



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 05:01 PM JST

PDB ID : 7XNX / pdb_00007xnx
EMDB ID : EMD-33329
Title : High resolution cry-EM structure of the human 80S ribosome from
SNORD127+/+ Kasumi-1 cells
Authors : Cheng, J.; Beckmann, R.
Deposited on : 2022-04-30
Resolution : 2.70 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

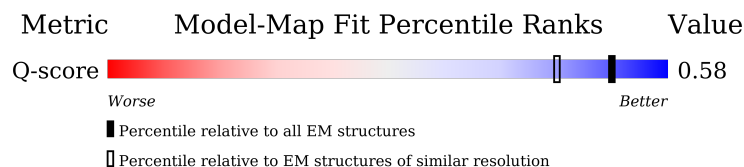
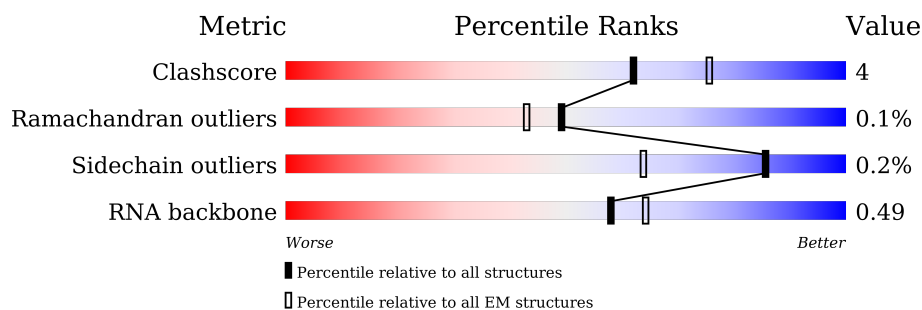
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



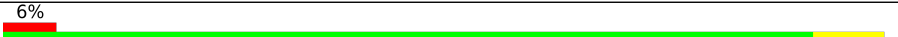
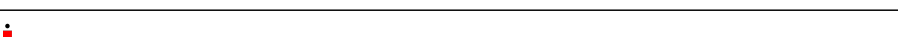
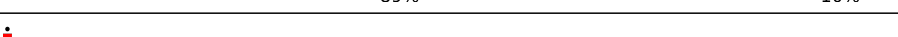
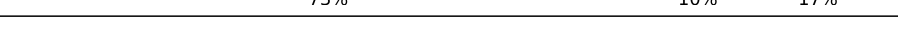
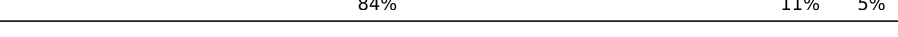
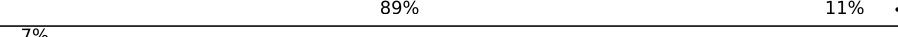
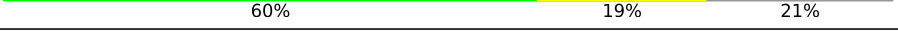
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	L1	5070	
2	L2	121	
3	L3	157	

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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	282	

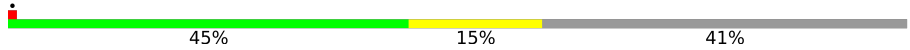
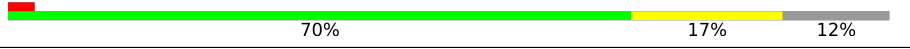
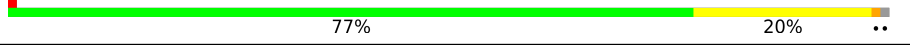
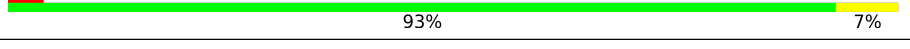
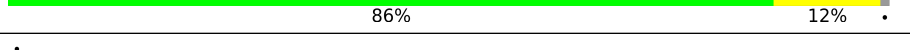
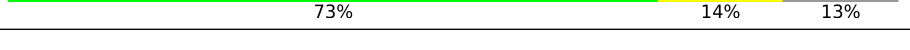
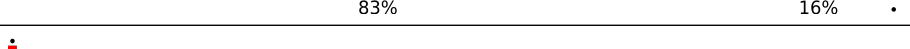
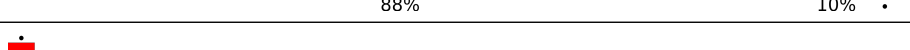
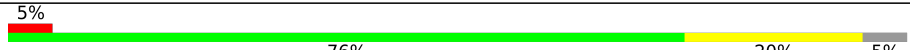
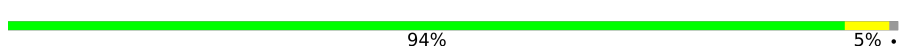
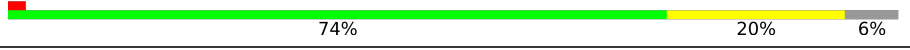
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Mol	Chain	Length	Quality of chain
28	La	282	
29	Lb	159	
30	Lc	115	
31	Ld	125	
32	Le	135	
33	Lf	110	
34	Lg	117	
35	Lh	123	
36	Li	105	
37	Lj	97	
38	Lk	70	
39	Ll	51	
40	Lm	128	
41	Ln	25	
42	Lo	106	
43	Lp	92	
44	Lr	137	
45	S2	1869	
46	SA	295	
47	SB	264	
48	SD	243	
49	SE	263	
50	SF	204	
51	SH	194	
52	SI	208	

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Mol	Chain	Length	Quality of chain
53	SK	165	
54	SL	158	
55	SP	145	
56	SQ	146	
57	SR	135	
58	SS	152	
59	ST	145	
60	SU	119	
61	SV	83	
62	SX	143	
63	Sa	115	
64	Sc	69	
65	Sd	56	
66	Sg	317	
67	SC	293	
68	SG	249	
69	SJ	194	
70	SM	132	
71	SN	151	
72	SO	151	
73	SW	130	
74	SY	133	
75	SZ	125	
76	Sb	84	
77	Se	59	

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Mol	Chain	Length	Quality of chain
78	CE	133	8%48%6%46%
78	Sf	133	39%7%54%
79	CC	75	67%37%48%15%

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 218434 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	3773	Total	C	N	O	P	0	0
			80211	35727	14590	26122	3772		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	220	Total	C	N	O	S	0	0
			1765	1136	334	291	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	227	Total	C	N	O	S	0	0
			1835	1171	353	307	4		

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

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

- Molecule 12 is a protein called Ribosomal protein L10 isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	169	Total	C	N	O	S	0	0
			1353	856	253	238	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		
28	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L29.

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

- Molecule 30 is a protein called 60S ribosomal protein L30.

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

- Molecule 31 is a protein called 60S ribosomal protein L31.

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

- Molecule 32 is a protein called 60S ribosomal protein L32.

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

- Molecule 33 is a protein called 60S ribosomal protein L35a.

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

- Molecule 34 is a protein called 60S ribosomal protein L34.

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

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

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

- Molecule 36 is a protein called 60S ribosomal protein L36.

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

- Molecule 37 is a protein called 60S ribosomal protein L37.

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

- Molecule 38 is a protein called 60S ribosomal protein L38.

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

- Molecule 39 is a protein called 60S ribosomal protein L39.

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

- Molecule 40 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 41 is a protein called 60S ribosomal protein L41.

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

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	103	Total	C	N	O	S	0	0
			843	529	172	136	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

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

- Molecule 44 is a protein called 60S ribosomal protein L28.

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

- Molecule 45 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S2	1740	Total	C	N	O	P	0	0
			36959	16515	6600	12105	1739		

- Molecule 46 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

- Molecule 47 is a protein called 40S ribosomal protein S3a.

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

- Molecule 48 is a protein called 40S ribosomal protein S3.

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

- Molecule 49 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 50 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 51 is a protein called 40S ribosomal protein S7.

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

- Molecule 52 is a protein called 40S ribosomal protein S8.

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

- Molecule 53 is a protein called 40S ribosomal protein S10.

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

- Molecule 54 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 55 is a protein called 40S ribosomal protein S15.

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

- Molecule 56 is a protein called 40S ribosomal protein S16.

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

- Molecule 57 is a protein called 40S ribosomal protein S17.

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

- Molecule 58 is a protein called 40S ribosomal protein S18.

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

- Molecule 59 is a protein called 40S ribosomal protein S19.

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

- Molecule 60 is a protein called 40S ribosomal protein S20.

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

- Molecule 61 is a protein called 40S ribosomal protein S21.

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

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

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

- Molecule 63 is a protein called 40S ribosomal protein S26.

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

- Molecule 64 is a protein called 40S ribosomal protein S28.

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

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called 40S ribosomal protein S9.

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

- Molecule 70 is a protein called 40S ribosomal protein S12.

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

- Molecule 71 is a protein called 40S ribosomal protein S13.

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

- Molecule 72 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SY	125	Total	C	N	O	S	0	0
			1022	645	200	172	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S27.

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

- Molecule 77 is a protein called 40S ribosomal protein S30.

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

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		
78	CE	72	Total	C	N	O		0	0
			603	395	105	103			

- Molecule 79 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	CC	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	L1	264	Total	Mg	0
			264	264	
80	L2	3	Total	Mg	0
			3	3	
80	L3	5	Total	Mg	0
			5	5	
80	LA	1	Total	Mg	0
			1	1	
80	LC	2	Total	Mg	0
			2	2	
80	LI	1	Total	Mg	0
			1	1	
80	LN	1	Total	Mg	0
			1	1	
80	LP	1	Total	Mg	0
			1	1	
80	LV	1	Total	Mg	0
			1	1	
80	Le	1	Total	Mg	0
			1	1	
80	Lf	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	Lg	1	Total 1	Mg 1	0
80	S2	135	Total 135	Mg 135	0
80	Sd	1	Total 1	Mg 1	0
80	SG	1	Total 1	Mg 1	0
80	SJ	1	Total 1	Mg 1	0
80	CC	1	Total 1	Mg 1	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
81	L1	12	Total 12	K 12	0

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 83 is water.

Mol	Chain	Residues	Atoms	AltConf
83	L1	762	Total O 762 762	0
83	L2	3	Total O 3 3	0
83	L3	6	Total O 6 6	0
83	LA	6	Total O 6 6	0
83	LB	3	Total O 3 3	0
83	LC	13	Total O 13 13	0
83	LD	1	Total O 1 1	0
83	LI	2	Total O 2 2	0
83	LL	1	Total O 1 1	0
83	LN	1	Total O 1 1	0
83	LP	1	Total O 1 1	0
83	LR	1	Total O 1 1	0
83	LX	2	Total O 2 2	0
83	LY	2	Total O 2 2	0
83	La	8	Total O 8 8	0
83	Lb	1	Total O 1 1	0
83	Le	2	Total O 2 2	0
83	Lg	2	Total O 2 2	0
83	Lj	4	Total O 4 4	0
83	Ll	2	Total O 2 2	0
83	Lo	1	Total O 1 1	0
83	S2	10	Total O 10 10	0

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Mol	Chain	Residues	Atoms		AltConf
83	SX	1	Total	O	0
			1	1	
83	CE	1	Total	O	0
			1	1	

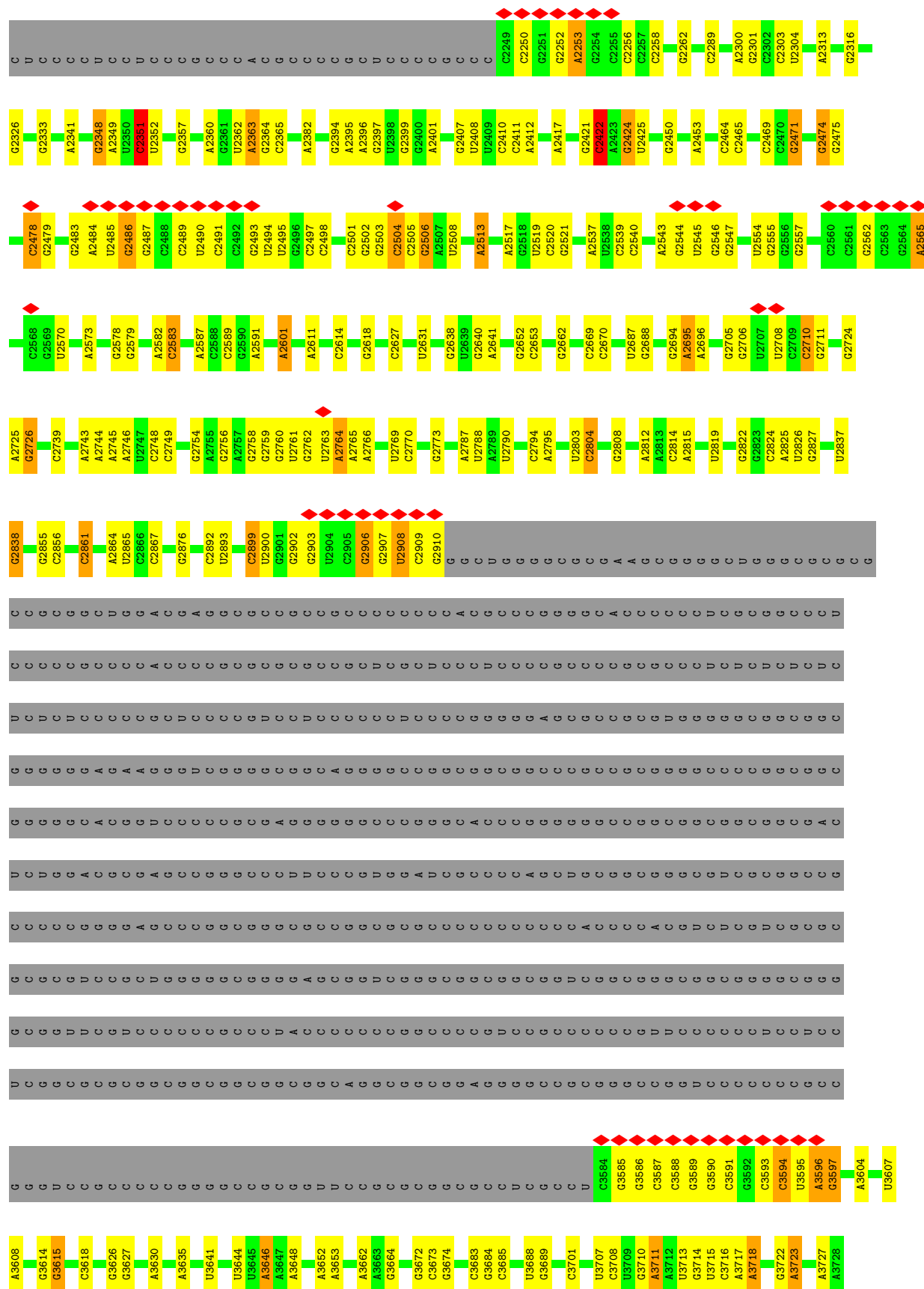
3 Residue-property plots [i](#)

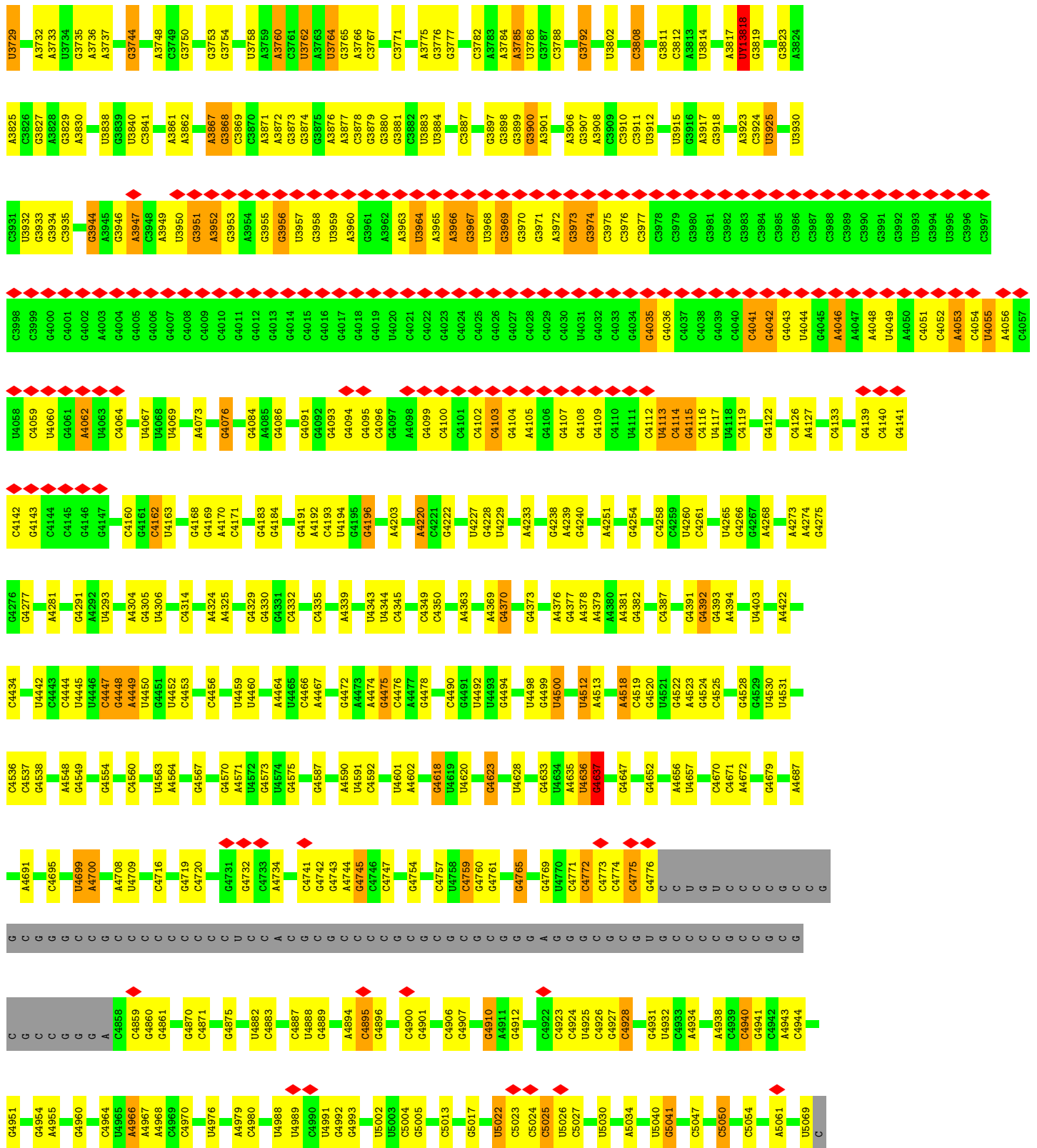
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S rRNA

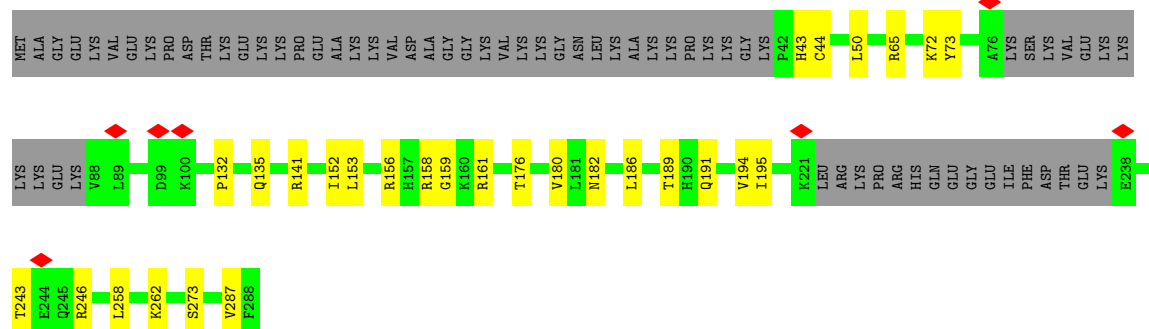




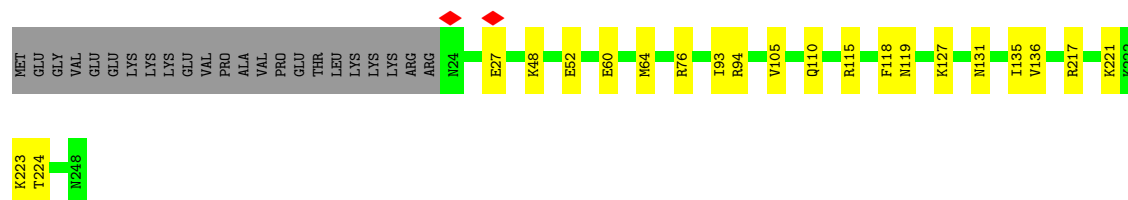




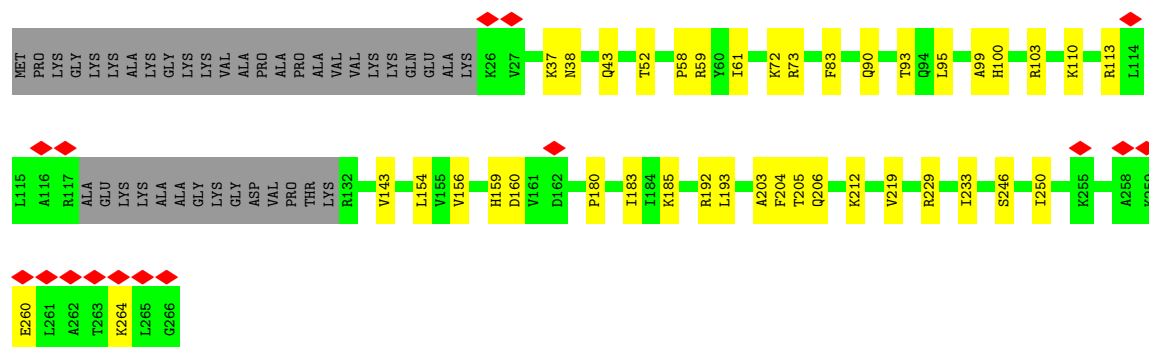
Chain LE:



Chain LF: 82% 8% 9%



Chain LG:

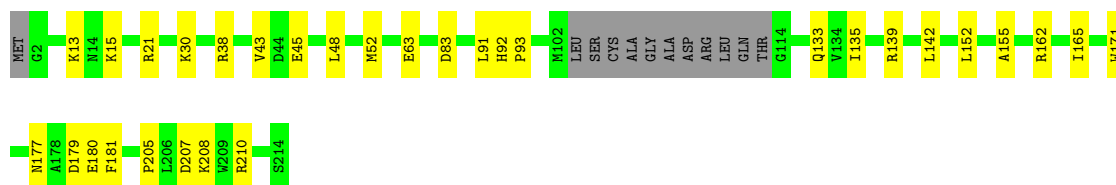


Chain LH: 84% 15%



- Molecule 12: Ribosomal protein L10 isoform A

Chain LI: 80% 14% 6%



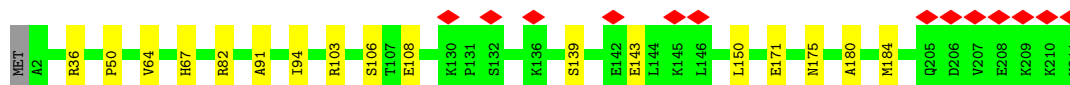
- Molecule 13: 60S ribosomal protein L11

Chain LJ: 84% 11% 5%



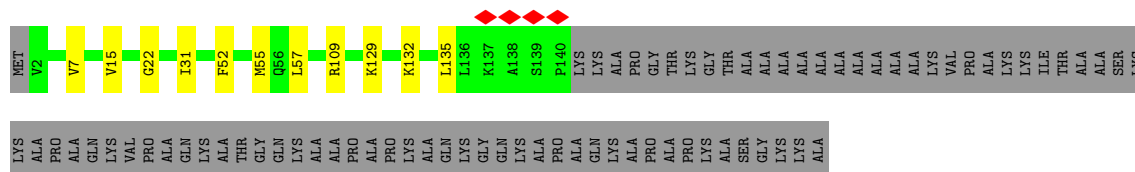
- Molecule 14: 60S ribosomal protein L13

Chain LL: 6% 91% 8%



- Molecule 15: 60S ribosomal protein L14

Chain LM: 60% 5% 35%



- Molecule 16: 60S ribosomal protein L15

Chain LN: 85% 14%

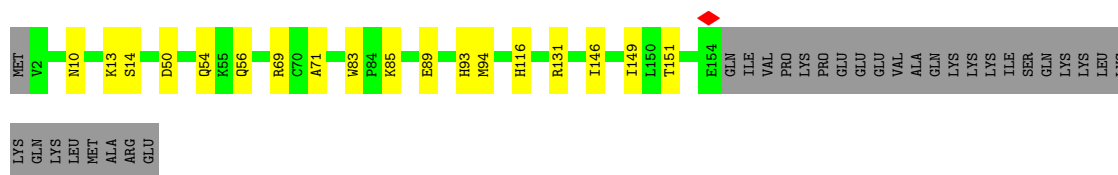
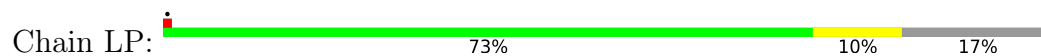


- Molecule 17: 60S ribosomal protein L13a

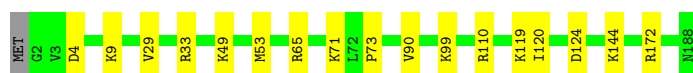
Chain LO: 89% 10%



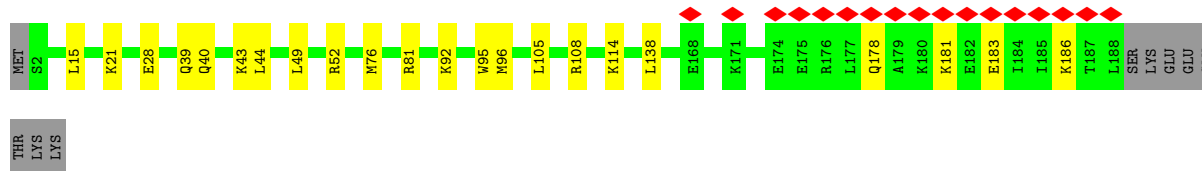
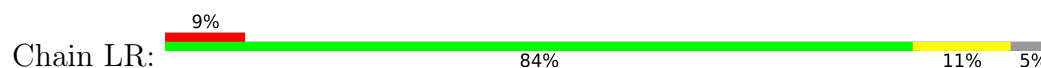
- Molecule 18: 60S ribosomal protein L17



- Molecule 19: 60S ribosomal protein L18



- Molecule 20: 60S ribosomal protein L19



- Molecule 21: 60S ribosomal protein L18a



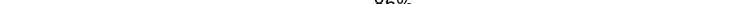
- Molecule 22: 60S ribosomal protein L21

