



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 06:58 AM EDT

PDB ID : 8G6J / pdb_00008g6j
EMDB ID : EMD-29771
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (GA state 2)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-15
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

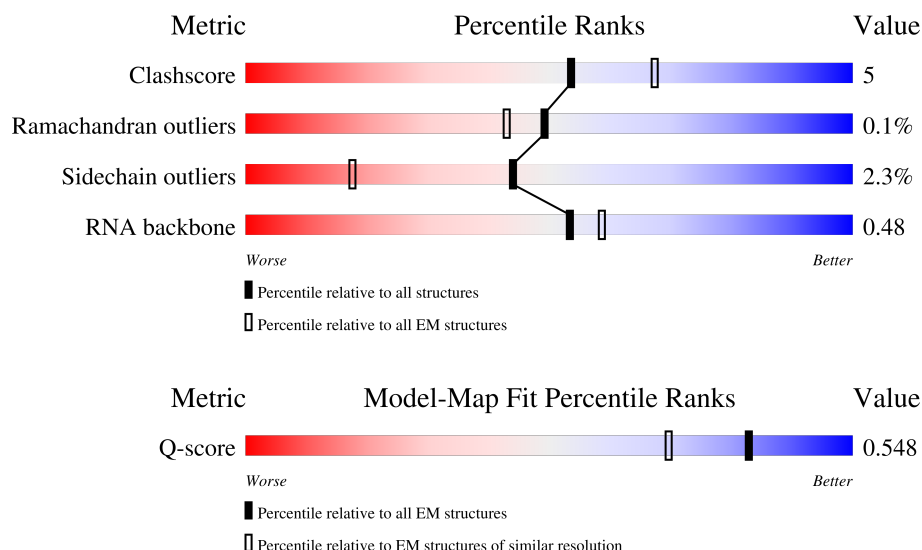
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	S2	1869	
2	L8	156	
3	L5	5069	

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SG	249	
12	SF	204	
13	SH	194	
14	SW	130	
15	SI	208	
16	SQ	146	
17	SU	119	
18	SK	165	
19	SO	151	
20	SX	143	
21	SM	132	
22	SS	152	
23	Sd	56	
24	SN	151	
25	SL	158	
26	SR	135	
27	SP	145	
28	ST	145	

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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	Lq	317	
47	LK	165	
48	LO	203	
49	LL	270	
50	LV	140	
51	LM	215	
52	La	148	
53	LN	204	

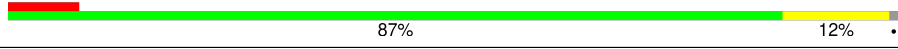
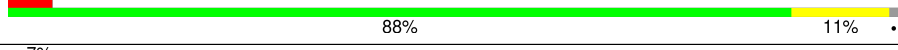
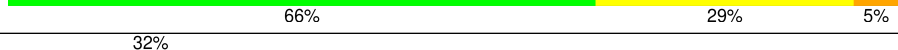
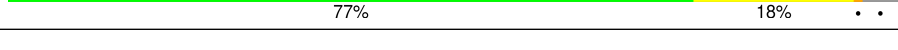
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Mol	Chain	Length	Quality of chain
54	LI	214	
55	LD	297	
56	LQ	188	
57	LR	196	
58	LS	176	
59	LT	160	
60	LP	184	
61	LU	128	
62	LX	156	
63	LY	145	
64	LW	157	
65	LZ	136	
66	Lr	137	
67	Lh	123	
68	Lb	159	
69	LF	248	
70	Lc	115	
71	Ld	125	
72	Le	135	
73	Lf	110	
74	Lg	117	
75	Li	105	
76	Lj	97	
77	Lk	70	
78	Ll	51	

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Mol	Chain	Length	Quality of chain
79	Lm	128	
80	Ln	25	
81	Lo	106	
82	Lp	92	
83	mR	60	
84	At	76	
85	Pt	77	
86	EF	462	

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
66	SAC	Lr	2	-	X	-	-
90	PUT	L5	5119	-	-	X	-

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 225765 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1701	Total	C	N	O	P	0	0
			36364	16257	6517	11889	1701		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3687	Total	C	N	O	P	1	0
			79146	35282	14478	25698	3688		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2562	1141	456	845	120		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

- Molecule 6 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	222	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

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

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

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 11 is a protein called 40S ribosomal protein S6.

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

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SF	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 18 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 19 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 20 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SX	142	Total	C	N	O	S	0	0
			1105	696	220	186	3		

- Molecule 21 is a protein called 40S ribosomal protein S12.

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

- Molecule 22 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 23 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	143	Total	C	N	O	S	0	0
			1171	746	221	198	6		

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1083	680	201	198	4		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	133	Total	C	N	O	S	0	0
			1093	695	206	185	7		

- Molecule 28 is a protein called 40S ribosomal protein S19.

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

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SV	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 30 is a protein called 40S ribosomal protein S24.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 34 is a protein called 40S ribosomal protein S28.

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

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	75	Total	C	N	O	S	0	0
			615	388	118	102	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	211	Total	C	N	O	S	0	0
			1701	1089	307	297	8		

- Molecule 39 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LA	251	Total	C	N	O	S	0	0
			1922	1204	393	319	6		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 41 is a protein called 60S ribosomal protein L4.

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

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	169	Total	C	N	O	S	0	0
			1358	859	253	240	6		

- Molecule 43 is a protein called 60S ribosomal protein L9.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	223	Total	C	N	O	S	1	0
			1793	1155	340	294	4		

- Molecule 45 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LG	239	Total	C	N	O	S	0	0
			1910	1217	368	321	4		

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lq	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LK	147	Total	C	N	O	S	0	0
			1121	700	211	207	3		

- Molecule 48 is a protein called 60S ribosomal protein L13a.

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

- Molecule 49 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 50 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LV	140	Total	C	N	O	S	0	0
			1042	653	200	183	6		

- Molecule 51 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 52 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 53 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 54 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LI	205	Total	C	N	O	S	0	0
			1660	1054	319	274	13		

- Molecule 55 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 56 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 57 is a protein called 60S ribosomal protein L19.

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

- Molecule 58 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 59 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 62 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 63 is a protein called 60S ribosomal protein L26.

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

- Molecule 64 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		

- Molecule 66 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lr	125	Total	C	N	O	S	0	0
			1005	624	207	169	5		

- Molecule 67 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lb	109	Total	C	N	O	S	0	0
			885	552	192	137	4		

- Molecule 69 is a protein called 60S ribosomal protein L7.

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

- Molecule 70 is a protein called 60S ribosomal protein L30.

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

- Molecule 71 is a protein called 60S ribosomal protein L31.

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

- Molecule 72 is a protein called 60S ribosomal protein L32.

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

- Molecule 73 is a protein called 60S ribosomal protein L35a.

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

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called 60S ribosomal protein L36.

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

- Molecule 76 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 77 is a protein called 60S ribosomal protein L38.

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

- Molecule 78 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 79 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 80 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 81 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 82 is a protein called 60S ribosomal protein L37a.

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

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	mR	11	Total	C	N	O	P	1	0
			252	113	41	86	12		

- Molecule 84 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	At	76	Total	C	N	O	P	S	0	0
			1630	730	290	532	76	2		

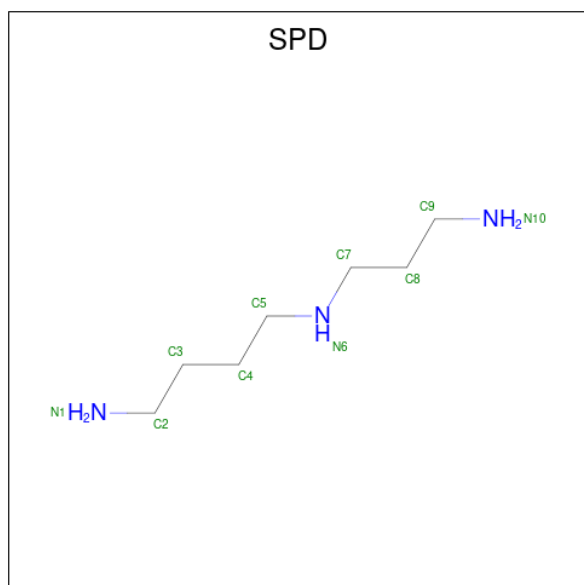
- Molecule 85 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 86 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	EF	444	Total	C	N	O	S	0	0
			3405	2167	585	636	17		

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
87	S2	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
88	S2	6	Total	K	0
			6	6	
88	L5	25	Total	K	0
			25	25	
88	LA	1	Total	K	0
			1	1	
88	Lf	1	Total	K	0
			1	1	
88	mR	1	Total	K	0
			1	1	

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

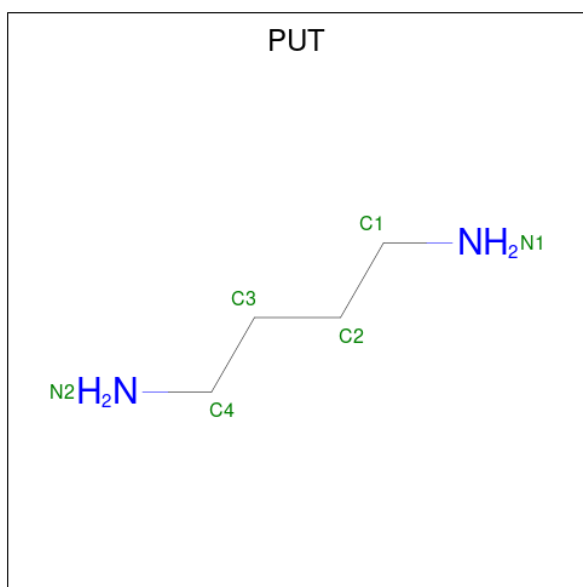
Mol	Chain	Residues	Atoms		AltConf
89	S2	83	Total	Mg	0
			83	83	
89	L8	3	Total	Mg	0
			3	3	
89	L5	225	Total	Mg	0
			225	225	
89	L7	5	Total	Mg	0
			5	5	
89	SE	1	Total	Mg	0
			1	1	
89	SO	1	Total	Mg	0
			1	1	

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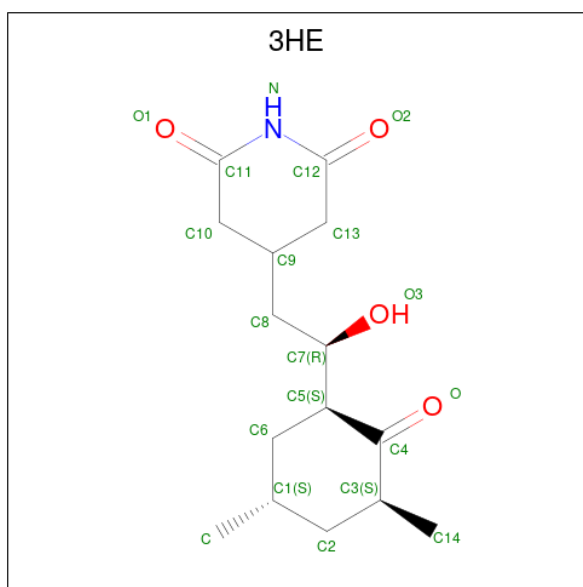
Mol	Chain	Residues	Atoms		AltConf
89	SX	1	Total 1	Mg 1	0
89	Sd	1	Total 1	Mg 1	0
89	ST	1	Total 1	Mg 1	0
89	LA	1	Total 1	Mg 1	0
89	LB	1	Total 1	Mg 1	0
89	LH	1	Total 1	Mg 1	0
89	LV	1	Total 1	Mg 1	0
89	LN	1	Total 1	Mg 1	0
89	LI	2	Total 2	Mg 2	0
89	LS	2	Total 2	Mg 2	0
89	LP	1	Total 1	Mg 1	0
89	Le	1	Total 1	Mg 1	0
89	Lg	1	Total 1	Mg 1	0
89	Lj	1	Total 1	Mg 1	0
89	Pt	1	Total 1	Mg 1	0
89	EF	2	Total 2	Mg 2	0

- Molecule 90 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



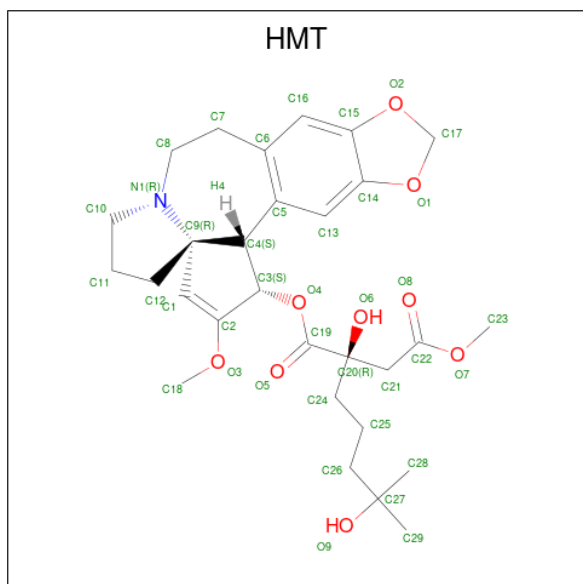
Mol	Chain	Residues	Atoms			AltConf
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	

- Molecule 91 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄).



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

- Molecule 92 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano yl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$).

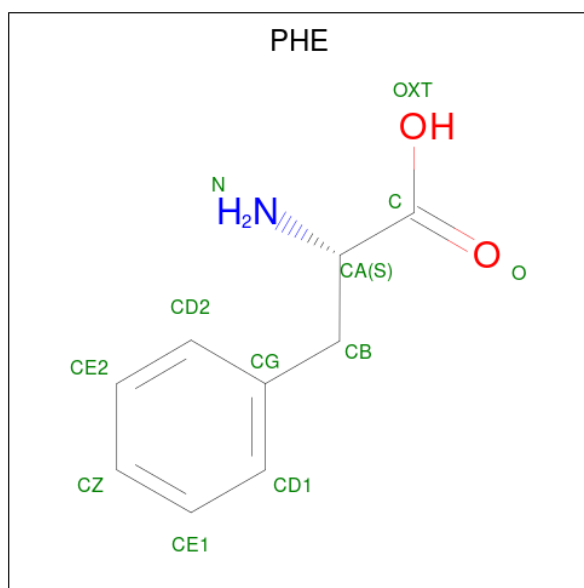


Mol	Chain	Residues	Atoms				AltConf
92	L5	1	Total	C	N	O	0
			39	29	1	9	

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

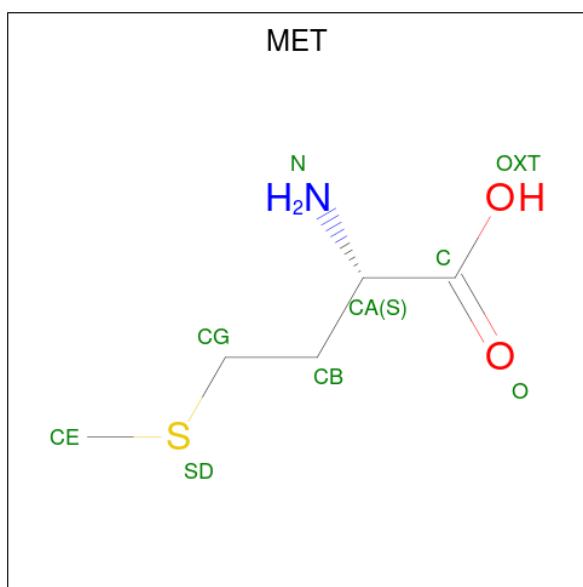
Mol	Chain	Residues	Atoms		AltConf
93	Sd	1	Total	Zn	0
			1	1	
93	Sa	1	Total	Zn	0
			1	1	
93	Sf	1	Total	Zn	0
			1	1	
93	Lg	1	Total	Zn	0
			1	1	
93	Lj	1	Total	Zn	0
			1	1	
93	Lm	1	Total	Zn	0
			1	1	
93	Lo	1	Total	Zn	0
			1	1	
93	Lp	1	Total	Zn	0
			1	1	

- Molecule 94 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



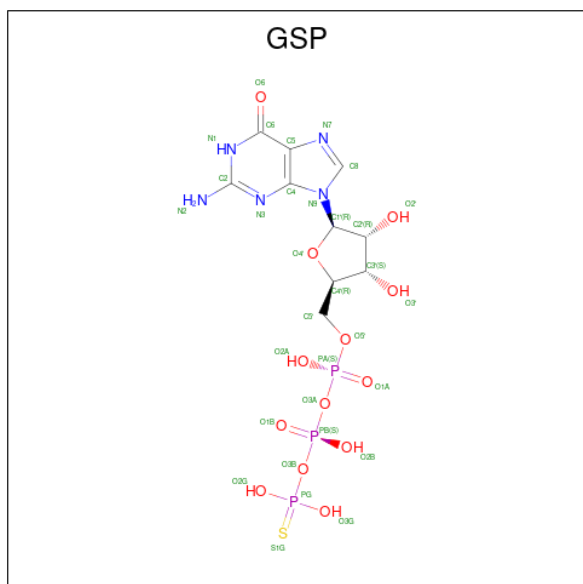
Mol	Chain	Residues	Atoms				AltConf
94	At	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 95 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
95	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

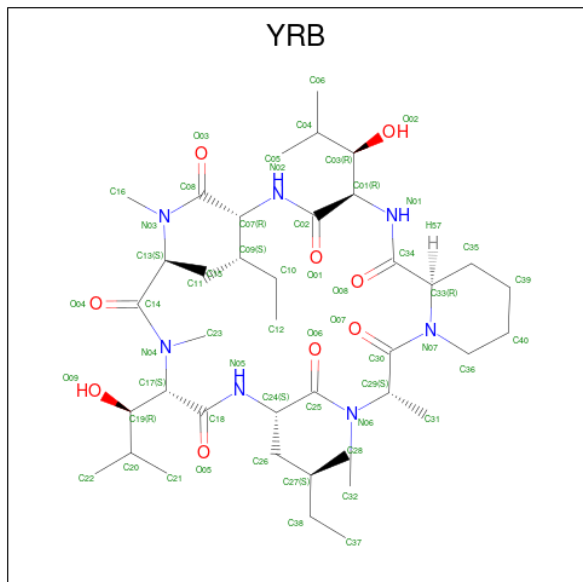
- Molecule 96 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms					AltConf
96	EF	1	Total	C	N	O	P	S
			32	10	5	13	3	1

- Molecule 97 is (3R,6R,9S,12S,15S,18S,20R,24aR)-6-[(2S)-butan-2-yl]-3,12-bis[(1R)-1-hydroxy-2-methylpropyl]-8,9,11,17,18-pentamethyl-15-[(2S)-2-methylbutyl]hexadecahydropyrido[

1,2-a)[1,4,7,10,13,16,19]heptaazacyclohenicosine-1,4,7,10,13,16,19(21H)-heptone (CCD ID: YRB) (formula: C₄₀H₇₁N₇O₉) (labeled as "Ligand of Interest" by depositor).

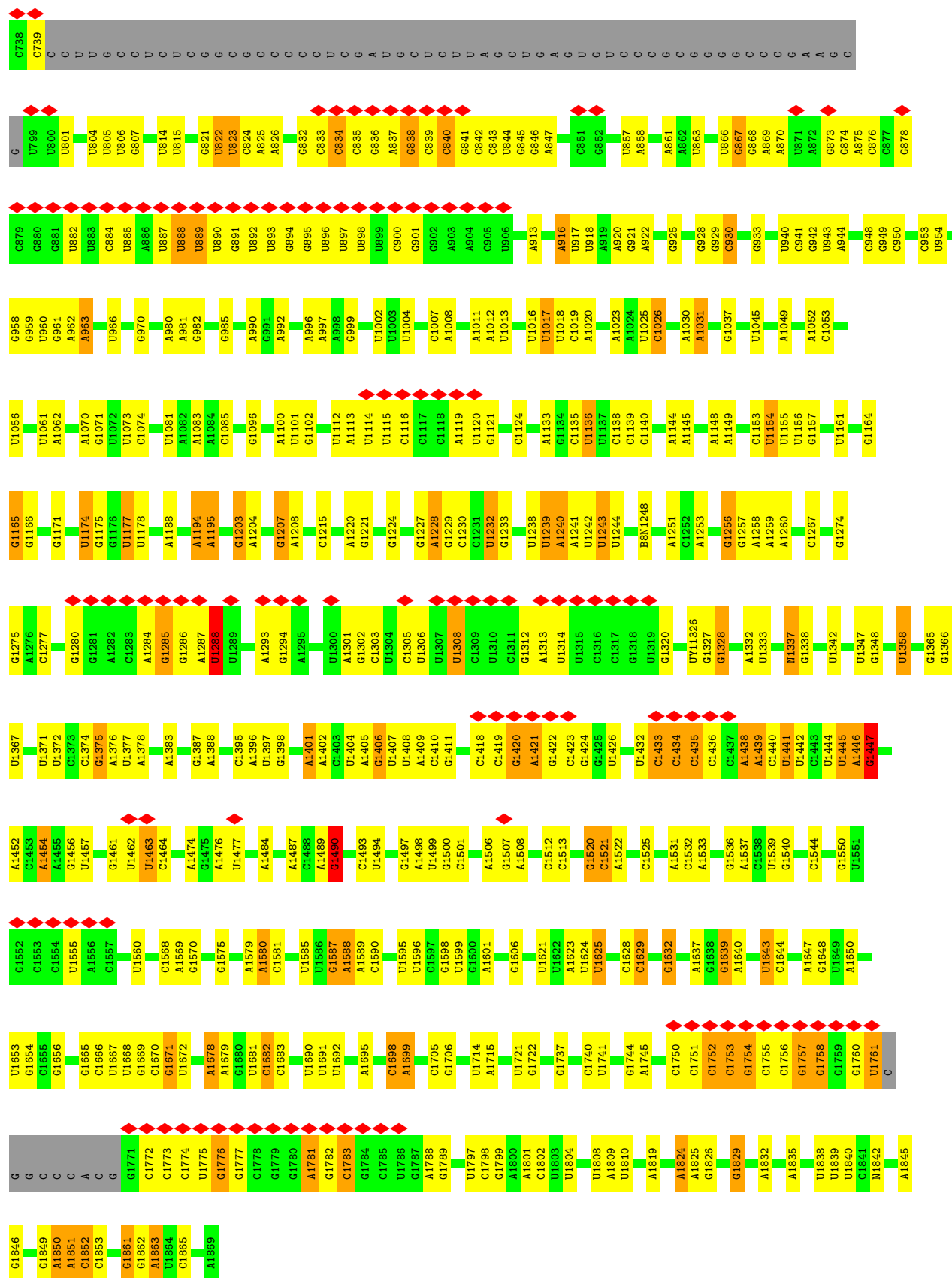


Mol	Chain	Residues	Atoms				AltConf
97	EF	1	Total	C	N	O	0
			56	40	7	9	

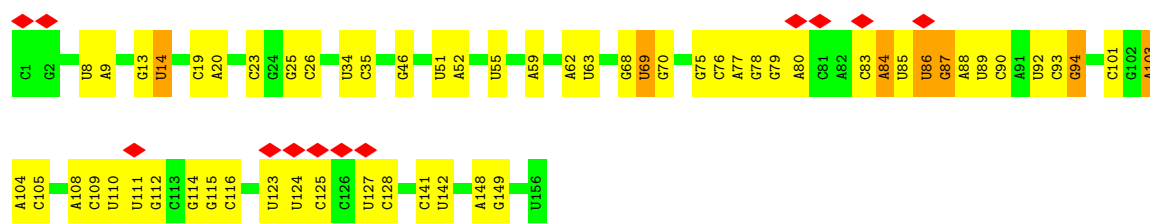
- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
98	EF	3	Total	O	0
			3	3	

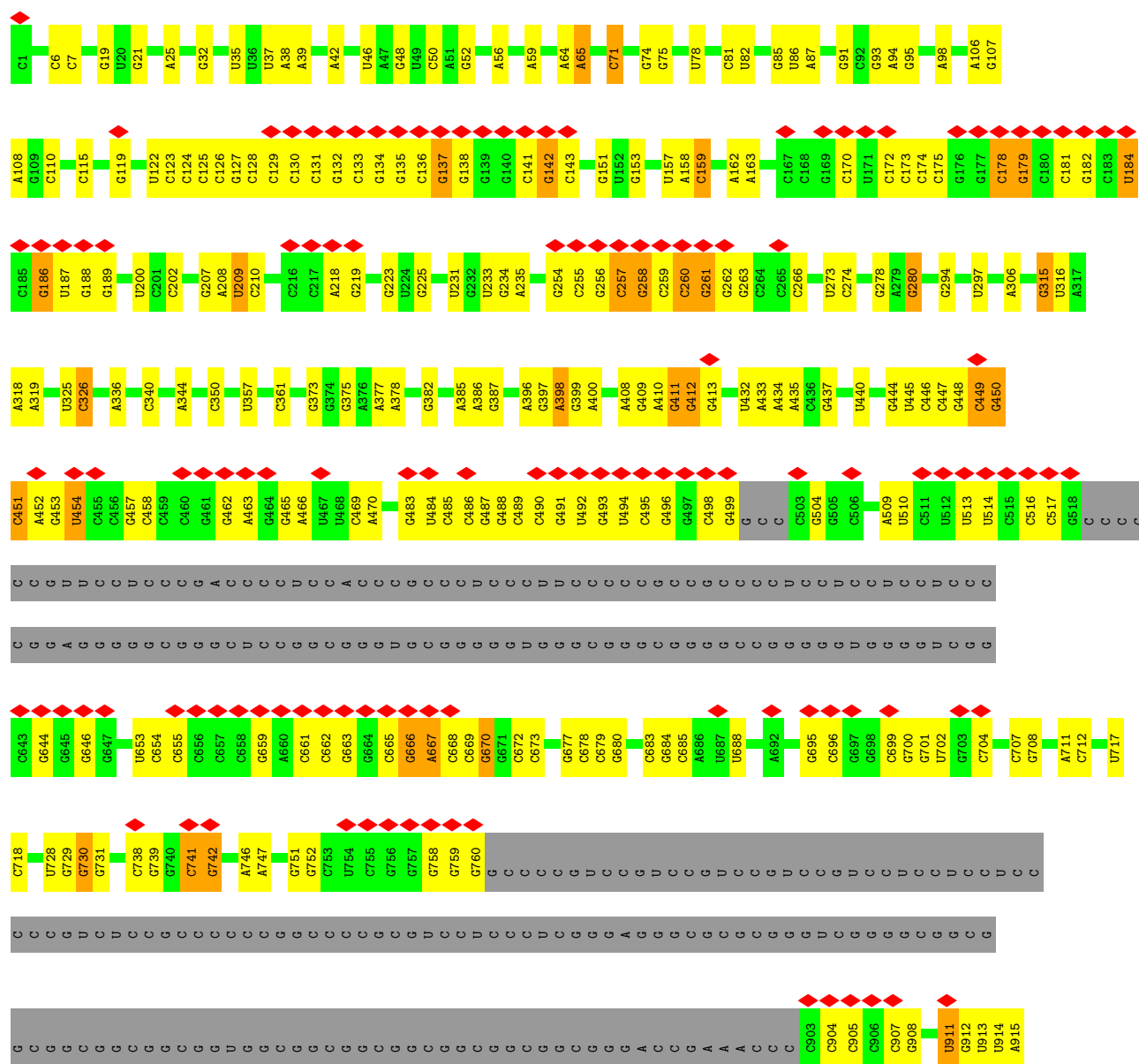


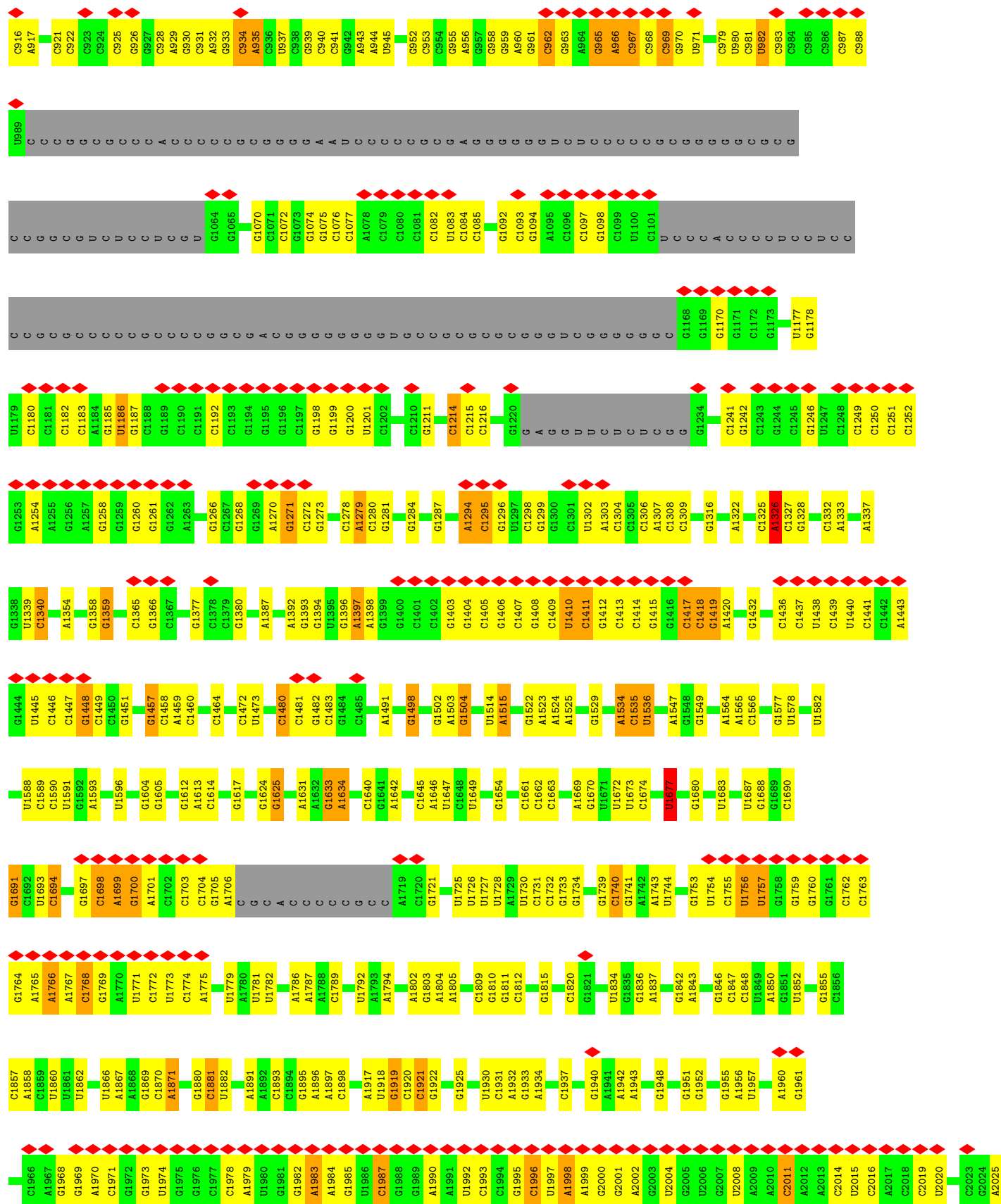


• Molecule 2: 5.8S rRNA

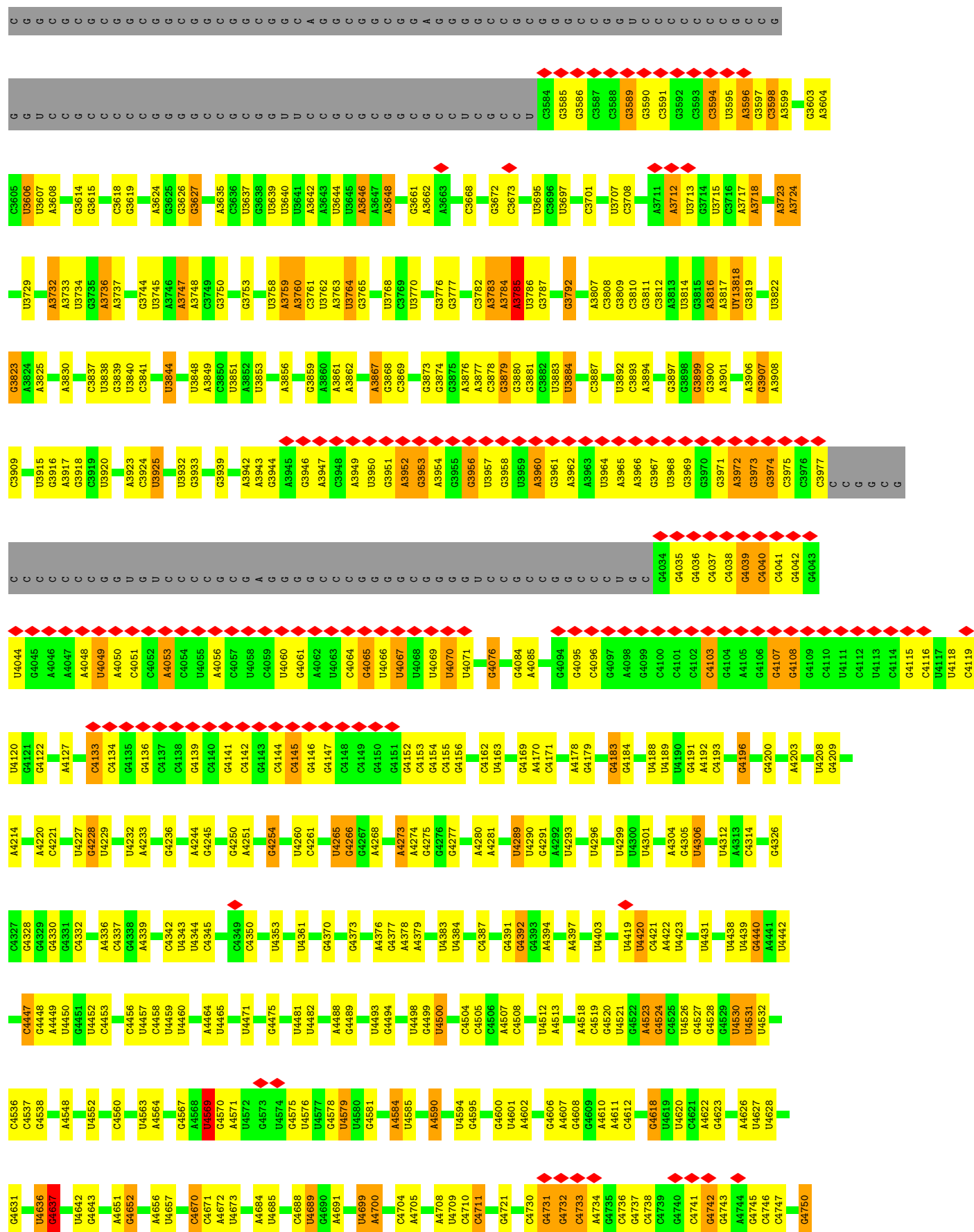


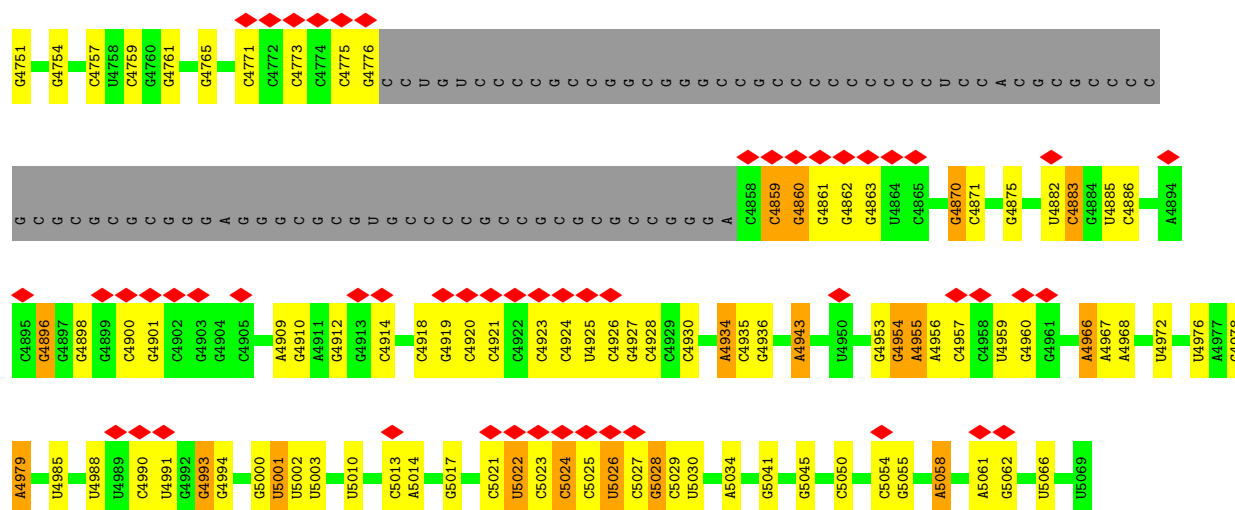
• Molecule 3: 28S rRNA



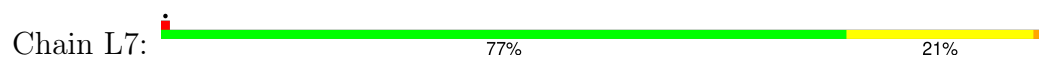




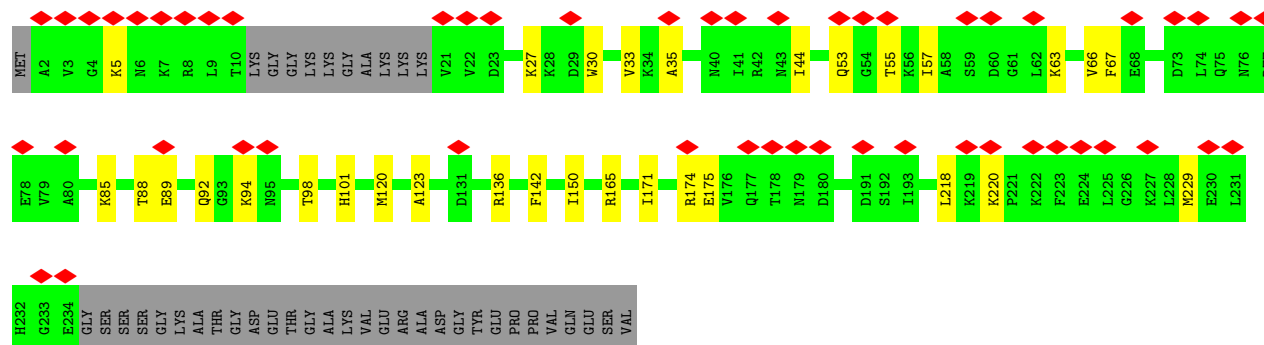
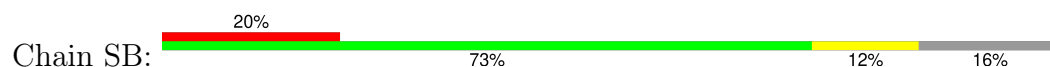




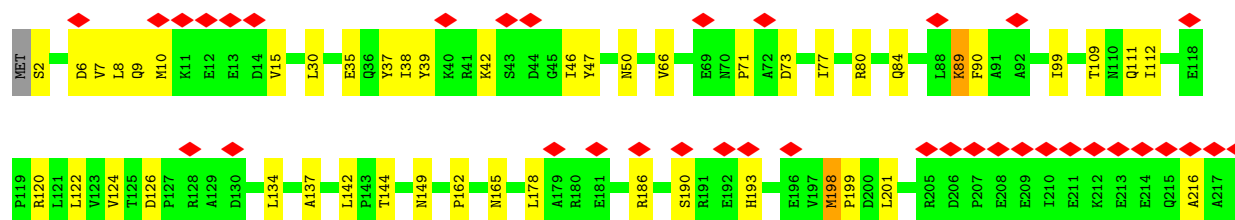
• Molecule 4: 5S rRNA

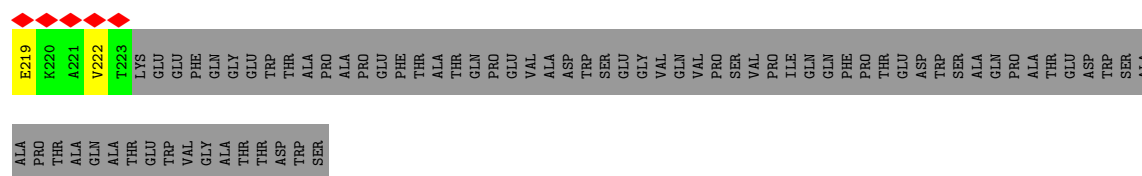


• Molecule 5: 40S ribosomal protein S3a

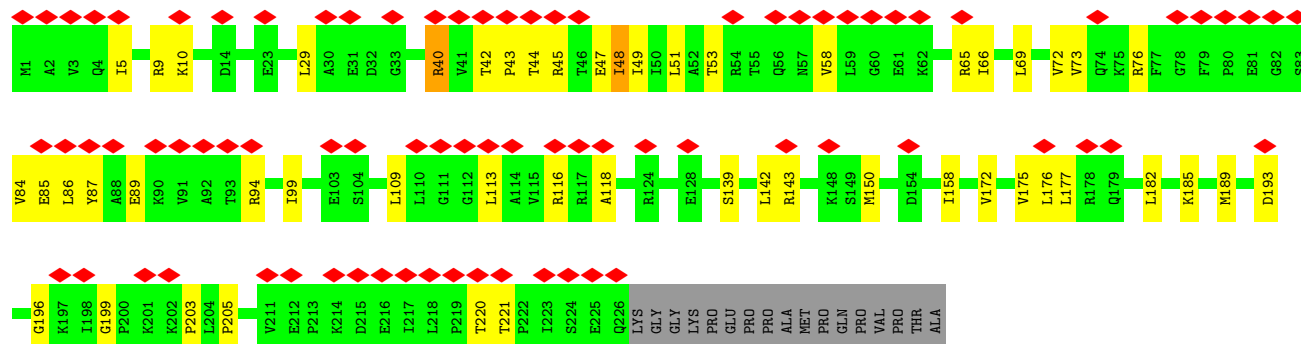
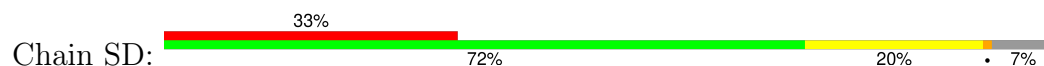


• Molecule 6: 40S ribosomal protein SA

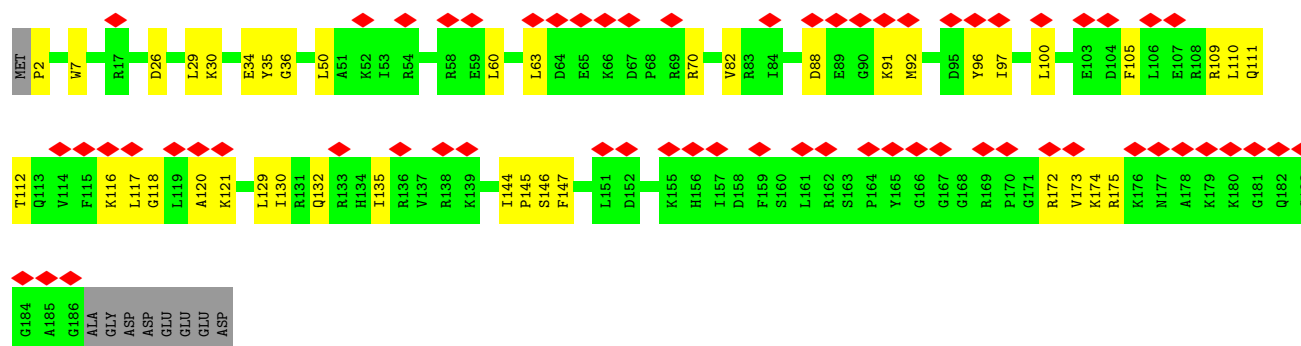
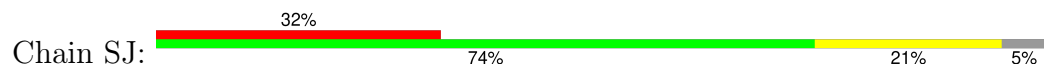




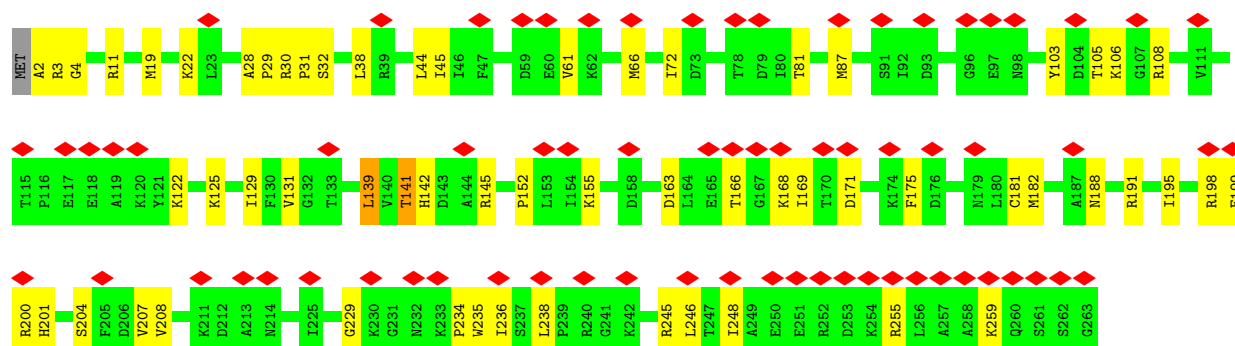
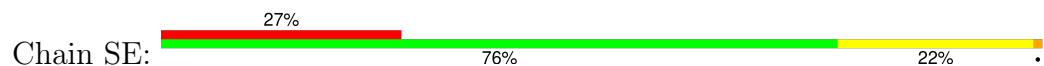
• Molecule 7: 40S ribosomal protein S3



• Molecule 8: 40S ribosomal protein S9

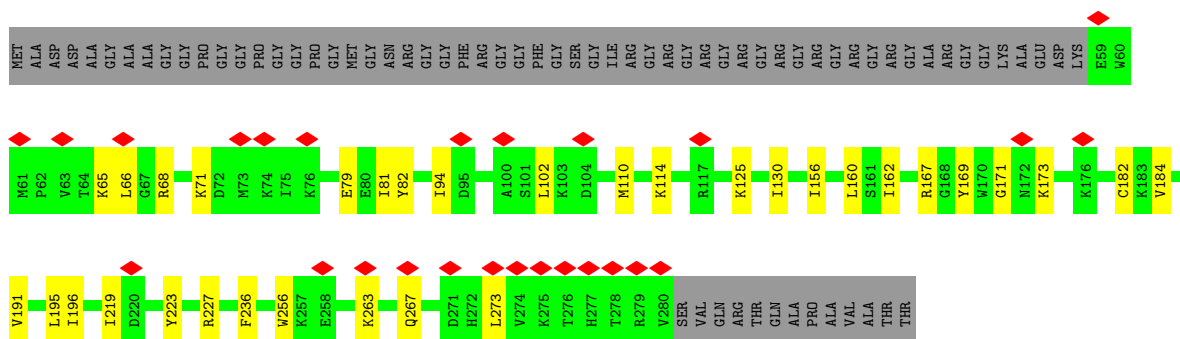


• Molecule 9: 40S ribosomal protein S4, X isoform



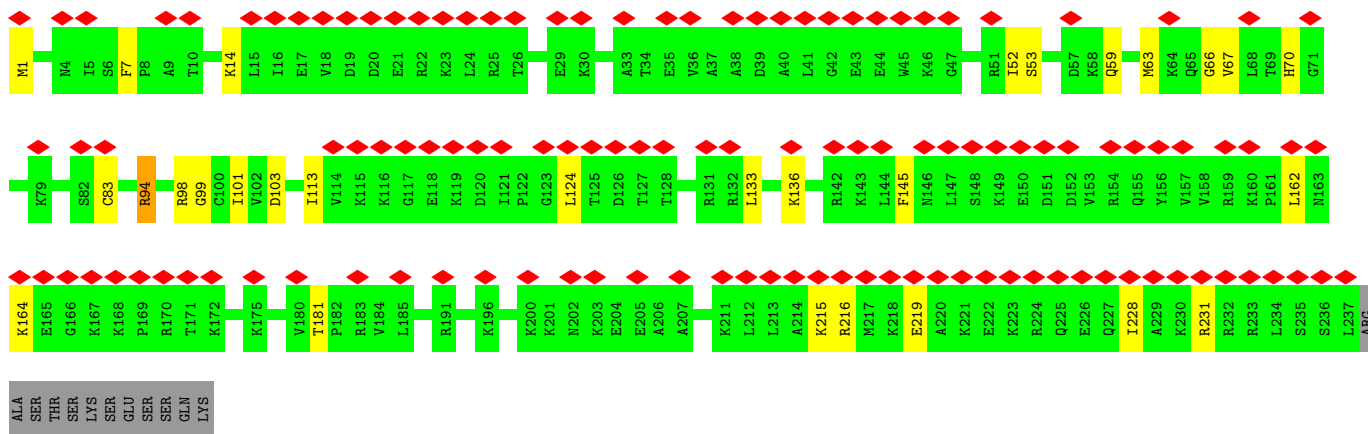
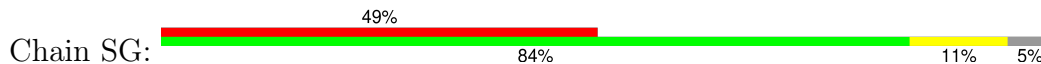
- Molecule 10: 40S ribosomal protein S2

Chain SC:



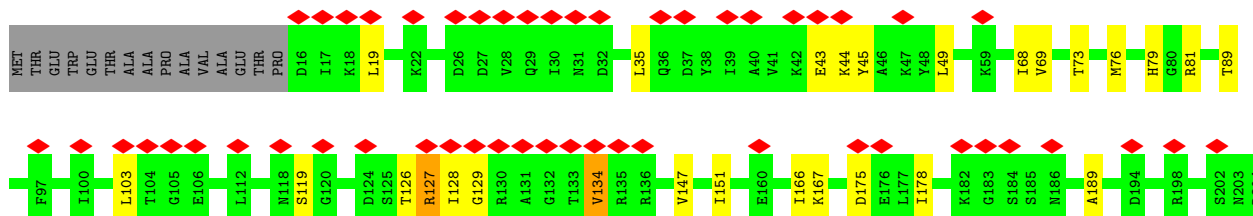
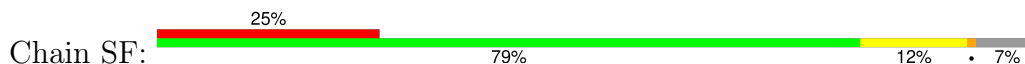
- Molecule 11: 40S ribosomal protein S6

Chain SG:



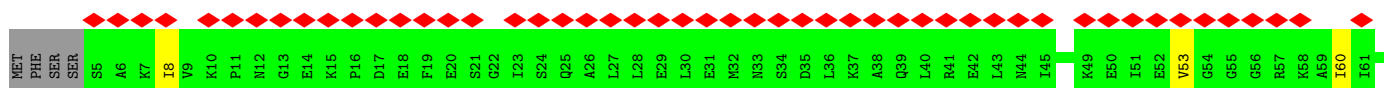
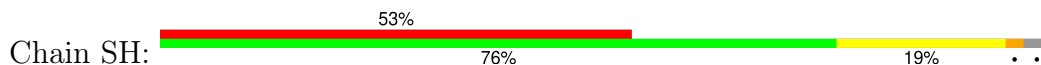
- Molecule 12: 40S ribosomal protein S5

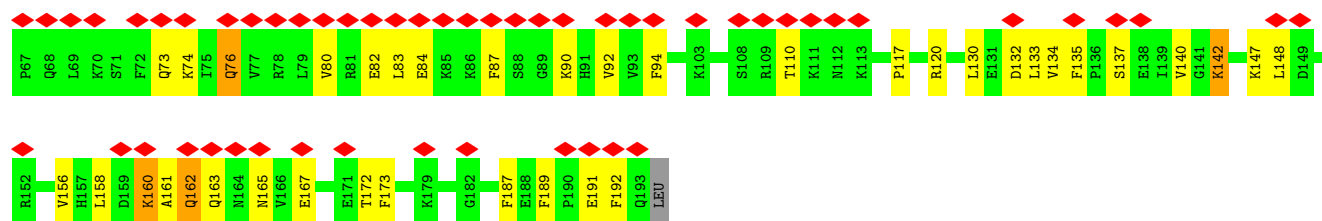
Chain SF:



- Molecule 13: 40S ribosomal protein S7

Chain SH:





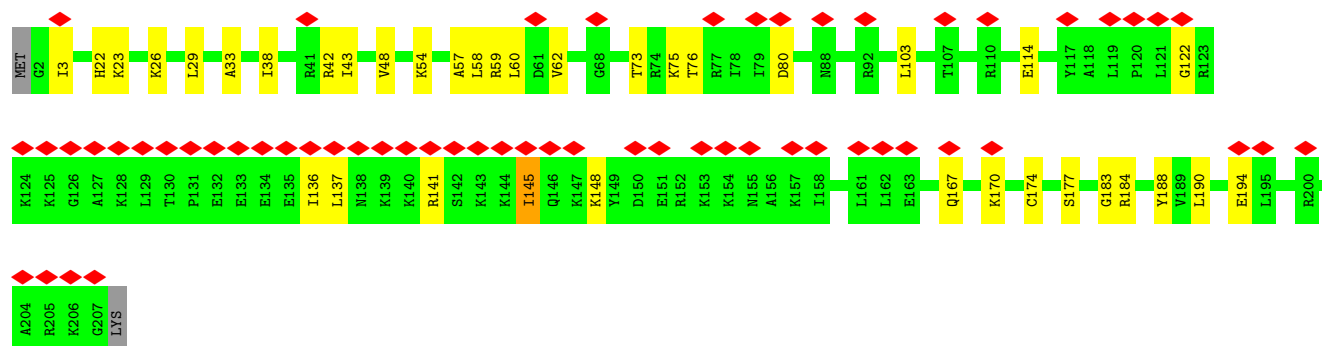
- Molecule 14: 40S ribosomal protein S15a

Chain SW: 86% 12% ..



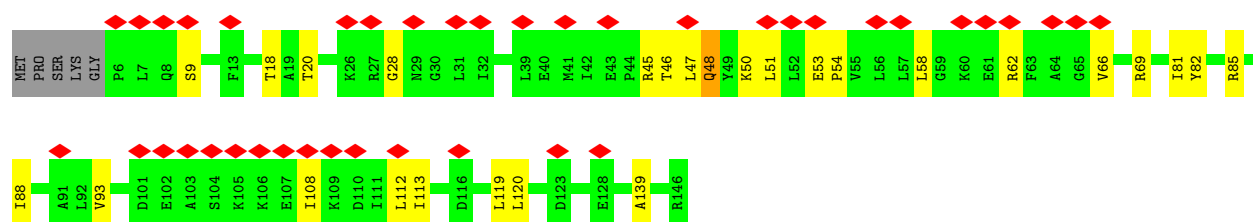
- Molecule 15: 40S ribosomal protein S8

Chain SI: 28% 81% 17% .



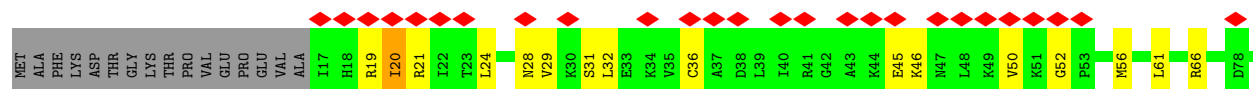
- Molecule 16: 40S ribosomal protein S16

Chain SQ: 27% 78% 18% ..

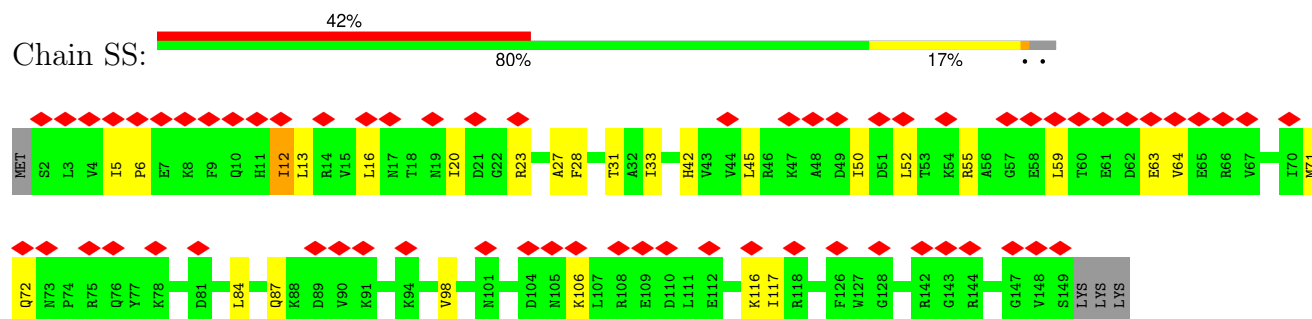


- Molecule 17: 40S ribosomal protein S20

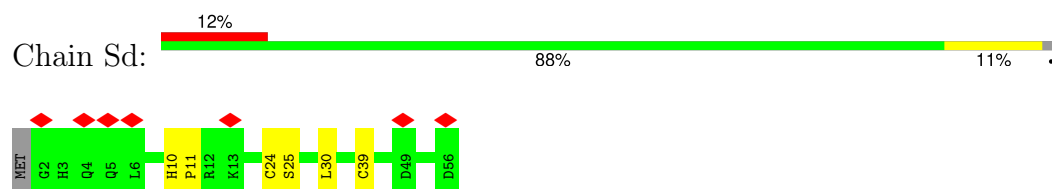
Chain SU: 46% 63% 20% 15% .



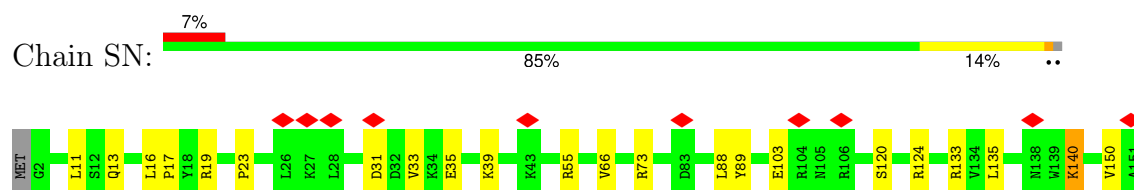
- Molecule 22: 40S ribosomal protein S18



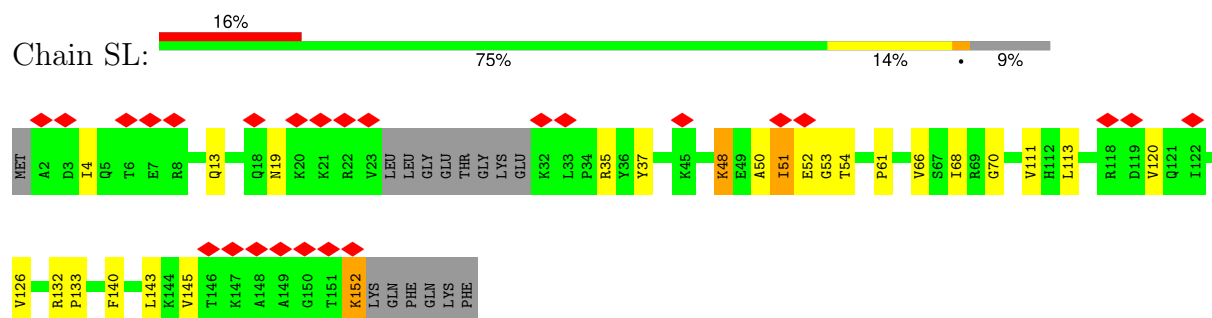
- Molecule 23: 40S ribosomal protein S29



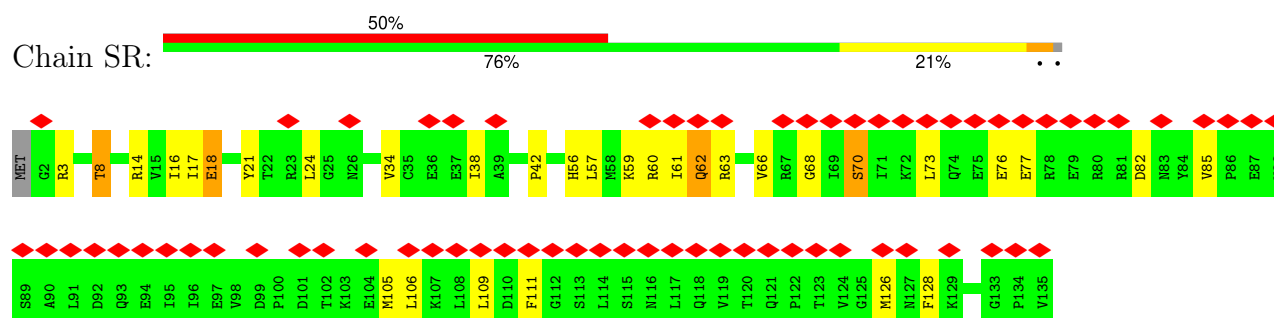
- Molecule 24: 40S ribosomal protein S13



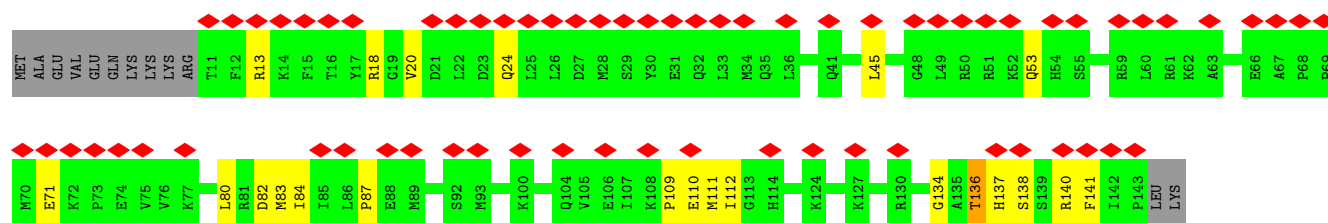
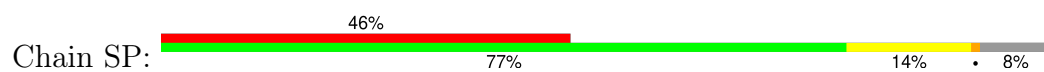
- Molecule 25: 40S ribosomal protein S11



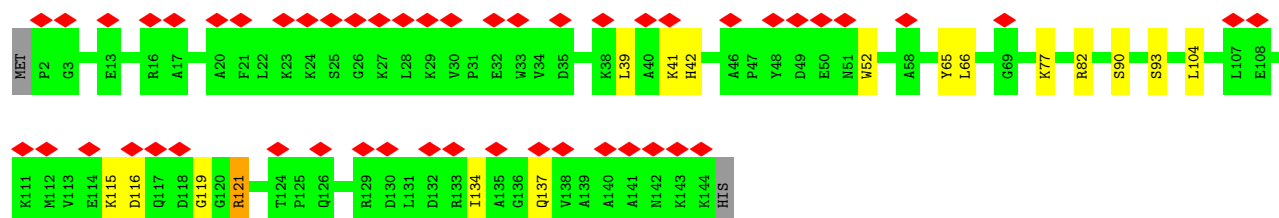
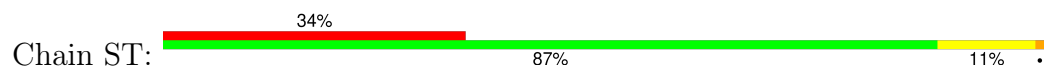
- Molecule 26: 40S ribosomal protein S17



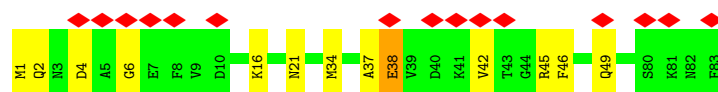
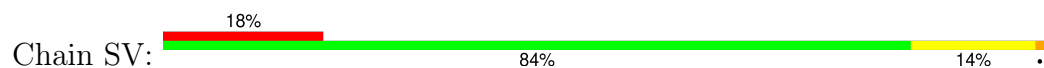
- Molecule 27: 40S ribosomal protein S15



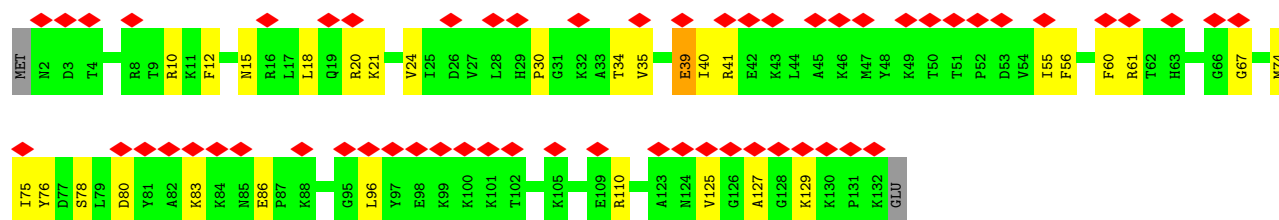
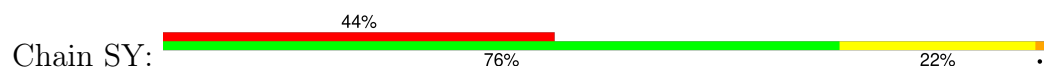
• Molecule 28: 40S ribosomal protein S19



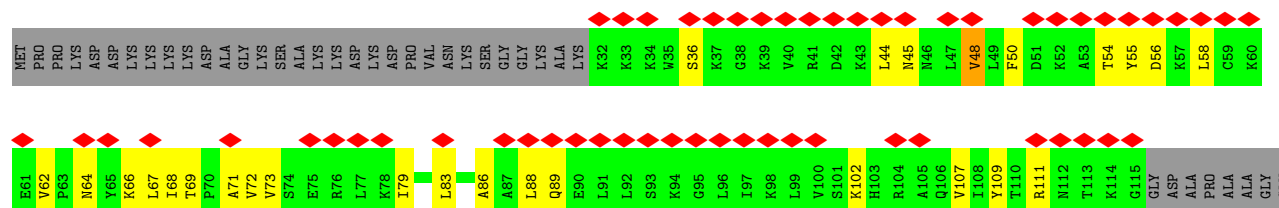
• Molecule 29: 40S ribosomal protein S21



• Molecule 30: 40S ribosomal protein S24

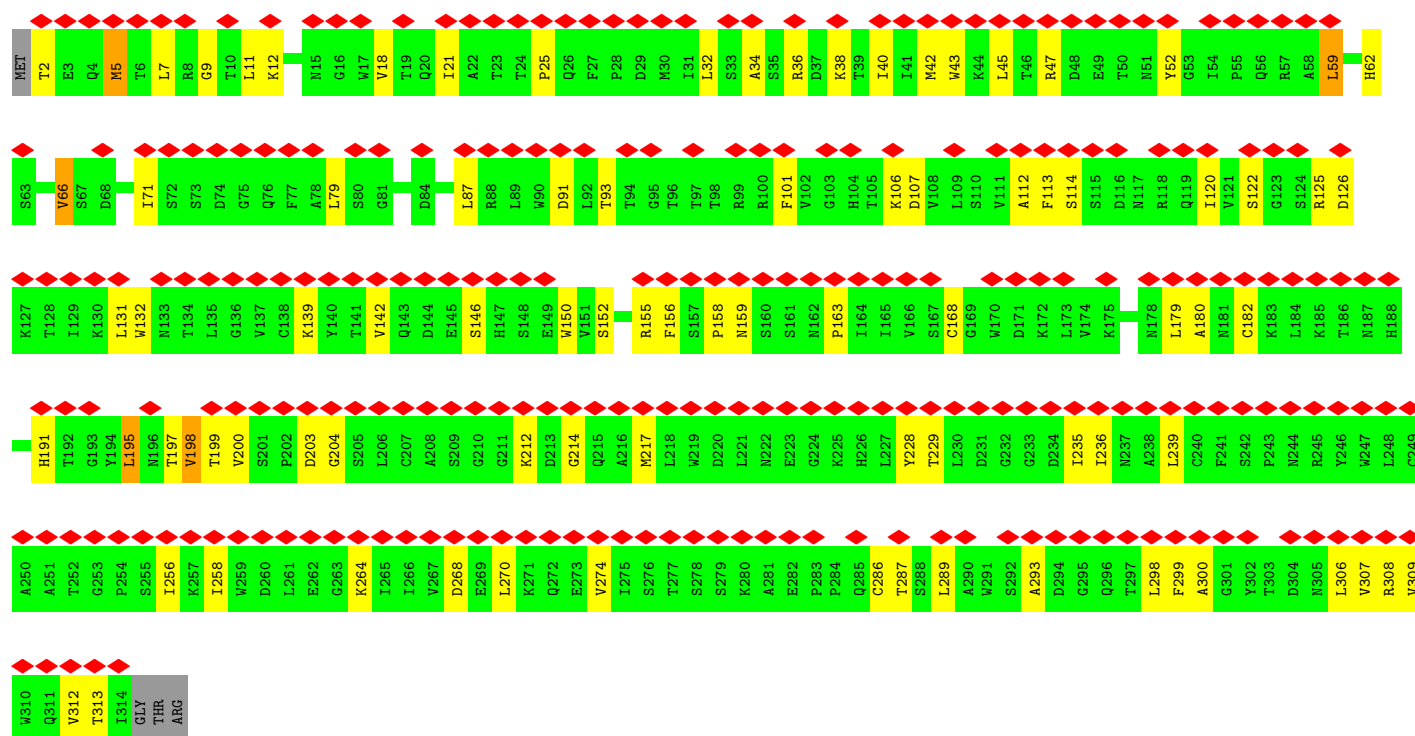


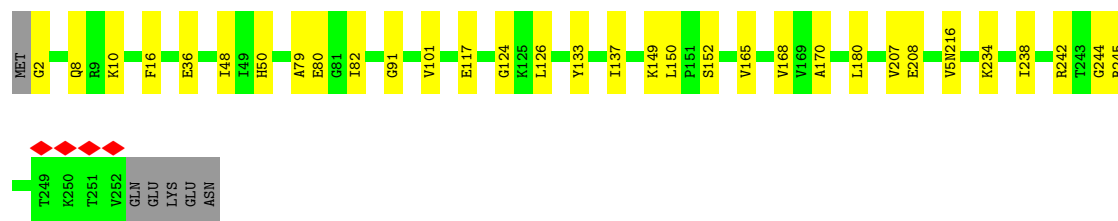
• Molecule 31: 40S ribosomal protein S25



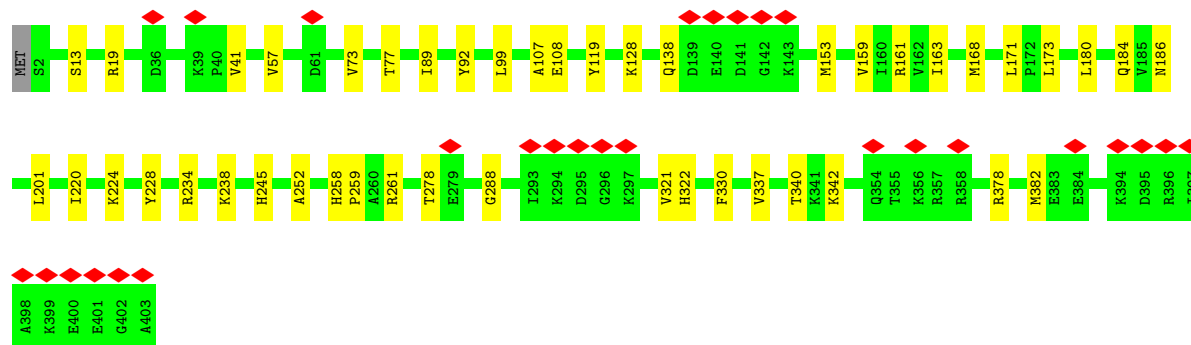
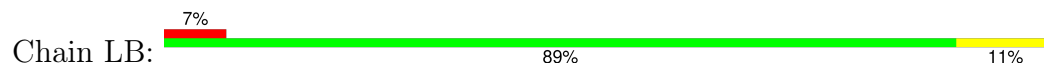
- Molecule 37: Receptor of activated protein C kinase 1

Chain Sg: 

