY	14	ASN
29	La	66	ASN
29	La	93	ASN
30	Lb	19	ASN
32	Ld	79	ASN
33	Le	43	ASN
33	Le	117	GLN
34	Lf	56	ASN
44	Lp	56	HIS
45	Lr	6	GLN
45	Lr	41	ASN
45	Lr	100	ASN
46	Lz	35	GLN
46	Lz	40	ASN
46	Lz	72	GLN
46	Lz	96	ASN
46	Lz	184	HIS
49	SA	50	ASN
50	SB	186	ASN
51	SD	159	HIS
52	SE	98	ASN
52	SE	112	HIS
52	SE	214	ASN
53	SF	79	HIS
54	SH	91	HIS
54	SH	186	ASN
55	SI	88	ASN
55	SI	138	ASN
57	SL	65	ASN
58	SP	41	GLN
58	SP	103	ASN
59	SQ	80	GLN
59	SQ	86	GLN
61	SS	11	HIS
61	SS	17	ASN
63	SU	81	GLN
64	SV	21	ASN
65	SX	23	HIS

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Mol	Chain	Res	Type
68	Sd	26	ASN
69	Sg	14	HIS
69	Sg	64	HIS
69	Sg	117	ASN
69	Sg	162	ASN
70	SC	115	GLN
71	SG	13	GLN
71	SG	81	HIS
73	SM	19	GLN
73	SM	52	GLN
74	SN	5	HIS
76	SW	90	GLN
78	SZ	46	ASN
81	Sf	91	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3677/5070 (72%)	1083 (29%)	23 (0%)
2	L7	119/120 (99%)	16 (13%)	0
3	L8	155/156 (99%)	33 (21%)	1 (0%)
47	S2	1708/1869 (91%)	452 (26%)	7 (0%)
48	S6	74/75 (98%)	32 (43%)	1 (1%)
All	All	5733/7290 (78%)	1616 (28%)	32 (0%)

All (1616) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	4	G
1	L5	6	C
1	L5	17	A
1	L5	25	A
1	L5	26	C
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	58	G
1	L5	59	A

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Mol	Chain	Res	Type
1	L5	64	A
1	L5	65	A
1	L5	66	A
1	L5	67	C
1	L5	69	A
1	L5	72	C
1	L5	73	A
1	L5	74	G
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	106	A
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	117	C
1	L5	119	G
1	L5	120	A
1	L5	132	G
1	L5	133	C
1	L5	134	G
1	L5	135	G
1	L5	136	C
1	L5	137	G
1	L5	139	G
1	L5	141	C
1	L5	142	G
1	L5	143	C
1	L5	144	G
1	L5	152	U
1	L5	158	A
1	L5	159	C
1	L5	165	A
1	L5	172	C
1	L5	177	G
1	L5	180	C
1	L5	181	C
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	186	G
1	L5	188	G

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Mol	Chain	Res	Type
1	L5	189	G
1	L5	200	U
1	L5	207	G
1	L5	209	U
1	L5	210	C
1	L5	212	A
1	L5	216	C
1	L5	218	A
1	L5	219	G
1	L5	225	G
1	L5	233	U
1	L5	234	G
1	L5	255	C
1	L5	256	G
1	L5	259	C
1	L5	261	G
1	L5	262	G
1	L5	265	C
1	L5	269	G
1	L5	274	C
1	L5	276	C
1	L5	278	G
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	341	G
1	L5	344	A
1	L5	345	C
1	L5	349	A
1	L5	350	C
1	L5	363	A
1	L5	387	G
1	L5	388	A
1	L5	398	A2M
1	L5	407	A
1	L5	408	A
1	L5	409	G
1	L5	410	A
1	L5	411	G

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Mol	Chain	Res	Type
1	L5	412	G
1	L5	413	G
1	L5	415	G
1	L5	432	U
1	L5	440	U
1	L5	449	C
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	461	G
1	L5	465	G
1	L5	467	U
1	L5	473	C
1	L5	478	G
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	492	U
1	L5	493	G
1	L5	494	U
1	L5	496	G
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	504	G
1	L5	505	G
1	L5	509	A
1	L5	510	U
1	L5	511	C
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	516	C
1	L5	517	C

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Mol	Chain	Res	Type
1	L5	518	G
1	L5	519	C
1	L5	643	C
1	L5	644	G
1	L5	646	G
1	L5	653	U
1	L5	654	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	670	G
1	L5	673	C
1	L5	676	C
1	L5	685	C
1	L5	686	A
1	L5	687	U
1	L5	693	C
1	L5	696	C
1	L5	697	G
1	L5	703	G
1	L5	704	C
1	L5	708	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	740	G
1	L5	742	G
1	L5	746	A
1	L5	747	A
1	L5	753	C
1	L5	754	U
1	L5	757	G
1	L5	758	G
1	L5	760	G
1	L5	904	C
1	L5	905	C
1	L5	912	G
1	L5	913	U

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Mol	Chain	Res	Type
1	L5	914	U
1	L5	915	A
1	L5	916	C
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	934	C
1	L5	935	A
1	L5	936	C
1	L5	942	G
1	L5	943	A
1	L5	945	U
1	L5	946	C
1	L5	955	G
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	963	G
1	L5	964	A
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	969	C
1	L5	970	G
1	L5	971	U
1	L5	977	C
1	L5	982	U
1	L5	984	C
1	L5	988	C
1	L5	989	U
1	L5	990	C
1	L5	991	C
1	L5	992	C
1	L5	993	G
1	L5	995	C
1	L5	1048	G
1	L5	1051	G

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Mol	Chain	Res	Type
1	L5	1069	G
1	L5	1070	G
1	L5	1074	G
1	L5	1083	U
1	L5	1095	A
1	L5	1096	C
1	L5	1168	G
1	L5	1170	G
1	L5	1171	G
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1184	A
1	L5	1187	G
1	L5	1191	C
1	L5	1192	C
1	L5	1193	C
1	L5	1195	G
1	L5	1197	C
1	L5	1198	G
1	L5	1200	G
1	L5	1202	C
1	L5	1203	G
1	L5	1205	G
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1216	C
1	L5	1217	G
1	L5	1218	G
1	L5	1219	G
1	L5	1220	G
1	L5	1222	A
1	L5	1241	C
1	L5	1243	C
1	L5	1245	C
1	L5	1254	A

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Mol	Chain	Res	Type
1	L5	1255	A
1	L5	1260	G
1	L5	1261	G
1	L5	1266	G
1	L5	1267	C
1	L5	1269	G
1	L5	1270	A
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1274	A
1	L5	1275	G
1	L5	1277	G
1	L5	1279	A
1	L5	1280	C
1	L5	1284	G
1	L5	1287	G
1	L5	1293	G
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1302	U
1	L5	1303	A
1	L5	1312	A
1	L5	1313	C
1	L5	1324	A
1	L5	1326	A2M
1	L5	1337	A
1	L5	1344	C
1	L5	1353	G
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1360	G
1	L5	1365	C
1	L5	1367	C
1	L5	1376	C
1	L5	1378	C
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A

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Mol	Chain	Res	Type
1	L5	1399	G
1	L5	1402	C
1	L5	1403	G
1	L5	1405	C
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1416	G
1	L5	1417	C
1	L5	1420	A
1	L5	1435	G
1	L5	1439	C
1	L5	1440	U
1	L5	1441	C
1	L5	1442	C
1	L5	1444	G
1	L5	1446	C
1	L5	1453	G
1	L5	1457	G
1	L5	1472	C
1	L5	1482	G
1	L5	1483	C
1	L5	1486	C
1	L5	1493	G
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1513	U
1	L5	1515	A
1	L5	1518	A
1	L5	1525	A
1	L5	1534	A2M
1	L5	1547	A
1	L5	1549	G
1	L5	1550	G
1	L5	1566	C
1	L5	1571	G
1	L5	1578	U
1	L5	1582	PSU
1	L5	1586	G
1	L5	1591	U
1	L5	1596	U

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Mol	Chain	Res	Type
1	L5	1624	G
1	L5	1625	OMG
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1661	C
1	L5	1662	C
1	L5	1663	C
1	L5	1676	C
1	L5	1677	PSU
1	L5	1678	C
1	L5	1680	G
1	L5	1681	G
1	L5	1691	G
1	L5	1694	C
1	L5	1697	G
1	L5	1699	A
1	L5	1700	G
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G
1	L5	1707	C
1	L5	1716	G
1	L5	1719	A
1	L5	1726	U
1	L5	1729	A
1	L5	1734	G
1	L5	1740	C
1	L5	1742	A
1	L5	1743	A
1	L5	1750	G
1	L5	1753	G
1	L5	1755	C
1	L5	1756	U
1	L5	1757	U
1	L5	1758	G
1	L5	1760	G
1	L5	1761	G

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Mol	Chain	Res	Type
1	L5	1762	C
1	L5	1763	C
1	L5	1764	G
1	L5	1765	A
1	L5	1766	A
1	L5	1768	C
1	L5	1769	G
1	L5	1770	A
1	L5	1775	A
1	L5	1787	A
1	L5	1803	G
1	L5	1804	A
1	L5	1810	G
1	L5	1819	G
1	L5	1821	G
1	L5	1822	U
1	L5	1823	G
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1852	U
1	L5	1855	G
1	L5	1865	G
1	L5	1866	UR3
1	L5	1869	G
1	L5	1876	U
1	L5	1881	C
1	L5	1882	U
1	L5	1889	U
1	L5	1890	G
1	L5	1892	A
1	L5	1897	A
1	L5	1898	C
1	L5	1917	A
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1930	U

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Mol	Chain	Res	Type
1	L5	1931	C
1	L5	1932	A
1	L5	1935	C
1	L5	1936	C
1	L5	1940	G
1	L5	1945	G
1	L5	1947	U
1	L5	1948	G
1	L5	1951	G
1	L5	1953	U
1	L5	1954	U
1	L5	1959	U
1	L5	1960	A
1	L5	1961	G
1	L5	1962	A
1	L5	1965	G
1	L5	1966	C
1	L5	1968	G
1	L5	1969	G
1	L5	1971	C
1	L5	1974	U
1	L5	1975	G
1	L5	1976	G
1	L5	1977	C
1	L5	1980	U
1	L5	1981	G
1	L5	1982	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1987	C
1	L5	1988	G
1	L5	1989	G
1	L5	1991	A
1	L5	1995	G
1	L5	1996	C
1	L5	1997	U
1	L5	1998	A
1	L5	1999	A
1	L5	2001	G
1	L5	2002	A
1	L5	2003	G

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Mol	Chain	Res	Type
1	L5	2004	U
1	L5	2006	U
1	L5	2007	G
1	L5	2008	U
1	L5	2009	A
1	L5	2010	A
1	L5	2011	C
1	L5	2012	A
1	L5	2013	A
1	L5	2015	U
1	L5	2016	C
1	L5	2018	C
1	L5	2019	C
1	L5	2020	U
1	L5	2025	A
1	L5	2026	A
1	L5	2033	A
1	L5	2034	G
1	L5	2038	U
1	L5	2044	U
1	L5	2046	G
1	L5	2048	U
1	L5	2055	G
1	L5	2056	G
1	L5	2062	C
1	L5	2068	C
1	L5	2069	A
1	L5	2072	C
1	L5	2084	C
1	L5	2085	G
1	L5	2089	G
1	L5	2090	U
1	L5	2091	C
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2102	G
1	L5	2106	G

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Mol	Chain	Res	Type
1	L5	2107	C
1	L5	2110	C
1	L5	2111	G
1	L5	2112	G
1	L5	2252	G
1	L5	2253	A
1	L5	2256	C
1	L5	2257	C
1	L5	2258	C
1	L5	2259	G
1	L5	2260	C
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2306	G
1	L5	2313	A
1	L5	2316	G
1	L5	2331	G
1	L5	2332	A
1	L5	2333	G
1	L5	2337	C
1	L5	2338	C
1	L5	2345	G
1	L5	2346	C
1	L5	2348	G
1	L5	2351	C
1	L5	2352	U
1	L5	2357	G
1	L5	2360	A
1	L5	2370	A
1	L5	2382	A
1	L5	2389	A
1	L5	2395	A
1	L5	2396	A
1	L5	2397	G
1	L5	2408	U
1	L5	2416	G
1	L5	2417	A
1	L5	2418	A
1	L5	2421	G
1	L5	2422	OMC
1	L5	2425	U

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Mol	Chain	Res	Type
1	L5	2437	C
1	L5	2440	U
1	L5	2441	C
1	L5	2447	U
1	L5	2450	G
1	L5	2453	A
1	L5	2464	C
1	L5	2465	C
1	L5	2469	C
1	L5	2471	G
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2482	C
1	L5	2483	G
1	L5	2485	U
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U
1	L5	2491	C
1	L5	2493	G
1	L5	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2511	A
1	L5	2513	A
1	L5	2519	U
1	L5	2529	A
1	L5	2533	C
1	L5	2537	A
1	L5	2543	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G
1	L5	2554	U
1	L5	2556	G
1	L5	2559	G
1	L5	2564	G
1	L5	2566	G
1	L5	2573	A
1	L5	2583	C

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Mol	Chain	Res	Type
1	L5	2587	A
1	L5	2589	C
1	L5	2600	A
1	L5	2601	A
1	L5	2602	G
1	L5	2606	G
1	L5	2611	A
1	L5	2612	G
1	L5	2616	C
1	L5	2618	G
1	L5	2622	G
1	L5	2627	C
1	L5	2637	U
1	L5	2651	C
1	L5	2652	G
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2670	C
1	L5	2673	G
1	L5	2675	G
1	L5	2676	A
1	L5	2680	G
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G
1	L5	2707	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2712	G
1	L5	2721	G
1	L5	2724	G
1	L5	2726	G
1	L5	2732	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2756	G
1	L5	2761	U

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Mol	Chain	Res	Type
1	L5	2763	U
1	L5	2764	A
1	L5	2770	C
1	L5	2772	C
1	L5	2787	A
1	L5	2788	U
1	L5	2790	U
1	L5	2794	C
1	L5	2801	U
1	L5	2812	A
1	L5	2814	C
1	L5	2815	A
1	L5	2826	U
1	L5	2827	G
1	L5	2838	G
1	L5	2842	G
1	L5	2848	G
1	L5	2855	G
1	L5	2856	C
1	L5	2867	C
1	L5	2877	G
1	L5	2892	C
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G
1	L5	2904	U
1	L5	2905	C
1	L5	2906	G
1	L5	2907	G
1	L5	2908	U
1	L5	2910	G
1	L5	3585	G
1	L5	3586	G
1	L5	3587	C
1	L5	3588	C
1	L5	3589	G
1	L5	3590	G
1	L5	3591	C
1	L5	3593	C
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A

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Mol	Chain	Res	Type
1	L5	3597	G
1	L5	3598	C
1	L5	3602	C
1	L5	3604	A
1	L5	3605	C
1	L5	3606	U
1	L5	3615	G
1	L5	3616	U
1	L5	3618	C
1	L5	3619	G
1	L5	3626	G
1	L5	3630	A
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3648	A
1	L5	3650	C
1	L5	3662	A
1	L5	3663	A
1	L5	3673	C
1	L5	3674	G
1	L5	3680	U
1	L5	3691	G
1	L5	3692	A
1	L5	3710	G
1	L5	3711	A
1	L5	3713	U
1	L5	3714	G
1	L5	3726	A
1	L5	3727	A
1	L5	3729	PSU
1	L5	3734	U
1	L5	3735	G
1	L5	3736	A
1	L5	3748	A
1	L5	3750	G
1	L5	3753	G
1	L5	3754	G
1	L5	3758	U
1	L5	3759	A
1	L5	3760	A
1	L5	3764	PSU

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Mol	Chain	Res	Type
1	L5	3771	C
1	L5	3775	A
1	L5	3776	G
1	L5	3777	G
1	L5	3784	A
1	L5	3785	A2M
1	L5	3786	U
1	L5	3799	A
1	L5	3801	U
1	L5	3802	U
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3851	U
1	L5	3867	A2M
1	L5	3870	C
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3885	G
1	L5	3890	A
1	L5	3892	U
1	L5	3898	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3916	G
1	L5	3922	G
1	L5	3925	U
1	L5	3926	C
1	L5	3942	A
1	L5	3943	A
1	L5	3944	G
1	L5	3945	A