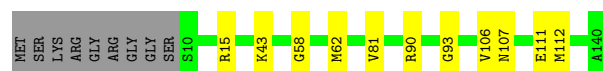


- Molecule 23: 60S ribosomal protein L22



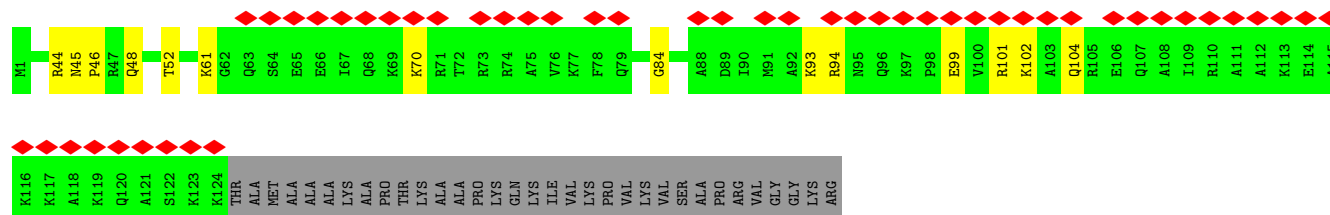
- Molecule 24: 60S ribosomal protein L23

Chain LV: 



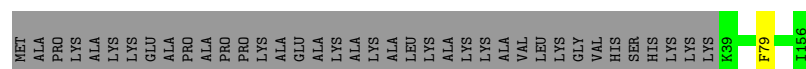
- Molecule 25: 60S ribosomal protein L24

Chain LW: 31% 70% 9% 21%



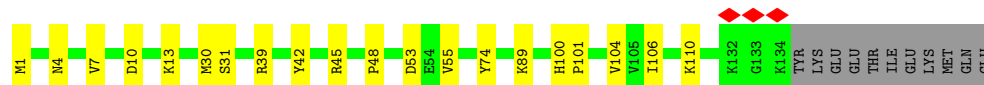
- Molecule 26: 60S ribosomal protein L23a

Chain LX: 75% 24%

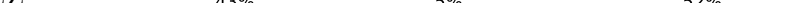


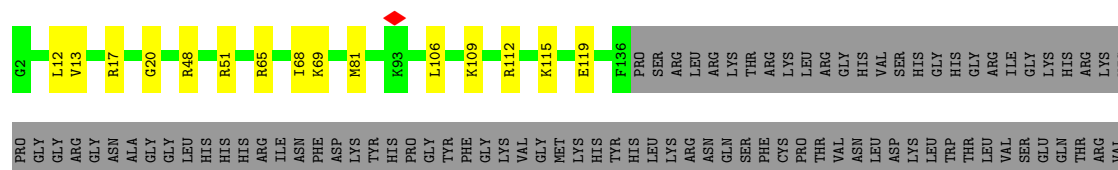
- Molecule 27: 60S ribosomal protein L26

Chain LY: 79% 14% 8%



- Molecule 28: 60S ribosomal protein L27

Chain LZ:  43% 5% 52%



ASN
ALA
ALA
LYS
LYS
MET
GLY
ASN
LYS
LYS
THR
GLY
ALA
ALA
PRO
PRO
ILE
ILE
ASP
VAL
VAL
ARG
SER
SER
GLY
TYR
TYR
LYS
LYS
VAL
VAL
GLY
LYS
LYS
LYS
LEU
PRO
LYS
LYS
GLN
PRO
VAL
ILE
ILE
VAL
LYS
ALA
LYS
PHE
PHE
SER
SER
ARG
ARG
ALA
GLU
GLU
LYS
LYS
ILE
LYS
LYS
SER
VAL
GLY
GLY
ALA
CYS
VAL
VAL
LYS
LYS
ALA

• Molecule 28: 60S ribosomal protein L27

Chain La: 45% 7% 48%

GLY
LYS
PHE
MET
GLY
LYS
PRO
LYS
LYS
GLY
LYS
VAL
VAL
VAL
GLN
LEU
VAL
VAL
LEU
ALA
GLY
ARG
TYR
ASN
TYR
HIS
HIS
SER
GLY
ARG
LYS
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ALA
VAL
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SER
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LYS
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ASP
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GLY
THR
SER
VAL
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ARG
PRO
LYS
LYS
ASP
ASP
SER
SER
HIS
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PHE
LEU
VAL
VAL
PRO
ASP
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GLY
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ASP
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ARG

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GLN
PHE
LYS
VAL
VAL
TYR
ASN
TYR
HIS
HIS
SER
GLY
MET
PRO
THR
ARG
TYR
SER
VAL
VAL
ASP
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PRO
LEU
ASP
GLY
LYS
THR
VAL
VAL
ASN
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ASP
ASP
VAL
PHE
PHE
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VAL
ALA
LYS
PHE
GLU
GLU
ARG

TYR
LYS
THR
THR
ASN
LYS
ASN
LYS
TRP
PHE
PHE
GLN
PHE
LYS
ARG
PHE
P2
S3
R4
K7
V56
P71
T72
V73
N74
L75
L78
W79
T80
L81
V82
S83
E84
R87
K94
I101
Y108
G115
K116
L117
R132
E135
K136
A148

• Molecule 29: 60S ribosomal protein L29

Chain Lb: 9% 62% 7% 31%

MET
A2
K3
K23
D36
R41
R44
H49
A62
M65
S66
A67
A69
E70
A71
I72
K73
A74
L75
V76
LYS
PRO
LYS
GLU
VAL
LYS
PRO
LYS
ILE
PRO
LYS
GLY
V89
G115
L116
R117
L118
C119
K122
LYS
LYS
ALA
ALA
LYS
LYS
LYS
LYS
ASP
GLN
THR

LYS
ALA
GLN
ALA
ALA
LYS
PRO
ALA
ALA
VAL
VAL
ALA
ALA
PRO
LYS
THR
GLN
ALA
PRO
LYS
SER
GLU

• Molecule 30: 60S ribosomal protein L30

Chain Lc: 73% 12% 15%

MET
VAL
ALA
ALA
LYS
LYS
THR
LYS
K9
V28
T34
L35
M37
I38
Q40
A43
I47
L48
K57
Y63
L94
A95
I96
I97
R106
SER
MET
PRO
GLU
GLN
THR
GLY
GLU
LYS

• Molecule 31: 60S ribosomal protein L31

Chain Ld: 6% 81% 5% 14%

MET
ALA
PRO
ALA
ALA
LYS
LYS
GLY
GLY
GLU
LYS
LYS
LYS
GLY
ARG
SER
ALA
ALA
ILE
N18
E19
I29
I33
V62
R63
I64
L68
E94
D95
E96
D97
S98
T104
D123
E124
ASN

• Molecule 32: 60S ribosomal protein L32

Chain Le: 84% 11% 5%

MET
A2
D26
W35
P38
R46
P56
E84
V87
L88
L89
N92
V103
S104
R108
L118
N124
A127
R128
L129
ARG
SER
GLU
GLU
ASN
GLU

• Molecule 33: 60S ribosomal protein L35a

Chain Lf:  92% 7%



- Molecule 34: 60S ribosomal protein L34

Chain Lg:  85% 13%

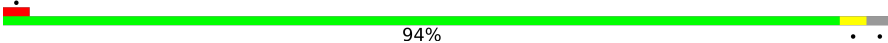


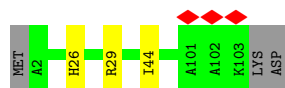
- Molecule 35: 60S ribosomal protein L35

Chain Lh:  85% 14%



- Molecule 36: 60S ribosomal protein L36

Chain Li:  94%



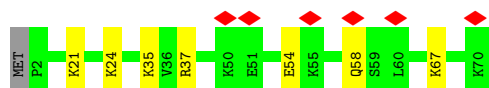
- Molecule 37: 60S ribosomal protein L37

Chain Lj:  77% 11% 11%



- Molecule 38: 60S ribosomal protein L38

Chain Lk:  9% 89% 10%

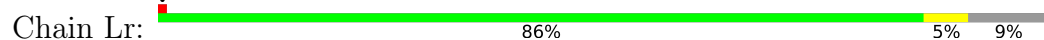


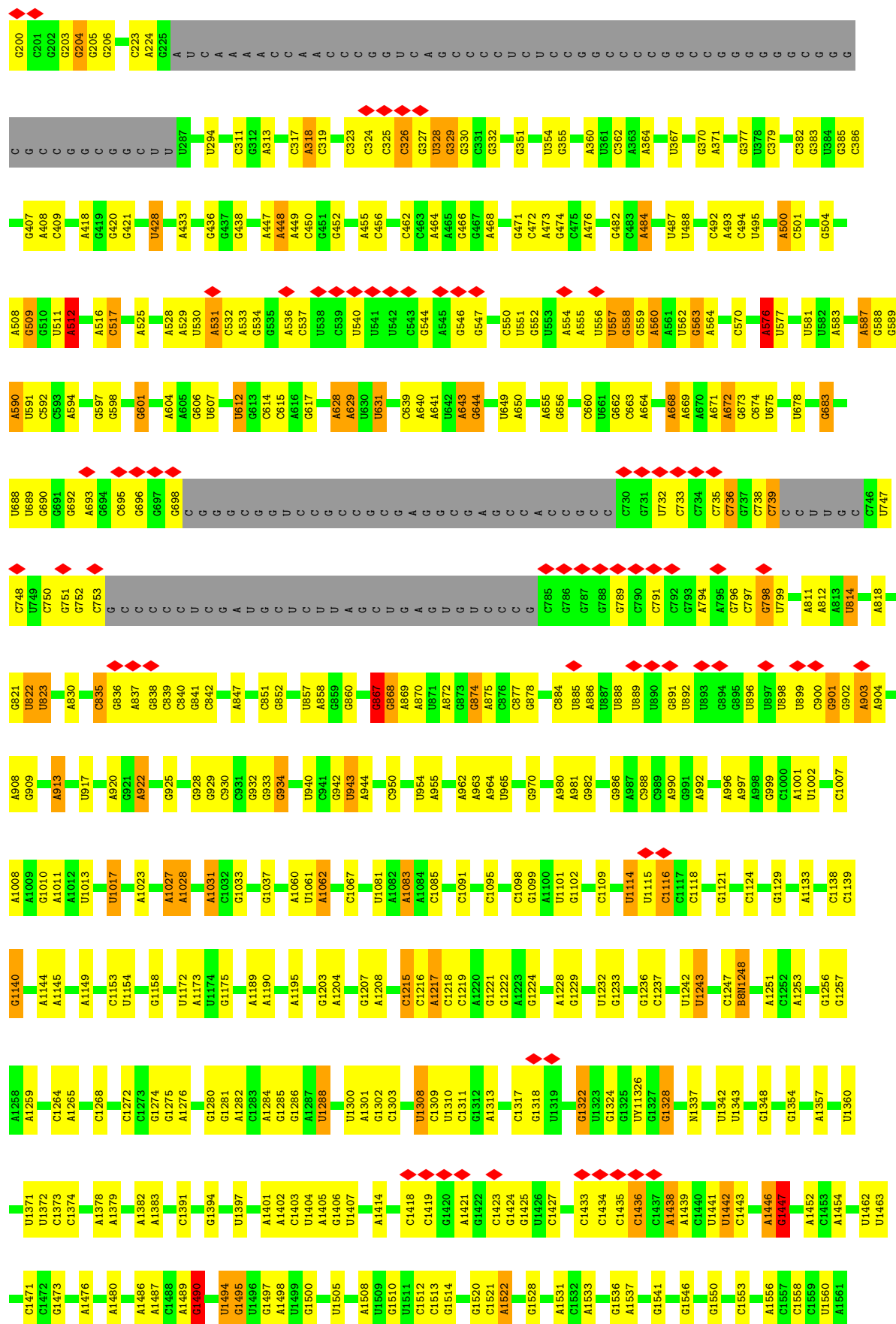
- Molecule 39: 60S ribosomal protein L39

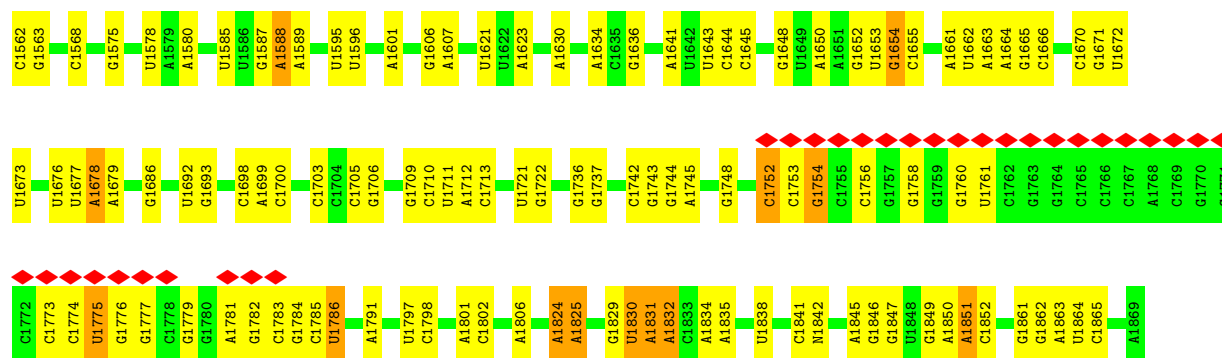
Chain Ll:  86% 12%



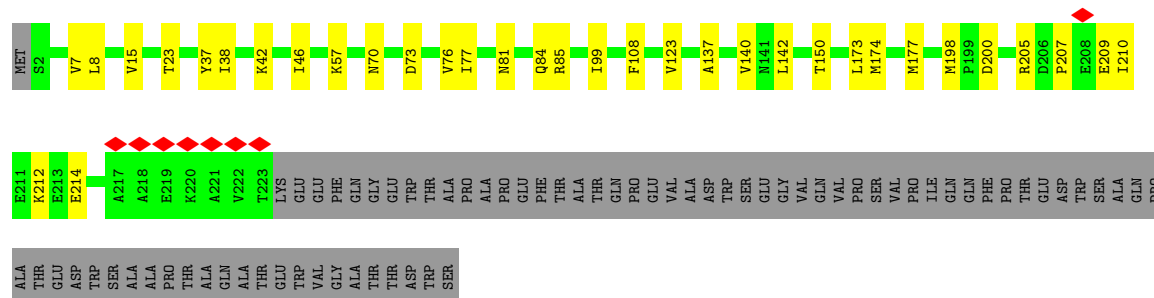
- Chain Lm:



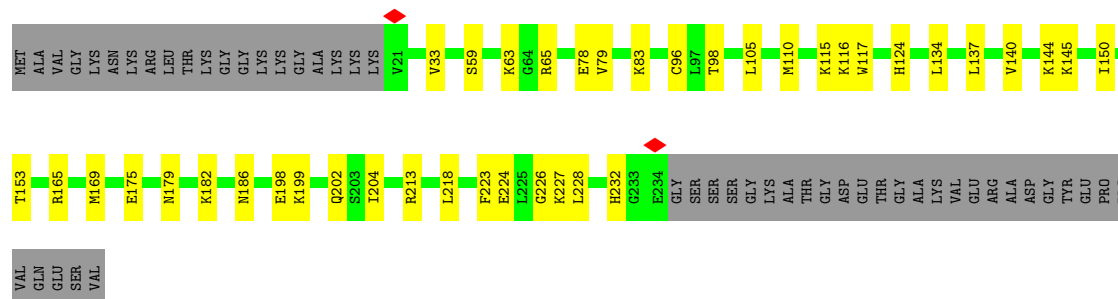




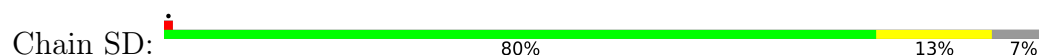
• Molecule 46: 40S ribosomal protein SA



• Molecule 47: 40S ribosomal protein S3a

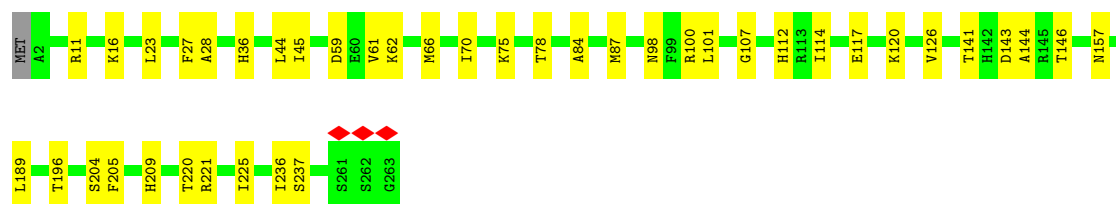


• Molecule 48: 40S ribosomal protein S3



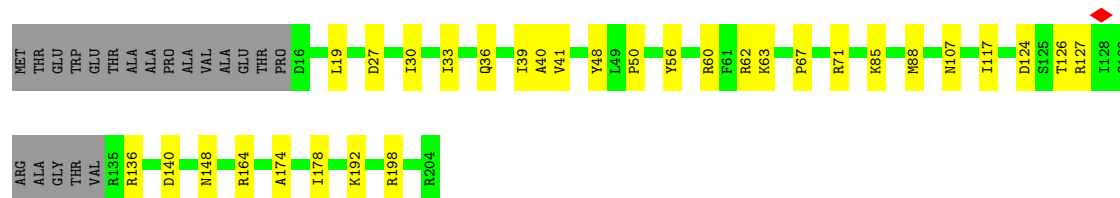
• Molecule 49: 40S ribosomal protein S4, X isoform

Chain SE:  84% 16%



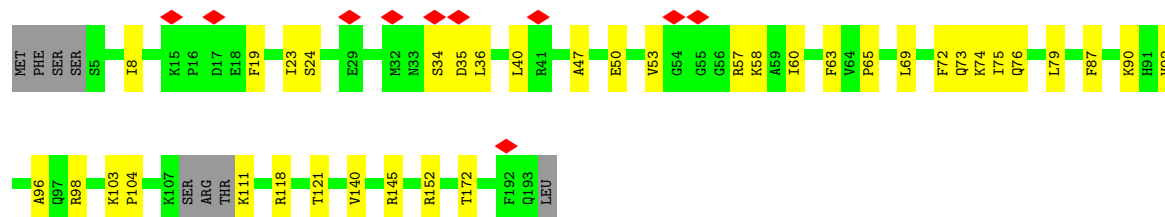
- Molecule 50: 40S ribosomal protein S5

Chain SF:  75% 15% 10%



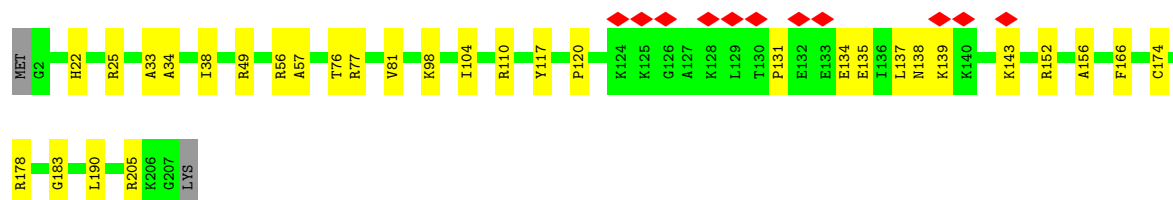
- Molecule 51: 40S ribosomal protein S7

Chain SH:  5% 77% 19%



- Molecule 52: 40S ribosomal protein S8

Chain SI:  5% 84% 15%



- Molecule 53: 40S ribosomal protein S10

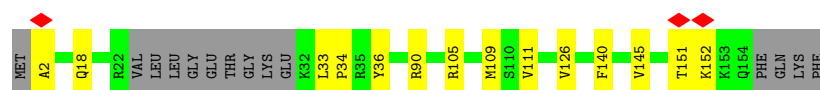
Chain SK:  45% 15% 41%



PRO ALA ARG LEU THR ARG GLY GLU ALA ASP ARG ASP THR TYR ARG ARG SER ALA VAL PRO PRO GLY ALA ASP LYS LYS ALA GLU ALA GLY ALA GLY GLY SER SER THR PHE GLU PHE GLN PHE ARG GLY GLY GLY ARG GLY GLY PRO PRO GLN

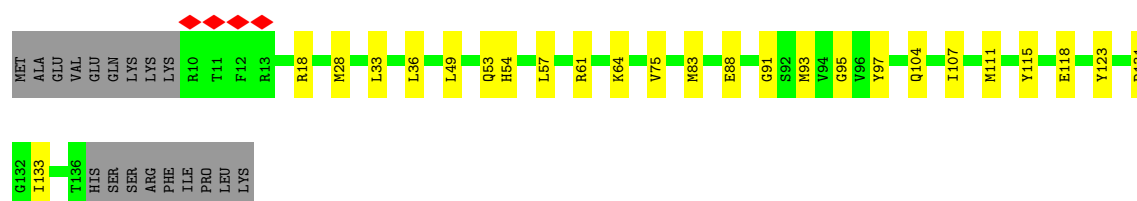
- Molecule 54: 40S ribosomal protein S11

Chain SL:  82% 9% 9%



- Molecule 55: 40S ribosomal protein S15

Chain SP:  70% 17% 12%

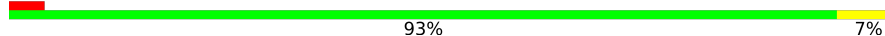


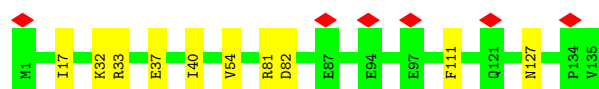
- Molecule 56: 40S ribosomal protein S16

Chain SQ:  77% 20% 3%



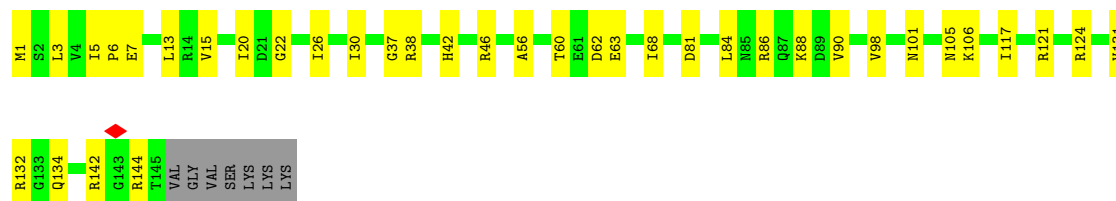
- Molecule 57: 40S ribosomal protein S17

Chain SR:  93% 7%



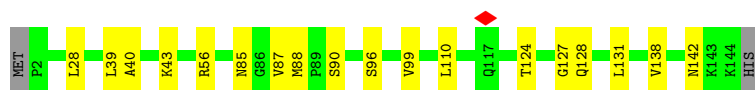
- Molecule 58: 40S ribosomal protein S18

Chain SS:  71% 24% 5%

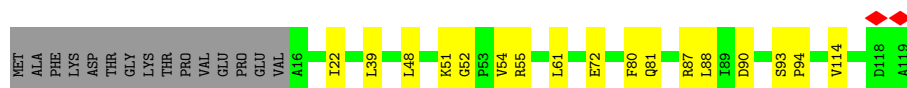
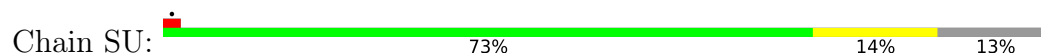


- Molecule 59: 40S ribosomal protein S19

Chain ST:  86% 12% 2%



- Molecule 60: 40S ribosomal protein S20



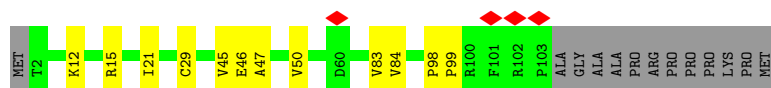
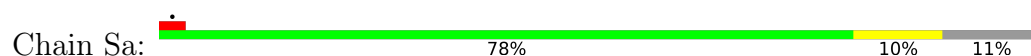
- Molecule 61: 40S ribosomal protein S21



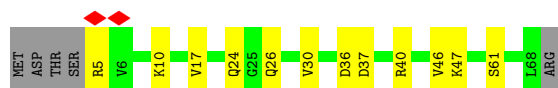
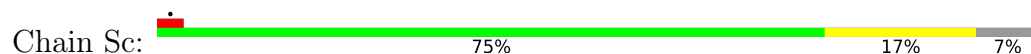
- Molecule 62: 40S ribosomal protein S23



- Molecule 63: 40S ribosomal protein S26



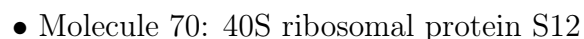
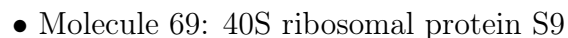
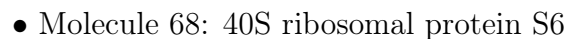
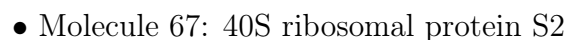
- Molecule 64: 40S ribosomal protein S28

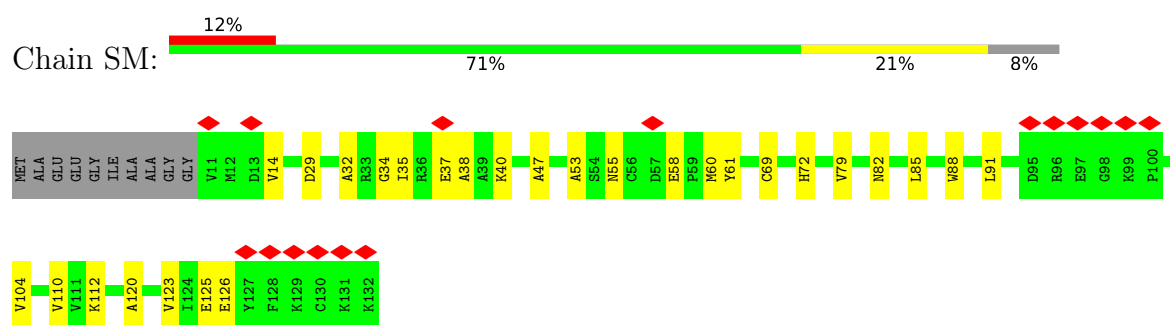


- Molecule 65: 40S ribosomal protein S29

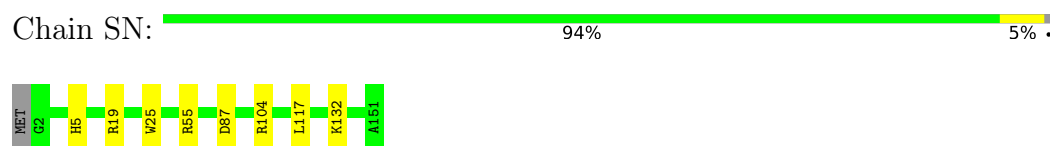


- Molecule 66: Receptor of activated protein C kinase 1

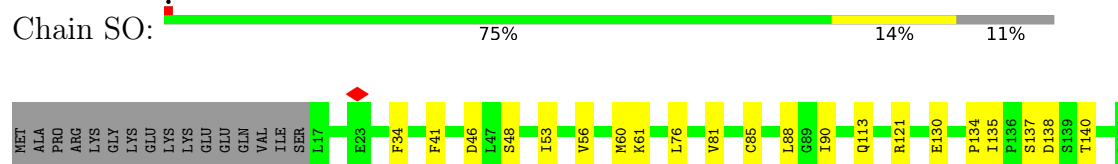




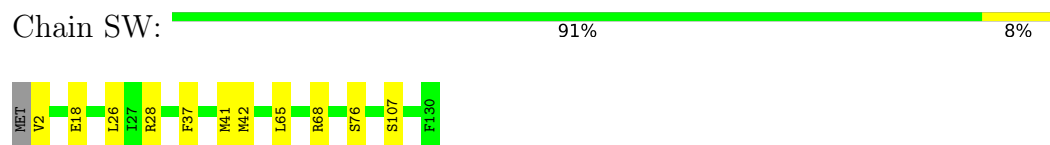
- Molecule 71: 40S ribosomal protein S13