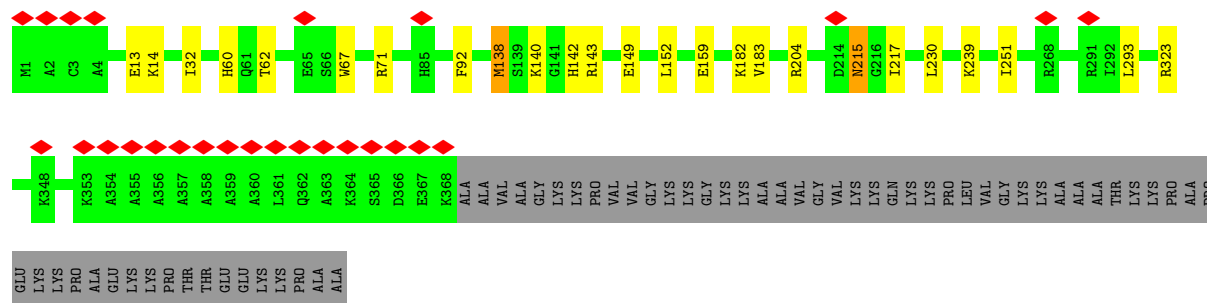
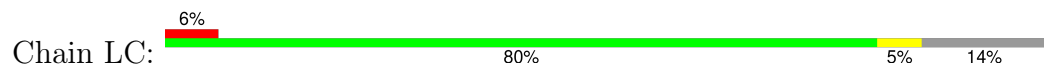




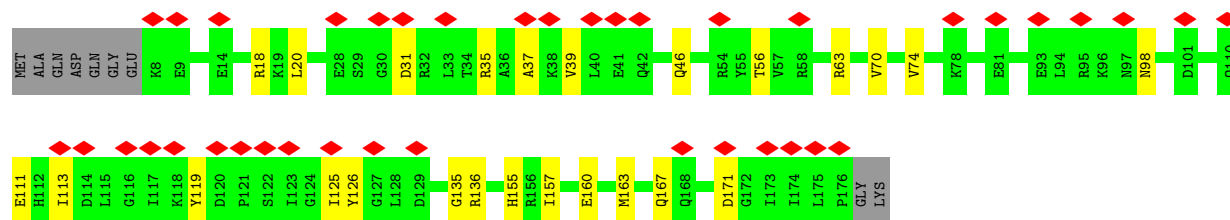
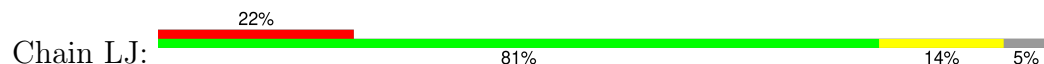
• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4

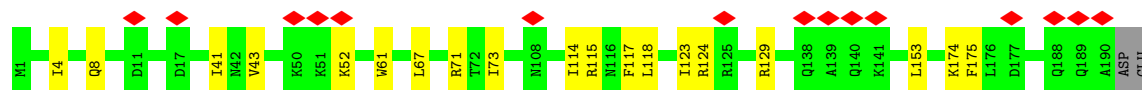


• Molecule 42: 60S ribosomal protein L11

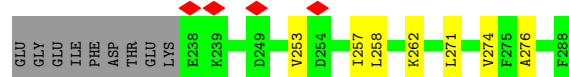
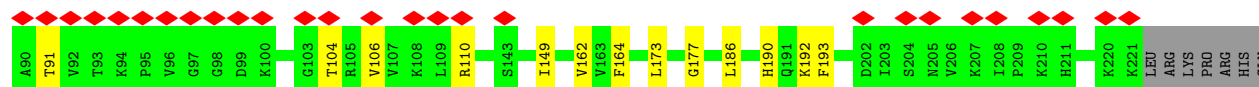
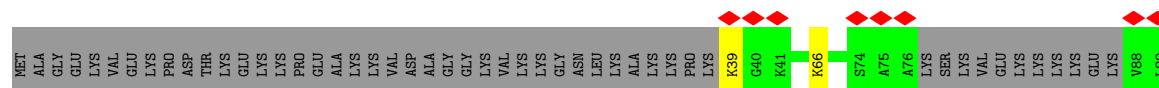


• Molecule 43: 60S ribosomal protein L9

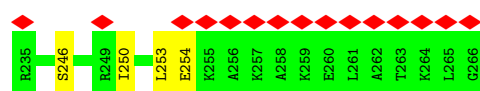
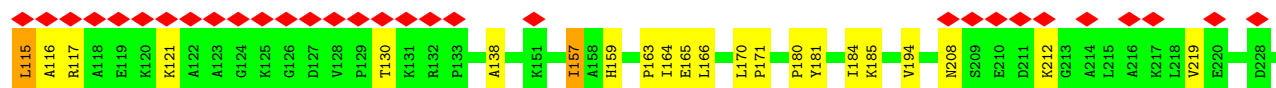
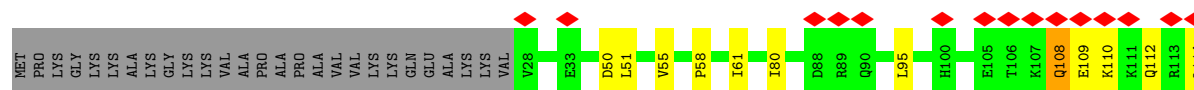
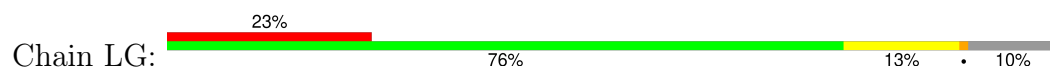




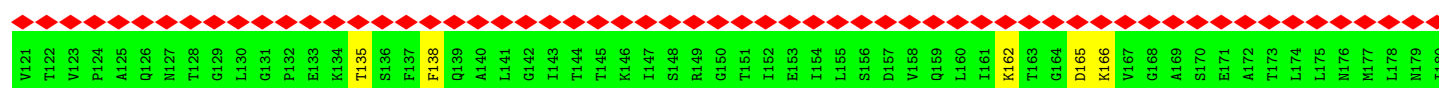
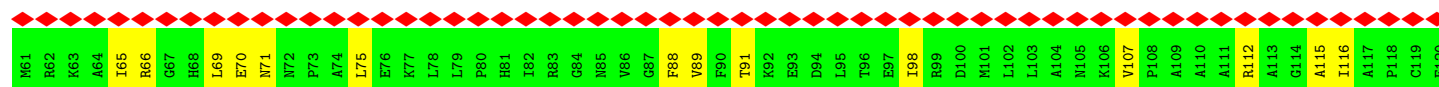
• Molecule 44: 60S ribosomal protein L6

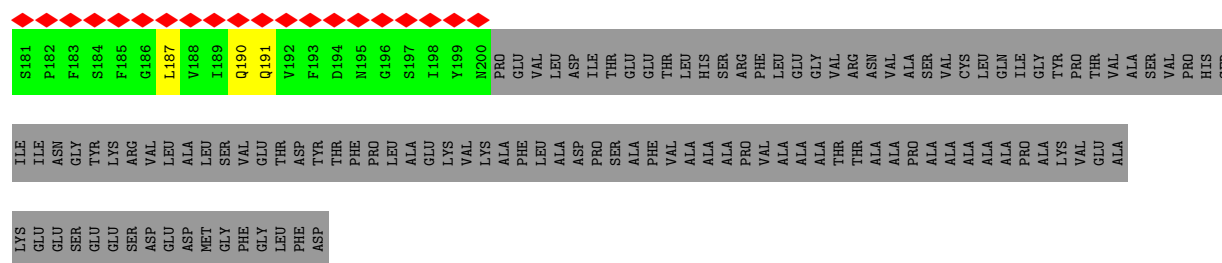


• Molecule 45: 60S ribosomal protein L7a

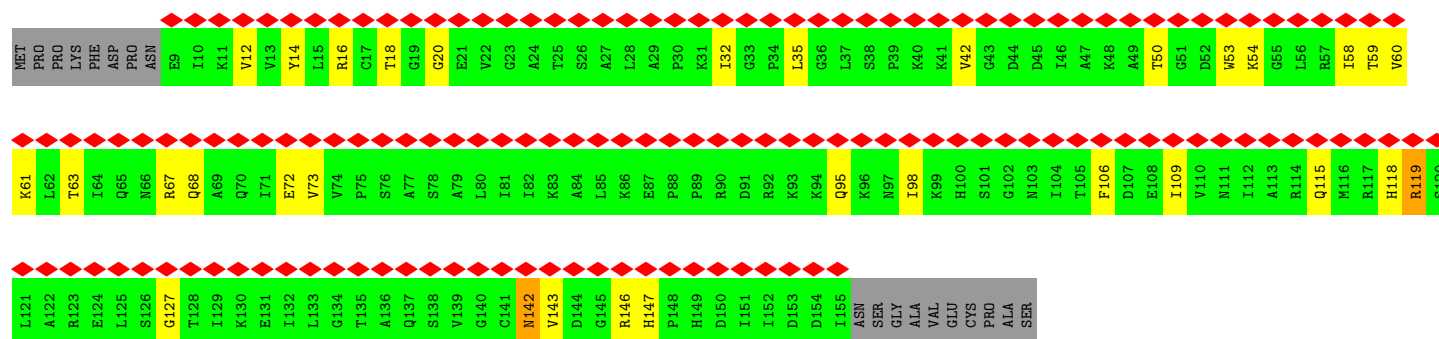
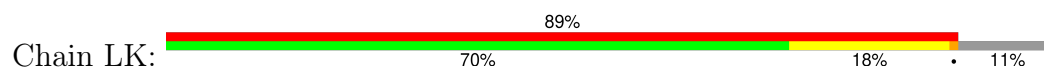


• Molecule 46: 60S acidic ribosomal protein P0

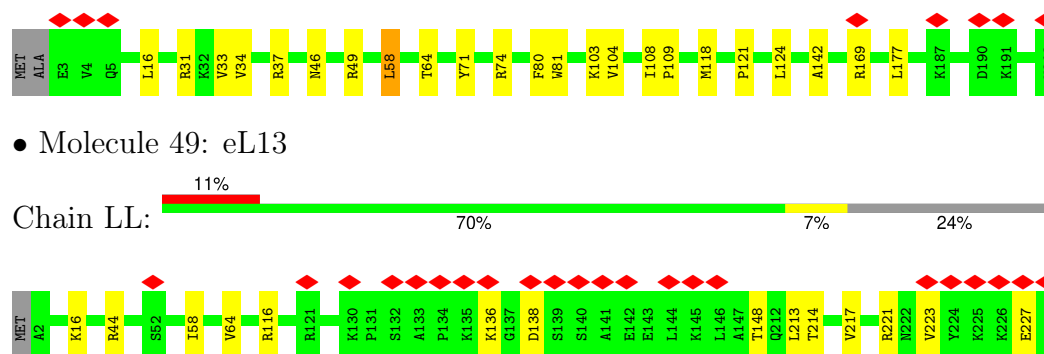




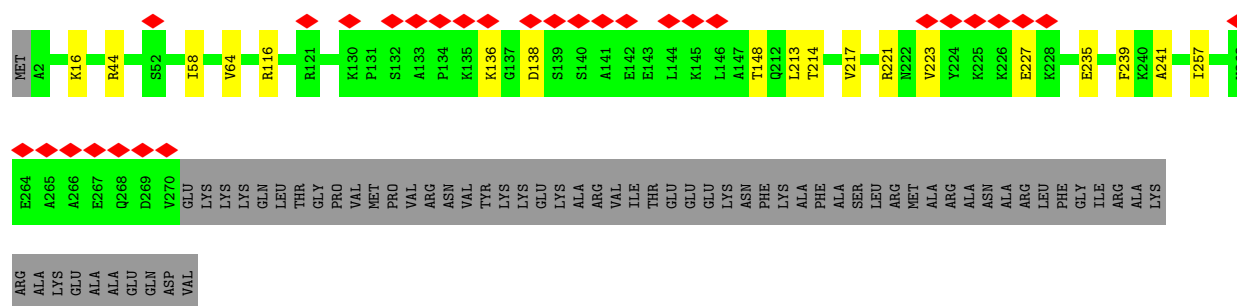
• Molecule 47: 60S ribosomal protein L12



• Molecule 48: 60S ribosomal protein L13a

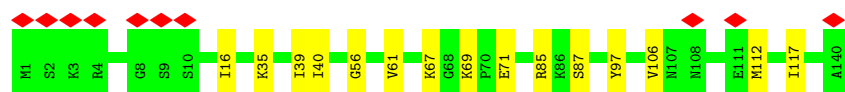


• Molecule 49: eL13



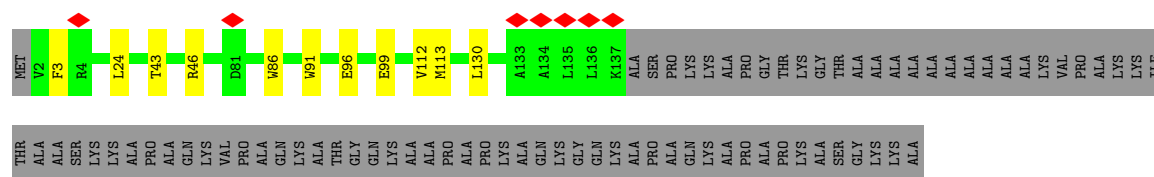
• Molecule 50: 60S ribosomal protein L23





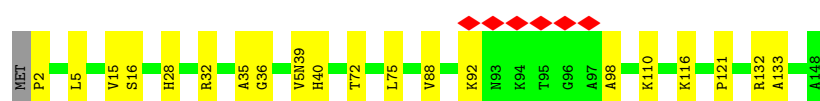
- Molecule 51: 60S ribosomal protein L14

Chain LM: 58% 5% 37%



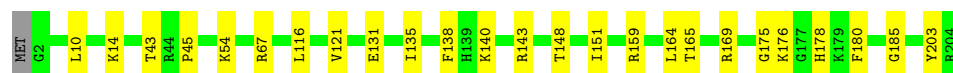
- Molecule 52: 60S ribosomal protein L27a

Chain La: 86% 14%



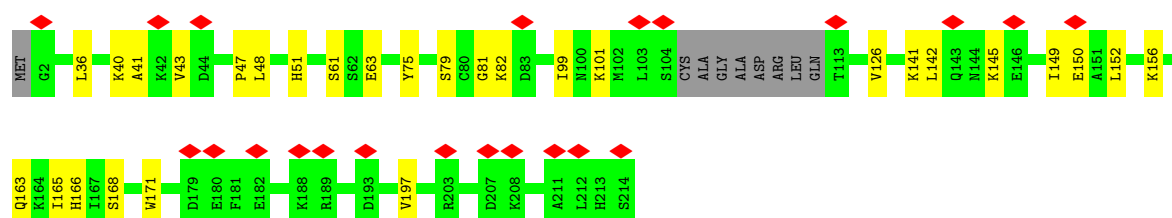
- Molecule 53: 60S ribosomal protein L15

Chain LN: 87% 12%



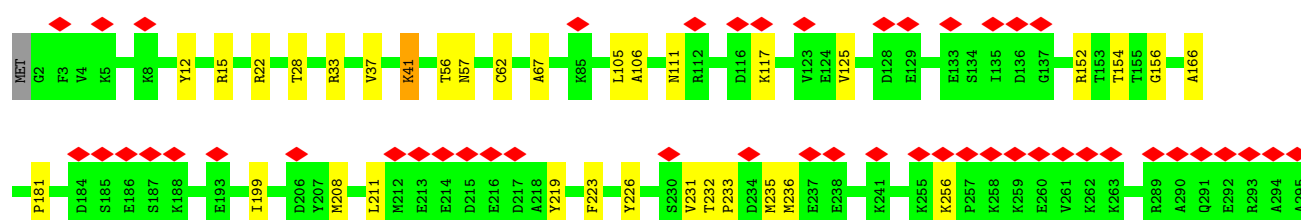
- Molecule 54: 60S ribosomal protein L10

Chain LI: 10% 82% 14%



- Molecule 55: 60S ribosomal protein L5

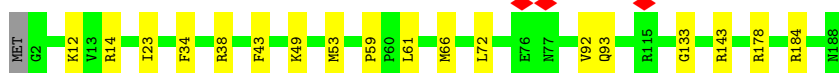
Chain LD: 16% 88% 11%



GLU
SER

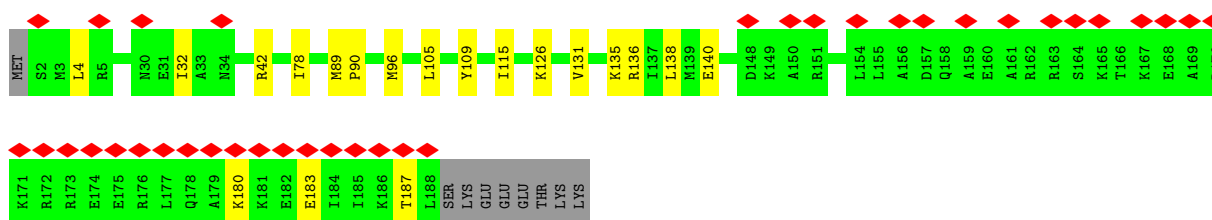
- Molecule 56: 60S ribosomal protein L18

Chain LQ: 



- Molecule 57: 60S ribosomal protein L19

Chain LR: 



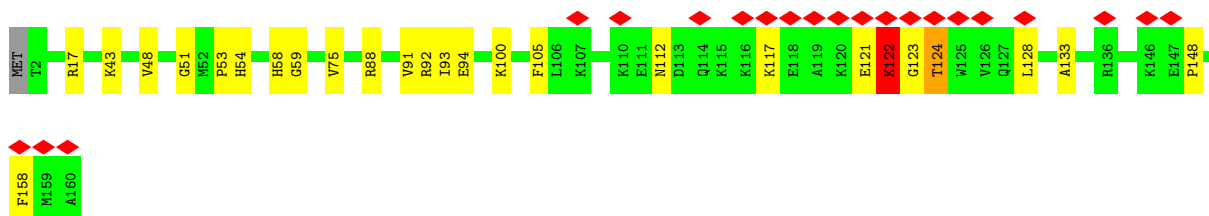
- Molecule 58: 60S ribosomal protein L18a

Chain LS: 



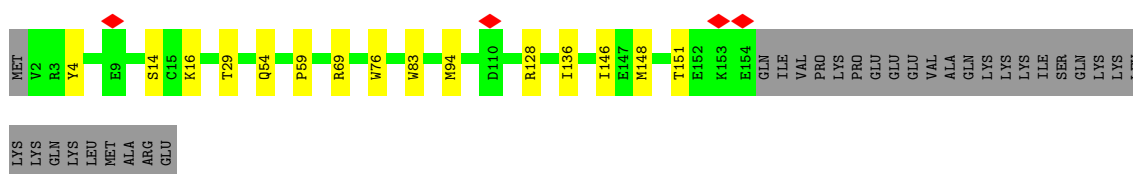
- Molecule 59: 60S ribosomal protein L21

Chain LT: 

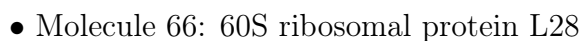


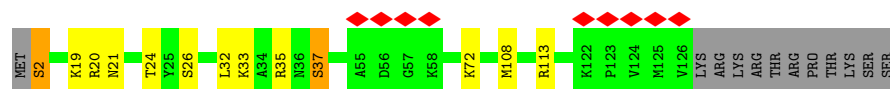
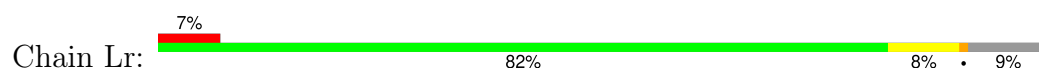
- Molecule 60: 60S ribosomal protein L17

Chain LP: 

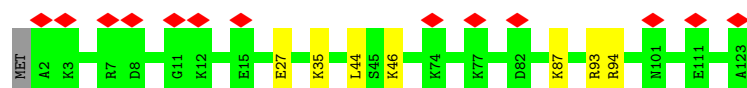


- Chain LU:

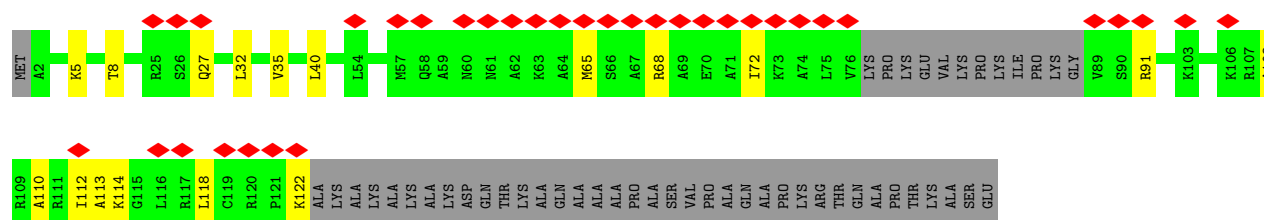




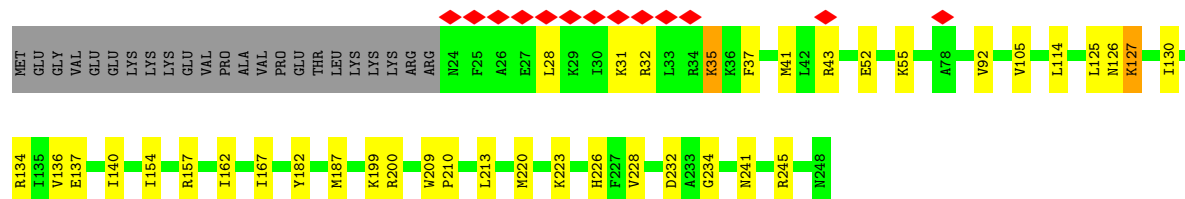
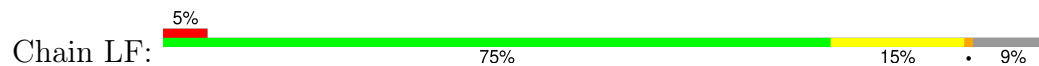
- Molecule 67: 60S ribosomal protein L35



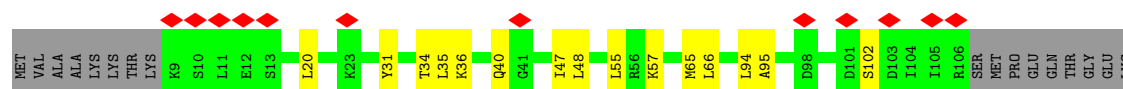
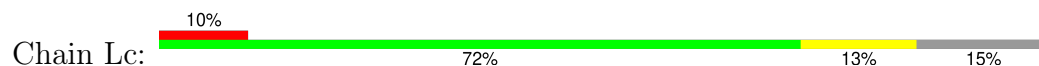
- Molecule 68: 60S ribosomal protein L29



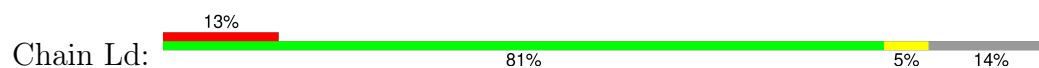
- Molecule 69: 60S ribosomal protein L7



- Molecule 70: 60S ribosomal protein L30



- Molecule 71: 60S ribosomal protein L31



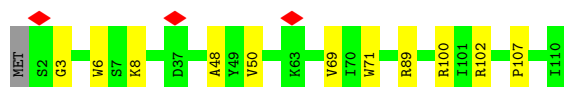
- Molecule 72: 60S ribosomal protein L32

Chain Le:  88% 6% • 5%



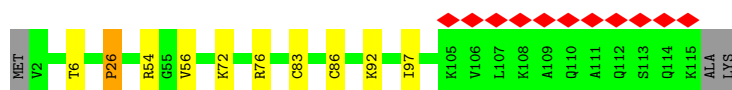
- Molecule 73: 60S ribosomal protein L35a

Chain Lf:  89% 10% •



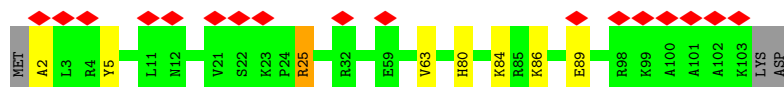
- Molecule 74: 60S ribosomal protein L34

Chain Lg:  9% 89% 8% • •



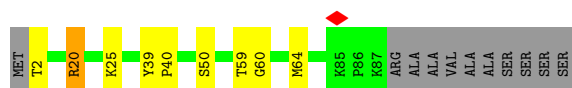
- Molecule 75: 60S ribosomal protein L36

Chain Li:  16% 90% 7% • •

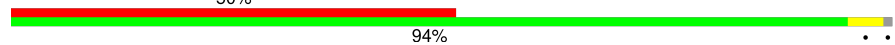


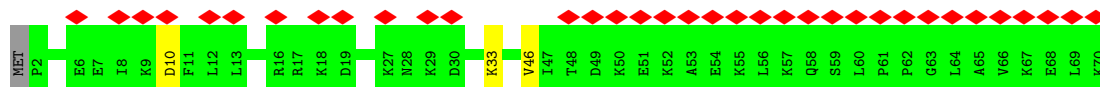
- Molecule 76: 60S ribosomal protein L37

Chain Lj:  79% 8% • 11%



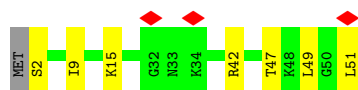
- Molecule 77: 60S ribosomal protein L38

Chain Lk:  50% 94% • •

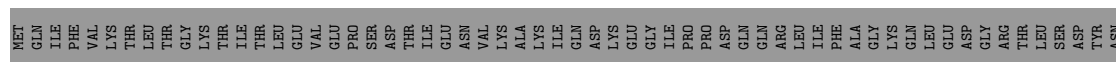


- Molecule 78: 60S ribosomal protein L39

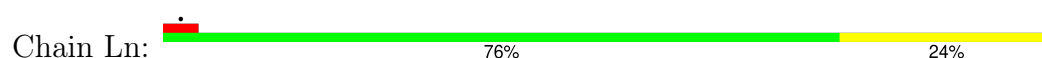
Chain Ll:  6% 84% 14% •



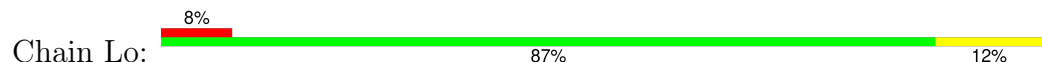
- Molecule 79: eL40



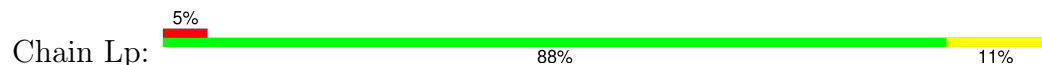
- Molecule 80: 60S ribosomal protein L41



- Molecule 81: 60S ribosomal protein L36a



- Molecule 82: 60S ribosomal protein L37a



- Molecule 83: mRNA



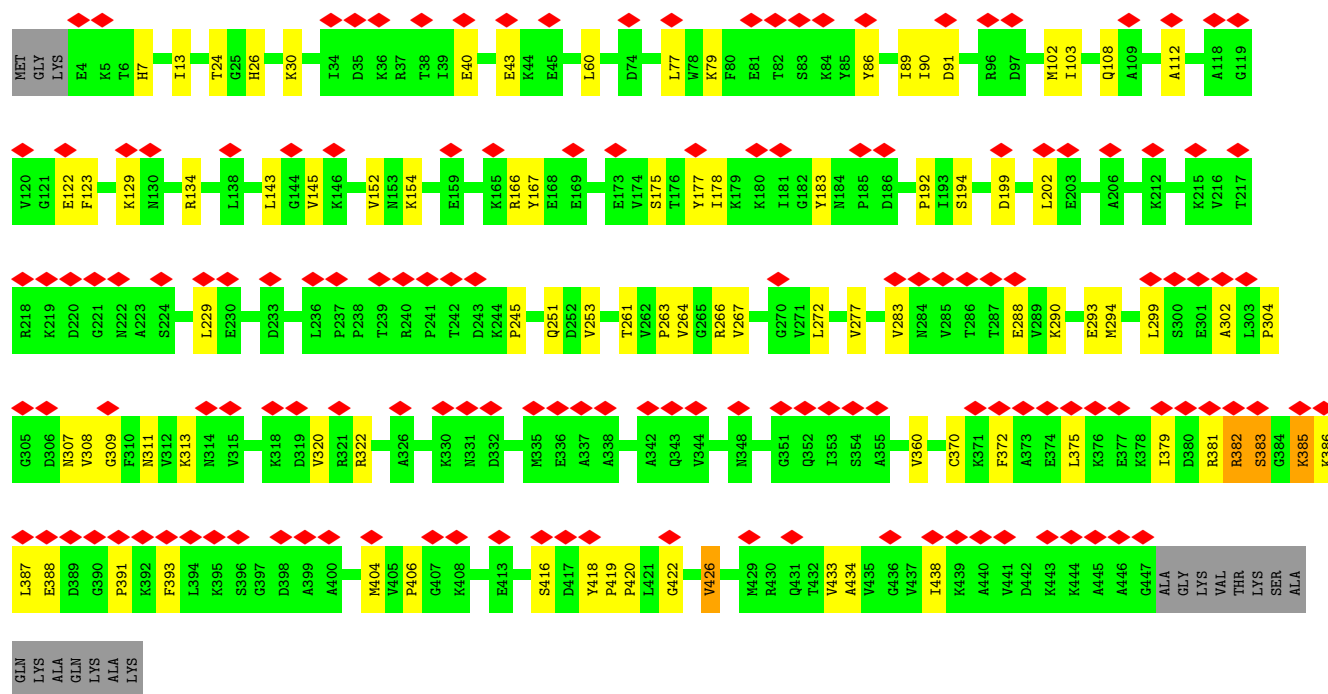
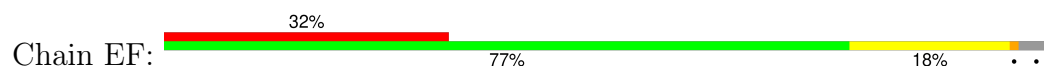
- Molecule 84: A-site tRNA



- Molecule 85: P-site tRNA



- Molecule 86: Elongation factor 1-alpha 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80708	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	579.8912, 579.8912, 579.8912	wwPDB
Map dimensions	896, 896, 896	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.6472, 0.6472, 0.6472	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, HY3, 4AC, PSU, K, ZN, 1MA, PUT, A2M, SPD, 4SU, H2U, HIC, OMG, UY1, OMC, MLZ, MIA, OMU, AME, 3HE, V5N, YRB, GSP, HMT, M3L, G7M, 5MC, MA6, 6MZ, UR3, MLY, MG, SAC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	S2	0.38	5/38635 (0.0%)	0.56	0/60214
2	L8	0.36	0/3613	0.51	0/5627
3	L5	0.36	7/85472 (0.0%)	0.51	1/133344 (0.0%)
4	L7	0.33	0/2862	0.46	0/4459
5	SB	0.34	0/1832	0.51	0/2449
6	SA	0.39	0/1778	0.54	0/2416
7	SD	0.54	0/1784	0.72	0/2403
8	SJ	0.54	0/1550	0.90	0/2069
9	SE	0.51	0/2118	0.80	0/2849
10	SC	0.47	0/1762	0.69	0/2381
11	SG	0.47	0/1946	0.74	0/2590
12	SF	0.46	0/1515	0.69	0/2037
13	SH	0.61	0/1540	0.89	0/2064
14	SW	0.50	0/1051	0.72	0/1406
15	SI	0.40	0/1715	0.64	0/2287
16	SQ	0.63	0/1141	0.86	0/1528
17	SU	0.71	0/813	1.01	0/1092
18	SK	0.53	0/834	0.83	0/1125
19	SO	0.57	0/1022	0.92	2/1372 (0.1%)
20	SX	0.55	0/1113	0.79	0/1483
21	SM	0.69	0/950	0.93	0/1275
22	SS	0.54	0/1232	0.84	0/1651
23	Sd	0.51	0/469	0.78	0/623
24	SN	0.52	0/1242	0.76	0/1671
25	SL	0.47	0/1191	0.69	1/1593 (0.1%)
26	SR	0.61	0/1098	0.97	0/1474
27	SP	0.48	0/1116	0.69	0/1493
28	ST	0.56	0/1131	0.83	0/1515
29	SV	0.48	0/635	0.73	0/850
30	SY	0.30	0/1083	0.54	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SZ	0.61	0/682	0.95	0/911
32	Sa	0.28	0/805	0.46	0/1079
33	Sb	0.35	0/664	0.54	0/891
34	Sc	0.60	0/508	0.94	0/680
35	Se	0.50	0/473	0.76	0/623
36	Sf	0.77	0/627	1.07	0/829
37	Sg	0.57	0/2493	0.84	0/3394
38	Lz	0.86	0/1729	1.17	0/2320
39	LA	0.49	0/1947	0.69	1/2609 (0.0%)
40	LB	0.38	0/3294	0.55	0/4406
41	LC	0.39	0/2981	0.57	0/4002
42	LJ	0.40	0/1381	0.63	0/1847
43	LH	0.40	0/1537	0.61	0/2066
44	LE	0.40	0/1830	0.57	0/2453
45	LG	0.57	0/1943	0.78	0/2616
46	Lq	0.25	0/1529	0.42	0/2063
47	LK	0.45	0/1135	0.64	0/1529
48	LO	0.49	0/1682	0.71	1/2250 (0.0%)
49	LL	0.57	0/1695	0.79	0/2270
50	LV	0.48	0/1056	0.69	1/1412 (0.1%)
51	LM	0.36	0/1142	0.52	0/1527
52	La	0.42	0/1179	0.61	0/1573
53	LN	0.44	0/1745	0.64	0/2338
54	LI	0.58	0/1698	0.86	1/2266 (0.0%)
55	LD	0.42	0/2437	0.61	0/3263
56	LQ	0.39	0/1536	0.60	0/2052
57	LR	0.35	0/1582	0.55	0/2091
58	LS	0.44	0/1500	0.63	0/2013
59	LT	0.35	0/1325	0.54	0/1770
60	LP	0.42	0/1268	0.66	0/1701
61	LU	0.53	0/822	0.76	0/1103
62	LX	0.29	0/984	0.43	0/1323
63	LY	0.47	0/1132	0.68	0/1504
64	LW	0.54	0/964	0.77	0/1278
65	LZ	0.53	0/1129	0.81	0/1507
66	Lr	0.46	0/1011	0.70	0/1356
67	Lh	0.42	0/1022	0.61	0/1351
68	Lb	0.48	0/887	0.75	0/1171
69	LF	0.36	0/1905	0.54	0/2539
70	Lc	0.25	0/774	0.39	0/1038
71	Ld	0.50	0/903	0.76	0/1216
72	Le	0.52	0/1071	0.66	0/1429
73	Lf	0.34	0/895	0.45	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Lg	0.43	0/916	0.63	0/1220
75	Li	0.62	0/843	0.91	0/1115
76	Lj	0.41	0/731	0.63	0/967
77	Lk	0.40	0/575	0.65	0/761
78	Ll	0.65	0/453	0.86	0/599
79	Lm	0.39	0/426	0.76	0/564
80	Ln	0.45	0/240	0.86	0/305
81	Lo	0.40	0/877	0.60	0/1156
82	Lp	0.38	0/718	0.58	0/953
83	mR	0.22	0/280	0.33	0/433
84	At	0.37	1/1650 (0.1%)	0.48	0/2566
85	Pt	0.44	1/1721 (0.1%)	0.56	0/2679
86	EF	0.39	0/3428	0.60	0/4644
All	All	0.42	14/236003 (0.0%)	0.60	8/345597 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	Pt	47	G7M	O3'-P	9.65	1.66	1.56
1	S2	166	A2M	O3'-P	7.69	1.64	1.56
3	L5	3785	A2M	O3'-P	6.74	1.62	1.56
1	S2	1288	OMU	O3'-P	6.52	1.62	1.56
84	At	8	4SU	O3'-P	6.01	1.62	1.56
3	L5	3825	A2M	O3'-P	5.99	1.62	1.56
3	L5	3718	A2M	O3'-P	5.89	1.62	1.56
1	S2	668	A2M	O3'-P	5.84	1.62	1.56
3	L5	3867	A2M	O3'-P	5.69	1.61	1.56
3	L5	398	A2M	O3'-P	5.57	1.61	1.56
3	L5	4571	A2M	O3'-P	5.54	1.61	1.56
3	L5	1326	A2M	O3'-P	5.46	1.61	1.56
1	S2	484	A2M	O3'-P	5.28	1.61	1.56
1	S2	27	A2M	O3'-P	5.17	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	LI	81	GLY	CA-C-O	-6.68	117.49	122.37
50	LV	40	ILE	N-CA-C	-6.51	107.53	113.71
19	SO	138	ASP	CB-CA-C	6.21	122.79	110.42
19	SO	137	SER	N-CA-C	-5.66	103.66	111.81
39	LA	244	GLY	CA-C-O	-5.61	118.09	122.52
3	L5	2098	G	C4'-C3'-O3'	-5.23	101.56	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	SL	50	ALA	N-CA-C	-5.18	107.09	113.41
48	LO	109	PRO	CB-CA-C	-5.16	104.63	110.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36364	0	18406	351	0
2	L8	3320	0	1686	26	0
3	L5	79146	0	40068	611	0
4	L7	2562	0	1295	14	0
5	SB	1806	0	1888	17	0
6	SA	1750	0	1755	28	0
7	SD	1756	0	1852	34	0
8	SJ	1525	0	1640	29	0
9	SE	2076	0	2177	39	0
10	SC	1725	0	1813	22	0
11	SG	1923	0	2089	26	0
12	SF	1494	0	1549	21	0
13	SH	1517	0	1605	29	0
14	SW	1034	0	1080	17	0
15	SI	1686	0	1772	21	0
16	SQ	1123	0	1193	17	0
17	SU	803	0	873	16	0
18	SK	810	0	836	22	0
19	SO	1009	0	1034	9	0
20	SX	1105	0	1167	13	0
21	SM	940	0	965	33	0
22	SS	1214	0	1275	23	0
23	Sd	458	0	448	3	0
24	SN	1214	0	1300	15	0
25	SL	1171	0	1241	13	0
26	SR	1083	0	1137	22	0
27	SP	1093	0	1139	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	ST	1112	0	1146	11	0
29	SV	639	0	638	6	0
30	SY	1065	0	1142	20	0
31	SZ	674	0	748	18	0
32	Sa	792	0	841	12	0
33	Sb	650	0	672	7	0
34	Sc	506	0	536	7	0
35	Se	467	0	516	9	0
36	Sf	615	0	639	13	0
37	Sg	2436	0	2393	48	0
38	Lz	1701	0	1810	69	0
39	LA	1922	0	2015	17	0
40	LB	3239	0	3377	31	0
41	LC	2927	0	3104	19	0
42	LJ	1358	0	1396	13	0
43	LH	1518	0	1601	10	0
44	LE	1793	0	1958	17	0
45	LG	1910	0	2052	23	0
46	Lq	1506	0	1562	21	0
47	LK	1121	0	1184	19	0
48	LO	1650	0	1794	14	0
49	LL	1664	0	1773	11	0
50	LV	1042	0	1109	9	0
51	LM	1120	0	1187	7	0
52	La	1163	0	1206	13	0
53	LN	1700	0	1749	16	0
54	LI	1660	0	1710	15	0
55	LD	2391	0	2426	22	0
56	LQ	1512	0	1628	10	0
57	LR	1566	0	1729	13	0
58	LS	1460	0	1502	13	0
59	LT	1297	0	1366	20	0
60	LP	1242	0	1269	10	0
61	LU	808	0	831	10	0
62	LX	967	0	1040	10	0
63	LY	1115	0	1205	8	0
64	LW	950	0	999	16	0
65	LZ	1106	0	1182	10	0
66	Lr	1005	0	1072	8	0
67	Lh	1014	0	1148	4	0
68	Lb	885	0	967	11	0
69	LF	1870	0	1996	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Lc	764	0	804	10	0
71	Ld	888	0	930	4	0
72	Le	1053	0	1147	5	0
73	Lf	876	0	910	9	0
74	Lg	906	0	998	8	0
75	Li	832	0	917	6	0
76	Lj	712	0	744	9	0
77	Lk	569	0	637	1	0
78	Ll	443	0	483	5	0
79	Lm	432	0	470	2	0
80	Ln	239	0	289	4	0
81	Lo	870	0	936	10	0
82	Lp	708	0	756	6	0
83	mR	252	0	127	8	0
84	At	1630	0	839	12	0
85	Pt	1645	0	843	6	0
86	EF	3405	0	3465	55	0
87	L5	90	0	171	3	0
87	S2	10	0	19	0	0
88	L5	25	0	0	0	0
88	LA	1	0	0	0	0
88	Lf	1	0	0	0	0
88	S2	6	0	0	0	0
88	mR	1	0	0	0	0
89	EF	2	0	0	0	0
89	L5	225	0	0	0	0
89	L7	5	0	0	0	0
89	L8	3	0	0	0	0
89	LA	1	0	0	0	0
89	LB	1	0	0	0	0
89	LH	1	0	0	0	0
89	LI	2	0	0	0	0
89	LN	1	0	0	0	0
89	LP	1	0	0	0	0
89	LS	2	0	0	0	0
89	LV	1	0	0	0	0
89	Le	1	0	0	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Pt	1	0	0	0	0
89	S2	83	0	0	0	0
89	SE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	SO	1	0	0	0	0
89	ST	1	0	0	0	0
89	SX	1	0	0	0	0
89	Sd	1	0	0	0	0
90	L5	48	0	96	8	0
91	L5	20	0	23	0	0
92	L5	39	0	39	6	0
93	Lg	1	0	0	0	0
93	Lj	1	0	0	0	0
93	Lm	1	0	0	0	0
93	Lo	1	0	0	0	0
93	Lp	1	0	0	0	0
93	Sa	1	0	0	0	0
93	Sd	1	0	0	0	0
93	Sf	1	0	0	0	0
94	At	11	0	8	0	0
95	Pt	8	0	8	1	0
96	EF	32	0	12	1	0
97	EF	56	0	0	0	0
98	EF	3	0	0	0	0
All	All	225765	0	169172	2051	0