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Mol	Chain	Res	Type
1	L5	3947	A
1	L5	3949	A
1	L5	3950	U
1	L5	3951	G
1	L5	3952	A
1	L5	3953	G
1	L5	3955	G
1	L5	3956	G
1	L5	3957	U
1	L5	3958	G
1	L5	3960	A
1	L5	3961	G
1	L5	3962	A
1	L5	3963	A
1	L5	3964	U
1	L5	3965	A
1	L5	3966	A
1	L5	3967	G
1	L5	3968	U
1	L5	3969	G
1	L5	3970	G
1	L5	3971	G
1	L5	3972	A
1	L5	3973	G
1	L5	3974	G
1	L5	3975	C
1	L5	3977	C
1	L5	4034	G
1	L5	4035	G
1	L5	4036	G
1	L5	4039	G
1	L5	4041	C
1	L5	4042	G
1	L5	4043	G
1	L5	4044	U
1	L5	4045	G
1	L5	4046	A
1	L5	4047	A
1	L5	4048	A
1	L5	4049	U
1	L5	4051	C
1	L5	4052	C

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Mol	Chain	Res	Type
1	L5	4053	A
1	L5	4054	C
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C
1	L5	4058	U
1	L5	4059	C
1	L5	4060	U
1	L5	4061	G
1	L5	4062	A
1	L5	4064	C
1	L5	4065	G
1	L5	4066	U
1	L5	4067	U
1	L5	4068	U
1	L5	4069	U
1	L5	4076	G
1	L5	4086	G
1	L5	4088	C
1	L5	4091	G
1	L5	4096	C
1	L5	4099	G
1	L5	4100	C
1	L5	4101	C
1	L5	4102	C
1	L5	4104	G
1	L5	4107	G
1	L5	4108	G
1	L5	4109	G
1	L5	4110	C
1	L5	4113	U
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4119	C
1	L5	4121	G
1	L5	4122	G
1	L5	4127	A
1	L5	4132	C
1	L5	4133	C
1	L5	4134	C
1	L5	4135	G

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Mol	Chain	Res	Type
1	L5	4137	C
1	L5	4138	C
1	L5	4139	G
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4145	C
1	L5	4146	G
1	L5	4150	G
1	L5	4155	C
1	L5	4156	G
1	L5	4162	C
1	L5	4163	U
1	L5	4168	G
1	L5	4170	A
1	L5	4180	G
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4193	C
1	L5	4195	G
1	L5	4201	G
1	L5	4203	A
1	L5	4212	A
1	L5	4213	A
1	L5	4214	A
1	L5	4222	G
1	L5	4225	G
1	L5	4228	G
1	L5	4229	U
1	L5	4232	U
1	L5	4233	A
1	L5	4242	U
1	L5	4249	G
1	L5	4251	A
1	L5	4254	G
1	L5	4257	A
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A

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Mol	Chain	Res	Type
1	L5	4280	A
1	L5	4281	A
1	L5	4291	G
1	L5	4293	PSU
1	L5	4295	U
1	L5	4302	U
1	L5	4304	A
1	L5	4305	G
1	L5	4306	OMU
1	L5	4314	C
1	L5	4329	G
1	L5	4330	G
1	L5	4332	C
1	L5	4338	G
1	L5	4348	A
1	L5	4349	C
1	L5	4354	U
1	L5	4372	U
1	L5	4373	G
1	L5	4374	U
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A
1	L5	4380	A
1	L5	4381	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4400	G
1	L5	4415	1MA
1	L5	4416	G
1	L5	4420	U
1	L5	4422	A
1	L5	4427	G
1	L5	4437	U
1	L5	4444	C
1	L5	4448	G
1	L5	4449	A
1	L5	4450	PSU
1	L5	4452	U
1	L5	4453	C

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Mol	Chain	Res	Type
1	L5	4464	A
1	L5	4466	C
1	L5	4475	G
1	L5	4488	A
1	L5	4494	OMG
1	L5	4500	PSU
1	L5	4510	A
1	L5	4512	U
1	L5	4513	A
1	L5	4518	A
1	L5	4519	C
1	L5	4523	A2M
1	L5	4524	G
1	L5	4530	UR3
1	L5	4531	PSU
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4554	G
1	L5	4556	U
1	L5	4560	C
1	L5	4567	G
1	L5	4570	G
1	L5	4573	G
1	L5	4575	G
1	L5	4584	A
1	L5	4589	A
1	L5	4590	A
1	L5	4599	A
1	L5	4600	G
1	L5	4601	U
1	L5	4606	G
1	L5	4611	A
1	L5	4617	G
1	L5	4627	U
1	L5	4633	G
1	L5	4635	A
1	L5	4636	PSU
1	L5	4637	OMG
1	L5	4652	G
1	L5	4656	A
1	L5	4657	U

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Mol	Chain	Res	Type
1	L5	4658	G
1	L5	4659	G
1	L5	4670	C
1	L5	4679	G
1	L5	4687	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4732	G
1	L5	4734	A
1	L5	4735	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4746	C
1	L5	4747	C
1	L5	4750	G
1	L5	4751	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4772	C
1	L5	4773	C
1	L5	4775	C
1	L5	4776	G
1	L5	4859	C
1	L5	4860	G
1	L5	4862	G
1	L5	4870	OMG
1	L5	4871	C
1	L5	4875	G
1	L5	4876	U
1	L5	4881	U
1	L5	4882	U
1	L5	4883	C
1	L5	4885	U
1	L5	4888	U

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Mol	Chain	Res	Type
1	L5	4889	G
1	L5	4895	C
1	L5	4896	G
1	L5	4897	G
1	L5	4899	G
1	L5	4900	C
1	L5	4901	G
1	L5	4903	G
1	L5	4910	G
1	L5	4911	A
1	L5	4912	G
1	L5	4913	G
1	L5	4914	C
1	L5	4916	G
1	L5	4921	C
1	L5	4923	C
1	L5	4925	U
1	L5	4926	C
1	L5	4927	G
1	L5	4928	C
1	L5	4931	G
1	L5	4934	A
1	L5	4937	C
1	L5	4938	A
1	L5	4940	C
1	L5	4941	G
1	L5	4942	C
1	L5	4943	A
1	L5	4947	U
1	L5	4950	U
1	L5	4951	G
1	L5	4955	A
1	L5	4960	G
1	L5	4966	A
1	L5	4967	A
1	L5	4975	G
1	L5	4976	U
1	L5	4979	A
1	L5	4985	U
1	L5	4988	U
1	L5	4989	U
1	L5	4990	C

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Mol	Chain	Res	Type
1	L5	4991	U
1	L5	5014	A
1	L5	5016	A
1	L5	5017	G
1	L5	5022	U
1	L5	5023	C
1	L5	5024	C
1	L5	5025	C
1	L5	5028	G
1	L5	5029	C
1	L5	5030	U
1	L5	5034	A
1	L5	5041	G
1	L5	5047	C
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5058	A
1	L5	5061	A
1	L5	5069	U
2	L7	4	U
2	L7	22	A
2	L7	31	G
2	L7	33	U
2	L7	38	U
2	L7	52	C
2	L7	53	U
2	L7	54	A
2	L7	62	U
2	L7	63	C
2	L7	64	G
2	L7	66	G
2	L7	71	G
2	L7	100	A
2	L7	103	A
2	L7	110	G
3	L8	23	C
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	38	U
3	L8	39	G

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Mol	Chain	Res	Type
3	L8	48	A
3	L8	50	C
3	L8	59	A
3	L8	60	G
3	L8	62	A
3	L8	63	U
3	L8	75	G
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	106	G
3	L8	110	U
3	L8	111	U
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	135	C
3	L8	150	C
3	L8	156	U
47	S2	2	A
47	S2	17	C
47	S2	32	U
47	S2	33	G
47	S2	41	G
47	S2	45	A
47	S2	46	A
47	S2	56	G
47	S2	58	C
47	S2	59	U
47	S2	62	G
47	S2	64	A
47	S2	67	C
47	S2	68	A
47	S2	72	C

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Mol	Chain	Res	Type
47	S2	73	C
47	S2	74	G
47	S2	76	U
47	S2	79	A
47	S2	92	A
47	S2	102	A
47	S2	103	A
47	S2	110	U
47	S2	112	U
47	S2	113	G
47	S2	114	G
47	S2	115	U
47	S2	116	OMU
47	S2	120	U
47	S2	121	OMU
47	S2	126	G
47	S2	139	C
47	S2	143	U
47	S2	149	A
47	S2	155	G
47	S2	160	U
47	S2	161	U
47	S2	162	C
47	S2	170	A
47	S2	184	G
47	S2	190	G
47	S2	192	C
47	S2	196	C
47	S2	198	U
47	S2	199	C
47	S2	200	G
47	S2	202	G
47	S2	203	G
47	S2	204	G
47	S2	205	G
47	S2	206	G
47	S2	211	G
47	S2	213	G
47	S2	214	U
47	S2	219	U
47	S2	225	G
47	S2	290	U

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Mol	Chain	Res	Type
47	S2	291	G
47	S2	292	A
47	S2	293	C
47	S2	295	C
47	S2	306	C
47	S2	307	G
47	S2	308	G
47	S2	309	G
47	S2	310	C
47	S2	311	C
47	S2	313	A
47	S2	318	A
47	S2	319	C
47	S2	321	C
47	S2	322	C
47	S2	323	C
47	S2	324	C
47	S2	326	C
47	S2	328	U
47	S2	329	G
47	S2	332	G
47	S2	335	G
47	S2	339	A
47	S2	347	G
47	S2	360	A
47	S2	362	C
47	S2	364	A
47	S2	365	C
47	S2	368	U
47	S2	369	C
47	S2	370	G
47	S2	374	G
47	S2	380	G
47	S2	382	C
47	S2	385	G
47	S2	386	C
47	S2	398	A
47	S2	400	C
47	S2	407	G
47	S2	408	A
47	S2	409	C
47	S2	417	C

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Mol	Chain	Res	Type
47	S2	418	A
47	S2	421	G
47	S2	425	G
47	S2	429	C
47	S2	436	G
47	S2	438	G
47	S2	447	A
47	S2	448	A
47	S2	449	A
47	S2	450	C
47	S2	452	G
47	S2	464	A
47	S2	465	A
47	S2	471	G
47	S2	472	C
47	S2	473	A
47	S2	474	G
47	S2	482	G
47	S2	487	U
47	S2	488	U
47	S2	492	C
47	S2	493	A
47	S2	525	A
47	S2	530	U
47	S2	531	A
47	S2	532	C
47	S2	537	C
47	S2	538	U
47	S2	540	U
47	S2	542	U
47	S2	544	G
47	S2	545	A
47	S2	546	G
47	S2	547	G
47	S2	552	G
47	S2	554	A
47	S2	556	U
47	S2	557	U
47	S2	558	G
47	S2	563	G
47	S2	564	A
47	S2	566	U

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Mol	Chain	Res	Type
47	S2	569	A
47	S2	570	C
47	S2	576	A
47	S2	583	C
47	S2	587	A
47	S2	589	G
47	S2	590	A
47	S2	591	U
47	S2	594	A
47	S2	597	G
47	S2	598	G
47	S2	603	C
47	S2	606	G
47	S2	607	U
47	S2	608	C
47	S2	614	C
47	S2	620	G
47	S2	623	G
47	S2	627	U
47	S2	629	A
47	S2	631	U
47	S2	643	A
47	S2	655	A
47	S2	658	U
47	S2	660	C
47	S2	664	A
47	S2	668	A2M
47	S2	669	A
47	S2	671	A
47	S2	672	A
47	S2	673	G
47	S2	683	OMG
47	S2	684	G
47	S2	687	C
47	S2	688	U
47	S2	689	U
47	S2	691	G
47	S2	692	G
47	S2	694	G
47	S2	695	C
47	S2	696	G
47	S2	697	G

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Mol	Chain	Res	Type
47	S2	698	G
47	S2	731	G
47	S2	732	U
47	S2	733	C
47	S2	734	C
47	S2	736	C
47	S2	738	C
47	S2	739	C
47	S2	748	C
47	S2	751	G
47	S2	752	G
47	S2	753	C
47	S2	788	G
47	S2	789	G
47	S2	791	C
47	S2	792	C
47	S2	794	A
47	S2	798	A
47	S2	799	U
47	S2	808	A
47	S2	810	A
47	S2	811	A
47	S2	820	U
47	S2	821	G
47	S2	822	PSU
47	S2	830	A
47	S2	834	C
47	S2	835	C
47	S2	836	G
47	S2	837	A
47	S2	838	G
47	S2	839	C
47	S2	840	C
47	S2	841	G
47	S2	842	C
47	S2	847	A
47	S2	853	C
47	S2	869	A
47	S2	870	A
47	S2	872	A
47	S2	873	G
47	S2	874	G

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Mol	Chain	Res	Type
47	S2	875	A
47	S2	878	G
47	S2	879	C
47	S2	880	G
47	S2	883	U
47	S2	885	U
47	S2	887	U
47	S2	888	U
47	S2	889	U
47	S2	891	G
47	S2	892	U
47	S2	896	U
47	S2	897	U
47	S2	898	U
47	S2	899	U
47	S2	900	C
47	S2	901	G
47	S2	903	A
47	S2	904	A
47	S2	913	A
47	S2	914	U
47	S2	920	A
47	S2	933	G
47	S2	934	G
47	S2	963	A
47	S2	971	G
47	S2	972	A
47	S2	978	G
47	S2	990	A
47	S2	992	A
47	S2	999	G
47	S2	1001	A
47	S2	1002	U
47	S2	1008	A
47	S2	1017	U
47	S2	1021	U
47	S2	1023	A
47	S2	1027	A
47	S2	1028	A
47	S2	1045	U
47	S2	1061	U
47	S2	1062	A

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Mol	Chain	Res	Type
47	S2	1067	C
47	S2	1076	G
47	S2	1078	C
47	S2	1081	PSU
47	S2	1083	A
47	S2	1085	C
47	S2	1089	G
47	S2	1109	C
47	S2	1114	U
47	S2	1116	C
47	S2	1121	G
47	S2	1133	A
47	S2	1138	C
47	S2	1148	A
47	S2	1153	C
47	S2	1154	U
47	S2	1165	G
47	S2	1170	A
47	S2	1172	U
47	S2	1195	A
47	S2	1206	G
47	S2	1207	G
47	S2	1208	A
47	S2	1215	C
47	S2	1216	C
47	S2	1217	A
47	S2	1221	G
47	S2	1224	G
47	S2	1227	G
47	S2	1234	C
47	S2	1242	U
47	S2	1243	PSU
47	S2	1250	A
47	S2	1251	A
47	S2	1253	A
47	S2	1256	G
47	S2	1257	G
47	S2	1259	A
47	S2	1264	C
47	S2	1265	A
47	S2	1266	C
47	S2	1274	G

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Mol	Chain	Res	Type
47	S2	1275	G
47	S2	1283	C
47	S2	1286	G
47	S2	1294	G
47	S2	1295	A
47	S2	1300	U
47	S2	1301	A
47	S2	1302	G
47	S2	1308	U
47	S2	1330	G
47	S2	1332	A
47	S2	1341	C
47	S2	1342	U
47	S2	1348	G
47	S2	1354	G
47	S2	1371	U
47	S2	1372	U
47	S2	1373	C
47	S2	1378	A
47	S2	1382	A
47	S2	1393	G
47	S2	1401	A
47	S2	1404	U
47	S2	1406	G
47	S2	1408	U
47	S2	1412	C
47	S2	1415	C
47	S2	1416	C
47	S2	1417	C
47	S2	1419	C
47	S2	1421	A
47	S2	1422	G
47	S2	1423	C
47	S2	1424	G
47	S2	1433	C
47	S2	1434	C
47	S2	1435	C
47	S2	1436	C
47	S2	1437	C
47	S2	1438	A
47	S2	1440	C
47	S2	1448	A

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Mol	Chain	Res	Type
47	S2	1452	A
47	S2	1454	A
47	S2	1455	A
47	S2	1463	U
47	S2	1478	U
47	S2	1480	A
47	S2	1484	A
47	S2	1487	A
47	S2	1488	C
47	S2	1489	A
47	S2	1490	G
47	S2	1494	U
47	S2	1495	G
47	S2	1497	G
47	S2	1498	A
47	S2	1520	G
47	S2	1521	C
47	S2	1522	A
47	S2	1533	A
47	S2	1537	A
47	S2	1544	C
47	S2	1545	A
47	S2	1548	G
47	S2	1552	G
47	S2	1553	C
47	S2	1556	A
47	S2	1560	U
47	S2	1570	G
47	S2	1580	A
47	S2	1585	U
47	S2	1586	U
47	S2	1587	G
47	S2	1588	A
47	S2	1600	G
47	S2	1601	A
47	S2	1603	G
47	S2	1621	U
47	S2	1623	A
47	S2	1629	C
47	S2	1634	A
47	S2	1635	C
47	S2	1638	G