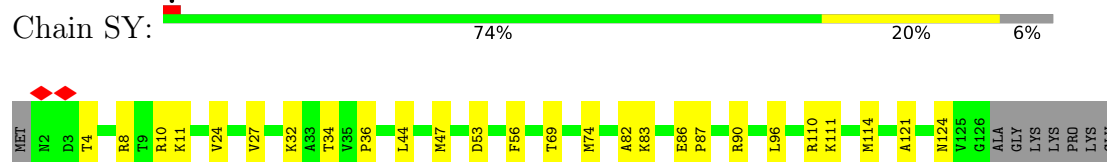
- Molecule 72: 40S ribosomal protein S14



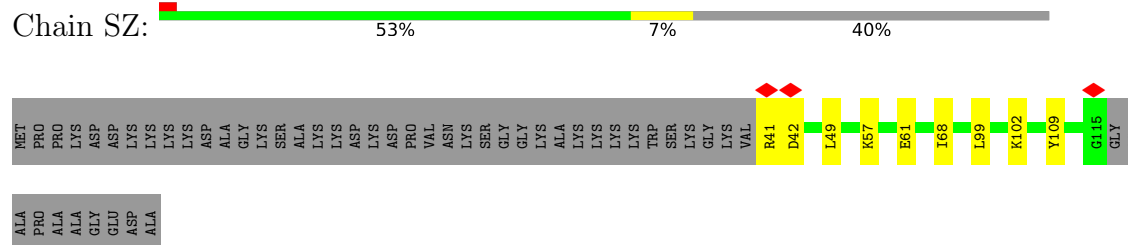
- Molecule 73: 40S ribosomal protein S15a



- Molecule 74: 40S ribosomal protein S24

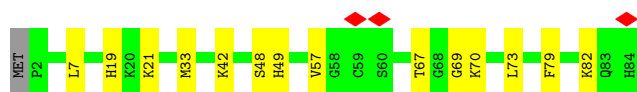


- Molecule 75: 40S ribosomal protein S25



- Molecule 76: 40S ribosomal protein S27

Chain Sb:  82% 17%



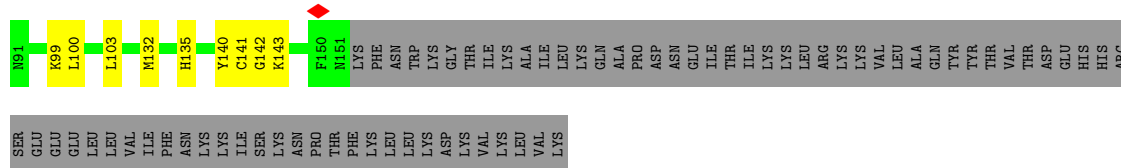
- Molecule 77: 40S ribosomal protein S30

Chain Se:  15% 86% 12%

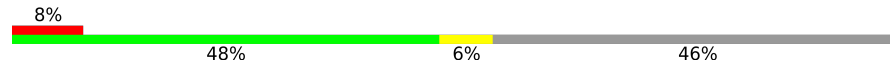


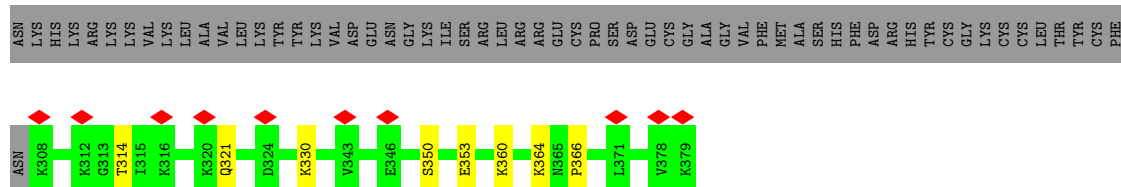
- Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  39% 7% 54%



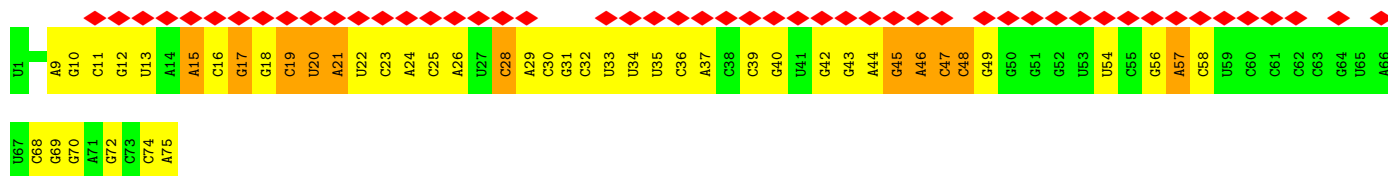
- Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain CE:  8% 48% 6% 46%



- Molecule 79: tRNA

Chain CC:  37% 67% 48% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	48.809	Depositor
Minimum map value	-19.709	Depositor
Average map value	0.030	Depositor
Map value standard deviation	1.171	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, 5MC, UY1, OMC, 1MA, B8T, PSU, A2M, MA6, 6MZ, K, UR3, ZN, MG, M7A, JMH, 4AC, OMG, 2MG, 5MU, B8N, B8H, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L1	0.27	2/87525 (0.0%)	0.37	1/136449 (0.0%)
2	L2	0.22	0/2858	0.32	0/4455
3	L3	0.25	0/3653	0.33	0/5691
4	LA	0.35	0/1936	0.66	0/2596
5	LB	0.27	0/3306	0.57	0/4424
6	LC	0.29	0/2962	0.55	0/3977
7	LD	0.20	0/2428	0.43	0/3252
8	LE	0.21	0/1799	0.52	0/2414
9	LF	0.30	0/1905	0.51	0/2539
10	LG	0.23	0/1866	0.50	0/2511
11	LH	0.22	0/1537	0.46	0/2066
12	LI	0.30	0/1677	0.51	0/2237
13	LJ	0.19	0/1376	0.52	0/1840
14	LL	0.24	0/1732	0.52	0/2315
15	LM	0.24	0/1161	0.53	0/1554
16	LN	0.32	0/1746	0.55	0/2338
17	LO	0.27	0/1682	0.50	1/2250 (0.0%)
18	LP	0.23	0/1268	0.50	0/1701
19	LQ	0.25	0/1537	0.49	0/2052
20	LR	0.28	0/1582	0.47	0/2091
21	LS	0.25	0/1501	0.45	0/2013
22	LT	0.25	0/1326	0.49	0/1770
23	LU	0.26	0/839	0.74	2/1126 (0.2%)
24	LV	0.25	0/993	0.52	0/1332
25	LW	0.21	0/1030	0.49	0/1364
26	LX	0.20	0/984	0.43	0/1323
27	LY	0.21	0/1132	0.46	0/1504
28	LZ	0.25	0/1129	0.55	1/1507 (0.1%)
28	La	0.28	0/1191	0.57	0/1591
29	Lb	0.24	0/889	0.54	0/1175
30	Lc	0.26	0/774	0.52	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Ld	0.23	0/903	0.48	0/1216
32	Le	0.26	0/1071	0.55	0/1429
33	Lf	0.26	0/895	0.54	0/1198
34	Lg	0.25	0/916	0.46	0/1220
35	Lh	0.24	0/1023	0.43	1/1351 (0.1%)
36	Li	0.19	0/843	0.42	0/1115
37	Lj	0.33	0/720	0.61	0/952
38	Lk	0.24	0/575	0.57	0/761
39	Ll	0.26	0/454	0.50	0/599
40	Lm	0.20	0/435	0.44	0/575
41	Ln	0.24	0/231	0.43	0/294
42	Lo	0.22	0/845	0.44	0/1113
43	Lp	0.26	0/718	0.52	0/953
44	Lr	0.23	0/1017	0.46	0/1364
45	S2	0.23	1/39961 (0.0%)	0.34	0/62247
46	SA	0.23	0/1784	0.47	0/2424
47	SB	0.24	0/1765	0.51	0/2362
48	SD	0.19	0/1793	0.44	0/2414
49	SE	0.21	0/2118	0.50	0/2849
50	SF	0.20	0/1481	0.50	0/1988
51	SH	0.54	0/1519	0.74	0/2033
52	SI	0.24	0/1715	0.54	0/2287
53	SK	0.20	0/851	0.52	0/1147
54	SL	0.22	0/1202	0.42	0/1606
55	SP	0.21	0/1065	0.55	0/1423
56	SQ	0.26	0/1160	0.66	2/1553 (0.1%)
57	SR	0.28	1/1105 (0.1%)	0.43	0/1484
58	SS	0.21	0/1216	0.57	0/1628
59	ST	0.19	0/1131	0.46	0/1515
60	SU	0.45	0/831	0.68	0/1115
61	SV	0.32	0/643	0.53	0/860
62	SX	0.22	0/1116	0.52	2/1490 (0.1%)
63	Sa	0.28	0/836	0.62	0/1121
64	Sc	0.23	0/508	0.55	0/680
65	Sd	0.20	0/470	0.56	0/623
66	Sg	0.19	0/2493	0.56	0/3394
67	SC	0.24	0/1762	0.50	0/2381
68	SG	0.26	0/1946	0.51	0/2590
69	SJ	0.23	0/1550	0.48	0/2069
70	SM	0.27	0/950	0.71	2/1275 (0.2%)
71	SN	0.21	0/1232	0.41	0/1656
72	SO	0.23	0/1023	0.51	0/1372
73	SW	0.23	0/1051	0.50	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	SY	0.20	0/1039	0.49	0/1381
75	SZ	0.17	0/604	0.49	0/810
76	Sb	0.19	0/665	0.45	0/891
77	Se	0.14	0/465	0.38	0/612
78	CE	0.16	0/613	0.48	0/819
78	Sf	0.17	0/507	0.55	0/673
79	CC	0.15	0/1773	0.34	0/2759
All	All	0.25	4/229913 (0.0%)	0.43	12/337572 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	LP	0	1
56	SQ	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SR	127	ASN	CA-CB	6.44	1.62	1.53
1	L1	4523	A2M	O3'-P	5.54	1.61	1.56
1	L1	3785	A2M	O3'-P	5.37	1.61	1.56
45	S2	668	A2M	O3'-P	5.09	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Lh	87	LYS	CB-CA-C	-5.96	109.69	116.54
17	LO	110	PRO	N-CA-C	5.92	117.92	110.70
23	LU	54	GLY	CA-C-N	5.92	132.84	121.54
23	LU	54	GLY	C-N-CA	5.92	132.84	121.54
70	SM	125	GLU	N-CA-CB	5.90	120.02	110.40
56	SQ	42	ILE	CA-C-N	5.56	129.11	120.60
56	SQ	42	ILE	C-N-CA	5.56	129.11	120.60
1	L1	1082	C	O4'-C1'-N1	5.36	116.24	108.20
70	SM	125	GLU	CA-CB-CG	5.24	124.58	114.10
28	LZ	112	ARG	CA-CB-CG	5.14	124.39	114.10
62	SX	60	LYS	CA-C-N	5.05	127.25	120.58
62	SX	60	LYS	C-N-CA	5.05	127.25	120.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	LP	131	ARG	Peptide
56	SQ	145	TYR	Peptide
56	SQ	43	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	80211	0	40469	456	0
2	L2	2558	0	1296	12	0
3	L3	3316	0	1687	16	0
4	LA	1898	0	1993	27	0
5	LB	3238	0	3376	28	0
6	LC	2908	0	3082	16	0
7	LD	2382	0	2410	13	0
8	LE	1765	0	1917	20	0
9	LF	1870	0	1996	15	0
10	LG	1835	0	1976	26	0
11	LH	1518	0	1601	17	0
12	LI	1639	0	1687	19	0
13	LJ	1353	0	1393	12	0
14	LL	1701	0	1818	13	0
15	LM	1138	0	1204	7	0
16	LN	1701	0	1749	20	0
17	LO	1650	0	1794	14	0
18	LP	1242	0	1269	10	0
19	LQ	1513	0	1628	13	0
20	LR	1566	0	1729	12	0
21	LS	1461	0	1502	12	0
22	LT	1298	0	1366	13	0
23	LU	825	0	850	13	0
24	LV	979	0	1039	6	0
25	LW	1015	0	1079	10	0
26	LX	967	0	1040	1	0
27	LY	1115	0	1205	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	LZ	1106	0	1182	8	0
28	La	1162	0	1213	15	0
29	Lb	876	0	948	10	0
30	Lc	764	0	804	8	0
31	Ld	888	0	930	3	0
32	Le	1053	0	1147	12	0
33	Lf	876	0	912	6	0
34	Lg	906	0	998	9	0
35	Lh	1015	0	1148	12	0
36	Li	832	0	917	2	0
37	Lj	705	0	737	8	0
38	Lk	569	0	637	4	0
39	Ll	444	0	483	4	0
40	Lm	429	0	465	8	0
41	Ln	230	0	276	2	0
42	Lo	843	0	912	6	0
43	Lp	708	0	756	9	0
44	Lr	1002	0	1068	5	0
45	S2	36959	0	18651	292	0
46	SA	1747	0	1751	22	0
47	SB	1738	0	1809	27	0
48	SD	1765	0	1865	20	0
49	SE	2076	0	2177	30	0
50	SF	1461	0	1511	21	0
51	SH	1497	0	1590	23	0
52	SI	1686	0	1772	21	0
53	SK	827	0	854	15	0
54	SL	1182	0	1253	9	0
55	SP	1045	0	1095	19	0
56	SQ	1142	0	1213	22	0
57	SR	1090	0	1149	9	0
58	SS	1198	0	1261	25	0
59	ST	1112	0	1146	12	0
60	SU	821	0	883	10	0
61	SV	636	0	637	6	0
62	SX	1098	0	1167	10	0
63	Sa	821	0	870	6	0
64	Sc	506	0	536	8	0
65	Sd	459	0	448	8	0
66	Sg	2436	0	2393	42	0
67	SC	1725	0	1813	19	0
68	SG	1923	0	2089	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	SJ	1525	0	1640	28	0
70	SM	940	0	965	19	0
71	SN	1208	0	1294	7	0
72	SO	1010	0	1034	15	0
73	SW	1034	0	1080	9	0
74	SY	1022	0	1088	17	0
75	SZ	598	0	656	5	0
76	Sb	651	0	670	8	0
77	Se	459	0	503	8	0
78	CE	603	0	660	9	0
78	Sf	497	0	495	7	0
79	CC	1589	0	810	34	0
80	CC	1	0	0	0	0
80	L1	264	0	0	0	0
80	L2	3	0	0	0	0
80	L3	5	0	0	0	0
80	LA	1	0	0	0	0
80	LC	2	0	0	0	0
80	LI	1	0	0	0	0
80	LN	1	0	0	0	0
80	LP	1	0	0	0	0
80	LV	1	0	0	0	0
80	Le	1	0	0	0	0
80	Lf	1	0	0	0	0
80	Lg	1	0	0	0	0
80	S2	135	0	0	0	0
80	SG	1	0	0	0	0
80	SJ	1	0	0	0	0
80	Sd	1	0	0	0	0
81	L1	12	0	0	0	0
82	Lg	1	0	0	0	0
82	Lj	1	0	0	0	0
82	Lm	1	0	0	0	0
82	Lo	1	0	0	0	0
82	Lp	1	0	0	0	0
82	Sa	1	0	0	0	0
82	Sb	1	0	0	0	0
82	Sd	1	0	0	0	0
82	Sf	1	0	0	0	0
83	CE	1	0	0	0	0
83	L1	762	0	0	5	0
83	L2	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	L3	6	0	0	0	0
83	LA	6	0	0	0	0
83	LB	3	0	0	0	0
83	LC	13	0	0	1	0
83	LD	1	0	0	0	0
83	LI	2	0	0	0	0
83	LL	1	0	0	0	0
83	LN	1	0	0	0	0
83	LP	1	0	0	0	0
83	LR	1	0	0	0	0
83	LX	2	0	0	0	0
83	LY	2	0	0	1	0
83	La	8	0	0	0	0
83	Lb	1	0	0	0	0
83	Le	2	0	0	0	0
83	Lg	2	0	0	0	0
83	Lj	4	0	0	0	0
83	Ll	2	0	0	0	0
83	Lo	1	0	0	0	0
83	S2	10	0	0	0	0
83	SX	1	0	0	0	0
All	All	218434	0	160516	1570	0