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

All (2051) 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)
1:S2:327:G:H2'	1:S2:329:G:H5''	1.40	1.02
9:SE:198:ARG:HG3	9:SE:208:VAL:HG22	1.48	0.94
21:SM:81:ASP:HB2	21:SM:84:LYS:HB2	1.50	0.93
3:L5:2097:U:H2'	3:L5:2098:G:H3'	1.49	0.90
3:L5:1688:G:H1'	90:L5:5119:PUT:H22	1.54	0.89
13:SH:160:LYS:HD2	13:SH:191:GLU:HA	1.53	0.88
17:SU:24:LEU:HB2	17:SU:87:ARG:HB2	1.60	0.83
21:SM:76:LEU:HD21	21:SM:78:LYS:HG3	1.60	0.82
1:S2:560:A:H5'	8:SJ:174:LYS:HB2	1.63	0.81
46:Lq:190:GLN:HG3	46:Lq:191:GLN:HG2	1.62	0.81
3:L5:1242:G:H4'	68:Lb:122:LYS:HA	1.63	0.80
21:SM:81:ASP:CB	21:SM:84:LYS:HB2	2.12	0.80
38:Lz:207:LYS:HG3	38:Lz:213:PRO:HD2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lz:90:LEU:HD21	38:Lz:124:LEU:HD12	1.62	0.79
37:Sg:87:LEU:HB2	37:Sg:101:PHE:HB2	1.64	0.79
38:Lz:68:LEU:HD11	38:Lz:77:ALA:HB2	1.65	0.79
21:SM:35:ILE:HD12	36:Sf:102:VAL:HG21	1.64	0.78
36:Sf:126:CYS:HB2	36:Sf:130:VAL:HG21	1.66	0.78
13:SH:137:SER:HA	13:SH:162:GLN:HG3	1.66	0.78
3:L5:3946:G:H1	3:L5:4067:U:H3	1.32	0.77
68:Lb:5:MLZ:HE3	68:Lb:8:THR:HB	1.66	0.77
1:S2:1285:G:O6	21:SM:56:CYS:HA	1.83	0.77
1:S2:16:G:H2'	1:S2:17:C:C6	2.21	0.76
38:Lz:77:ALA:HB3	38:Lz:84:HIS:HB3	1.69	0.75
3:L5:3759:A:H5'	3:L5:3765:G:H22	1.51	0.74
18:SK:21:MET:HG3	18:SK:49:MET:HE3	1.68	0.74
86:EF:245:PRO:HG2	86:EF:418:TYR:OH	1.89	0.73
1:S2:1639:G7M:H2'	1:S2:1640:A:C8	2.23	0.73
10:SC:171:GLY:HA2	14:SW:98:GLN:HE22	1.54	0.73
22:SS:98:VAL:HG11	22:SS:106:LYS:HG3	1.70	0.73
6:SA:134:LEU:HD22	6:SA:144:THR:HG21	1.71	0.72
1:S2:925:G:H1	1:S2:1017:U:H3	1.37	0.72
46:Lq:29:ILE:HB	46:Lq:191:GLN:HG3	1.72	0.71
46:Lq:91:THR:HG21	46:Lq:98:ILE:HG12	1.73	0.70
26:SR:17:ILE:HG21	26:SR:61:ILE:HD12	1.72	0.70
65:LZ:46:ILE:HG23	65:LZ:68:ILE:HG23	1.74	0.70
19:SO:53:ILE:HG23	19:SO:88:LEU:HD23	1.74	0.69
43:LH:115:ARG:HG2	43:LH:123:ILE:HG12	1.75	0.69
1:S2:944:A:H5''	19:SO:134:PRO:HB2	1.75	0.68
3:L5:1703:C:H2'	3:L5:1704:C:O4'	1.93	0.68
1:S2:928:G:H1	1:S2:1013:U:H3	1.41	0.68
3:L5:3697:U:H2'	39:LA:245:ARG:HH22	1.57	0.68
84:At:14:A:H61	84:At:21:A:H1'	1.59	0.68
86:EF:294:MET:HB2	86:EF:308:VAL:HG12	1.76	0.68
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.59	0.68
18:SK:84:HIS:ND1	21:SM:27:ILE:HG13	2.08	0.67
38:Lz:119:GLN:HG3	38:Lz:123:ILE:HB	1.76	0.67
86:EF:419:PRO:HB2	86:EF:420:PRO:HD3	1.76	0.67
37:Sg:79:LEU:HB2	37:Sg:113:PHE:CZ	2.28	0.67
38:Lz:14:VAL:HB	38:Lz:214:GLN:HE21	1.58	0.67
1:S2:327:G:H2'	1:S2:329:G:C5'	2.21	0.67
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.30	0.67
47:LK:50:THR:HB	47:LK:53:TRP:HD1	1.59	0.67
49:LL:58:ILE:HD12	49:LL:116:ARG:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:LD:211:LEU:HB3	55:LD:219:TYR:HB2	1.77	0.67
46:Lq:17:ILE:HG22	46:Lq:54:LEU:HD21	1.77	0.67
3:L5:37:U:H5''	52:La:32:ARG:HD3	1.76	0.66
37:Sg:32:LEU:HD21	37:Sg:42:MET:HG2	1.78	0.66
1:S2:328:U:H5'	64:LW:109:ILE:HD11	1.76	0.66
3:L5:4896:G:N2	3:L5:4926:C:H41	1.94	0.66
18:SK:1:MET:HE1	18:SK:43:LEU:HG	1.78	0.66
1:S2:190:G:H1'	1:S2:209:A:H61	1.62	0.65
1:S2:888:U:H1'	1:S2:889:U:H2'	1.79	0.65
3:L5:5025:C:H2'	3:L5:5026:U:H4'	1.79	0.65
13:SH:163:GLN:HG2	13:SH:167:GLU:HG3	1.78	0.65
1:S2:582:U:H2'	1:S2:583:A:H8	1.62	0.65
3:L5:1590:C:H4'	3:L5:2857:A:H5'	1.77	0.65
40:LB:107:ALA:HB2	40:LB:201:LEU:HD22	1.77	0.65
3:L5:4896:G:H21	3:L5:4926:C:H41	1.44	0.65
37:Sg:5:MET:HE2	37:Sg:312:VAL:HG12	1.78	0.65
3:L5:1447:C:H1'	3:L5:2098:G:H22	1.61	0.65
53:LN:138:PHE:HA	53:LN:143:ARG:HD2	1.78	0.64
3:L5:32:G:H21	3:L5:50:C:H5	1.45	0.64
64:LW:101:ARG:HA	64:LW:104:GLN:OE1	1.98	0.64
11:SG:70:HIS:HB3	11:SG:103:ASP:OD2	1.98	0.64
9:SE:105:THR:CG2	9:SE:245:ARG:HA	2.28	0.64
1:S2:1520:G:N3	1:S2:1520:G:H2'	2.13	0.64
27:SP:137:HIS:HA	27:SP:140:ARG:HG2	1.80	0.64
1:S2:1536:G:H2'	1:S2:1537:A:C8	2.32	0.64
59:LT:121:GLU:O	59:LT:122:LYS:HB2	1.97	0.63
66:Lr:35:ARG:HG3	66:Lr:37:SER:HB3	1.80	0.63
3:L5:4733:C:H4'	3:L5:4734:A:H5'	1.80	0.63
49:LL:58:ILE:CD1	49:LL:116:ARG:HD2	2.28	0.63
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.33	0.63
3:L5:2786:C:H5''	3:L5:2787:A2M:H5'	1.81	0.63
37:Sg:168:CYS:HB3	37:Sg:198:VAL:HG13	1.81	0.63
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.80	0.63
10:SC:196:ILE:HB	10:SC:223:TYR:HB2	1.81	0.63
9:SE:201:HIS:HB2	9:SE:204:SER:HB3	1.80	0.62
18:SK:7:ASN:ND2	18:SK:40:VAL:HG22	2.13	0.62
38:Lz:49:PHE:HB2	38:Lz:193:LEU:HD13	1.79	0.62
1:S2:92:A:O2'	9:SE:4:GLY:HA3	1.98	0.62
69:LF:182:TYR:HB3	69:LF:200:ARG:HG3	1.80	0.62
3:L5:451:C:H2'	3:L5:1294:A:C8	2.33	0.62
3:L5:3975:C:H2'	3:L5:4036:G:H1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SF:128:ILE:HD11	34:Sc:22:GLY:HA2	1.81	0.62
38:Lz:68:LEU:HD11	38:Lz:77:ALA:CB	2.29	0.62
1:S2:1650:A:H5''	16:SQ:139:ALA:HB2	1.80	0.62
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.34	0.62
22:SS:23:ARG:HG2	31:SZ:48:VAL:CG1	2.30	0.62
38:Lz:77:ALA:CB	38:Lz:84:HIS:HB3	2.28	0.62
7:SD:47:GLU:HG2	7:SD:87:TYR:HE2	1.64	0.62
1:S2:1824:A:OP1	20:SX:60:LYS:HA	1.99	0.62
9:SE:45:ILE:HG13	9:SE:61:VAL:HG21	1.82	0.62
11:SG:70:HIS:HA	11:SG:98:ARG:HH12	1.64	0.62
17:SU:21:ARG:HA	17:SU:89:ILE:O	2.00	0.62
40:LB:220:ILE:HG12	40:LB:278:THR:HG23	1.82	0.62
58:LS:15:ARG:HB3	58:LS:27:LEU:HD23	1.80	0.62
21:SM:58:GLU:HG2	21:SM:58:GLU:O	1.99	0.61
38:Lz:75:ASP:HA	38:Lz:78:LYS:HD2	1.81	0.61
1:S2:582:U:H2'	1:S2:583:A:C8	2.35	0.61
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.82	0.61
1:S2:190:G:H1'	1:S2:209:A:N6	2.15	0.61
3:L5:1850:A:N3	90:L5:5119:PUT:H31	2.16	0.61
37:Sg:87:LEU:HD21	37:Sg:122:SER:HB3	1.83	0.61
30:SY:15:ASN:HD21	30:SY:18:LEU:HD23	1.66	0.61
83:mR:36[A]:U:H2'	83:mR:37:A:C8	2.35	0.61
1:S2:1706:G:H5'	80:Ln:1:MET:HB2	1.83	0.61
5:SB:33:VAL:HG12	5:SB:44:ILE:HD13	1.82	0.61
7:SD:40:ARG:HA	7:SD:40:ARG:HH11	1.64	0.61
1:S2:1444:U:H2'	1:S2:1445:PSU:C6	2.36	0.61
20:SX:68:LYS:HE2	35:Se:83:ALA:HB2	1.81	0.61
20:SX:68:LYS:HE3	35:Se:80:LEU:HA	1.82	0.61
3:L5:184:U:H2'	3:L5:186:G:H1'	1.83	0.60
92:L5:5118:HMT:H23	95:Pt:78:MET:N	2.16	0.60
9:SE:175:PHE:HE2	9:SE:198:ARG:HD2	1.65	0.60
32:Sa:64:LEU:HD12	32:Sa:65:PRO:HD2	1.83	0.60
3:L5:1739:G:H5''	4:L7:102:U:H1'	1.83	0.60
13:SH:84:GLU:HG3	13:SH:92:VAL:HG22	1.82	0.60
39:LA:234:LYS:HG2	39:LA:238:ILE:HG12	1.82	0.60
81:Lo:56:PHE:HE2	81:Lo:59:LYS:HD3	1.67	0.60
1:S2:1444:U:H2'	1:S2:1445:PSU:H6	1.66	0.60
38:Lz:32:VAL:HG22	38:Lz:208:SER:HB3	1.82	0.60
37:Sg:113:PHE:O	37:Sg:156:PHE:HD2	1.84	0.60
69:LF:105:VAL:HG13	69:LF:136:VAL:HG12	1.83	0.60
2:L8:86:U:H3'	2:L8:87:G:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2458:C:H5''	53:LN:67:ARG:HD2	1.84	0.60
39:LA:36:GLU:HG3	39:LA:91:GLY:HA2	1.83	0.60
12:SF:76:MET:HB2	12:SF:89:THR:HG21	1.82	0.60
13:SH:73:GLN:HE21	13:SH:135:PHE:HD1	1.46	0.60
1:S2:1740:C:H5''	15:SI:58:LEU:HD21	1.83	0.60
70:Lc:20:LEU:HB3	70:Lc:102:SER:HB3	1.84	0.60
86:EF:77:LEU:HG	86:EF:90:ILE:HG13	1.82	0.60
3:L5:4731:G:H1'	3:L5:4732:G:C2	2.37	0.59
5:SB:171:ILE:HD13	5:SB:174:ARG:HH12	1.66	0.59
60:LP:128:ARG:HH21	60:LP:136:ILE:HD13	1.67	0.59
48:LO:37:ARG:HD2	48:LO:108:ILE:HD11	1.84	0.59
54:LI:51:HIS:CD2	54:LI:168:SER:HB2	2.37	0.59
1:S2:1587:G:H5''	28:ST:77:LYS:HD2	1.84	0.59
1:S2:543:C:H3'	1:S2:544:G:H8	1.68	0.59
3:L5:2008:U:H1'	3:L5:2011:C:H5	1.68	0.59
38:Lz:215:ARG:C	38:Lz:215:ARG:HD2	2.28	0.59
3:L5:4060:U:H2'	3:L5:4061:G:C8	2.38	0.59
18:SK:84:HIS:HB3	21:SM:27:ILE:HG23	1.83	0.59
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.37	0.59
12:SF:76:MET:HB2	12:SF:89:THR:CG2	2.32	0.59
38:Lz:120:ILE:HD12	38:Lz:124:LEU:HD13	1.83	0.59
21:SM:121:LYS:HA	21:SM:124:ILE:HG12	1.84	0.59
75:Li:80:HIS:HE2	75:Li:84:LYS:HE2	1.66	0.59
8:SJ:82:VAL:HG21	8:SJ:92:MET:HE1	1.83	0.59
15:SI:57:ALA:HB2	15:SI:183:GLY:HA2	1.85	0.59
37:Sg:25:PRO:HA	37:Sg:293:ALA:HB2	1.84	0.59
57:LR:109:TYR:HB3	57:LR:115:ILE:HG12	1.84	0.59
7:SD:220:THR:HG23	7:SD:221:THR:HG23	1.85	0.58
86:EF:108:GLN:HB2	86:EF:266:ARG:HD3	1.85	0.58
16:SQ:53:GLU:HB2	16:SQ:54:PRO:HD3	1.83	0.58
28:ST:115:LYS:HA	28:ST:121:ARG:HG3	1.85	0.58
47:LK:12:VAL:HG22	47:LK:63:THR:HG22	1.84	0.58
13:SH:130:LEU:HD21	13:SH:156:VAL:HG21	1.85	0.58
86:EF:272:LEU:HB3	86:EF:302:ALA:HB3	1.85	0.58
3:L5:1995:G:H5''	3:L5:1996:C:H5	1.68	0.58
1:S2:1401:A:H2'	1:S2:1402:A:C8	2.38	0.58
3:L5:260:C:H2'	3:L5:261:G:H5'	1.86	0.58
3:L5:667:A:H2'	3:L5:668:C:C6	2.38	0.58
21:SM:52:LEU:HD23	21:SM:78:LYS:HG2	1.85	0.58
32:Sa:59:PHE:HB2	32:Sa:62:TYR:HB2	1.86	0.58
37:Sg:236:ILE:HG21	37:Sg:239:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:31:PRO:HG2	9:SE:38:LEU:HG	1.85	0.58
46:Lq:66:ARG:HA	46:Lq:69:LEU:HD23	1.86	0.58
86:EF:266:ARG:HA	86:EF:307:ASN:HA	1.85	0.58
3:L5:4918:C:H2'	3:L5:4919:G:H8	1.69	0.58
6:SA:137:ALA:HB1	6:SA:142:LEU:HB3	1.84	0.58
1:S2:545:A:H2'	1:S2:546:G:C8	2.39	0.58
1:S2:1438:A:H2'	1:S2:1439:A:C8	2.39	0.58
3:L5:3603:G:H2'	3:L5:3604:A:C8	2.38	0.58
3:L5:3712:A:H2'	3:L5:3713:U:C6	2.38	0.58
3:L5:3950:U:H2'	3:L5:3951:G:C8	2.39	0.58
38:Lz:207:LYS:HG3	38:Lz:213:PRO:CD	2.34	0.58
40:LB:163:ILE:HG22	40:LB:180:LEU:HD11	1.86	0.58
47:LK:143:VAL:HG23	47:LK:147:HIS:CE1	2.38	0.58
1:S2:433:A:H5''	15:SI:22:HIS:HB3	1.85	0.58
1:S2:1017:U:H5'	24:SN:55:ARG:HD3	1.85	0.58
3:L5:930:G:H2'	3:L5:931:C:C6	2.39	0.58
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.39	0.57
3:L5:162:A:H2'	3:L5:163:A:C8	2.39	0.57
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.19	0.57
30:SY:125:VAL:HG12	30:SY:129:LYS:HE2	1.85	0.57
37:Sg:299:PHE:HD1	37:Sg:309:VAL:HG12	1.69	0.57
1:S2:1052:A:H2'	1:S2:1053:C:O4'	2.05	0.57
22:SS:117:ILE:HD13	27:SP:110:GLU:HB2	1.86	0.57
1:S2:546:G:H2'	1:S2:547:G:C8	2.40	0.57
3:L5:454:U:H3	3:L5:702:U:H3	1.52	0.57
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.40	0.57
27:SP:20:VAL:HG13	27:SP:24:GLN:HG3	1.86	0.57
3:L5:2478:C:H2'	3:L5:2479:G:C8	2.39	0.57
63:LY:10:ASP:HB3	63:LY:13:LYS:HB2	1.87	0.57
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.34	0.57
9:SE:181:CYS:HB3	9:SE:195:ILE:HD11	1.86	0.57
11:SG:145:PHE:HD2	64:LW:93:LYS:HB2	1.69	0.57
44:LE:192[A]:LYS:HE3	73:Lf:107:PRO:HB3	1.85	0.57
3:L5:1960:A:H4'	46:Lq:59:THR:HB	1.87	0.57
44:LE:149:ILE:HD12	44:LE:271:LEU:HD21	1.87	0.57
86:EF:386:LYS:O	86:EF:387:LEU:HD23	2.05	0.57
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.87	0.57
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.39	0.57
37:Sg:163:PRO:HB2	37:Sg:179:LEU:HB2	1.86	0.57
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.40	0.57
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SG:67:VAL:HB	11:SG:99:GLY:HA2	1.87	0.57
18:SK:31:LYS:HG2	18:SK:39:ASN:HA	1.87	0.57
13:SH:53:VAL:HG11	13:SH:172:THR:HA	1.86	0.57
1:S2:321:C:H2'	1:S2:322:C:C6	2.39	0.56
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.40	0.56
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.40	0.56
6:SA:77:ILE:HG12	6:SA:99:ILE:HB	1.86	0.56
26:SR:106:LEU:HA	26:SR:109:LEU:HB2	1.86	0.56
16:SQ:45:ARG:HG2	16:SQ:48:GLN:HE21	1.70	0.56
16:SQ:112:LEU:HD22	16:SQ:119:LEU:HD13	1.86	0.56
55:LD:208:MET:HB2	55:LD:233:PRO:HG3	1.87	0.56
55:LD:208:MET:HE2	55:LD:236:MET:HE1	1.86	0.56
3:L5:4859:C:H3'	3:L5:4860:G:H8	1.70	0.56
6:SA:7:VAL:HG13	6:SA:8:LEU:HG	1.86	0.56
10:SC:167:ARG:HG2	10:SC:219:ILE:HD13	1.87	0.56
1:S2:1101:U:H2'	1:S2:1102:G:C8	2.41	0.56
3:L5:1564:A:H2'	3:L5:1565:A:C8	2.40	0.56
39:LA:137:ILE:HD11	39:LA:149:LYS:HB2	1.87	0.56
43:LH:174:LYS:HG2	43:LH:175:PHE:H	1.71	0.56
45:LG:110:LYS:O	45:LG:114:LEU:HG	2.05	0.56
1:S2:328:U:H5'	64:LW:109:ILE:CD1	2.36	0.56
38:Lz:120:ILE:CG2	38:Lz:128:LEU:HD12	2.36	0.56
49:LL:227:GLU:O	49:LL:227:GLU:HG2	2.06	0.56
86:EF:426:VAL:HG22	86:EF:433:VAL:HB	1.88	0.56
27:SP:136:THR:HG21	85:Pt:30:G:OP1	2.05	0.56
75:Li:80:HIS:NE2	75:Li:84:LYS:HE2	2.20	0.56
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.41	0.56
22:SS:59:LEU:HG	22:SS:63:GLU:HG3	1.87	0.56
54:LI:152:LEU:HB3	54:LI:165:ILE:HD12	1.88	0.56
1:S2:944:A:H5''	19:SO:134:PRO:CB	2.34	0.56
1:S2:1824:A:H5''	20:SX:58:GLU:OE1	2.06	0.56
3:L5:495:C:H2'	3:L5:496:G:C8	2.41	0.56
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.05	0.56
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.41	0.56
6:SA:30:LEU:HB2	6:SA:47:TYR:CE2	2.40	0.56
25:SL:48:LYS:O	25:SL:52:GLU:HG2	2.05	0.56
48:LO:34:VAL:HG22	48:LO:103:LYS:HB2	1.88	0.56
3:L5:2583:C:OP1	74:Lg:54:ARG:HB2	2.06	0.56
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.70	0.56
11:SG:98:ARG:NH2	11:SG:103:ASP:HB2	2.21	0.56
37:Sg:11:LEU:HD12	37:Sg:43:TRP:CE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lz:120:ILE:HA	38:Lz:124:LEU:HB3	1.86	0.56
38:Lz:205:TYR:CE2	38:Lz:215:ARG:HD3	2.41	0.56
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.41	0.55
6:SA:6:ASP:HA	6:SA:9:GLN:HG2	1.89	0.55
6:SA:10:MET:HE2	6:SA:15:VAL:HG22	1.88	0.55
37:Sg:11:LEU:HB2	37:Sg:307:VAL:HB	1.87	0.55
69:LF:125:LEU:HD22	69:LF:130:ILE:HD11	1.86	0.55
3:L5:256:G:H2'	3:L5:257:C:C6	2.41	0.55
3:L5:1697:G:H2'	3:L5:1698:C:C2	2.41	0.55
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.40	0.55
40:LB:92:TYR:HB3	40:LB:99:LEU:HD22	1.88	0.55
3:L5:492:U:H2'	3:L5:493:G:C8	2.42	0.55
3:L5:1407:C:H2'	3:L5:1408:G:C8	2.42	0.55
19:SO:75:MET:HG3	19:SO:118:ALA:HB2	1.88	0.55
22:SS:23:ARG:HG2	31:SZ:48:VAL:HG12	1.89	0.55
57:LR:105:LEU:HD22	57:LR:135:LYS:HG2	1.87	0.55
3:L5:982:U:H2'	3:L5:983:C:C6	2.41	0.55
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.41	0.55
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.72	0.55
17:SU:36:CYS:SG	17:SU:87:ARG:HG3	2.47	0.55
26:SR:66:VAL:HG23	26:SR:68:GLY:H	1.72	0.55
55:LD:62:CYS:HB3	55:LD:105:LEU:HD22	1.88	0.55
79:Lm:99:CYS:HB2	79:Lm:114:LYS:HD2	1.88	0.55
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.41	0.55
8:SJ:34:GLU:HG3	8:SJ:35:TYR:CD2	2.41	0.55
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.05	0.55
3:L5:711:A:H2'	3:L5:712:C:C6	2.42	0.55
5:SB:92:GLN:HE22	5:SB:229:MET:HE1	1.72	0.55
9:SE:201:HIS:HE1	9:SE:207:VAL:HG23	1.70	0.55
16:SQ:50:LYS:HE2	16:SQ:50:LYS:HA	1.88	0.55
28:ST:42:HIS:HB3	28:ST:93:SER:HB3	1.88	0.55
57:LR:105:LEU:HD23	57:LR:138:LEU:HD23	1.87	0.55
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.41	0.55
3:L5:981:C:H4'	44:LE:39:LYS:HD2	1.88	0.55
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.41	0.55
3:L5:2019:C:H2'	3:L5:2020:U:C6	2.42	0.55
3:L5:2363:A2M:H2'	3:L5:2364:OMG:O4'	2.06	0.55
3:L5:2667:C:O4'	57:LR:96:MET:HG2	2.07	0.55
15:SI:141:ARG:HB2	15:SI:145:ILE:HD11	1.89	0.55
17:SU:96:GLU:HA	17:SU:99:LYS:HE2	1.88	0.55
37:Sg:32:LEU:HD12	37:Sg:71:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LH:114:ILE:HB	43:LH:124:ARG:HB2	1.87	0.55
1:S2:92:A:H4'	1:S2:93:PSU:OP2	2.07	0.55
3:L5:490:C:H2'	3:L5:491:G:C8	2.41	0.55
1:S2:948:C:H2'	1:S2:949:G:H8	1.71	0.55
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.42	0.55
2:L8:70:G:H5''	63:LY:27:ARG:CZ	2.37	0.55
3:L5:3961:G:H4'	3:L5:4049:U:H3	1.72	0.55
6:SA:80:ARG:HH21	6:SA:126:ASP:HB2	1.71	0.55
11:SG:63:MET:HG2	11:SG:99:GLY:O	2.07	0.55
59:LT:51:GLY:HA3	59:LT:92:ARG:HG3	1.89	0.55
1:S2:324:C:H2'	1:S2:325:C:C6	2.42	0.55
1:S2:681:PSU:H4'	20:SX:9:THR:HG22	1.89	0.55
3:L5:1688:G:C1'	90:L5:5119:PUT:H22	2.32	0.55
3:L5:1979:A:H2	3:L5:1987:C:H42	1.53	0.55
6:SA:71:PRO:HB3	6:SA:186:ARG:HH22	1.70	0.55
3:L5:1408:G:H21	3:L5:1409:C:H42	1.54	0.54
26:SR:56:HIS:HA	26:SR:59:LYS:HE3	1.88	0.54
29:SV:37:ALA:HB1	29:SV:46:PHE:CD1	2.42	0.54
59:LT:133:ALA:HB3	69:LF:127:LYS:HB2	1.88	0.54
45:LG:108:GLN:O	45:LG:112:GLN:HG3	2.06	0.54
1:S2:502:C:O4'	9:SE:66:MET:HG3	2.07	0.54
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.42	0.54
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.42	0.54
21:SM:81:ASP:CG	21:SM:84:LYS:HD2	2.32	0.54
50:LV:112:MET:HE1	50:LV:117:ILE:HG12	1.90	0.54
57:LR:136:ARG:O	57:LR:140:GLU:HG2	2.07	0.54
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.41	0.54
16:SQ:53:GLU:HG3	16:SQ:85:ARG:HH11	1.72	0.54
38:Lz:41:TYR:CE2	38:Lz:159:MET:HE2	2.42	0.54
75:Li:2:ALA:N	75:Li:5:TYR:HH	2.04	0.54
86:EF:375:LEU:HB3	86:EF:391:PRO:HD2	1.88	0.54
1:S2:28:U:H2'	1:S2:29:G:H8	1.72	0.54
1:S2:447:A:H4'	9:SE:3:ARG:HG2	1.90	0.54
1:S2:1454:A:H5''	26:SR:3:ARG:HD2	1.89	0.54
3:L5:131:C:H2'	3:L5:132:G:C8	2.42	0.54
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.43	0.54
41:LC:140:LYS:HB3	41:LC:142:HIS:HD2	1.72	0.54
1:S2:1536:G:H2'	1:S2:1537:A:H8	1.72	0.54
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.42	0.54
23:Sd:24:CYS:O	23:Sd:25:SER:OG	2.24	0.54
30:SY:15:ASN:ND2	30:SY:18:LEU:HD23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LH:4:ILE:HG12	43:LH:61:TRP:CH2	2.42	0.54
1:S2:5:U:H2'	1:S2:6:G:H8	1.73	0.54
1:S2:39:A:H5'	8:SJ:7:TRP:NE1	2.23	0.54
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.73	0.54
3:L5:1768:C:H3'	3:L5:1769:G:H8	1.73	0.54
4:L7:117:G:H5''	55:LD:256:LYS:HD2	1.90	0.54
41:LC:159:GLU:HA	41:LC:217:ILE:HB	1.90	0.54
69:LF:92:VAL:HG23	69:LF:114:LEU:HD11	1.90	0.54
70:Lc:47:ILE:HD12	70:Lc:94:LEU:HD11	1.89	0.54
70:Lc:55:LEU:HD11	74:Lg:92:LYS:HG3	1.89	0.54
1:S2:694:G:H3'	1:S2:695:C:H3'	1.89	0.54
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.42	0.54
7:SD:48:ILE:HD12	7:SD:73:VAL:HG11	1.89	0.54
7:SD:196:GLY:HA2	7:SD:199:GLY:O	2.08	0.54
9:SE:32:SER:HB3	9:SE:81:THR:OG1	2.08	0.54
38:Lz:155:ILE:HG13	38:Lz:167:VAL:CG1	2.37	0.54
78:Ll:42:ARG:HG3	78:Ll:47:THR:HG23	1.89	0.54
86:EF:267:VAL:HG13	86:EF:304:PRO:HA	1.90	0.54
1:S2:324:C:O2'	1:S2:325:C:H5'	2.08	0.54
3:L5:4145:C:H2'	3:L5:4146:G:C8	2.43	0.54
13:SH:140:VAL:HG12	24:SN:19:ARG:HD2	1.89	0.54
37:Sg:91:ASP:C	37:Sg:93:THR:H	2.16	0.54
3:L5:1983:A:H4'	3:L5:1983:A:OP1	2.07	0.53
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.43	0.53
3:L5:4966:A:H2'	3:L5:4967:A:O4'	2.08	0.53
3:L5:2673:G:N3	3:L5:2673:G:H5'	2.23	0.53
12:SF:127:ARG:HB2	12:SF:134:VAL:HG11	1.89	0.53
13:SH:60:ILE:HB	13:SH:92:VAL:HG12	1.90	0.53
50:LV:35:LYS:HB2	50:LV:67:LYS:HG3	1.90	0.53
52:La:2:PRO:HB2	52:La:5:LEU:HD12	1.90	0.53
1:S2:5:U:H2'	1:S2:6:G:C8	2.43	0.53
36:Sf:121:CYS:HB3	36:Sf:141:CYS:SG	2.47	0.53
68:Lb:35:VAL:HB	68:Lb:40:LEU:HD11	1.90	0.53
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.08	0.53
3:L5:280:G:H5''	53:LN:14:LYS:HE2	1.90	0.53
3:L5:1998:A:H2'	3:L5:1999:A:C8	2.42	0.53
3:L5:3823:G:N3	3:L5:3823:G:H5''	2.23	0.53
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.74	0.53
3:L5:3668:C:H5'	39:LA:8:GLN:O	2.08	0.53
3:L5:3952:A:H2'	3:L5:3953:G:C8	2.43	0.53
3:L5:4955:A:H2'	3:L5:4956:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:120:ALA:HB2	8:SJ:129:LEU:HD12	1.89	0.53
30:SY:110:ARG:HH12	30:SY:127:ALA:HA	1.73	0.53
48:LO:121:PRO:HA	48:LO:124:LEU:HD12	1.88	0.53
55:LD:106:ALA:HB2	55:LD:166:ALA:HA	1.90	0.53
1:S2:1337:4AC:H2'	1:S2:1338:G:C8	2.44	0.53
3:L5:1730:U:H4'	59:LT:100:LYS:HB2	1.91	0.53
3:L5:1881:OMC:C2	3:L5:1881:OMC:HM23	2.44	0.53
3:L5:3946:G:H2'	3:L5:3947:A:C8	2.44	0.53
3:L5:4959:U:H2'	3:L5:4960:G:C8	2.44	0.53
62:LX:89:LYS:HB3	62:LX:95:THR:HG23	1.90	0.53
3:L5:126:C:H2'	3:L5:127:G:H8	1.74	0.53
3:L5:3642:A:HO2'	76:Lj:2:THR:N	2.07	0.53
16:SQ:58:LEU:HB3	16:SQ:62:ARG:HD2	1.91	0.53
61:LU:56:LEU:O	61:LU:56:LEU:HD23	2.09	0.53
86:EF:264:VAL:HG12	86:EF:309:GLY:HA3	1.90	0.53
1:S2:640:A:H2'	1:S2:641:A:C8	2.44	0.53
1:S2:1030:A:H2'	1:S2:1031:A2M:H8	1.91	0.53
2:L8:101:C:O2'	76:Lj:20:ARG:HG3	2.09	0.53
10:SC:184:VAL:CG2	10:SC:195:LEU:HB2	2.39	0.53
54:LI:145:LYS:O	54:LI:149:ILE:HG13	2.08	0.53
27:SP:134:GLY:HA2	27:SP:140:ARG:HB3	1.91	0.53
42:LJ:39:VAL:HG21	42:LJ:126:TYR:HD2	1.75	0.53
45:LG:58:PRO:HD2	45:LG:61:ILE:HD12	1.89	0.53
54:LI:47:PRO:HB3	54:LI:171:TRP:CZ2	2.44	0.53
78:Ll:9:ILE:HD12	78:Ll:51:LEU:HD21	1.91	0.53
1:S2:388:U:H2'	1:S2:389:A:C8	2.44	0.52
1:S2:640:A:P	35:Se:115:ARG:HH22	2.32	0.52
15:SI:26:LYS:HD2	15:SI:29:LEU:HD23	1.91	0.52
17:SU:28:ASN:HB3	17:SU:31:SER:HB3	1.90	0.52
50:LV:106:VAL:HG12	50:LV:112:MET:HA	1.91	0.52
71:Ld:37:GLY:O	71:Ld:41:ARG:HG3	2.08	0.52
1:S2:35:C:H5''	1:S2:579:C:H5''	1.91	0.52
1:S2:189:U:H2'	1:S2:190:G:O4'	2.09	0.52
3:L5:1995:G:N3	3:L5:1995:G:H2'	2.24	0.52
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.08	0.52
22:SS:45:LEU:HB3	22:SS:52:LEU:HD21	1.91	0.52
41:LC:60:HIS:HA	41:LC:92:PHE:HE1	1.75	0.52
54:LI:166:HIS:HB2	59:LT:158:PHE:HE2	1.74	0.52
1:S2:168:C:O2'	11:SG:133:LEU:HB2	2.09	0.52
1:S2:323:C:H2'	1:S2:326:C:C6	2.45	0.52
1:S2:958:G:H2'	1:S2:959:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:318:A:H2'	3:L5:319:A:C8	2.44	0.52
3:L5:921:C:H2'	3:L5:922:C:C6	2.44	0.52
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.45	0.52
10:SC:191:VAL:HG11	10:SC:236:PHE:HA	1.90	0.52
46:Lq:39:GLN:HE22	46:Lq:107:VAL:HG11	1.74	0.52
3:L5:2283:G:H21	90:L5:5119:PUT:H41	1.75	0.52
3:L5:3661:G:N7	39:LA:152:SER:OG	2.38	0.52
21:SM:31:LEU:HD13	21:SM:109:VAL:HG13	1.90	0.52
64:LW:104:GLN:HA	64:LW:107:GLN:NE2	2.24	0.52
86:EF:152:VAL:HG21	86:EF:167:TYR:HD1	1.72	0.52
1:S2:186:C:H2'	1:S2:187:G:C8	2.45	0.52
1:S2:1499:U:H4'	7:SD:176:LEU:HD13	1.91	0.52
3:L5:260:C:C2'	3:L5:261:G:H5'	2.40	0.52
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.75	0.52
3:L5:2476:G:H2'	3:L5:2477:A:C8	2.44	0.52
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.44	0.52
18:SK:6:LYS:H	18:SK:6:LYS:CD	2.22	0.52
1:S2:455:A:H5'	11:SG:94:ARG:HH21	1.75	0.52
1:S2:857:U:H2'	1:S2:858:A:C8	2.44	0.52
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.44	0.52
22:SS:33:ILE:HD13	22:SS:71:MET:HE1	1.92	0.52
3:L5:717:U:H2'	3:L5:718:C:C6	2.45	0.52
31:SZ:86:ALA:O	31:SZ:89:GLN:HG2	2.09	0.52
34:Sc:32:VAL:HG11	34:Sc:56:LEU:HD12	1.90	0.52
41:LC:13:GLU:HG3	41:LC:14:LYS:HD2	1.91	0.52
1:S2:553:U:H2'	1:S2:555:A:H8	1.75	0.52
1:S2:562:U:H2'	1:S2:563:G:C8	2.45	0.52
3:L5:907:C:H2'	3:L5:908:G:C8	2.45	0.52
12:SF:103:LEU:HD21	31:SZ:67:LEU:HD22	1.91	0.52
25:SL:35:ARG:HD2	25:SL:53:GLY:O	2.10	0.52
38:Lz:206:ILE:HG12	38:Lz:214:GLN:CG	2.40	0.52
1:S2:981:A:H2'	1:S2:982:G:C8	2.45	0.52
1:S2:1672:U:OP1	16:SQ:18:THR:HG22	2.09	0.52
3:L5:4053:A:H4'	38:Lz:212:LYS:HG3	1.91	0.52
3:L5:4345:C:O2'	81:Lo:82:MET:HE3	2.10	0.52
11:SG:70:HIS:CE1	11:SG:101:ILE:HG21	2.44	0.52
16:SQ:51:LEU:HD11	16:SQ:81:ILE:HD12	1.92	0.52
17:SU:56:MET:HB2	17:SU:86:LYS:HB3	1.91	0.52
46:Lq:41:GLN:HG2	46:Lq:45:MET:HE1	1.90	0.52
65:LZ:87:VAL:HG22	65:LZ:89:ILE:HG13	1.92	0.52
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4923:C:H2'	3:L5:4924:C:C6	2.45	0.52
12:SF:19:LEU:HD21	12:SF:69:VAL:HG21	1.90	0.52
22:SS:45:LEU:HD22	22:SS:50:ILE:HD11	1.92	0.52
62:LX:119:ILE:HD12	62:LX:140:LEU:HD22	1.92	0.52
64:LW:81:ALA:HB2	64:LW:87:LEU:HB2	1.91	0.52
86:EF:103:ILE:HG23	86:EF:143:LEU:HD11	1.90	0.52
86:EF:129:LYS:HA	86:EF:134:ARG:NH2	2.25	0.52
1:S2:1461:G:H2'	1:S2:1464:C:H41	1.74	0.51
40:LB:92:TYR:HB2	40:LB:159:VAL:HB	1.92	0.51
3:L5:699:C:H2'	3:L5:700:G:H8	1.75	0.51
6:SA:89:LYS:HD3	6:SA:201:LEU:O	2.09	0.51
8:SJ:129:LEU:HB3	8:SJ:135:ILE:HD11	1.92	0.51
40:LB:261:ARG:HB2	48:LO:64:THR:HG21	1.91	0.51
1:S2:573:PSU:O4	1:S2:576:A2M:H8	2.11	0.51
1:S2:1119:A:H2'	1:S2:1120:U:O4'	2.10	0.51
3:L5:1472:C:H2'	3:L5:1473:U:C6	2.46	0.51
3:L5:2098:G:H1'	3:L5:2099:G:C8	2.45	0.51
3:L5:4200:G:H1	3:L5:4221:C:H42	1.58	0.51
12:SF:49:LEU:HD12	16:SQ:50:LYS:HG2	1.92	0.51
1:S2:201:C:H2'	1:S2:202:G:N3	2.26	0.51
3:L5:728:U:H2'	3:L5:730:G:H5'	1.91	0.51
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.75	0.51
5:SB:35:ALA:HB2	5:SB:44:ILE:HD11	1.93	0.51
12:SF:35:LEU:HD22	12:SF:147:VAL:HG23	1.93	0.51
15:SI:141:ARG:HB2	15:SI:145:ILE:CD1	2.41	0.51
38:Lz:34:LEU:HD12	38:Lz:206:ILE:HG22	1.92	0.51
38:Lz:155:ILE:HG13	38:Lz:167:VAL:HG11	1.92	0.51
46:Lq:135:THR:HA	46:Lq:138:PHE:HD2	1.75	0.51
48:LO:81:TRP:HB2	48:LO:104:VAL:HG21	1.93	0.51
50:LV:87:SER:HA	50:LV:97:TYR:HB3	1.91	0.51
52:La:98:ALA:HB2	52:La:121:PRO:HB2	1.90	0.51
1:S2:17:C:O2'	1:S2:1194:A:N1	2.40	0.51
3:L5:1593:A:H5''	3:L5:2839:PSU:H5'	1.92	0.51
8:SJ:30:LYS:O	8:SJ:34:GLU:HG2	2.11	0.51
64:LW:104:GLN:HA	64:LW:107:GLN:HE22	1.76	0.51
81:Lo:33:LEU:HA	81:Lo:38:LYS:HG2	1.91	0.51
1:S2:553:U:H2'	1:S2:555:A:C8	2.46	0.51
1:S2:1144:A:H2'	1:S2:1145:A:C8	2.46	0.51
1:S2:1698:C:H4'	1:S2:1699:A:OP2	2.10	0.51
3:L5:4530:UR3:H2'	3:L5:4531:PSU:H2'	1.92	0.51
26:SR:126:MET:HB2	26:SR:128:PHE:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:LK:20:GLY:HA3	47:LK:54:LYS:HA	1.92	0.51
3:L5:2558:C:H2'	3:L5:2559:G:C8	2.46	0.51
17:SU:19:ARG:H	17:SU:19:ARG:HD3	1.75	0.51
52:La:36:GLY:HA3	52:La:40:HIS:CE1	2.45	0.51
1:S2:65:C:OP1	11:SG:136:LYS:HE2	2.11	0.51
1:S2:536:A:H2'	1:S2:537:C:C6	2.46	0.51
1:S2:1207:G:N2	83:mR:36[B]:U:H3'	2.25	0.51
1:S2:1750:C:H2'	1:S2:1751:C:O4'	2.11	0.51
3:L5:1699:A:H8	3:L5:1706:A:H5''	1.75	0.51
3:L5:1971:C:C5	3:L5:2000:G:H2'	2.45	0.51
3:L5:4711:C:H5''	48:LO:58:LEU:HD23	1.91	0.51
25:SL:111:VAL:HG12	25:SL:140:PHE:HB2	1.91	0.51
28:ST:65:TYR:HD2	28:ST:66:LEU:HD23	1.76	0.51
37:Sg:131:LEU:HD12	37:Sg:139:LYS:HB2	1.92	0.51
1:S2:556:U:H2'	1:S2:557:U:O4'	2.11	0.51
33:Sb:33:MET:HE3	33:Sb:48:SER:HA	1.93	0.51
37:Sg:18:VAL:HG11	37:Sg:307:VAL:HG22	1.91	0.51
63:LY:24:HIS:CE1	63:LY:25:ILE:HG12	2.46	0.51
1:S2:627:OMU:H6	1:S2:627:OMU:H5''	1.91	0.51
3:L5:2000:G:H5''	3:L5:2001:G:H5'	1.92	0.51
3:L5:2361:G:O2'	3:L5:3859:G:O6	2.27	0.51
3:L5:4450:U:C5	92:L5:5118:HMT:H11A	2.46	0.51
10:SC:171:GLY:HA2	14:SW:98:GLN:NE2	2.22	0.51
21:SM:52:LEU:O	21:SM:78:LYS:HA	2.10	0.51
38:Lz:56:LYS:HE3	38:Lz:181:TYR:HB3	1.93	0.51
44:LE:190:HIS:HB3	44:LE:193:PHE:HD2	1.74	0.51
1:S2:329:G:H2'	1:S2:330:G:O4'	2.11	0.50
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.93	0.50
3:L5:4038:C:H5''	3:L5:4039:G:C8	2.47	0.50
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.93	0.50
26:SR:16:ILE:HG22	26:SR:24:LEU:HD11	1.94	0.50
31:SZ:79:ILE:HB	31:SZ:83:LEU:HD23	1.93	0.50
56:LQ:12:LYS:HB2	56:LQ:14:ARG:HH11	1.76	0.50
85:Pt:72:C:H2'	85:Pt:73:A:C8	2.47	0.50
1:S2:572:PSU:H4'	30:SY:61:ARG:HE	1.76	0.50
3:L5:3598:C:H2'	3:L5:3599:A:C8	2.47	0.50
8:SJ:109:ARG:HG2	8:SJ:146:SER:HA	1.93	0.50
32:Sa:4:LYS:HE3	32:Sa:92:ARG:CZ	2.41	0.50
37:Sg:125:ARG:HA	37:Sg:150:TRP:HB3	1.93	0.50
47:LK:115:GLN:HA	47:LK:118:HIS:ND1	2.26	0.50
1:S2:1445:PSU:O2'	1:S2:1446:A:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.47	0.50
3:L5:1766:A:H1'	22:SS:116:LYS:HA	1.93	0.50
38:Lz:36:ILE:HG12	38:Lz:165:LEU:H	1.76	0.50
38:Lz:76:GLU:O	38:Lz:79:ALA:HB3	2.11	0.50
38:Lz:194:LEU:HD21	38:Lz:200:ASN:HB2	1.94	0.50
46:Lq:30:VAL:HG21	46:Lq:187:LEU:CD1	2.40	0.50
9:SE:129:ILE:HD11	9:SE:139:LEU:HD12	1.94	0.50
13:SH:73:GLN:HB3	13:SH:135:PHE:CE1	2.46	0.50
37:Sg:158:PRO:HD2	37:Sg:204:GLY:HA2	1.92	0.50
38:Lz:85:MET:HG2	38:Lz:90:LEU:HD13	1.92	0.50
38:Lz:206:ILE:O	38:Lz:213:PRO:HG2	2.12	0.50
1:S2:323:C:H4'	1:S2:324:C:C5	2.46	0.50
2:L8:108:A:H2'	2:L8:109:C:O4'	2.12	0.50
3:L5:1074:G:H2'	3:L5:1075:G:H8	1.76	0.50
36:Sf:94:LYS:HA	36:Sf:94:LYS:HZ2	1.76	0.50
38:Lz:159:MET:HA	38:Lz:165:LEU:HD21	1.94	0.50
40:LB:288:GLY:HA3	40:LB:330:PHE:CZ	2.47	0.50
44:LE:186:LEU:HD21	44:LE:253:VAL:HG21	1.92	0.50
1:S2:1073:U:H2'	1:S2:1074:C:C6	2.47	0.50
1:S2:1643:PSU:H2'	1:S2:1644:C:C6	2.46	0.50
3:L5:141:C:O2'	3:L5:142:G:H5'	2.12	0.50
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.76	0.50
3:L5:4153:C:H2'	3:L5:4154:G:C8	2.46	0.50
7:SD:53:THR:HG21	7:SD:94:ARG:HG3	1.93	0.50
37:Sg:256:ILE:HB	37:Sg:270:LEU:HB2	1.94	0.50
47:LK:32:ILE:HG21	47:LK:42:VAL:HG21	1.94	0.50
72:Le:35:TRP:CZ2	72:Le:56:PRO:HD2	2.46	0.50
84:At:68:C:H2'	84:At:69:G:H8	1.75	0.50
1:S2:551:U:H2'	1:S2:552:G:C8	2.46	0.50
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.47	0.50
14:SW:14:ILE:HG13	14:SW:27:ILE:HD11	1.93	0.50
35:Se:75:LYS:HD3	84:At:37:MIA:H5''	1.93	0.50
86:EF:253:VAL:HG11	86:EF:320:VAL:HG23	1.94	0.50
1:S2:1419:C:H4'	1:S2:1420:G:H2'	1.94	0.50
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.47	0.50
3:L5:3973:G:H2'	3:L5:3975:C:N4	2.27	0.50
3:L5:4397:A:C2	92:L5:5118:HMT:H23A	2.46	0.50
42:LJ:113:ILE:HG21	42:LJ:119:TYR:HB2	1.94	0.50
45:LG:50:ASP:HB2	62:LX:40:ILE:HD12	1.93	0.50
59:LT:75:VAL:HG22	59:LT:88:ARG:HG2	1.92	0.50
72:Le:10:PRO:HG2	72:Le:69:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LB:378:ARG:HE	64:LW:32:LEU:HD21	1.76	0.50
77:Lk:33:LYS:HG2	77:Lk:46:VAL:HG22	1.93	0.50
3:L5:5045:G:H5'	71:Ld:82:TYR:HD2	1.77	0.49
15:SI:48:VAL:HG11	15:SI:54:LYS:HE3	1.94	0.49
15:SI:103:LEU:HD22	15:SI:170:LYS:HB3	1.94	0.49
39:LA:80:GLU:HB2	39:LA:170:ALA:HA	1.94	0.49
86:EF:79:M3L:HD3	86:EF:86:TYR:HE1	1.77	0.49
86:EF:388:GLU:OE2	86:EF:391:PRO:HA	2.12	0.49
1:S2:501:C:O2	1:S2:501:C:H2'	2.12	0.49
3:L5:1448:G:H2'	3:L5:1449:C:C6	2.48	0.49
3:L5:1688:G:H1'	90:L5:5119:PUT:C2	2.33	0.49
3:L5:2400:G:H21	74:Lg:6:THR:HG22	1.77	0.49
3:L5:2903:G:H5'	3:L5:2904:U:H5'	1.94	0.49
3:L5:5027:C:H4'	3:L5:5028:G:H5'	1.95	0.49
24:SN:13:GLN:HG3	33:Sb:21:LYS:HE3	1.92	0.49
31:SZ:66:LYS:HG3	31:SZ:111:ARG:HH12	1.77	0.49
60:LP:29:THR:HG21	60:LP:146:ILE:HD11	1.93	0.49
3:L5:71:C:H5'	49:LL:64:VAL:HG12	1.95	0.49
3:L5:490:C:H2'	3:L5:491:G:H8	1.75	0.49
3:L5:1097:C:H2'	3:L5:1098:G:H8	1.77	0.49
3:L5:1241:C:H2'	3:L5:1242:G:C8	2.48	0.49
3:L5:1771:U:H2'	3:L5:1772:C:C6	2.48	0.49
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.48	0.49
17:SU:20:ILE:HD12	17:SU:98:VAL:HG21	1.94	0.49
17:SU:24:LEU:HB3	17:SU:32:LEU:HD11	1.95	0.49
38:Lz:206:ILE:O	38:Lz:214:GLN:HB2	2.12	0.49
56:LQ:43:PHE:CD2	56:LQ:133:GLY:HA3	2.47	0.49
70:Lc:34:THR:HG23	70:Lc:95:ALA:HB2	1.94	0.49
75:Li:80:HIS:CD2	75:Li:84:LYS:HE2	2.47	0.49
1:S2:1754:G:H2'	1:S2:1755:C:C6	2.47	0.49
2:L8:141:C:H2'	2:L8:142:U:C6	2.47	0.49
22:SS:55:ARG:HG3	31:SZ:48:VAL:HG21	1.94	0.49
22:SS:59:LEU:HD23	22:SS:64:VAL:HG22	1.93	0.49
47:LK:32:ILE:O	47:LK:35:LEU:HG	2.11	0.49
3:L5:3974:G:H3'	3:L5:3975:C:H6	1.78	0.49
3:L5:5024:C:H2'	3:L5:5025:C:C6	2.48	0.49
8:SJ:111:GLN:HA	8:SJ:130:ILE:CD1	2.43	0.49
9:SE:141:THR:HG22	9:SE:145:ARG:H	1.76	0.49
10:SC:102:LEU:HD22	10:SC:130:ILE:HG13	1.94	0.49
22:SS:23:ARG:HG2	31:SZ:48:VAL:HG11	1.93	0.49
47:LK:142:ASN:HB3	47:LK:146:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:LR:89:MET:HE3	57:LR:90:PRO:HD2	1.93	0.49
1:S2:940:U:H3	1:S2:1002:U:H3	1.61	0.49
1:S2:1757:G:H1'	1:S2:1776:G:N1	2.27	0.49
3:L5:137:G:H2'	3:L5:138:G:H8	1.78	0.49
3:L5:4859:C:H3'	3:L5:4860:G:C8	2.47	0.49
7:SD:45:ARG:NH1	7:SD:85:GLU:HG3	2.28	0.49
13:SH:147:LYS:HA	14:SW:49:GLU:HG2	1.93	0.49
14:SW:57:ARG:HH22	24:SN:16:LEU:HB3	1.76	0.49
38:Lz:191:VAL:HG21	38:Lz:198:TRP:CE2	2.47	0.49
60:LP:54:GLN:HA	60:LP:83:TRP:CD1	2.48	0.49
82:Lp:51:ALA:HB3	82:Lp:54:ILE:HD12	1.94	0.49
1:S2:804:U:H2'	1:S2:805:U:C6	2.47	0.49
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.47	0.49
2:L8:84:A:C6	2:L8:88:A:H4'	2.48	0.49
3:L5:86:U:H2'	3:L5:87:A:C8	2.47	0.49
3:L5:1074:G:H2'	3:L5:1075:G:C8	2.47	0.49
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.47	0.49
3:L5:4860:G:H5'	48:LO:169:ARG:NE	2.28	0.49
5:SB:120:MET:HG3	5:SB:142:PHE:CE2	2.48	0.49
6:SA:77:ILE:HD12	6:SA:122:LEU:HD11	1.93	0.49
27:SP:83:MET:HA	27:SP:83:MET:HE3	1.95	0.49
37:Sg:258:ILE:HD12	37:Sg:268:ASP:HB3	1.94	0.49
51:LM:24:LEU:HD11	51:LM:86:TRP:CG	2.48	0.49
58:LS:84:TYR:HE1	58:LS:93:MET:HE3	1.77	0.49
84:At:66:U:H2'	84:At:67:C:C6	2.47	0.49
1:S2:527:C:H2'	1:S2:528:A:C8	2.47	0.49
1:S2:832:G:N2	1:S2:843:C:H1'	2.27	0.49
3:L5:78:U:H5''	53:LN:185:GLY:HA2	1.95	0.49
3:L5:1281:G:H5'	41:LC:323:ARG:HB2	1.95	0.49
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.47	0.49
9:SE:201:HIS:CE1	9:SE:207:VAL:HG23	2.47	0.49
40:LB:161:ARG:HG2	40:LB:184:GLN:HA	1.95	0.49
49:LL:136:LYS:HG2	49:LL:136:LYS:O	2.13	0.49
1:S2:67:C:C5	11:SG:162:LEU:HB3	2.48	0.49
1:S2:527:C:H4'	8:SJ:121:LYS:HD3	1.94	0.49
1:S2:1599:U:C4	12:SF:166:ILE:HA	2.48	0.49
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.13	0.49
9:SE:188:ASN:HB3	9:SE:191:ARG:HD3	1.95	0.49
30:SY:76:TYR:OH	30:SY:86:GLU:OE1	2.23	0.49
38:Lz:41:TYR:HE2	38:Lz:159:MET:HE2	1.77	0.49
39:LA:101:VAL:HG22	39:LA:165:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LV:39:ILE:HD12	50:LV:61:VAL:HG21	1.95	0.49
86:EF:277:VAL:HA	86:EF:288:GLU:HA	1.94	0.49
1:S2:496:C:OP1	9:SE:29:PRO:HD3	2.13	0.49
1:S2:1337:4AC:H2'	1:S2:1338:G:H8	1.75	0.49
3:L5:2656:U:H2'	3:L5:2657:G:O4'	2.13	0.49
70:Lc:48:LEU:HD13	70:Lc:57:LYS:HG3	1.94	0.49
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.48	0.48
3:L5:3972:A:H2	3:L5:4040:C:H2'	1.77	0.48
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.78	0.48
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.78	0.48
7:SD:42:THR:HB	7:SD:43:PRO:HD2	1.95	0.48
14:SW:57:ARG:NH2	24:SN:16:LEU:HB3	2.27	0.48
31:SZ:102:LYS:HG3	31:SZ:107:VAL:HG12	1.95	0.48
38:Lz:27:LYS:O	38:Lz:28:PHE:HB3	2.12	0.48
38:Lz:112:ALA:HB3	38:Lz:116:LEU:HB3	1.94	0.48
38:Lz:120:ILE:HG21	38:Lz:128:LEU:HD12	1.95	0.48
1:S2:929:G:H2'	1:S2:930:C:O4'	2.13	0.48
1:S2:1124:C:H5''	5:SB:150:ILE:HG12	1.95	0.48
3:L5:4606:G:H2'	3:L5:4607:A:C8	2.48	0.48
4:L7:112:U:H2'	4:L7:113:G:H8	1.77	0.48
8:SJ:91:LYS:HD2	8:SJ:96:TYR:HD2	1.77	0.48
16:SQ:82:TYR:O	16:SQ:85:ARG:HG2	2.13	0.48
1:S2:1256:G:H8	17:SU:66:ARG:HB2	1.79	0.48
3:L5:257:C:H2'	3:L5:258:G:C8	2.47	0.48
4:L7:39:C:O2'	42:LJ:46:GLN:HB3	2.13	0.48
4:L7:110:G:H2'	4:L7:111:C:C6	2.48	0.48
6:SA:111:GLN:HG2	6:SA:112:ILE:HG23	1.95	0.48
20:SX:90:CYS:HA	20:SX:93:PHE:HD2	1.78	0.48
21:SM:52:LEU:HD23	21:SM:78:LYS:CG	2.43	0.48
46:Lq:30:VAL:HG11	46:Lq:187:LEU:HD21	1.95	0.48
54:LI:43:VAL:HG21	54:LI:197:VAL:HG13	1.95	0.48
67:Lh:35:LYS:HA	67:Lh:44:LEU:HD21	1.94	0.48
1:S2:17:C:H2'	1:S2:18:C:C6	2.48	0.48
1:S2:1308:U:O2'	36:Sf:133:ALA:HB1	2.13	0.48
3:L5:493:G:H2'	3:L5:494:U:C6	2.48	0.48
3:L5:1417:C:H2'	3:L5:1418:C:O4'	2.14	0.48
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.14	0.48
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.48	0.48
3:L5:4301:U:H4'	59:LT:54:HIS:CD2	2.49	0.48
3:L5:4601:U:H2'	3:L5:4602:A:C8	2.47	0.48
3:L5:4684:A:H2'	3:L5:4685:U:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.48	0.48
7:SD:29:LEU:HD21	7:SD:69:LEU:HD11	1.95	0.48
13:SH:117:PRO:HG2	13:SH:120:ARG:HD3	1.95	0.48
18:SK:49:MET:HG3	18:SK:69:TRP:CE3	2.49	0.48
38:Lz:78:LYS:HA	38:Lz:84:HIS:CD2	2.48	0.48
55:LD:37:VAL:HB	55:LD:67:ALA:HB2	1.95	0.48
1:S2:434:G:H5''	15:SI:23:LYS:HE3	1.95	0.48
2:L8:80:A:H5''	2:L8:83:C:H5	1.79	0.48
3:L5:1082:C:H2'	3:L5:1083:U:O4'	2.13	0.48
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.13	0.48
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.49	0.48
3:L5:3942:A:H2'	3:L5:3943:A:C8	2.48	0.48
3:L5:4518:A:OP2	3:L5:4518:A:H8	1.97	0.48
38:Lz:35:GLN:HB2	38:Lz:205:TYR:HB2	1.95	0.48
1:S2:1745:A:H1'	11:SG:66:GLY:HA2	1.95	0.48
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.48	0.48
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.28	0.48
21:SM:55:ASN:HB2	21:SM:82:ASN:H	1.78	0.48
37:Sg:79:LEU:HD22	37:Sg:120:ILE:HD12	1.95	0.48
78:Ll:49:LEU:C	78:Ll:51:LEU:H	2.22	0.48
1:S2:115:U:H2'	1:S2:116:OMU:H6	1.96	0.48
1:S2:693:A:H1'	1:S2:694:G:H2'	1.96	0.48
1:S2:884:C:H2'	1:S2:885:U:C6	2.49	0.48
1:S2:953:C:H2'	1:S2:954:U:O4'	2.13	0.48
1:S2:1007:C:H2'	1:S2:1008:A:C8	2.49	0.48
1:S2:1293:A:H2'	1:S2:1294:G:C8	2.48	0.48
1:S2:1589:A:H2'	1:S2:1590:C:C6	2.49	0.48
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.49	0.48
3:L5:4039:G:H1'	3:L5:4040:C:H5	1.79	0.48
3:L5:4862:G:H2'	3:L5:4863:G:H8	1.79	0.48
6:SA:124:VAL:HG21	6:SA:134:LEU:HD21	1.95	0.48
8:SJ:29:LEU:HD21	35:Se:112:TYR:HA	1.95	0.48
9:SE:11:ARG:HA	9:SE:28:ALA:HB2	1.96	0.48
3:L5:106:A:H2'	3:L5:107:G:O4'	2.14	0.48
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.49	0.48
3:L5:1756:U:C2'	3:L5:1757:U:H5'	2.44	0.48
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.49	0.48
3:L5:2389:A:H4'	71:Ld:70:LYS:HG3	1.96	0.48
10:SC:110:MET:HE2	10:SC:125:LYS:HD2	1.94	0.48
15:SI:38:ILE:HD13	15:SI:80:ASP:HA	1.94	0.48
30:SY:12:PHE:HZ	30:SY:21:LYS:HD3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SZ:68:ILE:HB	31:SZ:109:TYR:HB2	1.94	0.48
1:S2:928:G:H2'	1:S2:929:G:C8	2.48	0.48
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.14	0.48
6:SA:198:MET:HG3	6:SA:199:PRO:HD2	1.96	0.48
18:SK:6:LYS:H	18:SK:6:LYS:HD2	1.78	0.48
25:SL:68:ILE:HG21	25:SL:143:LEU:HD11	1.95	0.48
40:LB:224:LYS:HG2	40:LB:340:THR:HG22	1.96	0.48
53:LN:121:VAL:HG11	53:LN:131:GLU:HG3	1.96	0.48
86:EF:426:VAL:CG2	86:EF:433:VAL:HB	2.43	0.48
1:S2:186:C:H2'	1:S2:187:G:H8	1.78	0.48
1:S2:302:A:H1'	15:SI:73:THR:OG1	2.13	0.48
2:L8:78:G:H2'	2:L8:79:G:C8	2.49	0.48
3:L5:411:G:H4'	3:L5:412:G:H5'	1.94	0.48
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.49	0.48
41:LC:67:TRP:HB3	41:LC:71:ARG:HD2	1.96	0.48
1:S2:379:C:H5'	15:SI:33:ALA:HA	1.96	0.47
1:S2:1432:U:H2'	1:S2:1438:A:C8	2.49	0.47
3:L5:462:G:H2'	3:L5:463:A:C8	2.49	0.47
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.13	0.47
3:L5:2096:G:H3'	3:L5:2096:G:N3	2.28	0.47
10:SC:184:VAL:HG23	10:SC:195:LEU:HB2	1.96	0.47
18:SK:92:ALA:HA	18:SK:95:ARG:NH2	2.29	0.47
22:SS:84:LEU:O	22:SS:87:GLN:HG3	2.14	0.47
39:LA:48:ILE:HG22	82:Lp:54:ILE:HG12	1.95	0.47
45:LG:114:LEU:O	45:LG:115:LEU:C	2.57	0.47
65:LZ:39:SER:HB2	65:LZ:77:TYR:CD2	2.48	0.47
69:LF:125:LEU:HD22	69:LF:130:ILE:CD1	2.44	0.47
3:L5:934:C:H4'	3:L5:935:A:O5'	2.14	0.47
3:L5:1325:C:C4	3:L5:3879:G:H5''	2.49	0.47
3:L5:3893:C:H2'	3:L5:3894:A:C8	2.49	0.47
7:SD:51:LEU:HD23	7:SD:89:GLU:HB2	1.96	0.47
9:SE:163:ASP:HB3	9:SE:166:THR:HG22	1.96	0.47
13:SH:76:GLN:NE2	13:SH:94:PHE:HB2	2.29	0.47
18:SK:1:MET:HE1	18:SK:43:LEU:CG	2.44	0.47
21:SM:55:ASN:ND2	21:SM:81:ASP:HA	2.29	0.47
45:LG:157:ILE:HG12	45:LG:170:LEU:HD23	1.96	0.47
60:LP:94:MET:SD	60:LP:148:MET:HE3	2.54	0.47
83:mR:36[A]:U:H2'	83:mR:37:A:H8	1.76	0.47
1:S2:39:A:H5'	8:SJ:7:TRP:HE1	1.78	0.47
1:S2:1434:C:H2'	1:S2:1435:C:C6	2.48	0.47
3:L5:1411:C:H2'	3:L5:1412:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3596:A:H1'	3:L5:3598:C:C4	2.49	0.47
3:L5:3701:OMC:N4	3:L5:3745:U:H2'	2.30	0.47
3:L5:3723:A2M:HM'3	3:L5:3723:A2M:H1'	1.55	0.47
14:SW:30:CYS:HB2	14:SW:61:ILE:HG13	1.95	0.47
22:SS:13:LEU:HB2	22:SS:20:ILE:HB	1.96	0.47
61:LU:101:ARG:HD2	61:LU:115:PHE:CE1	2.50	0.47
86:EF:134:ARG:HB3	86:EF:177:TYR:CZ	2.49	0.47
86:EF:422:GLY:HA2	86:EF:438:ILE:HD12	1.96	0.47
1:S2:12:U:H2'	1:S2:13:C:C6	2.49	0.47
1:S2:1760:G:H21	1:S2:1761:U:H4'	1.79	0.47
3:L5:448:G:H3'	3:L5:449:C:H5''	1.97	0.47
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.50	0.47
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.49	0.47
10:SC:79:GLU:HA	10:SC:82:TYR:HB2	1.96	0.47
13:SH:163:GLN:HG2	13:SH:167:GLU:CG	2.45	0.47
15:SI:136:ILE:HG13	15:SI:137:LEU:HD12	1.96	0.47
22:SS:117:ILE:HD11	27:SP:111:MET:HG3	1.96	0.47
31:SZ:69:THR:H	31:SZ:72:VAL:HG12	1.79	0.47
42:LJ:136:ARG:HG3	42:LJ:157:ILE:HD11	1.96	0.47
1:S2:1752:C:H2'	1:S2:1753:C:O4'	2.15	0.47
3:L5:231:U:H4'	63:LY:100:HIS:CD2	2.48	0.47
3:L5:707:C:O2'	3:L5:4943:A:N1	2.41	0.47
3:L5:2094:G:H2'	3:L5:2095:A:H2'	1.96	0.47
3:L5:2525:U:P	57:LR:42:ARG:HH22	2.37	0.47
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.78	0.47
11:SG:228:ILE:HA	11:SG:231:ARG:HG2	1.95	0.47
21:SM:23:LYS:O	21:SM:27:ILE:HD13	2.14	0.47
25:SL:13:GLN:HE22	25:SL:35:ARG:HG3	1.80	0.47
45:LG:180:PRO:HG3	45:LG:219:VAL:HG13	1.97	0.47
50:LV:16:ILE:HD11	50:LV:56:GLY:HA3	1.95	0.47
1:S2:685:A:H5''	14:SW:31:SER:OG	2.15	0.47
1:S2:1328:OMG:HM23	1:S2:1328:OMG:H1'	1.57	0.47
1:S2:1681:U:H2'	1:S2:1682:C:C6	2.49	0.47
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.49	0.47
13:SH:191:GLU:HG2	13:SH:192:PHE:CD1	2.50	0.47
21:SM:44:LYS:O	21:SM:44:LYS:HG2	2.14	0.47
46:Lq:190:GLN:HG3	46:Lq:191:GLN:CG	2.41	0.47
52:La:88:VAL:O	52:La:92:LYS:HG2	2.15	0.47
60:LP:59:PRO:HG3	60:LP:76:TRP:CG	2.49	0.47
69:LF:52:GLU:OE2	69:LF:55:LYS:HE2	2.14	0.47
86:EF:251:GLN:HA	86:EF:322:ARG:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:107:A:H2'	1:S2:108:G:C8	2.50	0.47
1:S2:382:C:H2'	1:S2:383:G:H8	1.79	0.47
1:S2:1670:C:H2'	1:S2:1671:G:C8	2.49	0.47
1:S2:1808:U:H2'	1:S2:1809:A:C8	2.50	0.47
1:S2:1809:A:H2'	1:S2:1810:U:C6	2.50	0.47
1:S2:1829:G:H1'	1:S2:1850:MA6:H2	1.97	0.47
3:L5:153:G:OP2	53:LN:54:LYS:NZ	2.41	0.47
3:L5:396:A:H2'	3:L5:397:G:C8	2.50	0.47
3:L5:963:G:H3'	3:L5:963:G:N3	2.30	0.47
3:L5:1396:G:H5''	52:La:132:ARG:HH12	1.80	0.47
3:L5:1697:G:N2	3:L5:2085:G:H5''	2.29	0.47
3:L5:1739:G:O2'	3:L5:1740:C:H5'	2.15	0.47
3:L5:1759:G:H1	3:L5:1773:U:H3	1.63	0.47
3:L5:3607:U:H2'	3:L5:3608:A:H8	1.80	0.47
3:L5:4133:C:H2'	3:L5:4134:C:H6	1.80	0.47
3:L5:4169:G:H4'	3:L5:4171:C:C2	2.49	0.47
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.50	0.47
9:SE:125:LYS:HB3	9:SE:142:HIS:HB3	1.97	0.47
10:SC:256:TRP:CE2	14:SW:68:ARG:HD3	2.50	0.47
12:SF:129:GLY:HA3	12:SF:134:VAL:HA	1.97	0.47
25:SL:113:LEU:HD11	25:SL:120:VAL:HG21	1.97	0.47
30:SY:41:ARG:HA	30:SY:55:ILE:HG21	1.97	0.47
36:Sf:94:LYS:HA	36:Sf:94:LYS:HD3	1.59	0.47
36:Sf:109:ASP:C	36:Sf:110:GLU:HG3	2.40	0.47
38:Lz:44:GLN:HE21	38:Lz:44:GLN:HB3	1.50	0.47
41:LC:230:LEU:HD11	41:LC:239:LYS:HB2	1.97	0.47
46:Lq:29:ILE:HG12	46:Lq:88:PHE:CE1	2.50	0.47
1:S2:825:A:H2'	1:S2:826:A:C8	2.50	0.47
1:S2:1462:U:H2'	1:S2:1463:U:C6	2.50	0.47
3:L5:653:U:H2'	3:L5:654:C:C6	2.49	0.47
3:L5:683:C:H2'	3:L5:684:G:O4'	2.15	0.47
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.58	0.47
5:SB:67:PHE:CE1	19:SO:48:SER:HB3	2.50	0.47
86:EF:60:LEU:HD13	86:EF:91:ASP:HB2	1.97	0.47
1:S2:943:U:H2'	1:S2:944:A:C8	2.50	0.47
1:S2:1387:G:N2	26:SR:8:THR:HG21	2.30	0.47
3:L5:294:G:O6	3:L5:315:G:H1'	2.15	0.47
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.15	0.47
7:SD:40:ARG:HB2	7:SD:47:GLU:HB2	1.96	0.47
22:SS:98:VAL:CG1	22:SS:106:LYS:HG3	2.44	0.47
38:Lz:116:LEU:HD21	38:Lz:137:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:LD:208:MET:HG2	55:LD:223:PHE:CE2	2.49	0.47
65:LZ:50:PRO:HD3	65:LZ:68:ILE:HG13	1.97	0.47
1:S2:562:U:H4'	8:SJ:132:GLN:HB3	1.95	0.47
1:S2:567:C:H2'	1:S2:568:C:H5''	1.97	0.47
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.15	0.47
1:S2:1599:U:O4	12:SF:166:ILE:HA	2.15	0.47
3:L5:488:G:H2'	3:L5:489:C:O4'	2.15	0.47
3:L5:1604:G:N7	87:L5:5107:SPD:H22	2.30	0.47
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.73	0.47
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.50	0.47
3:L5:4397:A:N1	92:L5:5118:HMT:H13	2.30	0.47
4:L7:3:C:H2'	4:L7:4:U:C6	2.50	0.47
8:SJ:91:LYS:HD2	8:SJ:96:TYR:CD2	2.50	0.47
42:LJ:160:GLU:HA	42:LJ:163:MET:HE2	1.96	0.47
63:LY:54:GLU:HB2	63:LY:108:ARG:HB3	1.97	0.47
66:Lr:32:LEU:O	66:Lr:33:LYS:HB2	2.15	0.47
1:S2:1447:OMG:H5''	17:SU:29:VAL:HG13	1.97	0.46
3:L5:209:U:C4	3:L5:233:U:C4	3.03	0.46
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.51	0.46
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.50	0.46
3:L5:3856:A:H5''	60:LP:83:TRP:O	2.15	0.46
9:SE:229:GLY:HA3	9:SE:234:PRO:HA	1.96	0.46
37:Sg:152:SER:HB3	37:Sg:168:CYS:SG	2.55	0.46
38:Lz:76:GLU:HG2	38:Lz:145:VAL:HG23	1.97	0.46
55:LD:41:LYS:HD2	59:LT:93:ILE:HD13	1.96	0.46
73:Lf:71:TRP:HB2	73:Lf:89:ARG:NH1	2.30	0.46
1:S2:321:C:H2'	1:S2:322:C:H6	1.78	0.46
1:S2:375:U:H2'	1:S2:376:A:C8	2.50	0.46
1:S2:522:A:H5''	8:SJ:145:PRO:HD2	1.97	0.46
3:L5:1809:C:H2'	3:L5:1810:G:H8	1.79	0.46
3:L5:1850:A:C4	90:L5:5119:PUT:H31	2.50	0.46
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.50	0.46
3:L5:1969:G:H4'	46:Lq:36:GLY:CA	2.45	0.46
3:L5:4178:A:H2'	3:L5:4179:G:C8	2.50	0.46
18:SK:42:ASN:O	18:SK:43:LEU:C	2.57	0.46
37:Sg:9:GLY:O	37:Sg:309:VAL:HG22	2.15	0.46
44:LE:258:LEU:O	44:LE:262:LYS:HG2	2.15	0.46
1:S2:532:C:H2'	1:S2:533:A:C8	2.50	0.46
1:S2:1539:U:H2'	1:S2:1540:G:O4'	2.15	0.46
3:L5:178:C:H2'	3:L5:258:G:H21	1.80	0.46
3:L5:1306:C:H2'	3:L5:1307:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1811:G:H2'	3:L5:1812:C:H6	1.80	0.46
3:L5:3640:U:H2'	3:L5:3646:A:N6	2.29	0.46
3:L5:3887:OMC:H5''	48:LO:71:TYR:CE2	2.51	0.46
3:L5:4885:U:H2'	3:L5:4886:C:H6	1.80	0.46
6:SA:66:VAL:HG11	29:SV:46:PHE:HB2	1.97	0.46
17:SU:61:LEU:HB2	17:SU:82:MET:HB3	1.97	0.46
35:Se:86:VAL:HA	35:Se:89:GLN:HG2	1.97	0.46
38:Lz:119:GLN:O	38:Lz:124:LEU:N	2.49	0.46
55:LD:56:THR:HG22	55:LD:57:ASN:H	1.80	0.46
55:LD:56:THR:HG22	55:LD:57:ASN:N	2.29	0.46
64:LW:107:GLN:HA	64:LW:110:ARG:HB2	1.95	0.46
1:S2:443:U:H2'	1:S2:444:G:O4'	2.15	0.46
3:L5:65:A:N6	3:L5:75:G:H1'	2.31	0.46
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.63	0.46
3:L5:700:G:H2'	3:L5:701:G:H8	1.81	0.46
3:L5:1732:C:H5''	59:LT:43:LYS:HD2	1.97	0.46
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.50	0.46
11:SG:215:LYS:O	11:SG:219:GLU:HG2	2.16	0.46
15:SI:3:ILE:H	15:SI:3:ILE:HD12	1.80	0.46
15:SI:43:ILE:HD11	15:SI:60:LEU:HD21	1.97	0.46
15:SI:177:SER:OG	15:SI:184:ARG:O	2.28	0.46
37:Sg:7:LEU:HD11	37:Sg:308:ARG:HG2	1.97	0.46
38:Lz:204:LEU:HB3	38:Lz:216:LEU:HB3	1.97	0.46
39:LA:126:LEU:HD12	39:LA:150:LEU:HD22	1.97	0.46
50:LV:69:LYS:HE2	50:LV:71:GLU:OE1	2.15	0.46
62:LX:73:HIS:ND1	62:LX:112:ALA:HA	2.30	0.46
76:Lj:39:TYR:CD1	76:Lj:40:PRO:HA	2.50	0.46
1:S2:494:C:H42	1:S2:509:OMG:HN22	1.63	0.46
1:S2:656:G:H5'	1:S2:662:G:N2	2.31	0.46
1:S2:960:U:H1'	1:S2:963:A:N7	2.31	0.46
3:L5:2858:A:H2'	3:L5:2859:G:O4'	2.16	0.46
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.80	0.46
4:L7:24:C:H2'	4:L7:25:G:O4'	2.16	0.46
48:LO:118:MET:HG2	58:LS:169:THR:HG22	1.98	0.46
54:LI:51:HIS:HD2	54:LI:168:SER:HB2	1.77	0.46
61:LU:63:ILE:HA	61:LU:71:THR:O	2.16	0.46
73:Lf:8:LYS:HB3	73:Lf:100:ARG:NH1	2.31	0.46
1:S2:67:C:H41	11:SG:164:LYS:H	1.62	0.46
3:L5:93:G:H2'	3:L5:94:A:C8	2.50	0.46
3:L5:315:G:C6	53:LN:178:HIS:HB2	2.50	0.46
3:L5:4145:C:H2'	3:L5:4146:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SH:148:LEU:HD22	14:SW:49:GLU:HG3	1.96	0.46
27:SP:53:GLN:HG3	27:SP:80:LEU:HD23	1.98	0.46
30:SY:10:ARG:HH21	30:SY:24:VAL:HG11	1.79	0.46
86:EF:123:PHE:HB3	86:EF:166:ARG:NH2	2.31	0.46
1:S2:293:C:O2'	1:S2:294:U:H3'	2.15	0.46
1:S2:948:C:H2'	1:S2:949:G:C8	2.51	0.46
1:S2:1401:A:H4'	17:SU:52:GLY:HA3	1.98	0.46
1:S2:1624:U:H2'	1:S2:1625:PSU:O4'	2.15	0.46
3:L5:126:C:H2'	3:L5:127:G:C8	2.51	0.46
3:L5:179:G:C5	3:L5:258:G:N2	2.84	0.46
3:L5:967:C:H5'	3:L5:969:C:H5	1.80	0.46
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.51	0.46
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.16	0.46
18:SK:16:PHE:HB2	18:SK:79:LEU:HD23	1.97	0.46
21:SM:18:LEU:HA	21:SM:21:VAL:HG12	1.98	0.46
31:SZ:58:LEU:HD12	31:SZ:62:VAL:HG21	1.97	0.46
37:Sg:286:CYS:SG	37:Sg:300:ALA:HB1	2.56	0.46
45:LG:95:LEU:HD23	45:LG:184:ILE:HD12	1.97	0.46
54:LI:48:LEU:HD22	54:LI:142:LEU:HA	1.98	0.46
56:LQ:34:PHE:CE1	56:LQ:38:ARG:HG3	2.51	0.46
56:LQ:49:LYS:HG2	56:LQ:53:MET:HE3	1.97	0.46
81:Lo:104:ILE:HG23	81:Lo:106:PHE:H	1.80	0.46
83:mR:36[A]:U:H4'	83:mR:36[A]:U:OP1	2.15	0.46
1:S2:1426:U:P	16:SQ:69:ARG:HH21	2.39	0.46
3:L5:677:G:H2'	3:L5:678:C:C6	2.50	0.46
3:L5:2326:G:H5''	72:Le:127:ALA:HB2	1.97	0.46
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.80	0.46
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	1.97	0.46
6:SA:73:ASP:HB3	6:SA:120:ARG:HB2	1.98	0.46
9:SE:22:LYS:HB2	9:SE:22:LYS:HE3	1.83	0.46
16:SQ:28:GLY:H	16:SQ:66:VAL:HA	1.80	0.46
26:SR:57:LEU:O	26:SR:61:ILE:HG13	2.16	0.46
27:SP:45:LEU:HD21	27:SP:84:ILE:HD11	1.97	0.46
30:SY:30:PRO:HA	30:SY:67:GLY:HA2	1.98	0.46
47:LK:95:GLN:HB3	47:LK:98:ILE:HG22	1.97	0.46
53:LN:148:THR:O	53:LN:151:ILE:HG22	2.15	0.46
57:LR:126:LYS:O	57:LR:131:VAL:HG22	2.15	0.46
60:LP:94:MET:HE1	60:LP:146:ILE:HB	1.98	0.46
69:LF:157:ARG:HD2	69:LF:213:LEU:HD23	1.98	0.46
69:LF:226:HIS:ND1	69:LF:228:VAL:HG22	2.31	0.46
76:Lj:59:THR:CG2	76:Lj:64:MET:HE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Lj:60:GLY:HA2	76:Lj:64:MET:HE3	1.98	0.46
84:At:5:G:H2'	84:At:6:G:H8	1.80	0.46
84:At:18:G:N2	84:At:57:G:H2'	2.30	0.46
1:S2:163:U:O3'	11:SG:83:CYS:HA	2.16	0.46
3:L5:1186:U:H2'	3:L5:1187:G:N3	2.31	0.46
3:L5:1756:U:H2'	3:L5:1757:U:H5'	1.97	0.46
3:L5:3763:A:H2'	3:L5:3764:PSU:O4'	2.16	0.46
22:SS:5:ILE:HD12	22:SS:6:PRO:HD2	1.97	0.46
42:LJ:20:LEU:HB3	42:LJ:74:VAL:HG23	1.97	0.46
42:LJ:31:ASP:HB3	42:LJ:35:ARG:NH1	2.31	0.46
49:LL:235:GLU:CD	49:LL:235:GLU:H	2.24	0.46
1:S2:324:C:C2'	1:S2:325:C:H5'	2.46	0.46
1:S2:327:G:C6	1:S2:329:G:C5	3.04	0.46
3:L5:1177:U:H2'	3:L5:1178:G:C8	2.50	0.46
3:L5:2477:A:H2'	3:L5:2478:C:C6	2.51	0.46
3:L5:2602:G:H2'	3:L5:2603:C:H6	1.80	0.46
3:L5:3974:G:H3'	3:L5:3975:C:C6	2.51	0.46
3:L5:4611:A:H2'	3:L5:4612:C:C6	2.51	0.46
3:L5:4618:OMG:HM23	3:L5:4618:OMG:H1'	1.69	0.46
4:L7:23:A:H2'	4:L7:24:C:C6	2.51	0.46
18:SK:31:LYS:CG	18:SK:39:ASN:HA	2.46	0.46
37:Sg:168:CYS:HB2	37:Sg:195:LEU:HB3	1.97	0.46
62:LX:129:ARG:HG2	62:LX:133:GLU:O	2.15	0.46
65:LZ:95:VAL:HG12	65:LZ:110:ALA:HA	1.98	0.46
86:EF:79:M3L:HD3	86:EF:86:TYR:CE1	2.51	0.46
1:S2:575:A:H2'	1:S2:576:A2M:O4'	2.16	0.45
1:S2:1112:U:H2'	1:S2:1113:A:C8	2.51	0.45
3:L5:4265:U:OP1	55:LD:12:TYR:OH	2.28	0.45
3:L5:4746:C:H2'	3:L5:4747:C:C6	2.51	0.45
7:SD:116:ARG:NE	7:SD:150:MET:HE2	2.30	0.45
9:SE:103:TYR:HB2	9:SE:182:MET:HE2	1.98	0.45
10:SC:263:LYS:HA	10:SC:267:GLN:HE21	1.81	0.45
11:SG:145:PHE:CD2	64:LW:93:LYS:HB2	2.51	0.45
13:SH:80:VAL:HG22	13:SH:92:VAL:HG23	1.98	0.45
21:SM:61:TYR:OH	21:SM:108:CYS:HB2	2.16	0.45
25:SL:126:VAL:HG12	25:SL:145:VAL:HG22	1.98	0.45
48:LO:177:LEU:HD11	51:LM:130:LEU:HB3	1.98	0.45
1:S2:1113:A:H2'	1:S2:1114:U:O4'	2.17	0.45
1:S2:1606:G:N2	1:S2:1632:G:H1'	2.31	0.45
2:L8:76:C:H2'	2:L8:77:A:O4'	2.16	0.45
3:L5:174:C:H2'	3:L5:175:C:C6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2323:C:H2'	3:L5:2324:C:H6	1.80	0.45
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.69	0.45
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.80	0.45
8:SJ:110:LEU:HB2	8:SJ:147:PHE:HB3	1.97	0.45
65:LZ:84:ARG:HA	70:Lc:66:LEU:HD21	1.98	0.45
82:Lp:13:LYS:HE3	82:Lp:14:TYR:CZ	2.51	0.45
1:S2:287:U:O2	9:SE:131:VAL:HG21	2.16	0.45
1:S2:554:A:H62	1:S2:589:G:N2	2.14	0.45
1:S2:961:G:C4	83:mR:34:C:H1'	2.51	0.45
1:S2:1540:G:OP1	28:ST:39:LEU:HD12	2.16	0.45
2:L8:93:C:O2'	2:L8:94:G:H8	1.99	0.45
3:L5:516:C:H2'	3:L5:517:C:C6	2.51	0.45
3:L5:1766:A:H2'	3:L5:1767:A:C8	2.51	0.45
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.16	0.45
3:L5:2521:G:H4'	74:Lg:26:PRO:HD2	1.97	0.45
3:L5:3747:A:C8	39:LA:245:ARG:HG2	2.51	0.45
38:Lz:11:TYR:CE1	38:Lz:12:GLU:HG2	2.51	0.45
58:LS:30:MET:HE1	58:LS:47:PHE:HB3	1.98	0.45
1:S2:71:G:H2'	1:S2:72:C:O4'	2.16	0.45
1:S2:1781:A:H2'	1:S2:1783:C:C4	2.51	0.45
3:L5:1432:G:H2'	3:L5:1451:G:N2	2.31	0.45
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.51	0.45
3:L5:4861:G:H2'	3:L5:4862:G:C8	2.51	0.45
12:SF:128:ILE:HG13	34:Sc:68:LEU:CD1	2.46	0.45
16:SQ:45:ARG:O	16:SQ:48:GLN:HB2	2.16	0.45
32:Sa:39:PHE:CD2	32:Sa:41:ILE:HD11	2.51	0.45
51:LM:96:GLU:HA	51:LM:99:GLU:HG3	1.99	0.45
68:Lb:65:MET:HA	68:Lb:68:ARG:HG2	1.98	0.45
73:Lf:71:TRP:HB2	73:Lf:89:ARG:HH12	1.82	0.45
1:S2:93:PSU:OP1	9:SE:2:ALA:HB1	2.17	0.45
3:L5:125:C:OP1	53:LN:140:LYS:HG3	2.16	0.45
3:L5:911:U:H2'	3:L5:912:G:O4'	2.16	0.45
3:L5:980:U:H2'	3:L5:981:C:C6	2.51	0.45
3:L5:1730:U:H2'	3:L5:1731:C:C6	2.51	0.45
3:L5:1850:A:C2	90:L5:5119:PUT:H31	2.50	0.45
3:L5:1982:G:H3'	3:L5:1983:A:H5''	1.99	0.45
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.82	0.45
3:L5:4155:C:H2'	3:L5:4156:G:O4'	2.17	0.45
14:SW:23:ARG:HG3	33:Sb:4:ALA:HB2	1.99	0.45
16:SQ:93:VAL:HA	16:SQ:108:ILE:HD11	1.98	0.45
27:SP:109:PRO:O	27:SP:112:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lz:41:TYR:CD1	38:Lz:195:LYS:HD3	2.51	0.45
40:LB:321:VAL:HG12	40:LB:322:HIS:ND1	2.32	0.45
85:Pt:24:C:H2'	85:Pt:25:U:C6	2.51	0.45
1:S2:428:OMU:O3'	8:SJ:2:PRO:HD2	2.16	0.45
1:S2:1520:G:H5''	1:S2:1521:C:OP2	2.17	0.45
2:L8:92:U:H2'	2:L8:93:C:O4'	2.16	0.45
3:L5:967:C:H42	3:L5:2261:G:H21	1.64	0.45
3:L5:1397:A:OP1	52:La:132:ARG:HD2	2.15	0.45
3:L5:2498:C:H2'	3:L5:2499:C:C6	2.52	0.45
3:L5:2689:C:H2'	3:L5:2690:C:C6	2.51	0.45
3:L5:3907:G:O6	92:L5:5118:HMT:H4	2.16	0.45
3:L5:4254:G:H2'	3:L5:4254:G:N3	2.31	0.45
3:L5:4861:G:H2'	3:L5:4862:G:H8	1.81	0.45
5:SB:171:ILE:O	5:SB:175:GLU:HG2	2.16	0.45
6:SA:219:GLU:HA	6:SA:222:VAL:HG12	1.99	0.45
7:SD:76:ARG:HB2	18:SK:22:VAL:HG11	1.99	0.45
37:Sg:180:ALA:C	37:Sg:182:CYS:H	2.24	0.45
39:LA:10:LYS:HA	39:LA:16:PHE:CD2	2.52	0.45
86:EF:290:LYS:HB3	86:EF:311:ASN:HB3	1.98	0.45
1:S2:326:C:H1'	1:S2:327:G:C6	2.52	0.45
1:S2:466:G:H1'	11:SG:59:GLN:HE21	1.82	0.45
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.52	0.45
1:S2:1852:C:H2'	1:S2:1853:C:C6	2.51	0.45
1:S2:1863:A:H1'	32:Sa:79:ILE:HD13	1.97	0.45
2:L8:127:U:H2'	2:L8:128:C:O4'	2.17	0.45
3:L5:700:G:H2'	3:L5:701:G:C8	2.52	0.45
3:L5:2518:G:H1'	3:L5:2539:C:H1'	1.98	0.45
3:L5:3595:U:H4'	3:L5:3596:A:H5'	1.99	0.45
3:L5:3724:A2M:HM'3	3:L5:3724:A2M:H1'	1.74	0.45
3:L5:3907:G:C6	92:L5:5118:HMT:H3	2.52	0.45
3:L5:4993:G:H22	3:L5:5058:A:H2	1.64	0.45
18:SK:6:LYS:HG2	18:SK:7:ASN:H	1.81	0.45
23:Sd:30:LEU:HA	23:Sd:39:CYS:HA	1.97	0.45
41:LC:32:ILE:O	56:LQ:23:ILE:HD11	2.15	0.45
42:LJ:56:THR:HG23	42:LJ:63:ARG:HA	1.99	0.45
86:EF:391:PRO:O	86:EF:393:PHE:N	2.49	0.45
86:EF:426:VAL:HG13	86:EF:434:ALA:O	2.17	0.45
1:S2:113:G:N2	1:S2:292:A:H2'	2.31	0.45
1:S2:1232:PSU:H2'	1:S2:1233:G:C8	2.52	0.45
1:S2:1512:C:H2'	1:S2:1513:C:C6	2.51	0.45
3:L5:928:C:H2'	3:L5:929:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:979:C:OP2	44:LE:66:LYS:HD3	2.17	0.45
3:L5:2560:C:H2'	3:L5:2561:C:C6	2.51	0.45
13:SH:137:SER:HA	13:SH:162:GLN:CG	2.40	0.45
19:SO:28:PHE:HZ	32:Sa:58:VAL:HG21	1.82	0.45
53:LN:116:LEU:HD22	53:LN:135:ILE:HD11	1.98	0.45
56:LQ:61:LEU:HD21	56:LQ:66:MET:HB2	1.99	0.45
61:LU:25:CYS:C	61:LU:28:PRO:HD2	2.41	0.45
64:LW:101:ARG:C	64:LW:103:ALA:N	2.74	0.45
65:LZ:16:GLY:O	74:Lg:76:ARG:HG3	2.16	0.45
80:Ln:20:MET:HE2	80:Ln:20:MET:HA	1.98	0.45
1:S2:195:C:H2'	1:S2:196:C:C6	2.52	0.45
1:S2:388:U:H2'	1:S2:389:A:H8	1.80	0.45
1:S2:542:U:H6	1:S2:542:U:H2'	1.65	0.45
1:S2:838:G:N3	1:S2:841:G:H1'	2.32	0.45
3:L5:325:U:H2'	3:L5:326:C:C6	2.52	0.45
5:SB:85:LYS:HB2	5:SB:101:HIS:HB3	1.99	0.45
9:SE:19:MET:SD	9:SE:108:ARG:HD2	2.57	0.45
38:Lz:35:GLN:HE21	38:Lz:35:GLN:HB3	1.55	0.45
46:Lq:162:LYS:HG3	46:Lq:165:ASP:HB2	1.98	0.45
86:EF:370:CYS:HA	86:EF:406:PRO:HA	1.97	0.45
86:EF:418:TYR:O	86:EF:419:PRO:C	2.59	0.45
1:S2:538:U:H2'	1:S2:539:C:C6	2.52	0.45
1:S2:874:G:H2'	1:S2:875:A:H8	1.81	0.45
1:S2:1305:C:H2'	1:S2:1306:U:H6	1.82	0.45
2:L8:115:G:H2'	2:L8:116:C:H6	1.82	0.45
3:L5:159:C:OP2	75:Li:25:ARG:HG2	2.17	0.45
3:L5:207:G:H2'	3:L5:208:A:C8	2.52	0.45
3:L5:469:C:H2'	3:L5:470:A:C8	2.52	0.45
3:L5:1250:C:H2'	3:L5:1251:C:C6	2.52	0.45
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.52	0.45
3:L5:1437:C:H1'	3:L5:2098:G:O2'	2.17	0.45
3:L5:1440:U:H2'	3:L5:1441:C:H6	1.82	0.45
3:L5:2310:C:H2'	3:L5:2311:C:H6	1.82	0.45
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.52	0.45
3:L5:3627:OMG:HM23	3:L5:3627:OMG:H1'	1.75	0.45
18:SK:16:PHE:CE2	18:SK:76:ILE:HG23	2.52	0.45
45:LG:166:LEU:HD21	53:LN:45:PRO:HG2	1.99	0.45
45:LG:246:SER:O	45:LG:250:ILE:HG12	2.17	0.45
52:La:72:THR:HG22	52:La:110:LYS:HB3	1.98	0.45
67:Lh:94:ARG:HE	67:Lh:94:ARG:HB3	1.53	0.45
69:LF:187:MET:HE3	69:LF:187:MET:HB3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:Ln:2:ARG:HD3	80:Ln:5:TRP:NE1	2.31	0.45
1:S2:1653:U:H2'	1:S2:1654:G:C8	2.52	0.44
2:L8:148:A:H2'	2:L8:149:G:C8	2.52	0.44
3:L5:699:C:H2'	3:L5:700:G:C8	2.52	0.44
3:L5:1409:C:C4	3:L5:1410:U:H1'	2.52	0.44
3:L5:1762:C:H2'	3:L5:1763:C:C6	2.52	0.44
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.32	0.44
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.52	0.44
7:SD:72:VAL:HB	18:SK:20:VAL:HG21	1.99	0.44
12:SF:167:LYS:HA	31:SZ:71:ALA:HB1	1.99	0.44
21:SM:52:LEU:HD23	21:SM:78:LYS:HD3	1.99	0.44
28:ST:134:ILE:O	28:ST:137:GLN:HG2	2.17	0.44
32:Sa:39:PHE:CE2	32:Sa:41:ILE:HD11	2.52	0.44
46:Lq:116:ILE:HG22	46:Lq:166:LYS:HA	1.99	0.44
54:LI:63:GLU:H	54:LI:63:GLU:CD	2.26	0.44
55:LD:156:GLY:HA2	55:LD:181:PRO:HG3	1.98	0.44
58:LS:1:MET:HG3	58:LS:39:VAL:HG11	1.99	0.44
80:Ln:2:ARG:HB3	80:Ln:5:TRP:CD1	2.52	0.44
1:S2:115:U:H2'	1:S2:116:OMU:C6	2.46	0.44
1:S2:806:U:H2'	1:S2:807:G:C8	2.51	0.44
1:S2:1229:G:H2'	1:S2:1230:C:O4'	2.16	0.44
3:L5:46:U:OP1	49:LL:16:LYS:HE2	2.17	0.44
3:L5:4107:G:C6	3:L5:4108:G:H1'	2.53	0.44
5:SB:89:GLU:OE2	5:SB:220:LYS:NZ	2.49	0.44
24:SN:23:PRO:HB3	33:Sb:84:HIS:HB2	1.99	0.44
25:SL:37:TYR:CE1	25:SL:51:ILE:HG23	2.52	0.44
27:SP:137:HIS:HD1	27:SP:141:PHE:HE2	1.64	0.44
41:LC:183:VAL:HA	41:LC:204:ARG:HG2	1.99	0.44
69:LF:137:GLU:OE1	69:LF:234:GLY:HA2	2.15	0.44
70:Lc:36:LYS:O	70:Lc:40:GLN:HG3	2.16	0.44
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.52	0.44
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.52	0.44
4:L7:18:C:H2'	4:L7:19:C:C6	2.53	0.44
37:Sg:299:PHE:CD1	37:Sg:309:VAL:HG12	2.50	0.44
45:LG:171:PRO:HB3	45:LG:181:TYR:CE2	2.53	0.44
51:LM:3:PHE:CZ	58:LS:155:PRO:HB3	2.52	0.44
59:LT:112:ASN:HD22	59:LT:128:LEU:HD22	1.81	0.44
69:LF:28:LEU:HA	69:LF:31:LYS:HG2	1.99	0.44
1:S2:344:U:H2'	1:S2:345:U:C6	2.52	0.44
1:S2:484:A2M:HM'3	1:S2:484:A2M:H1'	1.70	0.44
1:S2:1207:G:H22	83:mR:36[B]:U:H3'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1240:A:H1'	1:S2:1267:C:HO2'	1.82	0.44
1:S2:1520:G:N3	1:S2:1520:G:C2'	2.78	0.44
1:S2:1801:A:H2'	1:S2:1802:C:C6	2.53	0.44
3:L5:1414:C:H2'	3:L5:1415:G:C8	2.52	0.44
3:L5:4518:A:O5'	3:L5:4520:G:H4'	2.17	0.44
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.53	0.44
3:L5:4967:A:H5''	40:LB:119:TYR:HE1	1.83	0.44
12:SF:73:THR:O	12:SF:89:THR:HG21	2.17	0.44
37:Sg:142:VAL:HG12	37:Sg:146:SER:HB2	1.99	0.44
37:Sg:289:LEU:HD22	37:Sg:298:LEU:HD11	1.99	0.44
38:Lz:151:VAL:O	38:Lz:154:THR:HG23	2.17	0.44
54:LI:156:LYS:HG3	54:LI:163:GLN:HB2	1.99	0.44
59:LT:48:VAL:HG21	59:LT:94:GLU:HG2	1.99	0.44
69:LF:209:TRP:CD1	69:LF:210:PRO:HD2	2.52	0.44
1:S2:1654:G:OP1	28:ST:90:SER:HB2	2.17	0.44
2:L8:19:C:H2'	2:L8:20:A:C8	2.52	0.44
3:L5:1673:U:H2'	3:L5:1674:C:C6	2.53	0.44
13:SH:161:ALA:C	13:SH:163:GLN:H	2.25	0.44
40:LB:258:HIS:HA	40:LB:259:PRO:C	2.41	0.44
58:LS:84:TYR:CE1	58:LS:93:MET:HE3	2.53	0.44
63:LY:56:GLN:HG3	63:LY:67:ILE:HD13	2.00	0.44
86:EF:385:LYS:HB3	86:EF:385:LYS:HE3	1.58	0.44
1:S2:996:A:H2'	1:S2:997:A:C8	2.52	0.44
1:S2:1277:C:H4'	18:SK:55:ARG:HG3	1.99	0.44
1:S2:1839:U:H2'	1:S2:1840:U:C6	2.52	0.44
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.52	0.44
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.53	0.44
3:L5:1920:C:H3'	3:L5:1921:C:H5''	1.99	0.44
8:SJ:50:LEU:HD13	8:SJ:105:PHE:CE2	2.52	0.44
10:SC:182:CYS:HB2	14:SW:95:PRO:HB2	1.98	0.44
12:SF:128:ILE:HG13	34:Sc:68:LEU:HD12	1.99	0.44
25:SL:4:ILE:HG12	25:SL:54:THR:O	2.18	0.44
53:LN:159:ARG:HB3	53:LN:164:LEU:HB2	1.99	0.44
67:Lh:27:GLU:OE2	67:Lh:46:LYS:HE3	2.17	0.44
68:Lb:113:ALA:HB1	69:LF:37:PHE:HZ	1.83	0.44
76:Lj:25:LYS:HD2	76:Lj:25:LYS:O	2.18	0.44
1:S2:624:C:H41	20:SX:63:ASN:ND2	2.16	0.44
1:S2:639:C:H2'	1:S2:640:A:C8	2.53	0.44
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.18	0.44
2:L8:46:G:OP2	78:Ll:15:LYS:HD2	2.18	0.44
3:L5:106:A:H1'	3:L5:336:A:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:758:G:H5''	43:LH:52:LYS:HE3	2.00	0.44
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.53	0.44
3:L5:2091:C:H1'	3:L5:2094:G:H1'	1.99	0.44
3:L5:2714:G:C2'	3:L5:2715:G:H5'	2.48	0.44
3:L5:3648:A:H1'	3:L5:3785:A2M:N6	2.32	0.44
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.52	0.44
24:SN:88:LEU:HD22	24:SN:135:LEU:HD11	1.98	0.44
29:SV:38:GLU:CG	29:SV:49:GLN:HB2	2.48	0.44
30:SY:40:ILE:HD13	30:SY:60:PHE:CE2	2.53	0.44
39:LA:79:ALA:O	39:LA:82:ILE:HG12	2.18	0.44
44:LE:164:PHE:CE1	44:LE:173:LEU:HB3	2.52	0.44
51:LM:43:THR:O	51:LM:43:THR:HG22	2.18	0.44
59:LT:43:LYS:HG3	59:LT:58:HIS:NE2	2.32	0.44
62:LX:89:LYS:HD3	62:LX:93:ASN:HD22	1.83	0.44
66:Lr:20:ARG:HG2	66:Lr:21:ASN:OD1	2.17	0.44
82:Lp:46:LYS:HD3	82:Lp:59:SER:OG	2.16	0.44
1:S2:1240:A:H1'	1:S2:1267:C:O2'	2.17	0.44
1:S2:1714:U:H2'	1:S2:1715:A:C8	2.53	0.44
1:S2:1754:G:H2'	1:S2:1755:C:H6	1.81	0.44
3:L5:907:C:H2'	3:L5:908:G:H8	1.83	0.44
3:L5:1250:C:H2'	3:L5:1251:C:H6	1.82	0.44
3:L5:1772:C:H2'	3:L5:1773:U:C6	2.53	0.44
3:L5:2258:C:O2	44:LE:91:THR:HG22	2.16	0.44
7:SD:29:LEU:HD23	7:SD:65:ARG:HH21	1.83	0.44
7:SD:47:GLU:O	7:SD:49:ILE:HG13	2.18	0.44
8:SJ:91:LYS:O	8:SJ:92:MET:HE2	2.18	0.44
13:SH:134:VAL:O	13:SH:135:PHE:C	2.61	0.44
19:SO:44:VAL:HG11	19:SO:85:CYS:SG	2.57	0.44
24:SN:35:GLU:OE2	24:SN:39:LYS:HE3	2.18	0.44
34:Sc:44:ARG:HD3	34:Sc:44:ARG:HA	1.66	0.44
42:LJ:111:GLU:HB3	42:LJ:125:ILE:HD11	1.99	0.44
55:LD:152:ARG:HG3	55:LD:154:THR:HG23	1.99	0.44
63:LY:38:LEU:HD22	63:LY:42:TYR:HE2	1.81	0.44
76:Lj:59:THR:HG23	76:Lj:64:MET:HE1	2.00	0.44
1:S2:653:A:H2'	1:S2:654:A:O4'	2.18	0.44
1:S2:867:OMG:HM23	1:S2:867:OMG:H1'	1.53	0.44
1:S2:874:G:H2'	1:S2:875:A:C8	2.52	0.44
1:S2:1740:C:H2'	1:S2:1741:U:C6	2.53	0.44
3:L5:6:C:H2'	3:L5:7:C:C6	2.53	0.44
3:L5:131:C:H2'	3:L5:132:G:H8	1.82	0.44
3:L5:741:C:OP2	3:L5:742:G:H5''	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2298:U:H5''	41:LC:204:ARG:HH21	1.83	0.44
3:L5:3883:U:H2'	3:L5:3884:PSU:C6	2.53	0.44
3:L5:4978:G:H2'	3:L5:4979:A:H5''	2.00	0.44
6:SA:80:ARG:O	6:SA:84:GLN:HG3	2.18	0.44
8:SJ:26:ASP:HB2	35:Se:116:PHE:HZ	1.82	0.44
14:SW:102:ILE:HB	14:SW:113:HIS:HB3	1.99	0.44
22:SS:20:ILE:HD11	22:SS:33:ILE:HG13	1.99	0.44
28:ST:39:LEU:HD21	28:ST:52:TRP:CZ3	2.53	0.44
30:SY:12:PHE:CZ	30:SY:21:LYS:HD3	2.52	0.44
32:Sa:94:ASP:OD1	32:Sa:96:THR:HG22	2.18	0.44
37:Sg:45:LEU:HB3	37:Sg:47:ARG:HD2	1.99	0.44
43:LH:41:ILE:HG22	43:LH:43:VAL:HG13	1.99	0.44
44:LE:253:VAL:O	44:LE:257:ILE:HG12	2.18	0.44
47:LK:61:LYS:O	47:LK:72:GLU:HG3	2.18	0.44
50:LV:85:ARG:HG2	50:LV:85:ARG:HH11	1.82	0.44
82:Lp:30:GLU:OE2	82:Lp:34:HIS:HE1	2.00	0.44
1:S2:203:G:H2'	1:S2:204:G:H8	1.83	0.43
1:S2:1037:G:H4'	1:S2:1845:A:H4'	2.00	0.43
1:S2:1490:OMG:H1'	1:S2:1490:OMG:HM23	1.60	0.43
1:S2:1690:U:H2'	1:S2:1691:U:C6	2.53	0.43
3:L5:968:C:H5'	44:LE:110:ARG:NH1	2.33	0.43
3:L5:1397:A:OP1	52:La:132:ARG:HB2	2.19	0.43
3:L5:1445:U:H2'	3:L5:1446:C:C6	2.53	0.43
3:L5:2029:A:H2'	3:L5:2030:A:H8	1.81	0.43
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.83	0.43
16:SQ:113:ILE:HD11	16:SQ:120:LEU:HB2	1.99	0.43
21:SM:44:LYS:O	21:SM:46:GLN:HG2	2.18	0.43
24:SN:33:VAL:HG21	24:SN:66:VAL:HG11	2.00	0.43
32:Sa:13:LYS:HD3	32:Sa:13:LYS:HA	1.82	0.43
40:LB:322:HIS:O	40:LB:342:LYS:NZ	2.40	0.43
41:LC:149:GLU:HG3	66:Lr:72:LYS:HG2	2.00	0.43
68:Lb:108:ALA:O	68:Lb:112:ILE:HG12	2.18	0.43
69:LF:41:MET:HA	69:LF:41:MET:HE2	1.99	0.43
69:LF:241:ASN:O	69:LF:245:ARG:HG2	2.18	0.43
74:Lg:83:CYS:SG	74:Lg:86:CYS:HB2	2.57	0.43
86:EF:202:LEU:HG	86:EF:229:LEU:HD22	1.99	0.43
1:S2:121:OMU:HM23	1:S2:121:OMU:H1'	1.80	0.43
1:S2:128:U:H3'	1:S2:129:C:C6	2.52	0.43
1:S2:644:OMG:H1'	1:S2:644:OMG:HM23	1.68	0.43
1:S2:941:C:H2'	1:S2:942:G:C8	2.53	0.43
1:S2:1666:C:H2'	1:S2:1667:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:273:U:H2'	3:L5:274:C:H6	1.82	0.43
3:L5:966:A:H2'	3:L5:2092:G:N1	2.33	0.43
3:L5:1464:C:H5''	68:Lb:32:LEU:HD12	1.99	0.43
3:L5:1970:A:H4'	3:L5:2000:G:C8	2.53	0.43
7:SD:10:LYS:HB2	7:SD:10:LYS:HE2	1.84	0.43
20:SX:130:LEU:HD12	20:SX:130:LEU:HA	1.81	0.43
26:SR:62:GLN:O	26:SR:62:GLN:HG2	2.18	0.43
40:LB:168:MET:HA	40:LB:171:LEU:HD12	2.00	0.43
41:LC:152:LEU:HD23	41:LC:251:ILE:HG12	1.99	0.43
45:LG:80:ILE:HG23	45:LG:164:ILE:HD13	1.99	0.43
69:LF:199:LYS:HA	69:LF:199:LYS:HD3	1.74	0.43
85:Pt:72:C:H2'	85:Pt:73:A:H8	1.83	0.43
3:L5:1457:G:H5'	56:LQ:72:LEU:HD13	2.00	0.43
3:L5:1700:G:N2	3:L5:2097:U:H5'	2.33	0.43
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.53	0.43
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.18	0.43
3:L5:4232:U:OP2	81:Lo:2:VAL:HA	2.19	0.43
3:L5:4289:U:H2'	3:L5:4290:U:C6	2.53	0.43
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.53	0.43
7:SD:109:LEU:HD23	7:SD:182:LEU:HD23	1.99	0.43
8:SJ:88:ASP:HB3	8:SJ:91:LYS:HG2	2.00	0.43
21:SM:53:ALA:C	21:SM:55:ASN:N	2.76	0.43
32:Sa:89:ARG:HD2	32:Sa:89:ARG:HA	1.81	0.43
40:LB:238:LYS:HE2	40:LB:238:LYS:HB2	1.78	0.43
41:LC:215:ASN:HD22	41:LC:215:ASN:HA	1.49	0.43
42:LJ:167:GLN:O	42:LJ:171:ASP:HA	2.18	0.43
61:LU:84:LYS:HB2	61:LU:110:TYR:CE2	2.52	0.43
72:Le:82:VAL:HG13	72:Le:114:ARG:HG2	2.00	0.43
86:EF:122:GLU:OE2	86:EF:154:LYS:NZ	2.36	0.43
86:EF:175:SER:HA	86:EF:178:ILE:HG12	2.00	0.43
1:S2:916:A:C5	24:SN:73:ARG:HD3	2.53	0.43
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.18	0.43
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.18	0.43
1:S2:1328:OMG:H4'	36:Sf:78:LYS:HE3	2.01	0.43
1:S2:1808:U:H2'	1:S2:1809:A:H8	1.82	0.43
3:L5:38:A:H5''	52:La:35:ALA:HB2	2.00	0.43
3:L5:81:C:H2'	3:L5:82:U:O4'	2.18	0.43
3:L5:679:C:H2'	3:L5:680:G:C8	2.53	0.43
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.99	0.43
3:L5:2461:G:H2'	3:L5:2462:C:C6	2.53	0.43
3:L5:4208:U:H2'	3:L5:4209:G:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4342:C:O3'	81:Lo:37:GLY:HA3	2.19	0.43
3:L5:4651:A:H2'	3:L5:4652:G:O4'	2.19	0.43
7:SD:40:ARG:HA	7:SD:40:ARG:HD2	1.38	0.43
7:SD:49:ILE:HG12	7:SD:87:TYR:HB2	2.00	0.43
8:SJ:116:LYS:C	8:SJ:118:GLY:N	2.75	0.43
26:SR:57:LEU:HD23	26:SR:57:LEU:HA	1.90	0.43
34:Sc:67:ARG:HD3	34:Sc:67:ARG:HA	1.85	0.43
37:Sg:12:LYS:HG2	37:Sg:306:LEU:HD22	2.00	0.43
41:LC:293:LEU:HD22	56:LQ:34:PHE:CD2	2.53	0.43
51:LM:24:LEU:H	51:LM:43:THR:HG21	1.83	0.43
61:LU:26:THR:HA	61:LU:29:VAL:HG22	1.99	0.43
64:LW:109:ILE:O	64:LW:113:LYS:HG2	2.18	0.43
83:mR:34:C:H2'	83:mR:35:G:O4'	2.18	0.43
1:S2:37:C:H2'	1:S2:38:A:O4'	2.18	0.43
1:S2:1408:U:H2'	1:S2:1409:A:C8	2.54	0.43
1:S2:1654:G:OP1	28:ST:82:ARG:HD2	2.18	0.43
2:L8:86:U:C3'	2:L8:87:G:H5'	2.48	0.43
3:L5:137:G:H2'	3:L5:138:G:C8	2.54	0.43
3:L5:1377:G:H21	3:L5:1380:G:H5'	1.82	0.43
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	2.00	0.43
3:L5:4622:A:H4'	40:LB:13:SER:HB2	2.00	0.43
5:SB:136:ARG:HB2	5:SB:218:LEU:HD11	1.99	0.43
8:SJ:60:LEU:HD22	8:SJ:70:ARG:HA	2.01	0.43
12:SF:43:GLU:C	12:SF:45:TYR:H	2.26	0.43
12:SF:175:ASP:HA	12:SF:178:ILE:HB	2.00	0.43
21:SM:26:LEU:HA	21:SM:30:GLY:HA2	1.99	0.43
26:SR:126:MET:HB2	26:SR:128:PHE:CE1	2.52	0.43
36:Sf:78:LYS:HG3	36:Sf:79:LYS:N	2.33	0.43
44:LE:276:ALA:HB1	73:Lf:3:GLY:HA3	2.01	0.43
69:LF:154:ILE:HG22	69:LF:187:MET:HE1	2.00	0.43
85:Pt:4:G:H2'	85:Pt:5:G:H8	1.82	0.43
1:S2:77:A:H2'	1:S2:78:C:C6	2.54	0.43
1:S2:823:U:O2'	1:S2:824:C:H5'	2.18	0.43
1:S2:1440:C:O2'	1:S2:1441:U:H5'	2.18	0.43
3:L5:377:A:H2'	3:L5:378:A:O4'	2.19	0.43
3:L5:1251:C:H2'	3:L5:1252:C:C6	2.53	0.43
3:L5:1459:A:H2'	3:L5:1460:C:O4'	2.19	0.43
3:L5:1918:U:O3'	3:L5:1919:G:H3'	2.18	0.43
3:L5:3939:G:HO2'	3:L5:4076:G:H1	1.65	0.43
12:SF:68:ILE:HD11	12:SF:151:ILE:HD11	2.01	0.43
13:SH:73:GLN:O	13:SH:76:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SH:134:VAL:O	13:SH:134:VAL:HG23	2.17	0.43
37:Sg:214:GLY:HA2	37:Sg:236:ILE:HG12	2.00	0.43
40:LB:77:THR:HG21	40:LB:337:VAL:HG22	2.00	0.43
42:LJ:18:ARG:HG3	42:LJ:135:GLY:HA3	2.01	0.43
69:LF:162:ILE:HD12	69:LF:167:ILE:HB	1.99	0.43
79:Lm:97:ARG:HG3	79:Lm:122:ARG:HG2	1.99	0.43
86:EF:152:VAL:HG23	86:EF:192:PRO:HA	2.01	0.43
86:EF:372:PHE:CE1	86:EF:404:MET:HE2	2.53	0.43
1:S2:381:C:H2'	1:S2:382:C:C6	2.54	0.43
1:S2:440:G:H5''	1:S2:1798:C:O2'	2.19	0.43
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.54	0.43
3:L5:2900:U:H2'	3:L5:2901:G:C8	2.54	0.43
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.54	0.43
4:L7:3:C:H2'	4:L7:4:U:H6	1.83	0.43
7:SD:113:LEU:HD22	7:SD:118:ALA:HB2	2.00	0.43
14:SW:83:LEU:HD22	14:SW:83:LEU:HA	1.80	0.43
24:SN:120:SER:O	24:SN:124:ARG:HG3	2.18	0.43
38:Lz:41:TYR:CE1	38:Lz:46:ASP:HB3	2.53	0.43
38:Lz:117:ILE:HG23	38:Lz:118:LYS:HG3	2.01	0.43
39:LA:117:GLU:HG2	39:LA:124:GLY:H	1.84	0.43
54:LI:40:LYS:O	54:LI:41:ALA:C	2.62	0.43
86:EF:24:THR:HG23	86:EF:89:ILE:HD13	2.00	0.43
86:EF:40:GLU:HA	86:EF:43:GLU:HB3	2.00	0.43
1:S2:99:A2M:H1'	1:S2:99:A2M:HM'3	1.82	0.43
1:S2:888:U:H3	1:S2:900:C:H1'	1.82	0.43
1:S2:960:U:H2'	1:S2:962:A:OP2	2.19	0.43
1:S2:1148:A:H4'	1:S2:1149:A:O4'	2.18	0.43
1:S2:1580:A:H8	17:SU:56:MET:HE1	1.84	0.43
3:L5:1973:G:H2'	3:L5:1974:U:C5	2.53	0.43
3:L5:2109:G:H22	3:L5:2252:G:N2	2.17	0.43
3:L5:2876:OMG:HM22	3:L5:2877:G:O5'	2.18	0.43
4:L7:2:U:H2'	4:L7:3:C:C6	2.53	0.43
6:SA:90:PHE:HE2	6:SA:178:LEU:HG	1.84	0.43
7:SD:58:VAL:HA	7:SD:65:ARG:HD3	2.01	0.43
19:SO:34:PHE:HB3	19:SO:41:PHE:HB2	2.00	0.43
21:SM:53:ALA:C	21:SM:55:ASN:H	2.27	0.43
29:SV:34:MET:HE2	29:SV:34:MET:HB3	1.85	0.43
30:SY:55:ILE:HD13	30:SY:75:ILE:HD12	2.01	0.43
31:SZ:73:VAL:HG21	31:SZ:88:LEU:HD21	2.01	0.43
38:Lz:205:TYR:CZ	38:Lz:215:ARG:HD3	2.53	0.43
41:LC:60:HIS:HA	41:LC:92:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LG:163:PRO:HG3	53:LN:43:THR:O	2.18	0.43
86:EF:264:VAL:HG12	86:EF:309:GLY:CA	2.48	0.43
1:S2:921:G:H5'	33:Sb:21:LYS:HD2	2.01	0.43
1:S2:1194:A:H4'	1:S2:1195:A:OP1	2.18	0.43
1:S2:1568:C:H2'	1:S2:1569:A:C8	2.54	0.43
1:S2:1788:A:H2'	1:S2:1789:G:O4'	2.19	0.43
3:L5:444:G:H2'	3:L5:445:U:C6	2.53	0.43
3:L5:1249:C:H2'	3:L5:1250:C:C6	2.53	0.43
3:L5:1249:C:H2'	3:L5:1250:C:H6	1.83	0.43
3:L5:1971:C:H41	3:L5:2001:G:P	2.42	0.43
3:L5:2906:G:O2'	3:L5:3589:G:O6	2.34	0.43
3:L5:4670:C:O3'	3:L5:4671:C:H3'	2.19	0.43
9:SE:155:LYS:HA	9:SE:155:LYS:HD3	1.81	0.43
12:SF:119:SER:OG	12:SF:189:ALA:HB1	2.19	0.43
16:SQ:47:LEU:O	16:SQ:50:LYS:HB2	2.18	0.43
24:SN:89:TYR:CE1	24:SN:150:VAL:HG12	2.54	0.43
39:LA:2:GLY:HA2	39:LA:207:VAL:HG23	2.01	0.43
40:LB:378:ARG:HD3	64:LW:11:TYR:CD2	2.54	0.43
63:LY:126:ARG:HG3	63:LY:130:LYS:NZ	2.34	0.43
70:Lc:65:MET:HE3	70:Lc:65:MET:HB3	1.88	0.43
82:Lp:38:THR:HA	82:Lp:45:THR:HA	2.01	0.43
1:S2:392:A:C2'	1:S2:393:U:H5'	2.49	0.43
1:S2:1177:PSU:H2'	1:S2:1178:U:C6	2.54	0.43
3:L5:129:C:H2'	3:L5:130:C:C6	2.54	0.43
3:L5:450:G:H3'	3:L5:451:C:H6	1.83	0.43
3:L5:1727:U:H2'	3:L5:1728:U:C6	2.54	0.43
3:L5:4337:C:N3	81:Lo:61:LYS:HE3	2.34	0.43
3:L5:4524:G:C2	40:LB:252:ALA:HB1	2.54	0.43
14:SW:62:VAL:HG11	33:Sb:8:LEU:HD22	2.01	0.43
22:SS:28:PHE:HA	22:SS:31:THR:HG23	1.99	0.43
38:Lz:70:ASP:HB3	38:Lz:73:HIS:HB2	2.01	0.43
43:LH:43:VAL:HG21	43:LH:73:ILE:HD13	2.01	0.43
52:La:28:HIS:CD2	52:La:32:ARG:HG2	2.54	0.43
58:LS:76:LYS:HE2	58:LS:78:PHE:CZ	2.53	0.43
86:EF:112:ALA:HB2	86:EF:145:VAL:HG11	2.01	0.43
1:S2:833:C:H2'	1:S2:834:C:C6	2.54	0.42
1:S2:949:G:H2'	1:S2:950:C:C6	2.54	0.42
2:L8:88:A:H2'	2:L8:89:U:O4'	2.19	0.42
3:L5:1214:C:N3	68:Lb:91:ARG:HA	2.34	0.42
3:L5:3717:A:N1	3:L5:3933:G:H1'	2.34	0.42
3:L5:3792:OMG:HM23	3:L5:3792:OMG:H1'	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4085:A:H3'	62:LX:44:PRO:HB2	2.00	0.42
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.53	0.42
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.54	0.42
15:SI:188:TYR:OH	15:SI:194:GLU:OE2	2.33	0.42
18:SK:11:ILE:HG12	18:SK:45:VAL:HG22	1.99	0.42
20:SX:143:SER:O	86:EF:283:VAL:HG12	2.18	0.42
24:SN:140:LYS:HE3	24:SN:140:LYS:HB3	1.56	0.42
26:SR:17:ILE:O	26:SR:21:TYR:HB2	2.19	0.42
27:SP:82:ASP:OD1	27:SP:82:ASP:N	2.45	0.42
30:SY:55:ILE:CD1	30:SY:75:ILE:HD12	2.48	0.42
36:Sf:119:ARG:O	36:Sf:132:MET:HB2	2.19	0.42
38:Lz:34:LEU:HD11	38:Lz:204:LEU:HD21	2.00	0.42
58:LS:98:ARG:HG3	58:LS:142:VAL:HG13	2.01	0.42
84:At:68:C:H2'	84:At:69:G:C8	2.54	0.42
86:EF:264:VAL:HA	86:EF:309:GLY:HA2	2.01	0.42
1:S2:176:U:H2'	1:S2:177:G:C8	2.53	0.42
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.54	0.42
1:S2:1256:G:C8	17:SU:66:ARG:HB2	2.55	0.42
1:S2:1285:G:C6	21:SM:56:CYS:HA	2.54	0.42
1:S2:1446:A:O2'	1:S2:1447:OMG:H8	2.02	0.42
3:L5:4208:U:H4'	3:L5:4274:A:H2	1.84	0.42
3:L5:4569:PSU:H1'	60:LP:69:ARG:NH1	2.34	0.42
9:SE:30:ARG:HD2	9:SE:31:PRO:HD2	2.01	0.42
20:SX:40:PRO:HA	20:SX:79:LYS:HD2	2.01	0.42
38:Lz:8:ASP:O	38:Lz:12:GLU:HB2	2.17	0.42
40:LB:288:GLY:HA3	40:LB:330:PHE:CE2	2.54	0.42
46:Lq:28:PHE:HB2	46:Lq:89:VAL:HG23	2.00	0.42
48:LO:74:ARG:O	48:LO:142:ALA:HB1	2.19	0.42
61:LU:63:ILE:HG23	61:LU:70:ILE:HG23	2.01	0.42
66:Lr:32:LEU:HD23	66:Lr:113:ARG:HD3	2.01	0.42
76:Lj:39:TYR:CG	76:Lj:40:PRO:HA	2.54	0.42
86:EF:194:SER:HB3	86:EF:199:ASP:HB2	2.01	0.42
1:S2:554:A:H62	1:S2:589:G:H21	1.66	0.42
1:S2:1305:C:H2'	1:S2:1306:U:C6	2.54	0.42
1:S2:1861:G:H5''	32:Sa:3:LYS:HA	2.01	0.42
3:L5:94:A:C5	3:L5:95:G:H1'	2.53	0.42
3:L5:123:C:H2'	3:L5:124:C:H6	1.84	0.42
3:L5:208:A:H2	3:L5:233:U:H5''	1.85	0.42
3:L5:952:G:H2'	3:L5:953:C:C6	2.54	0.42
3:L5:968:C:H5'	44:LE:110:ARG:HH11	1.84	0.42
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1418:C:H2'	3:L5:1419:G:O4'	2.19	0.42
3:L5:2859:G:H21	3:L5:3837:C:H1'	1.85	0.42
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.54	0.42
3:L5:4736:C:H2'	3:L5:4737:G:C8	2.54	0.42
9:SE:44:LEU:HD21	9:SE:72:ILE:HD11	2.00	0.42
15:SI:42:ARG:HH21	15:SI:59:ARG:NH1	2.17	0.42
18:SK:1:MET:HE1	18:SK:43:LEU:CD2	2.49	0.42
38:Lz:39:LYS:HB2	38:Lz:202:ARG:HB2	2.01	0.42
41:LC:138:MET:HE3	41:LC:138:MET:HB3	1.69	0.42
55:LD:223:PHE:HB3	55:LD:226:TYR:HB2	2.02	0.42
58:LS:39:VAL:HG22	69:LF:228:VAL:HA	2.00	0.42
60:LP:14:SER:OG	60:LP:151:THR:HG22	2.19	0.42
73:Lf:6:TRP:CE2	73:Lf:102:ARG:HD3	2.55	0.42
1:S2:63:U:H2'	1:S2:64:A:H5''	2.02	0.42
1:S2:326:C:O2	64:LW:116:LYS:HE2	2.18	0.42
1:S2:455:A:H2'	1:S2:456:C:C6	2.53	0.42
1:S2:543:C:H3'	1:S2:544:G:C8	2.51	0.42
3:L5:1730:U:H2'	3:L5:1731:C:H6	1.85	0.42
3:L5:1956:A:H2'	3:L5:1957:U:H6	1.85	0.42
3:L5:2014:C:H2'	3:L5:2015:U:O4'	2.19	0.42
3:L5:2310:C:H2'	3:L5:2311:C:C6	2.54	0.42
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.54	0.42
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.54	0.42
5:SB:88:THR:HA	5:SB:98:THR:HA	2.02	0.42
7:SD:99:ILE:H	7:SD:99:ILE:HD12	1.84	0.42
13:SH:163:GLN:HG3	13:SH:189:PHE:CD2	2.54	0.42
37:Sg:156:PHE:CE1	37:Sg:179:LEU:HD21	2.54	0.42
37:Sg:212:LYS:HA	37:Sg:235:ILE:HG13	2.00	0.42
45:LG:117:ARG:HE	45:LG:117:ARG:HB3	1.58	0.42
47:LK:50:THR:HG21	47:LK:58:ILE:HD13	2.01	0.42
54:LI:47:PRO:HB3	54:LI:171:TRP:CE2	2.53	0.42
57:LR:180:LYS:HA	57:LR:183:GLU:HG3	2.01	0.42
62:LX:77:ILE:HD13	62:LX:100:VAL:HG12	2.00	0.42
68:Lb:110:ALA:O	68:Lb:114:LYS:HG2	2.19	0.42
70:Lc:20:LEU:HD12	70:Lc:20:LEU:HA	1.90	0.42
1:S2:1757:G:C4	1:S2:1758:G:N2	2.86	0.42
3:L5:1480:C:H1'	3:L5:1482:G:H21	1.84	0.42
3:L5:1480:C:H1'	3:L5:1482:G:N2	2.35	0.42
3:L5:1649:U:O2'	87:L5:5109:SPD:H92	2.19	0.42
3:L5:1700:G:C2	3:L5:2097:U:H5'	2.54	0.42
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4120:U:C4	74:Lg:97:ILE:HG12	2.55	0.42
3:L5:4523:A2M:HM'3	3:L5:4523:A2M:H1'	1.70	0.42
7:SD:142:LEU:HD12	7:SD:143:ARG:N	2.33	0.42
8:SJ:97:ILE:HG23	8:SJ:100:LEU:HD12	2.01	0.42
8:SJ:116:LYS:C	8:SJ:118:GLY:H	2.27	0.42
10:SC:68:ARG:NH2	10:SC:71:LYS:HD3	2.35	0.42
13:SH:158:LEU:HD11	13:SH:187:PHE:HD2	1.84	0.42
37:Sg:34:ALA:HB1	37:Sg:66:VAL:HG22	2.01	0.42
38:Lz:38:LEU:HB2	38:Lz:163:LEU:HD22	2.00	0.42
38:Lz:55:LEU:HD13	38:Lz:182:ASN:HD22	1.85	0.42
54:LI:99:ILE:HG12	54:LI:101:LYS:HD2	2.00	0.42
70:Lc:31:TYR:O	70:Lc:35:LEU:HD23	2.19	0.42
1:S2:674:C:H2'	1:S2:675:U:C6	2.55	0.42
1:S2:1525:C:H4'	27:SP:137:HIS:NE2	2.34	0.42
3:L5:172:C:H2'	3:L5:173:C:C6	2.54	0.42
3:L5:382:G:N1	3:L5:385:A:OP2	2.49	0.42
3:L5:965:G:O6	3:L5:2093:A:H5''	2.20	0.42
3:L5:2590:G:H2'	3:L5:2754:G:N2	2.34	0.42
3:L5:4439:U:H2'	3:L5:4440:G:O4'	2.19	0.42
21:SM:45:ARG:HD3	21:SM:72:HIS:HD2	1.85	0.42
25:SL:61:PRO:HA	25:SL:66:VAL:HG13	2.01	0.42
37:Sg:274:VAL:O	37:Sg:274:VAL:HG13	2.20	0.42
41:LC:140:LYS:HB3	41:LC:142:HIS:CD2	2.52	0.42
59:LT:58:HIS:HD2	59:LT:59:GLY:N	2.18	0.42
61:LU:100:LEU:HD13	61:LU:112:LEU:HD23	2.01	0.42
84:At:16:H2U:H61	84:At:16:H2U:H2'	1.81	0.42
86:EF:24:THR:HB	86:EF:60:LEU:HD11	2.02	0.42
1:S2:440:G:O2'	1:S2:1737:G:H1'	2.20	0.42
1:S2:1388:A:C2	7:SD:205:PRO:HG2	2.54	0.42
1:S2:1454:A:H2	1:S2:1476:A:H1'	1.83	0.42
1:S2:1579:A:H4'	1:S2:1581:C:C5	2.55	0.42
3:L5:223:G:H4'	3:L5:225:G:N7	2.35	0.42
3:L5:666:G:H2'	3:L5:666:G:N3	2.34	0.42
3:L5:965:G:N2	3:L5:2092:G:H1'	2.35	0.42
3:L5:2323:C:H2'	3:L5:2324:C:C6	2.55	0.42
3:L5:5021:C:H2'	3:L5:5022:U:H4'	2.00	0.42
5:SB:27:LYS:HD2	5:SB:53:GLN:HE22	1.85	0.42
5:SB:123:ALA:HB2	5:SB:165:ARG:HG3	2.02	0.42
6:SA:39:TYR:CE2	26:SR:105:MET:HB2	2.54	0.42
9:SE:129:ILE:HD13	9:SE:139:LEU:HA	2.02	0.42
11:SG:14:LYS:HB3	11:SG:124:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LB:89:ILE:HG22	40:LB:153:MET:HE1	2.02	0.42
64:LW:106:GLU:O	64:LW:110:ARG:HG3	2.20	0.42
1:S2:583:A:H2'	1:S2:584:A:C8	2.55	0.42
1:S2:601:OMG:HM23	1:S2:601:OMG:H1'	1.81	0.42
1:S2:643:A:H4'	1:S2:644:OMG:H5'	2.02	0.42
1:S2:1154:U:O4	10:SC:227:ARG:HD2	2.19	0.42
1:S2:1500:G:H2'	1:S2:1501:C:O4'	2.20	0.42
1:S2:1569:A:H5'	28:ST:41:LYS:HD3	2.02	0.42
3:L5:457:G:H2'	3:L5:458:C:C6	2.55	0.42
3:L5:678:C:H2'	3:L5:679:C:C6	2.55	0.42
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.55	0.42
3:L5:2390:G:H22	3:L5:2825:A:H2	1.68	0.42
3:L5:4065:G:H2'	3:L5:4066:U:C6	2.55	0.42
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.20	0.42
3:L5:4526:U:C5	3:L5:4527:G:C6	3.07	0.42
7:SD:175:VAL:HG12	7:SD:177:LEU:HG	2.00	0.42
10:SC:94:ILE:HG21	10:SC:162:ILE:HD12	2.01	0.42
30:SY:20:ARG:HB3	30:SY:76:TYR:CD1	2.55	0.42
31:SZ:50:PHE:HD1	31:SZ:54:THR:OG1	2.02	0.42
49:LL:213:LEU:HD23	49:LL:217:VAL:HG22	2.01	0.42
55:LD:233:PRO:HA	55:LD:236:MET:HE2	2.02	0.42
86:EF:382:ARG:O	86:EF:383:SER:C	2.61	0.42
1:S2:223:C:H2'	1:S2:224:A:C8	2.55	0.42
1:S2:1395:C:H1'	1:S2:1474:A:C5	2.55	0.42
1:S2:1410:C:H2'	1:S2:1411:G:C8	2.55	0.42
3:L5:52:G:H4'	3:L5:1529:G:H4'	2.01	0.42
3:L5:2741:U:H2'	39:LA:50:HIS:CD2	2.55	0.42
3:L5:2902:G:H22	3:L5:3596:A:P	2.43	0.42
3:L5:3899:OMG:HM23	3:L5:3899:OMG:H1'	1.88	0.42
3:L5:4524:G:OP2	3:L5:4524:G:H4'	2.20	0.42
3:L5:5000:G:O3'	40:LB:382:MET:HE1	2.20	0.42
6:SA:35:GLU:O	6:SA:38:ILE:HG12	2.19	0.42
6:SA:50:ASN:HA	26:SR:105:MET:HE3	2.02	0.42
7:SD:139:SER:O	7:SD:182:LEU:HD12	2.19	0.42
11:SG:7:PHE:HB2	11:SG:113:ILE:HD12	2.02	0.42
19:SO:88:LEU:HA	19:SO:88:LEU:HD12	1.70	0.42
30:SY:83:LYS:HD3	30:SY:96:LEU:HD21	2.02	0.42
44:LE:258:LEU:HD12	44:LE:262:LYS:HE3	2.02	0.42
44:LE:276:ALA:CB	73:Lf:3:GLY:HA3	2.50	0.42
47:LK:53:TRP:HB2	47:LK:58:ILE:HD11	2.02	0.42
68:Lb:72:ILE:HD13	68:Lb:72:ILE:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1456:G:H2'	1:S2:1457:U:C6	2.55	0.42
3:L5:71:C:H5'	49:LL:64:VAL:CG1	2.50	0.42
3:L5:123:C:H2'	3:L5:124:C:C6	2.55	0.42
3:L5:254:G:H2'	3:L5:255:C:O4'	2.20	0.42
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.55	0.42
3:L5:1672:U:H2'	3:L5:1673:U:C6	2.54	0.42
3:L5:1677:PSU:H4'	3:L5:1680:G:N1	2.35	0.42
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.85	0.42
3:L5:1952:G:H4'	58:LS:93:MET:HB3	2.01	0.42
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.55	0.42
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.20	0.42
3:L5:4488:A:H4'	3:L5:4489:G:H8	1.84	0.42
6:SA:42:LYS:HD3	6:SA:46:ILE:HB	2.02	0.42
9:SE:152:PRO:HG2	11:SG:216:ARG:HG3	2.00	0.42
9:SE:199:GLU:HG3	9:SE:201:HIS:CE1	2.55	0.42
13:SH:142:LYS:HB3	13:SH:142:LYS:HE2	1.49	0.42
24:SN:11:LEU:O	24:SN:13:GLN:HG2	2.20	0.42
28:ST:116:ASP:HB3	28:ST:119:GLY:O	2.19	0.42
32:Sa:10:ARG:HB2	32:Sa:33:ASP:OD2	2.19	0.42
37:Sg:228:TYR:CD2	37:Sg:264:LYS:HD3	2.55	0.42
38:Lz:43:PRO:O	38:Lz:159:MET:HE1	2.20	0.42
49:LL:239:PHE:CE2	49:LL:241:ALA:HA	2.54	0.42
58:LS:29:ARG:HB2	59:LT:148:PRO:HB2	2.01	0.42
69:LF:220:MET:HB3	69:LF:232:ASP:OD2	2.19	0.42
84:At:65:G:H5'	86:EF:360:VAL:HG21	2.01	0.42
1:S2:1433:C:H2'	1:S2:1434:C:C2	2.54	0.41
1:S2:1705:C:H2'	1:S2:1706:G:C8	2.55	0.41
3:L5:962:C:O4'	3:L5:963:G:C2	2.73	0.41
3:L5:1359:G:H4'	53:LN:203:TYR:HB2	2.02	0.41
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.20	0.41
3:L5:1805:A:N6	68:Lb:27:GLN:HA	2.35	0.41
3:L5:1881:OMC:H5''	3:L5:2281:U:H1'	2.02	0.41
3:L5:1882:U:C4	3:L5:2279:A:C2	3.08	0.41
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.75	0.41
3:L5:4438:U:H2'	3:L5:4439:U:O4'	2.20	0.41
5:SB:30:TRP:O	5:SB:94:LYS:HD2	2.20	0.41
9:SE:103:TYR:HA	9:SE:108:ARG:O	2.19	0.41
22:SS:55:ARG:NE	31:SZ:48:VAL:HG23	2.35	0.41
33:Sb:33:MET:HG2	33:Sb:46:VAL:O	2.20	0.41
40:LB:168:MET:HE1	40:LB:173:LEU:HD12	2.01	0.41
44:LE:162:VAL:HG12	44:LE:177:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:LK:67:ARG:HG2	47:LK:68:GLN:N	2.35	0.41
52:La:75:LEU:HD11	52:La:133:ALA:HA	2.02	0.41
1:S2:128:U:H3'	1:S2:129:C:H6	1.84	0.41
1:S2:1135:C:H2'	1:S2:1136:PSU:C6	2.54	0.41
1:S2:1232:PSU:H2'	1:S2:1233:G:H8	1.85	0.41
1:S2:1464:C:H5''	26:SR:60:ARG:NE	2.35	0.41
2:L8:89:U:H2'	2:L8:90:C:C6	2.56	0.41
3:L5:19:G:P	67:Lh:93:ARG:HE	2.43	0.41
3:L5:445:U:H2'	3:L5:446:C:O4'	2.20	0.41
3:L5:446:C:H2'	3:L5:447:C:C6	2.55	0.41
3:L5:1880:G:C8	3:L5:1881:OMC:HM22	2.55	0.41
4:L7:7:G:OP1	55:LD:33:ARG:HD2	2.20	0.41
13:SH:134:VAL:HG12	13:SH:173:PHE:CD2	2.55	0.41
26:SR:70:SER:OG	26:SR:73:LEU:HD12	2.20	0.41
37:Sg:191:HIS:CE1	37:Sg:217:MET:HG3	2.56	0.41
43:LH:117:PHE:O	43:LH:118:LEU:HB2	2.21	0.41
46:Lq:65:ILE:HG23	46:Lq:75:LEU:HB3	2.02	0.41
61:LU:25:CYS:O	61:LU:28:PRO:HD2	2.20	0.41
62:LX:87:MET:HE1	62:LX:155:ILE:HG22	2.02	0.41
66:Lr:2:SAC:H2A1	66:Lr:2:SAC:HA	1.75	0.41
73:Lf:48:ALA:HB2	73:Lf:71:TRP:CZ3	2.55	0.41
81:Lo:56:PHE:CE2	81:Lo:59:LYS:HD3	2.52	0.41
1:S2:111:A:H5'	25:SL:70:GLY:HA2	2.03	0.41
1:S2:329:G:H5'	1:S2:329:G:H8	1.85	0.41
1:S2:382:C:H2'	1:S2:383:G:C8	2.55	0.41
1:S2:428:OMU:H6	1:S2:428:OMU:H2'	1.78	0.41
1:S2:555:A:H2'	1:S2:555:A:N3	2.35	0.41
1:S2:1365:G:H2'	1:S2:1366:G:H8	1.86	0.41
1:S2:1376:A:H2'	1:S2:1377:U:O4'	2.21	0.41
3:L5:122:U:H2'	3:L5:123:C:H6	1.85	0.41
3:L5:434:A:H2'	3:L5:435:A:O4'	2.20	0.41
3:L5:654:C:H2'	3:L5:655:C:C6	2.56	0.41
3:L5:939:G:H2'	3:L5:940:C:C6	2.56	0.41
3:L5:962:C:O2	69:LF:32:ARG:NH2	2.53	0.41
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.83	0.41
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.20	0.41
3:L5:2861:OMC:H2'	3:L5:2862:G:O4'	2.20	0.41
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.54	0.41
9:SE:103:TYR:HB2	9:SE:182:MET:CE	2.50	0.41
12:SF:44:LYS:HE2	12:SF:44:LYS:HB3	1.89	0.41
23:Sd:10:HIS:HA	23:Sd:11:PRO:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SZ:54:THR:O	31:SZ:55:TYR:C	2.63	0.41
36:Sf:118:ARG:HB2	36:Sf:131:PHE:HB3	2.01	0.41
38:Lz:14:VAL:HB	38:Lz:214:GLN:NE2	2.30	0.41
40:LB:19:ARG:HB2	40:LB:234:ARG:NH2	2.35	0.41
46:Lq:70:GLU:HG2	46:Lq:71:ASN:N	2.34	0.41
47:LK:106:PHE:CD1	47:LK:109:ILE:HD11	2.55	0.41
65:LZ:51:ARG:HB3	65:LZ:65:ARG:NH2	2.35	0.41
86:EF:7:HIS:HA	86:EF:86:TYR:O	2.20	0.41
1:S2:509:OMG:H1'	1:S2:509:OMG:HM23	1.68	0.41
1:S2:846:G:OP1	9:SE:106:LYS:HE2	2.20	0.41
1:S2:1070:A:H2'	1:S2:1071:G:O4'	2.20	0.41
1:S2:1174:PSU:H2'	1:S2:1175:G:C8	2.56	0.41
1:S2:1239:PSU:O4	1:S2:1241:A:H8	2.04	0.41
3:L5:273:U:H2'	3:L5:274:C:C6	2.55	0.41
3:L5:1995:G:O2'	47:LK:127:GLY:HA3	2.21	0.41
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.86	0.41
3:L5:2815:A2M:H2'	3:L5:2816:G:C8	2.55	0.41
3:L5:3816:A:OP1	3:L5:3818:UY1:N1	2.53	0.41
3:L5:3942:A:H2'	3:L5:3943:A:H8	1.85	0.41
7:SD:203:PRO:HG2	26:SR:42:PRO:HB3	2.02	0.41
13:SH:133:LEU:O	13:SH:173:PHE:CE1	2.74	0.41
20:SX:87:ASN:HB3	20:SX:134:TYR:CE1	2.55	0.41
21:SM:52:LEU:HD13	21:SM:65:VAL:HG21	2.02	0.41
21:SM:123:VAL:O	21:SM:126:GLU:HG2	2.19	0.41
37:Sg:106:LYS:HB2	37:Sg:126:ASP:HB3	2.03	0.41
39:LA:133:TYR:HB3	39:LA:168:VAL:HG12	2.02	0.41
45:LG:163:PRO:HB2	45:LG:165:GLU:OE2	2.20	0.41
45:LG:170:LEU:HD12	45:LG:170:LEU:HA	1.92	0.41
45:LG:208:ASN:O	45:LG:212:LYS:HG3	2.20	0.41
46:Lq:112:ARG:HG3	46:Lq:115:ALA:HB3	2.01	0.41
48:LO:16:LEU:HD12	48:LO:80:PHE:HD1	1.84	0.41
69:LF:35:LYS:HB3	69:LF:35:LYS:HE2	1.86	0.41
69:LF:136:VAL:O	69:LF:140:ILE:HG12	2.21	0.41
73:Lf:50:VAL:HG22	73:Lf:69:VAL:HG22	2.02	0.41
86:EF:290:LYS:HE3	86:EF:313:LYS:HG2	2.02	0.41
1:S2:383:G:H4'	25:SL:132:ARG:HD2	2.02	0.41
1:S2:429:C:H2'	1:S2:430:C:H6	1.85	0.41
1:S2:731:G:H21	1:S2:733:C:H5''	1.84	0.41
3:L5:669:C:H2'	3:L5:670:G:C8	2.55	0.41
3:L5:987:C:H2'	3:L5:988:C:H6	1.85	0.41
3:L5:1458:C:H2'	3:L5:1459:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.56	0.41
3:L5:1703:C:O2'	69:LF:43:ARG:NH1	2.53	0.41
3:L5:1763:C:H2'	3:L5:1764:G:O4'	2.21	0.41
3:L5:2283:G:O2'	90:L5:5119:PUT:H32	2.20	0.41
3:L5:2424:OMG:HM23	3:L5:2424:OMG:H1'	1.58	0.41
3:L5:4277:G:H5''	59:LT:17:ARG:HG2	2.02	0.41
3:L5:4860:G:H2'	3:L5:4861:G:H8	1.85	0.41
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.20	0.41
6:SA:15:VAL:HG21	26:SR:111:PHE:CD2	2.56	0.41
7:SD:66:ILE:HD11	7:SD:86:LEU:HB3	2.03	0.41
10:SC:66:LEU:HD11	10:SC:81:ILE:HG12	2.02	0.41
10:SC:169:TYR:CG	10:SC:173:LYS:HA	2.55	0.41
11:SG:1:MET:HE3	11:SG:1:MET:HB2	1.95	0.41
18:SK:14:LEU:HD12	18:SK:14:LEU:HA	1.88	0.41
30:SY:56:PHE:HE2	30:SY:86:GLU:HG2	1.85	0.41
38:Lz:156:LYS:NZ	38:Lz:158:GLN:HB2	2.35	0.41
38:Lz:207:LYS:CG	38:Lz:213:PRO:HD2	2.44	0.41
40:LB:108:GLU:OE2	40:LB:138:GLN:NE2	2.42	0.41
47:LK:119:ARG:HE	47:LK:119:ARG:HB3	1.51	0.41
69:LF:134:ARG:HA	69:LF:137:GLU:HG2	2.02	0.41
1:S2:584:A:H2'	1:S2:585:C:O4'	2.21	0.41
1:S2:606:G:H1'	35:Se:132:ASN:ND2	2.35	0.41
1:S2:824:C:C2	8:SJ:144:ILE:HG12	2.55	0.41
1:S2:841:G:H2'	1:S2:842:C:C6	2.56	0.41
1:S2:1595:U:H2'	1:S2:1596:U:C6	2.55	0.41
2:L8:103:A:N3	3:L5:21:G:H1'	2.36	0.41
3:L5:260:C:N4	3:L5:261:G:O6	2.54	0.41
3:L5:1411:C:H2'	3:L5:1412:G:C8	2.56	0.41
3:L5:1687:U:H2'	3:L5:1688:G:C8	2.56	0.41
3:L5:3594:C:H2'	3:L5:3595:U:H2'	2.01	0.41
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.86	0.41
3:L5:4704:C:H2'	3:L5:4705:A:C8	2.56	0.41
15:SI:174:CYS:HB2	15:SI:190:LEU:HD11	2.02	0.41
38:Lz:93:LEU:HD13	38:Lz:93:LEU:HA	1.88	0.41
45:LG:115:LEU:HD12	45:LG:116:ALA:N	2.35	0.41
45:LG:138:ALA:HB2	45:LG:194:VAL:HG11	2.01	0.41
57:LR:180:LYS:O	57:LR:183:GLU:HG3	2.20	0.41
59:LT:122:LYS:O	59:LT:122:LYS:HD2	2.20	0.41
66:Lr:19:LYS:HG2	66:Lr:24:THR:HG23	2.03	0.41
1:S2:116:OMU:H6	1:S2:116:OMU:O5'	2.20	0.41
1:S2:518:G:H8	1:S2:518:G:O5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:839:C:H3'	1:S2:840:C:C5'	2.51	0.41
1:S2:873:G:C5	25:SL:152:LYS:HG3	2.55	0.41
1:S2:940:U:H2'	1:S2:941:C:C6	2.55	0.41
1:S2:1026:C:H4'	1:S2:1161:U:H4'	2.02	0.41
1:S2:1358:U:OP1	10:SC:114:LYS:HB2	2.21	0.41
1:S2:1418:C:N3	1:S2:1421:A:H2	2.19	0.41
2:L8:8:U:H2'	2:L8:9:A:C8	2.56	0.41
3:L5:218:A:H2'	3:L5:218:A:N3	2.36	0.41
3:L5:449:C:H4'	3:L5:450:G:C5'	2.51	0.41
3:L5:469:C:H2'	3:L5:470:A:H8	1.86	0.41
3:L5:661:C:H2'	3:L5:662:C:C6	2.56	0.41
3:L5:1669:A:N3	3:L5:1852:U:O2'	2.46	0.41
3:L5:1762:C:H2'	3:L5:1763:C:H6	1.86	0.41
3:L5:1809:C:H2'	3:L5:1810:G:C8	2.56	0.41
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.21	0.41
3:L5:2538:U:H2'	3:L5:2539:C:H6	1.82	0.41
3:L5:4870:G:H5''	51:LM:91:TRP:CD2	2.56	0.41
3:L5:4953:G:O2'	3:L5:4954:G:H5'	2.20	0.41
9:SE:171:ASP:OD2	9:SE:235:TRP:HH2	2.03	0.41
9:SE:255:ARG:HG2	9:SE:259:LYS:NZ	2.36	0.41
17:SU:45:GLU:OE2	17:SU:46:LYS:HG3	2.21	0.41
21:SM:50:CYS:HB2	21:SM:110:VAL:HG22	2.01	0.41
21:SM:86:GLY:HA2	21:SM:89:VAL:HG22	2.02	0.41
36:Sf:121:CYS:HB2	36:Sf:146:LEU:HD23	2.03	0.41
38:Lz:96:ASN:O	38:Lz:97:LYS:C	2.64	0.41
42:LJ:37:ALA:HA	42:LJ:70:VAL:HG11	2.02	0.41
47:LK:16:ARG:HG2	47:LK:59:THR:OG1	2.21	0.41
48:LO:31:ARG:O	48:LO:33:VAL:HG23	2.21	0.41
50:LV:112:MET:HE1	50:LV:117:ILE:CG1	2.50	0.41
55:LD:125:VAL:HG11	55:LD:199:ILE:HG21	2.03	0.41
58:LS:45:TRP:NE1	58:LS:56:LYS:HG3	2.35	0.41
86:EF:26:HIS:NE2	86:EF:30:LYS:HE2	2.36	0.41
86:EF:299:LEU:HD23	86:EF:299:LEU:HA	1.91	0.41
3:L5:375:G:OP1	41:LC:62:THR:OG1	2.33	0.41
3:L5:465:G:H2'	3:L5:466:A:C8	2.55	0.41
3:L5:1397:A:C2	3:L5:1498:G:N3	2.89	0.41
3:L5:1647:U:OP1	87:L5:5109:SPD:H52	2.20	0.41
3:L5:4336:A:H5''	3:L5:4337:C:H5'	2.03	0.41
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.56	0.41
3:L5:4966:A:H5''	40:LB:128:LYS:HG3	2.03	0.41
4:L7:111:C:H2'	4:L7:112:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SA:216:ALA:O	6:SA:219:GLU:HG3	2.20	0.41
15:SI:122:GLY:HA2	15:SI:167:GLN:HA	2.03	0.41
20:SX:56:GLY:HA3	35:Se:80:LEU:HD21	2.03	0.41
26:SR:14:ARG:O	26:SR:18:GLU:HG2	2.20	0.41
30:SY:78:SER:OG	30:SY:80:ASP:OD1	2.33	0.41
31:SZ:64:ASN:O	31:SZ:111:ARG:NE	2.52	0.41
37:Sg:52:TYR:CD2	37:Sg:309:VAL:HG11	2.55	0.41
38:Lz:120:ILE:HG23	38:Lz:124:LEU:HD22	2.03	0.41
38:Lz:206:ILE:HG12	38:Lz:214:GLN:CD	2.46	0.41
86:EF:13:ILE:CG2	86:EF:102:MET:HE3	2.51	0.41
86:EF:178:ILE:HB	86:EF:183:TYR:HB2	2.03	0.41
1:S2:434:G:H2'	1:S2:435:A:C8	2.56	0.41
1:S2:512:A2M:HM'3	1:S2:512:A2M:H1'	1.88	0.41
1:S2:1018:U:H2'	1:S2:1019:C:C6	2.56	0.41
1:S2:1161:U:OP2	20:SX:4:CYS:HB3	2.21	0.41
1:S2:1220:A:H2'	1:S2:1221:G:O4'	2.21	0.41
1:S2:1667:U:H2'	1:S2:1668:U:C6	2.56	0.41
2:L8:68:G:H2'	2:L8:69:PSU:O4'	2.21	0.41
2:L8:109:C:N3	76:Lj:20:ARG:NH1	2.69	0.41
3:L5:1535:C:H2'	3:L5:1536:PSU:O4'	2.21	0.41
3:L5:1690:C:H2'	3:L5:1691:G:O4'	2.20	0.41
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.35	0.41
3:L5:1765:A:H5'	3:L5:1767:A:H62	1.86	0.41
3:L5:1772:C:H2'	3:L5:1773:U:H6	1.85	0.41
3:L5:1802:A:H4'	59:LT:105:PHE:CE1	2.56	0.41
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.56	0.41
3:L5:2015:U:H2'	3:L5:2016:C:H6	1.86	0.41
3:L5:2249:C:H2'	3:L5:2250:C:C5	2.56	0.41
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.56	0.41
3:L5:3956:G:H21	3:L5:3960:A:H61	1.68	0.41
3:L5:4208:U:H4'	3:L5:4274:A:C2	2.56	0.41
3:L5:4250:G:H5''	42:LJ:98:ASN:OD1	2.21	0.41
4:L7:11:A:N1	4:L7:66:G:O2'	2.50	0.41
6:SA:190:SER:HB3	6:SA:193:HIS:HB3	2.02	0.41
7:SD:158:ILE:HG12	7:SD:189:MET:SD	2.61	0.41
10:SC:156:ILE:O	10:SC:160:LEU:HD23	2.21	0.41
26:SR:61:ILE:HG12	26:SR:66:VAL:HG21	2.03	0.41
27:SP:87:PRO:HG3	27:SP:112:ILE:HD13	2.03	0.41
34:Sc:18:LEU:HD13	34:Sc:18:LEU:HA	1.89	0.41
37:Sg:40:ILE:HB	37:Sg:59:LEU:HB2	2.03	0.41
37:Sg:112:ALA:HB2	37:Sg:155:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:217:MET:HA	37:Sg:229:THR:HA	2.03	0.41
43:LH:129:ARG:HB3	43:LH:153:LEU:HD22	2.02	0.41
45:LG:159:HIS:CE1	45:LG:185:LYS:HD3	2.55	0.41
47:LK:14:TYR:CZ	47:LK:59:THR:HG21	2.56	0.41
49:LL:257:ILE:HD12	49:LL:257:ILE:HA	1.94	0.41
53:LN:175:GLY:O	53:LN:180:PHE:HB2	2.20	0.41
55:LD:235:MET:HE2	55:LD:235:MET:HB2	1.75	0.41
57:LR:78:ILE:HD13	57:LR:78:ILE:HA	1.91	0.41
59:LT:117:LYS:HD3	59:LT:117:LYS:HA	1.88	0.41
83:mR:36[A]:U:O2	85:Pt:38:A:H2	2.04	0.41
84:At:5:G:H2'	84:At:6:G:C8	2.55	0.41
84:At:11:C:H2'	84:At:12:U:C6	2.55	0.41
84:At:44:G:H1'	84:At:45:U:H2'	2.01	0.41
1:S2:1227:G:N3	1:S2:1227:G:H2'	2.37	0.41
3:L5:672:C:H2'	3:L5:673:C:C6	2.56	0.41
3:L5:741:C:H3'	3:L5:742:G:C5'	2.51	0.41
3:L5:751:G:H2'	3:L5:752:G:O4'	2.21	0.41
3:L5:1410:U:H4'	3:L5:1411:C:O4'	2.20	0.41
3:L5:1432:G:H2'	3:L5:1451:G:H22	1.86	0.41
3:L5:1743:A:O4'	55:LD:15:ARG:HD2	2.20	0.41
3:L5:2370:A:C8	71:Ld:39:LYS:HD2	2.56	0.41
3:L5:2406:G:N7	78:Ll:2:SER:N	2.69	0.41
3:L5:2836:A:H1'	40:LB:228:TYR:HD2	1.86	0.41
15:SI:42:ARG:HH21	15:SI:59:ARG:HH12	1.69	0.41
22:SS:12:ILE:C	22:SS:13:LEU:HD12	2.45	0.41
30:SY:35:VAL:HG13	30:SY:39:GLU:HB3	2.03	0.41
37:Sg:5:MET:HB3	37:Sg:270:LEU:HD21	2.03	0.41
38:Lz:72:GLN:H	38:Lz:72:GLN:CD	2.29	0.41
38:Lz:74:CYS:C	38:Lz:78:LYS:HZ2	2.28	0.41
47:LK:60:VAL:HG12	47:LK:73:VAL:HG22	2.02	0.41
48:LO:46:ASN:ND2	48:LO:49:ARG:HG3	2.36	0.41
1:S2:28:U:H2'	1:S2:29:G:C8	2.53	0.40
1:S2:844:U:H2'	1:S2:845:G:H8	1.85	0.40
3:L5:86:U:H2'	3:L5:87:A:H8	1.85	0.40
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.84	0.40
3:L5:1437:C:C2	3:L5:2098:G:C8	3.09	0.40
3:L5:3783:A:O5'	3:L5:3784:A:H5'	2.21	0.40
3:L5:5029:C:H2'	3:L5:5030:U:C6	2.56	0.40
7:SD:47:GLU:HG2	7:SD:87:TYR:CE2	2.48	0.40
9:SE:168:LYS:HD2	9:SE:169:ILE:H	1.86	0.40
37:Sg:36:ARG:C	37:Sg:38:LYS:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LH:8:GLN:OE1	43:LH:71:ARG:HG3	2.21	0.40
53:LN:165:THR:O	53:LN:169:ARG:HG2	2.21	0.40
54:LI:75:TYR:CZ	54:LI:150:GLU:HG3	2.56	0.40
56:LQ:178:ARG:HA	56:LQ:184:ARG:O	2.21	0.40
61:LU:61:VAL:HG22	61:LU:74:SER:HB2	2.03	0.40
64:LW:3:VAL:HG11	64:LW:12:LYS:HE2	2.04	0.40
65:LZ:25:ILE:HA	65:LZ:43:VAL:HG12	2.03	0.40
81:Lo:33:LEU:HD23	81:Lo:33:LEU:O	2.21	0.40
1:S2:35:C:H2'	1:S2:36:PSU:H6	1.85	0.40
1:S2:118:C:H1'	1:S2:445:A:C5	2.56	0.40
1:S2:174:OMC:H1'	1:S2:174:OMC:HM23	1.79	0.40
1:S2:429:C:H2'	1:S2:430:C:C6	2.56	0.40
1:S2:1288:OMU:HM23	1:S2:1288:OMU:H1'	1.82	0.40
3:L5:35:U:H4'	3:L5:1525:A:C2	2.56	0.40
3:L5:489:C:H2'	3:L5:490:C:C6	2.57	0.40
3:L5:729:G:N3	3:L5:729:G:H5'	2.35	0.40
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.87	0.40
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.56	0.40
3:L5:3923:A:H2'	3:L5:3924:C:H6	1.85	0.40
3:L5:4152:G:H2'	3:L5:4153:C:O4'	2.22	0.40
3:L5:4883:C:OP2	44:LE:274:VAL:HG22	2.21	0.40
6:SA:37:TYR:CD1	6:SA:162:PRO:HG3	2.56	0.40
7:SD:172:VAL:HG22	7:SD:185:LYS:HG2	2.04	0.40
37:Sg:7:LEU:HD12	37:Sg:309:VAL:O	2.21	0.40
38:Lz:120:ILE:HG23	38:Lz:128:LEU:HD12	2.03	0.40
41:LC:143:ARG:HG2	41:LC:182:LYS:HD2	2.02	0.40
54:LI:61:SER:HA	54:LI:126:VAL:HG12	2.02	0.40
59:LT:53:PRO:HB3	59:LT:91:VAL:HG11	2.03	0.40
69:LF:126:ASN:O	69:LF:127:LYS:C	2.63	0.40
74:Lg:56:VAL:HG13	74:Lg:72:LYS:HA	2.03	0.40
1:S2:921:G:C6	14:SW:28:ARG:HD2	2.57	0.40
1:S2:1019:C:H2'	1:S2:1020:A:O4'	2.21	0.40
1:S2:1678:A2M:H1'	1:S2:1678:A2M:HM'3	1.60	0.40
2:L8:14:OMU:HM23	2:L8:14:OMU:H1'	1.62	0.40
3:L5:143:C:H5'	45:LG:108:GLN:HG3	2.03	0.40
3:L5:2804:OMC:HM23	3:L5:2804:OMC:H1'	1.84	0.40
3:L5:4183:G:N3	3:L5:4183:G:H2'	2.36	0.40
3:L5:4343:U:H2'	3:L5:4344:U:C6	2.56	0.40
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.86	0.40
5:SB:66:VAL:HG11	5:SB:85:LYS:HE2	2.02	0.40
9:SE:87:MET:O	9:SE:122:LYS:HE3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SC:65:LYS:HG2	10:SC:273:LEU:HD22	2.03	0.40
10:SC:171:GLY:HA3	14:SW:97:ARG:HH21	1.86	0.40
11:SG:70:HIS:C	11:SG:98:ARG:NH1	2.79	0.40
22:SS:16:LEU:HD11	22:SS:72:GLN:NE2	2.36	0.40
22:SS:27:ALA:HB1	22:SS:42:HIS:CE1	2.56	0.40
29:SV:2:GLN:HB3	29:SV:6:GLY:HA2	2.02	0.40
29:SV:16:LYS:HD2	29:SV:21:ASN:OD1	2.22	0.40
30:SY:74:MET:O	30:SY:75:ILE:HD13	2.21	0.40
38:Lz:49:PHE:HB2	38:Lz:193:LEU:CD1	2.47	0.40
45:LG:51:LEU:O	45:LG:55:VAL:HG23	2.21	0.40
57:LR:4:LEU:HD22	57:LR:32:ILE:HG22	2.03	0.40
60:LP:4:TYR:CE1	60:LP:16:LYS:HD3	2.55	0.40
62:LX:73:HIS:CE1	62:LX:115:LYS:HE3	2.56	0.40
65:LZ:26:VAL:HG12	65:LZ:93:LYS:HE3	2.03	0.40
1:S2:327:G:H3'	1:S2:327:G:H8	1.86	0.40
1:S2:441:C:H2'	1:S2:442:C:C6	2.57	0.40
1:S2:888:U:H4'	1:S2:889:U:H5'	2.04	0.40
1:S2:893:U:H3'	1:S2:894:G:H8	1.86	0.40
1:S2:980:A:H2'	1:S2:981:A:C8	2.57	0.40
1:S2:1011:A:H2'	1:S2:1012:A:O4'	2.21	0.40
2:L8:87:G:H8	2:L8:87:G:OP2	2.04	0.40
3:L5:162:A:H2'	3:L5:163:A:H8	1.85	0.40
3:L5:175:C:H42	3:L5:260:C:H42	1.68	0.40
3:L5:1271:G:N3	3:L5:1271:G:H2'	2.37	0.40
3:L5:1969:G:H4'	46:Lq:36:GLY:HA2	2.02	0.40
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.56	0.40
3:L5:4103:C:H42	3:L5:4108:G:H1	1.69	0.40
3:L5:4524:G:N3	40:LB:252:ALA:HB1	2.36	0.40
6:SA:149:ASN:HB2	6:SA:165:ASN:OD1	2.21	0.40
7:SD:5:ILE:HG22	7:SD:9:ARG:HB2	2.03	0.40
13:SH:87:PHE:HB3	13:SH:90:LYS:HE2	2.04	0.40
24:SN:16:LEU:HD12	24:SN:17:PRO:HD2	2.04	0.40
26:SR:34:VAL:HG12	26:SR:38:ILE:HD13	2.04	0.40
38:Lz:110:PHE:HB2	38:Lz:135:PRO:HA	2.01	0.40
55:LD:117:LYS:HD3	55:LD:117:LYS:HA	1.78	0.40
56:LQ:59:PRO:HG3	56:LQ:143:ARG:HA	2.04	0.40
59:LT:123:GLY:O	59:LT:124:THR:O	2.38	0.40
75:Li:86:LYS:O	75:Li:89:GLU:HG3	2.22	0.40
1:S2:67:C:C4	11:SG:162:LEU:HB3	2.56	0.40
1:S2:193:C:H2'	1:S2:194:C:C6	2.57	0.40
1:S2:1285:G:H1	21:SM:57:ASP:CG	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.53	0.40
2:L8:26:C:H4'	3:L5:357:U:OP1	2.21	0.40
3:L5:128:C:H2'	3:L5:129:C:C6	2.56	0.40
3:L5:437:G:H5'	72:Le:53:ILE:HD13	2.03	0.40
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.85	0.40
3:L5:1419:G:C6	52:La:116:LYS:HD2	2.56	0.40
3:L5:2263:A:H5''	66:Lr:108:MET:HG3	2.03	0.40
3:L5:2474:G:N2	3:L5:2503:G:H5''	2.37	0.40
3:L5:2889:G:H2'	3:L5:2890:C:C6	2.57	0.40
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.44	0.40
3:L5:4383:U:H2'	3:L5:4384:U:C6	2.55	0.40
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.86	0.40
5:SB:63:LYS:HA	5:SB:88:THR:HG23	2.02	0.40
8:SJ:63:LEU:O	8:SJ:70:ARG:NH1	2.49	0.40
8:SJ:111:GLN:HA	8:SJ:130:ILE:HD11	2.03	0.40
11:SG:70:HIS:CA	11:SG:98:ARG:HH12	2.31	0.40
11:SG:228:ILE:O	11:SG:231:ARG:HG2	2.22	0.40
12:SF:79:HIS:O	12:SF:81:ARG:N	2.52	0.40
13:SH:158:LEU:HD11	13:SH:187:PHE:CD2	2.56	0.40
21:SM:96:ARG:H	21:SM:96:ARG:HG3	1.42	0.40
36:Sf:90:LYS:HD2	36:Sf:90:LYS:HA	1.93	0.40
40:LB:41:VAL:HA	40:LB:186:ASN:O	2.22	0.40
40:LB:57:VAL:HG22	40:LB:73:VAL:HG22	2.04	0.40
45:LG:109:GLU:HA	45:LG:112:GLN:OE1	2.22	0.40
55:LD:22:ARG:HB3	55:LD:28:THR:HG22	2.04	0.40
57:LR:183:GLU:O	57:LR:187:THR:HG22	2.21	0.40
81:Lo:32:SER:C	81:Lo:34:TYR:H	2.28	0.40
86:EF:154:LYS:HG2	96:EF:501:GSP:C6	2.56	0.40
86:EF:261:THR:HG22	86:EF:263:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SB	219/264 (83%)	213 (97%)	6 (3%)	0	100	100
6	SA	220/295 (75%)	210 (96%)	10 (4%)	0	100	100
7	SD	224/243 (92%)	217 (97%)	6 (3%)	1 (0%)	30	60
8	SJ	183/194 (94%)	173 (94%)	8 (4%)	2 (1%)	11	36
9	SE	260/263 (99%)	247 (95%)	13 (5%)	0	100	100
10	SC	220/293 (75%)	212 (96%)	8 (4%)	0	100	100
11	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
12	SF	187/204 (92%)	180 (96%)	7 (4%)	0	100	100
13	SH	187/194 (96%)	182 (97%)	5 (3%)	0	100	100
14	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
15	SI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
16	SQ	139/146 (95%)	137 (99%)	2 (1%)	0	100	100
17	SU	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
18	SK	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
20	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
21	SM	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	16	44
22	SS	146/152 (96%)	140 (96%)	6 (4%)	0	100	100
23	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
24	SN	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
25	SL	139/158 (88%)	131 (94%)	8 (6%)	0	100	100
26	SR	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
27	SP	131/145 (90%)	126 (96%)	5 (4%)	0	100	100
28	ST	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
29	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
30	SY	129/133 (97%)	124 (96%)	5 (4%)	0	100	100
31	SZ	82/125 (66%)	79 (96%)	3 (4%)	0	100	100
32	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
33	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
34	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
35	Se	57/133 (43%)	56 (98%)	1 (2%)	0	100	100
36	Sf	73/156 (47%)	59 (81%)	14 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Sg	311/317 (98%)	287 (92%)	24 (8%)	0	100	100
38	Lz	209/217 (96%)	181 (87%)	26 (12%)	2 (1%)	12	38
39	LA	248/257 (96%)	241 (97%)	7 (3%)	0	100	100
40	LB	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
41	LC	366/427 (86%)	357 (98%)	9 (2%)	0	100	100
42	LJ	167/178 (94%)	164 (98%)	3 (2%)	0	100	100
43	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
44	LE	218/288 (76%)	207 (95%)	11 (5%)	0	100	100
45	LG	237/266 (89%)	231 (98%)	6 (2%)	0	100	100
46	Lq	194/317 (61%)	184 (95%)	10 (5%)	0	100	100
47	LK	145/165 (88%)	132 (91%)	13 (9%)	0	100	100
48	LO	199/203 (98%)	194 (98%)	5 (2%)	0	100	100
49	LL	204/270 (76%)	200 (98%)	4 (2%)	0	100	100
50	LV	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
51	LM	134/215 (62%)	128 (96%)	6 (4%)	0	100	100
52	La	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	47
53	LN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
54	LI	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
55	LD	292/297 (98%)	287 (98%)	5 (2%)	0	100	100
56	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
57	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
58	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
59	LT	157/160 (98%)	152 (97%)	3 (2%)	2 (1%)	9	31
60	LP	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
61	LU	97/128 (76%)	92 (95%)	5 (5%)	0	100	100
62	LX	116/156 (74%)	116 (100%)	0	0	100	100
63	LY	132/145 (91%)	132 (100%)	0	0	100	100
64	LW	114/157 (73%)	109 (96%)	5 (4%)	0	100	100
65	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
66	Lr	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
67	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Lb	104/159 (65%)	97 (93%)	7 (7%)	0	100	100
69	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
70	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
71	Ld	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
72	Le	126/135 (93%)	126 (100%)	0	0	100	100
73	Lf	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
74	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
75	Li	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
76	Lj	85/97 (88%)	84 (99%)	1 (1%)	0	100	100
77	Lk	67/70 (96%)	67 (100%)	0	0	100	100
78	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
79	Lm	49/128 (38%)	49 (100%)	0	0	100	100
80	Ln	23/25 (92%)	23 (100%)	0	0	100	100
81	Lo	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
82	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
86	EF	438/462 (95%)	420 (96%)	18 (4%)	0	100	100
All	All	12300/13982 (88%)	11856 (96%)	435 (4%)	9 (0%)	49	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	SM	58	GLU
59	LT	122	LYS
59	LT	124	THR
8	SJ	117	LEU
52	La	15	VAL
7	SD	48	ILE
8	SJ	36	GLY
38	Lz	65	VAL
38	Lz	87	ILE