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Mol	Chain	Res	Type
47	S2	1640	A
47	S2	1644	C
47	S2	1646	C
47	S2	1648	G
47	S2	1654	G
47	S2	1661	A
47	S2	1663	A
47	S2	1664	A
47	S2	1665	G
47	S2	1671	G
47	S2	1680	G
47	S2	1686	G
47	S2	1698	C
47	S2	1699	A
47	S2	1719	A
47	S2	1721	U
47	S2	1722	G
47	S2	1744	G
47	S2	1745	A
47	S2	1748	G
47	S2	1752	C
47	S2	1753	C
47	S2	1754	G
47	S2	1757	G
47	S2	1758	G
47	S2	1759	G
47	S2	1760	G
47	S2	1761	U
47	S2	1771	G
47	S2	1773	C
47	S2	1774	C
47	S2	1775	U
47	S2	1776	G
47	S2	1777	G
47	S2	1778	C
47	S2	1779	G
47	S2	1783	C
47	S2	1784	G
47	S2	1786	U
47	S2	1798	C
47	S2	1800	A
47	S2	1804	U

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Mol	Chain	Res	Type
47	S2	1813	A
47	S2	1822	A
47	S2	1823	A
47	S2	1824	A
47	S2	1829	G
47	S2	1831	A
47	S2	1835	A
47	S2	1837	G
47	S2	1838	U
47	S2	1849	G
47	S2	1852	C
47	S2	1861	G
47	S2	1862	G
47	S2	1863	A
47	S2	1864	U
47	S2	1865	C
47	S2	1867	U
48	S6	8	G
48	S6	9	U
48	S6	10	G
48	S6	18	G
48	S6	19	G
48	S6	20	A
48	S6	29	G
48	S6	31	G
48	S6	32	C
48	S6	33	C
48	S6	34	C
48	S6	36	U
48	S6	37	A
48	S6	39	C
48	S6	40	C
48	S6	41	C
48	S6	42	A
48	S6	44	A
48	S6	46	G
48	S6	47	U
48	S6	50	A
48	S6	51	U
48	S6	54	A
48	S6	55	U
48	S6	58	A

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Mol	Chain	Res	Type
48	S6	59	A
48	S6	65	C
48	S6	66	C
48	S6	69	U
48	S6	74	C
48	S6	75	C
48	S6	76	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	185	C
1	L5	255	C
1	L5	406	C
1	L5	504	G
1	L5	914	U
1	L5	981	C
1	L5	1082	C
1	L5	1625	OMG
1	L5	2019	C
1	L5	2033	A
1	L5	2084	C
1	L5	2416	G
1	L5	2675	G
1	L5	2760	G
1	L5	3597	G
1	L5	3614	G
1	L5	3673	C
1	L5	3876	A
1	L5	4378	A
1	L5	4699	U
1	L5	4870	OMG
1	L5	4913	G
1	L5	4949	G
3	L8	83	C
47	S2	112	U
47	S2	291	G
47	S2	417	C
47	S2	420	G
47	S2	563	G
47	S2	688	U
47	S2	1434	C

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Mol	Chain	Res	Type
48	S6	54	A

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

138 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
1	OMG	L5	1316	1	18,26,27	1.24	3 (16%)	22,38,41	2.30	7 (31%)
1	1MA	L5	1322	1,82	16,25,26	1.55	4 (25%)	13,37,40	1.34	2 (15%)
1	A2M	L5	1326	1	18,25,26	0.91	1 (5%)	20,36,39	1.80	2 (10%)
1	P4U	L5	1348	1	18,24,25	1.03	1 (5%)	20,33,36	2.06	1 (5%)
1	B8Q	L5	1456	1	16,22,23	1.30	2 (12%)	19,32,35	1.08	2 (10%)
1	2MG	L5	1517	1	19,26,27	1.02	2 (10%)	20,38,41	2.48	8 (40%)
1	OMG	L5	1522	1	18,26,27	1.26	3 (16%)	22,38,41	2.18	6 (27%)
1	A2M	L5	1524	1	18,25,26	1.11	2 (11%)	20,36,39	1.73	3 (15%)
1	A2M	L5	1534	1,82	18,25,26	1.02	1 (5%)	20,36,39	1.75	2 (10%)
1	B9B	L5	1574	1	21,28,29	1.00	2 (9%)	23,40,43	1.80	5 (21%)
1	PSU	L5	1582	1	16,21,22	1.58	5 (31%)	20,30,33	3.34	5 (25%)
1	7MG	L5	1605	1	20,26,27	1.42	2 (10%)	22,39,42	2.57	5 (22%)
1	OMG	L5	1625	1	18,26,27	1.20	3 (16%)	22,38,41	2.06	6 (27%)
1	I4U	L5	1659	1,82	17,24,25	0.89	1 (5%)	19,34,37	2.62	3 (15%)
1	PSU	L5	1677	1	16,21,22	1.90	5 (31%)	20,30,33	3.51	7 (35%)
1	PSU	L5	1683	1	16,21,22	1.93	5 (31%)	20,30,33	3.31	6 (30%)
1	E7G	L5	1797	1	20,27,28	1.36	2 (10%)	24,40,43	2.63	6 (25%)
1	B8H	L5	1860	1	16,22,23	1.33	2 (12%)	21,32,35	2.33	3 (14%)
1	UR3	L5	1866	1	14,22,23	0.84	0	16,32,35	0.88	1 (6%)
1	A2M	L5	1871	1,82	18,25,26	1.01	2 (11%)	20,36,39	1.82	2 (10%)
1	OMG	L5	1883	1	18,26,27	1.18	3 (16%)	22,38,41	1.99	6 (27%)
1	P7G	L5	1909	1	21,28,29	1.28	2 (9%)	26,41,44	3.00	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L5	2050	1	18,26,27	1.08	2 (11%)	22,38,41	1.99	6 (27%)
1	E7G	L5	2297	1	20,27,28	1.33	2 (10%)	24,40,43	2.66	7 (29%)
1	A2M	L5	2363	1,82	18,25,26	1.06	2 (11%)	20,36,39	1.62	2 (10%)
1	OMG	L5	2364	1	18,26,27	1.06	2 (11%)	22,38,41	2.00	6 (27%)
1	OMC	L5	2365	1,82	15,22,23	1.01	0	19,31,34	1.09	1 (5%)
1	B9B	L5	237	1	21,28,29	1.24	3 (14%)	23,40,43	1.86	6 (26%)
1	B8W	L5	2380	1	18,26,27	0.97	1 (5%)	19,38,41	1.76	4 (21%)
1	A2M	L5	2401	1	18,25,26	1.01	2 (11%)	20,36,39	1.67	2 (10%)
1	OMC	L5	2422	1,82	15,22,23	1.14	2 (13%)	19,31,34	0.73	0
1	OMG	L5	2424	1	18,26,27	1.24	3 (16%)	22,38,41	2.04	7 (31%)
1	PSU	L5	2508	1	16,21,22	1.57	3 (18%)	20,30,33	3.37	6 (30%)
1	7MG	L5	2522	1	20,26,27	1.41	2 (10%)	22,39,42	2.68	4 (18%)
1	B9B	L5	2754	1	21,28,29	1.10	2 (9%)	23,40,43	2.04	6 (26%)
1	OMG	L5	2773	1	18,26,27	1.22	2 (11%)	22,38,41	2.14	6 (27%)
1	B9H	L5	2786	1	19,25,26	1.23	3 (15%)	20,35,38	1.87	4 (20%)
1	OMC	L5	2804	1	15,22,23	1.07	1 (6%)	19,31,34	0.96	0
1	OMC	L5	2861	1	15,22,23	1.03	1 (6%)	19,31,34	0.77	0
1	OMC	L5	3701	1,82	15,22,23	1.03	1 (6%)	19,31,34	0.97	0
1	PSU	L5	3715	1,82	16,21,22	1.41	4 (25%)	20,30,33	3.41	6 (30%)
1	A2M	L5	3718	1	18,25,26	0.93	1 (5%)	20,36,39	1.63	2 (10%)
1	A2M	L5	3723	1	18,25,26	1.08	1 (5%)	20,36,39	1.53	2 (10%)
1	PSU	L5	3729	1	16,21,22	1.59	4 (25%)	20,30,33	3.42	5 (25%)
1	OMG	L5	373	1	18,26,27	1.20	3 (16%)	22,38,41	2.22	6 (27%)
1	B8H	L5	3762	1	16,22,23	1.60	3 (18%)	21,32,35	2.46	6 (28%)
1	PSU	L5	3764	1	16,21,22	1.51	3 (18%)	20,30,33	3.45	5 (25%)
1	5MC	L5	3782	1,82	15,22,23	1.21	1 (6%)	17,32,35	0.94	1 (5%)
1	A2M	L5	3785	1	18,25,26	0.95	1 (5%)	20,36,39	1.67	3 (15%)
1	OMG	L5	3792	1	18,26,27	1.16	2 (11%)	22,38,41	2.10	6 (27%)
1	A2M	L5	3825	1	18,25,26	1.05	2 (11%)	20,36,39	1.83	2 (10%)
1	A2M	L5	3867	1	18,25,26	1.01	1 (5%)	20,36,39	1.65	3 (15%)
1	OMC	L5	3869	1	15,22,23	1.10	1 (6%)	19,31,34	1.19	1 (5%)
1	P7G	L5	3880	1	21,28,29	1.24	3 (14%)	26,41,44	3.18	8 (30%)
1	OMC	L5	3887	1	15,22,23	1.03	1 (6%)	19,31,34	1.12	1 (5%)
1	B8K	L5	3897	1	22,28,29	1.63	3 (13%)	25,42,45	2.44	5 (20%)
1	BGH	L5	3899	1	22,29,30	2.30	4 (18%)	24,43,46	2.76	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	L5	3909	1	15,22,23	1.05	1 (6%)	19,31,34	0.82	0
1	A2M	L5	398	1	18,25,26	1.06	1 (5%)	20,36,39	1.81	2 (10%)
1	5MU	L5	4083	1	14,22,23	0.89	1 (7%)	16,32,35	2.28	2 (12%)
1	B8W	L5	4129	1	18,26,27	1.07	1 (5%)	19,38,41	1.95	4 (21%)
1	B8W	L5	4185	1	18,26,27	0.97	2 (11%)	19,38,41	1.92	4 (21%)
1	I4U	L5	4194	1	17,24,25	0.82	0	19,34,37	3.08	3 (15%)
1	OMG	L5	4196	1,82	18,26,27	1.16	2 (11%)	22,38,41	2.04	6 (27%)
1	6MZ	L5	4220	1	18,25,26	0.97	2 (11%)	16,36,39	2.61	4 (25%)
1	PSU	L5	4293	1	16,21,22	1.62	3 (18%)	20,30,33	3.41	6 (30%)
1	B8H	L5	4296	1	16,22,23	1.54	3 (18%)	21,32,35	2.25	3 (14%)
1	OMU	L5	4306	1	14,22,23	1.14	2 (14%)	18,31,34	2.29	2 (11%)
1	5MC	L5	4335	1	15,22,23	1.46	2 (13%)	17,32,35	0.97	2 (11%)
1	E6G	L5	4355	1	20,27,28	1.25	3 (15%)	22,39,42	1.97	6 (27%)
1	OMG	L5	4370	1	18,26,27	1.08	2 (11%)	22,38,41	1.99	5 (22%)
1	MHG	L5	4371	1	25,32,33	1.19	2 (8%)	29,46,49	2.79	8 (27%)
1	PSU	L5	4403	1	16,21,22	1.56	5 (31%)	20,30,33	3.61	8 (40%)
1	1MA	L5	4415	1	16,25,26	1.67	5 (31%)	13,37,40	1.34	2 (15%)
1	PSU	L5	4442	1	16,21,22	1.64	4 (25%)	20,30,33	3.37	7 (35%)
1	5MC	L5	4447	1,82	15,22,23	1.34	3 (20%)	17,32,35	1.99	4 (23%)
1	PSU	L5	4450	1,82	16,21,22	2.02	4 (25%)	20,30,33	3.39	6 (30%)
1	B8W	L5	4472	1	18,26,27	1.07	1 (5%)	19,38,41	2.04	4 (21%)
1	B8T	L5	4483	1	16,22,23	0.91	0	16,31,34	1.12	2 (12%)
1	OMG	L5	4494	1	18,26,27	1.19	3 (16%)	22,38,41	2.21	6 (27%)
1	PSU	L5	4500	1	16,21,22	1.74	5 (31%)	20,30,33	3.33	5 (25%)
1	A2M	L5	4523	1,82	18,25,26	0.96	1 (5%)	20,36,39	1.78	2 (10%)
1	B8W	L5	4529	1,82	18,26,27	1.03	2 (11%)	19,38,41	2.04	4 (21%)
1	UR3	L5	4530	1	14,22,23	0.93	1 (7%)	16,32,35	0.76	0
1	PSU	L5	4531	1	16,21,22	1.77	4 (25%)	20,30,33	3.41	6 (30%)
1	OMC	L5	4536	1	15,22,23	1.15	1 (6%)	19,31,34	1.21	2 (10%)
1	7MG	L5	4550	1	20,26,27	1.30	2 (10%)	22,39,42	2.53	5 (22%)
1	M7A	L5	4564	1	20,25,26	1.01	2 (10%)	23,37,40	2.26	5 (21%)
1	A2M	L5	4571	1	18,25,26	1.04	2 (11%)	20,36,39	1.73	2 (10%)
1	UR3	L5	4597	1	14,22,23	0.68	0	16,32,35	0.73	0
1	OMU	L5	4620	1	14,22,23	1.06	2 (14%)	18,31,34	2.54	4 (22%)
1	OMG	L5	4623	1	18,26,27	1.15	3 (16%)	22,38,41	2.13	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	4628	1	16,21,22	1.57	4 (25%)	20,30,33	3.35	7 (35%)
1	PSU	L5	4636	1	16,21,22	1.77	4 (25%)	20,30,33	3.38	6 (30%)
1	OMG	L5	4637	1	18,26,27	1.23	3 (16%)	22,38,41	2.19	7 (31%)
1	B8T	L5	4671	1	16,22,23	0.93	1 (6%)	16,31,34	1.11	2 (12%)
1	B8K	L5	4690	1	22,28,29	1.75	3 (13%)	25,42,45	2.71	6 (24%)
1	OMG	L5	4870	1	18,26,27	1.29	3 (16%)	22,38,41	2.08	6 (27%)
1	2MG	L5	4872	1	19,26,27	1.22	2 (10%)	20,38,41	3.29	10 (50%)
1	2MG	L5	729	1	19,26,27	1.06	2 (10%)	20,38,41	2.27	7 (35%)
1	2MG	L5	978	1	19,26,27	1.11	2 (10%)	20,38,41	2.43	8 (40%)
3	OMU	L8	14	1,3	14,22,23	1.15	2 (14%)	18,31,34	1.85	1 (5%)
6	MLZ	LC	333	6	9,9,10	1.30	1 (11%)	6,9,11	1.34	1 (16%)
41	MLZ	Lm	98	41	9,9,10	1.81	1 (11%)	6,9,11	1.61	2 (33%)
47	A2M	S2	1031	47	18,25,26	1.04	1 (5%)	20,36,39	1.76	3 (15%)
47	PSU	S2	1081	47	16,21,22	1.51	5 (31%)	20,30,33	3.71	8 (40%)
47	OMU	S2	116	47	14,22,23	1.09	1 (7%)	18,31,34	2.39	2 (11%)
47	PSU	S2	119	47	16,21,22	1.54	4 (25%)	20,30,33	3.27	5 (25%)
47	OMU	S2	121	47	14,22,23	1.32	2 (14%)	18,31,34	2.33	2 (11%)
47	B8Q	S2	1219	82,47	16,22,23	1.27	2 (12%)	19,32,35	0.97	2 (10%)
47	PSU	S2	1243	47	16,21,22	1.71	5 (31%)	20,30,33	3.49	6 (30%)
47	B8N	S2	1248	47	16,29,30	1.34	2 (12%)	20,42,45	0.83	1 (5%)
47	4AC	S2	1337	47	18,24,25	1.23	5 (27%)	20,34,37	1.41	3 (15%)
47	5MC	S2	1374	47	15,22,23	1.34	1 (6%)	17,32,35	1.00	1 (5%)
47	A2M	S2	159	47	18,25,26	1.07	1 (5%)	20,36,39	1.50	2 (10%)
47	A2M	S2	166	47	18,25,26	1.20	2 (11%)	20,36,39	1.70	2 (10%)
47	A2M	S2	1678	47	18,25,26	0.97	1 (5%)	20,36,39	1.68	2 (10%)
47	OMC	S2	1703	47	15,22,23	1.01	0	19,31,34	0.91	0
47	OMC	S2	1710	47	15,22,23	1.12	1 (6%)	19,31,34	0.85	0
47	OMC	S2	174	82,47	15,22,23	0.98	0	19,31,34	0.87	1 (5%)
47	M7A	S2	1806	47	20,25,26	1.07	2 (10%)	23,37,40	2.22	5 (21%)
47	UR3	S2	1830	47	14,22,23	0.82	0	16,32,35	0.78	0
47	6MZ	S2	1832	82,47	18,25,26	0.99	1 (5%)	16,36,39	2.47	3 (18%)
47	4AC	S2	1842	47	18,24,25	1.38	4 (22%)	20,34,37	1.54	5 (25%)
47	MA6	S2	1850	47	16,26,27	0.88	1 (6%)	18,38,41	2.35	3 (16%)
47	MA6	S2	1851	47	16,26,27	0.84	1 (6%)	18,38,41	2.24	3 (16%)
47	A2M	S2	27	82,47	18,25,26	1.04	1 (5%)	20,36,39	1.81	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	A2M	S2	484	47	18,25,26	1.00	1 (5%)	20,36,39	1.58	2 (10%)
47	OMG	S2	509	82,47	18,26,27	1.16	2 (11%)	22,38,41	2.06	6 (27%)
47	OMC	S2	517	47	15,22,23	1.03	0	19,31,34	0.97	0
47	E3C	S2	568	47	17,23,24	1.30	3 (17%)	19,33,36	1.58	3 (15%)
47	PSU	S2	612	47	16,21,22	1.72	4 (25%)	20,30,33	3.27	7 (35%)
47	OMG	S2	644	47	18,26,27	1.13	2 (11%)	22,38,41	2.15	6 (27%)
47	A2M	S2	668	82,47	18,25,26	1.06	2 (11%)	20,36,39	1.74	2 (10%)
47	OMG	S2	683	47	18,26,27	1.19	3 (16%)	22,38,41	2.25	6 (27%)
47	5MU	S2	814	47	14,22,23	0.90	1 (7%)	16,32,35	2.27	2 (12%)
47	PSU	S2	822	47	16,21,22	1.74	4 (25%)	20,30,33	3.39	6 (30%)
47	PSU	S2	823	47	16,21,22	1.62	4 (25%)	20,30,33	3.28	7 (35%)