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

All (1570) 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)
45:S2:814:5MU:C4	45:S2:814:5MU:C5	1.79	1.63
1:L1:3762:B8H:C6	1:L1:3762:B8H:N1	1.67	1.52
1:L1:3762:B8H:C4	1:L1:3762:B8H:C5	1.84	1.50
1:L1:1:C:N4	3:L3:156:U:H3	1.46	1.12
45:S2:628:A:N6	45:S2:1500:G:H21	1.47	1.10
1:L1:471:A:N6	1:L1:683:C:H42	1.51	1.07
1:L1:1176:C:N4	1:L1:1184:A:H61	1.51	1.07
1:L1:1176:C:H42	1:L1:1184:A:N6	1.50	1.07
1:L1:471:A:H61	1:L1:683:C:N4	1.51	1.06
1:L1:3951:G:C2	1:L1:4062:A:N6	2.27	1.03
1:L1:3951:G:N2	1:L1:4062:A:C6	2.28	1.01
45:S2:1756:C:N4	45:S2:1775:U:H3	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1761:G:N2	1:L1:1768:C:C2	2.32	0.97
45:S2:140:C:N4	45:S2:313:A:H61	1.64	0.96
45:S2:885:U:H3	45:S2:901:G:H1	1.10	0.95
45:S2:140:C:H42	45:S2:313:A:N6	1.64	0.95
1:L1:1759:G:H1	1:L1:1773:U:H3	1.03	0.94
1:L1:1094:G:H1	1:L1:1201:U:H3	0.98	0.94
45:S2:628:A:N6	45:S2:1500:G:N2	2.17	0.92
63:Sa:21:ILE:O	63:Sa:29:CYS:HA	1.70	0.91
1:L1:1175:A:H2	1:L1:1185:G:H1	1.00	0.91
1:L1:1443:A:H2	1:L1:2103:G:H1	1.16	0.91
45:S2:925:G:H1	45:S2:1017:U:H3	1.17	0.91
45:S2:886:A:N6	45:S2:901:G:C2	2.39	0.90
51:SH:53:VAL:O	51:SH:57:ARG:HB3	1.72	0.90
1:L1:1175:A:C2	1:L1:1185:G:N1	2.39	0.90
1:L1:3951:G:C2	1:L1:4062:A:C6	2.60	0.89
1:L1:1175:A:H2	1:L1:1185:G:N1	1.71	0.89
79:CC:11:C:H42	79:CC:24:A:N6	1.71	0.88
51:SH:72:PHE:O	51:SH:76:GLN:HB2	1.73	0.88
1:L1:1976:G:N1	1:L1:1991:A:C2	2.42	0.88
45:S2:533:A:H61	45:S2:550:C:N4	1.73	0.85
1:L1:2520:C:O2	1:L1:2640:G:N2	2.10	0.85
45:S2:1546:G:N2	45:S2:1670:C:O2	2.10	0.85
1:L1:1174:G:H1	1:L1:1186:U:H3	1.22	0.84
46:SA:205:ARG:HE	46:SA:210:ILE:HG12	1.43	0.83
1:L1:1095:A:H2	1:L1:1200:G:H1	1.24	0.82
1:L1:3596:A:HO2'	54:SL:2:ALA:N	1.76	0.82
79:CC:11:C:N4	79:CC:24:A:H61	1.78	0.81
45:S2:39:A:H5'	69:SJ:7:TRP:HE1	1.46	0.80
56:SQ:97:GLN:HB3	56:SQ:105:LYS:HD3	1.61	0.79
2:L2:27:G:H21	2:L2:55:A:N6	1.79	0.79
1:L1:1764:G:N2	1:L1:1770:A:C6	2.51	0.79
1:L1:4887:C:H42	1:L1:4932:U:H3	1.31	0.78
1:L1:751:G:O6	1:L1:912:G:N2	2.16	0.78
45:S2:1756:C:H42	45:S2:1775:U:H3	0.81	0.78
79:CC:12:G:C6	79:CC:24:A:N6	2.53	0.77
1:L1:4467:A:H61	1:L1:4490:C:H42	1.33	0.77
79:CC:12:G:N1	79:CC:24:A:N6	2.32	0.76
1:L1:1761:G:C2	1:L1:1768:C:O2	2.38	0.76
1:L1:1764:G:N2	1:L1:1770:A:N6	2.33	0.76
45:S2:1091:C:HO2'	73:SW:2:VAL:N	1.84	0.76
79:CC:11:C:H42	79:CC:24:A:H61	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SI:135:GLU:O	52:SI:139:LYS:HB3	1.86	0.75
1:L1:1761:G:C2	1:L1:1768:C:C2	2.74	0.75
1:L1:4970:C:H5''	18:LP:71:ALA:HB1	1.68	0.75
1:L1:1764:G:C2	1:L1:1770:A:N6	2.55	0.74
1:L1:1976:G:C6	1:L1:1991:A:N1	2.55	0.74
45:S2:140:C:H42	45:S2:313:A:H61	0.84	0.74
45:S2:1288:OMU:HN3	45:S2:1311:C:H42	1.36	0.74
1:L1:5022:U:O2	1:L1:5025:C:N3	2.21	0.74
79:CC:11:C:N3	79:CC:24:A:N1	2.36	0.74
1:L1:3951:G:N2	1:L1:4062:A:N6	2.36	0.73
1:L1:3762:B8H:N1	1:L1:3762:B8H:C5	2.36	0.72
1:L1:1443:A:C2	1:L1:2103:G:N1	2.52	0.72
2:L2:27:G:N2	2:L2:55:A:N6	2.37	0.72
12:LI:177:ASN:O	12:LI:181:PHE:HB2	1.89	0.71
1:L1:1095:A:C2	1:L1:1200:G:N1	2.57	0.71
78:CE:360:LYS:O	78:CE:364:LYS:HB2	1.89	0.71
1:L1:471:A:N1	1:L1:683:C:N3	2.38	0.71
1:L1:2611:A:H5'	1:L1:2688:G:H4'	1.73	0.71
6:LC:218:ILE:O	6:LC:222:ARG:HB2	1.91	0.70
14:LL:64:VAL:HA	14:LL:67:HIS:HD2	1.55	0.70
45:S2:140:C:N3	45:S2:313:A:N1	2.39	0.70
1:L1:1940:G:H22	1:L1:4434:C:H5''	1.55	0.70
68:SG:34:THR:O	68:SG:51:ARG:HA	1.92	0.70
45:S2:1652:G:H1	45:S2:1672:U:H3	1.39	0.70
45:S2:628:A:H61	45:S2:1500:G:N2	1.89	0.70
4:LA:28:ARG:HH21	4:LA:123:ARG:HD3	1.55	0.70
64:Sc:24:GLN:OE1	64:Sc:26:GLN:NE2	2.25	0.69
1:L1:1176:C:N3	1:L1:1184:A:N1	2.39	0.69
16:LN:200:LEU:HD22	16:LN:204:ARG:HD3	1.72	0.69
68:SG:142:ARG:HG2	68:SG:147:LEU:HB2	1.75	0.69
51:SH:140:VAL:HG12	71:SN:19:ARG:HD3	1.74	0.69
45:S2:628:A:H61	45:S2:1500:G:H21	1.40	0.68
1:L1:2486:G:C6	1:L1:2494:U:O2	2.47	0.68
45:S2:533:A:N6	45:S2:550:C:H42	1.89	0.68
1:L1:3762:B8H:C6	1:L1:3762:B8H:C2	2.67	0.68
45:S2:1754:G:O6	45:S2:1779:G:N3	2.25	0.68
1:L1:3762:B8H:C6	1:L1:3762:B8H:CN1	2.69	0.68
45:S2:1748:G:H1	45:S2:1786:U:H3	1.39	0.68
1:L1:1368:A:H1'	27:LY:1:MET:HE2	1.76	0.68
22:LT:37:GLY:N	22:LT:64:VAL:O	2.27	0.68
27:LY:31:SER:HA	27:LY:48:PRO:HA	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SD:163:PRO:O	48:SD:167:TYR:HB2	1.94	0.68
45:S2:1546:G:H1	45:S2:1655:C:H1'	1.59	0.67
1:L1:152:U:OP2	16:LN:49:ARG:NH2	2.27	0.67
45:S2:377:G:H5'	52:SI:98:LYS:HB3	1.75	0.67
44:Lr:63:VAL:HG22	44:Lr:79:ARG:HG2	1.76	0.67
70:SM:47:ALA:HA	70:SM:112:LYS:HA	1.76	0.67
4:LA:147:ARG:HG2	4:LA:157:VAL:HG22	1.75	0.67
24:LV:107:ASN:HD21	24:LV:111:GLU:HB3	1.60	0.67
79:CC:10:G:N7	79:CC:45:G:N1	2.42	0.67
1:L1:160:G:OP1	14:LL:82:ARG:NH2	2.29	0.66
50:SF:127:ARG:HB3	50:SF:136:ARG:HB2	1.76	0.66
45:S2:1007:C:O2'	71:SN:104:ARG:NH2	2.29	0.66
1:L1:2474:G:N2	1:L1:2502:G:O2'	2.28	0.66
58:SS:22:GLY:HA2	58:SS:56:ALA:HB3	1.77	0.66
1:L1:1440:U:O2	1:L1:2106:G:C2	2.48	0.66
1:L1:3951:G:N3	1:L1:4062:A:N1	2.43	0.66
22:LT:43:LYS:O	22:LT:58:HIS:ND1	2.28	0.66
70:SM:58:GLU:HB3	70:SM:61:TYR:HB3	1.77	0.66
14:LL:139:SER:O	14:LL:143:GLU:HB2	1.96	0.66
45:S2:533:A:N6	45:S2:550:C:N4	2.44	0.66
55:SP:91:GLY:HA2	55:SP:107:ILE:O	1.94	0.66
66:Sg:107:ASP:HB2	66:Sg:125:ARG:HD2	1.78	0.66
1:L1:2486:G:O6	1:L1:2494:U:O2	2.14	0.65
79:CC:13:U:O2	79:CC:23:C:N3	2.30	0.65
70:SM:79:VAL:HG11	70:SM:85:LEU:HB2	1.78	0.65
14:LL:64:VAL:HA	14:LL:67:HIS:CD2	2.32	0.65
74:SY:83:LYS:HE2	74:SY:96:LEU:HB3	1.79	0.65
79:CC:25:C:H2'	79:CC:26:A:H8	1.62	0.65
45:S2:1418:C:H2'	45:S2:1419:C:H2'	1.78	0.65
79:CC:15:A:N6	79:CC:47:C:O2	2.30	0.65
72:SO:56:VAL:HG23	72:SO:60:MET:HE2	1.78	0.65
45:S2:533:A:H61	45:S2:550:C:H42	1.41	0.65
45:S2:1825:A:H4'	78:CE:364:LYS:HB3	1.78	0.65
47:SB:59:SER:O	47:SB:63:LYS:HB2	1.97	0.65
50:SF:140:ASP:HB2	64:Sc:46:VAL:HG12	1.79	0.65
45:S2:1446:A:H1'	60:SU:55:ARG:HD2	1.79	0.65
1:L1:1974:U:O4	1:L1:1993:C:N3	2.30	0.64
23:LU:44:GLN:HB2	23:LU:56:LEU:HD21	1.77	0.64
1:L1:1443:A:H2	1:L1:2103:G:N1	1.93	0.64
1:L1:5022:U:O2	1:L1:5025:C:C4	2.50	0.64
8:LE:152:ILE:HD12	8:LE:189:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3711:A:C6	45:S2:970:G:C2	2.86	0.64
1:L1:4940:C:OP1	8:LE:156:ARG:NH1	2.30	0.64
45:S2:1752:C:N3	45:S2:1779:G:N1	2.44	0.64
58:SS:6:PRO:HD3	75:SZ:49:LEU:HD11	1.78	0.64
47:SB:175:GLU:OE2	47:SB:179:ASN:ND2	2.30	0.64
60:SU:80:PHE:HB3	65:Sd:52:PHE:HB3	1.79	0.64
1:L1:1094:G:O6	1:L1:1201:U:O4	2.16	0.64
3:L3:93:C:OP1	37:Lj:76:HIS:NE2	2.28	0.64
48:SD:42:THR:HB	48:SD:45:ARG:O	1.97	0.64
1:L1:234:G:O6	1:L1:2304:U:O2	2.16	0.63
1:L1:1100:U:H3	1:L1:1195:G:H1	1.46	0.63
1:L1:1801:A:H4'	22:LT:102:ARG:HD3	1.79	0.63
1:L1:2562:G:N2	1:L1:2565:A:OP2	2.32	0.63
25:LW:93:LYS:O	25:LW:101:ARG:NH2	2.32	0.63
45:S2:1414:A:N6	45:S2:1427:C:H42	1.96	0.63
1:L1:1764:G:N3	1:L1:1770:A:N1	2.46	0.63
5:LB:223:THR:O	5:LB:274:TYR:HA	1.97	0.63
46:SA:77:ILE:HG12	46:SA:99:ILE:HB	1.79	0.63
66:Sg:89:LEU:HB3	66:Sg:99:ARG:HB3	1.80	0.63
66:Sg:87:LEU:HB2	66:Sg:101:PHE:HB2	1.81	0.63
1:L1:1509:C:H5''	28:La:2:PRO:HD2	1.82	0.62
1:L1:3589:G:N2	1:L1:3590:G:N7	2.48	0.62
66:Sg:257:LYS:NZ	66:Sg:269:GLU:OE2	2.31	0.62
56:SQ:112:LEU:O	56:SQ:115:TYR:O	2.17	0.62
76:Sb:49:HIS:ND1	76:Sb:69:GLY:O	2.32	0.62
6:LC:254:GLU:OE2	6:LC:258:ARG:NE	2.32	0.62
17:LO:85:ARG:HG3	17:LO:99:LEU:HD11	1.81	0.62
1:L1:1764:G:C2	1:L1:1770:A:C6	2.87	0.62
45:S2:433:A:H5''	52:SI:22:HIS:HB3	1.81	0.62
50:SF:198:ARG:NH1	79:CC:40:G:O2'	2.32	0.62
68:SG:33:ALA:N	68:SG:52:ILE:O	2.33	0.62
38:Lk:54:GLU:O	38:Lk:58:GLN:NE2	2.32	0.62
53:SK:42:ASN:ND2	53:SK:46:MET:SD	2.72	0.62
1:L1:3967:G:O6	1:L1:4055:U:O4	2.17	0.62
1:L1:3946:G:H21	1:L1:3947:A:H62	1.48	0.62
58:SS:38:ARG:O	58:SS:42:HIS:ND1	2.32	0.62
1:L1:1238:A:O2'	9:LF:52:GLU:OE1	2.18	0.62
1:L1:3711:A:N1	45:S2:970:G:C2	2.67	0.61
46:SA:198:MET:HE3	46:SA:200:ASP:HB2	1.81	0.61
49:SE:126:VAL:O	49:SE:157:ASN:HA	2.00	0.61
47:SB:182:LYS:O	47:SB:186:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:100:ARG:NH2	83:LC:602:HOH:O	2.33	0.61
30:Lc:36:LYS:O	30:Lc:40:GLN:NE2	2.33	0.61
45:S2:1756:C:N4	45:S2:1775:U:N3	2.32	0.61
1:L1:2557:G:H1	1:L1:2570:U:H3	1.48	0.61
66:Sg:166:VAL:HG12	66:Sg:176:VAL:HG22	1.83	0.61
28:La:75:LEU:HB3	28:La:117:LEU:HD21	1.82	0.61
67:SC:166:ARG:HB2	67:SC:248:TYR:HD1	1.66	0.61
1:L1:512:U:H3	1:L1:647:G:H1	1.49	0.61
1:L1:1175:A:N1	1:L1:1185:G:O6	2.33	0.61
45:S2:1414:A:H61	45:S2:1427:C:N4	1.98	0.61
1:L1:1095:A:H2	1:L1:1200:G:N1	1.96	0.61
30:Lc:34:THR:HG23	30:Lc:95:ALA:HB2	1.83	0.61
45:S2:1401:A:H4'	60:SU:52:GLY:HA3	1.81	0.61
1:L1:1095:A:N1	1:L1:1200:G:O6	2.34	0.60
1:L1:1759:G:O6	1:L1:1773:U:O4	2.18	0.60
45:S2:940:U:H3	45:S2:1002:U:H3	1.50	0.60
50:SF:85:LYS:HB3	50:SF:88:MET:HB3	1.83	0.60
3:L3:150:C:N4	10:LG:52:THR:O	2.35	0.60
9:LF:93:ILE:HA	9:LF:119:ASN:O	2.01	0.60
19:LQ:99:LYS:HE2	19:LQ:119:LYS:HD2	1.83	0.60
1:L1:2469:C:H5	1:L1:2471:G:H1	1.49	0.60
45:S2:1276:A:H1'	53:SK:50:GLN:HE22	1.66	0.60
69:SJ:88:ASP:HB3	69:SJ:91:LYS:HG2	1.82	0.60
1:L1:138:G:H2'	1:L1:139:G:C8	2.37	0.60
1:L1:1974:U:H3	1:L1:1993:C:N4	1.99	0.60
27:LY:39:ARG:O	27:LY:42:TYR:O	2.19	0.60
58:SS:98:VAL:HG11	58:SS:106:LYS:HG3	1.82	0.60
1:L1:1761:G:N2	1:L1:1768:C:O2	2.32	0.60
63:Sa:45:VAL:O	72:SO:113:GLN:NE2	2.34	0.60
60:SU:22:ILE:HG22	60:SU:114:VAL:HG22	1.84	0.60
1:L1:1174:G:O6	1:L1:1186:U:O4	2.20	0.60
1:L1:2578:G:N7	28:LZ:17:ARG:NH1	2.49	0.59
59:ST:96:SER:HB3	59:ST:99:VAL:HG12	1.82	0.59
1:L1:3688:U:OP2	4:LA:198:ARG:NH2	2.35	0.59
1:L1:4041:C:H5'	1:L1:4042:G:H5''	1.83	0.59
45:S2:1322:G:O6	45:S2:1505:U:O2	2.20	0.59
1:L1:4258:C:H5'	13:LJ:68:ILE:HD11	1.84	0.59
61:SV:15:ARG:NH1	61:SV:33:GLN:OE1	2.34	0.59
22:LT:93:ILE:HA	22:LT:96:ILE:HG12	1.83	0.59
23:LU:65:ARG:HG2	23:LU:67:LYS:H	1.66	0.59
45:S2:329:G:H2'	45:S2:330:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:CC:12:G:N1	79:CC:24:A:C6	2.70	0.59
1:L1:67:C:OP2	1:L1:312:G:N2	2.35	0.59
1:L1:1976:G:C6	1:L1:1991:A:C2	2.90	0.59
24:LV:58:GLY:N	24:LV:81:VAL:O	2.36	0.59
45:S2:886:A:N6	45:S2:901:G:N1	2.51	0.59
56:SQ:8:GLN:HB2	56:SQ:27:ARG:HE	1.68	0.59
68:SG:32:MET:HE3	68:SG:54:GLY:HA2	1.84	0.59
12:LI:38:ARG:NH1	12:LI:45:GLU:OE2	2.35	0.59
45:S2:1424:G:H2'	45:S2:1425:G:H8	1.67	0.59
8:LE:153:LEU:HD11	8:LE:195:ILE:HG13	1.85	0.59
28:La:73:VAL:HG21	28:La:81:LEU:HD11	1.84	0.59
15:LM:52:PHE:HA	15:LM:55:MET:HG2	1.85	0.59
22:LT:39:ILE:HG13	22:LT:102:ARG:HG3	1.84	0.59
45:S2:886:A:C6	45:S2:901:G:C2	2.91	0.59
45:S2:1636:G:O2'	50:SF:164:ARG:NH2	2.36	0.59
45:S2:1743:G:H21	45:S2:1791:A:H62	1.51	0.59
66:Sg:176:VAL:HB	66:Sg:186:THR:HB	1.83	0.59
46:SA:70:ASN:HB3	46:SA:73:ASP:HB2	1.85	0.58
1:L1:5027:C:H2'	52:SI:77:ARG:HH12	1.68	0.58
48:SD:16:ILE:HD11	65:Sd:36:LEU:HD23	1.86	0.58
62:SX:67:ARG:HG3	62:SX:115:ILE:HG12	1.83	0.58
45:S2:818:A:OP1	69:SJ:80:ARG:NH1	2.36	0.58
46:SA:37:TYR:OH	46:SA:57:LYS:NZ	2.36	0.58
1:L1:1465:G:OP1	29:Lb:44:ARG:NH1	2.37	0.58
1:L1:2601:A:N6	1:L1:2744:A:OP2	2.36	0.58
1:L1:3967:G:H1	1:L1:4055:U:H3	0.76	0.58
27:LY:101:PRO:HA	27:LY:104:VAL:HG22	1.85	0.58
59:ST:40:ALA:HB3	59:ST:43:LYS:HE3	1.85	0.58
46:SA:42:LYS:HD3	46:SA:46:ILE:HB	1.86	0.58
70:SM:53:ALA:HA	70:SM:79:VAL:HB	1.86	0.58
47:SB:124:HIS:HA	47:SB:137:LEU:O	2.02	0.58
1:L1:654:C:H4'	6:LC:269:LYS:HB3	1.86	0.58
1:L1:4096:C:N4	1:L1:4113:U:O2'	2.37	0.58
17:LO:7:LEU:HD22	17:LO:31:ARG:HH11	1.67	0.58
45:S2:1630:A:H5''	58:SS:37:GLY:H	1.68	0.58
1:L1:3689:G:O2'	1:L1:3818:UY1:OP2	2.21	0.58
1:L1:495:C:N4	1:L1:496:G:O6	2.37	0.58
1:L1:1480:C:O2'	1:L1:1482:G:OP2	2.21	0.58
1:L1:2520:C:H2'	1:L1:2521:G:H8	1.69	0.58
45:S2:1237:C:OP1	78:CE:321:GLN:NE2	2.36	0.58
45:S2:1546:G:N2	45:S2:1655:C:O2	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sf:100:LEU:HB3	78:Sf:103:LEU:HB3	1.86	0.58
31:Ld:64:ILE:HG23	31:Ld:68:LEU:HD23	1.86	0.58
57:SR:37:GLU:OE1	66:Sg:150:TRP:NE1	2.37	0.58
1:L1:2362:U:H2'	1:L1:2363:A2M:H8	1.85	0.57
1:L1:2795:A:N6	83:L1:5483:HOH:O	2.37	0.57
20:LR:28:GLU:HG3	20:LR:49:LEU:HD22	1.85	0.57
45:S2:94:G:O2'	45:S2:508:A:O2'	2.22	0.57
45:S2:851:C:H5''	45:S2:852:G:H5'	1.86	0.57
19:LQ:90:VAL:HB	28:La:80:THR:HG21	1.86	0.57
25:LW:104:GLN:NE2	68:SG:155:GLN:OE1	2.32	0.57
45:S2:1512:C:H5''	65:Sd:8:TRP:HZ3	1.69	0.57
51:SH:19:PHE:HZ	51:SH:60:ILE:HG23	1.69	0.57
1:L1:757:G:H2'	1:L1:758:G:C8	2.38	0.57
1:L1:2486:G:O6	1:L1:2494:U:C2	2.56	0.57
66:Sg:245:ARG:NH2	66:Sg:295:GLY:O	2.37	0.57
67:SC:191:VAL:HG11	67:SC:236:PHE:HA	1.85	0.57
79:CC:10:G:N7	79:CC:45:G:C2	2.72	0.57
1:L1:1:C:H42	3:L3:156:U:H3	0.69	0.57
1:L1:4343:U:O2'	42:Lo:31:ASP:OD1	2.22	0.57
51:SH:87:PHE:HB3	51:SH:90:LYS:HD2	1.85	0.57
46:SA:205:ARG:HH21	46:SA:210:ILE:HA	1.69	0.57
55:SP:91:GLY:CA	55:SP:107:ILE:O	2.51	0.57
58:SS:1:MET:HG2	58:SS:3:LEU:H	1.70	0.57
66:Sg:99:ARG:HE	66:Sg:100:ARG:H	1.53	0.57
4:LA:102:LEU:HB2	4:LA:107:MET:HE3	1.85	0.57
11:LH:59:LYS:HE3	11:LH:66:GLU:HG2	1.87	0.57
14:LL:106:SER:OG	14:LL:108:GLU:OE1	2.23	0.57
50:SF:71:ARG:NH2	50:SF:148:ASN:OD1	2.38	0.57
59:ST:28:LEU:HA	59:ST:110:LEU:HD21	1.86	0.57
1:L1:2351:OMC:HM22	1:L1:2352:U:H5'	1.85	0.57
1:L1:4910:G:N2	17:LO:106:ASP:O	2.37	0.57
45:S2:1490:OMG:N2	60:SU:72:GLU:OE1	2.36	0.57
69:SJ:182:GLN:O	69:SJ:185:ALA:C	2.48	0.57
1:L1:962:C:OP2	1:L1:1702:C:N4	2.38	0.57
11:LH:44:GLU:HB3	11:LH:58:ASP:HB2	1.87	0.57
1:L1:4691:A:OP1	11:LH:71:ARG:NH1	2.38	0.56
10:LG:103:ARG:NH2	10:LG:192:ARG:O	2.38	0.56
55:SP:54:HIS:HA	55:SP:57:LEU:HD12	1.87	0.56
66:Sg:256:ILE:HB	66:Sg:270:LEU:HB2	1.87	0.56
1:L1:1100:U:O3'	1:L1:1167:C:N4	2.38	0.56
1:L1:1785:C:OP1	12:LI:133:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:2695:A:OP1	38:Lk:35:LYS:NZ	2.36	0.56
1:L1:4888:U:O2	1:L1:4931:G:N2	2.36	0.56
13:LJ:13:ARG:O	13:LJ:136:ARG:NH1	2.38	0.56
18:LP:10:ASN:HD22	18:LP:13:LYS:HE2	1.70	0.56
22:LT:26:PRO:O	22:LT:29:THR:OG1	2.21	0.56
27:LY:4:ASN:HB3	27:LY:7:VAL:HG22	1.87	0.56
56:SQ:112:LEU:O	56:SQ:115:TYR:C	2.48	0.56
67:SC:200:ARG:O	69:SJ:54:ARG:NH1	2.37	0.56
1:L1:435:A:O2'	32:Le:26:ASP:OD2	2.22	0.56
1:L1:4103:C:C2	1:L1:4105:A:C6	2.92	0.56
10:LG:58:PRO:HD2	10:LG:61:ILE:HD12	1.88	0.56
45:S2:121:OMU:HM23	49:SE:144:ALA:HB3	1.87	0.56
13:LJ:120:ASP:HB3	13:LJ:123:ILE:HG12	1.87	0.56
45:S2:1634:A:O2'	58:SS:142:ARG:NH1	2.39	0.56
1:L1:72:C:H5	14:LL:67:HIS:HD1	1.53	0.56
43:Lp:26:VAL:O	43:Lp:30:GLU:HB2	2.06	0.56
45:S2:1228:A:H2'	45:S2:1229:G:C8	2.41	0.56
48:SD:71:ALA:HB2	53:SK:96:ARG:HH12	1.69	0.56
1:L1:1443:A:N1	1:L1:2103:G:O6	2.38	0.56
1:L1:3868:G:H22	1:L1:3900:G:H1'	1.70	0.56
45:S2:466:G:O2'	68:SG:72:ARG:NH2	2.38	0.56
45:S2:1536:G:H2'	45:S2:1537:A:C8	2.41	0.56
45:S2:1754:G:O6	45:S2:1779:G:C2	2.59	0.56
52:SI:57:ALA:HB2	52:SI:183:GLY:HA2	1.88	0.56
1:L1:3968:U:O4	1:L1:3969:G:N2	2.38	0.56
10:LG:205:THR:HG22	10:LG:206:GLN:HG2	1.88	0.56
34:Lg:63:VAL:HA	34:Lg:66:ARG:HG2	1.88	0.56
8:LE:152:ILE:O	8:LE:159:GLY:N	2.38	0.56
45:S2:928:G:H2'	45:S2:929:G:C8	2.41	0.56
45:S2:1471:C:H42	45:S2:1476:A:N6	2.04	0.56
1:L1:4966:A:H5'	5:LB:128:LYS:HG3	1.88	0.56
16:LN:116:LEU:HD22	16:LN:135:ILE:HD11	1.88	0.56
45:S2:1678:A2M:OP2	50:SF:63:LYS:NZ	2.37	0.56
1:L1:265:C:O2	35:Lh:112:ARG:NH2	2.39	0.55
21:LS:15:ARG:HB3	21:LS:27:LEU:HD23	1.87	0.55
45:S2:615:C:O2	77:Se:11:LYS:NZ	2.39	0.55
45:S2:1317:C:H2'	45:S2:1318:G:H8	1.71	0.55
51:SH:69:LEU:HD22	51:SH:96:ALA:HB2	1.89	0.55
1:L1:407:A:O2'	1:L1:410:A:OP1	2.22	0.55
1:L1:3823:G:OP2	1:L1:3823:G:N2	2.34	0.55
15:LM:7:VAL:HG12	15:LM:57:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:508:A:H3'	45:S2:509:OMG:H8	1.71	0.55
45:S2:1830:UR3:H6	45:S2:1831:A:H62	1.70	0.55
8:LE:287:VAL:O	15:LM:109:ARG:NH2	2.39	0.55
12:LI:91:LEU:HD12	12:LI:135:ILE:HG23	1.88	0.55
15:LM:31:ILE:HD13	21:LS:100:LEU:HD11	1.88	0.55
45:S2:317:C:OP2	68:SG:183:ARG:NH2	2.37	0.55
53:SK:77:GLN:OE1	53:SK:80:ARG:NH1	2.39	0.55
67:SC:110:MET:HB3	67:SC:125:LYS:HB3	1.89	0.55
1:L1:1730:U:H4'	22:LT:100:LYS:HB2	1.87	0.55
45:S2:886:A:C6	45:S2:901:G:N2	2.75	0.55
46:SA:81:ASN:HA	46:SA:84:GLN:HB2	1.89	0.55
46:SA:207:PRO:HA	46:SA:210:ILE:HB	1.89	0.55
53:SK:85:LEU:HD23	53:SK:89:ILE:HG21	1.88	0.55
1:L1:132:G:N2	1:L1:136:C:O2'	2.40	0.55
1:L1:907:C:H2'	1:L1:908:G:H8	1.71	0.55
12:LI:207:ASP:OD1	12:LI:210:ARG:NH2	2.38	0.55
79:CC:54:U:N3	79:CC:57:A:OP2	2.39	0.55
1:L1:178:C:H2'	1:L1:179:G:H8	1.72	0.55
1:L1:513:U:H1'	1:L1:516:C:H5	1.72	0.55
1:L1:4769:G:H5'	17:LO:176:ARG:HE	1.71	0.55
6:LC:340:ILE:HG21	8:LE:50:LEU:HD13	1.89	0.55
1:L1:1339:U:H2'	1:L1:1340:OMC:C6	2.42	0.55
1:L1:1365:C:H41	1:L1:1370:G:H22	1.55	0.55
1:L1:4472:G:O2'	40:Lm:100:TYR:O	2.25	0.55
33:Lf:43:LEU:O	33:Lf:109:ARG:NH2	2.40	0.55
56:SQ:85:ARG:NH2	56:SQ:116:ASP:OD2	2.40	0.55
66:Sg:168:CYS:HB2	66:Sg:195:LEU:HD13	1.89	0.55
1:L1:3758:U:O2	1:L1:3766:A:N6	2.40	0.54
1:L1:4623:OMG:N2	5:LB:279:GLU:OE2	2.34	0.54
45:S2:1324:G:O2'	45:S2:1510:G:O2'	2.25	0.54
55:SP:123:TYR:OH	58:SS:124:ARG:NH1	2.40	0.54
56:SQ:5:GLY:O	56:SQ:27:ARG:NH2	2.40	0.54
30:Lc:38:ILE:HG21	30:Lc:63:TYR:HB3	1.88	0.54
55:SP:75:VAL:HG12	55:SP:93:MET:HB3	1.90	0.54
58:SS:60:THR:OG1	58:SS:62:ASP:OD1	2.24	0.54
18:LP:116:HIS:HB3	18:LP:149:ILE:HB	1.88	0.54
45:S2:1745:A:H1'	68:SG:66:GLY:HA2	1.90	0.54
1:L1:1443:A:C6	1:L1:2104:G:N1	2.76	0.54
45:S2:511:U:H2'	45:S2:512:A2M:H8	1.90	0.54
49:SE:87:MET:HE1	49:SE:236:ILE:HD13	1.90	0.54
1:L1:114:G:OP1	16:LN:49:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Le:103:VAL:O	32:Le:108:ARG:NH2	2.40	0.54
44:Lr:28:GLU:OE2	44:Lr:31:ASN:ND2	2.40	0.54
45:S2:1441:U:O2	45:S2:1443:C:N4	2.40	0.54
79:CC:12:G:C2	79:CC:24:A:C6	2.96	0.54
1:L1:62:A:N3	1:L1:77:U:O2'	2.37	0.54
1:L1:2501:C:N4	1:L1:2502:G:O6	2.40	0.54
1:L1:3762:B8H:C5	1:L1:3762:B8H:C2	2.85	0.54
1:L1:4860:G:H2'	1:L1:4861:G:H8	1.73	0.54
5:LB:49:TYR:OH	5:LB:179:HIS:ND1	2.38	0.54
49:SE:98:ASN:HB2	49:SE:114:ILE:HG13	1.89	0.54
52:SI:110:ARG:NH2	52:SI:166:PHE:O	2.41	0.54
53:SK:7:ASN:HD22	53:SK:40:VAL:HG22	1.71	0.54
1:L1:2724:G:O2'	1:L1:2726:G:OP2	2.23	0.54
23:LU:100:LEU:HD23	23:LU:112:LEU:HD23	1.90	0.54
32:Le:84:GLU:HA	32:Le:87:VAL:HG12	1.90	0.54
40:Lm:99:CYS:HB2	40:Lm:114:LYS:HE2	1.89	0.54
45:S2:326:C:O2	45:S2:327:G:N2	2.40	0.54
45:S2:1095:C:N3	45:S2:1149:A:N1	2.56	0.54
70:SM:69:CYS:O	70:SM:72:HIS:O	2.25	0.54
1:L1:1594:C:N4	83:L1:5514:HOH:O	2.41	0.54
1:L1:4537:C:H2'	1:L1:4538:G:C8	2.42	0.54
4:LA:116:LEU:HB2	4:LA:126:LEU:HB2	1.90	0.54
45:S2:1536:G:H2'	45:S2:1537:A:H8	1.73	0.54
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.89	0.54
48:SD:114:ALA:HB3	48:SD:117:ARG:HG2	1.90	0.54
1:L1:173:C:N3	1:L1:264:C:N4	2.57	0.53
1:L1:4103:C:N3	1:L1:4105:A:C6	2.76	0.53
32:Le:89:LEU:O	32:Le:92:ASN:ND2	2.41	0.53
50:SF:124:ASP:OD1	64:Sc:47:LYS:NZ	2.38	0.53
55:SP:133:ILE:HD11	78:CE:314:THR:HG23	1.89	0.53
1:L1:3946:G:O6	1:L1:4067:U:O4	2.27	0.53
45:S2:695:C:H41	45:S2:736:C:H1'	1.72	0.53
65:Sd:21:CYS:HB3	65:Sd:26:ASN:H	1.72	0.53
1:L1:1976:G:O6	1:L1:1991:A:N1	2.41	0.53
45:S2:448:A:H5''	52:SI:25:ARG:HA	1.91	0.53
45:S2:1247:C:OP1	78:CE:330:LYS:NZ	2.39	0.53
45:S2:1280:G:H2'	45:S2:1281:G:C8	2.43	0.53
1:L1:132:G:N2	1:L1:137:G:N7	2.56	0.53
33:Lf:36:ARG:NH1	33:Lf:79:GLY:O	2.39	0.53
45:S2:318:A:N6	68:SG:186:GLN:OE1	2.41	0.53
45:S2:798:G:N2	51:SH:103:LYS:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:1700:C:N3	45:S2:1834:A:N1	2.57	0.53
74:SY:4:THR:OG1	74:SY:32:LYS:NZ	2.37	0.53
45:S2:913:A:N6	51:SH:98:ARG:O	2.35	0.53
45:S2:1414:A:N6	45:S2:1427:C:N4	2.56	0.53
54:SL:18:GLN:HG2	54:SL:33:LEU:HD11	1.90	0.53
53:SK:55:ARG:NH1	53:SK:78:TYR:OH	2.42	0.53
1:L1:3711:A:N6	45:S2:970:G:N1	2.57	0.53
1:L1:3717:A:H2'	1:L1:3718:A2M:H8	1.91	0.53
4:LA:49:ILE:HD13	4:LA:60:LYS:HE3	1.89	0.53
18:LP:94:MET:HE1	18:LP:146:ILE:HB	1.91	0.53
45:S2:988:C:H5''	47:SB:116:LYS:HG2	1.90	0.53
45:S2:1752:C:N4	45:S2:1779:G:N2	2.57	0.53
45:S2:1756:C:N4	45:S2:1775:U:C4	2.76	0.53
1:L1:1699:A:OP1	1:L1:2085:G:O2'	2.27	0.53
11:LH:92:MET:HE2	11:LH:179:ILE:HG22	1.90	0.53
50:SF:30:ILE:HG23	50:SF:117:ILE:HD11	1.90	0.53
1:L1:2520:C:H2'	1:L1:2521:G:C8	2.44	0.53
1:L1:2906:G:N2	1:L1:3586:G:O6	2.42	0.53
1:L1:3711:A:C6	45:S2:970:G:N1	2.77	0.53
1:L1:3951:G:N2	1:L1:4062:A:C5	2.75	0.53
79:CC:13:U:H3	79:CC:23:C:H42	1.57	0.53
1:L1:2407:G:O6	39:L1:2:SER:N	2.42	0.52
7:LD:41:LYS:NZ	22:LT:32:ARG:O	2.40	0.52
7:LD:223:PHE:HB3	7:LD:226:TYR:HB2	1.91	0.52
19:LQ:49:LYS:HG2	19:LQ:53:MET:HE3	1.91	0.52
28:LZ:12:LEU:HB2	28:LZ:81:MET:HB3	1.90	0.52
54:SL:33:LEU:HD12	54:SL:34:PRO:HD2	1.91	0.52
69:SJ:182:GLN:O	69:SJ:185:ALA:O	2.27	0.52
1:L1:1468:C:OP1	28:La:132:ARG:NH2	2.42	0.52
1:L1:1726:U:H5'	9:LF:135:ILE:HD11	1.91	0.52
1:L1:3717:A:H2'	1:L1:3718:A2M:C8	2.39	0.52
45:S2:1673:U:H5''	56:SQ:78:VAL:HG22	1.91	0.52
62:SX:28:LYS:O	62:SX:32:LEU:HB2	2.10	0.52
55:SP:115:TYR:HB2	55:SP:118:GLU:HG3	1.90	0.52
1:L1:73:A:N7	14:LL:103:ARG:NH2	2.58	0.52
8:LE:132:PRO:HG2	8:LE:135:GLN:HG3	1.91	0.52
25:LW:94:ARG:NH1	68:SG:144:LEU:O	2.42	0.52
45:S2:672:A:N6	45:S2:1027:A:OP1	2.35	0.52
45:S2:1522:A:OP2	58:SS:144:ARG:NE	2.42	0.52
66:Sg:82:SER:OG	66:Sg:83:TRP:N	2.42	0.52
1:L1:1273:G:N7	29:Lb:117:ARG:NH1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3765:G:O2'	1:L1:3767:C:N4	2.42	0.52
1:L1:4887:C:N4	1:L1:4932:U:H3	2.01	0.52
45:S2:878:G:H1	45:S2:908:A:H2	1.57	0.52
45:S2:1650:A:H5''	56:SQ:139:ALA:HB2	1.91	0.52
74:SY:121:ALA:HA	74:SY:124:ASN:HB2	1.92	0.52
5:LB:354:GLN:HB3	5:LB:359:ALA:HB1	1.90	0.52
32:Le:104:SER:O	32:Le:108:ARG:HB2	2.10	0.52
45:S2:964:A:H2'	45:S2:965:U:H6	1.74	0.52
45:S2:1679:A:H2'	50:SF:60:ARG:HD2	1.92	0.52
66:Sg:174:VAL:HB	66:Sg:188:HIS:HB2	1.91	0.52
1:L1:137:G:H2'	1:L1:138:G:C8	2.45	0.52
1:L1:233:U:H2'	1:L1:234:G:C8	2.44	0.52
1:L1:1870:C:H2'	1:L1:1871:A2M:H8	1.92	0.52
1:L1:4274:A:H2'	1:L1:4275:G:C8	2.45	0.52
16:LN:68:ARG:NH1	16:LN:124:ASP:O	2.37	0.52
28:LZ:13:VAL:O	28:LZ:20:GLY:N	2.40	0.52
45:S2:1560:U:O2	45:S2:1575:G:O6	2.28	0.52
49:SE:204:SER:OG	49:SE:205:PHE:N	2.43	0.52
18:LP:50:ASP:OD2	18:LP:56:GLN:NE2	2.37	0.52
46:SA:7:VAL:HG13	46:SA:8:LEU:HD12	1.91	0.52
47:SB:65:ARG:NH2	72:SO:46:ASP:OD2	2.43	0.52
56:SQ:42:ILE:HG13	56:SQ:43:GLU:H	1.75	0.52
1:L1:1459:A:OP1	19:LQ:65:ARG:NH1	2.43	0.52
9:LF:115:ARG:NH1	19:LQ:4:ASP:O	2.42	0.52
45:S2:146:G:OP1	68:SG:143:LYS:NZ	2.42	0.52
46:SA:38:ILE:HD11	46:SA:150:THR:HG22	1.92	0.52
46:SA:85:ARG:NH2	57:SR:82:ASP:O	2.43	0.52
1:L1:2745:A:H2'	1:L1:2746:A:C8	2.45	0.51
1:L1:5022:U:C2	1:L1:5025:C:N3	2.78	0.51
27:LY:30:MET:HB3	27:LY:101:PRO:HG3	1.92	0.51
45:S2:1513:C:H2'	45:S2:1514:G:H8	1.75	0.51
64:Sc:17:VAL:HA	64:Sc:30:VAL:HG12	1.91	0.51
1:L1:4992:G:H2'	1:L1:4993:G:C8	2.45	0.51
66:Sg:29:ASP:OD1	66:Sg:47:ARG:NH1	2.42	0.51
1:L1:452:A:H4'	1:L1:453:G:H5'	1.91	0.51
1:L1:4745:G:H1	1:L1:4955:A:H61	1.58	0.51
1:L1:4771:C:H2'	1:L1:4772:C:C6	2.44	0.51
6:LC:134:PRO:HA	6:LC:150:LEU:HD22	1.93	0.51
45:S2:1661:A:OP2	65:Sd:19:ARG:NH1	2.42	0.51
1:L1:4765:G:OP1	11:LH:23:ARG:NH1	2.43	0.51
13:LJ:96:LYS:HE3	13:LJ:163:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LL:50:PRO:HB3	14:LL:150:LEU:HB3	1.93	0.51
58:SS:121:ARG:HG3	58:SS:131:VAL:HB	1.92	0.51
79:CC:9:A:N6	79:CC:22:U:OP2	2.42	0.51
23:LU:56:LEU:HD12	23:LU:61:VAL:HG23	1.92	0.51
1:L1:2504:C:O2'	1:L1:2506:G:OP1	2.27	0.51
43:Lp:10:ILE:HD13	43:Lp:30:GLU:HG3	1.93	0.51
45:S2:1471:C:N4	45:S2:1476:A:H62	2.09	0.51
68:SG:30:LYS:HB3	68:SG:34:THR:HG21	1.93	0.51
74:SY:10:ARG:HG3	74:SY:24:VAL:HG13	1.92	0.51
1:L1:4093:G:C6	1:L1:4114:C:O2	2.64	0.51
1:L1:4633:G:O2'	1:L1:4635:A:OP2	2.22	0.51
3:L3:141:C:H5''	16:LN:60:VAL:HG11	1.93	0.51
8:LE:72:LYS:HG3	29:Lb:119:CYS:HB3	1.93	0.51
11:LH:176:LEU:HB3	40:Lm:86:ALA:HB1	1.93	0.51
45:S2:367:U:H4'	45:S2:371:A:C8	2.46	0.51
45:S2:747:U:N3	45:S2:796:G:N1	2.59	0.51
45:S2:944:A:H5''	72:SO:134:PRO:HB3	1.92	0.51
45:S2:981:A:H2'	45:S2:982:G:C8	2.46	0.51
47:SB:105:LEU:HD13	47:SB:213:ARG:HA	1.92	0.51
49:SE:117:GLU:HA	49:SE:120:LYS:HE2	1.93	0.51
52:SI:152:ARG:O	52:SI:156:ALA:HB2	2.11	0.51
66:Sg:10:THR:HB	66:Sg:306:LEU:HD12	1.93	0.51
1:L1:2838:G:H5'	5:LB:247:GLY:HA2	1.93	0.51
16:LN:158:HIS:HB3	16:LN:161:MET:HB2	1.92	0.51
30:Lc:43:ALA:HA	30:Lc:97:ILE:HG22	1.90	0.51
1:L1:386:A:OP2	27:LY:89:LYS:NZ	2.35	0.51
1:L1:2583:C:OP2	34:Lg:76:ARG:NH1	2.38	0.51
1:L1:4467:A:N1	1:L1:4490:C:N3	2.59	0.51
5:LB:213:GLN:NE2	5:LB:285:TYR:O	2.37	0.51
45:S2:495:U:O2'	49:SE:27:PHE:O	2.26	0.51
45:S2:902:G:O2'	45:S2:903:A:O4'	2.28	0.51
45:S2:1281:G:H2'	45:S2:1282:A:C8	2.46	0.51
45:S2:1709:G:H1	45:S2:1824:A:H2	1.57	0.51
49:SE:11:ARG:HA	49:SE:28:ALA:HB2	1.92	0.51
53:SK:95:ARG:HD2	53:SK:98:ARG:HH22	1.75	0.51
1:L1:1419:G:OP1	19:LQ:71:LYS:NZ	2.44	0.51
1:L1:2906:G:H2'	1:L1:2908:U:H1'	1.93	0.51
23:LU:24:ASP:HB3	23:LU:69:LYS:HG2	1.93	0.51
51:SH:8:ILE:HG23	51:SH:24:SER:HB3	1.93	0.51
68:SG:1:MET:HE2	68:SG:109:LEU:HB2	1.93	0.51
1:L1:963:G:N7	1:L1:964:A:N6	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LD:79:TYR:HB2	7:LD:82:GLU:HG2	1.94	0.50
10:LG:180:PRO:HG3	10:LG:219:VAL:HG13	1.93	0.50
45:S2:1228:A:H2'	45:S2:1229:G:H8	1.76	0.50
62:SX:68:LYS:HB3	62:SX:91:LEU:HD13	1.93	0.50
11:LH:163:GLN:HA	11:LH:166:THR:HG23	1.93	0.50
31:Ld:62:VAL:HG12	31:Ld:104:THR:HB	1.93	0.50
45:S2:1785:C:O2'	45:S2:1786:U:O4'	2.29	0.50
52:SI:131:PRO:O	52:SI:134:GLU:HG3	2.11	0.50
75:SZ:41:ARG:NH1	75:SZ:42:ASP:O	2.44	0.50
1:L1:156:G:N7	83:L1:5469:HOH:O	2.35	0.50
1:L1:1974:U:N3	1:L1:1993:C:N4	2.60	0.50
1:L1:4103:C:N3	1:L1:4105:A:N1	2.59	0.50