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	
5	SB	202/231 (87%)	199 (98%)	3 (2%)	57	84
6	SA	183/242 (76%)	180 (98%)	3 (2%)	55	83
7	SD	189/202 (94%)	185 (98%)	4 (2%)	47	79
8	SJ	161/168 (96%)	157 (98%)	4 (2%)	42	76
9	SE	224/225 (100%)	217 (97%)	7 (3%)	35	70
10	SC	188/225 (84%)	188 (100%)	0	100	100
11	SG	207/218 (95%)	203 (98%)	4 (2%)	50	81
12	SF	159/170 (94%)	156 (98%)	3 (2%)	50	81
13	SH	168/174 (97%)	157 (94%)	11 (6%)	15	43
14	SW	112/113 (99%)	110 (98%)	2 (2%)	51	82
15	SI	178/180 (99%)	172 (97%)	6 (3%)	32	68
16	SQ	117/121 (97%)	112 (96%)	5 (4%)	26	60
17	SU	93/107 (87%)	87 (94%)	6 (6%)	15	43
18	SK	87/136 (64%)	81 (93%)	6 (7%)	14	41
19	SO	105/119 (88%)	101 (96%)	4 (4%)	29	64
20	SX	113/114 (99%)	108 (96%)	5 (4%)	25	59
21	SM	102/108 (94%)	94 (92%)	8 (8%)	11	35
22	SS	128/132 (97%)	127 (99%)	1 (1%)	73	90
23	Sd	48/49 (98%)	48 (100%)	0	100	100
24	SN	131/131 (100%)	127 (97%)	4 (3%)	35	70
25	SL	129/142 (91%)	124 (96%)	5 (4%)	28	64
26	SR	121/122 (99%)	112 (93%)	9 (7%)	13	37
27	SP	119/130 (92%)	114 (96%)	5 (4%)	26	61
28	ST	113/115 (98%)	111 (98%)	2 (2%)	51	82
29	SV	66/66 (100%)	62 (94%)	4 (6%)	17	46
30	SY	113/115 (98%)	111 (98%)	2 (2%)	51	82
31	SZ	74/103 (72%)	69 (93%)	5 (7%)	14	42
32	Sa	86/98 (88%)	86 (100%)	0	100	100
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Sc	57/62 (92%)	56 (98%)	1 (2%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Se	48/104 (46%)	47 (98%)	1 (2%)	47	79
36	Sf	67/140 (48%)	60 (90%)	7 (10%)	7	22
37	Sg	272/275 (99%)	254 (93%)	18 (7%)	15	43
38	Lz	190/196 (97%)	168 (88%)	22 (12%)	5	18
39	LA	192/198 (97%)	189 (98%)	3 (2%)	55	83
40	LB	347/348 (100%)	347 (100%)	0	100	100
41	LC	306/348 (88%)	304 (99%)	2 (1%)	76	91
42	LJ	143/149 (96%)	142 (99%)	1 (1%)	76	91
43	LH	169/171 (99%)	168 (99%)	1 (1%)	78	92
44	LE	197/252 (78%)	195 (99%)	2 (1%)	68	88
45	LG	201/223 (90%)	194 (96%)	7 (4%)	32	67
46	Lq	164/258 (64%)	164 (100%)	0	100	100
47	LK	122/137 (89%)	119 (98%)	3 (2%)	42	76
48	LO	173/174 (99%)	172 (99%)	1 (1%)	78	92
49	LL	172/224 (77%)	166 (96%)	6 (4%)	32	67
50	LV	107/107 (100%)	107 (100%)	0	100	100
51	LM	116/161 (72%)	113 (97%)	3 (3%)	40	75
52	La	119/120 (99%)	118 (99%)	1 (1%)	73	90
53	LN	171/172 (99%)	169 (99%)	2 (1%)	63	87
54	LI	175/181 (97%)	171 (98%)	4 (2%)	44	78
55	LD	247/250 (99%)	243 (98%)	4 (2%)	55	83
56	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	87
57	LR	166/175 (95%)	166 (100%)	0	100	100
58	LS	157/157 (100%)	157 (100%)	0	100	100
59	LT	139/140 (99%)	138 (99%)	1 (1%)	76	91
60	LP	134/163 (82%)	134 (100%)	0	100	100
61	LU	89/115 (77%)	85 (96%)	4 (4%)	24	58
62	LX	106/133 (80%)	106 (100%)	0	100	100
63	LY	124/135 (92%)	122 (98%)	2 (2%)	55	83
64	LW	95/126 (75%)	93 (98%)	2 (2%)	47	79
65	LZ	117/118 (99%)	114 (97%)	3 (3%)	40	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	Lr	108/120 (90%)	106 (98%)	2 (2%)	50	81
67	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	89
68	Lb	89/125 (71%)	88 (99%)	1 (1%)	65	87
69	LF	194/215 (90%)	191 (98%)	3 (2%)	57	84
70	Lc	83/97 (86%)	83 (100%)	0	100	100
71	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	88
72	Le	114/121 (94%)	112 (98%)	2 (2%)	51	82
73	Lf	88/89 (99%)	88 (100%)	0	100	100
74	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	88
75	Li	86/89 (97%)	84 (98%)	2 (2%)	44	78
76	Lj	74/80 (92%)	72 (97%)	2 (3%)	39	74
77	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	83
78	Ll	47/48 (98%)	47 (100%)	0	100	100
79	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	79
80	Ln	24/24 (100%)	22 (92%)	2 (8%)	10	32
81	Lo	93/93 (100%)	92 (99%)	1 (1%)	65	87
82	Lp	74/75 (99%)	74 (100%)	0	100	100
86	EF	363/375 (97%)	355 (98%)	8 (2%)	45	78
All	All	10690/11860 (90%)	10441 (98%)	249 (2%)	44	78