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
1	OMG	L5	1316	1	-	0/5/27/28	0/3/3/3
1	1MA	L5	1322	1,82	-	0/3/25/26	0/3/3/3
1	A2M	L5	1326	1	-	0/5/27/28	0/3/3/3
1	P4U	L5	1348	1	-	0/7/29/30	0/2/2/2
1	B8Q	L5	1456	1	1/1/9/11	0/7/42/43	0/2/2/2
1	2MG	L5	1517	1	-	0/5/27/28	0/3/3/3
1	OMG	L5	1522	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	1524	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	1534	1,82	-	0/5/27/28	0/3/3/3
1	B9B	L5	1574	1	-	2/7/29/30	0/3/3/3
1	PSU	L5	1582	1	-	0/7/25/26	0/2/2/2
1	7MG	L5	1605	1	-	0/7/37/38	0/3/3/3
1	OMG	L5	1625	1	-	0/5/27/28	0/3/3/3
1	I4U	L5	1659	1,82	-	1/7/29/30	0/2/2/2
1	PSU	L5	1677	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1683	1	-	0/7/25/26	0/2/2/2
1	E7G	L5	1797	1	-	0/9/39/40	0/3/3/3
1	B8H	L5	1860	1	-	0/7/25/26	0/2/2/2
1	UR3	L5	1866	1	-	0/3/25/26	0/2/2/2
1	A2M	L5	1871	1,82	-	0/5/27/28	0/3/3/3
1	OMG	L5	1883	1	-	0/5/27/28	0/3/3/3
1	P7G	L5	1909	1	-	0/10/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L5	2050	1	-	0/5/27/28	0/3/3/3
1	E7G	L5	2297	1	-	0/9/39/40	0/3/3/3
1	A2M	L5	2363	1,82	-	0/5/27/28	0/3/3/3
1	OMG	L5	2364	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	2365	1,82	-	0/5/27/28	0/2/2/2
1	B9B	L5	237	1	-	1/7/29/30	0/3/3/3
1	B8W	L5	2380	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	2401	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	2422	1,82	-	0/5/27/28	0/2/2/2
1	OMG	L5	2424	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
1	7MG	L5	2522	1	-	0/7/37/38	0/3/3/3
1	B9B	L5	2754	1	-	0/7/29/30	0/3/3/3
1	OMG	L5	2773	1	-	0/5/27/28	0/3/3/3
1	B9H	L5	2786	1	1/1/9/11	0/12/47/48	0/2/2/2
1	OMC	L5	2804	1	-	0/5/27/28	0/2/2/2
1	OMC	L5	2861	1	-	0/5/27/28	0/2/2/2
1	OMC	L5	3701	1,82	-	0/5/27/28	0/2/2/2
1	PSU	L5	3715	1,82	-	0/7/25/26	0/2/2/2
1	A2M	L5	3718	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	3723	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	3729	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	373	1	-	0/5/27/28	0/3/3/3
1	B8H	L5	3762	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3764	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	3782	1,82	-	0/3/25/26	0/2/2/2
1	A2M	L5	3785	1	-	0/5/27/28	0/3/3/3
1	OMG	L5	3792	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	3825	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	3867	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	3869	1	-	0/5/27/28	0/2/2/2
1	P7G	L5	3880	1	-	0/10/40/41	0/3/3/3
1	OMC	L5	3887	1	-	0/5/27/28	0/2/2/2
1	B8K	L5	3897	1	-	0/11/41/42	0/3/3/3
1	BGH	L5	3899	1	-	0/13/43/44	0/3/3/3
1	OMC	L5	3909	1	-	0/5/27/28	0/2/2/2
1	A2M	L5	398	1	-	0/5/27/28	0/3/3/3
1	5MU	L5	4083	1	-	0/3/25/26	0/2/2/2
1	B8W	L5	4129	1	-	2/5/27/28	0/3/3/3
1	B8W	L5	4185	1	-	2/5/27/28	0/3/3/3
1	I4U	L5	4194	1	-	1/7/29/30	0/2/2/2
1	OMG	L5	4196	1,82	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	L5	4220	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
1	B8H	L5	4296	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4306	1	-	0/5/27/28	0/2/2/2
1	5MC	L5	4335	1	-	0/3/25/26	0/2/2/2
1	E6G	L5	4355	1	-	2/6/28/29	0/3/3/3
1	OMG	L5	4370	1	-	0/5/27/28	0/3/3/3
1	MHG	L5	4371	1	-	0/16/46/47	0/3/3/3
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	1MA	L5	4415	1	-	0/3/25/26	0/3/3/3
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	4447	1,82	-	0/3/25/26	0/2/2/2
1	PSU	L5	4450	1,82	-	0/7/25/26	0/2/2/2
1	B8W	L5	4472	1	-	2/5/27/28	0/3/3/3
1	B8T	L5	4483	1	-	0/5/27/28	0/2/2/2
1	OMG	L5	4494	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4500	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	4523	1,82	-	0/5/27/28	0/3/3/3
1	B8W	L5	4529	1,82	-	2/5/27/28	0/3/3/3
1	UR3	L5	4530	1	-	0/3/25/26	0/2/2/2
1	PSU	L5	4531	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/5/27/28	0/2/2/2
1	7MG	L5	4550	1	-	0/7/37/38	0/3/3/3
1	M7A	L5	4564	1	-	0/7/37/38	0/3/3/3
1	A2M	L5	4571	1	-	0/5/27/28	0/3/3/3
1	UR3	L5	4597	1	-	0/3/25/26	0/2/2/2
1	OMU	L5	4620	1	-	0/5/27/28	0/2/2/2
1	OMG	L5	4623	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1	-	0/5/27/28	0/3/3/3
1	B8T	L5	4671	1	-	0/5/27/28	0/2/2/2
1	B8K	L5	4690	1	-	0/11/41/42	0/3/3/3
1	OMG	L5	4870	1	-	0/5/27/28	0/3/3/3
1	2MG	L5	4872	1	-	0/5/27/28	0/3/3/3
1	2MG	L5	729	1	-	0/5/27/28	0/3/3/3
1	2MG	L5	978	1	-	0/5/27/28	0/3/3/3
3	OMU	L8	14	1,3	-	0/5/27/28	0/2/2/2
6	MLZ	LC	333	6	-	0/6/8/10	0/0/0/0
41	MLZ	Lm	98	41	-	0/6/8/10	0/0/0/0
47	A2M	S2	1031	47	-	0/5/27/28	0/3/3/3
47	PSU	S2	1081	47	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	OMU	S2	116	47	-	0/5/27/28	0/2/2/2
47	PSU	S2	119	47	-	0/7/25/26	0/2/2/2
47	OMU	S2	121	47	-	0/5/27/28	0/2/2/2
47	B8Q	S2	1219	82,47	1/1/9/11	0/7/42/43	0/2/2/2
47	PSU	S2	1243	47	-	0/7/25/26	0/2/2/2
47	B8N	S2	1248	47	-	0/12/34/35	0/2/2/2
47	4AC	S2	1337	47	-	2/7/29/30	0/2/2/2
47	5MC	S2	1374	47	-	0/3/25/26	0/2/2/2
47	A2M	S2	159	47	-	0/5/27/28	0/3/3/3
47	A2M	S2	166	47	-	0/5/27/28	0/3/3/3
47	A2M	S2	1678	47	-	0/5/27/28	0/3/3/3
47	OMC	S2	1703	47	-	0/5/27/28	0/2/2/2
47	OMC	S2	1710	47	-	0/5/27/28	0/2/2/2
47	OMC	S2	174	82,47	-	0/5/27/28	0/2/2/2
47	M7A	S2	1806	47	-	0/7/37/38	0/3/3/3
47	UR3	S2	1830	47	-	0/3/25/26	0/2/2/2
47	6MZ	S2	1832	82,47	-	0/5/27/28	0/3/3/3
47	4AC	S2	1842	47	-	0/7/29/30	0/2/2/2
47	MA6	S2	1850	47	-	0/7/29/30	0/3/3/3
47	MA6	S2	1851	47	-	0/7/29/30	0/3/3/3
47	A2M	S2	27	82,47	-	0/5/27/28	0/3/3/3
47	A2M	S2	484	47	-	0/5/27/28	0/3/3/3
47	OMG	S2	509	82,47	-	0/5/27/28	0/3/3/3
47	OMC	S2	517	47	-	0/5/27/28	0/2/2/2
47	E3C	S2	568	47	1/1/9/11	0/9/44/45	0/2/2/2
47	PSU	S2	612	47	-	0/7/25/26	0/2/2/2
47	OMG	S2	644	47	-	0/5/27/28	0/3/3/3
47	A2M	S2	668	82,47	-	0/5/27/28	0/3/3/3
47	OMG	S2	683	47	-	0/5/27/28	0/3/3/3
47	5MU	S2	814	47	-	0/3/25/26	0/2/2/2
47	PSU	S2	822	47	-	0/7/25/26	0/2/2/2
47	PSU	S2	823	47	-	0/7/25/26	0/2/2/2