10:LG:159:HIS:ND1	10:LG:185:LYS:HA	2.25	0.50
38:Lk:21:LYS:N	38:Lk:37:ARG:O	2.44	0.50
45:S2:1158:G:H5''	73:SW:76:SER:HB3	1.92	0.50
45:S2:1562:C:H2'	45:S2:1563:G:H8	1.77	0.50
70:SM:120:ALA:HA	70:SM:123:VAL:HG22	1.93	0.50
1:L1:3910:C:H2'	1:L1:3911:C:C6	2.47	0.50
34:Lg:83:CYS:SG	34:Lg:86:CYS:HB2	2.51	0.50
45:S2:533:A:H2'	45:S2:534:G:C8	2.47	0.50
45:S2:1452:A:OP2	57:SR:32:LYS:NZ	2.45	0.50
69:SJ:136:ARG:HA	69:SJ:141:VAL:HA	1.92	0.50
1:L1:135:G:N7	35:Lh:97:LYS:NZ	2.50	0.50
1:L1:4277:G:H5''	22:LT:17:ARG:HG2	1.93	0.50
12:LI:43:VAL:O	12:LI:171:TRP:NE1	2.30	0.50
28:LZ:68:ILE:O	28:LZ:115:LYS:NZ	2.39	0.50
45:S2:860:G:H21	73:SW:107:SER:HB2	1.76	0.50
45:S2:1268:C:O2	55:SP:97:TYR:OH	2.27	0.50
45:S2:1662:U:O4	45:S2:1663:A:N6	2.44	0.50
45:S2:1752:C:C4	45:S2:1779:G:N2	2.79	0.50
45:S2:1825:A:H1'	78:CE:366:PRO:HD3	1.92	0.50
50:SF:19:LEU:HD11	50:SF:50:PRO:HD3	1.94	0.50
53:SK:15:LEU:HD21	53:SK:71:LEU:HD13	1.93	0.50
55:SP:28:MET:HE1	55:SP:36:LEU:HD12	1.93	0.50
55:SP:111:MET:HG3	58:SS:117:ILE:HD11	1.92	0.50
13:LJ:151:ILE:HD11	13:LJ:156:ARG:HG2	1.93	0.50
23:LU:111:GLU:OE2	23:LU:113:ARG:NE	2.45	0.50
29:Lb:62:ALA:HA	29:Lb:65:MET:HE2	1.94	0.50
39:Ll:16:LYS:HD3	39:Ll:19:GLN:HE21	1.77	0.50
43:Lp:46:LYS:HG3	43:Lp:59:SER:HB2	1.92	0.50
45:S2:1513:C:OP1	65:Sd:12:ARG:NH1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SI:117:TYR:HD1	52:SI:152:ARG:HB3	1.76	0.50
1:L1:691:C:H2'	1:L1:692:A:H8	1.77	0.50
1:L1:3736:A:H2'	1:L1:3737:A:C8	2.47	0.50
21:LS:127:MET:HG2	22:LT:153:PRO:HB2	1.93	0.50
45:S2:205:G:H2'	45:S2:206:G:C8	2.47	0.50
45:S2:1403:C:N4	45:S2:1433:C:OP1	2.45	0.50
58:SS:5:ILE:HG22	58:SS:7:GLU:H	1.77	0.50
66:Sg:39:THR:HG22	66:Sg:60:ARG:HG2	1.93	0.50
1:L1:3615:G:H1'	25:LW:44:ARG:HD2	1.93	0.50
57:SR:17:ILE:HD11	57:SR:54:VAL:HA	1.94	0.50
70:SM:85:LEU:HA	70:SM:88:TRP:HE3	1.77	0.50
45:S2:640:A:H2'	45:S2:641:A:C8	2.46	0.50
70:SM:34:GLY:O	70:SM:38:ALA:HB2	2.11	0.50
1:L1:679:C:H2'	1:L1:680:G:H8	1.76	0.49
1:L1:216:C:OP2	1:L1:219:G:O2'	2.27	0.49
1:L1:1175:A:N1	1:L1:1185:G:C6	2.80	0.49
1:L1:1456:JMH:O2'	19:LQ:73:PRO:O	2.29	0.49
1:L1:1591:U:OP2	1:L1:2856:C:O2'	2.26	0.49
8:LE:191:GLN:HA	8:LE:194:VAL:HG12	1.94	0.49
10:LG:246:SER:O	10:LG:250:ILE:HG12	2.12	0.49
70:SM:69:CYS:O	70:SM:72:HIS:C	2.55	0.49
1:L1:65:A:N6	1:L1:74:G:N2	2.59	0.49
5:LB:291:TYR:HB3	5:LB:297:LYS:HD2	1.95	0.49
21:LS:98:ARG:HG3	21:LS:142:VAL:HG13	1.94	0.49
32:Le:87:VAL:HG23	44:Lr:34:ALA:HB1	1.94	0.49
48:SD:62:LYS:O	48:SD:67:ARG:NH1	2.42	0.49
74:SY:53:ASP:OD2	74:SY:53:ASP:N	2.43	0.49
1:L1:1756:U:O2'	1:L1:1758:G:OP2	2.31	0.49
3:L3:87:G:OP2	35:Lh:5:LYS:NZ	2.41	0.49
67:SC:275:LYS:HG3	67:SC:276:THR:HG23	1.92	0.49
12:LI:48:LEU:HD12	12:LI:142:LEU:HD13	1.95	0.49
25:LW:84:GLY:HA2	68:SG:161:PRO:HD2	1.93	0.49
45:S2:1221:G:O2'	45:S2:1676:U:O2	2.29	0.49
58:SS:13:LEU:N	58:SS:20:ILE:O	2.43	0.49
66:Sg:148:SER:OG	66:Sg:149:GLU:OE1	2.26	0.49
1:L1:184:U:O2	1:L1:254:G:C6	2.65	0.49
1:L1:1079:C:H2'	1:L1:1080:C:C6	2.48	0.49
1:L1:3672:G:H4'	16:LN:67:ARG:HH12	1.77	0.49
1:L1:4478:G:O2'	1:L1:4602:A:N1	2.45	0.49
11:LH:95:VAL:HG22	40:Lm:82:LEU:HD23	1.95	0.49
34:Lg:42:PRO:HB2	34:Lg:53:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SH:69:LEU:O	51:SH:73:GLN:HG2	2.13	0.49
58:SS:132:ARG:HB2	58:SS:134:GLN:HE22	1.78	0.49
67:SC:194:ARG:HD3	67:SC:196:ILE:HD11	1.93	0.49
1:L1:982:U:OP1	8:LE:73:TYR:OH	2.28	0.49
1:L1:3976:C:N4	1:L1:4035:G:OP2	2.46	0.49
10:LG:264:LYS:HE3	47:SB:226:GLY:H	1.77	0.49
32:Le:89:LEU:HD13	32:Le:118:LEU:HD22	1.93	0.49
45:S2:943:U:O2'	72:SO:135:ILE:O	2.29	0.49
66:Sg:68:ASP:HB3	66:Sg:111:VAL:HG22	1.95	0.49
1:L1:184:U:O2	1:L1:254:G:O6	2.30	0.49
1:L1:2394:G:O2'	1:L1:2819:U:O4	2.28	0.49
1:L1:3707:U:H2'	1:L1:3708:C:C6	2.48	0.49
1:L1:4076:G:OP1	10:LG:73:ARG:NE	2.40	0.49
1:L1:4084:G:O6	4:LA:72:ARG:NH2	2.45	0.49
1:L1:4369:A:H2'	1:L1:4370:OMG:H8	1.78	0.49
3:L3:39:G:C2	3:L3:104:A:C2	3.00	0.49
54:SL:111:VAL:HG12	54:SL:140:PHE:HB2	1.93	0.49
1:L1:215:C:OP1	1:L1:219:G:N2	2.46	0.49
1:L1:453:G:H4'	1:L1:454:U:H5'	1.93	0.49
1:L1:718:C:OP1	9:LF:217:ARG:NH1	2.44	0.49
1:L1:4196:OMG:HM23	1:L1:4196:OMG:H1'	1.64	0.49
3:L3:75:OMG:OP2	27:LY:74:TYR:OH	2.29	0.49
13:LJ:89:VAL:HG11	13:LJ:109:ILE:HG23	1.95	0.49
45:S2:1007:C:H2'	45:S2:1008:A:C8	2.48	0.49
74:SY:11:LYS:HB2	74:SY:24:VAL:HG12	1.95	0.49
1:L1:2101:C:N3	1:L1:2102:G:N2	2.51	0.49
1:L1:4774:C:O2'	1:L1:4775:C:O4'	2.29	0.49
45:S2:942:G:H21	72:SO:137:SER:HB2	1.78	0.49
68:SG:181:THR:HG22	68:SG:183:ARG:H	1.77	0.49
1:L1:3917:A:H2'	1:L1:3918:G:H8	1.78	0.48
1:L1:4522:G:O2'	1:L1:4525:C:OP2	2.30	0.48
58:SS:86:ARG:HH22	58:SS:90:VAL:HG12	1.78	0.48
69:SJ:152:ASP:OD1	69:SJ:152:ASP:N	2.46	0.48
72:SO:53:ILE:HG23	72:SO:88:LEU:HD23	1.95	0.48
1:L1:1514:U:H2'	1:L1:1515:A:C8	2.48	0.48
5:LB:154:LYS:HG3	5:LB:194:LEU:HD23	1.94	0.48
34:Lg:110:GLN:NE2	34:Lg:114:GLN:OE1	2.46	0.48
45:S2:484:A2M:O5'	45:S2:484:A2M:H8	2.12	0.48
45:S2:874:G:H2'	45:S2:875:A:H8	1.78	0.48
46:SA:214:GLU:HG3	57:SR:81:ARG:HH12	1.78	0.48
55:SP:18:ARG:HD3	58:SS:88:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SY:27:VAL:HB	74:SY:69:THR:HB	1.94	0.48
1:L1:10:A:H2'	1:L1:11:G:C8	2.48	0.48
1:L1:1444:G:N2	1:L1:2102:G:O6	2.46	0.48
1:L1:4363:A:H5''	42:Lo:36:GLN:HG2	1.95	0.48
16:LN:138:PHE:HA	16:LN:143:ARG:HD2	1.95	0.48
49:SE:126:VAL:HA	49:SE:141:THR:HA	1.94	0.48
62:SX:74:LEU:O	62:SX:78:GLY:CA	2.61	0.48
68:SG:118:GLU:HG2	68:SG:119:LYS:HG3	1.96	0.48
1:L1:1328:G:O2'	1:L1:2349:A:OP1	2.30	0.48
1:L1:2303:C:H5''	32:Le:104:SER:HB3	1.94	0.48
16:LN:9:GLU:HB2	36:Li:44:ILE:HG13	1.95	0.48
45:S2:56:G:OP1	74:SY:111:LYS:NZ	2.38	0.48
45:S2:1436:C:O2'	45:S2:1438:A:OP2	2.30	0.48
53:SK:52:LEU:HD12	53:SK:55:ARG:HH21	1.78	0.48
66:Sg:86:THR:HG21	66:Sg:100:ARG:HH22	1.78	0.48
69:SJ:127:ARG:HD3	77:Se:31:ARG:HD3	1.94	0.48
79:CC:28:C:N4	79:CC:43:G:O6	2.46	0.48
1:L1:1857:C:H2'	1:L1:1858:A:H8	1.78	0.48
1:L1:2543:A:O2'	1:L1:2545:U:O4	2.30	0.48
1:L1:2758:G:O2'	1:L1:2765:A:N3	2.37	0.48
1:L1:4894:A:H5''	1:L1:4895:C:H2'	1.95	0.48
42:Lo:26:TYR:HB3	42:Lo:67:VAL:HB	1.95	0.48
45:S2:74:G:H5''	45:S2:76:U:H5	1.78	0.48
45:S2:812:A:H5''	49:SE:16:LYS:HD3	1.95	0.48
45:S2:878:G:O6	45:S2:908:A:N1	2.46	0.48
50:SF:30:ILE:HB	50:SF:36:GLN:HB3	1.94	0.48
70:SM:34:GLY:O	70:SM:38:ALA:CB	2.61	0.48
1:L1:29:G:H5''	16:LN:172:ARG:HG2	1.95	0.48
1:L1:4492:U:O2'	1:L1:4512:U:O2	2.25	0.48
4:LA:41:ILE:HG12	4:LA:63:PHE:HD2	1.79	0.48
15:LM:129:LYS:HA	15:LM:132:LYS:HG2	1.95	0.48
19:LQ:29:VAL:O	19:LQ:33:ARG:HB2	2.13	0.48
30:Lc:47:ILE:HD12	30:Lc:94:LEU:HD11	1.95	0.48
45:S2:107:A:H2'	45:S2:108:G:C8	2.49	0.48
45:S2:528:A:H2'	45:S2:529:A:C8	2.49	0.48
45:S2:1317:C:H2'	45:S2:1318:G:C8	2.48	0.48
49:SE:126:VAL:O	49:SE:157:ASN:N	2.46	0.48
49:SE:126:VAL:HG12	49:SE:141:THR:HG22	1.95	0.48
68:SG:57:ASP:OD1	68:SG:58:LYS:N	2.46	0.48
75:SZ:57:LYS:O	75:SZ:61:GLU:HB2	2.13	0.48
1:L1:68:U:OP1	16:LN:178:HIS:ND1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1095:A:N1	1:L1:1200:G:C6	2.81	0.48
25:LW:45:ASN:HD22	25:LW:48:GLN:HG3	1.78	0.48
45:S2:145:G:H2'	45:S2:146:G:C8	2.48	0.48
45:S2:165:G:OP2	45:S2:165:G:N2	2.39	0.48
45:S2:928:G:H1	45:S2:1013:U:H3	1.62	0.48
45:S2:1775:U:O2	45:S2:1776:G:N2	2.47	0.48
55:SP:91:GLY:N	55:SP:107:ILE:O	2.46	0.48
74:SY:44:LEU:HA	74:SY:47:MET:HG2	1.95	0.48
1:L1:1326:A2M:OP2	1:L1:4445:U:O2'	2.29	0.48
1:L1:1988:G:H2'	1:L1:1989:G:C8	2.48	0.48
1:L1:2543:A:H2	1:L1:2773:G:H22	1.61	0.48
9:LF:127:LYS:HB2	22:LT:133:ALA:HB3	1.95	0.48
12:LI:48:LEU:O	12:LI:139:ARG:HA	2.14	0.48
1:L1:1942:A:H2'	1:L1:1943:A:C8	2.49	0.48
1:L1:3861:A:H2'	1:L1:3862:A:C8	2.48	0.48
2:L2:120:U:H4'	7:LD:262:LYS:HG2	1.95	0.48
10:LG:154:LEU:HB3	10:LG:204:PHE:HB2	1.94	0.48
11:LH:26:ILE:HG13	11:LH:35:ARG:HG2	1.96	0.48
45:S2:530:U:N3	45:S2:531:A:N7	2.62	0.48
45:S2:1414:A:N1	45:S2:1427:C:N3	2.62	0.48
45:S2:1568:C:OP1	59:ST:96:SER:OG	2.27	0.48
47:SB:83:LYS:NZ	72:SO:130:GLU:OE2	2.40	0.48
49:SE:112:HIS:NE2	49:SE:237:SER:O	2.47	0.48
74:SY:82:ALA:O	74:SY:86:GLU:HB2	2.13	0.48
1:L1:1727:U:OP1	9:LF:131:ASN:ND2	2.46	0.48
1:L1:4759:C:O2	17:LO:165:LYS:NZ	2.37	0.48
4:LA:229:ALA:HB3	4:LA:234:LYS:HB3	1.94	0.48
8:LE:243:THR:HG23	8:LE:246:ARG:H	1.79	0.48
37:Lj:2:THR:HG22	37:Lj:4:GLY:H	1.79	0.48
45:S2:1447:OMG:HM23	45:S2:1447:OMG:H1'	1.67	0.48
45:S2:1845:A:H2'	45:S2:1846:G:C8	2.49	0.48
47:SB:223:PHE:HE1	47:SB:228:LEU:HD22	1.78	0.48
63:Sa:12:LYS:HG3	63:Sa:15:ARG:HB2	1.95	0.48
1:L1:93:G:H2'	1:L1:94:A:C8	2.49	0.47
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.96	0.47
45:S2:1825:A:H5'	78:CE:364:LYS:HD2	1.95	0.47
46:SA:209:GLU:HA	46:SA:212:LYS:HB3	1.95	0.47
62:SX:105:PHE:HD1	62:SX:121:LYS:HB3	1.79	0.47
66:Sg:207:CYS:HB2	66:Sg:221:LEU:HD11	1.96	0.47
1:L1:2705:G:H22	1:L1:2710:C:H5	1.61	0.47
1:L1:4093:G:N1	1:L1:4114:C:C2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:61:ARG:HA	17:LO:70:PRO:HD2	1.96	0.47
21:LS:142:VAL:HG12	21:LS:146:HIS:CE1	2.49	0.47
51:SH:50:GLU:HG2	51:SH:58:LYS:HE2	1.95	0.47
69:SJ:113:GLN:NE2	69:SJ:154:GLN:OE1	2.30	0.47
1:L1:106:A:H1'	1:L1:336:A:N3	2.29	0.47
1:L1:4467:A:N6	1:L1:4490:C:H42	2.07	0.47
5:LB:80:GLU:OE1	5:LB:323:TYR:OH	2.30	0.47
37:Lj:18:LEU:HG	39:Li:51:LEU:HD13	1.96	0.47
56:SQ:19:ALA:HB2	56:SQ:75:GLY:HA3	1.96	0.47
63:Sa:47:ALA:HA	63:Sa:50:VAL:HB	1.96	0.47
1:L1:512:U:O4	1:L1:647:G:O6	2.32	0.47
1:L1:1976:G:C2	1:L1:1991:A:C2	3.03	0.47
62:SX:74:LEU:O	62:SX:78:GLY:HA2	2.14	0.47
68:SG:33:ALA:CA	68:SG:52:ILE:O	2.62	0.47
72:SO:34:PHE:HB3	72:SO:41:PHE:HB2	1.96	0.47
1:L1:3880:G:H2'	1:L1:3881:G:C8	2.49	0.47
1:L1:751:G:O6	1:L1:912:G:C2	2.67	0.47
1:L1:1380:G:N2	1:L1:1381:U:O4	2.42	0.47
1:L1:1996:C:N4	1:L1:2000:G:H22	2.13	0.47
1:L1:4194:U:H3'	29:Lb:3:LYS:HD3	1.96	0.47
8:LE:161:ARG:O	8:LE:182:ASN:ND2	2.48	0.47
8:LE:180:VAL:HG21	8:LE:258:LEU:HD11	1.96	0.47
10:LG:260:GLU:O	10:LG:264:LYS:HG2	2.14	0.47
28:La:82:VAL:HG11	28:La:101:ILE:HG12	1.96	0.47
45:S2:122:G:H21	49:SE:146:THR:HG21	1.79	0.47
49:SE:126:VAL:O	49:SE:157:ASN:CA	2.62	0.47
59:ST:124:THR:OG1	59:ST:127:GLY:N	2.35	0.47
72:SO:85:CYS:HB3	72:SO:90:ILE:HB	1.96	0.47
1:L1:729:2MG:N2	21:LS:66:GLN:O	2.31	0.47
1:L1:3641:U:H5	1:L1:3646:A:N7	2.12	0.47
4:LA:140:ASN:OD1	4:LA:142:GLU:O	2.33	0.47
12:LI:152:LEU:HB3	12:LI:165:ILE:HD12	1.95	0.47
28:LZ:106:LEU:HD23	28:LZ:109:LYS:HD3	1.97	0.47
32:Le:38:PRO:HB2	32:Le:46:ARG:HB2	1.95	0.47
32:Le:124:ASN:HB2	32:Le:127:ALA:HB2	1.97	0.47
37:Lj:27:TYR:HA	37:Lj:34:CYS:HA	1.95	0.47
45:S2:382:C:H2'	45:S2:383:G:H8	1.80	0.47
45:S2:1203:G:H2'	45:S2:1204:A:C8	2.50	0.47
47:SB:33:VAL:HA	47:SB:96:CYS:HB2	1.96	0.47
54:SL:90:ARG:HD2	54:SL:109:MET:HE2	1.96	0.47
67:SC:184:VAL:HG21	67:SC:247:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:262:G:H2'	1:L1:263:G:C8	2.50	0.47
1:L1:1617:G:H1'	1:L1:2513:A:N6	2.30	0.47
8:LE:141:ARG:NH1	8:LE:191:GLN:O	2.45	0.47
45:S2:1528:G:O2'	45:S2:1666:C:OP1	2.31	0.47
64:Sc:5:ARG:O	64:Sc:5:ARG:NH1	2.47	0.47
79:CC:20:U:O2'	79:CC:46:A:N7	2.46	0.47
45:S2:10:G:O2'	67:SC:113:GLN:OE1	2.32	0.47
45:S2:639:C:H2'	45:S2:640:A:C8	2.50	0.47
46:SA:15:VAL:HG21	57:SR:111:PHE:HD2	1.79	0.47
70:SM:29:ASP:OD1	70:SM:29:ASP:N	2.46	0.47
5:LB:56:ILE:O	5:LB:73:VAL:HA	2.15	0.47
18:LP:85:LYS:O	18:LP:89:GLU:HG3	2.15	0.47
37:Lj:54:LYS:O	37:Lj:58:THR:HB	2.15	0.47
45:S2:557:U:H2'	45:S2:558:G:C8	2.50	0.47
56:SQ:110:ASP:O	56:SQ:114:GLN:HG3	2.15	0.47
79:CC:13:U:H3	79:CC:23:C:N4	2.12	0.47
1:L1:233:U:H2'	1:L1:234:G:H8	1.78	0.46
1:L1:746:A:H2'	1:L1:747:A:C8	2.50	0.46
1:L1:4591:U:H2'	1:L1:4592:C:C6	2.50	0.46
1:L1:4637:OMG:HM23	1:L1:4637:OMG:H1'	1.66	0.46
34:Lg:41:ALA:HB3	34:Lg:52:ARG:HB3	1.97	0.46
45:S2:379:C:H5'	52:SI:33:ALA:HA	1.96	0.46
49:SE:45:ILE:HA	49:SE:61:VAL:HG11	1.97	0.46
49:SE:107:GLY:HA2	49:SE:189:LEU:HG	1.97	0.46
64:Sc:10:LYS:HD3	64:Sc:61:SER:HB3	1.97	0.46
70:SM:55:ASN:HD21	70:SM:82:ASN:H	1.63	0.46
1:L1:1443:A:N1	1:L1:2103:G:C6	2.82	0.46
1:L1:1548:G:O2'	1:L1:2812:A:N3	2.41	0.46
11:LH:115:ARG:HD3	11:LH:123:ILE:HD12	1.96	0.46
20:LR:105:LEU:HD23	20:LR:138:LEU:HD23	1.96	0.46
51:SH:47:ALA:HB3	51:SH:63:PHE:HB2	1.98	0.46
1:L1:1857:C:H2'	1:L1:1858:A:C8	2.49	0.46
83:L1:5463:HOH:O	28:La:7:LYS:NZ	2.45	0.46
13:LJ:77:ALA:O	13:LJ:81:GLU:HG3	2.15	0.46
14:LL:91:ALA:HA	14:LL:94:ILE:HG22	1.96	0.46
43:Lp:46:LYS:O	43:Lp:57:CYS:HA	2.16	0.46
45:S2:932:G:O2'	45:S2:934:G:OP2	2.29	0.46
45:S2:1709:G:O6	45:S2:1824:A:N1	2.49	0.46
48:SD:53:THR:HG23	48:SD:54:ARG:HD3	1.95	0.46
50:SF:27:ASP:OD2	50:SF:107:ASN:ND2	2.48	0.46
58:SS:81:ASP:HA	58:SS:84:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SV:70:LEU:HD21	61:SV:83:PHE:CE1	2.50	0.46
79:CC:68:C:H2'	79:CC:69:G:H8	1.80	0.46
1:L1:3732:A:H2'	1:L1:3733:A:C8	2.51	0.46
2:L2:74:A:O2'	21:LS:53:LYS:NZ	2.41	0.46
45:S2:922:A:OP1	73:SW:28:ARG:NH2	2.48	0.46
45:S2:1328:OMG:HM23	45:S2:1328:OMG:H1'	1.71	0.46
45:S2:1705:C:H2'	45:S2:1706:G:C8	2.51	0.46
49:SE:66:MET:SD	49:SE:78:THR:OG1	2.73	0.46
53:SK:21:MET:HB2	53:SK:69:TRP:HB2	1.97	0.46
56:SQ:11:GLN:OE1	56:SQ:71:ARG:NH2	2.49	0.46
66:Sg:157:SER:OG	66:Sg:159:ASN:OD1	2.32	0.46
1:L1:2706:G:H2'	1:L1:2708:U:H3	1.81	0.46
28:La:75:LEU:HD23	28:La:78:LEU:HD13	1.97	0.46
45:S2:823:PSU:N3	69:SJ:143:ASN:OD1	2.42	0.46
45:S2:1013:U:OP1	45:S2:1129:G:O2'	2.33	0.46
45:S2:1101:U:H2'	45:S2:1102:G:C8	2.51	0.46
46:SA:76:VAL:HG12	46:SA:123:VAL:HB	1.98	0.46
47:SB:198:GLU:HG2	47:SB:202:GLN:HE21	1.80	0.46
1:L1:1443:A:N1	1:L1:2104:G:C2	2.84	0.46
1:L1:1443:A:C6	1:L1:2104:G:C2	3.04	0.46
1:L1:2652:G:N2	43:Lp:59:SER:O	2.48	0.46
1:L1:5002:U:OP2	5:LB:385:LYS:NZ	2.46	0.46
45:S2:570:C:O2'	74:SY:34:THR:O	2.32	0.46
45:S2:1745:A:O3'	68:SG:31:ARG:NH1	2.48	0.46
66:Sg:157:SER:HB2	66:Sg:164:ILE:HB	1.98	0.46
69:SJ:107:GLU:O	69:SJ:112:THR:OG1	2.34	0.46
77:Se:11:LYS:HE2	77:Se:15:GLN:HE22	1.80	0.46
1:L1:1308:C:H2'	1:L1:1309:C:C6	2.50	0.46
1:L1:4314:C:O2'	29:Lb:36:ASP:OD1	2.33	0.46
15:LM:132:LYS:HA	15:LM:135:LEU:HG	1.98	0.46
45:S2:447:A:OP1	52:SI:49:ARG:NH2	2.48	0.46
45:S2:1037:G:H4'	45:S2:1845:A:H4'	1.98	0.46
49:SE:112:HIS:NE2	49:SE:237:SER:OG	2.34	0.46
61:SV:14:PRO:HG2	61:SV:23:ILE:HD12	1.96	0.46
64:Sc:36:ASP:OD2	64:Sc:37:ASP:N	2.49	0.46
1:L1:4260:U:H2'	1:L1:4261:C:C6	2.51	0.46
1:L1:4587:G:OP1	17:LO:61:ARG:NH1	2.45	0.46
10:LG:100:HIS:HA	10:LG:103:ARG:HG3	1.98	0.46
19:LQ:124:ASP:N	19:LQ:124:ASP:OD1	2.48	0.46
22:LT:49:GLN:HA	22:LT:52:MET:HE3	1.98	0.46
45:S2:57:U:OP1	45:S2:504:G:O2'	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:1010:G:H2'	45:S2:1011:A:C8	2.51	0.46
45:S2:1407:U:O2'	56:SQ:11:GLN:OE1	2.33	0.46
47:SB:165:ARG:HG2	47:SB:169:MET:HE2	1.98	0.46
51:SH:60:ILE:HB	51:SH:92:VAL:HG22	1.97	0.46
71:SN:87:ASP:OD1	71:SN:87:ASP:N	2.49	0.46
1:L1:397:G:O6	18:LP:93:HIS:NE2	2.48	0.46
1:L1:1440:U:H3	1:L1:2105:A:H2	1.64	0.46
1:L1:2486:G:C6	1:L1:2495:U:C2	3.03	0.46
1:L1:4980:C:N3	18:LP:69:ARG:NH2	2.62	0.46
4:LA:101:VAL:HG22	4:LA:165:VAL:HG22	1.97	0.46
20:LR:44:LEU:HD22	20:LR:49:LEU:HD12	1.97	0.46
45:S2:223:C:H2'	45:S2:224:A:C8	2.51	0.46
45:S2:1424:G:H2'	45:S2:1425:G:C8	2.50	0.46
76:Sb:73:LEU:HD11	76:Sb:79:PHE:HB3	1.98	0.46
79:CC:21:A:H61	79:CC:46:A:H2'	1.81	0.46
1:L1:508:G:O2'	1:L1:510:U:OP2	2.20	0.46
1:L1:740:G:H21	1:L1:924:C:H41	1.64	0.46
1:L1:3925:OMU:HM23	1:L1:3925:OMU:H1'	1.80	0.46
1:L1:4192:A:H2'	1:L1:4193:C:H6	1.81	0.46
12:LI:30:LYS:HG2	12:LI:63:GLU:HA	1.98	0.46
28:La:79:TRP:HE1	28:La:117:LEU:HD22	1.81	0.46
45:S2:835:C:H41	74:SY:8:ARG:HH12	1.63	0.46
47:SB:144:LYS:NZ	47:SB:145:LYS:O	2.46	0.46
79:CC:30:C:H2'	79:CC:31:G:C8	2.50	0.46
1:L1:751:G:C6	1:L1:912:G:N2	2.84	0.45
1:L1:1996:C:H42	1:L1:2000:G:N2	2.14	0.45
45:S2:674:C:H2'	45:S2:675:U:C6	2.52	0.45
45:S2:1083:A:N7	45:S2:1841:C:O2'	2.48	0.45
48:SD:206:ASP:OD1	48:SD:206:ASP:N	2.49	0.45
56:SQ:39:LEU:HD23	56:SQ:52:LEU:HD23	1.98	0.45
61:SV:51:LYS:HG3	61:SV:78:ILE:HD11	1.98	0.45
67:SC:108:LYS:HE3	67:SC:233:LEU:HD22	1.98	0.45
79:CC:68:C:H2'	79:CC:69:G:C8	2.51	0.45
1:L1:1640:C:OP2	83:L1:5402:HOH:O	2.21	0.45
1:L1:1979:A:N6	1:L1:1984:A:OP1	2.43	0.45
1:L1:4537:C:H2'	1:L1:4538:G:H8	1.81	0.45
40:Lm:83:ARG:O	40:Lm:87:GLN:HG3	2.16	0.45
45:S2:428:OMU:H4'	69:SJ:2:PRO:HG2	1.97	0.45
45:S2:588:G:OP2	45:S2:588:G:N2	2.36	0.45
1:L1:382:G:N1	1:L1:385:A:OP2	2.44	0.45
1:L1:424:U:H2'	1:L1:425:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:508:A:H3'	45:S2:509:OMG:C8	2.50	0.45
46:SA:15:VAL:HG21	57:SR:111:PHE:CD2	2.51	0.45
49:SE:23:LEU:HD21	69:SJ:6:SER:HB3	1.98	0.45
68:SG:33:ALA:HA	68:SG:52:ILE:O	2.16	0.45
70:SM:60:MET:HG2	78:Sf:103:LEU:HD11	1.98	0.45
73:SW:18:GLU:HG2	73:SW:65:LEU:HD13	1.98	0.45
78:CE:350:SER:OG	78:CE:353:GLU:OE1	2.23	0.45
1:L1:691:C:H2'	1:L1:692:A:C8	2.51	0.45
1:L1:1207:C:H2'	1:L1:1208:G:H8	1.81	0.45
9:LF:94:ARG:O	9:LF:118:PHE:N	2.48	0.45
17:LO:190:ASP:OD1	17:LO:190:ASP:N	2.49	0.45
23:LU:74:SER:OG	23:LU:76:VAL:O	2.29	0.45
51:SH:65:PRO:O	51:SH:69:LEU:N	2.45	0.45
60:SU:54:VAL:HG22	60:SU:88:LEU:HB2	1.97	0.45
71:SN:5:HIS:HB3	71:SN:117:LEU:HD23	1.97	0.45
1:L1:1440:U:C2	1:L1:2106:G:C2	3.04	0.45
1:L1:2631:U:O4	23:LU:51:GLY:N	2.49	0.45
1:L1:4618:OMG:H5''	24:LV:15:ARG:HB2	1.98	0.45
2:L2:27:G:N2	2:L2:55:A:H61	2.14	0.45
4:LA:80:GLU:HB2	4:LA:170:ALA:HA	1.98	0.45
5:LB:223:THR:O	5:LB:274:TYR:CA	2.64	0.45
10:LG:95:LEU:HD21	10:LG:156:VAL:HG21	1.99	0.45
45:S2:1711:U:H2'	45:S2:1712:A:H8	1.82	0.45
58:SS:15:VAL:HG13	58:SS:68:ILE:HD11	1.99	0.45
62:SX:90:CYS:HA	62:SX:93:PHE:HD2	1.81	0.45
69:SJ:131:ARG:HD2	69:SJ:131:ARG:HA	1.77	0.45
72:SO:61:LYS:HE2	72:SO:76:LEU:HB3	1.98	0.45
1:L1:4474:A:OP2	1:L1:4476:C:N4	2.48	0.45
6:LC:298:ILE:O	6:LC:302:LEU:HG	2.17	0.45
7:LD:205:ALA:HB1	7:LD:233:PRO:HB3	1.98	0.45
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.51	0.45
25:LW:46:PRO:O	25:LW:52:THR:OG1	2.31	0.45
45:S2:643:A:OP1	69:SJ:38:ARG:NH1	2.49	0.45
66:Sg:125:ARG:HG2	66:Sg:150:TRP:CG	2.51	0.45
71:SN:25:TRP:CD2	76:Sb:82:LYS:HE2	2.51	0.45
78:CE:364:LYS:HA	78:CE:364:LYS:HD3	1.76	0.45
1:L1:2759:G:O2'	1:L1:2762:G:N2	2.50	0.45
10:LG:160:ASP:OD1	10:LG:160:ASP:N	2.50	0.45
33:Lf:37:ASP:OD1	33:Lf:37:ASP:N	2.49	0.45
45:S2:1189:A:H2'	45:S2:1190:A:C8	2.50	0.45
66:Sg:163:PRO:HB2	66:Sg:179:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sf:140:TYR:CZ	78:Sf:142:GLY:HA2	2.52	0.45
79:CC:11:C:N4	79:CC:24:A:N6	2.42	0.45
1:L1:1867:A:H2'	1:L1:1868:A:C8	2.52	0.45
1:L1:4238:G:H2'	1:L1:4239:A:C8	2.51	0.45
1:L1:4860:G:H2'	1:L1:4861:G:C8	2.52	0.45
12:LI:38:ARG:HD2	12:LI:83:ASP:HB2	1.99	0.45
45:S2:601:OMG:HM23	45:S2:601:OMG:H1'	1.70	0.45
45:S2:629:A:O2'	45:S2:631:U:OP1	2.34	0.45
50:SF:174:ALA:O	50:SF:178:ILE:HD12	2.16	0.45
1:L1:184:U:O2'	1:L1:189:G:O4'	2.30	0.45
1:L1:398:A2M:O5'	1:L1:398:A2M:H8	2.17	0.45
1:L1:1241:C:O2	29:Lb:115:GLY:HA2	2.16	0.45
1:L1:2764:A:H2'	1:L1:2765:A:H8	1.82	0.45
1:L1:4518:A:H5'	1:L1:4520:G:H4'	1.99	0.45
51:SH:145:ARG:O	51:SH:152:ARG:HA	2.17	0.45
66:Sg:201:SER:OG	66:Sg:203:ASP:O	2.32	0.45
78:Sf:132:MET:HG2	78:Sf:141:CYS:HB2	1.98	0.45
79:CC:17:G:O2'	79:CC:56:G:N2	2.50	0.45
8:LE:176:THR:HB	8:LE:186:LEU:HD23	1.99	0.45
16:LN:45:PRO:O	16:LN:49:ARG:HG3	2.16	0.45
28:La:84:GLU:OE2	28:La:87:ARG:NH2	2.50	0.45
45:S2:1354:G:N2	45:S2:1357:A:OP2	2.44	0.45
45:S2:1360:U:O2'	45:S2:1379:A:OP2	2.31	0.45
45:S2:1588:A:H2'	45:S2:1589:A:C8	2.51	0.45
49:SE:87:MET:N	49:SE:101:LEU:O	2.48	0.45
54:SL:151:THR:OG1	54:SL:152:LYS:N	2.49	0.45
60:SU:51:LYS:HB2	60:SU:90:ASP:HB2	1.99	0.45
69:SJ:104:ASP:OD1	69:SJ:104:ASP:N	2.48	0.45
1:L1:2326:G:H5'	32:Le:127:ALA:HB1	1.99	0.44
7:LD:65:ALA:HB2	7:LD:74:ILE:HD13	1.99	0.44
40:Lm:109:ASN:ND2	40:Lm:117:HIS:O	2.47	0.44
45:S2:570:C:H4'	74:SY:36:PRO:HG3	1.98	0.44
45:S2:644:OMG:HM23	45:S2:644:OMG:H1'	1.74	0.44
45:S2:1017:U:H5'	71:SN:55:ARG:HD3	1.98	0.44
48:SD:48:ILE:HB	48:SD:86:LEU:HG	1.99	0.44
54:SL:126:VAL:HG12	54:SL:145:VAL:HG22	1.99	0.44
76:Sb:19:HIS:CD2	76:Sb:21:LYS:H	2.34	0.44
1:L1:1492:G:H4'	29:Lb:41:ARG:HE	1.82	0.44
1:L1:3917:A:H2'	1:L1:3918:G:C8	2.52	0.44
1:L1:4967:A:H2'	1:L1:4968:A:C8	2.53	0.44
5:LB:54:THR:OG1	5:LB:55:HIS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:175:GLN:NE2	5:LB:177:LYS:O	2.45	0.44
6:LC:195:LYS:HA	6:LC:200:ARG:HG2	1.98	0.44
11:LH:31:ARG:HH21	11:LH:188:GLN:HG3	1.82	0.44
13:LJ:39:VAL:HG12	13:LJ:123:ILE:HD12	1.98	0.44
29:Lb:23:LYS:HE3	29:Lb:23:LYS:HB3	1.81	0.44
30:Lc:47:ILE:HB	30:Lc:94:LEU:HG	1.98	0.44
45:S2:857:U:H2'	45:S2:858:A:C8	2.51	0.44
45:S2:1360:U:O2	45:S2:1379:A:N7	2.50	0.44
55:SP:53:GLN:NE2	55:SP:83:MET:SD	2.78	0.44
68:SG:137:ARG:HG2	68:SG:140:ARG:HD2	1.99	0.44
69:SJ:60:LEU:HD22	69:SJ:70:ARG:HA	1.98	0.44
1:L1:1532:G:OP2	37:Lj:31:LYS:NZ	2.49	0.44
1:L1:1996:C:N4	1:L1:2000:G:N2	2.65	0.44
1:L1:2501:C:N4	1:L1:2502:G:C6	2.85	0.44
1:L1:4467:A:H61	1:L1:4490:C:N4	2.08	0.44
1:L1:4601:U:H2'	1:L1:4602:A:H8	1.81	0.44
5:LB:228:TYR:CE1	5:LB:270:GLY:HA2	2.52	0.44
10:LG:99:ALA:HB1	10:LG:193:LEU:HD21	1.99	0.44
21:LS:74:ARG:O	21:LS:76:LYS:NZ	2.47	0.44
45:S2:1115:U:H4'	45:S2:1116:C:H5'	2.00	0.44
62:SX:17:ARG:HG3	62:SX:21:LYS:HE2	1.99	0.44
1:L1:2748:C:O2'	34:Lg:61:PRO:O	2.31	0.44
7:LD:51:MET:HE3	7:LD:105:LEU:HD23	1.99	0.44
11:LH:41:ILE:HG22	11:LH:43:VAL:HG13	1.99	0.44
19:LQ:9:LYS:HA	19:LQ:9:LYS:HD3	1.74	0.44
20:LR:92:LYS:O	20:LR:96:MET:HG3	2.17	0.44
45:S2:72:C:O2'	45:S2:73:C:O4'	2.36	0.44
45:S2:1098:C:H2'	45:S2:1099:G:C8	2.53	0.44
45:S2:1801:A:H2'	45:S2:1802:C:C6	2.52	0.44
47:SB:110:MET:HE1	47:SB:140:VAL:HG21	1.99	0.44
79:CC:69:G:H2'	79:CC:70:G:C8	2.52	0.44
1:L1:1646:A:O2'	37:Lj:49:TRP:O	2.32	0.44
1:L1:2422:OMC:HM23	1:L1:2422:OMC:H1'	1.87	0.44
1:L1:2744:A:H2'	1:L1:2745:A:C8	2.52	0.44
1:L1:3946:G:H21	1:L1:3947:A:N6	2.15	0.44
1:L1:4475:G:H5''	1:L1:4476:C:H5''	1.99	0.44
1:L1:4699:U:H1'	1:L1:4700:A:H5''	1.99	0.44
1:L1:5047:C:O2'	1:L1:5050:C:OP2	2.28	0.44
2:L2:23:A:N3	2:L2:118:C:O2'	2.40	0.44
17:LO:9:LEU:HD23	17:LO:118:MET:HB2	1.98	0.44
20:LR:178:GLN:HA	20:LR:181:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LR:183:GLU:HA	20:LR:186:LYS:HG2	1.98	0.44
45:S2:494:C:N4	45:S2:509:OMG:HN22	2.14	0.44
49:SE:225:ILE:HD13	49:SE:225:ILE:HA	1.81	0.44
61:SV:17:CYS:O	61:SV:21:ASN:N	2.50	0.44
68:SG:227:GLN:OE1	68:SG:231:ARG:NH2	2.50	0.44
1:L1:3594:C:C2	1:L1:3597:G:C2	3.04	0.44
1:L1:4743:G:H2'	1:L1:4744:A:C8	2.52	0.44
1:L1:4910:G:H4'	5:LB:95:THR:HG22	1.99	0.44
9:LF:110:GLN:HG2	9:LF:115:ARG:CZ	2.46	0.44
13:LJ:89:VAL:HG21	13:LJ:115:LEU:HD23	1.98	0.44
16:LN:123:GLU:HB3	16:LN:128:LYS:HG3	1.99	0.44
42:Lo:11:PHE:O	42:Lo:81:ARG:NH1	2.46	0.44
47:SB:65:ARG:NH2	72:SO:48:SER:OG	2.48	0.44
49:SE:196:THR:OG1	49:SE:209:HIS:O	2.34	0.44
1:L1:906:C:H2'	1:L1:907:C:C6	2.53	0.44
1:L1:1802:A:H5''	1:L1:1803:G:H5'	2.00	0.44
1:L1:2864:A:H2'	1:L1:2865:U:C6	2.53	0.44
6:LC:5:ARG:NE	6:LC:24:LEU:O	2.49	0.44
45:S2:17:C:H2'	45:S2:18:C:C6	2.53	0.44
62:SX:74:LEU:O	62:SX:78:GLY:N	2.51	0.44
68:SG:181:THR:HB	68:SG:184:VAL:HG23	1.99	0.44
76:Sb:42:LYS:HE2	76:Sb:57:VAL:HG12	2.00	0.44
1:L1:2033:A:OP1	12:LI:162:ARG:NH2	2.39	0.44
1:L1:3744:OMG:HM23	1:L1:3744:OMG:H1'	1.81	0.44
1:L1:3911:C:H2'	1:L1:3912:U:H6	1.82	0.44
1:L1:3952:A:H2'	1:L1:3953:G:C8	2.53	0.44
4:LA:126:LEU:HD13	4:LA:150:LEU:HD21	2.00	0.44
35:Lh:80:PRO:HD2	35:Lh:83:LEU:HD12	2.00	0.44
41:Ln:21:ARG:NH2	45:S2:1175:G:OP1	2.51	0.44
42:Lo:12:CYS:HB3	42:Lo:15:CYS:HB2	1.99	0.44
45:S2:867:OMG:H3'	45:S2:868:G:N2	2.31	0.44
45:S2:1641:A:OP2	79:CC:34:U:O2'	2.35	0.44
66:Sg:18:VAL:O	66:Sg:287:THR:OG1	2.33	0.44
66:Sg:114:SER:HB3	66:Sg:119:GLN:HB2	1.99	0.44
1:L1:350:C:H3'	6:LC:197:ARG:HH12	1.82	0.44
1:L1:3911:C:H2'	1:L1:3912:U:C6	2.53	0.44
2:L2:4:U:H2'	2:L2:5:A:C8	2.53	0.44
5:LB:62:ARG:HG2	5:LB:65:SER:HB2	2.00	0.44
12:LI:177:ASN:HB2	12:LI:180:GLU:HG2	1.99	0.44
33:Lf:36:ARG:O	33:Lf:39:THR:OG1	2.32	0.44
45:S2:587:A:H5'	45:S2:592:C:H41	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:996:A:H2'	45:S2:997:A:C8	2.53	0.44
45:S2:1236:G:O2'	55:SP:131:PRO:O	2.36	0.44
45:S2:1700:C:O2	45:S2:1834:A:N6	2.51	0.44
47:SB:98:THR:O	47:SB:232:HIS:NE2	2.48	0.44
48:SD:75:LYS:HE2	53:SK:20:VAL:HG23	2.00	0.44
50:SF:56:TYR:HD1	50:SF:62:ARG:HG2	1.83	0.44
1:L1:2579:G:N2	1:L1:2582:A:OP2	2.42	0.43
1:L1:4392:OMG:H2'	1:L1:4447:5MC:HM51	1.99	0.43
6:LC:79:VAL:HG11	6:LC:86:ARG:HG3	1.98	0.43
12:LI:52:MET:HE1	12:LI:155:ALA:HB3	2.01	0.43
13:LJ:35:ARG:NH1	13:LJ:122:SER:O	2.47	0.43
19:LQ:172:ARG:NH1	28:La:56:VAL:O	2.48	0.43
35:Lh:52:LYS:HA	35:Lh:52:LYS:HD3	1.73	0.43
48:SD:103:GLU:HA	48:SD:106:ARG:HG2	1.99	0.43
69:SJ:111:GLN:HE21	69:SJ:123:ILE:HG13	1.82	0.43
1:L1:178:C:H2'	1:L1:179:G:C8	2.52	0.43
1:L1:1100:U:O2	1:L1:1195:G:N2	2.38	0.43
1:L1:3923:A:H2'	1:L1:3924:C:C6	2.53	0.43
1:L1:4369:A:H2'	1:L1:4370:OMG:C8	2.53	0.43
2:L2:4:U:H2'	2:L2:5:A:H8	1.83	0.43
2:L2:38:U:N3	2:L2:41:G:OP2	2.34	0.43
12:LI:205:PRO:O	12:LI:208:LYS:HG3	2.18	0.43
13:LJ:136:ARG:HG3	13:LJ:157:ILE:HD11	2.00	0.43
32:Le:35:TRP:CZ2	32:Le:56:PRO:HD2	2.53	0.43
45:S2:455:A:H2'	45:S2:456:C:C6	2.53	0.43
45:S2:649:U:H2'	45:S2:650:A:H8	1.83	0.43
45:S2:1215:C:O2'	45:S2:1645:C:OP2	2.35	0.43
58:SS:101:ASN:O	58:SS:105:ASN:ND2	2.50	0.43
74:SY:82:ALA:O	74:SY:86:GLU:CB	2.66	0.43
1:L1:137:G:H2'	1:L1:138:G:H8	1.82	0.43
1:L1:1175:A:H2	1:L1:1185:G:C2	2.35	0.43
1:L1:1972:G:N1	1:L1:1995:G:O6	2.51	0.43
3:L3:96:C:H5''	35:Lh:66:LYS:HG2	2.00	0.43
10:LG:110:LYS:HG3	10:LG:113:ARG:HH12	1.83	0.43
28:La:115:GLY:O	28:La:136:LYS:NZ	2.48	0.43