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SB	5	LYS
5	SB	55	THR
5	SB	57	ILE
6	SA	89	LYS
6	SA	109	THR
6	SA	198	MET
7	SD	40	ARG
7	SD	44	THR
7	SD	84	VAL
7	SD	193	ASP
8	SJ	112	THR
8	SJ	172	ARG
8	SJ	173	VAL

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Mol	Chain	Res	Type
8	SJ	175	ARG
9	SE	139	LEU
9	SE	141	THR
9	SE	200	ARG
9	SE	236	ILE
9	SE	238	LEU
9	SE	246	LEU
9	SE	248	ILE
11	SG	52	ILE
11	SG	53	SER
11	SG	94	ARG
11	SG	181	THR
12	SF	126	THR
12	SF	127	ARG
12	SF	134	VAL
13	SH	8	ILE
13	SH	74	LYS
13	SH	76	GLN
13	SH	82	GLU
13	SH	83	LEU
13	SH	110	THR
13	SH	132	ASP
13	SH	142	LYS
13	SH	160	LYS
13	SH	162	GLN
13	SH	165	ASN
14	SW	30	CYS
14	SW	83	LEU
15	SI	62	VAL
15	SI	75	LYS
15	SI	76	THR
15	SI	114	GLU
15	SI	145	ILE
15	SI	148	LYS
16	SQ	9	SER
16	SQ	20	THR
16	SQ	46	THR
16	SQ	48	GLN
16	SQ	88	ILE
17	SU	20	ILE
17	SU	50	VAL
17	SU	89	ILE

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Mol	Chain	Res	Type
17	SU	90	ASP
17	SU	91	LEU
17	SU	114	VAL
18	SK	2	LEU
18	SK	5	LYS
18	SK	6	LYS
18	SK	7	ASN
18	SK	9	ILE
18	SK	13	GLU
19	SO	53	ILE
19	SO	88	LEU
19	SO	104	ARG
19	SO	138	ASP
20	SX	105	PHE
20	SX	115	ILE
20	SX	129	SER
20	SX	142	ARG
20	SX	143	SER
21	SM	27	ILE
21	SM	52	LEU
21	SM	54	SER
21	SM	57	ASP
21	SM	58	GLU
21	SM	91	LEU
21	SM	96	ARG
21	SM	103	VAL
22	SS	12	ILE
24	SN	31	ASP
24	SN	103	GLU
24	SN	133	ARG
24	SN	140	LYS
25	SL	19	ASN
25	SL	48	LYS
25	SL	51	ILE
25	SL	133	PRO
25	SL	152	LYS
26	SR	8	THR
26	SR	18	GLU
26	SR	62	GLN
26	SR	63	ARG
26	SR	70	SER
26	SR	76	GLU

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Mol	Chain	Res	Type
26	SR	77	GLU
26	SR	82	ASP
26	SR	85	VAL
27	SP	13	ARG
27	SP	18	ARG
27	SP	71	GLU
27	SP	136	THR
27	SP	138	SER
28	ST	104	LEU
28	ST	121	ARG
29	SV	4	ASP
29	SV	38	GLU
29	SV	42	VAL
29	SV	45	ARG
30	SY	34	THR
30	SY	39	GLU
31	SZ	36	SER
31	SZ	44	LEU
31	SZ	45	ASN
31	SZ	48	VAL
31	SZ	56	ASP
34	Sc	18	LEU
35	Se	76	VAL
36	Sf	87	THR
36	Sf	92	LYS
36	Sf	94	LYS
36	Sf	97	LYS
36	Sf	98	VAL
36	Sf	108	VAL
36	Sf	132	MET
37	Sg	2	THR
37	Sg	5	MET
37	Sg	21	ILE
37	Sg	59	LEU
37	Sg	62	HIS
37	Sg	66	VAL
37	Sg	107	ASP
37	Sg	114	SER
37	Sg	132	TRP
37	Sg	159	ASN
37	Sg	195	LEU
37	Sg	197	THR

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Mol	Chain	Res	Type
37	Sg	198	VAL
37	Sg	199	THR
37	Sg	200	VAL
37	Sg	203	ASP
37	Sg	287	THR
37	Sg	313	THR
38	Lz	35	GLN
38	Lz	44	GLN
38	Lz	49	PHE
38	Lz	67	VAL
38	Lz	68	LEU
38	Lz	71	GLN
38	Lz	76	GLU
38	Lz	78	LYS
38	Lz	84	HIS
38	Lz	93	LEU
38	Lz	96	ASN
38	Lz	100	VAL
38	Lz	120	ILE
38	Lz	140	HIS
38	Lz	162	VAL
38	Lz	169	VAL
38	Lz	171	HIS
38	Lz	194	LEU
38	Lz	206	ILE
38	Lz	209	THR
38	Lz	214	GLN
38	Lz	215	ARG
39	LA	180	LEU
39	LA	208	GLU
39	LA	242	ARG
41	LC	138	MET
41	LC	215	ASN
42	LJ	155	HIS
43	LH	67	LEU
44	LE	104	THR
44	LE	106	VAL
45	LG	108	GLN
45	LG	115	LEU
45	LG	121	LYS
45	LG	130	THR
45	LG	157	ILE

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Mol	Chain	Res	Type
45	LG	253	LEU
45	LG	254	GLU
47	LK	18	THR
47	LK	119	ARG
47	LK	142	ASN
48	LO	58	LEU
49	LL	44	ARG
49	LL	138	ASP
49	LL	148	THR
49	LL	214	THR
49	LL	221	ARG
49	LL	223	VAL
51	LM	46	ARG
51	LM	112	VAL
51	LM	113	MET
52	La	16	SER
53	LN	10	LEU
53	LN	176	LYS
54	LI	36	LEU
54	LI	79	SER
54	LI	82	LYS
54	LI	141	LYS
55	LD	41	LYS
55	LD	111	ASN
55	LD	231	VAL
55	LD	232	THR
56	LQ	92	VAL
56	LQ	93	GLN
59	LT	122	LYS
61	LU	26	THR
61	LU	70	ILE
61	LU	105	ASN
61	LU	108	GLU
63	LY	46	SER
63	LY	130	LYS
64	LW	91	MET
64	LW	93	LYS
65	LZ	29	ILE
65	LZ	30	ASP
65	LZ	97	ASN
66	Lr	26	SER
66	Lr	37	SER

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Mol	Chain	Res	Type
67	Lh	87	LYS
68	Lb	118	LEU
69	LF	35	LYS
69	LF	127	LYS
69	LF	223	LYS
71	Ld	107	THR
72	Le	69	MET
72	Le	108	ARG
74	Lg	26	PRO
75	Li	25	ARG
75	Li	63	VAL
76	Lj	20	ARG
76	Lj	50	SER
77	Lk	10	ASP
79	Lm	119	ASN
80	Ln	15	ARG
80	Ln	16	LYS
81	Lo	103	VAL
86	EF	293	GLU
86	EF	379	ILE
86	EF	381	ARG
86	EF	382	ARG
86	EF	383	SER
86	EF	385	LYS
86	EF	416	SER
86	EF	426	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
5	SB	186	ASN
6	SA	9	GLN
7	SD	159	HIS
8	SJ	156	HIS
9	SE	67	GLN
9	SE	157	ASN
9	SE	201	HIS
12	SF	74	ASN
12	SF	137	GLN
12	SF	203	ASN
13	SH	44	ASN
13	SH	97	GLN

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Mol	Chain	Res	Type
13	SH	114	GLN
13	SH	168	HIS
14	SW	70	ASN
14	SW	98	GLN
15	SI	146	GLN
16	SQ	80	GLN
16	SQ	86	GLN
17	SU	28	ASN
18	SK	7	ASN
20	SX	16	HIS
20	SX	31	HIS
20	SX	73	GLN
21	SM	19	GLN
22	SS	135	HIS
23	Sd	3	HIS
24	SN	105	ASN
25	SL	13	GLN
25	SL	19	ASN
26	SR	26	ASN
27	SP	24	GLN
29	SV	35	ASN
30	SY	15	ASN
31	SZ	64	ASN
31	SZ	112	ASN
32	Sa	8	ASN
33	Sb	51	GLN
33	Sb	83	GLN
36	Sf	111	ASN
37	Sg	4	GLN
37	Sg	15	ASN
37	Sg	117	ASN
37	Sg	285	GLN
38	Lz	44	GLN
38	Lz	71	GLN
38	Lz	84	HIS
38	Lz	141	ASN
38	Lz	199	GLN
39	LA	38	HIS
39	LA	215	ASN
40	LB	145	GLN
40	LB	184	GLN
40	LB	186	ASN

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Mol	Chain	Res	Type
40	LB	203	GLN
41	LC	38	ASN
41	LC	43	ASN
41	LC	142	HIS
41	LC	215	ASN
41	LC	310	HIS
41	LC	329	ASN
41	LC	346	ASN
41	LC	347	HIS
42	LJ	65	ASN
43	LH	98	HIS
44	LE	245	GLN
45	LG	43	GLN
45	LG	66	GLN
45	LG	94	GLN
45	LG	206	GLN
45	LG	208	ASN
46	Lq	85	ASN
46	Lq	179	ASN
47	LK	142	ASN
48	LO	42	ASN
48	LO	50	ASN
49	LL	115	GLN
49	LL	238	ASN
51	LM	34	ASN
51	LM	48	GLN
51	LM	125	ASN
52	La	34	ASN
52	La	66	ASN
52	La	120	GLN
53	LN	117	ASN
53	LN	145	ASN
54	LI	133	GLN
55	LD	81	HIS
55	LD	122	GLN
55	LD	225	GLN
57	LR	118	HIS
58	LS	125	GLN
59	LT	54	HIS
59	LT	58	HIS
59	LT	112	ASN
59	LT	114	GLN

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Mol	Chain	Res	Type
60	LP	21	ASN
60	LP	34	GLN
60	LP	93	HIS
60	LP	97	ASN
60	LP	133	HIS
61	LU	27	HIS
61	LU	38	ASN
61	LU	105	ASN
63	LY	18	HIS
64	LW	95	ASN
64	LW	120	GLN
66	Lr	95	HIS
67	Lh	98	HIS
69	LF	39	GLN
69	LF	58	HIS
69	LF	239	GLN
70	Lc	72	HIS
72	Le	52	GLN
72	Le	80	HIS
72	Le	107	ASN
73	Lf	20	ASN
76	Lj	57	ASN
78	Ll	17	GLN
78	Ll	25	GLN
78	Ll	33	ASN
86	EF	307	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1695/1869 (90%)	365 (21%)	29 (1%)
2	L8	155/156 (99%)	25 (16%)	3 (1%)
3	L5	3673/5069 (72%)	693 (18%)	52 (1%)
4	L7	119/120 (99%)	13 (10%)	0
83	mR	9/60 (15%)	1 (11%)	0
84	At	75/76 (98%)	17 (22%)	0
85	Pt	76/77 (98%)	17 (22%)	0
All	All	5802/7427 (78%)	1131 (19%)	84 (1%)

All (1131) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	4	C
1	S2	17	C
1	S2	33	G
1	S2	41	G
1	S2	45	A
1	S2	46	A
1	S2	56	G
1	S2	58	C
1	S2	65	C
1	S2	67	C
1	S2	68	A
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	78	C
1	S2	103	A
1	S2	113	G
1	S2	115	U
1	S2	126	G
1	S2	127	C
1	S2	128	U
1	S2	129	C
1	S2	142	C
1	S2	143	U
1	S2	146	G
1	S2	147	A
1	S2	155	G
1	S2	163	U
1	S2	171	A
1	S2	173	A
1	S2	175	A
1	S2	182	C
1	S2	184	G
1	S2	186	C
1	S2	193	C
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	203	G
1	S2	204	G
1	S2	209	A
1	S2	211	G

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Mol	Chain	Res	Type
1	S2	214	U
1	S2	215	G
1	S2	224	A
1	S2	294	U
1	S2	302	A
1	S2	305	U
1	S2	306	C
1	S2	307	G
1	S2	312	G
1	S2	320	G
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	335	G
1	S2	347	G
1	S2	351	G
1	S2	362	C
1	S2	364	A
1	S2	369	C
1	S2	370	G
1	S2	377	G
1	S2	381	C
1	S2	382	C
1	S2	385	G
1	S2	386	C
1	S2	393	U
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	417	C
1	S2	418	A
1	S2	421	G
1	S2	429	C
1	S2	438	G
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	453	C

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Mol	Chain	Res	Type
1	S2	466	G
1	S2	467	G
1	S2	471	G
1	S2	472	C
1	S2	474	G
1	S2	476	A
1	S2	482	G
1	S2	487	U
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	500	A
1	S2	501	C
1	S2	508	A
1	S2	516	A
1	S2	517	OMC
1	S2	519	A
1	S2	525	A
1	S2	528	A
1	S2	533	A
1	S2	537	C
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	552	G
1	S2	554	A
1	S2	555	A
1	S2	556	U
1	S2	559	G
1	S2	562	U
1	S2	563	G
1	S2	568	C
1	S2	569	A
1	S2	573	PSU
1	S2	576	A2M
1	S2	578	C
1	S2	589	G
1	S2	590	A2M
1	S2	591	U
1	S2	598	G
1	S2	604	A
1	S2	606	G

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Mol	Chain	Res	Type
1	S2	607	U
1	S2	608	C
1	S2	614	C
1	S2	618	C
1	S2	626	G
1	S2	627	OMU
1	S2	628	A
1	S2	634	A
1	S2	643	A
1	S2	644	OMG
1	S2	655	A
1	S2	660	C
1	S2	664	A
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	688	U
1	S2	690	G
1	S2	691	G
1	S2	692	G
1	S2	694	G
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	735	C
1	S2	737	G
1	S2	739	C
1	S2	821	G
1	S2	822	PSU
1	S2	823	U
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	840	C

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Mol	Chain	Res	Type
1	S2	847	A
1	S2	861	A
1	S2	869	A
1	S2	870	A
1	S2	876	C
1	S2	878	G
1	S2	882	U
1	S2	887	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	895	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	901	G
1	S2	913	A
1	S2	916	A
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	930	C
1	S2	933	G
1	S2	963	A
1	S2	970	G
1	S2	985	G
1	S2	990	A
1	S2	992	A
1	S2	999	G
1	S2	1016	U
1	S2	1017	U
1	S2	1023	A
1	S2	1026	C
1	S2	1045	U
1	S2	1049	A
1	S2	1061	U
1	S2	1062	A
1	S2	1083	A
1	S2	1085	C
1	S2	1096	G

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Mol	Chain	Res	Type
1	S2	1100	A
1	S2	1115	U
1	S2	1116	C
1	S2	1121	G
1	S2	1133	A
1	S2	1138	C
1	S2	1153	C
1	S2	1154	U
1	S2	1155	U
1	S2	1156	U
1	S2	1157	G
1	S2	1165	G
1	S2	1166	G
1	S2	1171	G
1	S2	1188	A
1	S2	1195	A
1	S2	1203	G
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1224	G
1	S2	1228	A
1	S2	1240	A
1	S2	1242	U
1	S2	1243	PSU
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1258	A
1	S2	1259	A
1	S2	1260	A
1	S2	1274	G
1	S2	1275	G
1	S2	1280	G
1	S2	1284	A
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A
1	S2	1288	OMU
1	S2	1301	A
1	S2	1302	G

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Mol	Chain	Res	Type
1	S2	1303	C
1	S2	1308	U
1	S2	1312	G
1	S2	1313	A
1	S2	1314	U
1	S2	1320	G
1	S2	1327	G
1	S2	1332	A
1	S2	1333	U
1	S2	1342	U
1	S2	1348	G
1	S2	1358	U
1	S2	1371	U
1	S2	1372	U
1	S2	1375	G
1	S2	1378	A
1	S2	1397	U
1	S2	1401	A
1	S2	1404	U
1	S2	1405	A
1	S2	1406	G
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1438	A
1	S2	1439	A
1	S2	1441	U
1	S2	1447	OMG
1	S2	1452	A
1	S2	1454	A
1	S2	1463	U
1	S2	1477	U
1	S2	1484	A
1	S2	1487	A
1	S2	1489	A
1	S2	1490	OMG

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Mol	Chain	Res	Type
1	S2	1493	C
1	S2	1494	U
1	S2	1497	G
1	S2	1498	A
1	S2	1506	A
1	S2	1507	G
1	S2	1508	A
1	S2	1520	G
1	S2	1521	C
1	S2	1522	A
1	S2	1533	A
1	S2	1544	C
1	S2	1555	U
1	S2	1560	U
1	S2	1570	G
1	S2	1575	G
1	S2	1580	A
1	S2	1585	U
1	S2	1587	G
1	S2	1588	A
1	S2	1598	G
1	S2	1601	A
1	S2	1621	U
1	S2	1623	A
1	S2	1629	C
1	S2	1632	G
1	S2	1637	A
1	S2	1647	A
1	S2	1648	G
1	S2	1656	G
1	S2	1665	G
1	S2	1669	G
1	S2	1671	G
1	S2	1682	C
1	S2	1683	C
1	S2	1695	A
1	S2	1699	A
1	S2	1721	U
1	S2	1722	G
1	S2	1744	G
1	S2	1752	C
1	S2	1753	C

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Mol	Chain	Res	Type
1	S2	1754	G
1	S2	1756	C
1	S2	1757	G
1	S2	1758	G
1	S2	1761	U
1	S2	1772	C
1	S2	1773	C
1	S2	1774	C
1	S2	1775	U
1	S2	1776	G
1	S2	1777	G
1	S2	1781	A
1	S2	1782	G
1	S2	1783	C
1	S2	1819	A
1	S2	1824	A
1	S2	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1835	A
1	S2	1838	U
1	S2	1849	G
1	S2	1851	MA6
1	S2	1852	C
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1865	C
2	L8	13	G
2	L8	23	C
2	L8	25	G
2	L8	34	U
2	L8	35	C
2	L8	51	U
2	L8	52	A
2	L8	59	A
2	L8	62	A
2	L8	63	U
2	L8	84	A
2	L8	85	U
2	L8	86	U
2	L8	87	G

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Mol	Chain	Res	Type
2	L8	94	G
2	L8	103	A
2	L8	104	A
2	L8	105	C
2	L8	110	U
2	L8	111	U
2	L8	112	G
2	L8	114	G
2	L8	123	U
2	L8	124	U
2	L8	125	C
3	L5	25	A
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	71	C
3	L5	74	G
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	108	A
3	L5	110	C
3	L5	115	C
3	L5	119	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	136	C
3	L5	137	G
3	L5	142	G
3	L5	151	G
3	L5	158	A
3	L5	159	C
3	L5	170	C
3	L5	178	C
3	L5	179	G
3	L5	181	C
3	L5	182	G

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Mol	Chain	Res	Type
3	L5	184	U
3	L5	186	G
3	L5	187	U
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	202	C
3	L5	209	U
3	L5	210	C
3	L5	219	G
3	L5	234	G
3	L5	235	A
3	L5	257	C
3	L5	258	G
3	L5	259	C
3	L5	260	C
3	L5	261	G
3	L5	262	G
3	L5	263	G
3	L5	266	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	326	C
3	L5	340	C
3	L5	344	A
3	L5	350	C
3	L5	361	C
3	L5	373	G
3	L5	386	A
3	L5	387	G
3	L5	399	G
3	L5	408	A
3	L5	409	G
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	432	U
3	L5	440	U

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Mol	Chain	Res	Type
3	L5	449	C
3	L5	450	G
3	L5	451	C
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	483	G
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	487	G
3	L5	498	C
3	L5	499	G
3	L5	504	G
3	L5	510	U
3	L5	513	U
3	L5	514	U
3	L5	644	G
3	L5	646	G
3	L5	659	G
3	L5	663	G
3	L5	665	C
3	L5	666	G
3	L5	667	A
3	L5	670	G
3	L5	685	C
3	L5	688	U
3	L5	695	G
3	L5	696	C
3	L5	704	C
3	L5	708	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	741	C
3	L5	742	G
3	L5	746	A
3	L5	747	A
3	L5	759	G
3	L5	760	G
3	L5	904	C

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Mol	Chain	Res	Type
3	L5	905	C
3	L5	911	U
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	916	C
3	L5	917	A
3	L5	925	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	937	U
3	L5	941	C
3	L5	943	A
3	L5	944	A
3	L5	945	U
3	L5	955	G
3	L5	956	A
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	969	C
3	L5	970	G
3	L5	971	U
3	L5	982	U
3	L5	1070	G
3	L5	1072	C
3	L5	1092	G
3	L5	1093	C
3	L5	1094	G
3	L5	1170	G
3	L5	1180	C
3	L5	1182	C
3	L5	1183	C
3	L5	1185	G
3	L5	1186	U

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Mol	Chain	Res	Type
3	L5	1192	C
3	L5	1198	G
3	L5	1199	G
3	L5	1200	G
3	L5	1201	U
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1216	C
3	L5	1246	G
3	L5	1254	A
3	L5	1258	G
3	L5	1260	G
3	L5	1261	G
3	L5	1266	G
3	L5	1270	A
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1279	A
3	L5	1280	C
3	L5	1284	G
3	L5	1287	G
3	L5	1295	C
3	L5	1296	G
3	L5	1302	U
3	L5	1303	A
3	L5	1304	C
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1358	G
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1403	G
3	L5	1404	G
3	L5	1410	U

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Mol	Chain	Res	Type
3	L5	1411	C
3	L5	1413	C
3	L5	1417	C
3	L5	1418	C
3	L5	1419	G
3	L5	1420	A
3	L5	1436	C
3	L5	1438	U
3	L5	1439	C
3	L5	1443	A
3	L5	1448	G
3	L5	1457	G
3	L5	1480	C
3	L5	1481	C
3	L5	1483	C
3	L5	1491	A
3	L5	1498	G
3	L5	1502	G
3	L5	1504	G
3	L5	1515	A
3	L5	1523	A
3	L5	1534	A2M
3	L5	1535	C
3	L5	1547	A
3	L5	1549	G
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1613	A
3	L5	1614	C
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1640	C
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1670	G
3	L5	1677	PSU

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Mol	Chain	Res	Type
3	L5	1691	G
3	L5	1694	C
3	L5	1698	C
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1705	G
3	L5	1721	G
3	L5	1734	G
3	L5	1740	C
3	L5	1741	G
3	L5	1753	G
3	L5	1754	U
3	L5	1755	C
3	L5	1756	U
3	L5	1757	U
3	L5	1760	G
3	L5	1766	A
3	L5	1768	C
3	L5	1775	A
3	L5	1787	A
3	L5	1794	A
3	L5	1804	A
3	L5	1815	G
3	L5	1820	C
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
3	L5	1855	G
3	L5	1869	G
3	L5	1891	A
3	L5	1897	A
3	L5	1898	C
3	L5	1917	A
3	L5	1919	G
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1930	U
3	L5	1931	C

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Mol	Chain	Res	Type
3	L5	1932	A
3	L5	1940	G
3	L5	1948	G
3	L5	1951	G
3	L5	1955	G
3	L5	1961	G
3	L5	1968	G
3	L5	1983	A
3	L5	1984	A
3	L5	1985	G
3	L5	1987	C
3	L5	1990	A
3	L5	1992	U
3	L5	1993	C
3	L5	1996	C
3	L5	1997	U
3	L5	1998	A
3	L5	2002	A
3	L5	2004	U
3	L5	2011	C
3	L5	2025	A
3	L5	2026	A
3	L5	2042	A
3	L5	2043	A
3	L5	2044	U
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2094	G
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C
3	L5	2103	G
3	L5	2104	G
3	L5	2109	G

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Mol	Chain	Res	Type
3	L5	2110	C
3	L5	2111	G
3	L5	2112	G
3	L5	2250	C
3	L5	2253	A
3	L5	2255	C
3	L5	2256	C
3	L5	2259	G
3	L5	2260	C
3	L5	2268	A
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2314	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2357	G
3	L5	2360	A
3	L5	2395	A
3	L5	2396	A
3	L5	2397	G
3	L5	2417	A
3	L5	2421	G
3	L5	2425	U
3	L5	2447	U
3	L5	2453	A
3	L5	2474	G
3	L5	2486	G
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2492	C
3	L5	2503	G
3	L5	2504	C
3	L5	2506	G
3	L5	2513	A
3	L5	2514	G
3	L5	2519	U

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Mol	Chain	Res	Type
3	L5	2554	U
3	L5	2559	G
3	L5	2570	U
3	L5	2573	A
3	L5	2577	C
3	L5	2578	G
3	L5	2583	C
3	L5	2587	A
3	L5	2588	C
3	L5	2601	A
3	L5	2602	G
3	L5	2618	G
3	L5	2627	C
3	L5	2629	C
3	L5	2638	G
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2687	U
3	L5	2688	G
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2697	A
3	L5	2705	G
3	L5	2708	U
3	L5	2711	G
3	L5	2715	G
3	L5	2726	G
3	L5	2732	G
3	L5	2733	C
3	L5	2735	G
3	L5	2742	G
3	L5	2743	A
3	L5	2754	G
3	L5	2759	G
3	L5	2760	G
3	L5	2763	U
3	L5	2768	C
3	L5	2769	U
3	L5	2770	C
3	L5	2787	A2M

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Mol	Chain	Res	Type
3	L5	2788	U
3	L5	2790	U
3	L5	2798	A
3	L5	2814	C
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2830	G
3	L5	2855	G
3	L5	2903	G
3	L5	2904	U
3	L5	2906	G
3	L5	2907	G
3	L5	2909	C
3	L5	2910	G
3	L5	3585	G
3	L5	3586	G
3	L5	3589	G
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C
3	L5	3596	A
3	L5	3597	G
3	L5	3598	C
3	L5	3606	U
3	L5	3615	G
3	L5	3618	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3672	G
3	L5	3673	C
3	L5	3712	A
3	L5	3732	A
3	L5	3736	A
3	L5	3747	A
3	L5	3748	A
3	L5	3750	G
3	L5	3753	G

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Mol	Chain	Res	Type
3	L5	3759	A
3	L5	3760	A2M
3	L5	3761	C
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A2M
3	L5	3786	U
3	L5	3787	G
3	L5	3807	A
3	L5	3809	G
3	L5	3810	C
3	L5	3811	G
3	L5	3812	C
3	L5	3814	U
3	L5	3816	A
3	L5	3817	A
3	L5	3819	G
3	L5	3822	U
3	L5	3823	G
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3844	PSU
3	L5	3876	A
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3909	C
3	L5	3915	U
3	L5	3949	A
3	L5	3952	A
3	L5	3953	G
3	L5	3954	A
3	L5	3956	G

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Mol	Chain	Res	Type
3	L5	3957	U
3	L5	3958	G
3	L5	3960	A
3	L5	3962	A
3	L5	3964	U
3	L5	3965	A
3	L5	3966	A
3	L5	3967	G
3	L5	3968	U
3	L5	3969	G
3	L5	3971	G
3	L5	3972	A
3	L5	3973	G
3	L5	3974	G
3	L5	3977	C
3	L5	4035	G
3	L5	4037	C
3	L5	4039	G
3	L5	4040	C
3	L5	4041	C
3	L5	4042	G
3	L5	4044	U
3	L5	4048	A
3	L5	4049	U
3	L5	4050	A
3	L5	4051	C
3	L5	4053	A
3	L5	4056	A
3	L5	4064	C
3	L5	4065	G
3	L5	4067	U
3	L5	4069	U
3	L5	4070	U
3	L5	4076	G
3	L5	4084	G
3	L5	4095	G
3	L5	4096	C
3	L5	4103	C
3	L5	4107	G
3	L5	4108	G
3	L5	4115	G
3	L5	4116	C

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Mol	Chain	Res	Type
3	L5	4118	U
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4133	C
3	L5	4136	G
3	L5	4139	G
3	L5	4141	G
3	L5	4142	C
3	L5	4144	C
3	L5	4145	C
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4228	OMG
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4254	G
3	L5	4265	U
3	L5	4266	G
3	L5	4268	A
3	L5	4273	A
3	L5	4280	A
3	L5	4281	A
3	L5	4289	U
3	L5	4291	G
3	L5	4304	A
3	L5	4305	G
3	L5	4306	OMU
3	L5	4314	C
3	L5	4326	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4350	C
3	L5	4373	G
3	L5	4376	A

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Mol	Chain	Res	Type
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4419	U
3	L5	4420	PSU
3	L5	4421	C
3	L5	4422	A
3	L5	4440	G
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4453	C
3	L5	4464	A
3	L5	4465	U
3	L5	4475	G
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G
3	L5	4528	G
3	L5	4548	A
3	L5	4560	C
3	L5	4567	G
3	L5	4569	PSU
3	L5	4570	G
3	L5	4575	G
3	L5	4581	G
3	L5	4584	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4608	G
3	L5	4610	A
3	L5	4626	A
3	L5	4627	U
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A

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Mol	Chain	Res	Type
3	L5	4657	U
3	L5	4670	C
3	L5	4672	A
3	L5	4691	A
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4711	C
3	L5	4721	G
3	L5	4730	C
3	L5	4731	G
3	L5	4732	G
3	L5	4733	C
3	L5	4738	C
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4773	C
3	L5	4775	C
3	L5	4776	G
3	L5	4859	C
3	L5	4860	G
3	L5	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4882	U
3	L5	4883	C
3	L5	4896	G
3	L5	4898	G
3	L5	4900	C
3	L5	4901	G
3	L5	4909	A
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C

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Mol	Chain	Res	Type
3	L5	4928	C
3	L5	4930	C
3	L5	4934	A
3	L5	4943	A
3	L5	4954	G
3	L5	4955	A
3	L5	4957	C
3	L5	4966	A
3	L5	4976	U
3	L5	4979	A
3	L5	4985	U
3	L5	4988	U
3	L5	4990	C
3	L5	4991	U
3	L5	4993	G
3	L5	4994	G
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5026	U
3	L5	5028	G
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5055	G
3	L5	5058	A
3	L5	5061	A
3	L5	5062	G
3	L5	5066	U
4	L7	2	U
4	L7	3	C
4	L7	33	U
4	L7	42	A
4	L7	53	U
4	L7	63	C
4	L7	64	G
4	L7	76	U
4	L7	97	G
4	L7	100	A

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Mol	Chain	Res	Type
4	L7	106	G
4	L7	110	G
4	L7	120	U
83	mR	37	A
84	At	14	A
84	At	16	H2U
84	At	17	C
84	At	18	G
84	At	19	G
84	At	20	H2U
84	At	22	G
84	At	34	G
84	At	36	A
84	At	45	U
84	At	47	U
84	At	48	C
84	At	57	G
84	At	59	U
84	At	61	C
84	At	75	C
84	At	76	A
85	Pt	2	G
85	Pt	8	4SU
85	Pt	9	G
85	Pt	13	C
85	Pt	16	C
85	Pt	18	C
85	Pt	19	G
85	Pt	20	G
85	Pt	21	H2U
85	Pt	22	A
85	Pt	32	G
85	Pt	47	G7M
85	Pt	48	U
85	Pt	49	C
85	Pt	71	G
85	Pt	72	C
85	Pt	77	A

All (84) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	S2	3	C
1	S2	73	C
1	S2	127	C
1	S2	198	U
1	S2	203	G
1	S2	293	C
1	S2	370	G
1	S2	407	G
1	S2	417	C
1	S2	448	A
1	S2	500	A
1	S2	541	U
1	S2	553	U
1	S2	607	U
1	S2	868	G
1	S2	869	A
1	S2	1016	U
1	S2	1165	G
1	S2	1194	A
1	S2	1312	G
1	S2	1313	A
1	S2	1433	C
1	S2	1446	A
1	S2	1493	C
1	S2	1598	G
1	S2	1601	A
1	S2	1679	A
1	S2	1682	C
1	S2	1698	C
2	L8	51	U
2	L8	84	A
2	L8	85	U
3	L5	85	G
3	L5	157	U
3	L5	158	A
3	L5	178	C
3	L5	187	U
3	L5	235	A
3	L5	278	G
3	L5	412	G
3	L5	509	A

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Mol	Chain	Res	Type
3	L5	934	C
3	L5	955	G
3	L5	1199	G
3	L5	1214	C
3	L5	1215	C
3	L5	1268	G
3	L5	1294	A
3	L5	1359	G
3	L5	1419	G
3	L5	1613	A
3	L5	1633	G
3	L5	1677	PSU
3	L5	1698	C
3	L5	1740	C
3	L5	1984	A
3	L5	2042	A
3	L5	2055	G
3	L5	2259	G
3	L5	2313	A
3	L5	2470	C
3	L5	2487	G
3	L5	2587	A
3	L5	2687	U
3	L5	2696	A
3	L5	2759	G
3	L5	2903	G
3	L5	3614	G
3	L5	3672	G
3	L5	3809	G
3	L5	3876	A
3	L5	3952	A
3	L5	4049	U
3	L5	4115	G
3	L5	4452	U
3	L5	4464	A
3	L5	4626	A
3	L5	4699	U
3	L5	4909	A
3	L5	4925	U
3	L5	4927	G
3	L5	5022	U
3	L5	5023	C

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Mol	Chain	Res	Type
3	L5	5054	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3944	3	23,26,27	1.25	4 (17%)	32,38,41	2.09	7 (21%)
1	PSU	S2	119	1	18,21,22	1.47	4 (22%)	21,30,33	2.12	4 (19%)
3	A2M	L5	1871	3	22,25,26	1.49	5 (22%)	30,36,39	2.12	10 (33%)
1	B8N	S2	1248	1	25,29,30	0.92	1 (4%)	28,42,45	1.82	6 (21%)
3	OMG	L5	3744	3	23,26,27	1.25	4 (17%)	32,38,41	2.07	7 (21%)
3	A2M	L5	3785	3	22,25,26	1.43	5 (22%)	30,36,39	2.33	12 (40%)
3	OMG	L5	4228	3	23,26,27	1.19	4 (17%)	32,38,41	1.96	6 (18%)
3	A2M	L5	3723	3	22,25,26	1.46	4 (18%)	30,36,39	1.98	10 (33%)
1	OMU	S2	428	1	19,22,23	1.24	3 (15%)	25,31,34	1.93	6 (24%)
1	PSU	S2	815	1	18,21,22	1.41	2 (11%)	21,30,33	2.11	4 (19%)
1	A2M	S2	159	1	22,25,26	1.50	4 (18%)	30,36,39	1.99	9 (30%)
1	A2M	S2	512	1	22,25,26	1.48	4 (18%)	30,36,39	2.11	9 (30%)
3	PSU	L5	1792	3	18,21,22	1.56	4 (22%)	21,30,33	2.11	4 (19%)
1	A2M	S2	468	1	22,25,26	1.47	4 (18%)	30,36,39	2.11	9 (30%)
1	A2M	S2	99	1,89	22,25,26	1.44	4 (18%)	30,36,39	2.17	8 (26%)
3	PSU	L5	3764	3,89	18,21,22	1.58	4 (22%)	21,30,33	2.14	6 (28%)
86	MLY	EF	55	86	9,10,11	0.51	0	6,11,13	0.88	0
3	OMG	L5	3627	3	23,26,27	1.18	4 (17%)	32,38,41	2.04	6 (18%)
1	G7M	S2	1639	1,85	23,26,27	2.43	5 (21%)	34,39,42	3.13	12 (35%)
3	PSU	L5	4532	3	18,21,22	1.55	4 (22%)	21,30,33	2.16	4 (19%)
85	G7M	Pt	47	85	23,26,27	1.86	2 (8%)	34,39,42	1.10	1 (2%)
1	PSU	S2	918	1	18,21,22	1.52	3 (16%)	21,30,33	2.31	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	S2	27	1	22,25,26	1.46	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	S2	651	1	18,21,22	1.40	3 (16%)	21,30,33	2.06	4 (19%)
3	OMG	L5	1522	3	23,26,27	1.19	4 (17%)	32,38,41	1.97	6 (18%)
1	OMG	S2	601	1	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
3	PSU	L5	4531	3	18,21,22	1.41	3 (16%)	21,30,33	2.21	5 (23%)
3	PSU	L5	3695	3	18,21,22	1.40	3 (16%)	21,30,33	2.04	3 (14%)
84	4SU	At	8	84	18,21,22	1.85	4 (22%)	25,30,33	2.33	5 (20%)
1	OMG	S2	1490	1,89	23,26,27	1.27	3 (13%)	32,38,41	1.99	7 (21%)
1	OMC	S2	1703	1,89	19,22,23	0.78	0	25,31,34	0.75	0
3	PSU	L5	1677	3	18,21,22	1.52	4 (22%)	21,30,33	2.16	5 (23%)
3	PSU	L5	2839	3	18,21,22	1.37	4 (22%)	21,30,33	2.12	4 (19%)
1	PSU	S2	1367	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
3	A2M	L5	3760	3	22,25,26	1.52	5 (22%)	30,36,39	2.29	13 (43%)
39	V5N	LA	216	39	8,11,12	1.49	1 (12%)	8,14,16	1.82	1 (12%)
3	PSU	L5	4312	3	18,21,22	1.41	4 (22%)	21,30,33	2.10	4 (19%)
3	A2M	L5	3867	3	22,25,26	1.49	4 (18%)	30,36,39	2.04	8 (26%)
79	M3L	Lm	98	79	10,11,12	0.37	0	9,14,16	0.10	0
29	AME	SV	1	29	9,10,11	3.32	2 (22%)	9,11,13	3.86	3 (33%)
1	OMU	S2	172	1	19,22,23	1.33	4 (21%)	25,31,34	2.00	6 (24%)
3	OMC	L5	2804	3	19,22,23	0.82	0	25,31,34	0.79	0
66	SAC	Lr	2	66	7,8,9	3.74	2 (28%)	7,9,11	4.56	5 (71%)
3	PSU	L5	1582	3	18,21,22	1.51	4 (22%)	21,30,33	2.12	6 (28%)
3	OMG	L5	2364	3	23,26,27	1.18	3 (13%)	32,38,41	1.97	6 (18%)
3	A2M	L5	1534	3,89	22,25,26	1.48	5 (22%)	30,36,39	2.08	7 (23%)
1	PSU	S2	1004	1	18,21,22	1.40	4 (22%)	21,30,33	2.07	3 (14%)
1	A2M	S2	484	1	22,25,26	1.49	5 (22%)	30,36,39	2.05	7 (23%)
3	OMG	L5	4618	3	23,26,27	1.28	4 (17%)	32,38,41	2.03	7 (21%)
86	M3L	EF	318	86	10,11,12	0.43	0	9,14,16	0.13	0
3	OMC	L5	2365	3,89	19,22,23	0.80	0	25,31,34	0.76	0
1	PSU	S2	1243	1	18,21,22	1.42	2 (11%)	21,30,33	2.13	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
1	PSU	S2	1445	1	18,21,22	1.37	2 (11%)	21,30,33	2.18	5 (23%)
1	PSU	S2	109	1	18,21,22	1.53	4 (22%)	21,30,33	2.19	3 (14%)
3	PSU	L5	4552	3	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
3	PSU	L5	2508	3	18,21,22	1.40	3 (16%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3899	3	23,26,27	1.22	4 (17%)	32,38,41	2.02	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	649	1	18,21,22	1.51	4 (22%)	21,30,33	2.11	3 (14%)
1	PSU	S2	1238	1	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
1	A2M	S2	576	1	22,25,26	1.53	5 (22%)	30,36,39	2.00	10 (33%)
3	A2M	L5	3825	3	22,25,26	1.46	4 (18%)	30,36,39	2.08	10 (33%)
52	V5N	La	39	52	8,11,12	1.41	1 (12%)	8,14,16	1.70	2 (25%)
1	OMG	S2	683	1	23,26,27	1.21	4 (17%)	32,38,41	2.02	7 (21%)
1	PSU	S2	1347	1	18,21,22	1.50	4 (22%)	21,30,33	2.12	3 (14%)
1	PSU	S2	406	1	18,21,22	1.55	5 (27%)	21,30,33	2.10	4 (19%)
3	OMU	L5	3925	3	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
3	A2M	L5	3830	3	22,25,26	1.47	5 (22%)	30,36,39	2.15	10 (33%)
3	OMC	L5	4456	3	19,22,23	0.93	1 (5%)	25,31,34	1.09	2 (8%)
3	OMG	L5	1625	3	23,26,27	1.22	3 (13%)	32,38,41	2.01	6 (18%)
3	PSU	L5	4361	3	18,21,22	1.60	5 (27%)	21,30,33	2.20	6 (28%)
85	PSU	Pt	56	85	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
1	4AC	S2	1842	1	21,24,25	0.99	1 (4%)	28,34,37	1.17	4 (14%)
1	OMU	S2	1442	1,89	19,22,23	1.27	3 (15%)	25,31,34	1.88	4 (16%)
3	PSU	L5	3715	3	18,21,22	1.51	4 (22%)	21,30,33	2.04	5 (23%)
3	PSU	L5	1860	3	18,21,22	1.56	4 (22%)	21,30,33	2.09	5 (23%)
3	PSU	L5	3762	3	18,21,22	1.46	4 (22%)	21,30,33	2.21	5 (23%)
1	PSU	S2	573	1	18,21,22	1.45	3 (16%)	21,30,33	2.10	4 (19%)
3	OMG	L5	4499	3	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
1	OMU	S2	116	1	19,22,23	1.35	3 (15%)	25,31,34	1.76	5 (20%)
3	PSU	L5	5010	3	18,21,22	1.41	3 (16%)	21,30,33	2.09	4 (19%)
3	PSU	L5	4420	3	18,21,22	1.37	3 (16%)	21,30,33	1.97	4 (19%)
1	A2M	S2	668	1,89	22,25,26	1.47	4 (18%)	30,36,39	2.04	10 (33%)
3	A2M	L5	4590	3	22,25,26	1.48	5 (22%)	30,36,39	2.13	10 (33%)
1	PSU	S2	34	1	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	2415	3	19,22,23	1.38	4 (21%)	25,31,34	1.87	5 (20%)
3	PSU	L5	3884	3	18,21,22	1.64	4 (22%)	21,30,33	2.09	3 (14%)
1	OMC	S2	174	1	19,22,23	0.86	0	25,31,34	1.00	2 (8%)
1	OMU	S2	1804	1	19,22,23	1.27	3 (15%)	25,31,34	1.88	5 (20%)
3	UR3	L5	4530	3	19,22,23	0.90	0	26,32,35	1.92	4 (15%)
1	A2M	S2	1031	1	22,25,26	1.48	5 (22%)	30,36,39	2.03	9 (30%)
3	OMU	L5	4227	3	19,22,23	1.24	3 (15%)	25,31,34	1.82	4 (16%)
85	H2U	Pt	21	85	18,21,22	1.06	2 (11%)	19,30,33	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	866	1	18,21,22	1.45	3 (16%)	21,30,33	2.17	4 (19%)
3	PSU	L5	3920	3,89	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
3	PSU	L5	2843	3	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
3	A2M	L5	2363	3,89	22,25,26	1.49	5 (22%)	30,36,39	2.03	9 (30%)
3	PSU	L5	4500	3	18,21,22	1.42	2 (11%)	21,30,33	2.09	3 (14%)
84	H2U	At	20	84	18,21,22	1.04	2 (11%)	19,30,33	1.02	2 (10%)
2	OMG	L8	75	2	23,26,27	1.19	3 (13%)	32,38,41	2.14	7 (21%)
1	A2M	S2	166	1	22,25,26	1.47	4 (18%)	30,36,39	2.29	8 (26%)
3	OMG	L5	4392	3	23,26,27	1.30	4 (17%)	32,38,41	2.00	7 (21%)
3	OMG	L5	4370	3	23,26,27	1.18	3 (13%)	32,38,41	2.00	6 (18%)
1	PSU	S2	681	1	18,21,22	1.41	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
3	OMG	L5	2876	3	23,26,27	1.22	3 (13%)	32,38,41	2.04	6 (18%)
3	A2M	L5	3718	3	22,25,26	1.48	4 (18%)	30,36,39	1.95	9 (30%)
2	PSU	L8	69	2	18,21,22	1.60	5 (27%)	21,30,33	2.39	5 (23%)
3	PSU	L5	4689	3	18,21,22	1.47	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	3768	3	18,21,22	1.47	4 (22%)	21,30,33	2.04	4 (19%)
68	MLZ	Lb	5	68	8,9,10	0.35	0	4,9,11	0.19	0
3	PSU	L5	1744	3,88	18,21,22	1.50	4 (22%)	21,30,33	2.11	3 (14%)
3	OMU	L5	2837	3	19,22,23	1.29	3 (15%)	25,31,34	1.91	5 (20%)
3	5MC	L5	3782	3,89	19,22,23	1.55	3 (15%)	26,32,35	1.15	3 (11%)
3	OMC	L5	2824	3	19,22,23	0.79	0	25,31,34	0.82	0
3	PSU	L5	4636	3	18,21,22	1.57	4 (22%)	21,30,33	2.44	6 (28%)
1	PSU	S2	1177	1	18,21,22	1.40	3 (16%)	21,30,33	2.03	4 (19%)
3	OMC	L5	3701	3,88	19,22,23	0.90	0	25,31,34	1.07	0
1	PSU	S2	814	1	18,21,22	1.39	3 (16%)	21,30,33	2.12	4 (19%)
1	PSU	S2	863	1	18,21,22	1.49	4 (22%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1683	3,88	18,21,22	1.53	4 (22%)	21,30,33	1.93	3 (14%)
1	OMC	S2	462	1	19,22,23	0.87	0	25,31,34	0.93	1 (4%)
84	H2U	At	16	84	18,21,22	0.99	2 (11%)	19,30,33	0.82	1 (5%)
2	PSU	L8	55	2	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	S2	36	1	18,21,22	1.39	3 (16%)	21,30,33	2.13	4 (19%)
1	OMC	S2	1391	1	19,22,23	0.82	0	25,31,34	0.82	0
3	PSU	L5	3770	3	18,21,22	1.51	4 (22%)	21,30,33	2.23	5 (23%)
3	PSU	L5	4431	3	18,21,22	1.40	3 (16%)	21,30,33	2.13	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	L8	14	3,2	19,22,23	1.46	4 (21%)	25,31,34	2.05	5 (20%)
1	UY1	S2	1326	1,89	19,22,23	1.39	3 (15%)	21,31,34	2.25	4 (19%)
1	PSU	S2	609	1	18,21,22	1.50	4 (22%)	21,30,33	1.98	3 (14%)
1	MA6	S2	1850	1	23,26,27	1.48	4 (17%)	33,38,41	2.03	10 (30%)
3	PSU	L5	3844	3	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
3	A2M	L5	1326	3	22,25,26	1.47	4 (18%)	30,36,39	2.01	7 (23%)
3	OMC	L5	3869	3	19,22,23	0.89	1 (5%)	25,31,34	1.04	0
81	MLZ	Lo	53	81	8,9,10	0.78	0	4,9,11	0.67	0
3	OMC	L5	3887	3	19,22,23	0.81	0	25,31,34	0.83	0
3	A2M	L5	4571	3	22,25,26	1.45	3 (13%)	30,36,39	2.04	7 (23%)
3	1MA	L5	1322	3,89	21,25,26	1.38	4 (19%)	30,37,40	1.71	6 (20%)
85	4SU	Pt	8	85	18,21,22	2.07	4 (22%)	25,30,33	2.33	4 (16%)
3	A2M	L5	400	3	22,25,26	1.46	5 (22%)	30,36,39	2.11	9 (30%)
1	PSU	S2	1136	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	4 (19%)
1	OMU	S2	121	1	19,22,23	1.43	3 (15%)	25,31,34	1.88	5 (20%)
1	PSU	S2	218	1	18,21,22	1.46	3 (16%)	21,30,33	2.17	4 (19%)
3	PSU	L5	3729	3	18,21,22	1.53	5 (27%)	21,30,33	2.19	4 (19%)
1	OMG	S2	509	1	23,26,27	1.31	4 (17%)	32,38,41	2.08	7 (21%)
1	PSU	S2	1625	1	18,21,22	1.42	3 (16%)	21,30,33	2.17	3 (14%)
3	PSU	L5	4293	3	18,21,22	1.44	4 (22%)	21,30,33	2.12	4 (19%)
86	M3L	EF	79	86	10,11,12	0.55	0	9,14,16	0.51	0
3	PSU	L5	4353	3	18,21,22	1.54	4 (22%)	21,30,33	2.18	3 (14%)
3	PSU	L5	4569	3	18,21,22	1.49	3 (16%)	21,30,33	2.23	5 (23%)
20	HY3	SX	62	88,20	7,8,9	1.43	1 (14%)	7,10,12	1.28	1 (14%)
84	PSU	At	32	84	18,21,22	1.47	4 (22%)	21,30,33	2.18	4 (19%)
86	M3L	EF	36	86	10,11,12	0.53	0	9,14,16	0.46	0
3	A2M	L5	2401	3	22,25,26	1.47	5 (22%)	30,36,39	2.15	9 (30%)
1	PSU	S2	296	1	18,21,22	1.47	4 (22%)	21,30,33	2.17	3 (14%)
3	UY1	L5	3818	3,89	19,22,23	1.43	4 (21%)	21,31,34	2.00	4 (19%)
3	OMG	L5	1316	3	23,26,27	1.22	3 (13%)	32,38,41	2.00	6 (18%)
3	PSU	L5	1536	3	18,21,22	1.43	4 (22%)	21,30,33	2.06	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.46	5 (22%)	30,36,39	2.11	10 (33%)
3	PSU	L5	4521	3,89	18,21,22	1.54	5 (27%)	21,30,33	2.43	6 (28%)
3	OMG	L5	3792	3	23,26,27	1.19	3 (13%)	32,38,41	2.02	6 (18%)
3	PSU	L5	3639	3	18,21,22	1.45	4 (22%)	21,30,33	2.14	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OMC	Pt	33	85	19,22,23	0.92	1 (5%)	25,31,34	1.00	1 (4%)
3	PSU	L5	4296	3	18,21,22	1.38	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4498	3	19,22,23	1.25	3 (15%)	25,31,34	1.86	5 (20%)
3	PSU	L5	4493	3,88	18,21,22	1.43	4 (22%)	21,30,33	2.06	4 (19%)
3	OMG	L5	4623	3	23,26,27	1.22	3 (13%)	32,38,41	2.06	7 (21%)
3	A2M	L5	3724	3	22,25,26	1.45	4 (18%)	30,36,39	2.05	10 (33%)
1	OMG	S2	1328	1	23,26,27	1.26	3 (13%)	32,38,41	2.13	7 (21%)
3	PSU	L5	4579	3	18,21,22	1.61	6 (33%)	21,30,33	2.19	3 (14%)
1	PSU	S2	822	1	18,21,22	1.40	3 (16%)	21,30,33	2.36	5 (23%)
1	PSU	S2	1174	1,89	18,21,22	1.52	3 (16%)	21,30,33	2.20	5 (23%)
1	MA6	S2	1851	1	23,26,27	1.45	5 (21%)	33,38,41	2.04	10 (30%)
1	6MZ	S2	1832	1,89	22,25,26	1.49	5 (22%)	29,36,39	2.14	9 (31%)
3	PSU	L5	4442	3	18,21,22	1.55	4 (22%)	21,30,33	2.32	5 (23%)
3	PSU	L5	5001	3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	OMU	S2	627	1	19,22,23	1.31	3 (15%)	25,31,34	1.97	5 (20%)
3	OMC	L5	3841	3	19,22,23	0.78	0	25,31,34	0.97	2 (8%)
84	PSU	At	39	84	18,21,22	1.51	4 (22%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.53	4 (22%)	21,30,33	2.24	4 (19%)
3	PSU	L5	3853	3,89	18,21,22	1.43	4 (22%)	21,30,33	1.98	3 (14%)
3	OMC	L5	2351	3	19,22,23	0.94	1 (5%)	25,31,34	0.84	1 (4%)
3	PSU	L5	4423	3	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
3	A2M	L5	4523	3,89	22,25,26	1.44	4 (18%)	30,36,39	2.14	8 (26%)
3	OMU	L5	4306	3	19,22,23	1.29	3 (15%)	25,31,34	1.77	4 (16%)
3	OMG	L5	4637	3,88	23,26,27	1.28	4 (17%)	32,38,41	2.04	7 (21%)
40	HIC	LB	245	40	10,11,12	1.42	1 (10%)	9,14,16	1.30	2 (22%)
1	PSU	S2	105	1	18,21,22	1.54	4 (22%)	21,30,33	2.23	4 (19%)
3	A2M	L5	398	3	22,25,26	1.57	4 (18%)	30,36,39	2.02	7 (23%)
3	PSU	L5	4403	3	18,21,22	1.62	5 (27%)	21,30,33	2.32	5 (23%)
1	OMG	S2	436	1	23,26,27	1.26	3 (13%)	32,38,41	2.21	8 (25%)
3	PSU	L5	3734	3	18,21,22	1.50	4 (22%)	21,30,33	2.06	4 (19%)
1	A2M	S2	590	1	22,25,26	1.45	5 (22%)	30,36,39	2.10	7 (23%)
1	OMG	S2	867	1	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
3	OMC	L5	3808	3	19,22,23	0.93	0	25,31,34	1.06	1 (4%)
1	PSU	S2	1692	1	18,21,22	1.40	4 (22%)	21,30,33	2.06	4 (19%)
3	PSU	L5	2632	3	18,21,22	1.41	2 (11%)	21,30,33	2.01	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	2787	3	22,25,26	1.45	5 (22%)	30,36,39	2.05	9 (30%)
3	6MZ	L5	4220	3	22,25,26	1.41	5 (22%)	29,36,39	2.18	9 (31%)
1	PSU	S2	1643	1,89	18,21,22	1.39	4 (22%)	21,30,33	2.21	5 (23%)
3	5MC	L5	4447	3,88	19,22,23	1.56	3 (15%)	26,32,35	1.28	4 (15%)
3	OMG	L5	4494	3	23,26,27	1.28	4 (17%)	32,38,41	2.08	7 (21%)
3	OMU	L5	4620	3	19,22,23	1.39	3 (15%)	25,31,34	1.98	8 (32%)
84	MIA	At	37	84	28,31,32	2.47	7 (25%)	38,44,47	2.78	14 (36%)
1	PSU	S2	1081	1	18,21,22	1.46	5 (27%)	21,30,33	2.05	4 (19%)
1	PSU	S2	1239	1	18,21,22	1.39	3 (16%)	21,30,33	2.05	3 (14%)
3	OMC	L5	1881	3,89	19,22,23	0.91	0	25,31,34	1.13	2 (8%)
1	PSU	S2	686	1	18,21,22	1.51	4 (22%)	21,30,33	2.20	3 (14%)
1	PSU	S2	1232	1	18,21,22	1.57	4 (22%)	21,30,33	2.19	4 (19%)
1	A2M	S2	1678	1	22,25,26	1.48	4 (18%)	30,36,39	2.01	9 (30%)
3	OMC	L5	2422	3,89	19,22,23	0.87	0	25,31,34	1.07	2 (8%)
84	G7M	At	46	84	23,26,27	1.90	2 (8%)	34,39,42	1.10	1 (2%)
1	PSU	S2	1244	1	18,21,22	1.46	3 (16%)	21,30,33	2.18	4 (19%)
6	SAC	SA	2	6	7,8,9	3.45	2 (28%)	7,9,11	5.30	5 (71%)
1	PSU	S2	93	1	18,21,22	1.54	4 (22%)	21,30,33	2.20	4 (19%)
1	OMU	S2	354	1	19,22,23	1.45	3 (15%)	25,31,34	2.09	6 (24%)
1	PSU	S2	572	1	18,21,22	1.43	4 (22%)	21,30,33	1.98	4 (19%)
1	OMC	S2	517	1	19,22,23	0.92	0	25,31,34	1.00	2 (8%)
1	PSU	S2	966	1	18,21,22	1.46	2 (11%)	21,30,33	2.09	4 (19%)
1	4AC	S2	1337	1	21,24,25	1.17	3 (14%)	28,34,37	1.26	3 (10%)
3	OMG	L5	2424	3	23,26,27	1.32	3 (13%)	32,38,41	1.91	6 (18%)
3	PSU	L5	4457	3	18,21,22	1.53	4 (22%)	21,30,33	2.27	6 (28%)
3	PSU	L5	4471	3	18,21,22	1.49	3 (16%)	21,30,33	1.97	5 (23%)
1	A2M	S2	1383	1	22,25,26	1.46	4 (18%)	30,36,39	2.10	10 (33%)
1	PSU	S2	801	1	18,21,22	1.52	4 (22%)	21,30,33	1.99	4 (19%)
3	OMC	L5	1340	3	19,22,23	0.90	1 (5%)	25,31,34	0.84	0
3	PSU	L5	1779	3	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
1	OMG	S2	644	1	23,26,27	1.27	4 (17%)	32,38,41	2.03	7 (21%)
3	PSU	L5	4628	3	18,21,22	1.49	4 (22%)	21,30,33	2.40	5 (23%)
3	PSU	L5	4673	3,89	18,21,22	1.47	3 (16%)	21,30,33	1.98	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
1	OMG	S2	1447	1	23,26,27	1.24	3 (13%)	32,38,41	2.22	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	4196	3,85	23,26,27	1.30	4 (17%)	32,38,41	2.00	7 (21%)
3	A2M	L5	2815	3,89	22,25,26	1.49	4 (18%)	30,36,39	1.99	7 (23%)
3	OMC	L5	2861	3	19,22,23	0.80	0	25,31,34	0.83	1 (4%)
1	PSU	S2	1056	1	18,21,22	1.45	3 (16%)	21,30,33	2.25	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.43	4 (22%)	21,30,33	2.04	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.89	0	25,31,34	1.01	0
1	OMU	S2	1288	1	19,22,23	1.31	3 (15%)	25,31,34	1.84	5 (20%)
3	PSU	L5	3851	3	18,21,22	1.40	4 (22%)	21,30,33	2.08	5 (23%)
3	PSU	L5	3758	3	18,21,22	1.54	4 (22%)	21,30,33	2.26	5 (23%)
3	PSU	L5	4576	3	18,21,22	1.38	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	3637	3,89	18,21,22	1.51	3 (16%)	21,30,33	2.28	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	3	-	0/9/27/28	0/3/3/3
1	B8N	S2	1248	1	-	6/16/34/35	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	512	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	99	1,89	-	1/9/27/28	0/3/3/3
3	PSU	L5	3764	3,89	-	0/7/25/26	0/2/2/2
86	MLY	EF	55	86	-	1/8/9/11	-
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
1	G7M	S2	1639	1,85	-	0/7/25/26	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
85	G7M	Pt	47	85	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
84	4SU	At	8	84	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	1,89	-	2/9/27/28	0/3/3/3
1	OMC	S2	1703	1,89	-	0/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3760	3	-	2/9/27/28	0/3/3/3
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
79	M3L	Lm	98	79	-	0/9/10/12	-
29	AME	SV	1	29	-	2/9/10/12	-
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
66	SAC	Lr	2	66	-	3/7/8/10	-
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	1534	3,89	-	1/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
86	M3L	EF	318	86	-	0/9/10/12	-
3	OMC	L5	2365	3,89	-	0/9/27/28	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	V5N	La	39	52	-	0/9/10/12	0/1/1/1
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
85	PSU	Pt	56	85	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	OMU	S2	1442	1,89	-	0/9/27/28	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	4/7/25/26	0/2/2/2
1	A2M	S2	668	1,89	-	3/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	174	1	-	1/9/27/28	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
85	H2U	Pt	21	85	-	5/7/38/39	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3,89	-	0/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3,89	-	0/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	2/7/25/26	0/2/2/2
84	H2U	At	20	84	-	1/7/38/39	0/2/2/2
2	OMG	L8	75	2	-	1/9/27/28	0/3/3/3
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
68	MLZ	Lb	5	68	-	5/7/8/10	-
3	PSU	L5	1744	3,88	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	3,89	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3,88	-	4/9/27/28	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3,88	-	0/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
84	H2U	At	16	84	-	7/7/38/39	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
2	OMU	L8	14	3,2	-	1/9/27/28	0/2/2/2
1	UY1	S2	1326	1,89	-	1/9/27/28	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
3	PSU	L5	3844	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
81	MLZ	Lo	53	81	-	4/7/8/10	-
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	1MA	L5	1322	3,89	-	2/7/25/26	0/3/3/3
85	4SU	Pt	8	85	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
86	M3L	EF	79	86	-	3/9/10/12	-
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	2/7/25/26	0/2/2/2
20	HY3	SX	62	88,20	-	1/1/12/14	0/1/1/1
84	PSU	At	32	84	-	0/7/25/26	0/2/2/2
86	M3L	EF	36	86	-	0/9/10/12	-
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3,89	-	3/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4521	3,89	-	2/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
85	OMC	Pt	33	85	-	0/9/27/28	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4493	3,88	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
1	OMG	S2	1328	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1174	1,89	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	1/11/29/30	0/3/3/3
1	6MZ	S2	1832	1,89	-	2/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	4/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
84	PSU	At	39	84	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	3,89	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,89	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4306	3	-	2/9/27/28	0/2/2/2
3	OMG	L5	4637	3,88	-	2/9/27/28	0/3/3/3
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	2/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	2/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1643	1,89	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3,88	-	4/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
84	MIA	At	37	84	-	2/15/33/34	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	3,89	-	0/9/27/28	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
3	OMC	L5	2422	3,89	-	3/9/27/28	0/2/2/2
84	G7M	At	46	84	-	0/7/25/26	0/3/3/3
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
6	SAC	SA	2	6	-	2/7/8/10	-
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3,89	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	4196	3,85	-	1/9/27/28	0/3/3/3
3	A2M	L5	2815	3,89	-	1/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	1288	1	-	3/9/27/28	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3,89	-	0/7/25/26	0/2/2/2