All (299) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4450	PSU	C5-C1'	-6.22	1.46	1.52
1	L5	1677	PSU	C5-C1'	-5.65	1.47	1.52
1	L5	1683	PSU	C5-C1'	-5.59	1.47	1.52
1	L5	4690	B8K	C5-N7	-5.52	1.32	1.40
1	L5	4531	PSU	C5-C1'	-5.33	1.47	1.52
1	L5	4636	PSU	C5-C1'	-5.30	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4500	PSU	C5-C1'	-5.13	1.47	1.52
47	S2	612	PSU	C5-C1'	-5.10	1.47	1.52
1	L5	3897	B8K	C5-N7	-5.07	1.33	1.40
1	L5	3762	B8H	C5-C1'	-5.00	1.47	1.52
47	S2	822	PSU	C5-C1'	-4.93	1.48	1.52
1	L5	4442	PSU	C5-C1'	-4.83	1.48	1.52
1	L5	4296	B8H	C5-C1'	-4.71	1.48	1.52
1	L5	3729	PSU	C5-C1'	-4.67	1.48	1.52
47	S2	1243	PSU	C5-C1'	-4.61	1.48	1.52
47	S2	823	PSU	C5-C1'	-4.55	1.48	1.52
1	L5	4293	PSU	C5-C1'	-4.43	1.48	1.52
47	S2	1248	B8N	C5-C1'	-4.26	1.48	1.52
47	S2	119	PSU	C5-C1'	-4.15	1.48	1.52
1	L5	1582	PSU	C5-C1'	-4.12	1.48	1.52
1	L5	4628	PSU	C5-C1'	-4.09	1.48	1.52
1	L5	2508	PSU	C5-C1'	-3.99	1.48	1.52
1	L5	3764	PSU	C5-C1'	-3.95	1.48	1.52
1	L5	4403	PSU	C5-C1'	-3.93	1.48	1.52
1	L5	3899	BGH	C5-N7	-3.80	1.35	1.40
1	L5	1860	B8H	C5-C1'	-3.66	1.49	1.52
1	L5	3715	PSU	C5-C1'	-3.46	1.49	1.52
47	S2	1081	PSU	C2-N3	-3.02	1.32	1.38
47	S2	1081	PSU	C5-C1'	-2.99	1.49	1.52
1	L5	1683	PSU	C2-N3	-2.98	1.32	1.38
47	S2	1842	4AC	C6-N1	-2.96	1.31	1.35
47	S2	1243	PSU	C2-N1	-2.82	1.32	1.38
1	L5	1522	OMG	O5'-C5'	-2.80	1.40	1.44
47	S2	1081	PSU	C2-N1	-2.74	1.32	1.38
1	L5	4403	PSU	C2-N3	-2.73	1.32	1.38
1	L5	3762	B8H	C2-N3	-2.73	1.32	1.38
47	S2	121	OMU	O5'-C5'	-2.72	1.41	1.44
1	L5	4293	PSU	C2-N3	-2.69	1.32	1.38
1	L5	2786	B9H	O5'-C5'	-2.68	1.41	1.44
1	L5	1348	P4U	O5'-C5'	-2.66	1.41	1.44
47	S2	121	OMU	C2-N3	-2.65	1.32	1.38
1	L5	4628	PSU	C2-N1	-2.64	1.32	1.38
1	L5	1677	PSU	O4'-C1'	-2.62	1.40	1.44
3	L8	14	OMU	C2-N3	-2.61	1.33	1.38
1	L5	4293	PSU	C2-N1	-2.61	1.33	1.38
47	S2	166	A2M	O5'-C5'	-2.59	1.41	1.44
47	S2	822	PSU	O4'-C1'	-2.58	1.40	1.44
1	L5	1316	OMG	O5'-C5'	-2.57	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	1337	4AC	C4-N4	-2.56	1.35	1.40
47	S2	814	5MU	C2-N3	-2.54	1.33	1.38
47	S2	822	PSU	C2-N3	-2.54	1.33	1.38
1	L5	2508	PSU	C2-N1	-2.54	1.33	1.38
1	L5	3764	PSU	C2-N1	-2.52	1.33	1.38
1	L5	4636	PSU	C2-N3	-2.52	1.33	1.38
1	L5	4296	B8H	C2-N3	-2.52	1.33	1.38
1	L5	4450	PSU	C2-N3	-2.52	1.33	1.38
1	L5	1677	PSU	C2-N1	-2.52	1.33	1.38
1	L5	1683	PSU	C2-N1	-2.51	1.33	1.38
1	L5	4623	OMG	O5'-C5'	-2.50	1.41	1.44
1	L5	4564	M7A	C5-N7	-2.50	1.32	1.38
47	S2	1842	4AC	C2-N3	-2.49	1.33	1.38
1	L5	4530	UR3	O5'-C5'	-2.49	1.41	1.44
1	L5	1860	B8H	C2-N3	-2.48	1.33	1.38
1	L5	4403	PSU	C2-N1	-2.48	1.33	1.38
1	L5	4083	5MU	C2-N3	-2.47	1.33	1.38
1	L5	4636	PSU	O4'-C1'	-2.46	1.40	1.44
1	L5	4450	PSU	C2-N1	-2.45	1.33	1.38
1	L5	4306	OMU	C2-N3	-2.44	1.33	1.38
1	L5	2508	PSU	C2-N3	-2.44	1.33	1.38
1	L5	373	OMG	O5'-C5'	-2.44	1.41	1.44
47	S2	612	PSU	O4'-C1'	-2.43	1.40	1.44
1	L5	3764	PSU	C2-N3	-2.42	1.33	1.38
47	S2	119	PSU	C2-N3	-2.41	1.33	1.38
1	L5	2424	OMG	O5'-C5'	-2.41	1.41	1.44
47	S2	612	PSU	C2-N3	-2.41	1.33	1.38
47	S2	1243	PSU	C2-N3	-2.41	1.33	1.38
47	S2	822	PSU	C2-N1	-2.41	1.33	1.38
1	L5	4628	PSU	C2-N3	-2.41	1.33	1.38
47	S2	612	PSU	C2-N1	-2.39	1.33	1.38
1	L5	4500	PSU	O4'-C1'	-2.37	1.40	1.44
1	L5	4450	PSU	O4'-C1'	-2.35	1.40	1.44
1	L5	1582	PSU	C2-N1	-2.35	1.33	1.38
47	S2	823	PSU	C2-N3	-2.35	1.33	1.38
1	L5	2422	OMC	O5'-C5'	-2.34	1.41	1.44
1	L5	4531	PSU	O4'-C1'	-2.34	1.40	1.44
1	L5	4620	OMU	C2-N3	-2.33	1.33	1.38
1	L5	1524	A2M	O5'-C5'	-2.32	1.41	1.44
1	L5	2422	OMC	C2-N3	-2.32	1.33	1.38
47	S2	668	A2M	O5'-C5'	-2.32	1.41	1.44
1	L5	1582	PSU	O4'-C1'	-2.31	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	119	PSU	C2-N1	-2.30	1.33	1.38
1	L5	1677	PSU	O5'-C5'	-2.30	1.41	1.44
1	L5	4442	PSU	C2-N3	-2.29	1.33	1.38
1	L5	237	B9B	O5'-C5'	-2.29	1.41	1.44
1	L5	1683	PSU	O5'-C5'	-2.28	1.41	1.44
47	S2	823	PSU	C2-N1	-2.27	1.33	1.38
1	L5	4415	1MA	O5'-C5'	-2.27	1.41	1.44
1	L5	1582	PSU	C2-N3	-2.27	1.33	1.38
1	L5	3715	PSU	C2-N1	-2.27	1.33	1.38
1	L5	4442	PSU	O4'-C1'	-2.26	1.41	1.44
1	L5	4531	PSU	O5'-C5'	-2.25	1.41	1.44
47	S2	1710	OMC	O5'-C5'	-2.24	1.41	1.44
1	L5	1883	OMG	O5'-C5'	-2.24	1.41	1.44
1	L5	3762	B8H	O4'-C1'	-2.23	1.41	1.44
47	S2	1842	4AC	C4-N4	-2.23	1.35	1.40
47	S2	823	PSU	O4'-C1'	-2.22	1.41	1.44
1	L5	4500	PSU	C2-N1	-2.22	1.33	1.38
3	L8	14	OMU	C6-N1	-2.22	1.32	1.35
1	L5	4636	PSU	C2-N1	-2.21	1.33	1.38
1	L5	3715	PSU	C2-N3	-2.21	1.33	1.38
1	L5	1677	PSU	C2-N3	-2.21	1.33	1.38
47	S2	1337	4AC	C2-N3	-2.21	1.33	1.38
47	S2	1806	M7A	C5-N7	-2.21	1.33	1.38
1	L5	1659	I4U	C6-N1	-2.20	1.32	1.35
1	L5	4500	PSU	O5'-C5'	-2.20	1.41	1.44
47	S2	1081	PSU	O4'-C1'	-2.19	1.41	1.44
1	L5	4564	M7A	O5'-C5'	-2.19	1.41	1.44
1	L5	4494	OMG	O5'-C5'	-2.19	1.41	1.44
1	L5	4536	OMC	O5'-C5'	-2.19	1.41	1.44
1	L5	3715	PSU	O4'-C1'	-2.19	1.41	1.44
1	L5	3729	PSU	O4'-C1'	-2.18	1.41	1.44
1	L5	3825	A2M	O5'-C5'	-2.17	1.41	1.44
1	L5	3729	PSU	C2-N1	-2.17	1.33	1.38
47	S2	1248	B8N	O4'-C1'	-2.16	1.41	1.44
1	L5	4306	OMU	O5'-C5'	-2.16	1.41	1.44
1	L5	4355	E6G	O5'-C5'	-2.16	1.41	1.44
1	L5	4447	5MC	C2-N3	-2.16	1.33	1.38
1	L5	3869	OMC	O5'-C5'	-2.15	1.41	1.44
47	S2	1337	4AC	C6-N1	-2.14	1.32	1.35
1	L5	3880	P7G	O5'-C5'	-2.14	1.41	1.44
47	S2	683	OMG	O5'-C5'	-2.14	1.41	1.44
1	L5	2804	OMC	O5'-C5'	-2.14	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4500	PSU	C2-N3	-2.13	1.33	1.38
1	L5	1683	PSU	O4'-C1'	-2.13	1.41	1.44
47	S2	119	PSU	O4'-C1'	-2.12	1.41	1.44
1	L5	4637	OMG	O5'-C5'	-2.12	1.41	1.44
47	S2	1243	PSU	O4'-C1'	-2.11	1.41	1.44
1	L5	4185	B8W	O5'-C5'	-2.11	1.41	1.44
47	S2	1337	4AC	O5'-C5'	-2.10	1.41	1.44
1	L5	4403	PSU	O4'-C1'	-2.10	1.41	1.44
47	S2	116	OMU	C2-N3	-2.10	1.34	1.38
1	L5	4447	5MC	O5'-C5'	-2.10	1.41	1.44
47	S2	1243	PSU	O5'-C5'	-2.09	1.41	1.44
1	L5	4628	PSU	O4'-C1'	-2.09	1.41	1.44
1	L5	4671	B8T	C2-N3	-2.09	1.34	1.38
1	L5	4220	6MZ	O5'-C5'	-2.09	1.41	1.44
1	L5	3909	OMC	C2-N3	-2.08	1.34	1.38
1	L5	4529	B8W	O5'-C5'	-2.08	1.41	1.44
1	L5	2401	A2M	O5'-C5'	-2.07	1.41	1.44
1	L5	4872	2MG	C4-N3	-2.07	1.32	1.35
1	L5	4442	PSU	C2-N1	-2.07	1.34	1.38
1	L5	3729	PSU	C2-N3	-2.06	1.34	1.38
1	L5	1582	PSU	O5'-C5'	-2.06	1.41	1.44
1	L5	4296	B8H	O5'-C5'	-2.05	1.41	1.44
1	L5	1625	OMG	O5'-C5'	-2.05	1.41	1.44
1	L5	4620	OMU	O5'-C5'	-2.04	1.41	1.44
1	L5	4403	PSU	O5'-C5'	-2.04	1.41	1.44
1	L5	1322	1MA	O5'-C5'	-2.03	1.41	1.44
1	L5	4335	5MC	O5'-C5'	-2.03	1.41	1.44
1	L5	4571	A2M	O5'-C5'	-2.03	1.41	1.44
1	L5	4531	PSU	C2-N1	-2.03	1.34	1.38
47	S2	1842	4AC	O5'-C5'	-2.02	1.41	1.44
1	L5	3701	OMC	O5'-C5'	-2.02	1.41	1.44
1	L5	2861	OMC	C2-N3	-2.01	1.34	1.38
1	L5	1871	A2M	O5'-C5'	-2.01	1.42	1.44
1	L5	4870	OMG	O5'-C5'	-2.01	1.42	1.44
1	L5	3887	OMC	O5'-C5'	-2.00	1.42	1.44
47	S2	1337	4AC	C7-N4	-2.00	1.32	1.35
47	S2	1081	PSU	O5'-C5'	-2.00	1.42	1.44
1	L5	2363	A2M	O5'-C5'	-2.00	1.42	1.44
47	S2	1806	M7A	C5-C4	2.02	1.48	1.40
1	L5	4623	OMG	C5-C4	2.03	1.45	1.40
1	L5	1574	B9B	O6-C6	2.05	1.36	1.35
1	L5	1316	OMG	C5-C4	2.08	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	568	E3C	C2-N1	2.11	1.41	1.38
1	L5	4523	A2M	C5-C4	2.12	1.45	1.40
47	S2	568	E3C	C6-C5	2.16	1.38	1.32
1	L5	2050	OMG	C5-C4	2.17	1.45	1.40
1	L5	2364	OMG	C5-C4	2.18	1.45	1.40
47	S2	683	OMG	C5-C4	2.18	1.45	1.40
1	L5	2786	B9H	C6-C5	2.18	1.38	1.32
1	L5	4185	B8W	C5-C4	2.19	1.45	1.40
1	L5	3785	A2M	C5-C4	2.21	1.45	1.40
1	L5	1322	1MA	C5-C4	2.22	1.45	1.40
1	L5	1326	A2M	C5-C4	2.23	1.45	1.40
47	S2	509	OMG	C5-C4	2.24	1.45	1.40
1	L5	1522	OMG	C5-C4	2.25	1.45	1.40
1	L5	373	OMG	C5-C4	2.25	1.45	1.40
47	S2	1850	MA6	C5-C4	2.26	1.45	1.40
1	L5	2363	A2M	C5-C4	2.28	1.45	1.40
1	L5	1871	A2M	C5-C4	2.29	1.45	1.40
1	L5	1517	2MG	C5-C4	2.31	1.45	1.40
1	L5	978	2MG	C5-C4	2.32	1.45	1.40
1	L5	1883	OMG	C5-C4	2.33	1.45	1.40
47	S2	1678	A2M	C5-C4	2.33	1.45	1.40
1	L5	1574	B9B	C5-C4	2.33	1.45	1.40
47	S2	668	A2M	C5-C4	2.34	1.45	1.40
47	S2	1219	B8Q	C6-C5	2.34	1.38	1.32
1	L5	4220	6MZ	C5-C4	2.35	1.45	1.40
1	L5	729	2MG	C5-C4	2.35	1.45	1.40
1	L5	4415	1MA	C2-N3	2.37	1.34	1.30
47	S2	644	OMG	C5-C4	2.37	1.45	1.40
1	L5	2401	A2M	C5-C4	2.38	1.45	1.40
1	L5	1456	B8Q	C6-C5	2.39	1.38	1.32
1	L5	4494	OMG	C5-C4	2.39	1.45	1.40
1	L5	1524	A2M	C5-C4	2.43	1.46	1.40
1	L5	3867	A2M	C5-C4	2.44	1.46	1.40
1	L5	4370	OMG	C5-C4	2.44	1.46	1.40
1	L5	3718	A2M	C5-C4	2.45	1.46	1.40
1	L5	4623	OMG	C6-C5	2.45	1.46	1.41
1	L5	4637	OMG	C5-C4	2.46	1.46	1.40
47	S2	27	A2M	C5-C4	2.47	1.46	1.40
1	L5	3792	OMG	C5-C4	2.48	1.46	1.40
1	L5	4571	A2M	C5-C4	2.48	1.46	1.40
1	L5	2424	OMG	C5-C4	2.50	1.46	1.40
47	S2	1031	A2M	C5-C4	2.51	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4196	OMG	C5-C4	2.52	1.46	1.40
47	S2	484	A2M	C5-C4	2.53	1.46	1.40
1	L5	4371	MHG	C5-C4	2.54	1.46	1.39
1	L5	4550	7MG	C5-C4	2.55	1.46	1.39
47	S2	1851	MA6	C5-C4	2.56	1.46	1.40
1	L5	1534	A2M	C5-C4	2.56	1.46	1.40
1	L5	1625	OMG	C5-C4	2.59	1.46	1.40
1	L5	398	A2M	C5-C4	2.60	1.46	1.40
1	L5	1883	OMG	C6-C5	2.60	1.46	1.41
1	L5	2050	OMG	C6-C5	2.60	1.46	1.41
1	L5	2754	B9B	C5-C4	2.60	1.46	1.40
1	L5	1909	P7G	C5-C4	2.61	1.46	1.39
1	L5	4870	OMG	C5-C4	2.61	1.46	1.40
1	L5	3825	A2M	C5-C4	2.62	1.46	1.40
47	S2	166	A2M	C5-C4	2.63	1.46	1.40
1	L5	4529	B8W	C5-C4	2.66	1.46	1.40
47	S2	1832	6MZ	C5-C4	2.69	1.46	1.40
1	L5	237	B9B	C5-C4	2.69	1.46	1.40
1	L5	1797	E7G	C5-C4	2.71	1.46	1.39
1	L5	4355	E6G	C5-C4	2.71	1.46	1.40
1	L5	2773	OMG	C5-C4	2.71	1.46	1.40
1	L5	2380	B8W	C5-C4	2.72	1.46	1.40
1	L5	2364	OMG	C6-C5	2.72	1.46	1.41
1	L5	1605	7MG	C5-C4	2.73	1.46	1.39
1	L5	2297	E7G	C5-C4	2.74	1.46	1.39
1	L5	1316	OMG	C6-C5	2.77	1.46	1.41
1	L5	3723	A2M	C5-C4	2.78	1.46	1.40
47	S2	159	A2M	C5-C4	2.80	1.46	1.40
1	L5	3880	P7G	C5-C4	2.81	1.46	1.39
1	L5	2522	7MG	C5-C4	2.81	1.46	1.39
1	L5	4415	1MA	C5-C4	2.82	1.46	1.40
1	L5	4370	OMG	C6-C5	2.84	1.46	1.41
1	L5	3897	B8K	C5-C4	2.84	1.46	1.39
1	L5	2424	OMG	C6-C5	2.88	1.46	1.41
1	L5	4690	B8K	C5-C4	2.89	1.47	1.39
1	L5	4472	B8W	C5-C4	2.89	1.47	1.40
47	S2	1219	B8Q	C2-N3	2.91	1.40	1.35
1	L5	1625	OMG	C6-C5	2.94	1.47	1.41
47	S2	683	OMG	C6-C5	2.96	1.47	1.41
1	L5	1522	OMG	C6-C5	2.96	1.47	1.41
1	L5	2786	B9H	C2-N3	2.96	1.41	1.37
1	L5	1456	B8Q	C2-N3	2.97	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2754	B9B	O6-C6	3.01	1.37	1.35
1	L5	1517	2MG	C6-C5	3.03	1.47	1.41
1	L5	373	OMG	C6-C5	3.04	1.47	1.41
1	L5	4494	OMG	C6-C5	3.05	1.47	1.41
47	S2	568	E3C	C2-N3	3.05	1.41	1.37
47	S2	644	OMG	C6-C5	3.07	1.47	1.41
1	L5	3899	BGH	C5-C4	3.10	1.47	1.39
1	L5	4637	OMG	C6-C5	3.11	1.47	1.41
1	L5	3792	OMG	C6-C5	3.14	1.47	1.41
1	L5	978	2MG	C6-C5	3.14	1.47	1.41
1	L5	729	2MG	C6-C5	3.16	1.47	1.41
47	S2	509	OMG	C6-C5	3.16	1.47	1.41
1	L5	4129	B8W	C5-C4	3.20	1.47	1.40
1	L5	4196	OMG	C6-C5	3.22	1.47	1.41
6	LC	333	MLZ	CA-C	3.24	1.54	1.50
1	L5	4355	E6G	O6-C6	3.26	1.37	1.35
1	L5	4415	1MA	C6-N6	3.28	1.35	1.27
1	L5	1322	1MA	C6-N6	3.31	1.35	1.27
1	L5	2773	OMG	C6-C5	3.37	1.47	1.41
1	L5	237	B9B	O6-C6	3.41	1.37	1.35
1	L5	1322	1MA	C6-C5	3.47	1.47	1.41
1	L5	4870	OMG	C6-C5	3.61	1.48	1.41
1	L5	3782	5MC	C5-C4	3.63	1.46	1.41
1	L5	4872	2MG	C6-C5	3.64	1.48	1.41
1	L5	4415	1MA	C6-C5	3.70	1.47	1.41
1	L5	4447	5MC	C5-C4	3.71	1.46	1.41
1	L5	3880	P7G	C6-C5	3.95	1.46	1.41
1	L5	3897	B8K	C6-C5	4.20	1.46	1.41
1	L5	4550	7MG	C6-C5	4.32	1.46	1.41
47	S2	1374	5MC	C5-C4	4.33	1.47	1.41
1	L5	4690	B8K	C6-C5	4.46	1.46	1.41
1	L5	2297	E7G	C6-C5	4.55	1.46	1.41
1	L5	1909	P7G	C6-C5	4.58	1.46	1.41
1	L5	2522	7MG	C6-C5	4.63	1.46	1.41
1	L5	4371	MHG	C6-C5	4.84	1.47	1.41
1	L5	4335	5MC	C5-C4	4.84	1.48	1.41
41	Lm	98	MLZ	CA-C	4.90	1.56	1.50
1	L5	1797	E7G	C6-C5	4.97	1.47	1.41
1	L5	1605	7MG	C6-C5	5.04	1.47	1.41
1	L5	3899	BGH	C6-C5	6.06	1.48	1.41
1	L5	3899	BGH	C2-N2	6.65	1.47	1.34