45:S2:84:A:N3	45:S2:150:A:O2'	2.49	0.43
60:SU:61:LEU:O	60:SU:81:GLN:HA	2.18	0.43
66:Sg:84:ASP:OD1	66:Sg:84:ASP:N	2.51	0.43
75:SZ:68:ILE:HB	75:SZ:109:TYR:HB2	2.00	0.43
75:SZ:99:LEU:HD21	75:SZ:102:LYS:HB2	1.99	0.43
1:L1:1764:G:N2	1:L1:1768:C:O2'	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3722:G:H2'	1:L1:3723:A2M:H8	2.00	0.43
6:LC:209:ILE:HB	6:LC:229:LEU:HD13	2.00	0.43
28:LZ:48:ARG:HB2	28:LZ:69:LYS:HB3	2.00	0.43
45:S2:1308:U:H1'	78:Sf:135:HIS:HE1	1.82	0.43
45:S2:1711:U:H2'	45:S2:1712:A:C8	2.53	0.43
79:CC:43:G:H2'	79:CC:44:A:C8	2.53	0.43
1:L1:1359:G:H4'	16:LN:203:TYR:HB2	2.00	0.43
1:L1:3873:G:H2'	1:L1:3874:G:C8	2.53	0.43
1:L1:3932:U:H2'	1:L1:3933:G:C8	2.53	0.43
1:L1:3953:G:H22	1:L1:4060:U:H1'	1.83	0.43
3:L3:102:G:OP2	3:L3:104:A:O2'	2.31	0.43
8:LE:43:HIS:ND1	8:LE:44:CYS:O	2.43	0.43
10:LG:38:ASN:OD1	10:LG:43:GLN:NE2	2.51	0.43
17:LO:54:TYR:OH	17:LO:73:PHE:O	2.35	0.43
23:LU:22:THR:O	23:LU:109:SER:HA	2.18	0.43
45:S2:355:G:OP1	54:SL:105:ARG:NH1	2.43	0.43
45:S2:1144:A:H2'	45:S2:1145:A:C8	2.54	0.43
49:SE:220:THR:OG1	49:SE:221:ARG:N	2.51	0.43
55:SP:49:LEU:HD22	55:SP:53:GLN:HG2	1.99	0.43
66:Sg:42:MET:HE3	66:Sg:42:MET:HB3	1.79	0.43
1:L1:1662:C:H2'	1:L1:1663:C:C6	2.53	0.43
1:L1:3716:C:N4	1:L1:3735:G:O2'	2.48	0.43
1:L1:4162:C:C4	10:LG:72:LYS:HD3	2.54	0.43
5:LB:71:GLU:OE2	5:LB:366:LYS:NZ	2.36	0.43
16:LN:90:ASN:O	42:Lo:48:TYR:OH	2.36	0.43
51:SH:74:LYS:HG2	51:SH:75:ILE:HG23	1.99	0.43
52:SI:138:ASN:OD1	52:SI:139:LYS:N	2.50	0.43
59:ST:39:LEU:HD21	59:ST:56:ARG:HH22	1.83	0.43
76:Sb:33:MET:HE2	76:Sb:48:SER:HA	2.01	0.43
1:L1:468:U:C4	1:L1:686:A:N1	2.86	0.43
1:L1:4954:G:H2'	1:L1:4955:A:C8	2.54	0.43
11:LH:89:ARG:HG3	11:LH:145:ILE:HG23	2.01	0.43
45:S2:901:G:H2'	45:S2:902:G:C8	2.54	0.43
45:S2:1486:A:OP2	48:SD:151:LYS:NZ	2.46	0.43
45:S2:1653:U:H2'	45:S2:1654:G:C8	2.54	0.43
45:S2:1692:U:H2'	45:S2:1693:G:C8	2.54	0.43
45:S2:1797:U:H2'	45:S2:1798:C:C6	2.54	0.43
50:SF:126:THR:O	50:SF:126:THR:OG1	2.36	0.43
56:SQ:94:ALA:HA	56:SQ:97:GLN:HG2	2.00	0.43
1:L1:169:G:N2	1:L1:266:C:C2	2.79	0.43
1:L1:1070:G:OP2	8:LE:65:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:2253:A:N6	9:LF:27:GLU:OE1	2.45	0.43
1:L1:2614:C:O2'	1:L1:2808:G:OP1	2.32	0.43
1:L1:2640:G:H2'	1:L1:2641:A:C8	2.53	0.43
1:L1:2765:A:H2'	1:L1:2766:A:C8	2.54	0.43
1:L1:2803:U:H2'	1:L1:2804:OMC:H6	1.84	0.43
1:L1:4126:C:OP1	10:LG:37:LYS:NZ	2.49	0.43
3:L3:65:A:O2'	35:Lh:10:ARG:NH2	2.52	0.43
19:LQ:110:ARG:HG3	19:LQ:120:ILE:HD12	2.00	0.43
27:LY:10:ASP:HB3	27:LY:13:LYS:HB2	2.01	0.43
45:S2:71:G:H2'	45:S2:72:C:H4'	2.01	0.43
45:S2:1438:A:H2'	45:S2:1439:A:C8	2.53	0.43
53:SK:83:LEU:HD12	53:SK:85:LEU:HD13	2.01	0.43
67:SC:212:LYS:HE3	67:SC:212:LYS:HB2	1.77	0.43
1:L1:190:G:H2'	1:L1:191:G:H8	1.83	0.43
1:L1:1374:G:H1'	6:LC:234:LYS:HG3	2.01	0.43
1:L1:1443:A:N6	1:L1:2104:G:N1	2.67	0.43
1:L1:4563:U:H2'	1:L1:4564:A:C8	2.54	0.43
10:LG:83:PHE:HA	10:LG:183:ILE:HD13	2.01	0.43
11:LH:114:ILE:HB	11:LH:124:ARG:HB2	2.00	0.43
45:S2:986:G:O4'	72:SO:138:ASP:HB2	2.19	0.43
45:S2:1677:U:H2'	45:S2:1678:A2M:H8	2.01	0.43
55:SP:28:MET:HE3	55:SP:33:LEU:HD12	2.01	0.43
66:Sg:42:MET:HE2	66:Sg:92:LEU:HD22	2.01	0.43
1:L1:1333:A:H2'	1:L1:1334:A:C8	2.53	0.43
1:L1:1815:G:O6	29:Lb:49:HIS:NE2	2.42	0.43
1:L1:3718:A2M:H2	1:L1:3934:G:O4'	2.18	0.43
1:L1:3760:A:H62	45:S2:1825:A:H8	1.67	0.43
5:LB:77:THR:HG21	5:LB:337:VAL:HG22	2.01	0.43
10:LG:90:GLN:HA	10:LG:93:THR:HG22	2.01	0.43
36:Li:26:HIS:CE1	36:Li:29:ARG:HD3	2.53	0.43
40:Lm:114:LYS:H	40:Lm:114:LYS:HG2	1.70	0.43
45:S2:1172:U:H2'	45:S2:1173:A:H8	1.84	0.43
56:SQ:78:VAL:HA	56:SQ:81:ILE:HG12	2.00	0.43
70:SM:32:ALA:HB3	70:SM:110:VAL:HG23	2.01	0.43
79:CC:28:C:H2'	79:CC:29:A:C8	2.54	0.43
79:CC:28:C:H2'	79:CC:29:A:H8	1.84	0.43
1:L1:2348:G:OP1	1:L1:2351:OMC:N4	2.49	0.42
1:L1:2399:G:O2'	1:L1:2822:G:O2'	2.34	0.42
1:L1:3969:G:N2	1:L1:4053:A:O2'	2.52	0.42
2:L2:11:A:O2'	2:L2:13:A:OP2	2.32	0.42
4:LA:178:PRO:HD2	43:Lp:26:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LJ:42:GLN:HE21	13:LJ:117:ILE:HD12	1.83	0.42
45:S2:552:G:OP2	45:S2:552:G:N2	2.36	0.42
49:SE:75:LYS:HE2	49:SE:75:LYS:HB3	1.89	0.42
62:SX:68:LYS:HE3	77:Se:6:LEU:HA	2.01	0.42
1:L1:1405:C:N4	1:L1:1408:G:N3	2.56	0.42
1:L1:1761:G:N1	1:L1:1768:C:N3	2.67	0.42
1:L1:2471:G:H5''	10:LG:59:ARG:HD2	2.01	0.42
1:L1:3684:G:H2'	1:L1:3685:C:C6	2.54	0.42
1:L1:3788:C:N4	1:L1:3812:C:OP2	2.49	0.42
45:S2:649:U:H2'	45:S2:650:A:C8	2.54	0.42
48:SD:45:ARG:NH1	48:SD:82:GLY:O	2.52	0.42
65:Sd:54:LYS:HE3	65:Sd:54:LYS:HB3	1.88	0.42
69:SJ:3:VAL:HB	69:SJ:5:ARG:HD3	2.00	0.42
77:Se:2:VAL:HG22	77:Se:6:LEU:HD21	2.01	0.42
1:L1:318:A:H2'	1:L1:319:A:C8	2.55	0.42
1:L1:418:A:C2	3:L3:17:A:H1'	2.55	0.42
1:L1:1440:U:C2	1:L1:2106:G:N1	2.87	0.42
1:L1:2478:C:N3	1:L1:2591:A:O2'	2.51	0.42
3:L3:137:A:H2'	3:L3:138:C:C6	2.54	0.42
16:LN:51:LEU:O	16:LN:117:ASN:ND2	2.50	0.42
28:LZ:51:ARG:HB2	28:LZ:65:ARG:HB3	2.00	0.42
45:S2:1845:A:H2'	45:S2:1846:G:H8	1.83	0.42
52:SI:174:CYS:HB2	52:SI:190:LEU:HD21	2.02	0.42
69:SJ:153:SER:O	69:SJ:157:ILE:HG13	2.19	0.42
1:L1:351:C:OP2	6:LC:197:ARG:NH1	2.52	0.42
1:L1:4115:G:O2'	4:LA:93:LYS:NZ	2.36	0.42
1:L1:4760:G:OP1	17:LO:117:ARG:NH2	2.52	0.42
1:L1:4924:C:N4	1:L1:4925:U:O4	2.52	0.42
3:L3:46:G:O2'	3:L3:61:A:N1	2.49	0.42
4:LA:20:VAL:HA	4:LA:23:ARG:HG3	2.01	0.42
4:LA:117:GLU:HG2	4:LA:124:GLY:H	1.83	0.42
6:LC:47:ASN:ND2	6:LC:113:ARG:H	2.17	0.42
8:LE:158:ARG:HG2	33:Lf:5:LEU:HD13	2.01	0.42
14:LL:171:GLU:O	14:LL:175:ASN:ND2	2.53	0.42
20:LR:76:MET:O	20:LR:81:ARG:NH2	2.46	0.42
27:LY:39:ARG:NH2	83:LY:201:HOH:O	2.46	0.42
30:Lc:48:LEU:HD13	30:Lc:57:LYS:HG3	2.00	0.42
37:Lj:67:LEU:HD23	37:Lj:67:LEU:HA	1.89	0.42
45:S2:1308:U:H2'	45:S2:1309:C:C6	2.54	0.42
45:S2:1394:G:H5''	56:SQ:126:ARG:HE	1.83	0.42
53:SK:7:ASN:O	53:SK:11:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SV:70:LEU:HD21	61:SV:83:PHE:HE1	1.85	0.42
63:Sa:98:PRO:HA	63:Sa:99:PRO:HD3	1.93	0.42
74:SY:110:ARG:HG2	74:SY:114:MET:HE1	2.01	0.42
1:L1:1631:A:C2	4:LA:204:MET:HG2	2.54	0.42
25:LW:61:LYS:HD3	25:LW:61:LYS:HA	1.87	0.42
45:S2:166:A2M:HM'3	68:SG:13:GLN:HE21	1.84	0.42
45:S2:328:U:O2'	45:S2:329:G:O5'	2.37	0.42
45:S2:604:A:N3	45:S2:639:C:O2'	2.48	0.42
48:SD:17:PHE:HE2	48:SD:39:VAL:HG11	1.83	0.42
51:SH:118:ARG:O	51:SH:121:THR:OG1	2.30	0.42
58:SS:5:ILE:HA	58:SS:6:PRO:HD3	1.93	0.42
67:SC:166:ARG:HB2	67:SC:248:TYR:CD1	2.51	0.42
78:Sf:99:LYS:HG3	78:Sf:100:LEU:HD23	2.00	0.42
79:CC:19:C:O2'	79:CC:21:A:O4'	2.34	0.42
1:L1:238:C:OP2	27:LY:45:ARG:NH2	2.53	0.42
1:L1:2749:C:H5'	34:Lg:65:MET:HA	2.01	0.42
1:L1:4324:A:H2'	1:L1:4325:A:C8	2.54	0.42
3:L3:120:G:H2'	3:L3:121:G:H8	1.84	0.42
4:LA:180:LEU:HD23	43:Lp:18:TYR:CD2	2.55	0.42
27:LY:53:ASP:HB3	27:LY:110:LYS:H	1.84	0.42
28:La:132:ARG:HA	28:La:135:GLU:HG2	2.01	0.42
45:S2:155:G:H4'	68:SG:15:LEU:HD22	2.02	0.42
47:SB:83:LYS:HE3	47:SB:83:LYS:HB2	1.84	0.42
47:SB:198:GLU:O	47:SB:202:GLN:HG2	2.19	0.42
60:SU:22:ILE:HD12	60:SU:39:LEU:HD13	2.00	0.42
66:Sg:31:ILE:O	66:Sg:42:MET:HA	2.20	0.42
66:Sg:49:GLU:OE1	66:Sg:50:THR:HG23	2.20	0.42
1:L1:1442:C:H42	1:L1:2104:G:H2'	1.85	0.42
1:L1:1846:G:H2'	1:L1:1847:C:C6	2.54	0.42
1:L1:3966:A:O2'	1:L1:4046:A:N6	2.43	0.42
1:L1:4239:A:H2'	1:L1:4240:G:C8	2.54	0.42
4:LA:145:LYS:HD3	4:LA:145:LYS:HA	1.82	0.42
4:LA:150:LEU:HD11	4:LA:156:LYS:HD2	2.01	0.42
33:Lf:83:MET:HE3	33:Lf:83:MET:HB3	1.97	0.42
45:S2:1232:U:H2'	45:S2:1233:G:C8	2.54	0.42
47:SB:117:TRP:HB3	47:SB:153:THR:HG22	2.02	0.42
48:SD:123:LEU:HD22	48:SD:152:PHE:HB3	2.01	0.42
55:SP:57:LEU:HB3	55:SP:61:ARG:HH12	1.84	0.42
59:ST:85:ASN:HB2	59:ST:88:MET:HB2	2.01	0.42
66:Sg:248:LEU:HB2	66:Sg:261:LEU:HD11	2.01	0.42
67:SC:211:LYS:HG2	67:SC:215:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:138:G:H2'	1:L1:139:G:H8	1.81	0.42
1:L1:2822:G:OP2	20:LR:21:LYS:NZ	2.41	0.42
1:L1:3607:U:H2'	1:L1:3608:A:C8	2.55	0.42
1:L1:5004:C:H2'	1:L1:5005:G:O4'	2.20	0.42
5:LB:39:LYS:HA	5:LB:39:LYS:HD3	1.85	0.42
5:LB:258:HIS:HA	5:LB:259:PRO:C	2.43	0.42
6:LC:133:LEU:HD23	6:LC:133:LEU:HA	1.83	0.42
14:LL:180:ALA:O	14:LL:184:MET:HG3	2.20	0.42
23:LU:105:ASN:HB3	23:LU:111:GLU:HG2	2.02	0.42
43:Lp:26:VAL:O	43:Lp:30:GLU:CB	2.67	0.42
45:S2:12:U:H2'	45:S2:13:C:C6	2.55	0.42
52:SI:98:LYS:HG3	52:SI:178:ARG:HG3	2.01	0.42
56:SQ:53:GLU:HA	56:SQ:56:LEU:HB2	2.02	0.42
58:SS:62:ASP:OD1	58:SS:63:GLU:N	2.53	0.42
68:SG:137:ARG:HG3	68:SG:140:ARG:H	1.85	0.42
69:SJ:111:GLN:NE2	69:SJ:127:ARG:HB2	2.35	0.42
69:SJ:149:VAL:HG11	69:SJ:157:ILE:HD11	2.02	0.42
1:L1:268:G:H2'	1:L1:269:G:H8	1.85	0.42
1:L1:1789:C:OP1	12:LI:21:ARG:NH2	2.52	0.42
1:L1:2262:G:OP2	44:Lr:98:ARG:NH2	2.46	0.42
1:L1:2517:A:N3	1:L1:2539:C:O2'	2.53	0.42
1:L1:2893:U:H5''	52:SI:205:ARG:NH2	2.35	0.42
14:LL:139:SER:O	14:LL:143:GLU:CB	2.64	0.42
23:LU:26:THR:HG22	23:LU:68:SER:HB3	2.02	0.42
30:Lc:28:VAL:HG11	30:Lc:37:MET:HG3	2.01	0.42
45:S2:39:A:H5'	69:SJ:7:TRP:NE1	2.25	0.42
45:S2:942:G:H2'	45:S2:943:U:C6	2.54	0.42
45:S2:1288:OMU:HM23	45:S2:1288:OMU:H1'	1.93	0.42
45:S2:1403:C:OP2	45:S2:1405:A:N6	2.43	0.42
45:S2:1490:OMG:HM23	45:S2:1490:OMG:H1'	1.79	0.42
45:S2:1550:G:O2'	45:S2:1558:C:O2	2.32	0.42
52:SI:76:THR:HG21	52:SI:104:ILE:HD12	2.01	0.42
63:Sa:83:VAL:HG12	63:Sa:84:VAL:HG23	2.02	0.42
1:L1:461:G:H2'	1:L1:462:G:H8	1.85	0.42
1:L1:2899:C:OP1	20:LR:108:ARG:NH2	2.33	0.42
1:L1:3710:G:N3	1:L1:3711:A:N6	2.68	0.42
1:L1:3956:G:OP2	1:L1:3964:U:N3	2.41	0.42
1:L1:4108:G:H2'	1:L1:4109:G:C8	2.55	0.42
1:L1:4910:G:H22	17:LO:107:GLY:HA3	1.84	0.42
4:LA:206:PRO:HG3	4:LA:213:GLY:HA3	2.01	0.42
26:LX:79:PHE:CD2	35:Lh:36:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Lh:89:ARG:O	35:Lh:93:ARG:HG2	2.20	0.42
40:Lm:112:LYS:HB3	40:Lm:114:LYS:HG2	2.02	0.42
43:Lp:90:LYS:HE2	43:Lp:90:LYS:HB3	1.92	0.42
45:S2:166:A2M:HM'1	68:SG:11:GLY:HA2	2.02	0.42
49:SE:100:ARG:HB2	49:SE:114:ILE:HD13	2.01	0.42
53:SK:11:ILE:HG12	53:SK:45:VAL:HA	2.01	0.42
67:SC:253:PRO:HA	67:SC:256:TRP:CG	2.55	0.42
68:SG:201:LYS:HE3	68:SG:201:LYS:HB3	1.90	0.42
71:SN:132:LYS:HA	71:SN:132:LYS:HD3	1.89	0.42
79:CC:26:A:N6	79:CC:45:G:H1	2.18	0.42
1:L1:231:U:H4'	27:LY:100:HIS:CD2	2.55	0.41
1:L1:1364:U:OP2	14:LL:36:ARG:NH1	2.50	0.41
1:L1:1460:C:H5''	19:LQ:144:LYS:HG3	2.01	0.41
1:L1:1645:C:H2'	1:L1:1646:A:C8	2.54	0.41
1:L1:1921:C:C6	21:LS:161:ARG:HD3	2.55	0.41
1:L1:3827:G:O2'	1:L1:3829:G:OP2	2.33	0.41
2:L2:83:A:H4'	9:LF:224:THR:HB	2.01	0.41
4:LA:2:GLY:HA2	4:LA:207:VAL:HG23	2.02	0.41
12:LI:92:HIS:HA	12:LI:93:PRO:HD3	1.95	0.41
21:LS:11:LYS:HE2	21:LS:29:ARG:HD2	2.01	0.41
27:LY:39:ARG:O	27:LY:42:TYR:C	2.63	0.41
45:S2:28:U:H2'	45:S2:29:G:H8	1.85	0.41
45:S2:562:U:H2'	45:S2:563:G:C8	2.55	0.41
46:SA:173:LEU:HD11	46:SA:177:MET:HE2	2.02	0.41
49:SE:36:HIS:ND1	49:SE:84:ALA:O	2.53	0.41
55:SP:64:LYS:NZ	55:SP:88:GLU:O	2.46	0.41
66:Sg:302:TYR:CD2	66:Sg:308:ARG:HD3	2.55	0.41
70:SM:37:GLU:HA	70:SM:40:LYS:HD3	2.02	0.41
1:L1:280:G:H5''	16:LN:14:LYS:HE3	2.03	0.41
1:L1:3683:C:OP1	4:LA:132:ASN:ND2	2.44	0.41
1:L1:3792:OMG:HM23	1:L1:3792:OMG:H1'	1.90	0.41
1:L1:4716:C:OP2	5:LB:30:LYS:NZ	2.52	0.41
1:L1:4906:C:H2'	1:L1:4907:G:H8	1.85	0.41
1:L1:4927:G:H5''	1:L1:4928:C:H5	1.85	0.41
1:L1:5040:U:H4'	1:L1:5041:G:H5'	2.02	0.41
3:L3:67:U:H2'	3:L3:68:G:H8	1.85	0.41
7:LD:69:ILE:HD12	22:LT:32:ARG:NH1	2.34	0.41
17:LO:3:GLU:HG3	17:LO:31:ARG:HH21	1.85	0.41
34:Lg:100:GLN:HA	34:Lg:103:VAL:HG22	2.02	0.41
35:Lh:63:GLN:O	35:Lh:67:GLU:HG3	2.20	0.41
41:Ln:12:ARG:NH2	45:S2:1847:G:O6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:1308:U:H2'	45:S2:1309:C:H6	1.85	0.41
58:SS:26:ILE:O	58:SS:30:ILE:HG12	2.20	0.41
65:Sd:8:TRP:CZ2	65:Sd:12:ARG:HG3	2.55	0.41
70:SM:35:ILE:HG21	70:SM:61:TYR:HE1	1.84	0.41
74:SY:87:PRO:HB2	74:SY:90:ARG:HG3	2.02	0.41
77:Se:36:MET:HE2	77:Se:36:MET:HB3	1.99	0.41
1:L1:717:U:H2'	1:L1:718:C:C6	2.55	0.41
1:L1:1270:A:O2'	1:L1:1439:C:O2	2.36	0.41
1:L1:3871:A:H2'	1:L1:3872:A:C8	2.55	0.41
16:LN:80:THR:OG1	16:LN:87:HIS:HA	2.20	0.41
16:LN:113:LEU:HB2	16:LN:134:LEU:HD23	2.02	0.41
24:LV:90:ARG:O	24:LV:93:GLY:N	2.50	0.41
45:S2:796:G:N3	51:SH:111:LYS:NZ	2.68	0.41
47:SB:134:LEU:HG	47:SB:218:LEU:HD12	2.01	0.41
47:SB:224:GLU:HB2	47:SB:227:LYS:HE2	2.01	0.41
70:SM:14:VAL:HG22	70:SM:126:GLU:HG3	2.02	0.41
76:Sb:67:THR:OG1	76:Sb:70:LYS:O	2.24	0.41
1:L1:1563:A:N6	45:S2:1028:A:N1	2.68	0.41
1:L1:2411:C:H2'	1:L1:2412:A:C8	2.54	0.41
1:L1:3861:A:H2'	1:L1:3862:A:H8	1.86	0.41
1:L1:4169:G:H4'	1:L1:4171:C:C2	2.55	0.41
1:L1:4344:U:H2'	1:L1:4345:C:C6	2.56	0.41
4:LA:92:LYS:HB3	4:LA:92:LYS:HE2	1.76	0.41
4:LA:107:MET:HE2	4:LA:166:VAL:HG22	2.03	0.41
5:LB:50:LYS:O	5:LB:342:LYS:N	2.54	0.41
5:LB:220:ILE:HB	5:LB:346:THR:HB	2.02	0.41
24:LV:43:LYS:NZ	24:LV:62:MET:SD	2.93	0.41
27:LY:55:VAL:HG12	27:LY:106:ILE:HA	2.01	0.41
45:S2:560:A:H5'	69:SJ:174:LYS:HE2	2.03	0.41
45:S2:1060:A:O2'	45:S2:1062:A:N7	2.45	0.41
45:S2:1217:A:H2'	45:S2:1218:C:C6	2.56	0.41
57:SR:33:ARG:NE	66:Sg:107:ASP:OD2	2.52	0.41
64:Sc:40:ARG:NH2	72:SO:121:ARG:HH12	2.17	0.41
68:SG:50:VAL:HG12	68:SG:113:ILE:HG12	2.02	0.41
73:SW:26:LEU:HB2	76:Sb:7:LEU:HD23	2.02	0.41
1:L1:2861:OMC:HM23	1:L1:2861:OMC:H1'	1.88	0.41
5:LB:14:LEU:HA	5:LB:17:LEU:HB2	2.01	0.41
5:LB:165:HIS:HA	5:LB:179:HIS:O	2.21	0.41
11:LH:115:ARG:HD3	11:LH:115:ARG:HA	1.83	0.41
17:LO:186:GLU:HA	17:LO:189:ILE:HG12	2.02	0.41
21:LS:43:ARG:HD2	21:LS:43:ARG:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:576:A2M:HM'2	45:S2:577:U:H5'	2.03	0.41
45:S2:612:PSU:H4'	77:Se:15:GLN:NE2	2.35	0.41
45:S2:798:G:H21	51:SH:104:PRO:HA	1.84	0.41
48:SD:50:ILE:HD11	48:SD:86:LEU:HD23	2.02	0.41
48:SD:204:LEU:HB2	48:SD:207:HIS:HB3	2.03	0.41
66:Sg:152:SER:H	66:Sg:169:GLY:HA2	1.86	0.41
66:Sg:215:GLN:HB3	66:Sg:217:MET:HE3	2.03	0.41
67:SC:88:ILE:HG21	67:SC:94:ILE:HD11	2.02	0.41
67:SC:184:VAL:HG11	67:SC:247:THR:HA	2.03	0.41
68:SG:153:VAL:HA	68:SG:156:TYR:HB2	2.02	0.41
74:SY:56:PHE:O	74:SY:74:MET:N	2.47	0.41
1:L1:1572:U:H4'	20:LR:95:TRP:CE2	2.55	0.41
10:LG:212:LYS:HE3	10:LG:212:LYS:HB2	1.86	0.41
21:LS:53:LYS:HE3	21:LS:53:LYS:HB2	1.94	0.41
23:LU:63:ILE:HG13	23:LU:72:VAL:HG22	2.03	0.41
28:LZ:115:LYS:O	28:LZ:119:GLU:HG3	2.20	0.41
45:S2:382:C:H2'	45:S2:383:G:C8	2.56	0.41
45:S2:1221:G:H2'	45:S2:1222:G:C8	2.56	0.41
46:SA:38:ILE:HA	46:SA:38:ILE:HD13	1.85	0.41
46:SA:137:ALA:HB1	46:SA:142:LEU:HB3	2.03	0.41
48:SD:132:LYS:HG3	48:SD:191:PRO:HA	2.03	0.41
49:SE:141:THR:OG1	49:SE:143:ASP:OD1	2.35	0.41
50:SF:48:TYR:CZ	56:SQ:56:LEU:HD13	2.55	0.41
67:SC:243:ALA:O	67:SC:247:THR:HG23	2.20	0.41
68:SG:194:LEU:HD23	68:SG:197:GLN:HE21	1.85	0.41
1:L1:35:U:H4'	1:L1:1525:A:C2	2.55	0.41
1:L1:730:G:OP2	9:LF:76:ARG:NE	2.50	0.41
11:LH:12:ILE:HB	11:LH:53:LYS:O	2.20	0.41
12:LI:177:ASN:O	12:LI:181:PHE:CB	2.63	0.41
45:S2:294:U:OP1	54:SL:36:TYR:OH	2.37	0.41
45:S2:1630:A:H5''	58:SS:37:GLY:N	2.33	0.41
45:S2:1654:G:OP1	59:ST:90:SER:OG	2.27	0.41
47:SB:78:GLU:HG3	47:SB:79:VAL:H	1.86	0.41
47:SB:115:LYS:HE2	47:SB:115:LYS:HB3	1.89	0.41
51:SH:53:VAL:HG11	51:SH:172:THR:HA	2.01	0.41
1:L1:1406:G:N2	1:L1:1409:C:H41	2.19	0.41
1:L1:2497:C:H2'	1:L1:2498:C:H6	1.85	0.41
8:LE:161:ARG:NH1	8:LE:273:SER:OG	2.54	0.41
25:LW:99:GLU:HA	25:LW:102:LYS:HE2	2.03	0.41
44:Lr:101:LYS:HD3	44:Lr:101:LYS:HA	1.81	0.41
45:S2:581:U:OP1	69:SJ:133:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:1121:G:O2'	47:SB:204:ILE:O	2.29	0.41
45:S2:1473:G:N1	45:S2:1476:A:OP2	2.49	0.41
45:S2:1541:G:P	59:ST:56:ARG:HH21	2.44	0.41
45:S2:1736:G:H2'	45:S2:1737:G:C8	2.56	0.41
51:SH:40:LEU:HD21	51:SH:79:LEU:HD21	2.02	0.41
66:Sg:164:ILE:HD13	66:Sg:164:ILE:HA	1.94	0.41
73:SW:37:PHE:CE2	73:SW:41:MET:HE3	2.55	0.41
1:L1:1332:C:H2'	1:L1:1333:A:H8	1.85	0.41
1:L1:2112:G:H21	1:L1:2250:C:N4	2.18	0.41
1:L1:2411:C:H2'	1:L1:2412:A:H8	1.85	0.41
1:L1:3711:A:N1	45:S2:970:G:N2	2.69	0.41
1:L1:3934:G:H2'	1:L1:3935:C:C6	2.56	0.41
1:L1:4220:6MZ:O5'	1:L1:4220:6MZ:H8	2.21	0.41
4:LA:225:ILE:HG12	4:LA:234:LYS:HA	2.02	0.41
7:LD:216:GLU:O	7:LD:220:LYS:HG2	2.21	0.41
10:LG:143:VAL:HG22	10:LG:203:ALA:HB2	2.03	0.41
10:LG:229:ARG:O	10:LG:233:ILE:HG13	2.21	0.41
12:LI:179:ASP:OD1	12:LI:179:ASP:N	2.53	0.41
18:LP:14:SER:HB3	18:LP:151:THR:HG22	2.03	0.41
20:LR:114:LYS:HE3	20:LR:114:LYS:HB3	1.91	0.41
38:Lk:24:LYS:HA	38:Lk:67:LYS:O	2.21	0.41
45:S2:16:G:H2'	45:S2:17:C:C6	2.56	0.41
45:S2:76:U:O2	68:SG:159:ARG:NH2	2.48	0.41
45:S2:1124:C:H5''	47:SB:150:ILE:HG12	2.03	0.41
45:S2:1831:A:H2'	45:S2:1832:6MZ:H8	2.01	0.41
51:SH:23:ILE:HD13	51:SH:87:PHE:CE2	2.56	0.41
52:SI:120:PRO:HG3	52:SI:137:LEU:HD11	2.02	0.41
56:SQ:90:LYS:HA	56:SQ:93:VAL:HG22	2.03	0.41
58:SS:42:HIS:HB3	58:SS:46:ARG:NH1	2.36	0.41
60:SU:48:LEU:HD22	60:SU:93:SER:HB2	2.02	0.41
67:SC:210:PRO:HD3	67:SC:236:PHE:CE2	2.56	0.41
67:SC:256:TRP:CD2	73:SW:68:ARG:HD3	2.56	0.41
68:SG:45:TRP:HZ3	68:SG:113:ILE:HD11	1.86	0.41
70:SM:91:LEU:HD23	70:SM:104:VAL:HG13	2.02	0.41
79:CC:48:C:H2'	79:CC:49:G:C8	2.56	0.41
1:L1:267:G:H2'	1:L1:268:G:H8	1.86	0.41
1:L1:1320:U:O2'	1:L1:1891:A:N1	2.48	0.41
1:L1:2007:G:H21	1:L1:2012:A:H62	1.68	0.41
9:LF:48:LYS:O	9:LF:52:GLU:HG2	2.21	0.41
9:LF:60:GLU:HG2	9:LF:64:MET:HE3	2.03	0.41
11:LH:93:ARG:HD2	11:LH:143:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:29:G:H2'	45:S2:30:C:C6	2.57	0.41
45:S2:204:G:H2'	45:S2:205:G:C8	2.57	0.41
45:S2:656:G:H5'	45:S2:662:G:N2	2.36	0.41
45:S2:693:A:O2'	45:S2:739:C:O3'	2.36	0.41
46:SA:108:PHE:HB3	46:SA:140:VAL:HG21	2.02	0.41
49:SE:59:ASP:O	49:SE:62:LYS:HG3	2.21	0.41
52:SI:38:ILE:HD11	52:SI:81:VAL:HG23	2.03	0.41
55:SP:95:GLY:HA2	55:SP:104:GLN:HA	2.02	0.41
59:ST:138:VAL:O	59:ST:142:ASN:ND2	2.54	0.41
68:SG:44:GLU:HA	68:SG:119:LYS:HE2	2.03	0.41
73:SW:42:MET:HE2	73:SW:42:MET:HB3	1.89	0.41
1:L1:2341:A:OP2	28:La:4:ARG:NH1	2.51	0.40
1:L1:4563:U:H2'	1:L1:4564:A:H8	1.85	0.40
20:LR:15:LEU:HD13	20:LR:52:ARG:HB2	2.04	0.40
35:Lh:31:LEU:HB3	35:Lh:47:ILE:HG12	2.02	0.40
45:S2:1712:A:H2'	45:S2:1713:C:C6	2.57	0.40
48:SD:93:THR:HG21	48:SD:198:ILE:HG22	2.03	0.40
70:SM:79:VAL:HG21	70:SM:85:LEU:HD22	2.03	0.40
77:Se:52:LYS:HD3	77:Se:52:LYS:HA	1.89	0.40
1:L1:1415:G:H2'	1:L1:1416:G:H8	1.86	0.40
1:L1:3652:A:H2'	1:L1:3653:A:C5	2.57	0.40
1:L1:3883:U:H2'	1:L1:3884:U:C6	2.56	0.40
1:L1:3973:G:N2	1:L1:3974:G:O6	2.54	0.40
1:L1:4448:G:H5''	1:L1:4449:A:H5'	2.03	0.40
1:L1:4459:U:H2'	1:L1:4460:U:C6	2.57	0.40
2:L2:62:U:OP2	7:LD:276:LYS:NZ	2.44	0.40
7:LD:152:ARG:HG3	7:LD:154:THR:HG23	2.02	0.40
25:LW:70:LYS:HD3	25:LW:70:LYS:HA	1.91	0.40
28:La:71:PRO:HG2	28:La:108:TYR:HA	2.02	0.40
39:Ll:23:ILE:HG23	39:Ll:38:ASN:HB2	2.03	0.40
45:S2:102:A:H4'	45:S2:104:A:C8	2.56	0.40
45:S2:1114:U:H5''	47:SB:199:LYS:HE3	2.02	0.40
45:S2:1139:C:H2'	45:S2:1140:G:O4'	2.21	0.40
45:S2:1310:U:H4'	78:Sf:143:LYS:HG3	2.04	0.40
46:SA:23:THR:HG21	46:SA:174:MET:HE3	2.03	0.40
48:SD:209:SER:HB2	57:SR:40:ILE:HB	2.03	0.40
50:SF:33:ILE:HD13	50:SF:36:GLN:HE22	1.85	0.40
50:SF:40:ALA:HB3	50:SF:67:PRO:HA	2.03	0.40
52:SI:34:ALA:HB2	52:SI:56:ARG:HD2	2.03	0.40
56:SQ:110:ASP:HA	56:SQ:113:ILE:HG12	2.02	0.40
66:Sg:153:CYS:HB3	66:Sg:198:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sg:313:THR:HB	66:Sg:314:ILE:HD12	2.04	0.40
67:SC:68:ARG:HA	67:SC:68:ARG:HD3	1.88	0.40
72:SO:56:VAL:HG12	72:SO:81:VAL:HG23	2.02	0.40
1:L1:3707:U:H2'	1:L1:3708:C:H6	1.87	0.40
23:LU:80:LYS:HG2	23:LU:110:TYR:CE2	2.56	0.40
45:S2:639:C:H2'	45:S2:640:A:H8	1.85	0.40
45:S2:1494:U:H4'	45:S2:1495:G:H5''	2.04	0.40
45:S2:1653:U:H3	45:S2:1671:G:H1	1.69	0.40
51:SH:19:PHE:CZ	51:SH:60:ILE:HG23	2.53	0.40
52:SI:143:LYS:H	52:SI:143:LYS:HG2	1.69	0.40
56:SQ:43:GLU:HG2	56:SQ:44:PRO:HD3	2.02	0.40
1:L1:2539:C:H2'	1:L1:2540:C:C6	2.56	0.40
7:LD:116:ASP:N	7:LD:116:ASP:OD2	2.52	0.40
10:LG:72:LYS:HE2	10:LG:72:LYS:HB3	1.91	0.40
15:LM:15:VAL:O	15:LM:22:GLY:N	2.47	0.40
24:LV:106:VAL:HG12	24:LV:112:MET:HA	2.02	0.40
45:S2:1643:U:H2'	45:S2:1644:C:C6	2.56	0.40
49:SE:44:LEU:HD21	49:SE:70:ILE:HG21	2.03	0.40
50:SF:192:LYS:HD3	50:SF:192:LYS:HA	1.93	0.40
59:ST:128:GLN:HA	59:ST:131:LEU:HB2	2.03	0.40
66:Sg:24:THR:HG22	66:Sg:27:PHE:H	1.86	0.40
66:Sg:251:ALA:HB1	66:Sg:286:CYS:HB3	2.04	0.40
68:SG:194:LEU:HD23	68:SG:197:GLN:NE2	2.37	0.40
1:L1:756:G:H2'	1:L1:757:G:C8	2.57	0.40
1:L1:1097:C:H2'	1:L1:1098:G:C8	2.57	0.40
1:L1:1332:C:H2'	1:L1:1333:A:C8	2.57	0.40
1:L1:1820:C:H2'	1:L1:1822:U:H5'	2.02	0.40
5:LB:58:ARG:CZ	5:LB:60:VAL:HG12	2.52	0.40
8:LE:258:LEU:HD22	8:LE:262:LYS:HE3	2.04	0.40
31:Ld:29:ILE:O	31:Ld:33:ILE:HG12	2.21	0.40
35:Lh:105:LYS:HE3	35:Lh:105:LYS:HB2	1.89	0.40
45:S2:38:A:OP1	69:SJ:5:ARG:HG3	2.22	0.40
45:S2:500:A:H5'	45:S2:501:C:H5	1.85	0.40
45:S2:656:G:N2	45:S2:663:C:H5''	2.36	0.40
45:S2:980:A:H2'	45:S2:981:A:C8	2.56	0.40
45:S2:1031:A2M:HM'3	45:S2:1031:A2M:H1'	1.94	0.40
45:S2:1595:U:H2'	45:S2:1596:U:C6	2.57	0.40
45:S2:1607:A:H5'	59:ST:87:VAL:HG21	2.03	0.40
50:SF:39:ILE:HG22	50:SF:41:VAL:HG23	2.04	0.40
68:SG:24:LEU:HB3	68:SG:28:TYR:CZ	2.57	0.40
69:SJ:111:GLN:NE2	69:SJ:123:ILE:HG13	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	230 (94%)	16 (6%)	0	100	100
5	LB	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
6	LC	363/427 (85%)	354 (98%)	9 (2%)	0	100	100
7	LD	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
8	LE	214/288 (74%)	205 (96%)	9 (4%)	0	100	100
9	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
10	LG	223/266 (84%)	218 (98%)	5 (2%)	0	100	100
11	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
12	LI	198/214 (92%)	190 (96%)	8 (4%)	0	100	100
13	LJ	167/178 (94%)	161 (96%)	6 (4%)	0	100	100
14	LL	208/211 (99%)	196 (94%)	12 (6%)	0	100	100
15	LM	137/215 (64%)	132 (96%)	5 (4%)	0	100	100
16	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	LO	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
20	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
21	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
22	LT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
23	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
24	LV	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
25	LW	122/157 (78%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
27	LY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
28	LZ	133/282 (47%)	126 (95%)	7 (5%)	0	100	100
28	La	145/282 (51%)	139 (96%)	6 (4%)	0	100	100
29	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
30	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
31	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
32	Le	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
33	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
34	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
35	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
36	Li	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
37	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
38	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
39	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
40	Lm	50/128 (39%)	50 (100%)	0	0	100	100
41	Ln	22/25 (88%)	22 (100%)	0	0	100	100
42	Lo	100/106 (94%)	97 (97%)	3 (3%)	0	100	100
43	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
44	Lr	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
46	SA	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
47	SB	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
48	SD	225/243 (93%)	220 (98%)	5 (2%)	0	100	100
49	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
50	SF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
51	SH	182/194 (94%)	169 (93%)	11 (6%)	2 (1%)	11	29
52	SI	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
53	SK	96/165 (58%)	90 (94%)	5 (5%)	1 (1%)	12	32
54	SL	140/158 (89%)	131 (94%)	9 (6%)	0	100	100
55	SP	125/145 (86%)	120 (96%)	5 (4%)	0	100	100
56	SQ	142/146 (97%)	128 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	SR	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
58	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
59	ST	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
60	SU	102/119 (86%)	95 (93%)	6 (6%)	1 (1%)	12	32
61	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
62	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
63	Sa	100/115 (87%)	94 (94%)	5 (5%)	1 (1%)	12	32
64	Sc	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
65	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
66	Sg	311/317 (98%)	292 (94%)	18 (6%)	1 (0%)	36	60
67	SC	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
68	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
69	SJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	24	48
70	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
71	SN	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
72	SO	133/151 (88%)	126 (95%)	6 (4%)	1 (1%)	16	37
73	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
74	SY	123/133 (92%)	117 (95%)	6 (5%)	0	100	100
75	SZ	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
76	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
77	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
78	CE	70/133 (53%)	67 (96%)	3 (4%)	0	100	100
78	Sf	59/133 (44%)	52 (88%)	7 (12%)	0	100	100
All	All	11319/13078 (86%)	10904 (96%)	407 (4%)	8 (0%)	49	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	SU	94	PRO
51	SH	34	SER
51	SH	35	ASP
66	Sg	50	THR
69	SJ	122	SER
72	SO	140	THR