All (769) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	8.97	1.43	1.23
66	Lr	2	SAC	OAC-C1A	8.86	1.43	1.23
84	At	37	MIA	C2-S10	-8.64	1.68	1.75
6	SA	2	SAC	OAC-C1A	8.21	1.41	1.23
84	At	46	G7M	C8-N7	7.56	1.46	1.33
1	S2	1639	G7M	C8-N7	7.49	1.45	1.33
85	Pt	47	G7M	C8-N7	7.31	1.45	1.33
84	At	37	MIA	C13-C14	6.64	1.52	1.32
85	Pt	8	4SU	C4-S4	-5.45	1.59	1.68
3	L5	3782	5MC	C5-C4	5.44	1.48	1.44
3	L5	4447	5MC	C5-C4	5.29	1.48	1.44
1	S2	1639	G7M	C5-N7	-5.25	1.33	1.39
84	At	8	4SU	C4-S4	-4.94	1.59	1.68
3	L5	398	A2M	C5-C4	4.87	1.47	1.39
1	S2	576	A2M	C5-C4	4.72	1.47	1.39
1	S2	159	A2M	C5-C4	4.53	1.47	1.39
1	S2	1850	MA6	C5-C4	4.52	1.47	1.39
1	S2	1832	6MZ	C5-C4	4.50	1.47	1.39
1	S2	166	A2M	C5-C4	4.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1851	MA6	C5-C4	4.43	1.47	1.39
3	L5	3718	A2M	C5-C4	4.41	1.47	1.39
3	L5	3830	A2M	C5-C4	4.36	1.46	1.39
1	S2	1031	A2M	C5-C4	4.36	1.46	1.39
3	L5	400	A2M	C5-C4	4.33	1.46	1.39
3	L5	3825	A2M	C5-C4	4.33	1.46	1.39
1	S2	512	A2M	C5-C4	4.32	1.46	1.39
3	L5	1524	A2M	C5-C4	4.30	1.46	1.39
1	S2	590	A2M	C5-C4	4.29	1.46	1.39
3	L5	4523	A2M	C5-C4	4.28	1.46	1.39
3	L5	2363	A2M	C5-C4	4.27	1.46	1.39
3	L5	3724	A2M	C5-C4	4.27	1.46	1.39
3	L5	4571	A2M	C5-C4	4.26	1.46	1.39
3	L5	2815	A2M	C5-C4	4.25	1.46	1.39
3	L5	1534	A2M	C5-C4	4.25	1.46	1.39
3	L5	4590	A2M	C5-C4	4.24	1.46	1.39
1	S2	668	A2M	C5-C4	4.22	1.46	1.39
1	S2	468	A2M	C5-C4	4.21	1.46	1.39
1	S2	484	A2M	C5-C4	4.19	1.46	1.39
1	S2	1383	A2M	C5-C4	4.18	1.46	1.39
3	L5	2787	A2M	C5-C4	4.18	1.46	1.39
3	L5	4220	6MZ	C5-C4	4.17	1.46	1.39
66	Lr	2	SAC	C1A-N	4.16	1.47	1.34
84	At	37	MIA	C5-C4	4.13	1.46	1.39
3	L5	3723	A2M	C5-C4	4.12	1.46	1.39
1	S2	99	A2M	C5-C4	4.11	1.46	1.39
3	L5	3867	A2M	C5-C4	4.10	1.46	1.39
1	S2	1639	G7M	C8-N9	4.10	1.46	1.35
1	S2	1678	A2M	C5-C4	4.10	1.46	1.39
3	L5	3760	A2M	C5-C4	4.09	1.46	1.39
3	L5	2401	A2M	C5-C4	4.07	1.46	1.39
3	L5	3785	A2M	C5-C4	4.05	1.46	1.39
1	S2	27	A2M	C5-C4	4.04	1.46	1.39
85	Pt	8	4SU	C4-N3	-4.03	1.33	1.37
84	At	46	G7M	C8-N9	4.02	1.46	1.35
85	Pt	47	G7M	C8-N9	3.98	1.46	1.35
3	L5	1326	A2M	C5-C4	3.95	1.46	1.39
3	L5	1871	A2M	C5-C4	3.95	1.46	1.39
29	SV	1	AME	CT1-N	3.89	1.46	1.34
1	S2	1639	G7M	C5-C4	3.78	1.47	1.38
1	S2	966	PSU	C6-C5	3.72	1.39	1.35
84	At	8	4SU	C4-N3	-3.55	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L8	69	PSU	C4-N3	-3.54	1.32	1.38
3	L5	4521	PSU	C4-N3	-3.50	1.32	1.38
39	LA	216	V5N	CG-ND1	-3.49	1.34	1.37
2	L8	14	OMU	C4-N3	-3.47	1.32	1.38
20	SX	62	HY3	C3-CA	-3.46	1.51	1.55
1	S2	354	OMU	C4-N3	-3.45	1.32	1.38
1	S2	121	OMU	C4-N3	-3.45	1.32	1.38
3	L5	4403	PSU	C4-N3	-3.44	1.32	1.38
3	L5	3764	PSU	C6-C5	3.44	1.39	1.35
3	L5	4471	PSU	C6-C5	3.44	1.39	1.35
3	L5	3884	PSU	C4-N3	-3.43	1.32	1.38
1	S2	918	PSU	C6-C5	3.43	1.39	1.35
6	SA	2	SAC	C1A-N	3.43	1.45	1.34
85	Pt	8	4SU	C5-C4	-3.40	1.38	1.42
3	L5	1582	PSU	C4-N3	-3.40	1.32	1.38
1	S2	815	PSU	C6-C5	3.39	1.39	1.35
3	L5	1683	PSU	C4-N3	-3.36	1.32	1.38
1	S2	1243	PSU	C6-C5	3.36	1.39	1.35
3	L5	4620	OMU	C4-N3	-3.36	1.32	1.38
3	L5	1860	PSU	C4-N3	-3.35	1.32	1.38
3	L5	4673	PSU	C6-C5	3.35	1.39	1.35
52	La	39	V5N	CG-ND1	-3.34	1.34	1.37
3	L5	4457	PSU	C4-N3	-3.33	1.32	1.38
1	S2	1232	PSU	C4-N3	-3.32	1.32	1.38
3	L5	4636	PSU	C4-N3	-3.32	1.32	1.38
3	L5	3758	PSU	C4-N3	-3.31	1.32	1.38
1	S2	105	PSU	C4-N3	-3.30	1.32	1.38
3	L5	3637	PSU	C4-N3	-3.29	1.32	1.38
3	L5	4579	PSU	C4-N3	-3.29	1.32	1.38
3	L5	4431	PSU	C6-C5	3.29	1.38	1.35
3	L5	4361	PSU	C4-N3	-3.29	1.32	1.38
85	Pt	56	PSU	C6-C5	3.28	1.38	1.35
1	S2	573	PSU	C4-N3	-3.28	1.32	1.38
3	L5	4532	PSU	C4-N3	-3.27	1.32	1.38
1	S2	1174	PSU	C6-C5	3.26	1.38	1.35
3	L5	1683	PSU	C6-C5	3.25	1.38	1.35
3	L5	3734	PSU	C6-C5	3.25	1.38	1.35
1	S2	1337	4AC	C4-N4	-3.25	1.35	1.39
2	L8	14	OMU	C2-N3	-3.24	1.32	1.38
3	L5	4628	PSU	C6-C5	3.24	1.38	1.35
3	L5	1862	PSU	C4-N3	-3.24	1.32	1.38
1	S2	1625	PSU	C6-C5	3.22	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C4-N3	-3.21	1.32	1.38
3	L5	2415	OMU	C4-N3	-3.21	1.33	1.38
3	L5	2632	PSU	C6-C5	3.21	1.38	1.35
1	S2	406	PSU	C4-N3	-3.21	1.32	1.38
1	S2	1347	PSU	C4-N3	-3.20	1.32	1.38
3	L5	4569	PSU	C6-C5	3.20	1.38	1.35
84	At	39	PSU	C4-N3	-3.20	1.32	1.38
1	S2	1326	UY1	C4-N3	-3.19	1.32	1.38
1	S2	801	PSU	C6-C5	3.19	1.38	1.35
3	L5	3637	PSU	C6-C5	3.19	1.38	1.35
1	S2	1174	PSU	C4-N3	-3.19	1.32	1.38
1	S2	1056	PSU	C6-C5	3.19	1.38	1.35
3	L5	4531	PSU	C4-N3	-3.18	1.32	1.38
3	L5	4442	PSU	C4-N3	-3.17	1.32	1.38
1	S2	866	PSU	C4-N3	-3.17	1.32	1.38
1	S2	1445	PSU	C6-C5	3.17	1.38	1.35
1	S2	93	PSU	C4-N3	-3.16	1.32	1.38
1	S2	509	OMG	C6-N1	-3.16	1.32	1.38
1	S2	218	PSU	C4-N3	-3.16	1.32	1.38
3	L5	4500	PSU	C6-C5	3.15	1.38	1.35
3	L5	3715	PSU	C4-N3	-3.15	1.32	1.38
3	L5	4353	PSU	C4-N3	-3.15	1.32	1.38
1	S2	1239	PSU	C6-C5	3.15	1.38	1.35
3	L5	4689	PSU	C4-N3	-3.14	1.33	1.38
1	S2	1232	PSU	C6-C5	3.14	1.38	1.35
1	S2	651	PSU	C6-C5	3.13	1.38	1.35
1	S2	109	PSU	C4-N3	-3.13	1.33	1.38
3	L5	3770	PSU	C4-N3	-3.13	1.33	1.38
3	L5	5010	PSU	C6-C5	3.12	1.38	1.35
1	S2	609	PSU	C4-N3	-3.12	1.33	1.38
1	S2	1244	PSU	C4-N3	-3.12	1.33	1.38
1	S2	649	PSU	C4-N3	-3.12	1.33	1.38
1	S2	572	PSU	C6-C5	3.12	1.38	1.35
3	L5	1792	PSU	C4-N3	-3.12	1.33	1.38
1	S2	36	PSU	C6-C5	3.11	1.38	1.35
3	L5	4628	PSU	C4-N3	-3.11	1.33	1.38
1	S2	801	PSU	C4-N3	-3.11	1.33	1.38
1	S2	686	PSU	C6-C5	3.11	1.38	1.35
3	L5	1744	PSU	C4-N3	-3.10	1.33	1.38
3	L5	2424	OMG	C6-N1	-3.10	1.33	1.38
3	L5	4673	PSU	C4-N3	-3.09	1.33	1.38
3	L5	3639	PSU	C4-N3	-3.09	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L8	55	PSU	C6-C5	3.09	1.38	1.35
1	S2	1056	PSU	C4-N3	-3.08	1.33	1.38
1	S2	109	PSU	C6-C5	3.08	1.38	1.35
3	L5	2815	A2M	C5-N7	-3.07	1.33	1.39
1	S2	1177	PSU	C6-C5	3.06	1.38	1.35
3	L5	4293	PSU	C6-C5	3.06	1.38	1.35
3	L5	4392	OMG	C6-N1	-3.06	1.33	1.38
3	L5	4569	PSU	C4-N3	-3.05	1.33	1.38
84	At	32	PSU	C4-N3	-3.05	1.33	1.38
84	At	39	PSU	C6-C5	3.04	1.38	1.35
3	L5	3768	PSU	C4-N3	-3.04	1.33	1.38
3	L5	3768	PSU	C6-C5	3.04	1.38	1.35
1	S2	918	PSU	C4-N3	-3.03	1.33	1.38
3	L5	3920	PSU	C6-C5	3.03	1.38	1.35
1	S2	119	PSU	C4-N3	-3.03	1.33	1.38
1	S2	172	OMU	C4-N3	-3.03	1.33	1.38
3	L5	1536	PSU	C4-N3	-3.03	1.33	1.38
3	L5	1792	PSU	C6-C5	3.02	1.38	1.35
3	L5	3844	PSU	C4-N3	-3.02	1.33	1.38
3	L5	3734	PSU	C4-N3	-3.02	1.33	1.38
3	L5	4637	OMG	C6-N1	-3.02	1.33	1.38
1	S2	1238	PSU	C6-C5	3.02	1.38	1.35
3	L5	4493	PSU	C4-N3	-3.01	1.33	1.38
1	S2	681	PSU	C4-N3	-3.01	1.33	1.38
3	L5	4423	PSU	C6-C5	3.01	1.38	1.35
3	L5	4312	PSU	C4-N3	-3.01	1.33	1.38
3	L5	4196	OMG	C6-N1	-3.01	1.33	1.38
3	L5	4552	PSU	C4-N3	-3.01	1.33	1.38
1	S2	573	PSU	C6-C5	3.00	1.38	1.35
3	L5	2843	PSU	C4-N3	-3.00	1.33	1.38
1	S2	609	PSU	C6-C5	2.99	1.38	1.35
3	L5	4471	PSU	C4-N3	-2.99	1.33	1.38
3	L5	4293	PSU	C4-N3	-2.99	1.33	1.38
3	L5	1781	PSU	C6-C5	2.99	1.38	1.35
3	L5	2508	PSU	C4-N3	-2.99	1.33	1.38
1	S2	354	OMU	C2-N3	-2.98	1.32	1.38
3	L5	2424	OMG	C5-C4	2.98	1.46	1.38
3	L5	1862	PSU	C6-C5	2.98	1.38	1.35
3	L5	3764	PSU	C4-N3	-2.98	1.33	1.38
1	S2	1288	OMU	C4-N3	-2.98	1.33	1.38
3	L5	4306	OMU	C4-N3	-2.98	1.33	1.38
3	L5	2876	OMG	C5-C4	2.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4296	PSU	C4-N3	-2.97	1.33	1.38
1	S2	814	PSU	C6-C5	2.97	1.38	1.35
3	L5	4493	PSU	C6-C5	2.97	1.38	1.35
1	S2	121	OMU	C2-N3	-2.97	1.32	1.38
3	L5	3762	PSU	C6-C5	2.97	1.38	1.35
3	L5	5001	PSU	C6-C5	2.97	1.38	1.35
3	L5	3695	PSU	C4-N3	-2.97	1.33	1.38
1	S2	863	PSU	C6-C5	2.96	1.38	1.35
3	L5	5001	PSU	C4-N3	-2.95	1.33	1.38
3	L5	1625	OMG	C5-C4	2.95	1.46	1.38
3	L5	1779	PSU	C6-C5	2.95	1.38	1.35
3	L5	4494	OMG	C5-C4	2.95	1.46	1.38
3	L5	4689	PSU	C6-C5	2.95	1.38	1.35
1	S2	863	PSU	C4-N3	-2.95	1.33	1.38
3	L5	4972	PSU	C4-N3	-2.94	1.33	1.38
3	L5	2401	A2M	C5-N7	-2.94	1.33	1.39
3	L5	1781	PSU	C4-N3	-2.94	1.33	1.38
1	S2	1692	PSU	C6-C5	2.94	1.38	1.35
1	S2	1004	PSU	C6-C5	2.94	1.38	1.35
2	L8	75	OMG	C5-C4	2.94	1.46	1.38
3	L5	2632	PSU	C4-N3	-2.94	1.33	1.38
1	S2	822	PSU	C6-C5	2.93	1.38	1.35
3	L5	2837	OMU	C4-N3	-2.93	1.33	1.38
3	L5	4299	PSU	C6-C5	2.93	1.38	1.35
1	S2	296	PSU	C4-N3	-2.93	1.33	1.38
3	L5	1326	A2M	C5-N7	-2.93	1.33	1.39
3	L5	4576	PSU	C4-N3	-2.93	1.33	1.38
3	L5	2876	OMG	C6-N1	-2.93	1.33	1.38
2	L8	55	PSU	C4-N3	-2.93	1.33	1.38
3	L5	3867	A2M	C5-N7	-2.93	1.33	1.39
3	L5	3770	PSU	C6-C5	2.93	1.38	1.35
3	L5	3729	PSU	C4-N3	-2.92	1.33	1.38
3	L5	3744	OMG	C6-N1	-2.92	1.33	1.38
3	L5	3715	PSU	C6-C5	2.92	1.38	1.35
3	L5	3792	OMG	C5-C4	2.92	1.46	1.38
3	L5	1782	PSU	C4-N3	-2.92	1.33	1.38
1	S2	1136	PSU	C6-C5	2.92	1.38	1.35
1	S2	572	PSU	C4-N3	-2.92	1.33	1.38
3	L5	1779	PSU	C4-N3	-2.92	1.33	1.38
3	L5	4523	A2M	C5-N7	-2.91	1.33	1.39
1	S2	36	PSU	C4-N3	-2.91	1.33	1.38
1	S2	34	PSU	C6-C5	2.91	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	218	PSU	C6-C5	2.91	1.38	1.35
1	S2	867	OMG	C5-C4	2.91	1.46	1.38
1	S2	484	A2M	C5-N7	-2.91	1.33	1.39
3	L5	1782	PSU	C6-C5	2.90	1.38	1.35
1	S2	1004	PSU	C4-N3	-2.90	1.33	1.38
1	S2	1081	PSU	C4-N3	-2.90	1.33	1.38
3	L5	3695	PSU	C6-C5	2.90	1.38	1.35
3	L5	4499	OMG	C5-C4	2.90	1.46	1.38
1	S2	1367	PSU	C4-N3	-2.89	1.33	1.38
3	L5	4361	PSU	C2-N3	-2.89	1.32	1.37
3	L5	1582	PSU	C2-N3	-2.89	1.32	1.37
1	S2	1367	PSU	C6-C5	2.89	1.38	1.35
3	L5	4552	PSU	C6-C5	2.89	1.38	1.35
1	S2	814	PSU	C4-N3	-2.89	1.33	1.38
1	S2	866	PSU	C6-C5	2.89	1.38	1.35
1	S2	436	OMG	C6-N1	-2.89	1.33	1.38
3	L5	3851	PSU	C4-N3	-2.88	1.33	1.38
3	L5	4299	PSU	C4-N3	-2.88	1.33	1.38
1	S2	683	OMG	C5-C4	2.88	1.46	1.38
1	S2	1328	OMG	C6-N1	-2.88	1.33	1.38
3	L5	3762	PSU	C4-N3	-2.88	1.33	1.38
3	L5	3853	PSU	C4-N3	-2.88	1.33	1.38
1	S2	1490	OMG	C6-N1	-2.88	1.33	1.38
1	S2	601	OMG	C5-C4	2.88	1.46	1.38
3	L5	5010	PSU	C4-N3	-2.88	1.33	1.38
1	S2	644	OMG	C6-N1	-2.88	1.33	1.38
1	S2	966	PSU	C4-N3	-2.88	1.33	1.38
1	S2	681	PSU	C6-C5	2.88	1.38	1.35
1	S2	116	OMU	C4-N3	-2.88	1.33	1.38
1	S2	686	PSU	C4-N3	-2.88	1.33	1.38
1	S2	627	OMU	C4-N3	-2.87	1.33	1.38
3	L5	3925	OMU	C4-N3	-2.87	1.33	1.38
3	L5	4498	OMU	C4-N3	-2.87	1.33	1.38
3	L5	4457	PSU	C6-C5	2.87	1.38	1.35
3	L5	1316	OMG	C6-N1	-2.87	1.33	1.38
3	L5	3920	PSU	C4-N3	-2.87	1.33	1.38
1	S2	1643	PSU	C4-N3	-2.87	1.33	1.38
1	S2	1239	PSU	C4-N3	-2.87	1.33	1.38
1	S2	93	PSU	C6-C5	2.86	1.38	1.35
3	L5	4370	OMG	C5-C4	2.86	1.46	1.38
3	L5	1860	PSU	C6-C5	2.86	1.38	1.35
3	L5	4420	PSU	C6-C5	2.86	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1328	OMG	C5-C4	2.86	1.46	1.38
3	L5	3944	OMG	C5-C4	2.86	1.46	1.38
1	S2	99	A2M	C5-N7	-2.86	1.33	1.39
3	L5	4618	OMG	C6-N1	-2.85	1.33	1.38
3	L5	4447	5MC	C6-C5	2.85	1.39	1.34
3	L5	2843	PSU	C6-C5	2.85	1.38	1.35
3	L5	3884	PSU	C2-N3	-2.85	1.32	1.37
3	L5	2364	OMG	C5-C4	2.85	1.46	1.38
1	S2	1692	PSU	C4-N3	-2.85	1.33	1.38
3	L5	4353	PSU	C6-C5	2.84	1.38	1.35
1	S2	1177	PSU	C4-N3	-2.84	1.33	1.38
1	S2	105	PSU	C6-C5	2.84	1.38	1.35
84	At	8	4SU	C5-C4	-2.84	1.39	1.42
3	L5	4228	OMG	C5-C4	2.84	1.46	1.38
1	S2	1447	OMG	C5-C4	2.84	1.46	1.38
1	S2	406	PSU	C6-C5	2.84	1.38	1.35
3	L5	4494	OMG	C6-N1	-2.83	1.33	1.38
1	S2	1244	PSU	C6-C5	2.83	1.38	1.35
3	L5	2508	PSU	C6-C5	2.83	1.38	1.35
3	L5	3825	A2M	C5-N7	-2.82	1.33	1.39
1	S2	1804	OMU	C4-N3	-2.82	1.33	1.38
1	S2	649	PSU	C6-C5	2.82	1.38	1.35
85	Pt	21	H2U	C2-N3	-2.82	1.33	1.38
3	L5	3899	OMG	C5-C4	2.82	1.46	1.38
1	S2	34	PSU	C4-N3	-2.82	1.33	1.38
1	S2	651	PSU	C4-N3	-2.82	1.33	1.38
1	S2	1490	OMG	C5-C4	2.82	1.46	1.38
3	L5	2839	PSU	C4-N3	-2.81	1.33	1.38
3	L5	4623	OMG	C5-C4	2.81	1.46	1.38
3	L5	4500	PSU	C4-N3	-2.81	1.33	1.38
3	L5	4457	PSU	C2-N3	-2.81	1.32	1.37
3	L5	3944	OMG	C6-N1	-2.80	1.33	1.38
3	L5	1871	A2M	C5-N7	-2.80	1.34	1.39
3	L5	4576	PSU	C6-C5	2.80	1.38	1.35
3	L5	2424	OMG	C5-N7	-2.79	1.33	1.39
3	L5	4972	PSU	C6-C5	2.79	1.38	1.35
1	S2	822	PSU	C4-N3	-2.79	1.33	1.38
3	L5	4296	PSU	C6-C5	2.79	1.38	1.35
3	L5	4618	OMG	C5-C4	2.79	1.46	1.38
3	L5	4403	PSU	C2-N3	-2.79	1.32	1.37
1	S2	512	A2M	C5-N7	-2.78	1.34	1.39
1	S2	1347	PSU	C6-C5	2.78	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1536	PSU	C6-C5	2.78	1.38	1.35
3	L5	4227	OMU	C4-N3	-2.78	1.33	1.38
1	S2	644	OMG	C5-C4	2.78	1.46	1.38
1	S2	815	PSU	C4-N3	-2.78	1.33	1.38
3	L5	2415	OMU	C2-N3	-2.78	1.33	1.38
3	L5	4423	PSU	C4-N3	-2.78	1.33	1.38
3	L5	3627	OMG	C5-C4	2.77	1.46	1.38
3	L5	3899	OMG	C6-N1	-2.77	1.33	1.38
3	L5	1744	PSU	C6-C5	2.77	1.38	1.35
1	S2	1851	MA6	C5-C6	2.77	1.48	1.41
3	L5	4620	OMU	C2-N3	-2.77	1.33	1.38
1	S2	509	OMG	C5-C4	2.77	1.46	1.38
85	Pt	56	PSU	C4-N3	-2.76	1.33	1.38
1	S2	1243	PSU	C4-N3	-2.76	1.33	1.38
3	L5	4521	PSU	C6-C5	2.76	1.38	1.35
3	L5	1677	PSU	C4-N3	-2.76	1.33	1.38
3	L5	4431	PSU	C4-N3	-2.76	1.33	1.38
3	L5	1522	OMG	C5-C4	2.76	1.46	1.38
1	S2	1136	PSU	C4-N3	-2.76	1.33	1.38
3	L5	4361	PSU	C6-C5	2.76	1.38	1.35
3	L5	4571	A2M	C5-N7	-2.76	1.34	1.39
3	L5	1316	OMG	C5-C4	2.76	1.46	1.38
1	S2	1238	PSU	C4-N3	-2.75	1.33	1.38
1	S2	1081	PSU	C6-C5	2.75	1.38	1.35
3	L5	3744	OMG	C5-C4	2.75	1.46	1.38
3	L5	3853	PSU	C6-C5	2.74	1.38	1.35
3	L5	3844	PSU	C6-C5	2.74	1.38	1.35
3	L5	3637	PSU	C2-N3	-2.74	1.33	1.37
1	S2	428	OMU	C4-N3	-2.74	1.33	1.38
1	S2	1832	6MZ	C5-C6	2.74	1.48	1.41
1	S2	1445	PSU	C4-N3	-2.74	1.33	1.38
40	LB	245	HIC	CD2-CG	2.73	1.41	1.36
3	L5	1625	OMG	C6-N1	-2.73	1.33	1.38
1	S2	436	OMG	C5-C4	2.73	1.46	1.38
1	S2	1850	MA6	C5-C6	2.72	1.48	1.41
1	S2	601	OMG	C6-N1	-2.71	1.33	1.38
3	L5	3639	PSU	C6-C5	2.71	1.38	1.35
3	L5	1322	1MA	C6-N6	2.70	1.34	1.28
85	Pt	8	4SU	C2-N3	-2.70	1.33	1.38
1	S2	119	PSU	C6-C5	2.70	1.38	1.35
3	L5	3729	PSU	C6-C5	2.70	1.38	1.35
3	L5	4590	A2M	C5-N7	-2.69	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4312	PSU	C6-C5	2.69	1.38	1.35
3	L5	4392	OMG	C5-C4	2.69	1.46	1.38
3	L5	1860	PSU	C2-N3	-2.69	1.33	1.37
3	L5	2364	OMG	C6-N1	-2.69	1.33	1.38
3	L5	1522	OMG	C6-N1	-2.68	1.33	1.38
3	L5	4532	PSU	C2-N3	-2.67	1.33	1.37
3	L5	4623	OMG	C6-N1	-2.67	1.33	1.38
1	S2	1643	PSU	C6-C5	2.66	1.38	1.35
3	L5	4579	PSU	C6-C5	2.66	1.38	1.35
3	L5	3627	OMG	C6-N1	-2.66	1.33	1.38
3	L5	3884	PSU	C2-N1	-2.65	1.33	1.36
3	L5	2363	A2M	C5-N7	-2.64	1.34	1.39
3	L5	4637	OMG	C5-C4	2.64	1.46	1.38
3	L5	3851	PSU	C6-C5	2.64	1.38	1.35
3	L5	4442	PSU	C6-C5	2.64	1.38	1.35
3	L5	3718	A2M	C5-N7	-2.64	1.34	1.39
1	S2	509	OMG	C5-N7	-2.64	1.33	1.39
3	L5	3792	OMG	C6-N1	-2.63	1.33	1.38
3	L5	4228	OMG	C6-N1	-2.63	1.33	1.38
1	S2	1678	A2M	C5-N7	-2.63	1.34	1.39
3	L5	4636	PSU	C2-N3	-2.63	1.33	1.37
84	At	16	H2U	C2-N3	-2.63	1.33	1.38
1	S2	468	A2M	C5-N7	-2.62	1.34	1.39
3	L5	3758	PSU	C6-C5	2.62	1.38	1.35
1	S2	1639	G7M	C6-N1	-2.62	1.33	1.38
3	L5	1871	A2M	C4-N9	-2.62	1.32	1.37
3	L5	398	A2M	C5-C6	2.62	1.48	1.41
3	L5	1534	A2M	C5-N7	-2.62	1.34	1.39
3	L5	3723	A2M	C5-N7	-2.62	1.34	1.39
1	S2	1447	OMG	C6-N1	-2.62	1.33	1.38
3	L5	4196	OMG	C5-C4	2.62	1.45	1.38
84	At	32	PSU	C6-C5	2.62	1.38	1.35
3	L5	4370	OMG	C6-N1	-2.62	1.34	1.38
1	S2	27	A2M	C5-N7	-2.61	1.34	1.39
3	L5	4220	6MZ	C5-N7	-2.61	1.34	1.39
1	S2	119	PSU	C2-N3	-2.60	1.33	1.37
1	S2	1326	UY1	C6-C5	2.60	1.38	1.35
1	S2	159	A2M	C5-N7	-2.60	1.34	1.39
3	L5	1524	A2M	C5-N7	-2.60	1.34	1.39
1	S2	683	OMG	C6-N1	-2.60	1.34	1.38
84	At	20	H2U	C2-N3	-2.59	1.33	1.38
3	L5	2839	PSU	C6-C5	2.59	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1792	PSU	C2-N3	-2.59	1.33	1.37
1	S2	590	A2M	C5-N7	-2.59	1.34	1.39
1	S2	867	OMG	C6-N1	-2.58	1.34	1.38
3	L5	3724	A2M	C5-N7	-2.58	1.34	1.39
3	L5	4579	PSU	C2-N3	-2.58	1.33	1.37
3	L5	3782	5MC	C6-C5	2.58	1.38	1.34
3	L5	2787	A2M	C5-N7	-2.57	1.34	1.39
3	L5	400	A2M	C5-N7	-2.57	1.34	1.39
1	S2	801	PSU	C2-N3	-2.57	1.33	1.37
85	Pt	21	H2U	C4-N3	-2.56	1.33	1.37
3	L5	4471	PSU	C2-N3	-2.56	1.33	1.37
3	L5	3760	A2M	C5-N7	-2.55	1.34	1.39
1	S2	1288	OMU	C2-N3	-2.55	1.33	1.38
1	S2	1248	B8N	C6-C5	2.55	1.38	1.35
3	L5	3723	A2M	C4-N9	-2.55	1.32	1.37
1	S2	576	A2M	C5-C6	2.55	1.48	1.41
3	L5	1322	1MA	C5-C4	2.55	1.45	1.38
1	S2	1842	4AC	C4-N4	-2.55	1.36	1.39
3	L5	4532	PSU	C6-C5	2.55	1.38	1.35
2	L8	69	PSU	C6-C5	2.55	1.38	1.35
3	L5	3764	PSU	C2-N3	-2.54	1.33	1.37
3	L5	1524	A2M	C5-C6	2.54	1.48	1.41
1	S2	1383	A2M	C5-N7	-2.54	1.34	1.39
3	L5	3818	UY1	C2-N3	-2.54	1.33	1.37
3	L5	3830	A2M	C5-N7	-2.53	1.34	1.39
1	S2	218	PSU	C2-N3	-2.53	1.33	1.37
1	S2	576	A2M	C5-N7	-2.53	1.34	1.39
1	S2	1232	PSU	C2-N3	-2.53	1.33	1.37
3	L5	4499	OMG	C6-N1	-2.53	1.34	1.38
3	L5	3782	5MC	C6-N1	-2.53	1.33	1.38
3	L5	2837	OMU	C2-N3	-2.53	1.33	1.38
84	At	37	MIA	C5-N7	-2.53	1.34	1.39
1	S2	1832	6MZ	C5-N7	-2.52	1.34	1.39
1	S2	1031	A2M	C5-N7	-2.52	1.34	1.39
1	S2	1031	A2M	C5-C6	2.52	1.48	1.41
1	S2	159	A2M	C5-C6	2.52	1.48	1.41
3	L5	4579	PSU	C2-N1	-2.52	1.33	1.36
3	L5	3884	PSU	C6-C5	2.52	1.38	1.35
1	S2	166	A2M	C5-C6	2.51	1.48	1.41
3	L5	1322	1MA	C5-N7	-2.51	1.34	1.39
3	L5	4420	PSU	C4-N3	-2.51	1.34	1.38
3	L5	1677	PSU	C2-N1	-2.51	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	627	OMU	C2-N3	-2.50	1.33	1.38
1	S2	1490	OMG	C5-N7	-2.50	1.34	1.39
3	L5	3718	A2M	C4-N9	-2.50	1.32	1.37
1	S2	1442	OMU	C4-N3	-2.50	1.34	1.38
3	L5	1534	A2M	C5-C6	2.50	1.47	1.41
1	S2	116	OMU	C5-C4	-2.49	1.38	1.43
1	S2	668	A2M	C5-C6	2.49	1.47	1.41
84	At	39	PSU	C2-N3	-2.49	1.33	1.37
1	S2	436	OMG	C5-N7	-2.49	1.34	1.39
3	L5	4227	OMU	C2-N3	-2.49	1.33	1.38
1	S2	172	OMU	C2-N3	-2.48	1.33	1.38
3	L5	4392	OMG	C5-N7	-2.48	1.34	1.39
2	L8	69	PSU	C2-N3	-2.48	1.33	1.37
1	S2	918	PSU	C2-N3	-2.48	1.33	1.37
3	L5	1582	PSU	C6-C5	2.48	1.38	1.35
1	S2	105	PSU	C2-N3	-2.48	1.33	1.37
3	L5	4618	OMG	C5-N7	-2.47	1.34	1.39
3	L5	3770	PSU	C2-N1	-2.47	1.33	1.36
1	S2	863	PSU	C2-N1	-2.47	1.33	1.36
3	L5	3760	A2M	C5-C6	2.47	1.47	1.41
3	L5	2363	A2M	C5-C6	2.47	1.47	1.41
1	S2	166	A2M	C5-N7	-2.47	1.34	1.39
3	L5	4498	OMU	C2-N3	-2.47	1.33	1.38
1	S2	668	A2M	C5-N7	-2.46	1.34	1.39
2	L8	14	OMU	C5-C4	-2.46	1.38	1.43
1	S2	1347	PSU	C2-N3	-2.46	1.33	1.37
1	S2	863	PSU	C2-N3	-2.46	1.33	1.37
3	L5	3830	A2M	C5-C6	2.46	1.47	1.41
3	L5	1625	OMG	C5-N7	-2.46	1.34	1.39
3	L5	3770	PSU	C2-N3	-2.46	1.33	1.37
3	L5	4673	PSU	C2-N3	-2.46	1.33	1.37
3	L5	2415	OMU	C5-C4	-2.46	1.38	1.43
1	S2	1678	A2M	C5-C6	2.46	1.47	1.41
3	L5	3758	PSU	C2-N3	-2.45	1.33	1.37
3	L5	3785	A2M	C5-N7	-2.45	1.34	1.39
1	S2	590	A2M	C5-C6	2.45	1.47	1.41
3	L5	3764	PSU	C2'-C1'	-2.45	1.50	1.53
3	L5	400	A2M	C5-C6	2.45	1.47	1.41
3	L5	1326	A2M	C4-N9	-2.45	1.32	1.37
84	At	37	MIA	C5-C6	2.45	1.47	1.41
3	L5	3715	PSU	C2-N3	-2.45	1.33	1.37
3	L5	1322	1MA	C4-N9	-2.44	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4306	OMU	C2-N3	-2.44	1.33	1.38
1	S2	354	OMU	C5-C4	-2.44	1.38	1.43
1	S2	1804	OMU	C2-N3	-2.44	1.33	1.38
3	L5	3818	UY1	C6-C5	2.44	1.38	1.35
3	L5	4457	PSU	C2-N1	-2.43	1.33	1.36
1	S2	1678	A2M	C4-N9	-2.43	1.32	1.37
3	L5	4447	5MC	C6-N1	-2.43	1.33	1.38
3	L5	3785	A2M	C5-C6	2.43	1.47	1.41
1	S2	1625	PSU	C4-N3	-2.43	1.34	1.38
1	S2	609	PSU	C2-N3	-2.43	1.33	1.37
3	L5	4637	OMG	C5-N7	-2.43	1.34	1.39
3	L5	2787	A2M	C5-C6	2.42	1.47	1.41
3	L5	4220	6MZ	C5-C6	2.42	1.47	1.41
3	L5	2815	A2M	C5-C6	2.41	1.47	1.41
1	S2	649	PSU	C2-N1	-2.41	1.33	1.36
1	S2	27	A2M	C5-C6	2.41	1.47	1.41
3	L5	3925	OMU	C2-N3	-2.41	1.33	1.38
84	At	16	H2U	C4-N3	-2.41	1.33	1.37
1	S2	644	OMG	C5-N7	-2.41	1.34	1.39
3	L5	3825	A2M	C5-C6	2.41	1.47	1.41
1	S2	121	OMU	C5-C4	-2.41	1.38	1.43
3	L5	3867	A2M	C4-N9	-2.40	1.32	1.37
3	L5	4196	OMG	C5-N7	-2.40	1.34	1.39
1	S2	428	OMU	C2-N3	-2.40	1.33	1.38
3	L5	1683	PSU	C2-N3	-2.40	1.33	1.37
1	S2	668	A2M	C4-N9	-2.40	1.32	1.37
1	S2	468	A2M	C4-N9	-2.40	1.32	1.37
1	S2	1383	A2M	C4-N9	-2.40	1.32	1.37
3	L5	4493	PSU	C2-N3	-2.40	1.33	1.37
3	L5	398	A2M	C8-N7	2.39	1.36	1.31
3	L5	4571	A2M	C5-C6	2.39	1.47	1.41
3	L5	4521	PSU	C2-N3	-2.39	1.33	1.37
1	S2	406	PSU	C2-N3	-2.39	1.33	1.37
1	S2	484	A2M	C5-C6	2.39	1.47	1.41
84	At	37	MIA	C4-N9	-2.39	1.32	1.37
1	S2	1850	MA6	C5-N7	-2.38	1.34	1.39
3	L5	4590	A2M	C5-C6	2.38	1.47	1.41
3	L5	4403	PSU	C2-N1	-2.38	1.33	1.36
3	L5	1744	PSU	C2-N3	-2.38	1.33	1.37
1	S2	1081	PSU	O4'-C1'	-2.37	1.40	1.43
3	L5	3744	OMG	C5-N7	-2.37	1.34	1.39
84	At	20	H2U	C4-N3	-2.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4353	PSU	C2-N3	-2.37	1.33	1.37
1	S2	1383	A2M	C5-C6	2.37	1.47	1.41
3	L5	4353	PSU	C2-N1	-2.37	1.33	1.36
1	S2	1328	OMG	C5-N7	-2.37	1.34	1.39
1	S2	572	PSU	C2-N3	-2.37	1.33	1.37
1	S2	1850	MA6	C4-N9	-2.36	1.32	1.37
1	S2	649	PSU	C2-N3	-2.36	1.33	1.37
1	S2	686	PSU	C2-N1	-2.36	1.33	1.36
3	L5	4636	PSU	C6-C5	2.36	1.37	1.35
3	L5	4523	A2M	C5-C6	2.36	1.47	1.41
3	L5	4531	PSU	C6-C5	2.36	1.37	1.35
1	S2	1447	OMG	C5-N7	-2.35	1.34	1.39
3	L5	4442	PSU	C2-N3	-2.35	1.33	1.37
1	S2	1347	PSU	C2-N1	-2.35	1.33	1.36
1	S2	1851	MA6	C5-N7	-2.35	1.34	1.39
3	L5	3899	OMG	C5-N7	-2.35	1.34	1.39
1	S2	1174	PSU	C2-N3	-2.35	1.33	1.37
3	L5	1862	PSU	C2-N3	-2.35	1.33	1.37
1	S2	296	PSU	C6-C5	2.35	1.37	1.35
3	L5	398	A2M	C5-N7	-2.34	1.34	1.39
3	L5	4531	PSU	C2-N3	-2.34	1.33	1.37
3	L5	4403	PSU	C6-C5	2.34	1.37	1.35
1	S2	1244	PSU	C2-N3	-2.34	1.33	1.37
3	L5	3792	OMG	C5-N7	-2.34	1.34	1.39
3	L5	4494	OMG	C5-N7	-2.33	1.34	1.39
3	L5	3718	A2M	C5-C6	2.33	1.47	1.41
2	L8	75	OMG	C6-N1	-2.33	1.34	1.38
3	L5	1792	PSU	C2-N1	-2.33	1.33	1.36
3	L5	3734	PSU	C2-N3	-2.33	1.33	1.37
3	L5	4590	A2M	C4-N9	-2.33	1.32	1.37
1	S2	109	PSU	C2-N1	-2.33	1.33	1.36
1	S2	116	OMU	C2-N3	-2.33	1.33	1.38
3	L5	3724	A2M	C5-C6	2.32	1.47	1.41
3	L5	2876	OMG	C5-N7	-2.32	1.34	1.39
3	L5	5001	PSU	C2-N3	-2.31	1.33	1.37
3	L5	1316	OMG	C5-N7	-2.31	1.34	1.39
1	S2	296	PSU	C2-N1	-2.31	1.33	1.36
3	L5	4370	OMG	C5-N7	-2.30	1.34	1.39
1	S2	609	PSU	C2-N1	-2.30	1.33	1.36
1	S2	512	A2M	C5-C6	2.30	1.47	1.41
1	S2	93	PSU	C2-N3	-2.30	1.33	1.37
3	L5	3851	PSU	C2-N3	-2.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3853	PSU	C2-N3	-2.30	1.33	1.37
3	L5	3758	PSU	C2'-C1'	-2.30	1.50	1.53
3	L5	3724	A2M	C4-N9	-2.30	1.32	1.37
1	S2	1081	PSU	C2-N3	-2.30	1.33	1.37
1	S2	296	PSU	C2-N3	-2.30	1.33	1.37
1	S2	573	PSU	C2-N3	-2.30	1.33	1.37
1	S2	406	PSU	C2-N1	-2.29	1.33	1.36
3	L5	3825	A2M	C4-N9	-2.29	1.32	1.37
3	L5	4442	PSU	C2-N1	-2.29	1.33	1.36
3	L5	4623	OMG	C4-N9	-2.29	1.32	1.38
3	L5	4628	PSU	C2-N1	-2.29	1.33	1.36
3	L5	1860	PSU	C2-N1	-2.28	1.33	1.36
1	S2	822	PSU	C2-N3	-2.28	1.33	1.37
3	L5	2401	A2M	C5-C6	2.27	1.47	1.41
3	L5	2843	PSU	C2-N3	-2.27	1.33	1.37
3	L5	3762	PSU	C2-N3	-2.27	1.33	1.37
1	S2	1326	UY1	C2-N3	-2.27	1.33	1.37
3	L5	3785	A2M	C4-N9	-2.27	1.33	1.37
3	L5	3723	A2M	C5-C6	2.27	1.47	1.41
3	L5	2401	A2M	C4-N9	-2.27	1.33	1.37
3	L5	3844	PSU	C2-N3	-2.27	1.33	1.37
3	L5	4306	OMU	C5-C4	-2.27	1.38	1.43
1	S2	1643	PSU	C2-N3	-2.26	1.33	1.37
3	L5	3729	PSU	C2-N1	-2.26	1.33	1.36
1	S2	1442	OMU	C5-C4	-2.26	1.38	1.43
2	L8	69	PSU	C2-N1	-2.26	1.33	1.36
3	L5	3639	PSU	C2-N3	-2.26	1.33	1.37
3	L5	2837	OMU	C5-C4	-2.26	1.38	1.43
3	L5	3867	A2M	C5-C6	2.26	1.47	1.41
1	S2	1442	OMU	C2-N3	-2.26	1.34	1.38
3	L5	4361	PSU	C2-N1	-2.25	1.33	1.36
3	L5	1744	PSU	C2-N1	-2.25	1.33	1.36
1	S2	468	A2M	C5-C6	2.25	1.47	1.41
1	S2	172	OMU	C5-C4	-2.24	1.38	1.43
3	L5	3729	PSU	C2'-C1'	-2.24	1.50	1.53
1	S2	1851	MA6	C4-N9	-2.24	1.33	1.37
1	S2	681	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4532	PSU	C2'-C1'	-2.24	1.50	1.53
3	L5	1536	PSU	C2-N3	-2.24	1.33	1.37
3	L5	1779	PSU	C2-N3	-2.24	1.33	1.37
1	S2	627	OMU	C5-C4	-2.24	1.38	1.43
1	S2	1031	A2M	C4-N9	-2.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2787	A2M	C4-N9	-2.23	1.33	1.37
1	S2	1625	PSU	C2'-C1'	-2.23	1.50	1.53
3	L5	3729	PSU	C2-N3	-2.23	1.33	1.37
3	L5	4499	OMG	C5-N7	-2.23	1.34	1.39
1	S2	686	PSU	C2-N3	-2.22	1.33	1.37
3	L5	4228	OMG	C4-N9	-2.22	1.32	1.38
3	L5	4312	PSU	C2-N3	-2.22	1.33	1.37
3	L5	4498	OMU	C5-C4	-2.22	1.38	1.43
3	L5	3853	PSU	C2-N1	-2.22	1.33	1.36
3	L5	1522	OMG	C5-N7	-2.22	1.34	1.39
3	L5	4431	PSU	C2-N3	-2.21	1.33	1.37
1	S2	93	PSU	C2'-C1'	-2.21	1.50	1.53
1	S2	1288	OMU	C5-C4	-2.21	1.38	1.43
3	L5	1781	PSU	C2-N3	-2.21	1.33	1.37
3	L5	1677	PSU	C2-N3	-2.20	1.33	1.37
3	L5	2364	OMG	C5-N7	-2.20	1.34	1.39
3	L5	4689	PSU	C2-N3	-2.20	1.33	1.37
3	L5	1683	PSU	C2-N1	-2.20	1.33	1.36
3	L5	2839	PSU	C2-N3	-2.20	1.33	1.37
1	S2	99	A2M	C4-N9	-2.20	1.33	1.37
1	S2	601	OMG	C5-N7	-2.20	1.34	1.39
1	S2	814	PSU	C2-N3	-2.20	1.33	1.37
1	S2	512	A2M	C4-N9	-2.20	1.33	1.37
3	L5	2508	PSU	C2-N3	-2.20	1.33	1.37
3	L5	4569	PSU	C2-N3	-2.20	1.33	1.37
1	S2	484	A2M	C4-N9	-2.20	1.33	1.37
3	L5	2815	A2M	C4-N9	-2.19	1.33	1.37
3	L5	3760	A2M	C8-N7	2.19	1.35	1.31
1	S2	159	A2M	C4-N9	-2.19	1.33	1.37
3	L5	1326	A2M	C5-C6	2.19	1.47	1.41
3	L5	3785	A2M	C8-N7	2.19	1.35	1.31
1	S2	34	PSU	C2-N3	-2.19	1.33	1.37
3	L5	3768	PSU	C2-N3	-2.19	1.33	1.37
1	S2	105	PSU	C2-N1	-2.18	1.33	1.36
3	L5	4403	PSU	C2'-C1'	-2.18	1.50	1.53
3	L5	1862	PSU	C2-N1	-2.18	1.33	1.36
3	L5	3944	OMG	C5-N7	-2.18	1.34	1.39
3	L5	4196	OMG	C4-N9	-2.18	1.32	1.38
1	S2	576	A2M	C4-N9	-2.18	1.33	1.37
3	L5	4618	OMG	C4-N9	-2.18	1.32	1.38
3	L5	3627	OMG	C5-N7	-2.18	1.34	1.39
3	L5	1677	PSU	C6-C5	2.17	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	At	32	PSU	C2-N3	-2.17	1.33	1.37
3	L5	4620	OMU	C5-C4	-2.17	1.39	1.43
3	L5	4552	PSU	C2-N3	-2.17	1.33	1.37
3	L5	4299	PSU	C2-N3	-2.17	1.33	1.37
3	L5	3818	UY1	C2-N1	-2.16	1.33	1.36
3	L5	4228	OMG	C5-N7	-2.16	1.34	1.39
84	At	8	4SU	C2-N3	-2.16	1.34	1.38
1	S2	1239	PSU	C2-N3	-2.16	1.33	1.37
1	S2	1692	PSU	C2-N3	-2.16	1.33	1.37
2	L8	69	PSU	C2'-C1'	-2.16	1.50	1.53
85	Pt	33	OMC	C6-N1	-2.16	1.32	1.38
3	L5	3760	A2M	C4-N9	-2.16	1.33	1.37
1	S2	1232	PSU	C2-N1	-2.16	1.33	1.36
1	S2	1643	PSU	C2-N1	-2.16	1.33	1.36
1	S2	866	PSU	C2-N3	-2.15	1.33	1.37
84	At	32	PSU	C2'-C1'	-2.15	1.50	1.53
3	L5	2363	A2M	C4-N9	-2.15	1.33	1.37
3	L5	3639	PSU	C2-N1	-2.15	1.33	1.36
1	S2	867	OMG	C5-N7	-2.15	1.34	1.39
3	L5	2351	OMC	C5-C4	-2.15	1.37	1.42
1	S2	1004	PSU	C2-N3	-2.15	1.33	1.37
3	L5	4293	PSU	C2-N3	-2.14	1.33	1.37
3	L5	4579	PSU	C6-N1	-2.14	1.32	1.36
1	S2	109	PSU	C2-N3	-2.14	1.33	1.37
3	L5	4296	PSU	C2-N3	-2.14	1.33	1.37
3	L5	3830	A2M	C8-N7	2.14	1.35	1.31
3	L5	1782	PSU	C2-N3	-2.14	1.34	1.37
1	S2	428	OMU	C5-C4	-2.13	1.39	1.43
3	L5	3925	OMU	C5-C4	-2.13	1.39	1.43
1	S2	683	OMG	C5-N7	-2.13	1.34	1.39
3	L5	4521	PSU	C2'-C1'	-2.13	1.50	1.53
84	At	39	PSU	C2-N1	-2.13	1.33	1.36
1	S2	1056	PSU	C2-N3	-2.13	1.34	1.37
3	L5	4637	OMG	C4-N9	-2.13	1.32	1.38
1	S2	1804	OMU	C5-C4	-2.13	1.39	1.43
3	L5	4227	OMU	C5-C4	-2.12	1.39	1.43
3	L5	3695	PSU	C2-N3	-2.12	1.34	1.37
3	L5	4579	PSU	C2'-C1'	-2.12	1.50	1.53
3	L5	4392	OMG	C4-N9	-2.12	1.32	1.38
3	L5	4293	PSU	C2-N1	-2.12	1.33	1.36
1	S2	576	A2M	C8-N7	2.11	1.35	1.31
1	S2	27	A2M	C4-N9	-2.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3734	PSU	C2-N1	-2.11	1.33	1.36
1	S2	406	PSU	C2'-C1'	-2.11	1.50	1.53
3	L5	3762	PSU	C2-N1	-2.11	1.33	1.36
1	S2	1031	A2M	C8-N7	2.11	1.35	1.31
3	L5	3920	PSU	C2-N3	-2.11	1.34	1.37
1	S2	1136	PSU	C2-N3	-2.10	1.34	1.37
3	L5	4493	PSU	C2-N1	-2.10	1.33	1.36
1	S2	509	OMG	C4-N9	-2.10	1.32	1.38
1	S2	651	PSU	C2-N3	-2.10	1.34	1.37
3	L5	4361	PSU	C2'-C1'	-2.10	1.50	1.53
1	S2	119	PSU	C2-N1	-2.10	1.33	1.36
3	L5	1536	PSU	C2-N1	-2.10	1.33	1.36
3	L5	2787	A2M	C8-N7	2.09	1.35	1.31
1	S2	1337	4AC	C7-N4	-2.09	1.32	1.37
1	S2	172	OMU	C6-N1	-2.09	1.33	1.38
1	S2	99	A2M	C5-C6	2.09	1.46	1.41
3	L5	1871	A2M	C5-C6	2.09	1.46	1.41
3	L5	1582	PSU	C2-N1	-2.09	1.33	1.36
2	L8	75	OMG	C5-N7	-2.09	1.34	1.39
1	S2	36	PSU	C2-N3	-2.09	1.34	1.37
3	L5	4972	PSU	C2-N3	-2.09	1.34	1.37
1	S2	1692	PSU	C2-N1	-2.09	1.33	1.36
3	L5	4628	PSU	C2-N3	-2.08	1.34	1.37
3	L5	3851	PSU	C2-N1	-2.08	1.33	1.36
1	S2	484	A2M	C8-N9	-2.08	1.34	1.37
1	S2	801	PSU	C2-N1	-2.08	1.33	1.36
3	L5	4312	PSU	C2-N1	-2.08	1.33	1.36
3	L5	4220	6MZ	C4-N9	-2.08	1.33	1.37
3	L5	400	A2M	C8-N7	2.08	1.35	1.31
3	L5	3744	OMG	C4-N9	-2.08	1.32	1.38
3	L5	3830	A2M	C4-N9	-2.08	1.33	1.37
3	L5	4523	A2M	C4-N9	-2.07	1.33	1.37
3	L5	1781	PSU	C2-N1	-2.07	1.34	1.36
3	L5	4590	A2M	C8-N7	2.07	1.35	1.31
2	L8	55	PSU	C2-N3	-2.07	1.34	1.37
3	L5	1871	A2M	C8-N9	-2.07	1.34	1.37
1	S2	644	OMG	C4-N9	-2.07	1.32	1.38
3	L5	4576	PSU	C2-N3	-2.07	1.34	1.37
3	L5	2401	A2M	C8-N9	-2.07	1.34	1.37
3	L5	2839	PSU	C2-N1	-2.06	1.34	1.36
3	L5	2363	A2M	C8-N7	2.06	1.35	1.31
1	S2	1367	PSU	C2-N3	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	5010	PSU	C2-N3	-2.06	1.34	1.37
3	L5	3627	OMG	C4-N9	-2.06	1.32	1.38
3	L5	1524	A2M	C4-N9	-2.06	1.33	1.37
1	S2	1832	6MZ	C8-N7	2.06	1.35	1.31
3	L5	4420	PSU	C2-N1	-2.05	1.34	1.36
1	S2	683	OMG	C4-N9	-2.05	1.32	1.38
1	S2	1004	PSU	C2-N1	-2.05	1.34	1.36
3	L5	3768	PSU	C2-N1	-2.05	1.34	1.36
3	L5	4521	PSU	C2-N1	-2.05	1.34	1.36
3	L5	4636	PSU	C2-N1	-2.05	1.34	1.36
2	L8	14	OMU	C6-N1	-2.05	1.33	1.38
3	L5	1524	A2M	C8-N7	2.04	1.35	1.31
1	S2	1238	PSU	C2-N3	-2.04	1.34	1.37
3	L5	400	A2M	C4-N9	-2.04	1.33	1.37
3	L5	3869	OMC	C6-N1	-2.04	1.33	1.38
84	At	37	MIA	C8-N7	2.03	1.35	1.31
1	S2	166	A2M	C8-N7	2.03	1.35	1.31
3	L5	1534	A2M	C4-N9	-2.03	1.33	1.37
1	S2	1851	MA6	C8-N7	2.03	1.35	1.31
1	S2	1177	PSU	C2-N1	-2.03	1.34	1.36
1	S2	590	A2M	C4-N9	-2.03	1.33	1.37
1	S2	1081	PSU	C2-N1	-2.02	1.34	1.36
1	S2	572	PSU	C2-N1	-2.01	1.34	1.36
1	S2	1832	6MZ	C4-N9	-2.01	1.33	1.37
3	L5	4494	OMG	C4-N9	-2.01	1.32	1.38
3	L5	1522	OMG	C4-N9	-2.01	1.32	1.38
1	S2	1337	4AC	C6-N1	-2.01	1.33	1.38
1	S2	590	A2M	C8-N7	2.01	1.35	1.31
3	L5	3944	OMG	C4-N9	-2.01	1.32	1.38
3	L5	1534	A2M	C8-N7	2.01	1.35	1.31
3	L5	4220	6MZ	C8-N7	2.01	1.35	1.31
3	L5	4456	OMC	C6-N1	-2.00	1.33	1.38
3	L5	2415	OMU	C6-N1	-2.00	1.33	1.38
3	L5	3715	PSU	C2-N1	-2.00	1.34	1.36
3	L5	1340	OMC	C5-C4	-2.00	1.38	1.42
3	L5	3899	OMG	C4-N9	-2.00	1.33	1.38