All (543) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1081	PSU	N1-C2-N3	-9.71	121.41	128.40
1	L5	3715	PSU	N1-C2-N3	-9.58	121.51	128.40
1	L5	4403	PSU	N1-C2-N3	-9.18	121.79	128.40
1	L5	1677	PSU	C5-C4-N3	-9.08	117.98	125.43
1	L5	3764	PSU	N1-C2-N3	-9.08	121.87	128.40
1	L5	1582	PSU	N1-C2-N3	-9.01	121.92	128.40
1	L5	4636	PSU	N1-C2-N3	-8.94	121.97	128.40
1	L5	4293	PSU	N1-C2-N3	-8.90	122.00	128.40
1	L5	3729	PSU	N1-C2-N3	-8.90	122.00	128.40
47	S2	823	PSU	N1-C2-N3	-8.88	122.01	128.40
47	S2	1243	PSU	C5-C4-N3	-8.86	118.16	125.43
1	L5	4450	PSU	N1-C2-N3	-8.81	122.06	128.40
1	L5	4531	PSU	N1-C2-N3	-8.79	122.08	128.40
1	L5	3729	PSU	C5-C4-N3	-8.71	118.28	125.43
1	L5	2508	PSU	N1-C2-N3	-8.69	122.15	128.40
47	S2	822	PSU	C5-C4-N3	-8.68	118.31	125.43
1	L5	4531	PSU	C5-C4-N3	-8.64	118.34	125.43
47	S2	1243	PSU	N1-C2-N3	-8.63	122.19	128.40
47	S2	119	PSU	N1-C2-N3	-8.58	122.23	128.40
1	L5	4442	PSU	N1-C2-N3	-8.54	122.26	128.40
1	L5	3764	PSU	C5-C4-N3	-8.49	118.47	125.43
1	L5	4403	PSU	C5-C4-N3	-8.47	118.48	125.43
1	L5	4628	PSU	N1-C2-N3	-8.46	122.31	128.40
1	L5	4500	PSU	C5-C4-N3	-8.45	118.50	125.43
1	L5	4628	PSU	C5-C4-N3	-8.41	118.53	125.43
47	S2	1081	PSU	C5-C4-N3	-8.40	118.54	125.43
1	L5	4500	PSU	N1-C2-N3	-8.40	122.36	128.40
1	L5	1677	PSU	N1-C2-N3	-8.31	122.42	128.40
47	S2	612	PSU	C5-C4-N3	-8.29	118.62	125.43
47	S2	822	PSU	N1-C2-N3	-8.27	122.45	128.40
1	L5	4450	PSU	C5-C4-N3	-8.23	118.67	125.43
1	L5	1683	PSU	C5-C4-N3	-8.19	118.71	125.43
1	L5	4442	PSU	C5-C4-N3	-8.18	118.72	125.43
1	L5	2508	PSU	C5-C4-N3	-8.12	118.77	125.43
47	S2	612	PSU	N1-C2-N3	-8.06	122.60	128.40
1	L5	1683	PSU	N1-C2-N3	-8.04	122.61	128.40
47	S2	119	PSU	C5-C4-N3	-7.99	118.88	125.43
1	L5	4371	MHG	C8-N7-C71	-7.98	109.46	122.80
1	L5	1582	PSU	C5-C4-N3	-7.92	118.93	125.43
1	L5	4636	PSU	C5-C4-N3	-7.87	118.97	125.43
1	L5	4293	PSU	C5-C4-N3	-7.84	119.00	125.43
1	L5	3715	PSU	C5-C4-N3	-7.69	119.12	125.43
1	L5	1909	P7G	C8-N7-C71	-7.65	110.01	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3762	B8H	C5-C4-N3	-7.51	119.27	125.43
47	S2	823	PSU	C5-C4-N3	-7.44	119.33	125.43
1	L5	1860	B8H	C5-C4-N3	-7.18	119.54	125.43
1	L5	4296	B8H	C5-C4-N3	-7.10	119.61	125.43
1	L5	3825	A2M	N3-C2-N1	-7.03	122.74	128.86
47	S2	1850	MA6	N3-C2-N1	-6.95	122.81	128.86
1	L5	398	A2M	N3-C2-N1	-6.66	123.06	128.86
1	L5	1871	A2M	N3-C2-N1	-6.62	123.09	128.86
1	L5	4523	A2M	N3-C2-N1	-6.59	123.12	128.86
47	S2	1851	MA6	N3-C2-N1	-6.51	123.19	128.86
1	L5	4571	A2M	N3-C2-N1	-6.50	123.19	128.86
1	L5	3880	P7G	C8-N7-C71	-6.49	111.94	122.80
47	S2	1678	A2M	N3-C2-N1	-6.39	123.29	128.86
1	L5	2401	A2M	N3-C2-N1	-6.38	123.30	128.86
47	S2	27	A2M	N3-C2-N1	-6.37	123.31	128.86
47	S2	166	A2M	N3-C2-N1	-6.22	123.44	128.86
47	S2	1031	A2M	N3-C2-N1	-6.22	123.44	128.86
47	S2	814	5MU	C5-C4-N3	-6.02	118.60	125.24
1	L5	1534	A2M	N3-C2-N1	-6.02	123.62	128.86
1	L5	2363	A2M	N3-C2-N1	-5.99	123.64	128.86
1	L5	1326	A2M	N3-C2-N1	-5.96	123.67	128.86
47	S2	668	A2M	N3-C2-N1	-5.95	123.68	128.86
1	L5	4083	5MU	C5-C4-N3	-5.77	118.88	125.24
1	L5	4220	6MZ	N3-C2-N1	-5.72	123.87	128.86
1	L5	3718	A2M	N3-C2-N1	-5.66	123.92	128.86
1	L5	4447	5MC	CM5-C5-C4	-5.65	115.84	121.65
1	L5	1524	A2M	N3-C2-N1	-5.64	123.95	128.86
1	L5	3880	P7G	C5-C4-N3	-5.59	117.14	126.47
1	L5	4690	B8K	C5-C4-N3	-5.53	117.25	126.47
47	S2	1832	6MZ	N3-C2-N1	-5.50	124.06	128.86
1	L5	4872	2MG	CM2-N2-C2	-5.50	116.94	123.63
1	L5	3723	A2M	N3-C2-N1	-5.46	124.10	128.86
47	S2	484	A2M	N3-C2-N1	-5.42	124.14	128.86
1	L5	3785	A2M	N3-C2-N1	-5.33	124.22	128.86
1	L5	1797	E7G	C5-C4-N3	-5.24	117.73	126.47
1	L5	3867	A2M	N3-C2-N1	-5.03	124.48	128.86
1	L5	1909	P7G	C5-C4-N3	-5.01	118.10	126.47
1	L5	3880	P7G	C5-C6-N1	-5.01	115.51	123.37
1	L5	2522	7MG	C5-C6-N1	-4.98	115.56	123.37
1	L5	2297	E7G	C5-C4-N3	-4.93	118.24	126.47
1	L5	4872	2MG	C4-C5-N7	-4.90	104.67	109.41
1	L5	2522	7MG	C5-C4-N3	-4.90	118.30	126.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1605	7MG	C5-C4-N3	-4.87	118.34	126.47
1	L5	4872	2MG	C6-C5-C4	-4.86	116.02	120.84
1	L5	4550	7MG	C5-C4-N3	-4.76	118.53	126.47
1	L5	3899	BGH	C5-C6-N1	-4.74	115.94	123.37
1	L5	1605	7MG	C5-C6-N1	-4.72	115.96	123.37
1	L5	3897	B8K	C5-C6-N1	-4.71	115.99	123.37
47	S2	159	A2M	N3-C2-N1	-4.65	124.81	128.86
1	L5	1909	P7G	C5-C6-N1	-4.60	116.15	123.37
1	L5	4371	MHG	C5-C6-N1	-4.55	116.22	123.37
1	L5	4636	PSU	C5-C6-N1	-4.47	118.59	124.39
1	L5	1797	E7G	C5-C6-N1	-4.46	116.37	123.37
1	L5	2297	E7G	C5-C6-N1	-4.41	116.45	123.37
47	S2	1850	MA6	C4-C5-N7	-4.39	105.16	109.41
1	L5	4690	B8K	C5-C6-N1	-4.38	116.50	123.37
1	L5	4531	PSU	C5-C6-N1	-4.34	118.77	124.39
1	L5	3899	BGH	C5-C4-N3	-4.31	119.28	126.47
1	L5	4442	PSU	C5-C6-N1	-4.30	118.82	124.39
47	S2	1337	4AC	C4-N4-C7	-4.26	123.62	128.16
1	L5	4500	PSU	C5-C6-N1	-4.26	118.87	124.39
1	L5	4450	PSU	C5-C6-N1	-4.26	118.87	124.39
1	L5	1316	OMG	C6-C5-C4	-4.25	116.62	120.84
1	L5	1522	OMG	C6-C5-C4	-4.23	116.64	120.84
1	L5	4872	2MG	C1'-N9-C4	-4.20	119.37	126.64
1	L5	978	2MG	C6-C5-C4	-4.20	116.67	120.84
1	L5	2773	OMG	C6-C5-C4	-4.18	116.69	120.84
1	L5	4550	7MG	C5-C6-N1	-4.16	116.84	123.37
47	S2	1851	MA6	C4-C5-N7	-4.16	105.39	109.41
1	L5	4623	OMG	C6-C5-C4	-4.15	116.71	120.84
1	L5	373	OMG	C6-C5-C4	-4.14	116.73	120.84
1	L5	3792	OMG	C6-C5-C4	-4.08	116.79	120.84
1	L5	4529	B8W	C4-C5-N7	-4.07	105.48	109.41
1	L5	4371	MHG	C5-C4-N3	-4.05	119.70	126.47
1	L5	3897	B8K	C5-C4-N3	-4.04	119.73	126.47
1	L5	4494	OMG	C6-C5-C4	-4.01	116.86	120.84
47	S2	509	OMG	C5-C6-N1	-3.99	117.80	123.48
1	L5	729	2MG	C6-C5-C4	-3.99	116.87	120.84
1	L5	4870	OMG	C6-C5-C4	-3.97	116.89	120.84
47	S2	612	PSU	C5-C6-N1	-3.96	119.26	124.39
1	L5	2773	OMG	C5-C6-N1	-3.94	117.87	123.48
1	L5	1677	PSU	C5-C1'-C2'	-3.94	108.76	115.55
47	S2	568	E3C	O2-C2-N3	-3.93	117.27	122.12
1	L5	1625	OMG	C5-C6-N1	-3.91	117.91	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2364	OMG	C5-C6-N1	-3.90	117.94	123.48
47	S2	644	OMG	C5-C6-N1	-3.86	117.99	123.48
1	L5	3762	B8H	C5-C1'-C2'	-3.85	108.91	115.55
1	L5	4637	OMG	C6-C5-C4	-3.85	117.02	120.84
1	L5	4220	6MZ	C9-N6-C6	-3.83	119.57	122.85
47	S2	823	PSU	C5-C6-N1	-3.81	119.45	124.39
1	L5	2050	OMG	C6-C5-C4	-3.81	117.05	120.84
47	S2	683	OMG	C5-C6-N1	-3.81	118.06	123.48
1	L5	1883	OMG	C6-C5-C4	-3.79	117.07	120.84
1	L5	4494	OMG	C5-C6-N1	-3.79	118.08	123.48
1	L5	4870	OMG	C5-C6-N1	-3.78	118.10	123.48
47	S2	644	OMG	C6-C5-C4	-3.74	117.12	120.84
47	S2	822	PSU	C5-C6-N1	-3.71	119.58	124.39
47	S2	568	E3C	C1'-N1-C6	-3.69	112.67	120.78
47	S2	509	OMG	C6-C5-C4	-3.67	117.19	120.84
1	L5	4196	OMG	C5-C6-N1	-3.66	118.27	123.48
1	L5	4370	OMG	C6-C5-C4	-3.64	117.22	120.84
1	L5	978	2MG	C5-C6-N1	-3.64	118.30	123.48
1	L5	2424	OMG	C5-C6-N1	-3.60	118.36	123.48
1	L5	1524	A2M	C4'-O4'-C1'	-3.59	105.94	109.77
47	S2	683	OMG	N3-C2-N1	-3.58	122.24	127.46
1	L5	373	OMG	C5-C6-N1	-3.55	118.43	123.48
47	S2	683	OMG	C6-C5-C4	-3.53	117.33	120.84
1	L5	4403	PSU	C5-C6-N1	-3.52	119.82	124.39
1	L5	2508	PSU	C5-C6-N1	-3.52	119.83	124.39
1	L5	4196	OMG	C6-C5-C4	-3.51	117.36	120.84
1	L5	2424	OMG	C6-C5-C4	-3.51	117.36	120.84
1	L5	4623	OMG	N3-C2-N1	-3.50	122.34	127.46
1	L5	4637	OMG	C5-C6-N1	-3.50	118.50	123.48
1	L5	2364	OMG	C6-C5-C4	-3.49	117.37	120.84
1	L5	1316	OMG	C4-C5-N7	-3.49	106.04	109.41
47	S2	119	PSU	C5-C6-N1	-3.48	119.88	124.39
1	L5	1677	PSU	C5-C6-N1	-3.48	119.88	124.39
1	L5	1522	OMG	C5-C6-N1	-3.46	118.55	123.48
1	L5	3792	OMG	C5-C6-N1	-3.46	118.55	123.48
1	L5	1517	2MG	C6-C5-C4	-3.44	117.42	120.84
47	S2	1806	M7A	C5-C4-N3	-3.43	118.06	126.61
1	L5	4494	OMG	N3-C2-N1	-3.43	122.46	127.46
1	L5	1683	PSU	C5-C6-N1	-3.42	119.96	124.39
1	L5	2050	OMG	C5-C6-N1	-3.41	118.63	123.48
1	L5	978	2MG	CM2-N2-C2	-3.40	119.49	123.63
1	L5	4472	B8W	C4-C5-N7	-3.39	106.14	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1517	2MG	CM2-N2-C2	-3.38	119.52	123.63
1	L5	4293	PSU	C5-C6-N1	-3.38	120.01	124.39
1	L5	729	2MG	C5-C6-N1	-3.37	118.68	123.48
1	L5	4370	OMG	C5-C6-N1	-3.37	118.68	123.48
1	L5	4447	5MC	C5-C6-N1	-3.37	118.50	122.15
1	L5	1582	PSU	C5-C6-N1	-3.36	120.03	124.39
1	L5	1316	OMG	N3-C2-N1	-3.36	122.56	127.46
1	L5	4623	OMG	C5-C6-N1	-3.34	118.72	123.48
1	L5	4129	B8W	C4-C5-N7	-3.34	106.18	109.41
1	L5	1574	B9B	N3-C2-N1	-3.33	122.59	127.46
1	L5	1522	OMG	C4-C5-N7	-3.33	106.19	109.41
1	L5	373	OMG	N3-C2-N1	-3.33	122.60	127.46
47	S2	1243	PSU	C5-C1'-C2'	-3.32	109.81	115.55
1	L5	4564	M7A	C5-C4-N3	-3.32	118.32	126.61
1	L5	4296	B8H	C5-C1'-C2'	-3.32	109.82	115.55
1	L5	237	B9B	N3-C2-N1	-3.32	122.61	127.46
1	L5	4185	B8W	N3-C2-N1	-3.32	122.62	127.46
1	L5	2773	OMG	N3-C2-N1	-3.29	122.66	127.46
1	L5	4472	B8W	N3-C2-N1	-3.28	122.67	127.46
1	L5	4529	B8W	N3-C2-N1	-3.27	122.68	127.46
1	L5	1517	2MG	C5-C6-N1	-3.27	118.82	123.48
47	S2	1243	PSU	C5-C6-N1	-3.26	120.16	124.39
47	S2	509	OMG	C4-C5-N7	-3.26	106.26	109.41
1	L5	4872	2MG	C5-C6-N1	-3.25	118.85	123.48
1	L5	3764	PSU	C5-C6-N1	-3.25	120.17	124.39
1	L5	1625	OMG	C6-C5-C4	-3.24	117.62	120.84
1	L5	4196	OMG	N3-C2-N1	-3.23	122.74	127.46
1	L5	4370	OMG	N3-C2-N1	-3.22	122.75	127.46
1	L5	1316	OMG	C5-C6-N1	-3.22	118.90	123.48
1	L5	3729	PSU	C5-C6-N1	-3.20	120.24	124.39
1	L5	1683	PSU	C5-C1'-C2'	-3.20	110.04	115.55
1	L5	4129	B8W	N3-C2-N1	-3.19	122.80	127.46
1	L5	3792	OMG	N3-C2-N1	-3.17	122.83	127.46
1	L5	1326	A2M	C4-C5-N7	-3.16	106.36	109.41
1	L5	1883	OMG	C5-C6-N1	-3.12	119.04	123.48
1	L5	398	A2M	C4-C5-N7	-3.07	106.44	109.41
47	S2	1842	4AC	C5-C4-N3	-3.06	118.11	123.21
1	L5	4293	PSU	C5-C1'-C2'	-3.05	110.29	115.55
1	L5	1797	E7G	C8-N7-C71	-3.04	112.94	120.34
1	L5	4564	M7A	N1-C2-N3	-3.04	123.72	128.65
1	L5	4628	PSU	C5-C6-N1	-3.01	120.48	124.39
47	S2	1031	A2M	C4-C5-N7	-3.01	106.50	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1883	OMG	N3-C2-N1	-3.01	123.07	127.46
1	L5	2050	OMG	N3-C2-N1	-3.00	123.08	127.46
1	L5	4355	E6G	N3-C2-N1	-2.99	123.10	127.46
1	L5	4637	OMG	N3-C2-N1	-2.98	123.11	127.46
47	S2	27	A2M	C4-C5-N7	-2.97	106.54	109.41
1	L5	1522	OMG	N3-C2-N1	-2.97	123.12	127.46
1	L5	3715	PSU	C5-C6-N1	-2.94	120.57	124.39
1	L5	4442	PSU	C5-C1'-C2'	-2.94	110.48	115.55
41	Lm	98	MLZ	CB-CA-C	-2.90	106.86	111.65
47	S2	644	OMG	N3-C2-N1	-2.90	123.22	127.46
1	L5	2424	OMG	N3-C2-N1	-2.90	123.23	127.46
1	L5	1625	OMG	N3-C2-N1	-2.89	123.23	127.46
1	L5	1534	A2M	C4-C5-N7	-2.88	106.63	109.41
1	L5	4415	1MA	C4-C5-N7	-2.86	106.64	109.41
1	L5	4870	OMG	C4-C5-N7	-2.86	106.64	109.41
1	L5	3723	A2M	C4-C5-N7	-2.86	106.65	109.41
1	L5	978	2MG	C4-C5-N7	-2.81	106.69	109.41
47	S2	484	A2M	C4-C5-N7	-2.80	106.70	109.41
1	L5	2364	OMG	C4-C5-N7	-2.80	106.71	109.41
1	L5	4870	OMG	N3-C2-N1	-2.78	123.39	127.46
47	S2	1842	4AC	O7-C7-CM7	-2.78	116.99	122.06
1	L5	373	OMG	C4-C5-N7	-2.78	106.72	109.41
1	L5	1456	B8Q	O2-C2-N3	-2.77	118.86	122.95
1	L5	2380	B8W	C4-C5-N7	-2.77	106.74	109.41
1	L5	2380	B8W	N3-C2-N1	-2.76	123.42	127.46
1	L5	2364	OMG	N3-C2-N1	-2.75	123.44	127.46
1	L5	2401	A2M	C4-C5-N7	-2.75	106.75	109.41
1	L5	3792	OMG	C4-C5-N7	-2.75	106.75	109.41
1	L5	4355	E6G	C4-C5-N7	-2.74	106.76	109.41
1	L5	4637	OMG	C4-C5-N7	-2.72	106.78	109.41
1	L5	1860	B8H	C5-C1'-C2'	-2.72	110.86	115.55
47	S2	509	OMG	N3-C2-N1	-2.71	123.50	127.46
1	L5	2754	B9B	N3-C2-N1	-2.71	123.50	127.46
47	S2	1678	A2M	C4-C5-N7	-2.71	106.79	109.41
47	S2	1081	PSU	C5-C6-N1	-2.71	120.88	124.39
1	L5	3718	A2M	C4-C5-N7	-2.70	106.80	109.41
1	L5	1871	A2M	C4-C5-N7	-2.69	106.81	109.41
47	S2	159	A2M	C4-C5-N7	-2.68	106.83	109.41
1	L5	4872	2MG	N2-C2-N3	-2.66	114.37	116.95
47	S2	683	OMG	C4-C5-N7	-2.66	106.84	109.41
1	L5	4671	B8T	C41-N4-C4	-2.64	120.66	122.94
1	L5	4494	OMG	C4-C5-N7	-2.63	106.87	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	729	2MG	C4-C5-N7	-2.62	106.87	109.41
1	L5	3785	A2M	C4-C5-N7	-2.61	106.89	109.41
47	S2	1832	6MZ	C4-C5-N7	-2.61	106.89	109.41
47	S2	1219	B8Q	O2-C2-N3	-2.61	119.10	122.95
1	L5	2508	PSU	C5-C1'-C2'	-2.60	111.06	115.55
47	S2	644	OMG	C4-C5-N7	-2.59	106.91	109.41
1	L5	2773	OMG	C4-C5-N7	-2.59	106.91	109.41
1	L5	4872	2MG	N3-C2-N1	-2.57	122.34	126.23
1	L5	4628	PSU	C5-C1'-C2'	-2.56	111.13	115.55
1	L5	4196	OMG	C4-C5-N7	-2.55	106.95	109.41
1	L5	4571	A2M	C4-C5-N7	-2.55	106.95	109.41
1	L5	4220	6MZ	C4-C5-N7	-2.55	106.95	109.41
47	S2	1806	M7A	N1-C2-N3	-2.53	124.54	128.65
1	L5	3867	A2M	C4-C5-N7	-2.52	106.98	109.41
1	L5	4531	PSU	C5-C1'-C2'	-2.51	111.22	115.55
1	L5	4637	OMG	C4'-O4'-C1'	-2.50	107.10	109.77