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Mol	Chain	Res	Type
53	SK	64	TRP
63	Sa	46	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	189 (100%)	1 (0%)	81	92
5	LB	348/349 (100%)	347 (100%)	1 (0%)	86	94
6	LC	304/348 (87%)	303 (100%)	1 (0%)	86	94
7	LD	246/250 (98%)	246 (100%)	0	100	100
8	LE	194/252 (77%)	194 (100%)	0	100	100
9	LF	194/215 (90%)	192 (99%)	2 (1%)	68	86
10	LG	196/223 (88%)	196 (100%)	0	100	100
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	172/181 (95%)	170 (99%)	2 (1%)	63	84
13	LJ	142/149 (95%)	142 (100%)	0	100	100
14	LL	176/177 (99%)	176 (100%)	0	100	100
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	170 (99%)	1 (1%)	78	91
17	LO	173/174 (99%)	173 (100%)	0	100	100
18	LP	134/163 (82%)	134 (100%)	0	100	100
19	LQ	164/165 (99%)	164 (100%)	0	100	100
20	LR	166/175 (95%)	163 (98%)	3 (2%)	51	78
21	LS	157/157 (100%)	157 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	91 (100%)	0	100	100
24	LV	101/107 (94%)	101 (100%)	0	100	100
25	LW	103/126 (82%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	LX	106/133 (80%)	106 (100%)	0	100	100
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/237 (49%)	117 (100%)	0	100	100
28	La	120/237 (51%)	120 (100%)	0	100	100
29	Lb	88/126 (70%)	88 (100%)	0	100	100
30	Lc	83/97 (86%)	83 (100%)	0	100	100
31	Ld	98/110 (89%)	98 (100%)	0	100	100
32	Le	114/121 (94%)	114 (100%)	0	100	100
33	Lf	88/89 (99%)	88 (100%)	0	100	100
34	Lg	98/100 (98%)	98 (100%)	0	100	100
35	Lh	109/110 (99%)	109 (100%)	0	100	100
36	Li	86/89 (97%)	86 (100%)	0	100	100
37	Lj	73/80 (91%)	73 (100%)	0	100	100
38	Lk	64/65 (98%)	64 (100%)	0	100	100
39	Ll	47/48 (98%)	47 (100%)	0	100	100
40	Lm	48/116 (41%)	48 (100%)	0	100	100
41	Ln	23/24 (96%)	23 (100%)	0	100	100
42	Lo	90/93 (97%)	90 (100%)	0	100	100
43	Lp	74/75 (99%)	74 (100%)	0	100	100
44	Lr	109/121 (90%)	109 (100%)	0	100	100
46	SA	184/243 (76%)	184 (100%)	0	100	100
47	SB	195/231 (84%)	195 (100%)	0	100	100
48	SD	190/202 (94%)	190 (100%)	0	100	100
49	SE	224/225 (100%)	224 (100%)	0	100	100
50	SF	156/170 (92%)	156 (100%)	0	100	100
51	SH	166/174 (95%)	165 (99%)	1 (1%)	78	91
52	SI	178/180 (99%)	178 (100%)	0	100	100
53	SK	89/136 (65%)	89 (100%)	0	100	100
54	SL	130/142 (92%)	130 (100%)	0	100	100
55	SP	113/130 (87%)	113 (100%)	0	100	100
56	SQ	119/121 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	SR	122/122 (100%)	122 (100%)	0	100	100
58	SS	126/132 (96%)	126 (100%)	0	100	100
59	ST	113/115 (98%)	113 (100%)	0	100	100
60	SU	94/107 (88%)	93 (99%)	1 (1%)	65	85
61	SV	67/67 (100%)	62 (92%)	5 (8%)	12	31
62	SX	113/115 (98%)	113 (100%)	0	100	100
63	Sa	89/98 (91%)	89 (100%)	0	100	100
64	Sc	57/62 (92%)	57 (100%)	0	100	100
65	Sd	48/49 (98%)	48 (100%)	0	100	100
66	Sg	272/275 (99%)	272 (100%)	0	100	100
67	SC	188/225 (84%)	188 (100%)	0	100	100
68	SG	207/218 (95%)	203 (98%)	4 (2%)	50	77
69	SJ	161/168 (96%)	161 (100%)	0	100	100
70	SM	102/108 (94%)	102 (100%)	0	100	100
71	SN	130/131 (99%)	130 (100%)	0	100	100
72	SO	105/119 (88%)	105 (100%)	0	100	100
73	SW	112/113 (99%)	112 (100%)	0	100	100
74	SY	109/115 (95%)	109 (100%)	0	100	100
75	SZ	66/103 (64%)	66 (100%)	0	100	100
76	Sb	75/76 (99%)	75 (100%)	0	100	100
77	Se	47/48 (98%)	47 (100%)	0	100	100
78	CE	68/122 (56%)	68 (100%)	0	100	100
78	Sf	54/122 (44%)	54 (100%)	0	100	100
All	All	9876/11139 (89%)	9854 (100%)	22 (0%)	85	95