All (1183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SA	2	SAC	OAC-C1A-N	-10.15	104.05	121.98
84	At	37	MIA	C12-C13-C14	-8.54	111.68	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1639	G7M	CN7-N7-C8	-7.95	112.75	124.79
66	Lr	2	SAC	OAC-C1A-N	-7.84	108.12	121.98
3	L5	4628	PSU	N1-C2-N3	7.65	123.24	115.17
3	L5	4636	PSU	N1-C2-N3	7.51	123.09	115.17
29	SV	1	AME	OT-CT1-N	-7.48	108.77	121.98
84	At	37	MIA	C5-C4-N3	-7.46	119.32	127.18
2	L8	69	PSU	N1-C2-N3	7.33	122.90	115.17
3	L5	4521	PSU	N1-C2-N3	7.31	122.89	115.17
66	Lr	2	SAC	OAC-C1A-C2A	-7.30	109.05	122.05
1	S2	1056	PSU	N1-C2-N3	7.20	122.76	115.17
1	S2	1174	PSU	N1-C2-N3	7.19	122.75	115.17
3	L5	4442	PSU	N1-C2-N3	7.13	122.69	115.17
1	S2	918	PSU	N1-C2-N3	7.13	122.69	115.17
3	L5	4531	PSU	N1-C2-N3	7.12	122.68	115.17
3	L5	4530	UR3	C4-N3-C2	-7.10	118.86	124.58
84	At	8	4SU	C4-N3-C2	-7.10	120.51	127.31
1	S2	1232	PSU	N1-C2-N3	7.10	122.65	115.17
3	L5	3758	PSU	N1-C2-N3	7.02	122.58	115.17
1	S2	686	PSU	N1-C2-N3	7.02	122.58	115.17
1	S2	105	PSU	N1-C2-N3	7.00	122.56	115.17
1	S2	1639	G7M	N9-C4-N3	6.99	139.93	125.95
1	S2	822	PSU	N1-C2-N3	6.98	122.54	115.17
3	L5	1862	PSU	N1-C2-N3	6.97	122.52	115.17
3	L5	4403	PSU	N1-C2-N3	6.96	122.51	115.17
29	SV	1	AME	OT-CT1-CT2	-6.93	109.71	122.05
3	L5	4353	PSU	N1-C2-N3	6.92	122.47	115.17
3	L5	3637	PSU	N1-C2-N3	6.92	122.47	115.17
3	L5	4569	PSU	N1-C2-N3	6.92	122.46	115.17
1	S2	93	PSU	N1-C2-N3	6.89	122.44	115.17
3	L5	4579	PSU	N1-C2-N3	6.89	122.44	115.17
1	S2	866	PSU	N1-C2-N3	6.88	122.42	115.17
1	S2	109	PSU	N1-C2-N3	6.86	122.41	115.17
1	S2	1639	G7M	N9-C8-N7	-6.85	95.85	112.48
1	S2	1244	PSU	N1-C2-N3	6.81	122.35	115.17
1	S2	1243	PSU	N1-C2-N3	6.79	122.33	115.17
3	L5	4532	PSU	N1-C2-N3	6.75	122.29	115.17
3	L5	4293	PSU	N1-C2-N3	6.75	122.28	115.17
1	S2	573	PSU	N1-C2-N3	6.74	122.28	115.17
84	At	39	PSU	N1-C2-N3	6.74	122.28	115.17
6	SA	2	SAC	OAC-C1A-C2A	-6.72	110.09	122.05
3	L5	3764	PSU	N1-C2-N3	6.72	122.25	115.17
3	L5	4361	PSU	N1-C2-N3	6.72	122.25	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1326	UY1	N1-C2-N3	6.72	122.25	115.17
3	L5	3768	PSU	N1-C2-N3	6.71	122.25	115.17
3	L5	1779	PSU	N1-C2-N3	6.70	122.24	115.17
84	At	32	PSU	N1-C2-N3	6.70	122.24	115.17
3	L5	1860	PSU	N1-C2-N3	6.69	122.22	115.17
3	L5	3729	PSU	N1-C2-N3	6.68	122.22	115.17
3	L5	3770	PSU	N1-C2-N3	6.68	122.21	115.17
3	L5	3762	PSU	N1-C2-N3	6.67	122.21	115.17
3	L5	2876	OMG	C5-C4-N3	-6.66	117.79	128.39
1	S2	218	PSU	N1-C2-N3	6.66	122.19	115.17
1	S2	36	PSU	N1-C2-N3	6.65	122.19	115.17
1	S2	296	PSU	N1-C2-N3	6.65	122.18	115.17
1	S2	815	PSU	N1-C2-N3	6.64	122.17	115.17
1	S2	814	PSU	N1-C2-N3	6.64	122.17	115.17
1	S2	1367	PSU	N1-C2-N3	6.63	122.16	115.17
1	S2	1347	PSU	N1-C2-N3	6.62	122.15	115.17
1	S2	1625	PSU	N1-C2-N3	6.61	122.14	115.17
3	L5	4552	PSU	N1-C2-N3	6.60	122.13	115.17
3	L5	2424	OMG	C5-C4-N3	-6.57	117.93	128.39
3	L5	3639	PSU	N1-C2-N3	6.57	122.10	115.17
3	L5	5010	PSU	N1-C2-N3	6.56	122.09	115.17
1	S2	649	PSU	N1-C2-N3	6.55	122.08	115.17
3	L5	2508	PSU	N1-C2-N3	6.55	122.08	115.17
3	L5	3920	PSU	N1-C2-N3	6.55	122.08	115.17
2	L8	55	PSU	N1-C2-N3	6.55	122.08	115.17
3	L5	1744	PSU	N1-C2-N3	6.54	122.07	115.17
3	L5	4312	PSU	N1-C2-N3	6.54	122.07	115.17
3	L5	4457	PSU	N1-C2-N3	6.54	122.06	115.17
3	L5	4576	PSU	N1-C2-N3	6.54	122.06	115.17
3	L5	3734	PSU	N1-C2-N3	6.53	122.06	115.17
3	L5	4972	PSU	N1-C2-N3	6.53	122.05	115.17
1	S2	406	PSU	N1-C2-N3	6.52	122.05	115.17
1	S2	1639	G7M	C8-N7-C5	6.52	115.93	107.78
1	S2	34	PSU	N1-C2-N3	6.51	122.04	115.17
3	L5	3884	PSU	N1-C2-N3	6.51	122.03	115.17
1	S2	966	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	2839	PSU	N1-C2-N3	6.50	122.02	115.17
3	L5	4299	PSU	N1-C2-N3	6.50	122.02	115.17
1	S2	1445	PSU	N1-C2-N3	6.49	122.02	115.17
85	Pt	8	4SU	C4-N3-C2	-6.49	121.10	127.31
3	L5	2843	PSU	N1-C2-N3	6.49	122.01	115.17
3	L5	4689	PSU	N1-C2-N3	6.47	121.99	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4500	PSU	N1-C2-N3	6.47	121.99	115.17
3	L5	1792	PSU	N1-C2-N3	6.44	121.97	115.17
3	L5	3844	PSU	N1-C2-N3	6.43	121.95	115.17
3	L5	3715	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	1238	PSU	N1-C2-N3	6.43	121.95	115.17
3	L5	4423	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	651	PSU	N1-C2-N3	6.42	121.94	115.17
1	S2	609	PSU	N1-C2-N3	6.41	121.93	115.17
3	L5	3851	PSU	N1-C2-N3	6.41	121.93	115.17
3	L5	4493	PSU	N1-C2-N3	6.41	121.93	115.17
1	S2	681	PSU	N1-C2-N3	6.41	121.93	115.17
3	L5	4296	PSU	N1-C2-N3	6.39	121.91	115.17
3	L5	1625	OMG	C5-C4-N3	-6.38	118.23	128.39
3	L5	1781	PSU	N1-C2-N3	6.38	121.90	115.17
1	S2	1328	OMG	C5-C4-N3	-6.37	118.25	128.39
1	S2	1004	PSU	N1-C2-N3	6.36	121.88	115.17
85	Pt	8	4SU	C5-C4-N3	6.35	120.65	114.75
3	L5	5001	PSU	N1-C2-N3	6.34	121.86	115.17
1	S2	1177	PSU	N1-C2-N3	6.34	121.86	115.17
3	L5	1536	PSU	N1-C2-N3	6.34	121.86	115.17
3	L5	1782	PSU	N1-C2-N3	6.33	121.85	115.17
1	S2	1081	PSU	N1-C2-N3	6.33	121.85	115.17
1	S2	1239	PSU	N1-C2-N3	6.33	121.84	115.17
3	L5	1677	PSU	N1-C2-N3	6.32	121.83	115.17
3	L5	3695	PSU	N1-C2-N3	6.32	121.83	115.17
3	L5	3792	OMG	C5-C4-N3	-6.31	118.35	128.39
3	L5	1683	PSU	N1-C2-N3	6.31	121.82	115.17
85	Pt	56	PSU	N1-C2-N3	6.31	121.82	115.17
1	S2	863	PSU	N1-C2-N3	6.31	121.82	115.17
1	S2	436	OMG	C5-C4-N3	-6.30	118.36	128.39
1	S2	1692	PSU	N1-C2-N3	6.30	121.82	115.17
3	L5	1582	PSU	N1-C2-N3	6.29	121.81	115.17
3	L5	4673	PSU	N1-C2-N3	6.27	121.78	115.17
3	L5	2632	PSU	N1-C2-N3	6.25	121.76	115.17
3	L5	4471	PSU	N1-C2-N3	6.24	121.75	115.17
1	S2	1136	PSU	N1-C2-N3	6.24	121.75	115.17
3	L5	3818	UY1	N1-C2-N3	6.19	121.69	115.17
1	S2	1447	OMG	C5-C4-N3	-6.18	118.56	128.39
3	L5	4431	PSU	N1-C2-N3	6.17	121.67	115.17
1	S2	166	A2M	C5-C4-N3	-6.17	118.23	126.72
3	L5	4370	OMG	C5-C4-N3	-6.16	118.58	128.39
1	S2	1490	OMG	C5-C4-N3	-6.16	118.59	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	801	PSU	N1-C2-N3	6.15	121.65	115.17
1	S2	509	OMG	C5-C4-N3	-6.14	118.62	128.39
3	L5	3853	PSU	N1-C2-N3	6.13	121.64	115.17
1	S2	119	PSU	N1-C2-N3	6.11	121.61	115.17
3	L5	4523	A2M	C5-C4-N3	-6.10	118.31	126.72
2	L8	75	OMG	C5-C4-N3	-6.09	118.69	128.39
1	S2	867	OMG	C5-C4-N3	-6.09	118.70	128.39
3	L5	4392	OMG	C5-C4-N3	-6.09	118.70	128.39
3	L5	3899	OMG	C5-C4-N3	-6.08	118.72	128.39
1	S2	590	A2M	C5-C4-N3	-6.07	118.36	126.72
3	L5	1316	OMG	C5-C4-N3	-6.05	118.76	128.39
3	L5	3744	OMG	C5-C4-N3	-6.04	118.77	128.39
3	L5	4637	OMG	C5-C4-N3	-6.02	118.81	128.39
1	S2	644	OMG	C5-C4-N3	-6.00	118.84	128.39
84	At	8	4SU	C5-C4-N3	5.99	120.33	114.75
3	L5	4420	PSU	N1-C2-N3	5.99	121.49	115.17
3	L5	4196	OMG	C5-C4-N3	-5.99	118.85	128.39
3	L5	2364	OMG	C5-C4-N3	-5.98	118.87	128.39
1	S2	484	A2M	C5-C4-N3	-5.98	118.48	126.72
1	S2	601	OMG	C5-C4-N3	-5.97	118.89	128.39
3	L5	4571	A2M	C5-C4-N3	-5.97	118.50	126.72
3	L5	2401	A2M	C5-C4-N3	-5.95	118.53	126.72
3	L5	1524	A2M	C5-C4-N3	-5.95	118.53	126.72
3	L5	2363	A2M	C5-C4-N3	-5.91	118.59	126.72
1	S2	1643	PSU	N1-C2-N3	5.90	121.39	115.17
3	L5	4618	OMG	C5-C4-N3	-5.90	119.00	128.39
1	S2	27	A2M	C5-C4-N3	-5.90	118.60	126.72
1	S2	99	A2M	C5-C4-N3	-5.89	118.60	126.72
3	L5	4220	6MZ	C5-C4-N3	-5.89	118.60	126.72
3	L5	2815	A2M	C5-C4-N3	-5.88	118.62	126.72
3	L5	4494	OMG	C5-C4-N3	-5.87	119.04	128.39
84	At	37	MIA	N3-C4-N9	5.86	134.43	126.99
3	L5	3627	OMG	C5-C4-N3	-5.86	119.07	128.39
3	L5	3944	OMG	C5-C4-N3	-5.84	119.09	128.39
3	L5	4499	OMG	C5-C4-N3	-5.84	119.09	128.39
3	L5	3760	A2M	C5-C4-N3	-5.83	118.69	126.72
3	L5	1522	OMG	C5-C4-N3	-5.83	119.11	128.39
3	L5	1534	A2M	C5-C4-N3	-5.82	118.71	126.72
3	L5	3867	A2M	C5-C4-N3	-5.80	118.72	126.72
3	L5	398	A2M	C5-C4-N3	-5.80	118.74	126.72
1	S2	572	PSU	N1-C2-N3	5.80	121.28	115.17
1	S2	1832	6MZ	C5-C4-N3	-5.76	118.78	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1447	OMG	C2-N3-C4	5.74	122.19	112.30
3	L5	2787	A2M	C5-C4-N3	-5.74	118.82	126.72
1	S2	683	OMG	C5-C4-N3	-5.73	119.26	128.39
1	S2	1639	G7M	C5-C4-N3	-5.73	117.32	128.15
3	L5	400	A2M	C5-C4-N3	-5.70	118.87	126.72
1	S2	1678	A2M	C5-C4-N3	-5.68	118.90	126.72
1	S2	512	A2M	C5-C4-N3	-5.64	118.95	126.72
3	L5	3830	A2M	C5-C4-N3	-5.63	118.96	126.72
1	S2	159	A2M	C5-C4-N3	-5.61	118.99	126.72
3	L5	1326	A2M	C5-C4-N3	-5.60	119.00	126.72
1	S2	1031	A2M	C5-C4-N3	-5.58	119.03	126.72
3	L5	4228	OMG	C5-C4-N3	-5.52	119.60	128.39
3	L5	4590	A2M	C5-C4-N3	-5.52	119.12	126.72
3	L5	4623	OMG	C5-C4-N3	-5.48	119.67	128.39
3	L5	3724	A2M	C5-C4-N3	-5.47	119.18	126.72
3	L5	3785	A2M	C5-C4-N3	-5.46	119.20	126.72
1	S2	468	A2M	C5-C4-N3	-5.39	119.30	126.72
3	L5	3825	A2M	C5-C4-N3	-5.38	119.30	126.72
1	S2	1248	B8N	C4-N3-C2	-5.38	119.00	125.62
2	L8	75	OMG	C2-N3-C4	5.37	121.56	112.30
1	S2	1851	MA6	C5-C4-N3	-5.35	119.35	126.72
1	S2	1383	A2M	C5-C4-N3	-5.35	119.36	126.72
1	S2	436	OMG	C2-N3-C4	5.34	121.50	112.30
2	L8	14	OMU	C4-N3-C2	-5.31	120.02	126.61
3	L5	1871	A2M	C5-C4-N3	-5.31	119.41	126.72
1	S2	576	A2M	C5-C4-N3	-5.27	119.46	126.72
1	S2	668	A2M	C5-C4-N3	-5.19	119.56	126.72
1	S2	867	OMG	C2-N3-C4	5.19	121.24	112.30
3	L5	4392	OMG	C2-N3-C4	5.18	121.23	112.30
3	L5	3723	A2M	C5-C4-N3	-5.17	119.60	126.72
3	L5	2876	OMG	C2-N3-C4	5.17	121.20	112.30
3	L5	3744	OMG	C2-N3-C4	5.15	121.18	112.30
1	S2	1328	OMG	C2-N3-C4	5.15	121.17	112.30
3	L5	4196	OMG	C2-N3-C4	5.15	121.17	112.30
1	S2	683	OMG	C2-N3-C4	5.15	121.16	112.30
1	S2	627	OMU	C4-N3-C2	-5.13	120.24	126.61
3	L5	3792	OMG	C2-N3-C4	5.12	121.13	112.30
3	L5	3627	OMG	C2-N3-C4	5.11	121.09	112.30
1	S2	1850	MA6	C5-C4-N3	-5.10	119.69	126.72
3	L5	4370	OMG	C2-N3-C4	5.10	121.08	112.30
3	L5	3899	OMG	C2-N3-C4	5.08	121.05	112.30
1	S2	99	A2M	N3-C4-N9	5.06	135.76	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1490	OMG	C2-N3-C4	5.05	121.00	112.30
3	L5	3718	A2M	C5-C4-N3	-5.04	119.77	126.72
1	S2	601	OMG	C2-N3-C4	5.04	120.98	112.30
3	L5	2837	OMU	C4-N3-C2	-5.03	120.36	126.61
3	L5	2364	OMG	C2-N3-C4	5.02	120.95	112.30
3	L5	4498	OMU	C4-N3-C2	-5.02	120.38	126.61
3	L5	4618	OMG	C2-N3-C4	5.02	120.94	112.30
1	S2	1804	OMU	C4-N3-C2	-5.01	120.39	126.61
3	L5	1625	OMG	C2-N3-C4	5.01	120.92	112.30
3	L5	4499	OMG	C2-N3-C4	5.00	120.92	112.30
1	S2	354	OMU	C4-N3-C2	-5.00	120.41	126.61
3	L5	1522	OMG	C2-N3-C4	4.98	120.88	112.30
3	L5	4623	OMG	C2-N3-C4	4.98	120.87	112.30
3	L5	1625	OMG	N9-C4-N3	4.97	135.90	125.95
3	L5	3944	OMG	C2-N3-C4	4.97	120.86	112.30
3	L5	2876	OMG	N9-C4-N3	4.97	135.89	125.95
1	S2	644	OMG	C2-N3-C4	4.96	120.85	112.30
84	At	37	MIA	C11-S10-C2	-4.96	98.53	102.25
3	L5	4571	A2M	N3-C4-N9	4.96	135.60	127.17
3	L5	1316	OMG	C2-N3-C4	4.96	120.84	112.30
3	L5	4637	OMG	C2-N3-C4	4.94	120.81	112.30
3	L5	4523	A2M	N3-C4-N9	4.94	135.56	127.17
3	L5	4227	OMU	C4-N3-C2	-4.94	120.48	126.61
1	S2	590	A2M	N3-C4-N9	4.93	135.56	127.17
1	S2	166	A2M	N3-C4-N9	4.93	135.56	127.17
3	L5	2424	OMG	N9-C4-N3	4.92	135.79	125.95
3	L5	3867	A2M	N3-C4-N9	4.92	135.53	127.17
3	L5	4494	OMG	C2-N3-C4	4.92	120.77	112.30
3	L5	3925	OMU	C4-N3-C2	-4.90	120.52	126.61
1	S2	172	OMU	C4-N3-C2	-4.90	120.53	126.61
3	L5	3637	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L5	2815	A2M	N3-C4-N9	4.89	135.49	127.17
3	L5	4636	PSU	C4-N3-C2	-4.89	119.64	126.37
1	S2	428	OMU	C4-N3-C2	-4.85	120.59	126.61
3	L5	4228	OMG	C2-N3-C4	4.85	120.64	112.30
3	L5	3792	OMG	N9-C4-N3	4.84	135.63	125.95
6	SA	2	SAC	C-CA-N	-4.82	100.20	109.50
3	L5	4220	6MZ	N3-C4-N9	4.81	135.35	127.17
3	L5	4521	PSU	C4-N3-C2	-4.81	119.74	126.37
1	S2	436	OMG	N9-C4-N3	4.81	135.57	125.95
1	S2	509	OMG	C2-N3-C4	4.80	120.56	112.30
1	S2	1442	OMU	C4-N3-C2	-4.80	120.66	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3758	PSU	C4-N3-C2	-4.78	119.79	126.37
3	L5	2401	A2M	N3-C4-N9	4.77	135.27	127.17
1	S2	1326	UY1	C4-N3-C2	-4.76	119.81	126.37
3	L5	1524	A2M	N3-C4-N9	4.75	135.25	127.17
3	L5	2424	OMG	C2-N3-C4	4.74	120.47	112.30
1	S2	484	A2M	N3-C4-N9	4.72	135.19	127.17
3	L5	2415	OMU	C4-N3-C2	-4.71	120.77	126.61
3	L5	4531	PSU	C4-N3-C2	-4.69	119.91	126.37
3	L5	1534	A2M	N3-C4-N9	4.67	135.12	127.17
2	L8	14	OMU	C5-C4-N3	4.66	121.33	114.80
3	L5	4620	OMU	N3-C2-N1	4.66	120.96	114.89
3	L5	1322	1MA	C5-C4-N3	-4.66	120.41	127.27
3	L5	3762	PSU	C4-N3-C2	-4.65	119.97	126.37
3	L5	4628	PSU	O2-C2-N1	-4.64	118.00	122.79
3	L5	1326	A2M	N3-C4-N9	4.63	135.05	127.17
1	S2	218	PSU	C4-N3-C2	-4.63	119.99	126.37
1	S2	1244	PSU	C4-N3-C2	-4.62	120.01	126.37
3	L5	4370	OMG	N9-C4-N3	4.60	135.16	125.95
3	L5	2363	A2M	N3-C4-N9	4.60	134.99	127.17
2	L8	75	OMG	N9-C4-N3	4.60	135.15	125.95
1	S2	512	A2M	N3-C4-N9	4.60	134.99	127.17
3	L5	400	A2M	N3-C4-N9	4.60	134.99	127.17
84	At	32	PSU	C4-N3-C2	-4.60	120.03	126.37
1	S2	105	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	4532	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	1582	PSU	C4-N3-C2	-4.59	120.05	126.37
1	S2	27	A2M	N3-C4-N9	4.59	134.97	127.17
1	S2	1056	PSU	C4-N3-C2	-4.58	120.06	126.37
3	L5	3760	A2M	N3-C4-N9	4.58	134.95	127.17
3	L5	3785	A2M	O4'-C1'-N9	4.57	116.87	108.09
1	S2	867	OMG	N9-C4-N3	4.57	135.09	125.95
1	S2	1328	OMG	N9-C4-N3	4.57	135.09	125.95
1	S2	509	OMG	N9-C4-N3	4.56	135.06	125.95
1	S2	93	PSU	C4-N3-C2	-4.55	120.11	126.37
3	L5	4637	OMG	N9-C4-N3	4.54	135.04	125.95
3	L5	4442	PSU	C4-N3-C2	-4.54	120.12	126.37
3	L5	4196	OMG	N9-C4-N3	4.51	134.97	125.95
2	L8	69	PSU	C4-N3-C2	-4.51	120.16	126.37
3	L5	3639	PSU	C4-N3-C2	-4.50	120.17	126.37
3	L5	2364	OMG	N9-C4-N3	4.50	134.96	125.95
85	Pt	47	G7M	N9-C8-N7	-4.50	101.56	112.48
1	S2	681	PSU	C4-N3-C2	-4.49	120.18	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1678	A2M	N3-C4-N9	4.49	134.80	127.17
3	L5	4306	OMU	C4-N3-C2	-4.49	121.04	126.61
3	L5	3899	OMG	N9-C4-N3	4.48	134.91	125.95
3	L5	3830	A2M	N3-C4-N9	4.48	134.78	127.17
1	S2	822	PSU	C4-N3-C2	-4.48	120.21	126.37
3	L5	1316	OMG	N9-C4-N3	4.47	134.90	125.95
1	S2	121	OMU	C4-N3-C2	-4.47	121.06	126.61
1	S2	1832	6MZ	N3-C4-N9	4.47	134.76	127.17
3	L5	3830	A2M	C2'-C1'-N9	-4.46	106.41	113.75
3	L5	4403	PSU	C4-N3-C2	-4.45	120.24	126.37
3	L5	2787	A2M	N3-C4-N9	4.45	134.73	127.17
3	L5	4494	OMG	N9-C4-N3	4.45	134.84	125.95
1	S2	1639	G7M	C8-N9-C4	4.44	118.09	107.09
1	S2	121	OMU	N3-C2-N1	4.44	120.67	114.89
3	L5	1862	PSU	C4-N3-C2	-4.43	120.27	126.37
29	SV	1	AME	CT2-CT1-N	-4.43	108.77	116.12
3	L5	4498	OMU	N3-C2-N1	4.42	120.64	114.89
3	L5	4628	PSU	C4-N3-C2	-4.42	120.28	126.37
1	S2	354	OMU	N3-C2-N1	4.42	120.64	114.89
1	S2	1639	G7M	C2-N3-C4	4.42	119.91	112.30
3	L5	398	A2M	N3-C4-N9	4.41	134.68	127.17
85	Pt	8	4SU	C5-C4-S4	-4.41	119.26	124.31
1	S2	644	OMG	N9-C4-N3	4.41	134.78	125.95
3	L5	2843	PSU	C4-N3-C2	-4.41	120.30	126.37
3	L5	1322	1MA	C2-N3-C4	4.41	121.17	112.53
1	S2	296	PSU	C4-N3-C2	-4.41	120.30	126.37
1	S2	1850	MA6	C2-N1-C6	4.40	122.59	111.83
3	L5	2837	OMU	N3-C2-N1	4.40	120.62	114.89
1	S2	814	PSU	C4-N3-C2	-4.40	120.31	126.37
1	S2	1625	PSU	C4-N3-C2	-4.40	120.31	126.37
3	L5	4590	A2M	N3-C4-N9	4.40	134.64	127.17
84	At	46	G7M	N9-C8-N7	-4.39	101.81	112.48
3	L5	4296	PSU	C4-N3-C2	-4.38	120.33	126.37
1	S2	1031	A2M	N3-C4-N9	4.38	134.62	127.17
2	L8	14	OMU	N3-C2-N1	4.38	120.59	114.89
1	S2	36	PSU	C4-N3-C2	-4.38	120.34	126.37
3	L5	3920	PSU	C4-N3-C2	-4.38	120.34	126.37
1	S2	296	PSU	O2-C2-N1	-4.38	118.28	122.79
3	L5	1871	A2M	N3-C4-N9	4.38	134.61	127.17
1	S2	1288	OMU	C4-N3-C2	-4.37	121.18	126.61
3	L5	4457	PSU	C4-N3-C2	-4.37	120.35	126.37
1	S2	166	A2M	C2'-C1'-N9	-4.37	106.56	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	119	PSU	C4-N3-C2	-4.37	120.35	126.37
1	S2	1490	OMG	N9-C4-N3	4.37	134.69	125.95
1	S2	601	OMG	N9-C4-N3	4.36	134.68	125.95
1	S2	866	PSU	C4-N3-C2	-4.36	120.36	126.37
3	L5	4353	PSU	C4-N3-C2	-4.35	120.37	126.37
3	L5	5001	PSU	C4-N3-C2	-4.35	120.38	126.37
3	L5	1779	PSU	C4-N3-C2	-4.35	120.38	126.37
1	S2	159	A2M	N3-C4-N9	4.35	134.57	127.17
3	L5	4972	PSU	C4-N3-C2	-4.35	120.38	126.37
1	S2	468	A2M	N3-C4-N9	4.34	134.56	127.17
3	L5	2839	PSU	C4-N3-C2	-4.34	120.39	126.37
3	L5	3724	A2M	N3-C4-N9	4.34	134.55	127.17
1	S2	1367	PSU	C4-N3-C2	-4.33	120.40	126.37
3	L5	4361	PSU	C4-N3-C2	-4.33	120.40	126.37
1	S2	1243	PSU	C4-N3-C2	-4.33	120.41	126.37
3	L5	3844	PSU	C4-N3-C2	-4.32	120.42	126.37
3	L5	4312	PSU	C4-N3-C2	-4.32	120.42	126.37
3	L5	3925	OMU	N3-C2-N1	4.31	120.50	114.89
1	S2	34	PSU	C4-N3-C2	-4.31	120.44	126.37
1	S2	683	OMG	N9-C4-N3	4.31	134.57	125.95
1	S2	172	OMU	N3-C2-N1	4.31	120.50	114.89
3	L5	2508	PSU	C4-N3-C2	-4.31	120.44	126.37
1	S2	1288	OMU	N3-C2-N1	4.30	120.49	114.89
3	L5	4576	PSU	C4-N3-C2	-4.30	120.44	126.37
1	S2	686	PSU	C4-N3-C2	-4.30	120.45	126.37
3	L5	4552	PSU	C4-N3-C2	-4.30	120.45	126.37
1	S2	1851	MA6	C2-N1-C6	4.29	122.31	111.83
1	S2	1643	PSU	C4-N3-C2	-4.29	120.46	126.37
3	L5	4431	PSU	C4-N3-C2	-4.29	120.46	126.37
3	L5	3785	A2M	N3-C4-N9	4.29	134.47	127.17
1	S2	1804	OMU	N3-C2-N1	4.29	120.47	114.89
3	L5	1862	PSU	O2-C2-N1	-4.28	118.37	122.79
3	L5	3770	PSU	C4-N3-C2	-4.28	120.48	126.37
1	S2	354	OMU	C5-C4-N3	4.27	120.79	114.80
3	L5	4392	OMG	N9-C4-N3	4.27	134.50	125.95
3	L5	3818	UY1	C4-N3-C2	-4.27	120.48	126.37
2	L8	55	PSU	C4-N3-C2	-4.27	120.48	126.37
3	L5	4299	PSU	C4-N3-C2	-4.27	120.48	126.37
3	L5	4499	OMG	N9-C4-N3	4.26	134.48	125.95
1	S2	1239	PSU	C4-N3-C2	-4.26	120.50	126.37
3	L5	1782	PSU	C4-N3-C2	-4.26	120.50	126.37
3	L5	5010	PSU	C4-N3-C2	-4.26	120.50	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3723	A2M	N3-C4-N9	4.26	134.41	127.17
3	L5	3744	OMG	N9-C4-N3	4.26	134.47	125.95
3	L5	3851	PSU	C4-N3-C2	-4.25	120.51	126.37
1	S2	627	OMU	N3-C2-N1	4.25	120.43	114.89
1	S2	918	PSU	C4-N3-C2	-4.25	120.52	126.37
1	S2	651	PSU	C4-N3-C2	-4.25	120.52	126.37
3	L5	3944	OMG	N9-C4-N3	4.25	134.44	125.95
3	L5	1536	PSU	C4-N3-C2	-4.24	120.53	126.37
1	S2	1692	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	4227	OMU	N3-C2-N1	4.23	120.40	114.89
3	L5	4493	PSU	C4-N3-C2	-4.22	120.55	126.37
3	L5	1677	PSU	C4-N3-C2	-4.22	120.56	126.37
1	S2	1238	PSU	C4-N3-C2	-4.22	120.56	126.37
84	At	8	4SU	C5-C4-S4	-4.22	119.49	124.31
1	S2	815	PSU	C4-N3-C2	-4.21	120.57	126.37
1	S2	436	OMG	C2'-C1'-N9	-4.21	106.25	114.24
1	S2	1347	PSU	C4-N3-C2	-4.21	120.57	126.37
3	L5	3729	PSU	C4-N3-C2	-4.21	120.57	126.37
3	L5	4618	OMG	N9-C4-N3	4.21	134.37	125.95
3	L5	3944	OMG	C2'-C1'-N9	-4.20	106.26	114.24
1	S2	668	A2M	N3-C4-N9	4.20	134.31	127.17
1	S2	1004	PSU	C4-N3-C2	-4.20	120.59	126.37
3	L5	4306	OMU	N3-C2-N1	4.20	120.35	114.89
3	L5	3825	A2M	N3-C4-N9	4.20	134.30	127.17
3	L5	4579	PSU	C4-N3-C2	-4.20	120.59	126.37
3	L5	1744	PSU	C4-N3-C2	-4.19	120.59	126.37
84	At	39	PSU	C4-N3-C2	-4.19	120.60	126.37
84	At	8	4SU	N3-C2-N1	4.19	120.34	114.89
3	L5	3627	OMG	N9-C4-N3	4.18	134.32	125.95
3	L5	4569	PSU	C4-N3-C2	-4.18	120.61	126.37
3	L5	1522	OMG	N9-C4-N3	4.18	134.31	125.95
3	L5	4293	PSU	C4-N3-C2	-4.18	120.62	126.37
85	Pt	56	PSU	C4-N3-C2	-4.18	120.62	126.37
1	S2	686	PSU	O2-C2-N1	-4.18	118.48	122.79
1	S2	1081	PSU	C4-N3-C2	-4.17	120.62	126.37
1	S2	1442	OMU	C5-C4-N3	4.17	120.64	114.80
1	S2	1232	PSU	C4-N3-C2	-4.17	120.63	126.37
1	S2	1445	PSU	C4-N3-C2	-4.16	120.64	126.37
3	L5	4500	PSU	C4-N3-C2	-4.15	120.65	126.37
1	S2	109	PSU	C4-N3-C2	-4.15	120.66	126.37
3	L5	2415	OMU	N3-C2-N1	4.15	120.29	114.89
3	L5	4423	PSU	C4-N3-C2	-4.14	120.67	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4447	5MC	C5-C6-N1	-4.13	118.82	123.31
1	S2	649	PSU	C4-N3-C2	-4.13	120.68	126.37
3	L5	1781	PSU	C4-N3-C2	-4.13	120.68	126.37
1	S2	1177	PSU	C4-N3-C2	-4.13	120.68	126.37
3	L5	3695	PSU	C4-N3-C2	-4.13	120.68	126.37
1	S2	1447	OMG	N9-C4-N3	4.13	134.21	125.95
3	L5	3729	PSU	O2-C2-N1	-4.13	118.53	122.79
1	S2	1383	A2M	N3-C4-N9	4.13	134.19	127.17
1	S2	1174	PSU	C4-N3-C2	-4.12	120.69	126.37
1	S2	1639	G7M	C1'-N9-C8	-4.12	112.84	126.74
1	S2	627	OMU	C5-C4-N3	4.12	120.56	114.80
3	L5	2415	OMU	C5-C4-N3	4.11	120.56	114.80
3	L5	1860	PSU	C4-N3-C2	-4.11	120.70	126.37
1	S2	1625	PSU	O2-C2-N1	-4.11	118.55	122.79
1	S2	1136	PSU	C4-N3-C2	-4.11	120.72	126.37
1	S2	109	PSU	O2-C2-N1	-4.10	118.56	122.79
2	L8	69	PSU	O2-C2-N1	-4.10	118.56	122.79
3	L5	4620	OMU	C4-N3-C2	-4.10	121.53	126.61
3	L5	1677	PSU	O2-C2-N1	-4.09	118.57	122.79
3	L5	4442	PSU	O2-C2-N1	-4.09	118.57	122.79
1	S2	428	OMU	N3-C2-N1	4.08	120.20	114.89
1	S2	822	PSU	O2-C2-N1	-4.08	118.59	122.79
1	S2	573	PSU	C4-N3-C2	-4.06	120.78	126.37
1	S2	116	OMU	N3-C2-N1	4.06	120.17	114.89
84	At	37	MIA	C15-C14-C13	-4.05	110.50	122.66
1	S2	1804	OMU	C5-C4-N3	4.05	120.47	114.80
39	LA	216	V5N	CD2-CG-ND1	4.04	111.20	105.76
3	L5	3734	PSU	C4-N3-C2	-4.04	120.81	126.37
1	S2	1851	MA6	N3-C4-N9	4.04	134.03	127.17
3	L5	1792	PSU	C4-N3-C2	-4.03	120.82	126.37
3	L5	4228	OMG	N9-C4-N3	4.03	134.01	125.95
3	L5	2839	PSU	O2-C2-N1	-4.02	118.64	122.79
3	L5	3715	PSU	C4-N3-C2	-4.02	120.83	126.37
3	L5	4227	OMU	C5-C4-N3	4.01	120.41	114.80
1	S2	1850	MA6	N3-C4-N9	4.01	133.98	127.17
3	L5	4623	OMG	C6-C5-N7	4.00	137.57	130.29
1	S2	863	PSU	C4-N3-C2	-4.00	120.86	126.37
1	S2	509	OMG	C2'-C1'-N9	-3.99	106.66	114.24
1	S2	1248	B8N	C31-N3-C4	3.98	122.82	117.18
3	L5	2632	PSU	C4-N3-C2	-3.98	120.89	126.37
1	S2	572	PSU	C4-N3-C2	-3.98	120.89	126.37
3	L5	3925	OMU	C5-C4-N3	3.97	120.36	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	At	37	MIA	C16-C14-C13	-3.97	110.74	122.66
3	L5	3853	PSU	C4-N3-C2	-3.97	120.91	126.37
3	L5	2837	OMU	C5-C4-N3	3.96	120.35	114.80
3	L5	4579	PSU	O2-C2-N1	-3.96	118.70	122.79
1	S2	576	A2M	C2'-C1'-N9	-3.96	107.23	113.75
1	S2	428	OMU	C5-C4-N3	3.96	120.34	114.80
3	L5	4353	PSU	O2-C2-N1	-3.95	118.71	122.79
3	L5	1744	PSU	O2-C2-N1	-3.94	118.72	122.79
1	S2	166	A2M	C2-N3-C4	3.94	121.45	111.83
3	L5	3718	A2M	N3-C4-N9	3.94	133.87	127.17
3	L5	4500	PSU	O2-C2-N1	-3.93	118.73	122.79
3	L5	4689	PSU	C4-N3-C2	-3.93	120.95	126.37
3	L5	4498	OMU	C5-C4-N3	3.93	120.30	114.80
1	S2	121	OMU	C5-C4-N3	3.91	120.28	114.80
3	L5	4673	PSU	C4-N3-C2	-3.91	120.99	126.37
3	L5	4494	OMG	C2'-C1'-N9	-3.90	106.84	114.24
1	S2	576	A2M	N3-C4-N9	3.90	133.79	127.17
1	S2	866	PSU	O2-C2-N1	-3.89	118.77	122.79
3	L5	3770	PSU	O2-C2-N1	-3.89	118.77	122.79
1	S2	1442	OMU	N3-C2-N1	3.89	119.95	114.89
1	S2	172	OMU	C5-C4-N3	3.88	120.24	114.80
3	L5	4471	PSU	C4-N3-C2	-3.88	121.03	126.37
1	S2	590	A2M	C2-N3-C4	3.87	121.29	111.83
1	S2	1056	PSU	O2-C2-N1	-3.87	118.79	122.79
1	S2	1851	MA6	C4-C5-N7	-3.86	106.17	110.58
1	S2	512	A2M	C2'-C1'-N9	-3.86	107.40	113.75
84	At	32	PSU	O2-C2-N1	-3.86	118.81	122.79
1	S2	649	PSU	O2-C2-N1	-3.85	118.82	122.79
3	L5	4431	PSU	O2-C2-N1	-3.85	118.82	122.79
3	L5	4576	PSU	O2-C2-N1	-3.84	118.82	122.79
1	S2	99	A2M	C2'-C1'-N9	-3.84	107.42	113.75
3	L5	4521	PSU	C3'-C2'-C1'	3.84	106.22	101.69
3	L5	3884	PSU	C4-N3-C2	-3.83	121.09	126.37
1	S2	801	PSU	C4-N3-C2	-3.83	121.10	126.37
3	L5	4623	OMG	N9-C4-N3	3.81	133.58	125.95
3	L5	2401	A2M	C2-N3-C4	3.81	121.14	111.83
1	S2	1383	A2M	C2'-C1'-N9	-3.81	107.48	113.75
3	L5	4569	PSU	O2-C2-N1	-3.81	118.86	122.79
3	L5	3760	A2M	C2-N3-C4	3.80	121.12	111.83
1	S2	1850	MA6	C4-C5-N7	-3.80	106.23	110.58
3	L5	4590	A2M	C2'-C1'-N9	-3.80	107.50	113.75
3	L5	4293	PSU	O2-C2-N1	-3.80	118.87	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1643	PSU	O2-C2-N1	-3.80	118.88	122.79
1	S2	27	A2M	C2-N3-C4	3.79	121.08	111.83
3	L5	4420	PSU	O2-C2-N1	-3.78	118.89	122.79
1	S2	1136	PSU	O2-C2-N1	-3.78	118.89	122.79
3	L5	3920	PSU	O2-C2-N1	-3.78	118.89	122.79
3	L5	3762	PSU	O2-C2-N1	-3.78	118.89	122.79
3	L5	3768	PSU	C4-N3-C2	-3.78	121.17	126.37
3	L5	4220	6MZ	C2-N3-C4	3.78	121.06	111.83
1	S2	1832	6MZ	C4-C5-N7	-3.77	106.27	110.58
1	S2	99	A2M	C2-N3-C4	3.77	121.04	111.83
1	S2	966	PSU	C4-N3-C2	-3.77	121.18	126.37
1	S2	1248	B8N	N3-C2-N1	3.76	121.32	116.72
3	L5	3851	PSU	O2-C2-N1	-3.76	118.91	122.79
1	S2	354	OMU	C2'-C1'-N1	-3.76	107.10	114.24
3	L5	4299	PSU	O2-C2-N1	-3.76	118.91	122.79
3	L5	1524	A2M	C2-N3-C4	3.76	121.01	111.83
1	S2	1337	4AC	N4-C4-N3	3.75	119.96	113.87
1	S2	966	PSU	O2-C2-N1	-3.74	118.93	122.79
1	S2	406	PSU	C4-N3-C2	-3.74	121.22	126.37
1	S2	815	PSU	O2-C2-N1	-3.73	118.94	122.79
3	L5	1871	A2M	N3-C2-N1	-3.73	122.93	128.58
3	L5	3844	PSU	O2-C2-N1	-3.73	118.94	122.79
1	S2	1004	PSU	O2-C2-N1	-3.73	118.94	122.79
1	S2	484	A2M	C2-N3-C4	3.73	120.93	111.83
3	L5	4403	PSU	O2-C2-N1	-3.72	118.95	122.79
1	S2	576	A2M	C4-C5-N7	-3.72	106.33	110.58
1	S2	1445	PSU	O2-C2-N1	-3.72	118.95	122.79
3	L5	2363	A2M	C2-N3-C4	3.72	120.92	111.83
1	S2	918	PSU	O2-C2-N1	-3.72	118.95	122.79
1	S2	1832	6MZ	C2-N3-C4	3.72	120.91	111.83
1	S2	1447	OMG	C6-C5-N7	3.72	137.05	130.29
3	L5	3639	PSU	O2-C2-N1	-3.71	118.96	122.79
3	L5	3785	A2M	C2-N3-C4	3.71	120.90	111.83
3	L5	4523	A2M	C2-N3-C4	3.71	120.89	111.83
3	L5	4552	PSU	O2-C2-N1	-3.71	118.97	122.79
1	S2	1288	OMU	C5-C4-N3	3.71	119.99	114.80
3	L5	4306	OMU	C5-C4-N3	3.71	119.99	114.80
3	L5	4590	A2M	C2-N3-C4	3.70	120.87	111.83
85	Pt	8	4SU	N3-C2-N1	3.70	119.70	114.89
1	S2	27	A2M	C2'-C1'-N9	-3.70	107.67	113.75
1	S2	1347	PSU	O2-C2-N1	-3.69	118.98	122.79
1	S2	1243	PSU	O2-C2-N1	-3.69	118.99	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1692	PSU	O2-C2-N1	-3.68	118.99	122.79
3	L5	4420	PSU	C4-N3-C2	-3.68	121.30	126.37
3	L5	2787	A2M	C2-N3-C4	3.67	120.80	111.83
1	S2	1367	PSU	O2-C2-N1	-3.67	119.00	122.79
1	S2	1326	UY1	O2-C2-N1	-3.67	119.00	122.79
3	L5	2815	A2M	C2-N3-C4	3.67	120.79	111.83
3	L5	4228	OMG	C6-C5-N7	3.66	136.96	130.29
3	L5	1534	A2M	C2-N3-C4	3.66	120.77	111.83
3	L5	3825	A2M	C2-N3-C4	3.66	120.76	111.83
1	S2	468	A2M	C2'-C1'-N9	-3.65	107.74	113.75
1	S2	1678	A2M	C2-N3-C4	3.65	120.76	111.83
3	L5	3764	PSU	C4-N3-C2	-3.65	121.34	126.37
1	S2	918	PSU	C3'-C2'-C1'	3.65	106.00	101.69
3	L5	1871	A2M	C2-N3-C4	3.65	120.74	111.83
1	S2	609	PSU	O2-C2-N1	-3.64	119.03	122.79
1	S2	1238	PSU	O2-C2-N1	-3.64	119.03	122.79
1	S2	1832	6MZ	C6-C5-N7	3.64	136.40	132.43
3	L5	398	A2M	C2-N3-C4	3.64	120.73	111.83
3	L5	1871	A2M	C2'-C1'-N9	-3.64	107.76	113.75
3	L5	3825	A2M	N3-C2-N1	-3.64	123.07	128.58
3	L5	4972	PSU	O2-C2-N1	-3.64	119.04	122.79
1	S2	668	A2M	C4-C5-N7	-3.64	106.42	110.58
3	L5	1782	PSU	O2-C2-N1	-3.64	119.04	122.79
3	L5	4532	PSU	O2-C2-N1	-3.64	119.04	122.79
3	L5	3724	A2M	C2-N3-C4	3.64	120.71	111.83
84	At	37	MIA	C6-C5-N7	3.63	136.38	132.43
3	L5	4590	A2M	N3-C2-N1	-3.63	123.09	128.58
1	S2	1639	G7M	CN7-N7-C5	3.62	131.32	126.80
3	L5	1326	A2M	C2-N3-C4	3.62	120.68	111.83
3	L5	4636	PSU	O2-C2-N1	-3.62	119.06	122.79
1	S2	116	OMU	C4-N3-C2	-3.61	122.13	126.61
1	S2	863	PSU	O2-C2-N1	-3.61	119.06	122.79
3	L5	4689	PSU	O2-C2-N1	-3.61	119.07	122.79
3	L5	3627	OMG	C6-C5-N7	3.61	136.86	130.29
1	S2	36	PSU	O2-C2-N1	-3.60	119.07	122.79
3	L5	1792	PSU	O2-C2-N1	-3.60	119.07	122.79
3	L5	3734	PSU	O2-C2-N1	-3.60	119.07	122.79
3	L5	3830	A2M	C2-N3-C4	3.60	120.62	111.83
1	S2	512	A2M	C2-N3-C4	3.60	120.62	111.83
1	S2	1177	PSU	O2-C2-N1	-3.60	119.08	122.79
85	Pt	56	PSU	O2-C2-N1	-3.59	119.08	122.79
3	L5	4423	PSU	O2-C2-N1	-3.59	119.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4220	6MZ	C9-N6-C6	-3.59	119.52	122.85
1	S2	406	PSU	O2-C2-N1	-3.59	119.09	122.79
3	L5	1683	PSU	C4-N3-C2	-3.59	121.43	126.37
1	S2	814	PSU	O2-C2-N1	-3.59	119.09	122.79
3	L5	2363	A2M	C4-C5-N7	-3.58	106.49	110.58
1	S2	1031	A2M	C2-N3-C4	3.58	120.57	111.83
3	L5	3695	PSU	O2-C2-N1	-3.58	119.10	122.79
1	S2	1442	OMU	O4-C4-C5	-3.58	119.00	125.16
3	L5	1536	PSU	O2-C2-N1	-3.57	119.10	122.79
1	S2	1851	MA6	C2-N3-C4	3.57	120.56	111.83
3	L5	4571	A2M	C2-N3-C4	3.57	120.55	111.83
3	L5	4530	UR3	C5-C4-N3	3.57	119.74	115.04
1	S2	822	PSU	C3'-C2'-C1'	3.57	105.90	101.69
1	S2	609	PSU	C4-N3-C2	-3.57	121.46	126.37
3	L5	400	A2M	C2-N3-C4	3.57	120.54	111.83
3	L5	1779	PSU	O2-C2-N1	-3.56	119.11	122.79
3	L5	3853	PSU	O2-C2-N1	-3.56	119.11	122.79
2	L8	55	PSU	O2-C2-N1	-3.55	119.13	122.79
1	S2	99	A2M	N3-C2-N1	-3.55	123.21	128.58
3	L5	400	A2M	C2'-C1'-N9	-3.54	107.92	113.75
1	S2	1328	OMG	C2'-C1'-N9	-3.54	107.52	114.24
3	L5	3867	A2M	C2-N3-C4	3.54	120.47	111.83
3	L5	4403	PSU	C3'-C2'-C1'	3.53	105.86	101.69
3	L5	4312	PSU	O2-C2-N1	-3.53	119.14	122.79
3	L5	3944	OMG	C6-C5-N7	3.53	136.71	130.29
3	L5	1781	PSU	O2-C2-N1	-3.53	119.15	122.79
1	S2	1174	PSU	O2-C2-N1	-3.53	119.15	122.79
3	L5	3723	A2M	C2-N3-C4	3.52	120.44	111.83
3	L5	4521	PSU	O2-C2-N1	-3.52	119.16	122.79
1	S2	159	A2M	C4-C5-N7	-3.52	106.56	110.58
3	L5	3760	A2M	N3-C2-N1	-3.52	123.26	128.58
3	L5	2401	A2M	N3-C2-N1	-3.51	123.26	128.58
3	L5	3724	A2M	N3-C2-N1	-3.51	123.26	128.58
3	L5	3785	A2M	C4-C5-N7	-3.51	106.56	110.58
1	S2	468	A2M	C2-N3-C4	3.51	120.40	111.83
3	L5	5010	PSU	O2-C2-N1	-3.50	119.18	122.79
1	S2	93	PSU	O2-C2-N1	-3.50	119.18	122.79
3	L5	3782	5MC	C5-C6-N1	-3.49	119.52	123.31
1	S2	484	A2M	C4-C5-N7	-3.49	106.59	110.58
1	S2	1383	A2M	C2-N3-C4	3.48	120.33	111.83
3	L5	1522	OMG	C6-C5-N7	3.48	136.62	130.29
3	L5	3723	A2M	N3-C2-N1	-3.48	123.32	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	C4-C5-N7	-3.47	106.61	110.58
3	L5	4296	PSU	O2-C2-N1	-3.47	119.21	122.79
3	L5	2508	PSU	O2-C2-N1	-3.47	119.21	122.79
3	L5	4392	OMG	C6-C5-N7	3.46	136.59	130.29
3	L5	3785	A2M	N3-C2-N1	-3.46	123.35	128.58
1	S2	1031	A2M	C4-C5-N7	-3.45	106.63	110.58
3	L5	4618	OMG	C6-C5-N7	3.45	136.57	130.29
1	S2	105	PSU	O2-C2-N1	-3.44	119.24	122.79
3	L5	3760	A2M	C4-C5-N7	-3.44	106.65	110.58
1	S2	1081	PSU	O2-C2-N1	-3.43	119.25	122.79
1	S2	27	A2M	C4-C5-N7	-3.43	106.66	110.58
1	S2	1678	A2M	C4-C5-N7	-3.43	106.66	110.58
3	L5	3758	PSU	O2-C2-N1	-3.43	119.25	122.79
3	L5	2843	PSU	O2-C2-N1	-3.43	119.25	122.79
1	S2	683	OMG	C6-C5-N7	3.43	136.52	130.29
1	S2	668	A2M	C2-N3-C4	3.43	120.20	111.83
3	L5	1524	A2M	C4-C5-N7	-3.42	106.67	110.58
1	S2	27	A2M	N3-C2-N1	-3.42	123.40	128.58
66	Lr	2	SAC	CB-CA-C	-3.42	103.83	111.35
1	S2	601	OMG	C6-C5-N7	3.42	136.51	130.29
1	S2	1850	MA6	C2-N3-C4	3.42	120.18	111.83
3	L5	4499	OMG	C6-C5-N7	3.41	136.50	130.29
1	S2	34	PSU	O2-C2-N1	-3.41	119.27	122.79
1	S2	590	A2M	N3-C2-N1	-3.41	123.42	128.58
3	L5	3744	OMG	C6-C5-N7	3.41	136.49	130.29
3	L5	398	A2M	C4-C5-N7	-3.40	106.70	110.58
3	L5	400	A2M	C4-C5-N7	-3.40	106.70	110.58
1	S2	651	PSU	O2-C2-N1	-3.39	119.29	122.79
2	L8	75	OMG	C2'-C1'-N9	-3.39	107.81	114.24
3	L5	4531	PSU	O2-C2-N1	-3.39	119.30	122.79
6	SA	2	SAC	C2A-C1A-N	-3.39	110.50	116.12
1	S2	1832	6MZ	N1-C2-N3	-3.39	123.46	128.58
1	S2	468	A2M	N3-C2-N1	-3.38	123.46	128.58
1	S2	1383	A2M	C4-C5-N7	-3.38	106.72	110.58
1	S2	159	A2M	C2-N3-C4	3.37	120.07	111.83
1	S2	681	PSU	O2-C2-N1	-3.37	119.31	122.79
3	L5	1534	A2M	C4-C5-N7	-3.37	106.73	110.58
3	L5	398	A2M	N3-C2-N1	-3.37	123.49	128.58
52	La	39	V5N	CD2-CG-ND1	3.36	110.28	105.76
3	L5	3830	A2M	C4-C5-N7	-3.35	106.75	110.58
1	S2	1244	PSU	O2-C2-N1	-3.35	119.33	122.79
1	S2	512	A2M	N3-C2-N1	-3.35	123.51	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L8	75	OMG	C6-C5-N7	3.35	136.38	130.29
1	S2	166	A2M	N3-C2-N1	-3.35	123.52	128.58
1	S2	1239	PSU	O2-C2-N1	-3.34	119.34	122.79
84	At	37	MIA	C4-C5-N7	-3.34	106.76	110.58
3	L5	4457	PSU	C6-C5-C4	-3.34	115.92	118.17
66	Lr	2	SAC	C2A-C1A-N	-3.34	110.58	116.12
1	S2	119	PSU	O2-C2-N1	-3.33	119.35	122.79
3	L5	4494	OMG	C6-C5-N7	3.33	136.35	130.29
3	L5	3884	PSU	O2-C2-N1	-3.33	119.36	122.79
84	At	39	PSU	O2-C2-N1	-3.32	119.36	122.79
1	S2	1490	OMG	C6-C5-N7	3.32	136.33	130.29
3	L5	3818	UY1	O2-C2-N1	-3.32	119.37	122.79
3	L5	4220	6MZ	N1-C2-N3	-3.32	123.56	128.58
1	S2	1678	A2M	N3-C2-N1	-3.32	123.56	128.58
3	L5	1326	A2M	N3-C2-N1	-3.31	123.58	128.58
3	L5	3899	OMG	C6-C5-N7	3.31	136.31	130.29
1	S2	590	A2M	C4-C5-N7	-3.30	106.80	110.58
1	S2	1851	MA6	N1-C2-N3	-3.30	123.58	128.58
3	L5	3830	A2M	N3-C2-N1	-3.30	123.59	128.58
1	S2	1328	OMG	C6-C5-N7	3.29	136.28	130.29
3	L5	4523	A2M	C4-C5-N7	-3.29	106.82	110.58
3	L5	3724	A2M	C2'-C1'-N9	-3.29	108.34	113.75
3	L5	4196	OMG	C6-C5-N7	3.28	136.27	130.29
3	L5	4637	OMG	C2'-C1'-N9	-3.28	108.01	114.24
1	S2	166	A2M	C4-C5-N7	-3.28	106.83	110.58
3	L5	2364	OMG	C6-C5-N7	3.28	136.25	130.29
1	S2	668	A2M	C4-N9-C8	3.27	109.17	105.74
3	L5	2401	A2M	C4-C5-N7	-3.27	106.84	110.58
3	L5	4618	OMG	C2'-C1'-N9	-3.26	108.05	114.24
3	L5	2787	A2M	N3-C2-N1	-3.25	123.66	128.58
1	S2	1031	A2M	N3-C2-N1	-3.25	123.66	128.58
1	S2	1232	PSU	O2-C2-N1	-3.25	119.44	122.79
3	L5	4620	OMU	C5-C4-N3	3.25	119.35	114.80
1	S2	576	A2M	C2-N3-C4	3.25	119.76	111.83
3	L5	3825	A2M	C4-C5-N7	-3.24	106.87	110.58
1	S2	218	PSU	O2-C2-N1	-3.24	119.45	122.79
1	S2	1850	MA6	N1-C2-N3	-3.23	123.69	128.58
3	L5	1316	OMG	C6-C5-N7	3.22	136.16	130.29
1	S2	436	OMG	C6-C5-N7	3.22	136.15	130.29
1	S2	867	OMG	C6-C5-N7	3.22	136.15	130.29
3	L5	3718	A2M	C4-C5-N7	-3.22	106.91	110.58
3	L5	3744	OMG	C2'-C1'-N9	-3.21	108.14	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1383	A2M	N3-C2-N1	-3.21	123.72	128.58
1	S2	627	OMU	O4-C4-C5	-3.21	119.63	125.16
1	S2	683	OMG	C2'-C1'-N9	-3.21	108.15	114.24
84	At	37	MIA	C2-N3-C4	3.20	120.68	112.29
1	S2	668	A2M	N3-C2-N1	-3.18	123.76	128.58
3	L5	4590	A2M	C4-C5-N7	-3.18	106.94	110.58
3	L5	3715	PSU	O2-C2-N1	-3.18	119.51	122.79
1	S2	484	A2M	N3-C2-N1	-3.18	123.77	128.58
3	L5	3718	A2M	C2-N3-C4	3.17	119.58	111.83
1	S2	1643	PSU	C3'-C2'-C1'	3.17	105.43	101.69
3	L5	2837	OMU	O4-C4-C5	-3.17	119.69	125.16
3	L5	4637	OMG	C6-C5-N7	3.17	136.06	130.29
3	L5	1534	A2M	N3-C2-N1	-3.17	123.79	128.58
3	L5	4623	OMG	C2'-C1'-N9	-3.16	108.24	114.24
1	S2	1445	PSU	C3'-C2'-C1'	3.16	105.42	101.69
3	L5	4370	OMG	C6-C5-N7	3.16	136.04	130.29
3	L5	4442	PSU	C3'-C2'-C1'	3.16	105.41	101.69
3	L5	2632	PSU	O2-C2-N1	-3.16	119.53	122.79
3	L5	3825	A2M	C2'-C1'-N9	-3.15	108.56	113.75
3	L5	3768	PSU	O2-C2-N1	-3.15	119.54	122.79
1	S2	644	OMG	C6-C5-N7	3.15	136.02	130.29
3	L5	3764	PSU	O2-C2-N1	-3.14	119.55	122.79
1	S2	512	A2M	C4-C5-N7	-3.14	106.99	110.58
1	S2	1804	OMU	O4-C4-C5	-3.14	119.74	125.16
1	S2	468	A2M	C4-C5-N7	-3.14	106.99	110.58
3	L5	4361	PSU	O2-C2-N1	-3.14	119.55	122.79
3	L5	2363	A2M	N3-C2-N1	-3.14	123.83	128.58
3	L5	2815	A2M	N3-C2-N1	-3.13	123.84	128.58
3	L5	1524	A2M	N3-C2-N1	-3.13	123.85	128.58
3	L5	1322	1MA	N9-C4-N3	3.12	134.02	126.90
1	S2	116	OMU	C5-C4-N3	3.12	119.17	114.80
3	L5	4498	OMU	O4-C4-C5	-3.11	119.80	125.16
3	L5	4220	6MZ	C4-C5-N7	-3.11	107.03	110.58
3	L5	3718	A2M	C2'-C1'-N9	-3.10	108.64	113.75
3	L5	400	A2M	N3-C2-N1	-3.10	123.89	128.58
3	L5	2415	OMU	O4-C4-C5	-3.10	119.82	125.16
3	L5	4523	A2M	N3-C2-N1	-3.09	123.90	128.58
3	L5	5001	PSU	O2-C2-N1	-3.09	119.60	122.79
2	L8	14	OMU	O4-C4-C5	-3.08	119.85	125.16
1	S2	509	OMG	C6-C5-N7	3.07	135.88	130.29
3	L5	3785	A2M	C4-N9-C8	3.07	108.96	105.74
3	L5	1860	PSU	O2-C2-N1	-3.06	119.63	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4493	PSU	O2-C2-N1	-3.06	119.63	122.79
3	L5	4571	A2M	N3-C2-N1	-3.06	123.95	128.58
1	S2	1842	4AC	C6-C5-C4	3.06	120.68	117.00
3	L5	4306	OMU	O4-C4-C5	-3.05	119.90	125.16
1	S2	573	PSU	O2-C2-N1	-3.05	119.64	122.79
3	L5	4571	A2M	C4-C5-N7	-3.04	107.10	110.58
3	L5	4227	OMU	O4-C4-C5	-3.04	119.92	125.16
3	L5	4457	PSU	O2-C2-N1	-3.03	119.66	122.79
1	S2	1850	MA6	C4-N9-C8	3.03	108.92	105.74
3	L5	3925	OMU	O4-C4-C5	-3.02	119.95	125.16
1	S2	428	OMU	O4-C4-C5	-3.01	119.97	125.16
3	L5	4636	PSU	C5-C6-N1	-3.00	117.98	122.14
40	LB	245	HIC	NE2-CE1-ND1	-2.99	111.52	112.66
3	L5	2815	A2M	C4-C5-N7	-2.99	107.16	110.58
3	L5	3724	A2M	C4-C5-N7	-2.99	107.16	110.58
1	S2	572	PSU	O2-C2-N1	-2.99	119.70	122.79
1	S2	172	OMU	O4-C4-C5	-2.99	120.01	125.16
2	L8	69	PSU	C3'-C2'-C1'	2.99	105.22	101.69
3	L5	4220	6MZ	C6-C5-N7	2.98	135.68	132.43
1	S2	644	OMG	C2'-C1'-N9	-2.98	108.59	114.24
3	L5	1871	A2M	C4-C5-N7	-2.97	107.19	110.58
3	L5	3808	OMC	O2-C2-N3	-2.97	117.65	122.33
3	L5	3867	A2M	N3-C2-N1	-2.96	124.09	128.58
3	L5	3723	A2M	C4-C5-N7	-2.96	107.20	110.58
3	L5	4457	PSU	C3'-C2'-C1'	2.96	105.18	101.69
3	L5	3723	A2M	C4-N9-C8	2.95	108.84	105.74
3	L5	3758	PSU	C5-C6-N1	-2.94	118.05	122.14
1	S2	1643	PSU	C6-C5-C4	-2.94	116.19	118.17
84	At	37	MIA	C4-N9-C8	2.94	108.83	105.74
3	L5	4620	OMU	C2'-C1'-N1	-2.94	108.66	114.24
1	S2	354	OMU	O4-C4-C5	-2.93	120.11	125.16
3	L5	1871	A2M	C4-N9-C8	2.91	108.79	105.74
1	S2	966	PSU	C3'-C2'-C1'	2.90	105.11	101.69
3	L5	1683	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	2401	A2M	C2'-C1'-N9	-2.89	109.00	113.75
3	L5	4523	A2M	C2'-C1'-N9	-2.89	109.00	113.75
3	L5	3792	OMG	C6-C5-N7	2.89	135.54	130.29
1	S2	1288	OMU	O4-C4-C5	-2.88	120.19	125.16
3	L5	1326	A2M	C4-C5-N7	-2.87	107.30	110.58
3	L5	2876	OMG	C6-C5-N7	2.87	135.51	130.29
2	L8	14	OMU	C2'-C1'-N1	-2.87	108.80	114.24
1	S2	116	OMU	O4-C4-C5	-2.87	120.22	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4447	5MC	C5-C4-N3	-2.86	118.82	121.75
1	S2	119	PSU	C6-C5-C4	-2.86	116.25	118.17
1	S2	1639	G7M	O6-C6-C5	-2.86	121.63	128.01
3	L5	3718	A2M	N3-C2-N1	-2.85	124.27	128.58
3	L5	3760	A2M	C4-N9-C8	2.84	108.72	105.74
1	S2	863	PSU	C6-C5-C4	-2.84	116.26	118.17
1	S2	99	A2M	C4-N9-C8	2.84	108.72	105.74
3	L5	4532	PSU	C5-C6-N1	-2.83	118.21	122.14
1	S2	1248	B8N	C1'-C5-C4	2.83	121.90	117.61
1	S2	172	OMU	O2'-C2'-C1'	2.83	114.35	108.99
3	L5	3770	PSU	C3'-C2'-C1'	2.82	105.02	101.69
3	L5	1625	OMG	C6-C5-N7	2.82	135.42	130.29
1	S2	1288	OMU	C2'-C1'-N1	-2.81	108.91	114.24
3	L5	400	A2M	C4-N9-C8	2.80	108.68	105.74
6	SA	2	SAC	CB-CA-C	-2.80	105.18	111.35
1	S2	1678	A2M	C4-N9-C8	2.80	108.68	105.74
3	L5	3867	A2M	C4-N9-C8	2.79	108.67	105.74
1	S2	468	A2M	C4-N9-C8	2.78	108.65	105.74
3	L5	4623	OMG	C4-C5-N7	-2.77	106.29	110.67
3	L5	3782	5MC	C5-C4-N3	-2.76	118.92	121.75
3	L5	3867	A2M	C4-C5-N7	-2.75	107.44	110.58
1	S2	99	A2M	C4-C5-N7	-2.74	107.45	110.58
1	S2	590	A2M	C4-N9-C8	2.74	108.61	105.74
1	S2	159	A2M	N3-C2-N1	-2.74	124.44	128.58
1	S2	576	A2M	N3-C2-N1	-2.73	124.45	128.58
1	S2	668	A2M	C5-N7-C8	2.72	107.73	103.45
1	S2	1326	UY1	C5-C6-N1	-2.72	118.36	122.14
3	L5	1524	A2M	C4-N9-C8	2.72	108.59	105.74
3	L5	3637	PSU	C5-C6-N1	-2.72	118.37	122.14
3	L5	4220	6MZ	C4-N9-C8	2.71	108.59	105.74
1	S2	1832	6MZ	C5-N7-C8	2.71	107.71	103.45
1	S2	1031	A2M	C4-N9-C8	2.70	108.58	105.74
1	S2	1328	OMG	C4-C5-N7	-2.70	106.39	110.67
1	S2	93	PSU	C5-C6-N1	-2.70	118.40	122.14
1	S2	1851	MA6	C5-N7-C8	2.69	107.68	103.45
1	S2	1447	OMG	C4-C5-N7	-2.69	106.41	110.67
1	S2	1851	MA6	C4-N9-C8	2.69	108.56	105.74
3	L5	3830	A2M	C4-N9-C8	2.69	108.56	105.74
3	L5	4620	OMU	O4'-C4'-C3'	-2.68	99.83	105.15
3	L5	3627	OMG	C4-C5-N7	-2.68	106.42	110.67
3	L5	4590	A2M	C4-N9-C8	2.68	108.55	105.74
1	S2	1850	MA6	C5-N7-C8	2.68	107.66	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	572	PSU	C6-C5-C4	-2.67	116.37	118.17
1	S2	801	PSU	O2-C2-N1	-2.67	120.03	122.79
3	L5	2787	A2M	C4-N9-C8	2.66	108.54	105.74
3	L5	1534	A2M	C4-N9-C8	2.66	108.53	105.74
3	L5	3637	PSU	O2-C2-N1	-2.66	120.04	122.79
1	S2	1244	PSU	C5-C6-N1	-2.65	118.46	122.14
3	L5	2363	A2M	C4-N9-C8	2.65	108.52	105.74
1	S2	627	OMU	O2-C2-N1	-2.64	119.36	122.80
3	L5	3785	A2M	C4'-O4'-C1'	-2.62	103.68	109.47
3	L5	2422	OMC	O2-C2-N3	-2.62	118.20	122.33
3	L5	4499	OMG	C4-C5-N7	-2.62	106.52	110.67
3	L5	2363	A2M	C5-N7-C8	2.62	107.56	103.45
84	At	32	PSU	C5-C6-N1	-2.62	118.51	122.14
3	L5	1582	PSU	O2-C2-N1	-2.62	120.09	122.79
1	S2	1031	A2M	C2'-C1'-N9	-2.61	109.45	113.75
1	S2	116	OMU	C6-N1-C2	-2.61	117.82	121.00
3	L5	4531	PSU	C5-C6-N1	-2.60	118.53	122.14
2	L8	69	PSU	C5-C6-N1	-2.59	118.54	122.14
3	L5	4471	PSU	O2-C2-N1	-2.59	120.11	122.79
1	S2	121	OMU	O4-C4-C5	-2.59	120.70	125.16
1	S2	1490	OMG	C4-C5-N7	-2.58	106.57	110.67
1	S2	1832	6MZ	C4-N9-C8	2.58	108.45	105.74
3	L5	3785	A2M	C5-N7-C8	2.58	107.50	103.45
1	S2	1383	A2M	C4-N9-C8	2.58	108.44	105.74
1	S2	601	OMG	C4-C5-N7	-2.58	106.59	110.67
3	L5	1524	A2M	C5-N7-C8	2.58	107.50	103.45
3	L5	4530	UR3	C2'-C1'-N1	-2.57	106.10	113.25
3	L5	4523	A2M	C5-N7-C8	2.57	107.49	103.45
1	S2	484	A2M	C5-N7-C8	2.57	107.48	103.45
1	S2	1842	4AC	N4-C4-N3	2.57	118.03	113.87
3	L5	3760	A2M	C5-N7-C8	2.57	107.48	103.45
3	L5	2401	A2M	C4-N9-C8	2.56	108.42	105.74
3	L5	4628	PSU	C3'-C2'-C1'	2.56	104.71	101.69
3	L5	4618	OMG	C4-C5-N7	-2.56	106.62	110.67
3	L5	400	A2M	C5-N7-C8	2.56	107.47	103.45
3	L5	4530	UR3	C3U-N3-C4	2.56	121.41	117.87
3	L5	3944	OMG	C4-C5-N7	-2.55	106.63	110.67
3	L5	1326	A2M	C4-N9-C8	2.55	108.42	105.74
3	L5	1522	OMG	C4-C5-N7	-2.55	106.64	110.67
3	L5	3760	A2M	C5'-C4'-C3'	-2.54	106.06	115.21
3	L5	4228	OMG	C4-C5-N7	-2.54	106.64	110.67
1	S2	1248	B8N	C3'-C2'-C1'	2.54	104.69	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	512	A2M	C4-N9-C8	2.54	108.40	105.74
1	S2	27	A2M	C5-N7-C8	2.53	107.43	103.45
3	L5	4521	PSU	C5-C6-N1	-2.53	118.63	122.14
3	L5	3899	OMG	C4-C5-N7	-2.53	106.66	110.67
2	L8	75	OMG	O6-C6-C5	-2.52	119.88	126.53
3	L5	3764	PSU	C3'-C2'-C1'	2.52	104.66	101.69
3	L5	2787	A2M	C5-N7-C8	2.52	107.41	103.45
3	L5	4673	PSU	O2-C2-N1	-2.50	120.21	122.79
3	L5	1316	OMG	C4-C5-N7	-2.50	106.70	110.67
3	L5	3744	OMG	C4-C5-N7	-2.50	106.71	110.67
3	L5	4456	OMC	C2'-C1'-N1	-2.50	109.50	114.24
3	L5	1322	1MA	N1-C2-N3	-2.49	123.03	126.00
3	L5	3830	A2M	C5-N7-C8	2.49	107.37	103.45
3	L5	4392	OMG	C4-C5-N7	-2.49	106.72	110.67
1	S2	27	A2M	C4-N9-C8	2.49	108.35	105.74
1	S2	484	A2M	C4-N9-C8	2.49	108.35	105.74
3	L5	1534	A2M	C5-N7-C8	2.49	107.36	103.45
1	S2	1447	OMG	O4'-C1'-N9	2.49	113.99	108.36
3	L5	2876	OMG	C4-C5-N7	-2.48	106.74	110.67
1	S2	1842	4AC	C5-C4-N3	-2.48	118.72	122.60
1	S2	590	A2M	C5-N7-C8	2.48	107.35	103.45
3	L5	4370	OMG	C4-C5-N7	-2.47	106.75	110.67
1	S2	1678	A2M	C5-N7-C8	2.47	107.33	103.45
3	L5	3637	PSU	O2-C2-N3	-2.47	117.48	121.86
2	L8	75	OMG	C4-C5-N7	-2.46	106.78	110.67
84	At	37	MIA	C5-N7-C8	2.46	107.31	103.45
1	S2	1031	A2M	C5-N7-C8	2.45	107.31	103.45
1	S2	1243	PSU	C5-C6-N1	-2.44	118.75	122.14
3	L5	3825	A2M	C5-N7-C8	2.44	107.28	103.45
3	L5	2401	A2M	C5-N7-C8	2.44	107.28	103.45
3	L5	3818	UY1	C5-C6-N1	-2.44	118.76	122.14
52	La	39	V5N	O-C-CA	-2.44	118.50	124.77
3	L5	4498	OMU	O2-C2-N1	-2.43	119.64	122.80
1	S2	166	A2M	C5-N7-C8	2.43	107.26	103.45
3	L5	2364	OMG	C4-C5-N7	-2.42	106.83	110.67
3	L5	4571	A2M	C5-N7-C8	2.42	107.26	103.45
3	L5	1881	OMC	C2'-C1'-N1	2.42	118.84	114.24
1	S2	159	A2M	C2'-C1'-N9	-2.42	109.77	113.75
3	L5	2815	A2M	C4-N9-C8	2.41	108.27	105.74
1	S2	462	OMC	C2'-C1'-N1	-2.41	109.67	114.24
1	S2	509	OMG	C4-C5-N7	-2.41	106.85	110.67
3	L5	3792	OMG	O6-C6-C5	-2.41	120.17	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	668	A2M	N9-C8-N7	-2.40	110.53	113.94
1	S2	681	PSU	C5-C6-N1	-2.40	118.81	122.14
3	L5	4296	PSU	C5-C6-N1	-2.40	118.81	122.14
1	S2	867	OMG	C4-C5-N7	-2.40	106.87	110.67
3	L5	4523	A2M	C4-N9-C8	2.39	108.25	105.74
3	L5	4431	PSU	C6-C5-C4	-2.39	116.56	118.17
1	S2	166	A2M	C4-N9-C8	2.39	108.25	105.74
84	At	20	H2U	C5-C6-N1	-2.39	104.30	111.52
3	L5	3762	PSU	C5-C6-N1	-2.39	118.83	122.14
3	L5	1582	PSU	C5-C6-N1	-2.38	118.83	122.14
3	L5	5001	PSU	C5-C6-N1	-2.38	118.83	122.14
3	L5	3785	A2M	C6-C5-N7	2.38	136.68	132.09
3	L5	3825	A2M	C2-N1-C6	2.38	122.64	118.73
1	S2	1056	PSU	C5-C6-N1	-2.38	118.84	122.14
3	L5	3724	A2M	C4-N9-C8	2.38	108.23	105.74
1	S2	436	OMG	C4-C5-N7	-2.37	106.91	110.67
1	S2	644	OMG	C4-C5-N7	-2.37	106.91	110.67
1	S2	668	A2M	C6-C5-N7	2.37	136.66	132.09
3	L5	1779	PSU	C5-C6-N1	-2.37	118.86	122.14
1	S2	683	OMG	C4-C5-N7	-2.36	106.93	110.67
3	L5	4220	6MZ	C5-N7-C8	2.36	107.16	103.45
3	L5	4620	OMU	C6-N1-C2	-2.35	118.13	121.00
3	L5	3760	A2M	O4'-C1'-N9	2.35	112.61	108.09
3	L5	4590	A2M	C2-N1-C6	2.35	122.59	118.73
3	L5	1625	OMG	C4-C5-N7	-2.35	106.95	110.67
3	L5	3841	OMC	O2-C2-N3	-2.35	118.63	122.33
1	S2	1383	A2M	C5-N7-C8	2.34	107.14	103.45
3	L5	4637	OMG	C4-C5-N7	-2.34	106.96	110.67
3	L5	3729	PSU	C3'-C2'-C1'	2.34	104.45	101.69
3	L5	4590	A2M	C5-N7-C8	2.34	107.13	103.45
1	S2	159	A2M	C5-N7-C8	2.34	107.13	103.45
3	L5	3825	A2M	C4-N9-C8	2.34	108.19	105.74
3	L5	4972	PSU	C5-C6-N1	-2.34	118.90	122.14
3	L5	2843	PSU	C5-C6-N1	-2.33	118.91	122.14
3	L5	3718	A2M	C2-N1-C6	2.33	122.56	118.73
3	L5	3785	A2M	N9-C8-N7	-2.33	110.64	113.94
3	L5	1871	A2M	C2-N1-C6	2.33	122.55	118.73
3	L5	2422	OMC	C2'-C1'-N1	-2.32	109.83	114.24
3	L5	4571	A2M	C4-N9-C8	2.32	108.17	105.74
1	S2	1337	4AC	C6-C5-C4	2.32	119.80	117.00
3	L5	4494	OMG	C4-C5-N7	-2.32	107.00	110.67
3	L5	2364	OMG	O6-C6-C5	-2.32	120.42	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2815	A2M	C5-N7-C8	2.32	107.09	103.45
3	L5	1677	PSU	C4'-O4'-C1'	-2.31	102.64	108.44
66	Lr	2	SAC	C-CA-N	2.31	113.96	109.50
3	L5	3718	A2M	C4-N9-C8	2.31	108.16	105.74
1	S2	1174	PSU	C5-C6-N1	-2.31	118.94	122.14
1	S2	121	OMU	C2'-C1'-N1	-2.31	109.86	114.24
3	L5	1625	OMG	O6-C6-C5	-2.31	120.44	126.53
3	L5	2424	OMG	C6-C5-N7	2.31	134.49	130.29
1	S2	468	A2M	C5-N7-C8	2.31	107.07	103.45
1	S2	512	A2M	C5-N7-C8	2.31	107.07	103.45
3	L5	1316	OMG	O6-C6-C5	-2.30	120.45	126.53
3	L5	4636	PSU	C3'-C2'-C1'	2.30	104.41	101.69
3	L5	3792	OMG	C4-C5-N7	-2.30	107.02	110.67
1	S2	576	A2M	C5-N7-C8	2.30	107.06	103.45
1	S2	436	OMG	O6-C6-C5	-2.30	120.46	126.53
3	L5	3639	PSU	C5-C6-N1	-2.30	118.95	122.14
84	At	16	H2U	C5-C6-N1	-2.30	104.57	111.52
1	S2	517	OMC	C2'-C1'-N1	-2.29	109.89	114.24
3	L5	4420	PSU	O4'-C1'-C2'	2.29	108.32	105.15
3	L5	1322	1MA	C6-C5-N7	2.29	136.21	132.16
3	L5	4361	PSU	C3'-C2'-C1'	2.28	104.38	101.69
3	L5	4196	OMG	O6-C6-C5	-2.28	120.52	126.53
3	L5	4637	OMG	O6-C6-C5	-2.28	120.52	126.53
1	S2	1851	MA6	C6-C5-N7	2.28	137.07	133.43
3	L5	3782	5MC	O2-C2-N3	-2.28	118.74	122.33
3	L5	4312	PSU	C5-C6-N1	-2.27	118.99	122.14
3	L5	1677	PSU	C5-C6-N1	-2.27	118.99	122.14
84	At	37	MIA	C2-N1-C6	2.27	121.84	117.54
3	L5	3844	PSU	C5-C6-N1	-2.27	118.99	122.14
3	L5	4403	PSU	C5-C6-N1	-2.27	118.99	122.14
3	L5	3920	PSU	C5-C6-N1	-2.26	119.00	122.14
1	S2	517	OMC	O2-C2-N3	-2.26	118.77	122.33
3	L5	4636	PSU	O2-C2-N3	-2.25	117.86	121.86
3	L5	3762	PSU	C3'-C2'-C1'	2.25	104.35	101.69
1	S2	174	OMC	C2'-C1'-N1	-2.25	109.96	114.24
3	L5	4196	OMG	C4-C5-N7	-2.25	107.10	110.67
1	S2	867	OMG	O6-C6-C5	-2.25	120.60	126.53
1	S2	644	OMG	O6-C6-C5	-2.25	120.61	126.53
1	S2	918	PSU	C5-C6-N1	-2.25	119.02	122.14
3	L5	3851	PSU	C5-C6-N1	-2.24	119.03	122.14
1	S2	1850	MA6	C6-C5-N7	2.24	137.01	133.43
3	L5	2508	PSU	C5-C6-N1	-2.24	119.03	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	218	PSU	C5-C6-N1	-2.24	119.03	122.14
3	L5	398	A2M	C2-N1-C6	2.24	122.40	118.73
2	L8	55	PSU	C5-C6-N1	-2.23	119.04	122.14
1	S2	1490	OMG	C2'-C1'-N9	-2.23	110.01	114.24
1	S2	1232	PSU	O2-C2-N3	-2.23	117.90	121.86
3	L5	1524	A2M	C2'-C1'-N9	-2.23	110.08	113.75
3	L5	4228	OMG	O6-C6-C5	-2.23	120.65	126.53
3	L5	2837	OMU	O2-C2-N1	-2.22	119.90	122.80
3	L5	3627	OMG	O6-C6-C5	-2.22	120.67	126.53
84	At	8	4SU	O2-C2-N1	-2.22	119.90	122.80
1	S2	814	PSU	C5-C6-N1	-2.22	119.06	122.14
3	L5	4569	PSU	C5-C6-N1	-2.22	119.06	122.14
3	L5	3760	A2M	N9-C8-N7	-2.22	110.79	113.94
1	S2	576	A2M	C2-N1-C6	2.22	122.37	118.73
3	L5	3723	A2M	C2'-C1'-N9	-2.22	110.10	113.75
1	S2	159	A2M	C4-N9-C8	2.22	108.06	105.74
3	L5	4442	PSU	C5-C6-N1	-2.21	119.07	122.14
3	L5	1322	1MA	C4-C5-N7	-2.21	107.16	110.67
3	L5	398	A2M	C5-N7-C8	2.21	106.92	103.45
1	S2	34	PSU	C5-C6-N1	-2.21	119.07	122.14
3	L5	4620	OMU	O4-C4-C5	-2.21	121.35	125.16
1	S2	36	PSU	C5-C6-N1	-2.20	119.08	122.14
3	L5	4521	PSU	O2-C2-N3	-2.20	117.95	121.86
1	S2	99	A2M	C5-N7-C8	2.20	106.91	103.45
3	L5	2861	OMC	O2-C2-N3	-2.20	118.86	122.33
1	S2	651	PSU	C5-C6-N1	-2.20	119.09	122.14
3	L5	2415	OMU	C1'-N1-C2	2.19	121.53	117.59
1	S2	1447	OMG	O6-C6-C5	-2.19	120.76	126.53
3	L5	4576	PSU	C5-C6-N1	-2.18	119.12	122.14
3	L5	4569	PSU	C2'-C3'-C4'	-2.18	98.40	102.61
3	L5	1326	A2M	C5-N7-C8	2.18	106.87	103.45
3	L5	1881	OMC	O2'-C2'-C1'	2.18	113.12	108.99
3	L5	1792	PSU	C6-C5-C4	-2.17	116.71	118.17
3	L5	1522	OMG	O6-C6-C5	-2.17	120.80	126.53
84	At	37	MIA	N9-C8-N7	-2.17	110.85	113.94
3	L5	3723	A2M	C5-N7-C8	2.17	106.86	103.45
3	L5	4673	PSU	O2-C2-N3	-2.17	118.01	121.86
1	S2	1850	MA6	N9-C8-N7	-2.17	110.86	113.94
1	S2	601	OMG	O6-C6-C5	-2.17	120.81	126.53
3	L5	3770	PSU	C6-C5-C4	-2.17	116.71	118.17
3	L5	3899	OMG	O6-C6-C5	-2.17	120.82	126.53
3	L5	4456	OMC	O2-C2-N3	-2.16	118.92	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1782	PSU	C5-C6-N1	-2.16	119.14	122.14
3	L5	4531	PSU	O2-C2-N3	-2.16	118.02	121.86
3	L5	3760	A2M	O2'-C2'-C1'	2.16	113.09	108.99
1	S2	1031	A2M	C6-C5-N7	2.16	136.25	132.09
3	L5	3760	A2M	C6-C5-N7	2.16	136.25	132.09
1	S2	1490	OMG	O6-C6-C5	-2.15	120.85	126.53
3	L5	3718	A2M	C5-N7-C8	2.15	106.83	103.45
3	L5	3744	OMG	O6-C6-C5	-2.15	120.85	126.53
85	Pt	56	PSU	C5-C6-N1	-2.15	119.15	122.14
3	L5	3825	A2M	C6-C5-N7	2.15	136.24	132.09
1	S2	1238	PSU	C5-C6-N1	-2.15	119.16	122.14
85	Pt	33	OMC	O2-C2-N3	-2.15	118.94	122.33
3	L5	2632	PSU	C3'-C2'-C1'	2.15	104.22	101.69
3	L5	2632	PSU	C6-C5-C4	-2.15	116.72	118.17
1	S2	1832	6MZ	C2-N1-C6	2.15	122.36	115.24
3	L5	4623	OMG	O6-C6-C5	-2.15	120.86	126.53
1	S2	512	A2M	C2-N1-C6	2.15	122.25	118.73
3	L5	4494	OMG	O6-C6-C5	-2.14	120.88	126.53
1	S2	468	A2M	C2-N1-C6	2.14	122.25	118.73
3	L5	2424	OMG	O6-C6-C5	-2.14	120.89	126.53
3	L5	1871	A2M	C6-C5-N7	2.14	136.21	132.09
1	S2	1692	PSU	C5-C6-N1	-2.14	119.17	122.14
1	S2	576	A2M	C6-C5-N7	2.14	136.21	132.09
1	S2	573	PSU	O2-C2-N3	-2.13	118.07	121.86
1	S2	1367	PSU	C5-C6-N1	-2.13	119.18	122.14
3	L5	2363	A2M	C6-C5-N7	2.13	136.20	132.09
3	L5	1871	A2M	C5-N7-C8	2.13	106.80	103.45
3	L5	3724	A2M	C5-N7-C8	2.13	106.80	103.45
1	S2	866	PSU	C5-C6-N1	-2.13	119.18	122.14
3	L5	5010	PSU	C5-C6-N1	-2.13	119.18	122.14
3	L5	4370	OMG	O6-C6-C5	-2.13	120.92	126.53
3	L5	4618	OMG	O6-C6-C5	-2.13	120.92	126.53
3	L5	3867	A2M	C5-N7-C8	2.12	106.79	103.45
3	L5	4620	OMU	O2-C2-N3	-2.12	117.57	121.49
1	S2	801	PSU	C6-C5-C4	-2.12	116.74	118.17
1	S2	428	OMU	O2-C2-N1	-2.12	120.03	122.80
3	L5	2839	PSU	C5-C6-N1	-2.12	119.20	122.14
1	S2	1174	PSU	O2-C2-N3	-2.12	118.09	121.86
1	S2	668	A2M	C2-N1-C6	2.12	122.21	118.73
3	L5	1582	PSU	O2-C2-N3	-2.12	118.10	121.86
1	S2	1081	PSU	C5-C6-N1	-2.12	119.20	122.14
1	S2	1383	A2M	C6-C5-N7	2.11	136.17	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4361	PSU	C5-C6-N1	-2.11	119.21	122.14
1	S2	354	OMU	O2-C2-N1	-2.11	120.05	122.80
3	L5	4552	PSU	C5-C6-N1	-2.11	119.21	122.14
1	S2	406	PSU	O2'-C2'-C1'	-2.11	106.21	111.21
3	L5	4590	A2M	C6-C5-N7	2.11	136.15	132.09
1	S2	1804	OMU	O2-C2-N1	-2.11	120.06	122.80
84	At	39	PSU	C5-C6-N1	-2.10	119.22	122.14
3	L5	3723	A2M	C2-N1-C6	2.10	122.19	118.73
1	S2	1678	A2M	C6-C5-N7	2.10	136.14	132.09
3	L5	4471	PSU	O2-C2-N3	-2.10	118.13	121.86
3	L5	2424	OMG	C4-C5-N7	-2.10	107.35	110.67
3	L5	3715	PSU	C5-C6-N1	-2.10	119.23	122.14
3	L5	4299	PSU	C5-C6-N1	-2.10	119.23	122.14
3	L5	3760	A2M	CM'-O2'-C2'	-2.10	109.09	114.47
3	L5	3785	A2M	O4'-C1'-C2'	-2.10	102.98	106.59
1	S2	683	OMG	O6-C6-C5	-2.09	121.00	126.53
20	SX	62	HY3	O-C-CA	-2.09	119.32	124.86
3	L5	4493	PSU	C6-C5-C4	-2.09	116.76	118.17
1	S2	1639	G7M	C5-C6-N1	2.09	116.17	111.84
3	L5	1860	PSU	O2-C2-N3	-2.09	118.15	121.86
3	L5	3925	OMU	O2-C2-N1	-2.09	120.07	122.80
1	S2	1447	OMG	C2'-C1'-N9	-2.09	110.28	114.24
1	S2	1851	MA6	N9-C8-N7	-2.09	110.97	113.94
1	S2	1328	OMG	O6-C6-C5	-2.09	121.03	126.53
3	L5	2787	A2M	C6-C5-N7	2.09	136.11	132.09
3	L5	4447	5MC	O2-C2-N3	-2.09	119.04	122.33
3	L5	3841	OMC	C2'-C1'-N1	-2.09	110.28	114.24
1	S2	27	A2M	C6-C5-N7	2.08	136.11	132.09
1	S2	1383	A2M	C2-N1-C6	2.08	122.15	118.73
1	S2	172	OMU	O2-C2-N1	-2.08	120.09	122.80
3	L5	3758	PSU	O2-C2-N3	-2.08	118.17	121.86
84	At	37	MIA	N3-C2-N1	-2.08	123.21	127.00
1	S2	1445	PSU	C5-C6-N1	-2.08	119.26	122.14
3	L5	3830	A2M	C6-C5-N7	2.07	136.09	132.09
1	S2	174	OMC	O2-C2-N3	-2.07	119.06	122.33
3	L5	4689	PSU	C6-C5-C4	-2.07	116.77	118.17
1	S2	1447	OMG	C4'-O4'-C1'	-2.07	104.89	109.47
3	L5	4499	OMG	O6-C6-C5	-2.07	121.06	126.53
3	L5	2787	A2M	N9-C8-N7	-2.07	111.00	113.94
3	L5	400	A2M	N9-C8-N7	-2.07	111.00	113.94
3	L5	4361	PSU	O2-C2-N3	-2.06	118.19	121.86
1	S2	1248	B8N	O2-C2-N3	-2.06	119.20	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1536	PSU	C5-C6-N1	-2.06	119.28	122.14
3	L5	3764	PSU	O2-C2-N3	-2.06	118.20	121.86
3	L5	2363	A2M	N9-C8-N7	-2.06	111.01	113.94
3	L5	1781	PSU	C5-C6-N1	-2.06	119.28	122.14
1	S2	105	PSU	O2-C2-N3	-2.06	118.21	121.86
3	L5	3768	PSU	O2-C2-N3	-2.06	118.21	121.86
1	S2	1842	4AC	O7-C7-N4	2.06	125.13	121.90
3	L5	1524	A2M	N9-C8-N7	-2.05	111.02	113.94
3	L5	1860	PSU	C5-C6-N1	-2.05	119.29	122.14
3	L5	1524	A2M	C6-C5-N7	2.05	136.05	132.09
3	L5	1862	PSU	C5-C6-N1	-2.05	119.29	122.14
3	L5	4392	OMG	O6-C6-C5	-2.05	121.12	126.53
3	L5	3944	OMG	O6-C6-C5	-2.05	121.12	126.53
1	S2	436	OMG	C5-C6-N1	2.05	118.47	113.25
1	S2	576	A2M	C4-N9-C8	2.05	107.89	105.74
1	S2	822	PSU	C5-C6-N1	-2.05	119.30	122.14
3	L5	3724	A2M	C2-N1-C6	2.04	122.09	118.73
1	S2	428	OMU	C2'-C1'-N1	-2.04	110.36	114.24
1	S2	1678	A2M	N9-C8-N7	-2.04	111.04	113.94
3	L5	2401	A2M	C2-N1-C6	2.04	122.08	118.73
3	L5	3867	A2M	C3'-C2'-C1'	2.04	106.72	102.81
3	L5	4471	PSU	C5-C6-N1	-2.04	119.31	122.14
3	L5	4392	OMG	C5-C6-N1	2.04	118.44	113.25
40	LB	245	HIC	CB-CG-CD2	-2.04	125.05	129.96
3	L5	1582	PSU	C3'-C2'-C1'	2.04	104.09	101.69
1	S2	1639	G7M	C3'-C2'-C1'	2.03	105.31	101.46
3	L5	3851	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	S2	1136	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	S2	159	A2M	C6-C5-N7	2.03	136.00	132.09
84	At	20	H2U	O2-C2-N1	-2.02	120.67	123.10
3	L5	4196	OMG	C5-C6-N1	2.02	118.40	113.25
3	L5	2876	OMG	O6-C6-C5	-2.02	121.19	126.53
1	S2	1337	4AC	C3'-C2'-C1'	2.02	105.29	101.46
3	L5	3830	A2M	N9-C8-N7	-2.02	111.07	113.94
3	L5	4457	PSU	O2-C2-N3	-2.02	118.28	121.86
1	S2	509	OMG	O6-C6-C5	-2.02	121.21	126.53
3	L5	3764	PSU	O2'-C2'-C1'	-2.01	106.43	111.21
3	L5	4447	5MC	N1-C2-N3	2.01	122.30	118.80
3	L5	4628	PSU	C6-N1-C2	-2.01	120.82	122.69
3	L5	4293	PSU	C5-C6-N1	-2.01	119.35	122.14
3	L5	3723	A2M	C6-C5-N7	2.01	135.97	132.09
1	S2	1177	PSU	C5-C6-N1	-2.01	119.36	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2351	OMC	O2-C2-N3	-2.01	119.17	122.33
3	L5	3724	A2M	C6-C5-N7	2.00	135.96	132.09
3	L5	3715	PSU	C3'-C2'-C1'	2.00	104.05	101.69
1	S2	815	PSU	C5-C6-N1	-2.00	119.36	122.14
3	L5	3734	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
2	L8	75	OMG	C1'-C2'-O2'-CM2
6	SA	2	SAC	OAC-C1A-N-CA
6	SA	2	SAC	C-CA-CB-OG
66	Lr	2	SAC	C2A-C1A-N-CA
68	Lb	5	MLZ	N-CA-CB-CG
68	Lb	5	MLZ	C-CA-CB-CG
68	Lb	5	MLZ	O-C-CA-CB
81	Lo	53	MLZ	C-CA-CB-CG
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	121	OMU	C1'-C2'-O2'-CM2
1	S2	174	OMC	C1'-C2'-O2'-CM2
1	S2	462	OMC	C1'-C2'-O2'-CM2
1	S2	484	A2M	C1'-C2'-O2'-CM'
1	S2	509	OMG	C1'-C2'-O2'-CM2
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	867	OMG	C1'-C2'-O2'-CM2
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1248	B8N	C31-C32-C33-N34
1	S2	1288	OMU	O4'-C4'-C5'-O5'
1	S2	1328	OMG	C1'-C2'-O2'-CM2
1	S2	1337	4AC	N3-C4-N4-C7
1	S2	1337	4AC	C5-C4-N4-C7
1	S2	1447	OMG	C1'-C2'-O2'-CM2
1	S2	1490	OMG	C1'-C2'-O2'-CM2
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2415	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	2422	OMC	C1'-C2'-O2'-CM2
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	2815	A2M	C1'-C2'-O2'-CM'
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	3841	OMC	C1'-C2'-O2'-CM2
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4420	PSU	C2'-C1'-C5-C4
3	L5	4420	PSU	C2'-C1'-C5-C6
3	L5	4420	PSU	O4'-C4'-C5'-O5'
3	L5	4456	OMC	C1'-C2'-O2'-CM2
3	L5	4523	A2M	C1'-C2'-O2'-CM'
3	L5	4569	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	4618	OMG	C1'-C2'-O2'-CM2
3	L5	4620	OMU	C1'-C2'-O2'-CM2
3	L5	4637	OMG	C1'-C2'-O2'-CM2
39	LA	216	V5N	O-C-CA-CB
84	At	16	H2U	O4'-C4'-C5'-O5'
84	At	16	H2U	C3'-C4'-C5'-O5'
84	At	16	H2U	O4'-C1'-N1-C2
84	At	16	H2U	O4'-C1'-N1-C6
84	At	37	MIA	C12-C13-C14-C15
84	At	37	MIA	C12-C13-C14-C16
29	SV	1	AME	OT-CT1-N-CA
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	644	OMG	O4'-C4'-C5'-O5'
3	L5	3760	A2M	C3'-C4'-C5'-O5'
3	L5	4306	OMU	C3'-C4'-C5'-O5'
3	L5	4420	PSU	C3'-C4'-C5'-O5'
85	Pt	21	H2U	O4'-C4'-C5'-O5'
85	Pt	21	H2U	C3'-C4'-C5'-O5'
66	Lr	2	SAC	OAC-C1A-N-CA
1	S2	512	A2M	O4'-C4'-C5'-O5'
1	S2	1288	OMU	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C6
1	S2	590	A2M	C3'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	3760	A2M	O4'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
3	L5	4569	PSU	C3'-C4'-C5'-O5'
84	At	16	H2U	C2'-C1'-N1-C6
29	SV	1	AME	CB-CG-SD-CE
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	590	A2M	O4'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
3	L5	3944	OMG	C3'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
68	Lb	5	MLZ	CE-CD-CG-CB
1	S2	1248	B8N	C32-C33-C34-O36
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3844	PSU	O4'-C4'-C5'-O5'
3	L5	4306	OMU	O4'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
81	Lo	53	MLZ	CG-CD-CE-NZ
1	S2	1248	B8N	C32-C33-C34-O35
3	L5	4447	5MC	C2'-C1'-N1-C2
1	S2	512	A2M	C3'-C4'-C5'-O5'
66	Lr	2	SAC	C-CA-CB-OG
81	Lo	53	MLZ	CA-CB-CG-CD
3	L5	2422	OMC	C3'-C4'-C5'-O5'
1	S2	1288	OMU	C1'-C2'-O2'-CM2
3	L5	3718	A2M	C1'-C2'-O2'-CM'
20	SX	62	HY3	O-C-CA-C3
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	3944	OMG	O4'-C4'-C5'-O5'
68	Lb	5	MLZ	CG-CD-CE-NZ
1	S2	1248	B8N	C31-C32-C33-C34
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
1	S2	1248	B8N	N34-C33-C34-O36
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
84	At	16	H2U	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	1625	OMG	C3'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	3729	PSU	O4'-C4'-C5'-O5'
1	S2	428	OMU	C2'-C1'-N1-C6
86	EF	79	M3L	CD-CE-NZ-CM1
3	L5	4447	5MC	O4'-C1'-N1-C2
81	Lo	53	MLZ	N-CA-CB-CG
86	EF	79	M3L	CD-CE-NZ-CM3
85	Pt	21	H2U	C4'-C5'-O5'-P
86	EF	79	M3L	CD-CE-NZ-CM2
1	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
1	S2	627	OMU	C2'-C1'-N1-C6
3	L5	3818	UY1	O4'-C1'-C5-C4
3	L5	4500	PSU	O4'-C1'-C5-C4
3	L5	4521	PSU	O4'-C1'-C5-C4
3	L5	1326	A2M	C3'-C4'-C5'-O5'
84	At	16	H2U	C4'-C5'-O5'-P
86	EF	55	MLY	CD-CE-NZ-CH1
1	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	398	A2M	C3'-C4'-C5'-O5'
1	S2	1248	B8N	N34-C33-C34-O35
85	Pt	21	H2U	C2'-C1'-N1-C6
3	L5	1322	1MA	C2'-C1'-N9-C4
1	S2	644	OMG	C4'-C5'-O5'-P
3	L5	3844	PSU	C3'-C4'-C5'-O5'
1	S2	627	OMU	O4'-C1'-N1-C6
85	Pt	21	H2U	C2'-C1'-N1-C2
1	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	1322	1MA	C2'-C1'-N9-C8
1	S2	99	A2M	C1'-C2'-O2'-CM'
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	1383	A2M	C1'-C2'-O2'-CM'
3	L5	3830	A2M	C1'-C2'-O2'-CM'
1	S2	428	OMU	O4'-C1'-N1-C6
3	L5	3818	UY1	O4'-C1'-C5-C6
3	L5	4521	PSU	O4'-C1'-C5-C6
3	L5	4637	OMG	O4'-C4'-C5'-O5'
84	At	20	H2U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	1326	UY1	C2'-C1'-C5-C6
1	S2	627	OMU	O4'-C1'-N1-C2
1	S2	428	OMU	O4'-C1'-N1-C2
1	S2	668	A2M	C2'-C1'-N9-C8
3	L5	3887	OMC	C4'-C5'-O5'-P
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	627	OMU	C2'-C1'-N1-C2

There are no ring outliers.