1	L5	2297	E7G	C8-N7-C71	-2.49	114.28	120.34
1	L5	4620	OMU	C6-N1-C2	-2.49	117.25	121.28
1	L5	4185	B8W	C4-C5-N7	-2.48	107.01	109.41
1	L5	978	2MG	N3-C2-N1	-2.48	122.48	126.23
1	L5	4623	OMG	C4-C5-N7	-2.45	107.04	109.41
1	L5	729	2MG	N3-C2-N1	-2.45	122.53	126.23
1	L5	3825	A2M	C4-C5-N7	-2.45	107.04	109.41
1	L5	1517	2MG	N3-C2-N1	-2.43	122.55	126.23
1	L5	4371	MHG	C21-N2-C2	-2.43	120.67	123.63
6	LC	333	MLZ	CB-CA-C	-2.42	107.66	111.65
1	L5	2050	OMG	C4-C5-N7	-2.41	107.08	109.41
47	S2	116	OMU	C6-N1-C2	-2.41	117.37	121.28
47	S2	668	A2M	C4-C5-N7	-2.37	107.12	109.41
1	L5	1524	A2M	C4-C5-N7	-2.36	107.13	109.41
1	L5	4483	B8T	C5-C4-N3	-2.36	119.27	123.21
47	S2	166	A2M	C4-C5-N7	-2.35	107.14	109.41
1	L5	1883	OMG	C4-C5-N7	-2.33	107.16	109.41
47	S2	1337	4AC	C5-C4-N3	-2.32	119.33	123.21
1	L5	3899	BGH	C5'-C4'-C3'	-2.30	106.52	115.29
1	L5	1517	2MG	C4-C5-N7	-2.29	107.19	109.41
41	Lm	98	MLZ	O-C-CA	-2.29	118.71	125.02
1	L5	3899	BGH	O71-C71-N7	-2.27	116.08	120.65
1	L5	3715	PSU	C5-C1'-C2'	-2.27	111.63	115.55
1	L5	4536	OMC	O2'-C2'-C3'	-2.26	105.21	111.21
1	L5	2424	OMG	C5'-C4'-C3'	-2.24	106.75	115.29
1	L5	2424	OMG	C4-C5-N7	-2.24	107.25	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4671	B8T	C5-C4-N3	-2.23	119.48	123.21
1	L5	729	2MG	CM2-N2-C2	-2.16	121.00	123.63
1	L5	3762	B8H	C5-C6-N1	-2.15	118.55	121.51
1	L5	4483	B8T	C41-N4-C4	-2.15	121.09	122.94
1	L5	4335	5MC	C5-C6-N1	-2.13	119.84	122.15
1	L5	2297	E7G	C5-C4-N9	-2.12	103.22	106.31
1	L5	4523	A2M	C4-C5-N7	-2.12	107.36	109.41
1	L5	1574	B9B	C4-C5-N7	-2.11	107.37	109.41
1	L5	4371	MHG	N1-C2-N3	-2.11	123.05	126.23
1	L5	3880	P7G	C5-C4-N9	-2.11	103.25	106.31
1	L5	4306	OMU	C6-N1-C2	-2.10	117.88	121.28
1	L5	2363	A2M	C4-C5-N7	-2.09	107.39	109.41
1	L5	4450	PSU	C5-C1'-C2'	-2.09	111.94	115.55
1	L5	1322	1MA	C4-C5-N7	-2.09	107.39	109.41
1	L5	3869	OMC	O4'-C1'-C2'	-2.09	102.94	106.59
1	L5	1625	OMG	C4-C5-N7	-2.09	107.39	109.41
1	L5	237	B9B	C4-C5-N7	-2.08	107.40	109.41
1	L5	3899	BGH	O4'-C4'-C3'	-2.08	101.03	105.17
47	S2	823	PSU	C5-C1'-C2'	-2.06	112.00	115.55
1	L5	3785	A2M	C4'-O4'-C1'	-2.05	107.58	109.77
47	S2	1081	PSU	O2'-C2'-C1'	-2.05	107.56	112.21
47	S2	1842	4AC	C6-N1-C2	-2.03	117.99	121.28
1	L5	4620	OMU	O4'-C1'-C2'	-2.02	103.06	106.59
1	L5	4628	PSU	O2'-C2'-C1'	-2.02	107.64	112.21
47	S2	612	PSU	C5-C1'-C2'	-2.01	112.07	115.55
1	L5	1316	OMG	O4'-C1'-C2'	-2.01	103.08	106.59
47	S2	121	OMU	O4'-C1'-N1	2.01	112.10	108.08
47	S2	27	A2M	C2-N1-C6	2.02	122.30	118.77
1	L5	2365	OMC	N4-C4-N3	2.02	120.04	116.64
1	L5	3899	BGH	O3'-C3'-C2'	2.02	116.92	111.18
47	S2	823	PSU	O4'-C1'-C2'	2.02	107.70	104.45
47	S2	1031	A2M	C2-N1-C6	2.03	122.32	118.77
47	S2	1219	B8Q	C31-N3-C2	2.03	120.72	117.78
47	S2	1081	PSU	O4'-C1'-C2'	2.03	107.72	104.45
1	L5	3887	OMC	N4-C4-N3	2.04	120.08	116.64
1	L5	237	B9B	O6-C6-N1	2.04	122.33	120.23
47	S2	1337	4AC	N4-C4-N3	2.04	118.10	113.22
1	L5	3880	P7G	N2-C2-N3	2.07	120.55	117.24
1	L5	2297	E7G	C2-N3-C4	2.08	119.78	113.95
1	L5	1605	7MG	C2-N3-C4	2.08	119.81	113.95
1	L5	1677	PSU	O4'-C1'-C2'	2.09	107.81	104.45
1	L5	4550	7MG	C2-N3-C4	2.10	119.84	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4403	PSU	O4'-C1'-C2'	2.10	107.82	104.45
1	L5	2754	B9B	C1'-N9-C4	2.11	130.28	126.64
47	S2	1806	M7A	C2-N1-C6	2.11	122.49	118.78
47	S2	1248	B8N	O4'-C1'-C2'	2.14	107.88	104.45
1	L5	4335	5MC	N4-C4-N3	2.15	120.18	117.00
1	L5	4447	5MC	N4-C4-N3	2.16	120.19	117.00
1	L5	4536	OMC	N4-C4-N3	2.19	120.34	116.64
47	S2	174	OMC	N4-C4-N3	2.21	120.37	116.64
1	L5	4442	PSU	O4'-C1'-C2'	2.22	108.02	104.45
1	L5	4690	B8K	C2-N3-C4	2.23	120.20	113.95
1	L5	1909	P7G	C2-N3-C4	2.23	120.21	113.95
1	L5	2786	B9H	C32-C31-N3	2.23	115.56	112.65
1	L5	3899	BGH	C2-N3-C4	2.23	120.23	113.95
1	L5	1797	E7G	C2-N3-C4	2.24	120.25	113.95
47	S2	822	PSU	O4'-C1'-C2'	2.26	108.08	104.45
1	L5	3867	A2M	C4'-O4'-C1'	2.28	112.19	109.77
1	L5	3762	B8H	CN1-N1-C6	2.28	121.26	118.78
47	S2	1374	5MC	N4-C4-N3	2.29	120.39	117.00
1	L5	4636	PSU	O4'-C1'-C2'	2.32	108.17	104.45
47	S2	612	PSU	O4'-C1'-C2'	2.35	108.22	104.45
1	L5	3762	B8H	O4'-C1'-C2'	2.35	108.22	104.45
1	L5	3782	5MC	N4-C4-N3	2.43	120.59	117.00
1	L5	4403	PSU	C4-C5-C1'	2.44	125.86	121.15
1	L5	1456	B8Q	N3-C2-N1	2.44	120.07	117.16
1	L5	1866	UR3	C3U-N3-C4	2.48	121.44	118.15
1	L5	4620	OMU	O3'-C3'-C4'	2.72	119.03	111.09
47	S2	1842	4AC	C4-N4-C7	2.73	131.07	128.16
1	L5	2786	B9H	O3'-C3'-C4'	2.74	119.09	111.09
1	L5	4564	M7A	C2-N1-C6	2.83	123.76	118.78
1	L5	4447	5MC	CM5-C5-C6	2.92	124.49	118.67
1	L5	4403	PSU	O4'-C1'-C5	2.95	114.50	109.93
1	L5	4355	E6G	C61-O6-C6	2.98	120.64	117.58
47	S2	568	E3C	C32-C31-N3	3.00	120.47	112.65
1	L5	978	2MG	N2-C2-N1	3.08	119.95	116.95
1	L5	4872	2MG	C6-N1-C2	3.25	121.00	115.18
1	L5	4415	1MA	C2-N3-C4	3.32	121.50	116.41
1	L5	1574	B9B	O6-C6-C5	3.34	120.33	115.14
1	L5	1517	2MG	C6-N1-C2	3.40	121.27	115.18
47	S2	1842	4AC	O7-C7-N4	3.40	127.49	123.06
1	L5	2786	B9H	C31-N3-C2	3.42	122.42	117.31
47	S2	1806	M7A	C2-N3-C4	3.42	119.95	111.75
1	L5	4355	E6G	O6-C6-C5	3.46	120.51	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4564	M7A	C2-N3-C4	3.46	120.06	111.75
1	L5	237	B9B	O6-C6-C5	3.48	120.54	115.14
1	L5	2754	B9B	C2-N1-C6	3.48	121.22	116.18
1	L5	1517	2MG	N2-C2-N1	3.51	120.36	116.95
1	L5	1683	PSU	C6-N1-C2	3.61	121.14	115.36
1	L5	4628	PSU	C6-N1-C2	3.65	121.21	115.36
47	S2	1081	PSU	C4-C5-C1'	3.69	128.29	121.15
1	L5	1883	OMG	C6-N1-C2	3.70	121.38	116.06
1	L5	1677	PSU	C6-N1-C2	3.71	121.29	115.36
1	L5	2754	B9B	C61-O6-C6	3.74	125.03	117.39
1	L5	2380	B8W	C2-N1-C6	3.74	121.59	116.18
1	L5	729	2MG	C6-N1-C2	3.75	121.89	115.18
1	L5	3729	PSU	C6-N1-C2	3.80	121.43	115.36
1	L5	978	2MG	C6-N1-C2	3.84	122.06	115.18
47	S2	822	PSU	C6-N1-C2	3.84	121.51	115.36
1	L5	2424	OMG	C6-N1-C2	3.86	121.61	116.06
47	S2	1243	PSU	C6-N1-C2	3.91	121.61	115.36
1	L5	3897	B8K	C72-C71-N7	3.92	122.67	117.65
1	L5	3764	PSU	C6-N1-C2	3.93	121.66	115.36
47	S2	612	PSU	C6-N1-C2	3.94	121.67	115.36
1	L5	1322	1MA	C2-N3-C4	3.95	122.46	116.41
1	L5	1582	PSU	C6-N1-C2	3.96	121.69	115.36
1	L5	3715	PSU	C6-N1-C2	3.96	121.70	115.36
1	L5	2508	PSU	C6-N1-C2	3.97	121.71	115.36
1	L5	4293	PSU	C6-N1-C2	3.97	121.71	115.36
1	L5	1659	I4U	C4-O4-C41	4.00	123.34	117.86
47	S2	119	PSU	C6-N1-C2	4.00	121.76	115.36
1	L5	4870	OMG	C6-N1-C2	4.01	121.83	116.06
1	L5	1316	OMG	C6-N1-C2	4.04	121.87	116.06
1	L5	2050	OMG	C6-N1-C2	4.05	121.89	116.06
1	L5	4355	E6G	C2-N1-C6	4.06	122.04	116.18
1	L5	3792	OMG	C6-N1-C2	4.07	121.92	116.06
47	S2	823	PSU	C6-N1-C2	4.09	121.90	115.36
1	L5	4450	PSU	C6-N1-C2	4.09	121.91	115.36
1	L5	4370	OMG	C6-N1-C2	4.11	121.97	116.06
47	S2	1081	PSU	C6-N1-C2	4.12	121.95	115.36
1	L5	1574	B9B	C2-N3-C4	4.12	119.97	115.16
1	L5	4196	OMG	C6-N1-C2	4.15	122.03	116.06
1	L5	4185	B8W	C2-N1-C6	4.15	122.18	116.18
1	L5	4500	PSU	C6-N1-C2	4.16	122.02	115.36
1	L5	4637	OMG	C6-N1-C2	4.18	122.07	116.06
47	S2	509	OMG	C6-N1-C2	4.18	122.08	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4403	PSU	C6-N1-C2	4.19	122.07	115.36
1	L5	4623	OMG	C6-N1-C2	4.21	122.11	116.06
1	L5	2364	OMG	C2-N3-C4	4.21	120.08	115.16
1	L5	373	OMG	C6-N1-C2	4.23	122.14	116.06
1	L5	2364	OMG	C6-N1-C2	4.25	122.18	116.06
1	L5	1625	OMG	C6-N1-C2	4.26	122.18	116.06
1	L5	1522	OMG	C6-N1-C2	4.27	122.20	116.06
47	S2	683	OMG	C6-N1-C2	4.28	122.22	116.06
1	L5	4442	PSU	C6-N1-C2	4.29	122.22	115.36
47	S2	1851	MA6	C2-N1-C6	4.31	122.41	111.82
1	L5	4531	PSU	C6-N1-C2	4.32	122.27	115.36
1	L5	4636	PSU	C6-N1-C2	4.35	122.32	115.36
1	L5	3880	P7G	C71-N7-C5	4.36	132.34	122.09
47	S2	644	OMG	C6-N1-C2	4.37	122.35	116.06
1	L5	4550	7MG	C6-N1-C2	4.39	122.37	116.06
1	L5	1574	B9B	C2-N1-C6	4.41	122.55	116.18
1	L5	4690	B8K	C6-N1-C2	4.41	122.40	116.06
1	L5	2754	B9B	O6-C6-N1	4.55	124.90	120.23
1	L5	237	B9B	C2-N1-C6	4.56	122.77	116.18
1	L5	4690	B8K	C72-C71-N7	4.56	123.49	117.65
1	L5	1605	7MG	C6-N1-C2	4.58	122.65	116.06
1	L5	2773	OMG	C2-N3-C4	4.58	120.51	115.16
1	L5	4494	OMG	C6-N1-C2	4.60	122.68	116.06
1	L5	1909	P7G	C6-N1-C2	4.61	122.69	116.06
47	S2	1850	MA6	C2-N1-C6	4.61	123.14	111.82
1	L5	4371	MHG	C6-N1-C2	4.61	123.44	115.18
1	L5	4129	B8W	C2-N3-C4	4.64	120.57	115.16
47	S2	509	OMG	C2-N3-C4	4.66	120.59	115.16
1	L5	237	B9B	C2-N3-C4	4.66	120.60	115.16
1	L5	1797	E7G	C6-N1-C2	4.68	122.79	116.06
1	L5	4355	E6G	C2-N3-C4	4.68	120.62	115.16
1	L5	4472	B8W	C2-N3-C4	4.70	120.65	115.16
1	L5	2773	OMG	C6-N1-C2	4.71	122.83	116.06
47	S2	644	OMG	C2-N3-C4	4.71	120.66	115.16
1	L5	4529	B8W	C2-N1-C6	4.73	123.02	116.18
1	L5	1625	OMG	C2-N3-C4	4.76	120.71	115.16
1	L5	4870	OMG	C2-N3-C4	4.76	120.72	115.16
1	L5	2297	E7G	C6-N1-C2	4.77	122.92	116.06
1	L5	4529	B8W	C2-N3-C4	4.79	120.75	115.16
1	L5	4637	OMG	C2-N3-C4	4.87	120.84	115.16
1	L5	2380	B8W	C2-N3-C4	4.90	120.88	115.16
1	L5	1522	OMG	C2-N3-C4	4.90	120.88	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2754	B9B	C2-N3-C4	4.91	120.90	115.16
1	L5	4185	B8W	C2-N3-C4	4.93	120.91	115.16
1	L5	2050	OMG	C2-N3-C4	4.95	120.94	115.16
1	L5	2522	7MG	C6-N1-C2	4.97	123.21	116.06
1	L5	2424	OMG	C2-N3-C4	5.01	121.01	115.16
1	L5	1659	I4U	O4-C4-C5	5.01	121.82	115.74
1	L5	3897	B8K	C6-N1-C2	5.01	123.27	116.06
1	L5	4494	OMG	C2-N3-C4	5.03	121.03	115.16
1	L5	2786	B9H	O3'-C3'-C2'	5.04	125.51	111.18
1	L5	3880	P7G	C6-N1-C2	5.06	123.34	116.06
1	L5	4472	B8W	C2-N1-C6	5.06	123.50	116.18
1	L5	4129	B8W	C2-N1-C6	5.07	123.52	116.18
1	L5	4370	OMG	C2-N3-C4	5.13	121.15	115.16
1	L5	3899	BGH	C6-N1-C2	5.19	123.53	116.06
1	L5	978	2MG	C2-N3-C4	5.24	121.09	115.11
1	L5	4623	OMG	C2-N3-C4	5.30	121.35	115.16
1	L5	1883	OMG	C2-N3-C4	5.34	121.39	115.16
1	L5	4196	OMG	C2-N3-C4	5.35	121.41	115.16
1	L5	3792	OMG	C2-N3-C4	5.37	121.43	115.16
1	L5	4371	MHG	C71-N7-C5	5.41	134.81	122.09
1	L5	373	OMG	C2-N3-C4	5.47	121.55	115.16
1	L5	1909	P7G	C71-N7-C5	5.59	135.23	122.09
1	L5	4296	B8H	C4-N3-C2	5.63	120.08	115.16
1	L5	4500	PSU	C4-N3-C2	5.66	120.11	115.16
1	L5	3762	B8H	C4-N3-C2	5.68	120.12	115.16
1	L5	4442	PSU	C4-N3-C2	5.70	120.14	115.16
1	L5	1316	OMG	C2-N3-C4	5.71	121.83	115.16
1	L5	729	2MG	C2-N3-C4	5.71	121.63	115.11
1	L5	4531	PSU	C4-N3-C2	5.76	120.19	115.16
47	S2	683	OMG	C2-N3-C4	5.76	121.88	115.16
47	S2	612	PSU	C4-N3-C2	5.77	120.20	115.16
1	L5	4636	PSU	C4-N3-C2	5.87	120.30	115.16
47	S2	823	PSU	C4-N3-C2	5.87	120.30	115.16
47	S2	119	PSU	C4-N3-C2	6.00	120.41	115.16
1	L5	4450	PSU	C4-N3-C2	6.03	120.43	115.16
1	L5	3899	BGH	N3-C4-N9	6.09	134.76	126.98
47	S2	814	5MU	C4-N3-C2	6.10	120.49	115.16
47	S2	822	PSU	C4-N3-C2	6.22	120.60	115.16
1	L5	1683	PSU	C4-N3-C2	6.27	120.65	115.16
1	L5	2508	PSU	C4-N3-C2	6.30	120.67	115.16
1	L5	4872	2MG	C2-N3-C4	6.31	122.31	115.11
1	L5	4083	5MU	C4-N3-C2	6.34	120.70	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4194	I4U	C4-O4-C41	6.36	126.58	117.86
1	L5	4293	PSU	C4-N3-C2	6.37	120.73	115.16
1	L5	1582	PSU	C4-N3-C2	6.43	120.78	115.16
1	L5	1860	B8H	C4-N3-C2	6.43	120.79	115.16
1	L5	1677	PSU	C4-N3-C2	6.48	120.83	115.16
1	L5	4628	PSU	C4-N3-C2	6.50	120.84	115.16
1	L5	4872	2MG	N2-C2-N1	6.53	123.29	116.95
1	L5	3729	PSU	C4-N3-C2	6.57	120.91	115.16
1	L5	4194	I4U	O4-C4-C5	6.58	123.72	115.74
47	S2	1243	PSU	C4-N3-C2	6.63	120.96	115.16
1	L5	3899	BGH	C72-C71-N7	6.63	126.14	117.65
1	L5	3715	PSU	C4-N3-C2	6.69	121.01	115.16
1	L5	1517	2MG	C2-N3-C4	6.73	122.80	115.11
1	L5	3764	PSU	C4-N3-C2	6.76	121.07	115.16
1	L5	4371	MHG	N3-C4-N9	6.82	135.69	126.98
1	L5	4403	PSU	C4-N3-C2	6.95	121.24	115.16
3	L8	14	OMU	C4-N3-C2	7.04	120.18	114.13
1	L5	4220	6MZ	C2-N1-C6	7.08	121.14	116.53
47	S2	1832	6MZ	C2-N1-C6	7.35	121.32	116.53
1	L5	3897	B8K	N3-C4-N9	7.36	136.38	126.98
47	S2	1081	PSU	C4-N3-C2	7.48	121.70	115.16
1	L5	1909	P7G	N3-C4-N9	7.95	137.14	126.98
1	L5	4550	7MG	N3-C4-N9	8.12	137.35	126.98
1	L5	4564	M7A	N3-C4-N9	8.15	137.12	126.83
47	S2	121	OMU	C4-N3-C2	8.17	121.15	114.13
1	L5	1605	7MG	N3-C4-N9	8.19	137.44	126.98
47	S2	1806	M7A	N3-C4-N9	8.28	137.29	126.83
1	L5	1348	P4U	C2-N3-C4	8.39	121.34	114.13
1	L5	2522	7MG	N3-C4-N9	8.39	137.70	126.98
1	L5	1797	E7G	N3-C4-N9	8.60	137.97	126.98
1	L5	4306	OMU	C4-N3-C2	8.65	121.56	114.13
1	L5	1659	I4U	C2-N3-C4	8.83	121.72	114.13
1	L5	4690	B8K	N3-C4-N9	8.84	138.27	126.98
47	S2	116	OMU	C4-N3-C2	8.95	121.82	114.13
1	L5	2297	E7G	N3-C4-N9	9.04	138.53	126.98
1	L5	4620	OMU	C4-N3-C2	9.05	121.91	114.13
1	L5	4194	I4U	C2-N3-C4	9.31	122.13	114.13
1	L5	3880	P7G	N3-C4-N9	9.89	139.61	126.98