88 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1871	A2M	1	0
3	L5	3785	A2M	1	0
3	L5	3723	A2M	1	0
1	S2	428	OMU	2	0
1	S2	512	A2M	1	0
1	S2	99	A2M	1	0
3	L5	3764	PSU	1	0
3	L5	3627	OMG	1	0
1	S2	1639	G7M	1	0
1	S2	601	OMG	1	0
3	L5	4531	PSU	1	0
1	S2	1490	OMG	1	0
3	L5	1677	PSU	1	0
3	L5	2839	PSU	1	0
3	L5	3867	A2M	3	0
3	L5	2804	OMC	1	0
66	Lr	2	SAC	1	0
3	L5	2364	OMG	2	0
1	S2	484	A2M	1	0
3	L5	4618	OMG	1	0
1	S2	1445	PSU	3	0
3	L5	3899	OMG	1	0
1	S2	576	A2M	2	0
3	L5	3925	OMU	1	0
1	S2	573	PSU	1	0
1	S2	116	OMU	3	0
3	L5	3884	PSU	1	0
1	S2	174	OMC	1	0
3	L5	4530	UR3	1	0
1	S2	1031	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2363	A2M	2	0
3	L5	4392	OMG	1	0
1	S2	681	PSU	1	0
3	L5	2876	OMG	1	0
3	L5	3718	A2M	2	0
2	L8	69	PSU	1	0
3	L5	4689	PSU	1	0
68	Lb	5	MLZ	1	0
1	S2	1177	PSU	1	0
3	L5	3701	OMC	1	0
84	At	16	H2U	1	0
1	S2	36	PSU	1	0
2	L8	14	OMU	1	0
1	S2	1850	MA6	1	0
3	L5	1326	A2M	1	0
3	L5	3887	OMC	1	0
1	S2	1136	PSU	1	0
1	S2	121	OMU	1	0
1	S2	509	OMG	3	0
1	S2	1625	PSU	1	0
86	EF	79	M3L	2	0
3	L5	4569	PSU	1	0
3	L5	3818	UY1	1	0
3	L5	1536	PSU	1	0
3	L5	3792	OMG	1	0
3	L5	3724	A2M	1	0
1	S2	1328	OMG	2	0
3	L5	4579	PSU	2	0
1	S2	1174	PSU	1	0
3	L5	5001	PSU	1	0
1	S2	627	OMU	1	0
3	L5	2351	OMC	1	0
3	L5	4523	A2M	1	0
3	L5	4637	OMG	1	0
3	L5	398	A2M	1	0
1	S2	867	OMG	1	0
3	L5	2632	PSU	1	0
3	L5	2787	A2M	1	0
1	S2	1643	PSU	1	0
3	L5	4447	5MC	1	0
84	At	37	MIA	1	0
1	S2	1239	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1881	OMC	3	0
1	S2	1232	PSU	2	0
1	S2	1678	A2M	1	0
3	L5	2422	OMC	1	0
1	S2	93	PSU	2	0
1	S2	572	PSU	1	0
1	S2	1337	4AC	2	0
3	L5	2424	OMG	1	0
3	L5	1340	OMC	2	0
1	S2	644	OMG	2	0
1	S2	1447	OMG	2	0
3	L5	4196	OMG	1	0
3	L5	2815	A2M	1	0
3	L5	2861	OMC	1	0
3	L5	4536	OMC	1	0
1	S2	1288	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 403 ligands modelled in this entry, 379 are monoatomic - leaving 24 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	$\# Z > 2$
90	PUT	L5	5113	-	5,5,5	0.14	0	4,4,4	0.23	0
94	PHE	At	77	84	10,11,12	0.33	0	8,13,15	0.72	0
90	PUT	L5	5112	-	5,5,5	0.11	0	4,4,4	0.12	0
91	3HE	L5	5117	-	21,21,21	1.00	2 (9%)	23,30,30	1.42	4 (17%)
87	SPD	L5	5107	-	9,9,9	0.15	0	8,8,8	0.24	0
97	YRB	EF	503	-	57,57,57	2.75	14 (24%)	79,82,82	1.29	10 (12%)
87	SPD	L5	5109	-	9,9,9	0.32	0	8,8,8	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	L5	5106	-	9,9,9	0.18	0	8,8,8	0.40	0
87	SPD	L5	5108	-	9,9,9	0.32	0	8,8,8	0.90	0
87	SPD	L5	5105	-	9,9,9	0.31	0	8,8,8	0.89	0
90	PUT	L5	5116	-	5,5,5	0.16	0	4,4,4	0.25	0
90	PUT	L5	5110	-	5,5,5	0.08	0	4,4,4	0.16	0
96	GSP	EF	501	89	33,34,34	1.90	3 (9%)	47,54,54	1.71	9 (19%)
90	PUT	L5	5111	-	5,5,5	0.15	0	4,4,4	0.26	0
87	SPD	L5	5101	-	9,9,9	0.31	0	8,8,8	0.89	0
92	HMT	L5	5118	-	41,43,43	1.50	4 (9%)	43,66,66	1.72	10 (23%)
95	MET	Pt	78	85	6,7,8	0.57	0	2,7,9	1.52	1 (50%)
90	PUT	L5	5119	-	5,5,5	0.10	0	4,4,4	0.19	0
90	PUT	L5	5115	-	5,5,5	0.14	0	4,4,4	0.21	0
87	SPD	L5	5104	-	9,9,9	0.32	0	8,8,8	0.93	0
87	SPD	L5	5103	-	9,9,9	0.33	0	8,8,8	0.91	0
90	PUT	L5	5114	-	5,5,5	0.10	0	4,4,4	0.13	0
87	SPD	L5	5102	-	9,9,9	0.33	0	8,8,8	0.94	0
87	SPD	S2	1901	-	9,9,9	0.16	0	8,8,8	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	PUT	L5	5113	-	-	0/3/3/3	-
94	PHE	At	77	84	-	2/5/6/8	0/1/1/1
90	PUT	L5	5112	-	-	0/3/3/3	-
91	3HE	L5	5117	-	-	0/8/36/36	0/2/2/2
87	SPD	L5	5107	-	-	2/7/7/7	-
97	YRB	EF	503	-	-	13/96/107/107	0/1/2/2
87	SPD	L5	5109	-	-	2/7/7/7	-
87	SPD	L5	5106	-	-	2/7/7/7	-
87	SPD	L5	5108	-	-	1/7/7/7	-
87	SPD	L5	5105	-	-	0/7/7/7	-
90	PUT	L5	5116	-	-	1/3/3/3	-
90	PUT	L5	5110	-	-	1/3/3/3	-
96	GSP	EF	501	89	-	0/21/38/38	0/3/3/3
90	PUT	L5	5111	-	-	0/3/3/3	-
87	SPD	L5	5101	-	-	0/7/7/7	-
92	HMT	L5	5118	-	-	10/27/74/74	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	MET	Pt	78	85	-	2/5/6/8	-
90	PUT	L5	5119	-	-	1/3/3/3	-
90	PUT	L5	5115	-	-	3/3/3/3	-
87	SPD	L5	5104	-	-	2/7/7/7	-
87	SPD	L5	5103	-	-	3/7/7/7	-
90	PUT	L5	5114	-	-	0/3/3/3	-
87	SPD	L5	5102	-	-	3/7/7/7	-
87	SPD	S2	1901	-	-	3/7/7/7	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	EF	501	GSP	PG-S1G	-9.46	1.70	1.90
97	EF	503	YRB	C30-N07	7.80	1.52	1.34
97	EF	503	YRB	C02-N02	7.50	1.50	1.34
97	EF	503	YRB	C34-N01	7.42	1.49	1.34
97	EF	503	YRB	C25-N06	7.06	1.51	1.35
97	EF	503	YRB	C14-N04	6.94	1.50	1.35
97	EF	503	YRB	C18-N05	6.82	1.48	1.34
97	EF	503	YRB	C08-N03	6.11	1.48	1.35
92	L5	5118	HMT	O4-C19	5.25	1.44	1.34
92	L5	5118	HMT	O3-C2	5.06	1.45	1.35
92	L5	5118	HMT	O7-C22	3.80	1.44	1.33
97	EF	503	YRB	O06-C25	-2.94	1.17	1.22
97	EF	503	YRB	O08-C34	-2.89	1.17	1.23
91	L5	5117	3HE	C12-N	-2.69	1.33	1.37
97	EF	503	YRB	O01-C02	-2.61	1.18	1.23
91	L5	5117	3HE	C11-N	-2.59	1.33	1.37
97	EF	503	YRB	O07-C30	-2.50	1.17	1.22
92	L5	5118	HMT	C20-C19	-2.48	1.50	1.53
97	EF	503	YRB	O05-C18	-2.48	1.18	1.23
97	EF	503	YRB	O04-C14	-2.45	1.18	1.22
97	EF	503	YRB	O03-C08	-2.09	1.18	1.22
96	EF	501	GSP	C5-N7	-2.05	1.35	1.39
96	EF	501	GSP	C2-N3	2.02	1.38	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	L5	5118	HMT	O7-C22-C21	5.62	121.03	111.16
96	EF	501	GSP	C5-C4-N3	-5.02	120.40	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
96	EF	501	GSP	C2-N3-C4	4.60	120.23	112.30
97	EF	503	YRB	C30-C29-N06	-4.09	100.42	109.10
92	L5	5118	HMT	O4-C19-C20	3.83	118.26	111.24
96	EF	501	GSP	PB-O3B-PG	-3.64	119.84	133.17
96	EF	501	GSP	N9-C4-N3	3.19	132.33	125.95
92	L5	5118	HMT	O1-C17-O2	-3.17	103.12	108.09
91	L5	5117	3HE	C9-C13-C12	-3.12	109.21	114.46
92	L5	5118	HMT	C17-O1-C14	3.10	109.47	105.32
97	EF	503	YRB	C27-C26-C24	-3.04	107.43	114.17
96	EF	501	GSP	C2-N1-C6	-3.03	119.61	125.11
92	L5	5118	HMT	C9-C4-C5	-2.88	111.28	115.96
91	L5	5117	3HE	C10-C11-N	2.86	119.39	115.92
97	EF	503	YRB	C26-C24-N05	-2.85	104.15	110.58
91	L5	5117	3HE	C13-C12-N	2.79	119.30	115.92
91	L5	5117	3HE	C9-C10-C11	-2.67	109.97	114.46
92	L5	5118	HMT	C17-O2-C15	2.66	108.87	105.32
96	EF	501	GSP	N9-C8-N7	-2.61	108.56	113.40
96	EF	501	GSP	C5-C6-N1	2.57	119.80	113.25
97	EF	503	YRB	C23-N04-C17	2.51	123.09	118.46
97	EF	503	YRB	C36-N07-C33	2.49	120.98	115.81
96	EF	501	GSP	C8-N7-C5	2.47	108.66	104.26
96	EF	501	GSP	O6-C6-C5	-2.45	120.08	126.53
92	L5	5118	HMT	O4-C19-O5	-2.38	119.74	123.95
92	L5	5118	HMT	O7-C22-O8	-2.35	116.18	123.20
97	EF	503	YRB	C04-C03-C01	-2.33	108.54	113.62
97	EF	503	YRB	C03-C01-C02	-2.30	105.66	111.01
97	EF	503	YRB	C15-C13-N03	-2.27	108.16	112.02
97	EF	503	YRB	C32-N06-C29	2.20	122.10	118.08
95	Pt	78	MET	CE-SD-CG	2.12	111.29	100.32
92	L5	5118	HMT	C3-O4-C19	-2.09	113.95	117.24
92	L5	5118	HMT	C15-C16-C6	-2.08	117.98	121.10
97	EF	503	YRB	C35-C33-C34	-2.07	108.28	112.17

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	S2	1901	SPD	C4-C5-N6-C7
92	L5	5118	HMT	C1-C2-O3-C18
92	L5	5118	HMT	C3-C2-O3-C18
92	L5	5118	HMT	C21-C20-C24-C25
92	L5	5118	HMT	O6-C20-C24-C25

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Mol	Chain	Res	Type	Atoms
95	Pt	78	MET	N-CA-CB-CG
95	Pt	78	MET	C-CA-CB-CG
97	EF	503	YRB	C19-C17-N04-C23
97	EF	503	YRB	C17-C19-C20-C22
97	EF	503	YRB	O09-C19-C20-C21
97	EF	503	YRB	O09-C19-C20-C22
92	L5	5118	HMT	O8-C22-O7-C23
92	L5	5118	HMT	C21-C22-O7-C23
87	L5	5102	SPD	C3-C4-C5-N6
87	L5	5103	SPD	C3-C4-C5-N6
92	L5	5118	HMT	C25-C26-C27-C29
92	L5	5118	HMT	C20-C24-C25-C26
87	L5	5109	SPD	C3-C4-C5-N6
90	L5	5115	PUT	C1-C2-C3-C4
97	EF	503	YRB	O02-C03-C04-C05
92	L5	5118	HMT	C25-C26-C27-O9
90	L5	5116	PUT	C1-C2-C3-C4
97	EF	503	YRB	C17-C19-C20-C21
87	L5	5102	SPD	C8-C7-N6-C5
92	L5	5118	HMT	C25-C26-C27-C28
87	S2	1901	SPD	C3-C4-C5-N6
97	EF	503	YRB	O02-C03-C04-C06
87	L5	5107	SPD	N6-C7-C8-C9
94	At	77	PHE	CA-CB-CG-CD2
94	At	77	PHE	CA-CB-CG-CD1
97	EF	503	YRB	C01-C03-C04-C05
97	EF	503	YRB	C01-C03-C04-C06
90	L5	5115	PUT	N1-C1-C2-C3
87	L5	5108	SPD	C2-C3-C4-C5
87	L5	5103	SPD	C2-C3-C4-C5
87	L5	5106	SPD	N6-C7-C8-C9
87	L5	5104	SPD	C8-C7-N6-C5
87	L5	5107	SPD	N1-C2-C3-C4
97	EF	503	YRB	C18-C17-N04-C23
87	L5	5104	SPD	N6-C7-C8-C9
87	L5	5106	SPD	C8-C7-N6-C5
97	EF	503	YRB	C14-C13-N03-C16
90	L5	5110	PUT	C2-C3-C4-N2
87	L5	5103	SPD	C8-C7-N6-C5
87	L5	5102	SPD	C2-C3-C4-C5
97	EF	503	YRB	C07-C09-C10-C12
87	L5	5109	SPD	N6-C7-C8-C9

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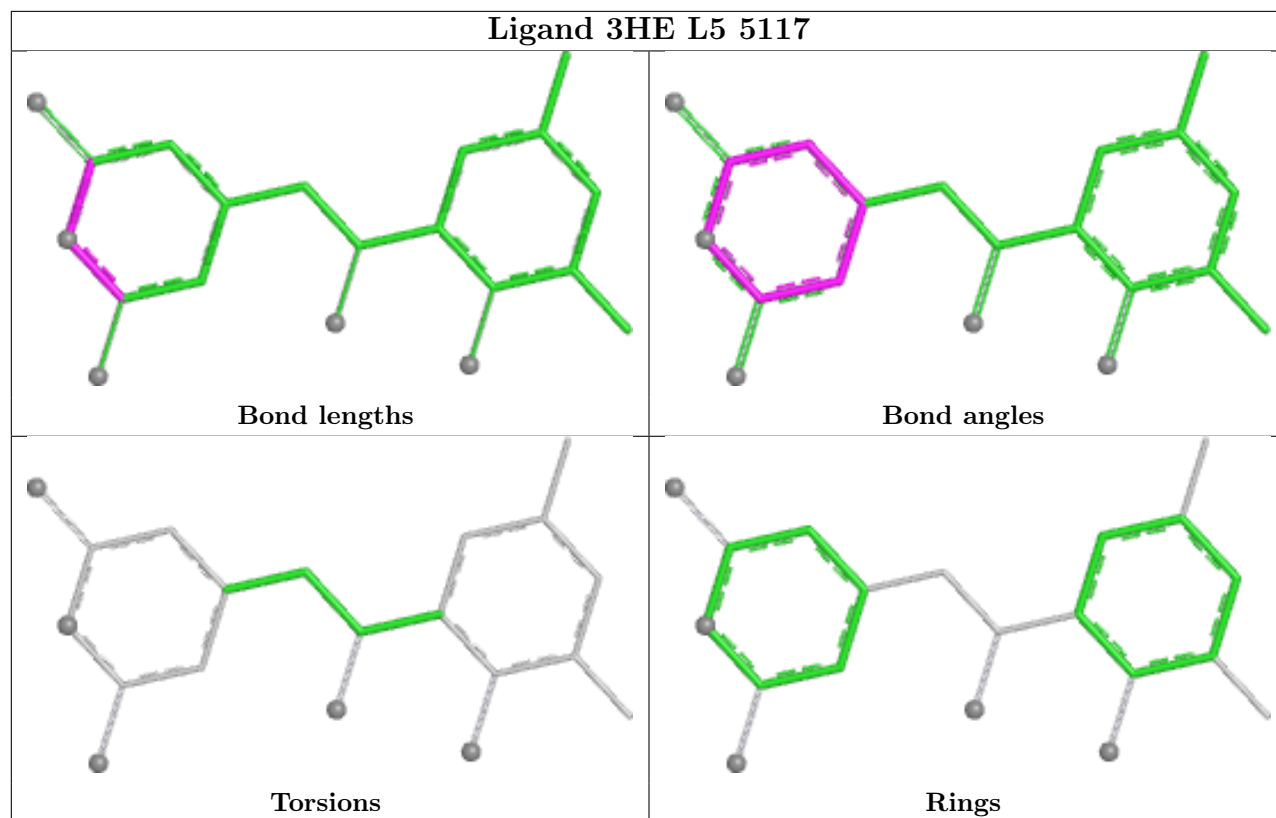
Mol	Chain	Res	Type	Atoms
90	L5	5115	PUT	C2-C3-C4-N2
87	S2	1901	SPD	C8-C7-N6-C5
90	L5	5119	PUT	C1-C2-C3-C4
97	EF	503	YRB	C11-C09-C10-C12

There are no ring outliers.

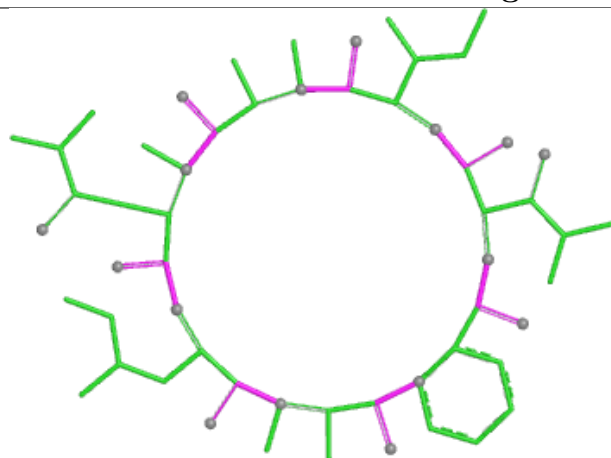
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5107	SPD	1	0
87	L5	5109	SPD	2	0
96	EF	501	GSP	1	0
92	L5	5118	HMT	6	0
95	Pt	78	MET	1	0
90	L5	5119	PUT	8	0

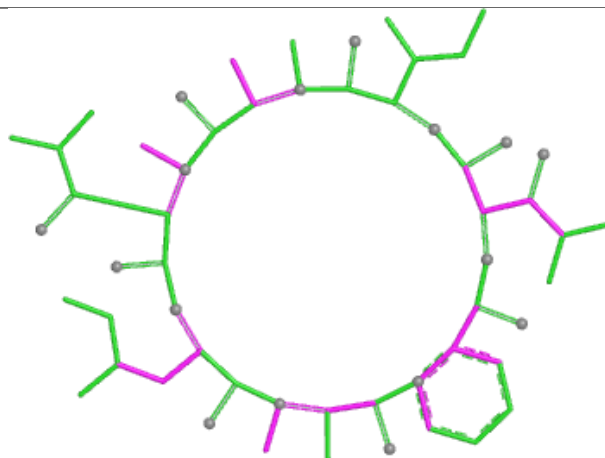
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



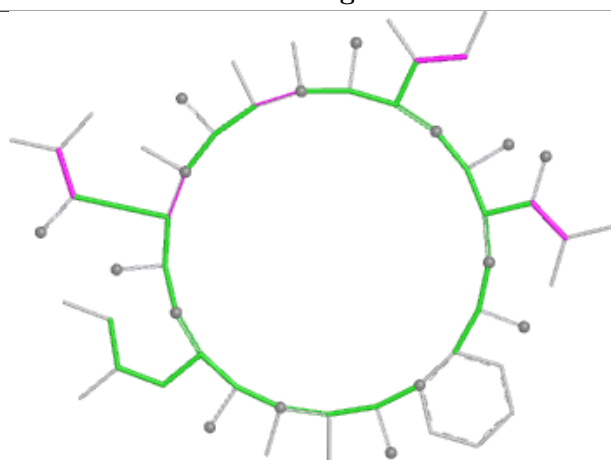
Ligand YRB EF 503



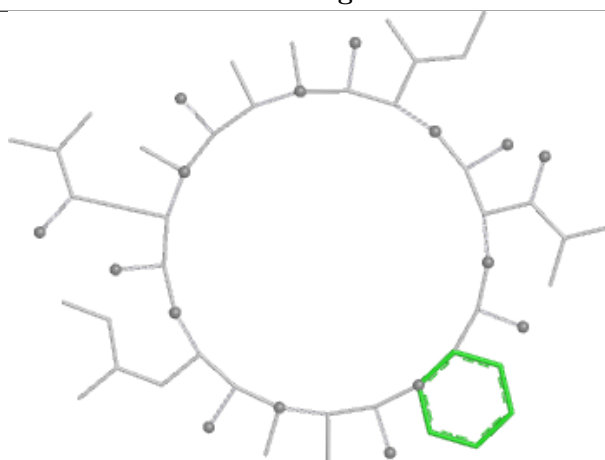
Bond lengths



Bond angles

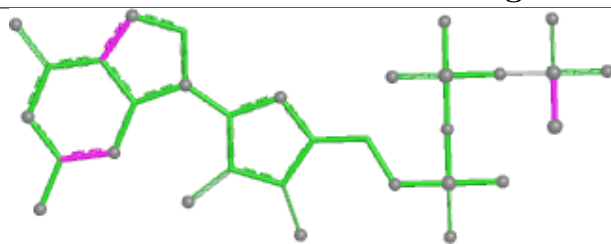


Torsions

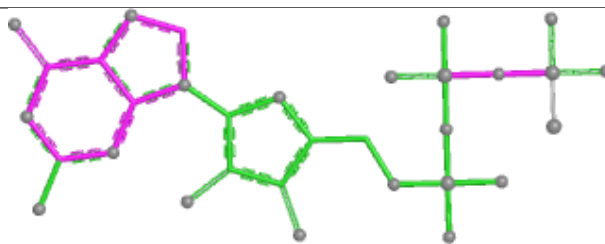


Rings

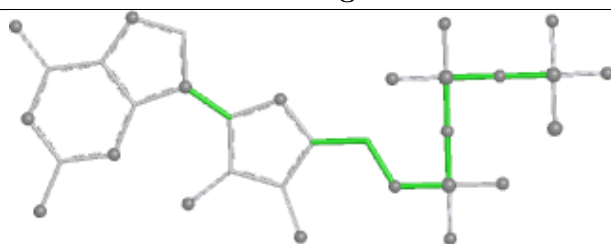
Ligand GSP EF 501



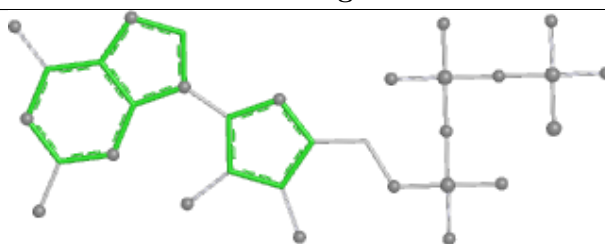
Bond lengths



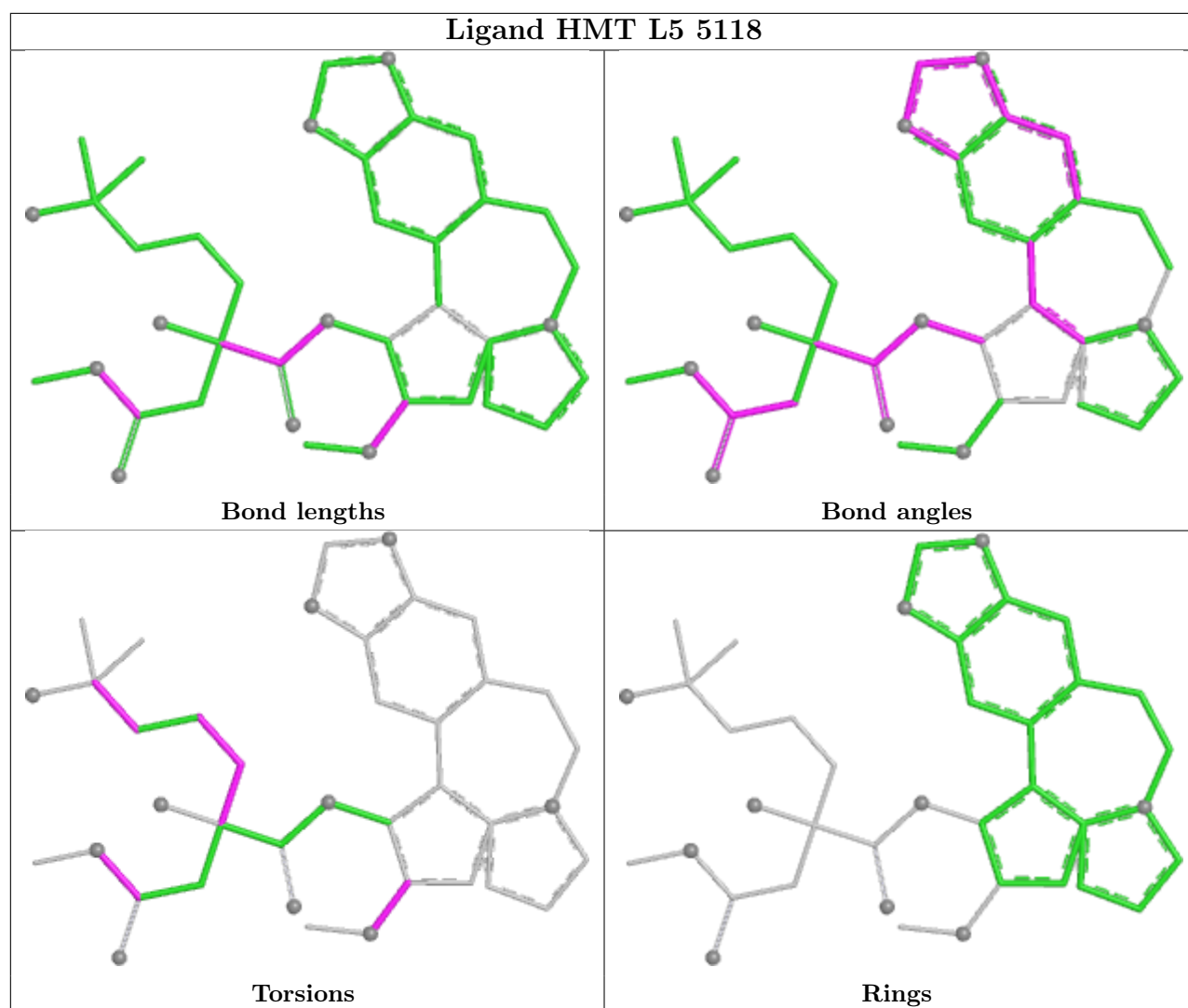
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

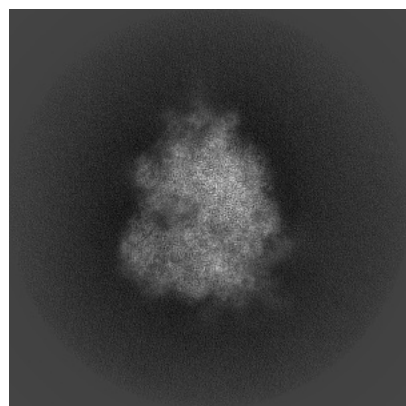
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29771. These allow visual inspection of the internal detail of the map and identification of artifacts.

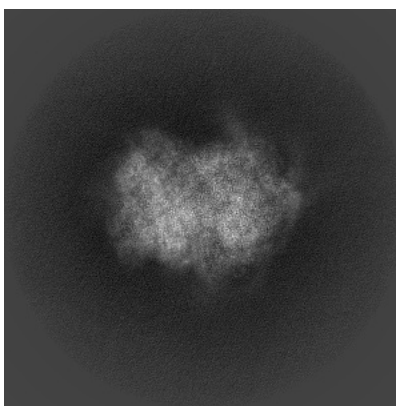
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

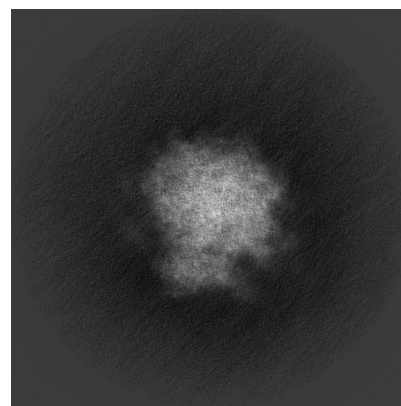
6.1.1 Primary map



X

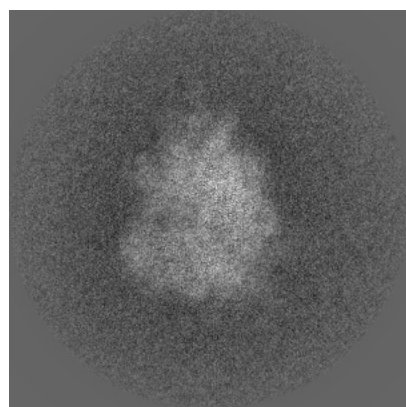


Y

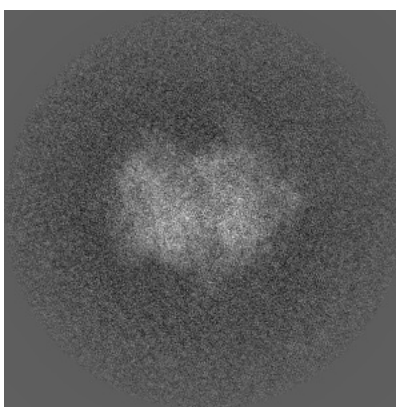


Z

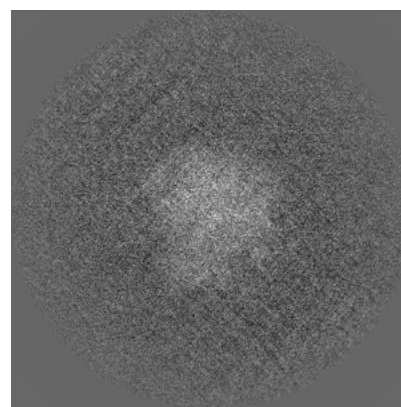
6.1.2 Raw map



X



Y

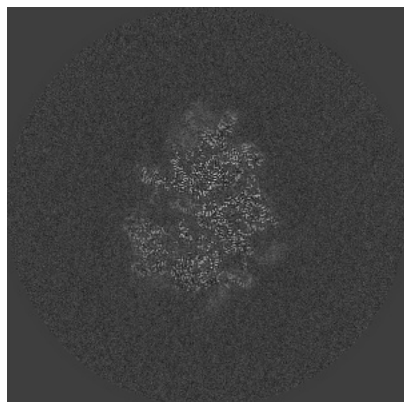


Z

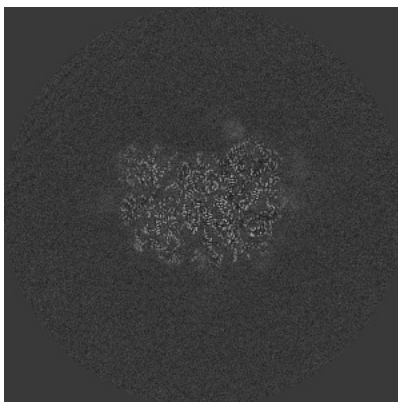
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

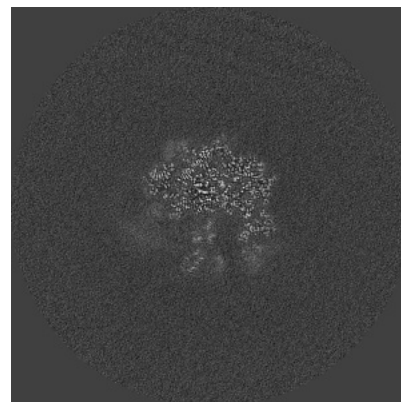
6.2.1 Primary map



X Index: 448

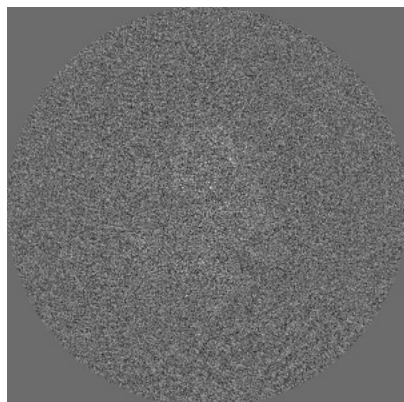


Y Index: 448

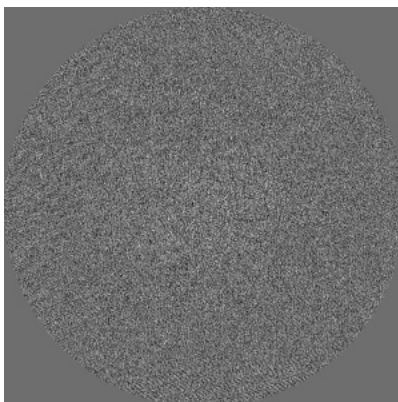


Z Index: 448

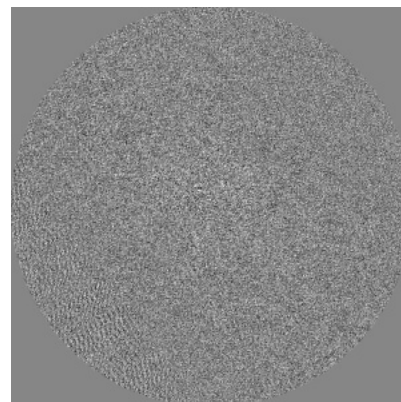
6.2.2 Raw map



X Index: 448



Y Index: 448

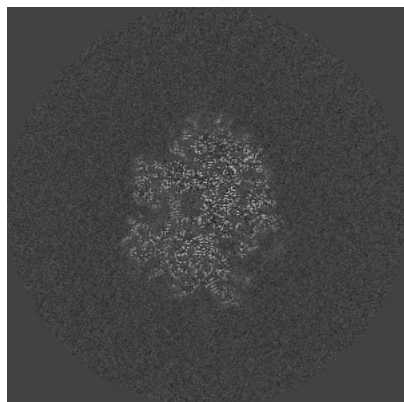


Z Index: 448

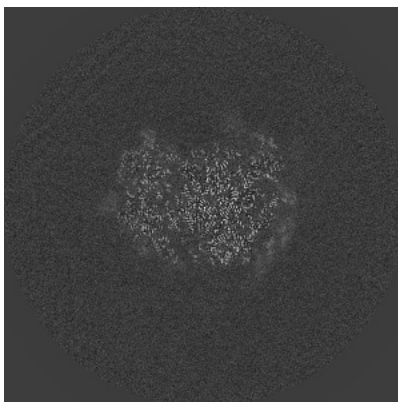
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

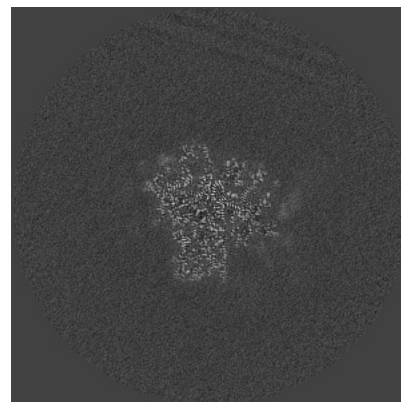
6.3.1 Primary map



X Index: 424

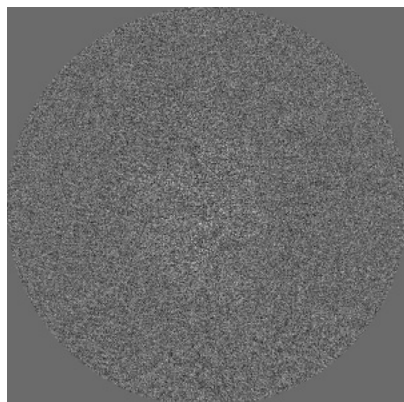


Y Index: 464

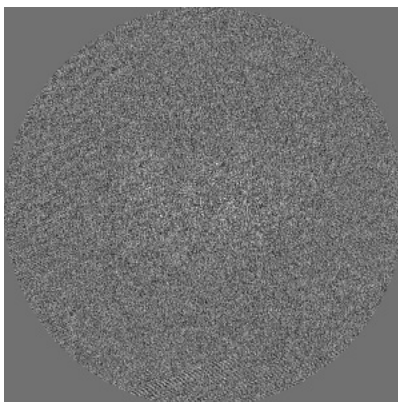


Z Index: 513

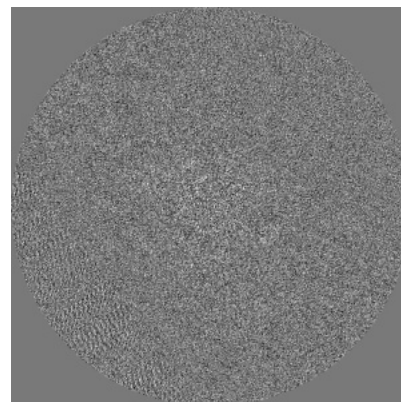
6.3.2 Raw map



X Index: 428



Y Index: 438

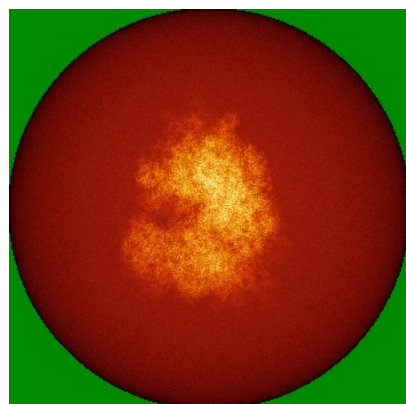


Z Index: 485

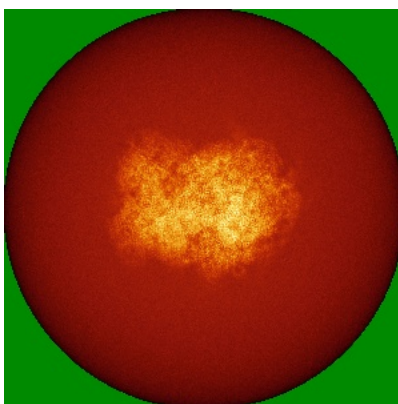
The images above show the largest variance slices of the map in three orthogonal directions.

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

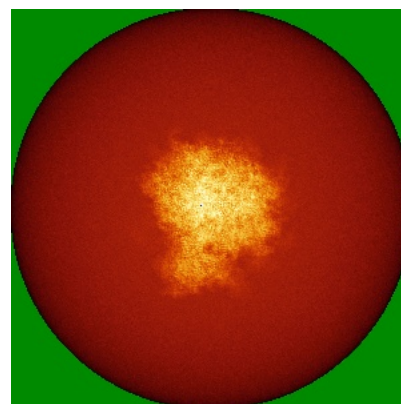
6.4.1 Primary map



X

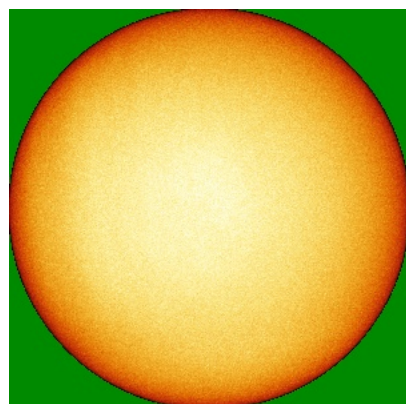


Y

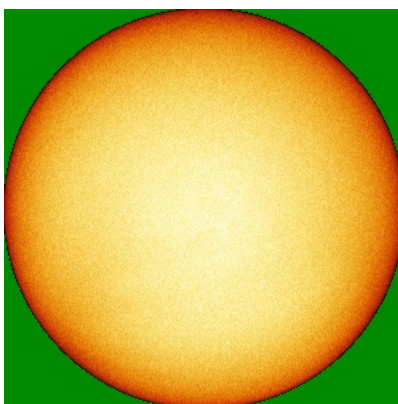


Z

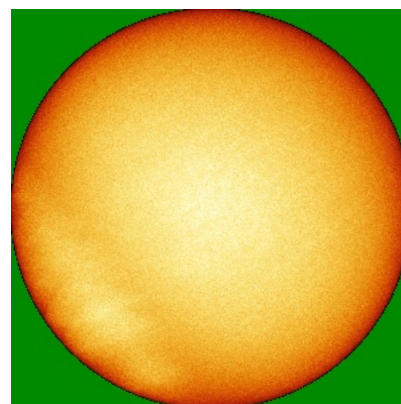
6.4.2 Raw map



X



Y

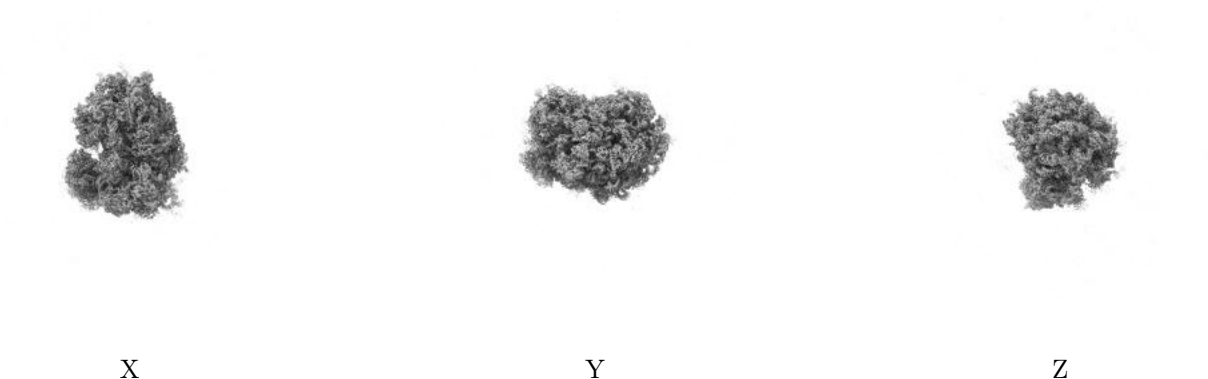


Z

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

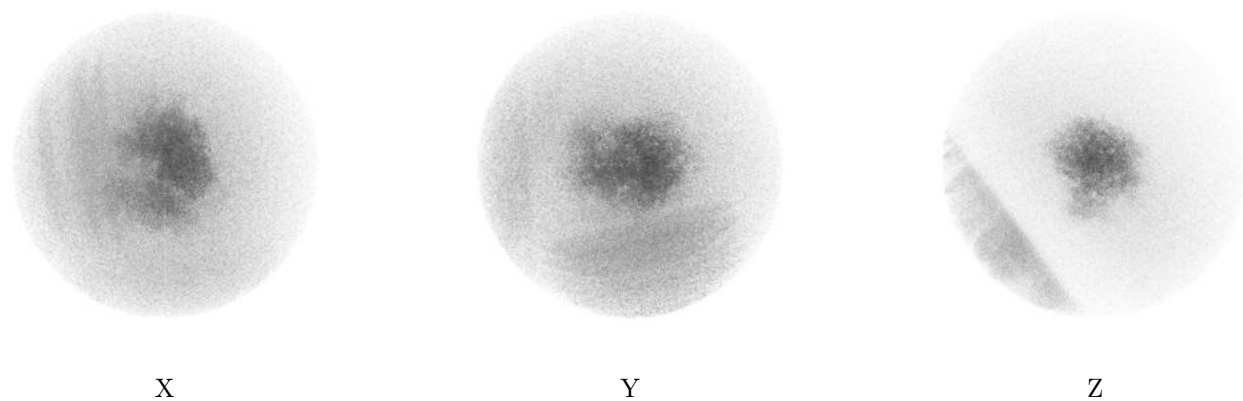
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

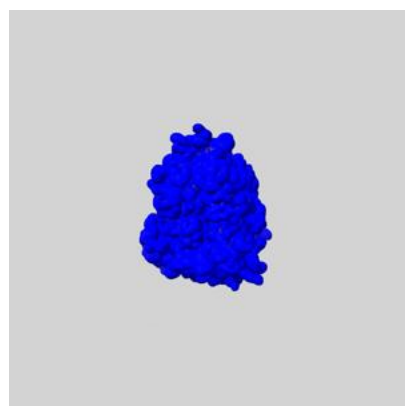
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

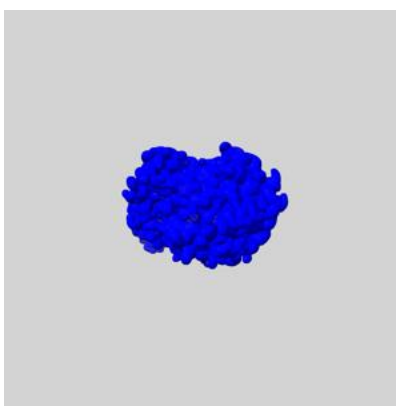
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

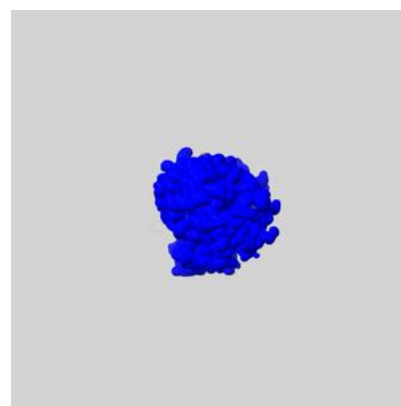
6.6.1 emd_29771_msk_1.map [i](#)



X



Y

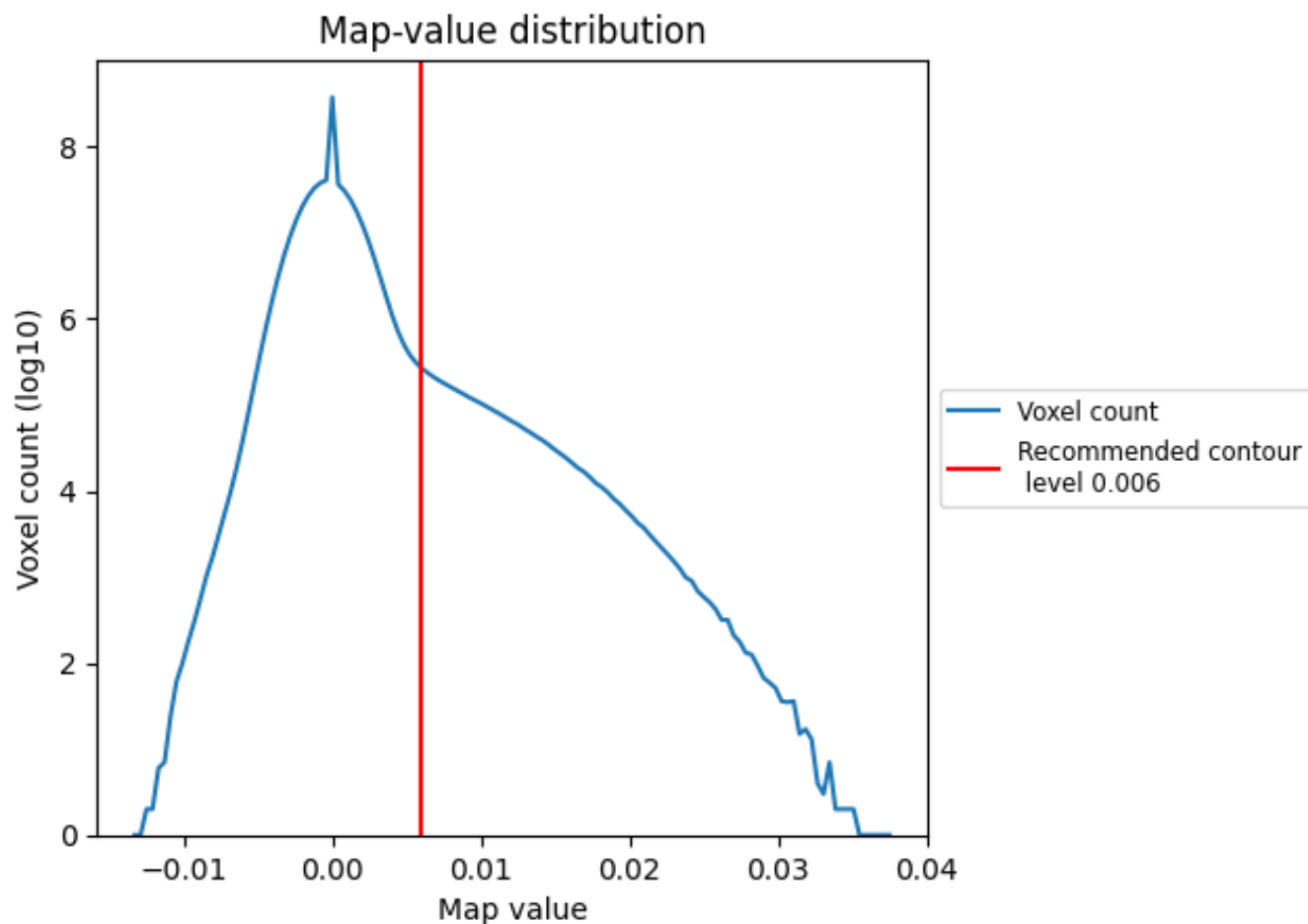


Z

7 Map analysis [i](#)

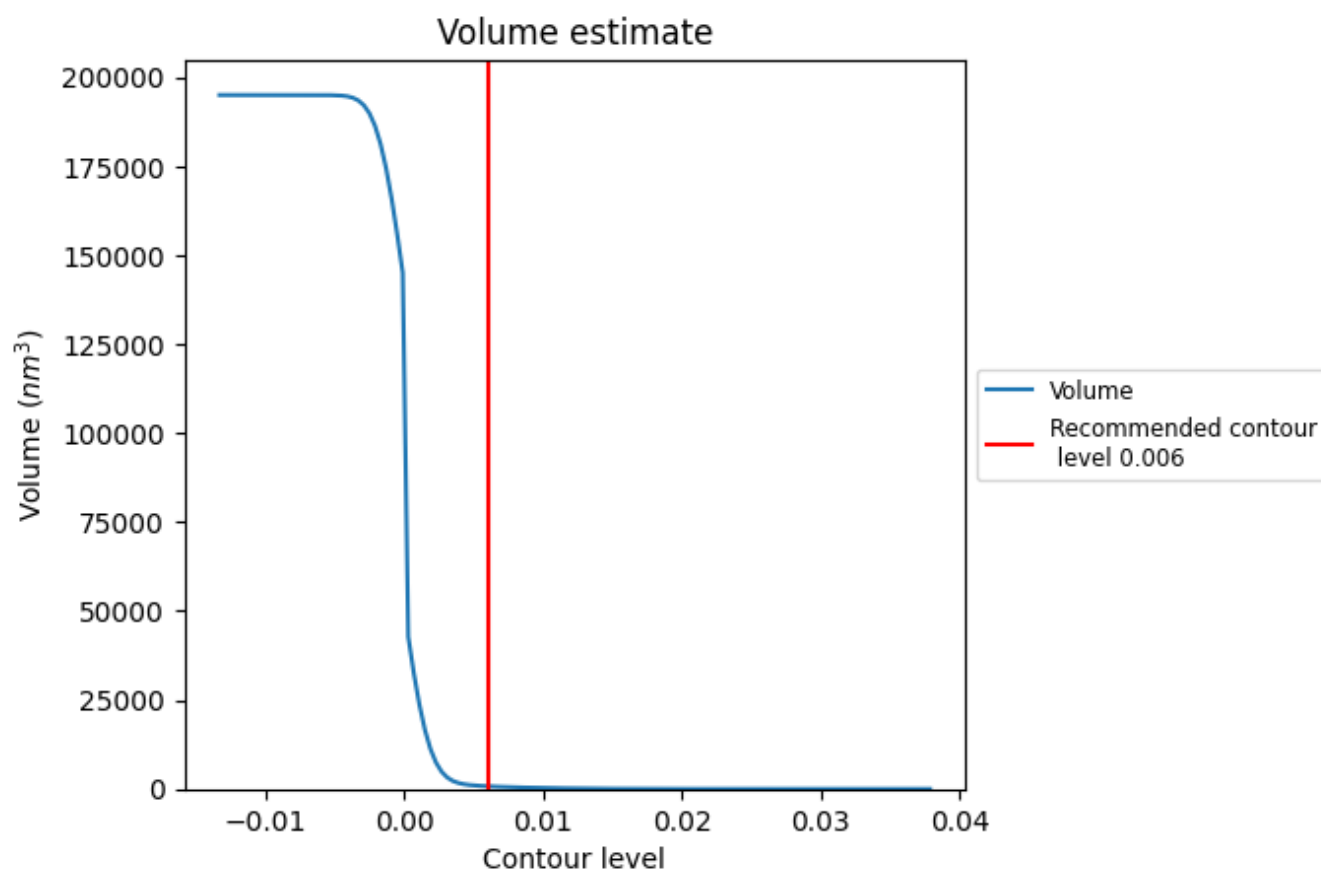
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

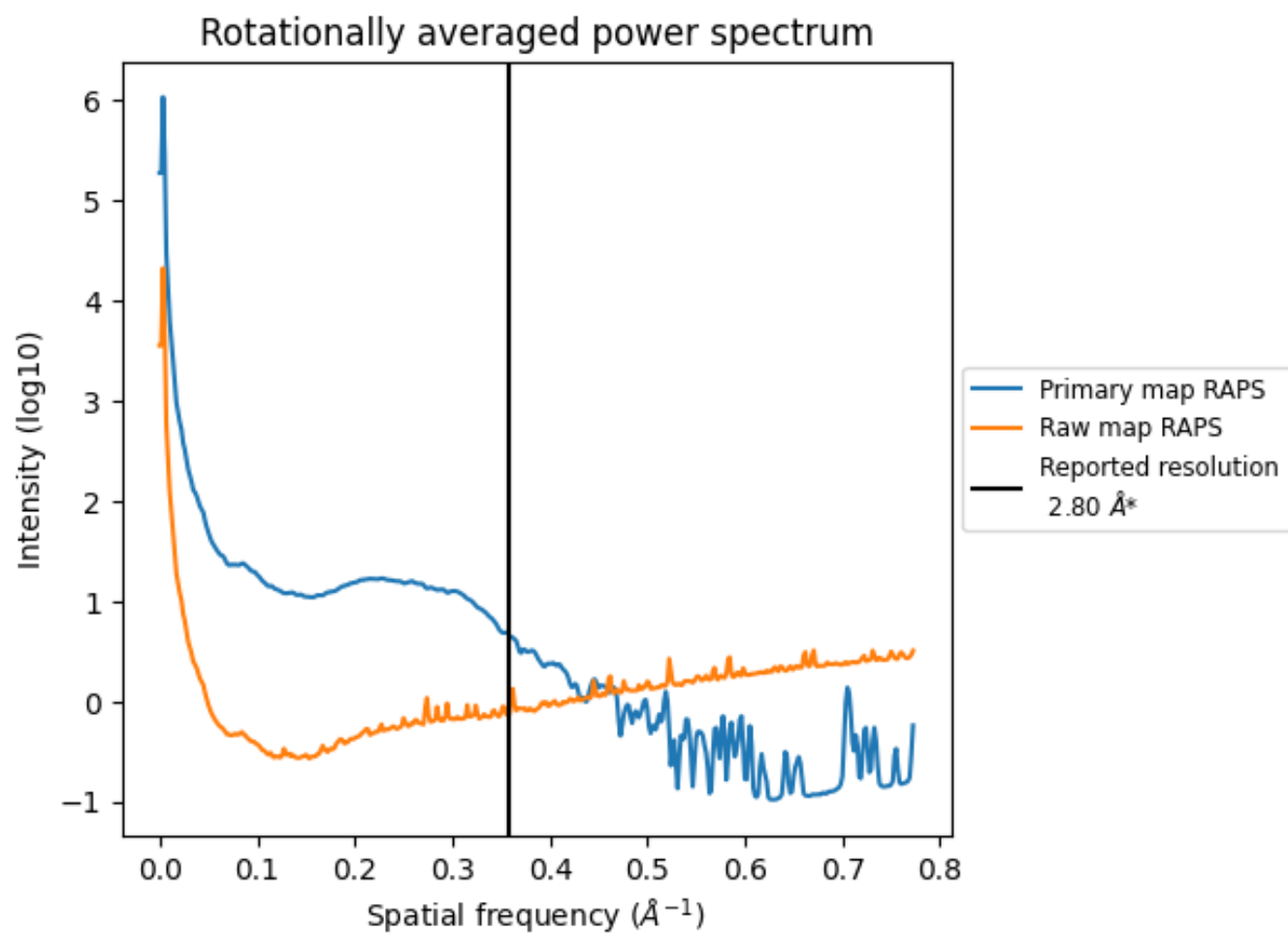
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 754 nm^3 ; this corresponds to an approximate mass of 682 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

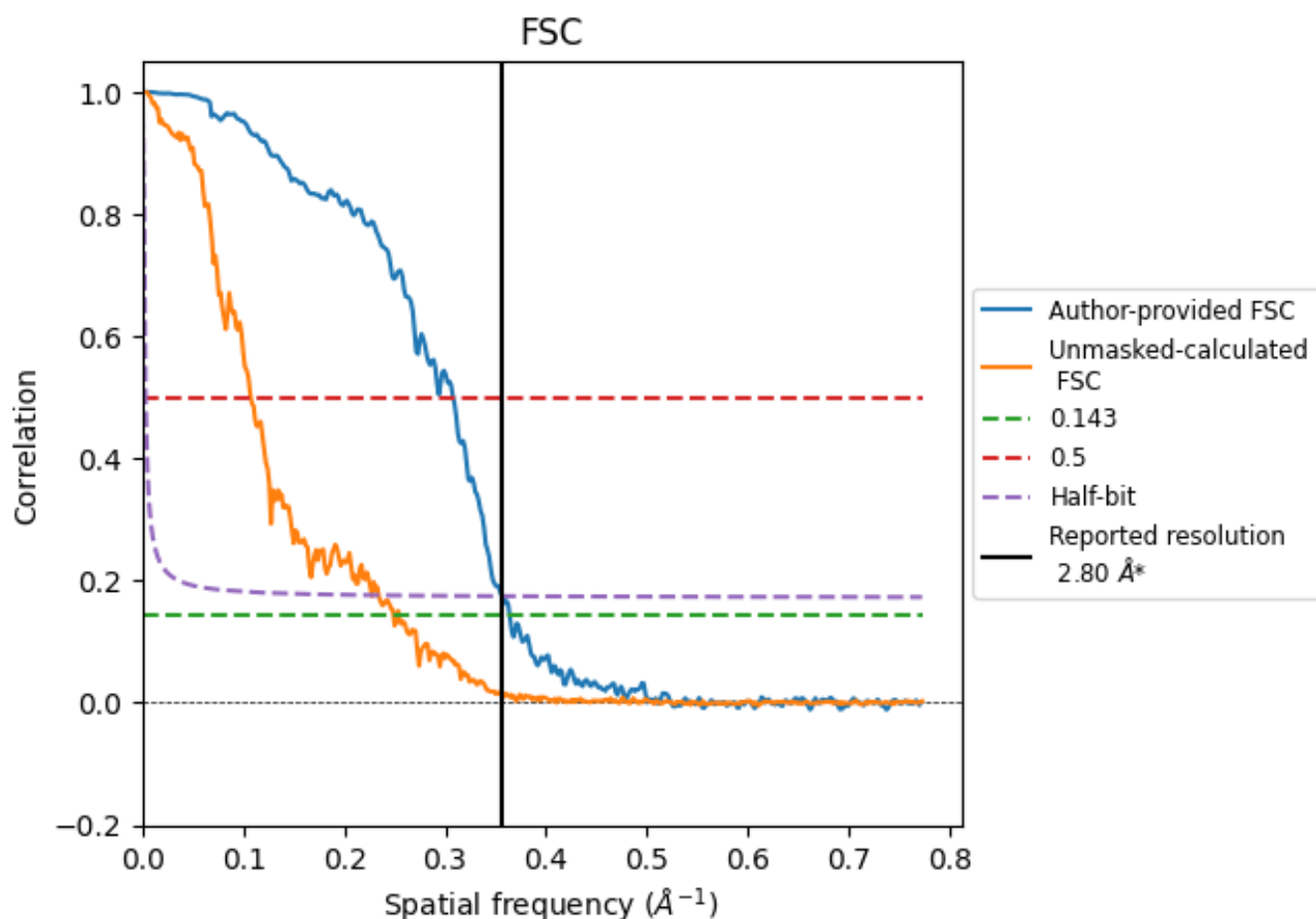


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

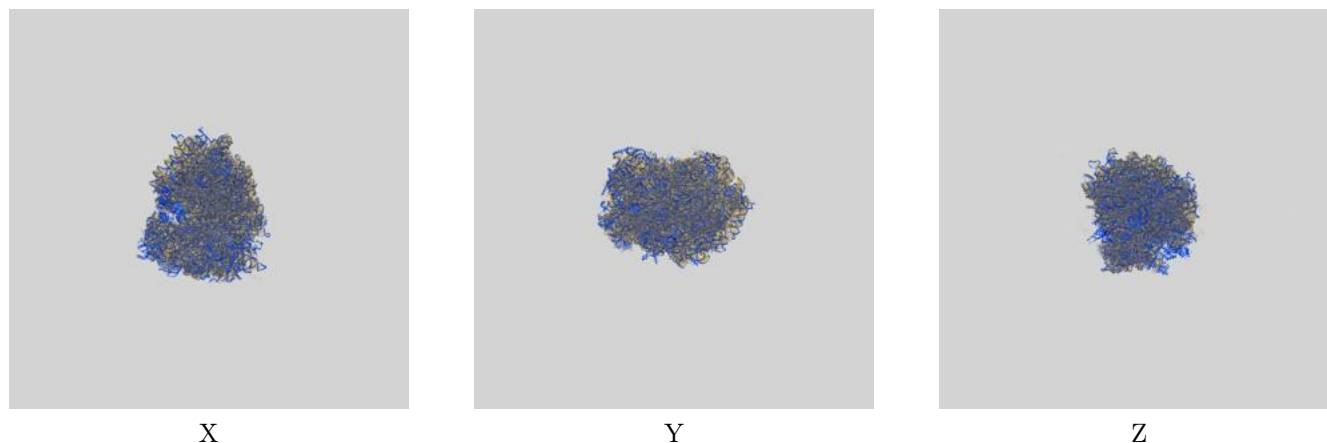
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.75	3.25	2.81
Unmasked-calculated*	4.02	9.29	4.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

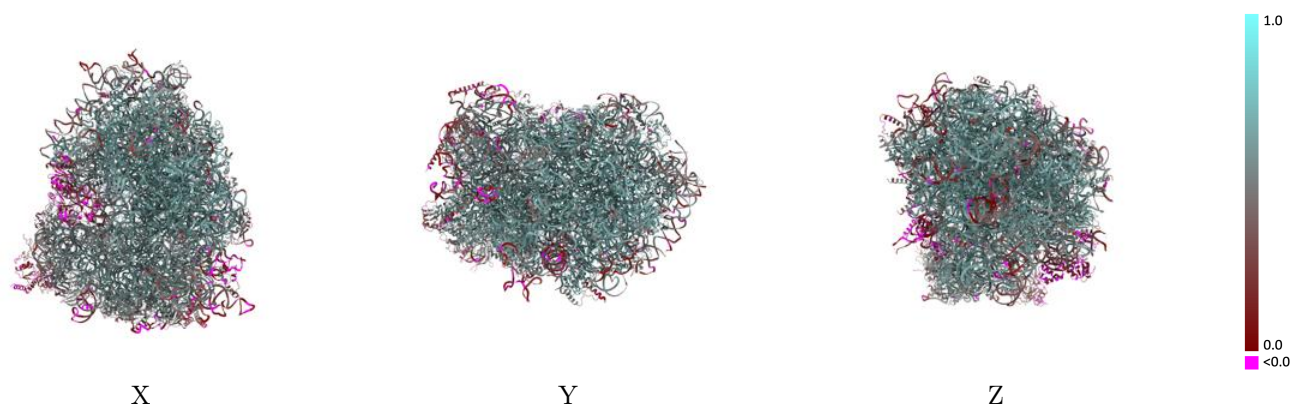
This section contains information regarding the fit between EMDB map EMD-29771 and PDB model 8G6J. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



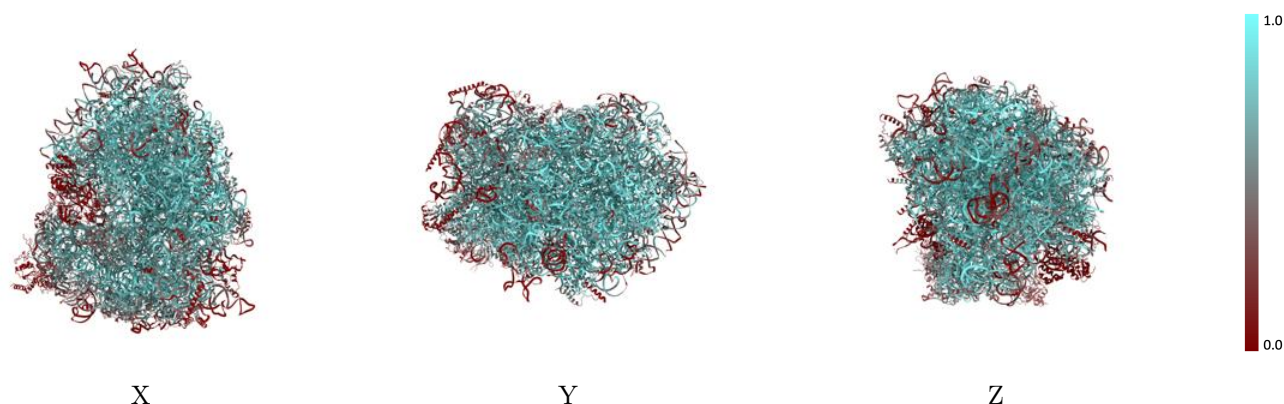
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



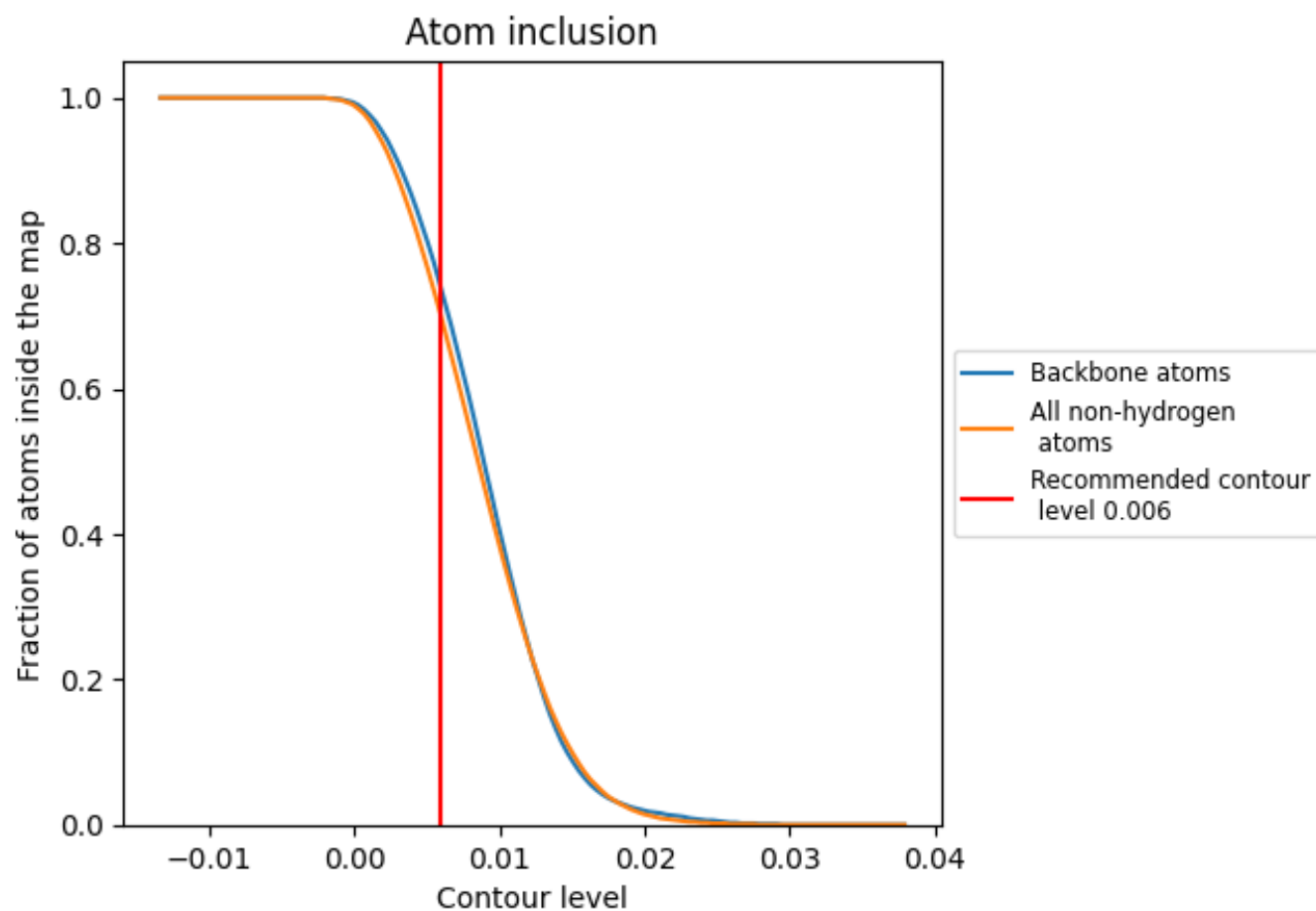
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.5480
At	 0.5340	 0.4730
EF	 0.5090	 0.5250
L5	 0.7730	 0.5680
L7	 0.9160	 0.6390
L8	 0.8520	 0.6090
LA	 0.8660	 0.6610
LB	 0.7950	 0.6310
LC	 0.8070	 0.6290
LD	 0.6740	 0.5660
LE	 0.6720	 0.5790
LF	 0.8420	 0.6420
LG	 0.6000	 0.5220
LH	 0.6980	 0.5930
LI	 0.7340	 0.5940
LJ	 0.5720	 0.5220
LK	 0.0010	 0.0390
LL	 0.7160	 0.5950
LM	 0.7330	 0.5930
LN	 0.9180	 0.6770
LO	 0.8180	 0.6280
LP	 0.8480	 0.6540
LQ	 0.8670	 0.6630
LR	 0.6830	 0.5640
LS	 0.8270	 0.6380
LT	 0.7650	 0.6080
LU	 0.4380	 0.4630
LV	 0.7770	 0.6330
LW	 0.4570	 0.4260
LX	 0.7420	 0.6030
LY	 0.7380	 0.5980
LZ	 0.7220	 0.5930
La	 0.8670	 0.6600
Lb	 0.5890	 0.5050
Lc	 0.7240	 0.5910



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Chain	Atom inclusion	Q-score
Ld	 0.7240	 0.5760
Le	 0.8630	 0.6600
Lf	 0.8770	 0.6590
Lg	 0.7880	 0.6190
Lh	 0.7010	 0.5920
Li	 0.6550	 0.5500
Lj	 0.8890	 0.6690
Lk	 0.4450	 0.4770
Ll	 0.8220	 0.6250
Lm	 0.7280	 0.6040
Ln	 0.7750	 0.6050
Lo	 0.7360	 0.6020
Lp	 0.8100	 0.6380
Lq	 0.0050	 0.0560
Lr	 0.8120	 0.6320
Lz	 0.0000	 0.0440
Pt	 0.6740	 0.5340
S2	 0.7530	 0.5450
SA	 0.5970	 0.5580
SB	 0.5820	 0.5410
SC	 0.6660	 0.5780
SD	 0.4700	 0.4720
SE	 0.5560	 0.5130
SF	 0.5500	 0.5190
SG	 0.4000	 0.4260
SH	 0.3710	 0.4300
SI	 0.5480	 0.5000
SJ	 0.5060	 0.4710
SK	 0.4330	 0.4480
SL	 0.6760	 0.5690
SM	 0.0040	 0.0910
SN	 0.6990	 0.5910
SO	 0.6820	 0.5850
SP	 0.4260	 0.4330
SQ	 0.5640	 0.5260
SR	 0.4120	 0.4620
SS	 0.4660	 0.4810
ST	 0.4980	 0.5050
SU	 0.3950	 0.4280
SV	 0.5900	 0.5560
SW	 0.7440	 0.6110
SX	 0.7280	 0.6040

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Chain	Atom inclusion	Q-score
SY	 0.4230	 0.4350
SZ	 0.3300	 0.4330
Sa	 0.6970	 0.5840
Sb	 0.5340	 0.5240
Sc	 0.4650	 0.4640
Sd	 0.7150	 0.5680
Se	 0.4340	 0.4110
Sf	 0.0250	 0.1680
Sg	 0.2380	 0.4030
mR	 0.6440	 0.5020