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	L5	2786	B9H	C4
47	S2	1219	B8Q	C4
1	L5	1456	B8Q	C4
47	S2	568	E3C	C4

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	S2	1337	4AC	CM7-C7-N4-C4
1	L5	237	B9B	C61-O6-C6-C5
47	S2	1337	4AC	O7-C7-N4-C4
1	L5	4185	B8W	C61-O6-C6-N1
1	L5	1574	B9B	C61-O6-C6-N1
1	L5	4355	E6G	C61-O6-C6-N1
1	L5	1574	B9B	C61-O6-C6-C5
1	L5	4355	E6G	C61-O6-C6-C5
1	L5	4185	B8W	C61-O6-C6-C5
1	L5	4194	I4U	C41-O4-C4-N3
1	L5	4472	B8W	C61-O6-C6-N1
1	L5	4529	B8W	C61-O6-C6-N1
1	L5	4129	B8W	C61-O6-C6-N1
1	L5	1659	I4U	C41-O4-C4-N3
1	L5	4472	B8W	C61-O6-C6-C5
1	L5	4529	B8W	C61-O6-C6-C5
1	L5	4129	B8W	C61-O6-C6-C5

There are no ring outliers.

25 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	1322	1MA	1	0
1	L5	1326	A2M	1	0
1	L5	1456	B8Q	1	0
1	L5	1522	OMG	1	0
1	L5	1625	OMG	1	0
1	L5	1797	E7G	1	0
1	L5	1871	A2M	1	0
1	L5	1909	P7G	1	0
1	L5	2363	A2M	1	0
1	L5	2422	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	2522	7MG	1	0
1	L5	3723	A2M	1	0
1	L5	4194	I4U	1	0
1	L5	4220	6MZ	1	0
1	L5	4415	1MA	1	0
1	L5	4523	A2M	1	0
1	L5	4571	A2M	1	0
1	L5	4623	OMG	1	0
1	L5	4671	B8T	1	0
1	L5	729	2MG	1	0
3	L8	14	OMU	1	0
47	S2	116	OMU	1	0
47	S2	121	OMU	1	0
47	S2	1337	4AC	1	0
47	S2	159	A2M	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 412 ligands modelled in this entry, 410 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
83	HMT	L5	5348	-	37,43,43	1.89	6 (16%)	47,66,66	1.61	10 (21%)
85	HYG	S2	2034	-	35,39,39	0.85	1 (2%)	41,60,60	1.59	7 (17%)

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
83	HMT	L5	5348	-	-	0/27/74/74	0/5/5/5
85	HYG	S2	2034	-	-	0/12/87/87	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	L5	5348	HMT	C5-C4	-6.68	1.39	1.51
83	L5	5348	HMT	C7-C6	-5.86	1.38	1.51
83	L5	5348	HMT	C3-C2	-3.45	1.40	1.50
83	L5	5348	HMT	C13-C14	-2.83	1.33	1.38
83	L5	5348	HMT	C16-C15	-2.80	1.33	1.38
83	L5	5348	HMT	C15-C14	-2.18	1.33	1.39
85	S2	2034	HYG	O28-C23	2.51	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	2034	HYG	O22-C17-C12	-4.78	96.03	103.60
83	L5	5348	HMT	C25-C24-C20	-4.31	109.68	115.91
83	L5	5348	HMT	C7-C6-C16	-3.45	111.77	119.29
83	L5	5348	HMT	C13-C5-C4	-3.37	109.43	119.08
85	S2	2034	HYG	O8-C1-C2	-3.06	104.17	109.82
85	S2	2034	HYG	C23-C24-C25	-3.06	107.43	110.53
83	L5	5348	HMT	C11-C12-C9	-2.79	100.58	105.05
83	L5	5348	HMT	C3-O4-C19	-2.62	112.95	117.22
83	L5	5348	HMT	O1-C17-O2	-2.13	104.78	108.10
85	S2	2034	HYG	C16-C17-C12	-2.13	108.20	113.40
83	L5	5348	HMT	C10-N1-C8	-2.08	106.07	112.02
85	S2	2034	HYG	C19-C15-C16	-2.06	108.17	113.00
83	L5	5348	HMT	C7-C6-C5	2.40	129.91	122.38
83	L5	5348	HMT	C4-C3-C2	3.17	106.59	102.73
83	L5	5348	HMT	C6-C5-C4	3.42	132.07	122.44
85	S2	2034	HYG	O18-C6-C1	3.73	116.17	107.19
85	S2	2034	HYG	C13-O18-C6	3.74	127.12	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	L5	5348	HMT	3	0

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
59	SQ	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SQ	2:PRO	C	3:SER	N	8.50