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	15	VAL
5	LB	261	ARG
6	LC	71	ARG
9	LF	221	LYS
9	LF	223	LYS
12	LI	13	LYS

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Mol	Chain	Res	Type
12	LI	15	LYS
16	LN	83	LYS
20	LR	39	GLN
20	LR	40	GLN
20	LR	43	LYS
51	SH	36	LEU
60	SU	87	ARG
61	SV	79	VAL
61	SV	80	SER
61	SV	81	LYS
61	SV	82	ASN
61	SV	83	PHE
68	SG	215	LYS
68	SG	217	MET
68	SG	218	LYS
68	SG	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	50	HIS
4	LA	194	ASN
5	LB	11	HIS
5	LB	121	ASN
5	LB	184	GLN
5	LB	203	GLN
6	LC	329	ASN
7	LD	267	ASN
8	LE	245	GLN
9	LF	119	ASN
9	LF	126	ASN
9	LF	206	ASN
9	LF	235	ASN
11	LH	39	ASN
11	LH	78	GLN
11	LH	102	ASN
11	LH	138	GLN
12	LI	59	GLN
12	LI	73	ASN
12	LI	147	HIS
13	LJ	104	ASN
14	LL	87	HIS

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Mol	Chain	Res	Type
14	LL	175	ASN
15	LM	20	HIS
15	LM	48	GLN
16	LN	32	GLN
17	LO	180	GLN
18	LP	25	HIS
18	LP	34	GLN
18	LP	97	ASN
20	LR	141	HIS
21	LS	173	ASN
22	LT	66	ASN
24	LV	27	ASN
26	LX	111	GLN
27	LY	56	GLN
28	La	19	HIS
32	Le	92	ASN
34	Lg	110	GLN
35	Lh	65	GLN
38	Lk	58	GLN
39	Ll	4	HIS
39	Ll	17	GLN
39	Ll	19	GLN
39	Ll	33	ASN
44	Lr	23	GLN
44	Lr	30	ASN
46	SA	131	HIS
46	SA	132	GLN
47	SB	159	GLN
47	SB	186	ASN
48	SD	226	GLN
49	SE	67	GLN
49	SE	142	HIS
50	SF	36	GLN
50	SF	101	HIS
51	SH	168	HIS
53	SK	42	ASN
53	SK	50	GLN
53	SK	84	HIS
54	SL	19	ASN
54	SL	94	HIS
54	SL	100	ASN
55	SP	24	GLN

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Mol	Chain	Res	Type
56	SQ	80	GLN
56	SQ	86	GLN
57	SR	62	GLN
58	SS	11	HIS
58	SS	19	ASN
59	ST	42	HIS
59	ST	63	HIS
59	ST	142	ASN
60	SU	28	ASN
66	Sg	20	GLN
66	Sg	76	GLN
66	Sg	117	ASN
66	Sg	285	GLN
66	Sg	296	GLN
67	SC	277	HIS
68	SG	110	ASN
68	SG	202	ASN
71	SN	62	GLN
71	SN	105	ASN
72	SO	113	GLN
73	SW	70	ASN
74	SY	106	GLN
76	Sb	65	GLN
77	Se	15	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3705/5070 (73%)	746 (20%)	12 (0%)
2	L2	119/121 (98%)	11 (9%)	0
3	L3	155/157 (98%)	34 (21%)	0
45	S2	1715/1869 (91%)	335 (19%)	9 (0%)
79	CC	74/75 (98%)	23 (31%)	2 (2%)
All	All	5768/7292 (79%)	1149 (19%)	23 (0%)

All (1149) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	39	A
1	L1	48	G
1	L1	56	A

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Mol	Chain	Res	Type
1	L1	59	A
1	L1	64	A
1	L1	65	A
1	L1	66	A
1	L1	69	A
1	L1	73	A
1	L1	91	G
1	L1	98	A
1	L1	108	A
1	L1	109	G
1	L1	110	C
1	L1	116	G
1	L1	117	C
1	L1	119	G
1	L1	120	A
1	L1	133	C
1	L1	134	G
1	L1	135	G
1	L1	136	C
1	L1	159	C
1	L1	169	G
1	L1	172	C
1	L1	178	C
1	L1	183	C
1	L1	184	U
1	L1	185	C
1	L1	188	G
1	L1	189	G
1	L1	200	U
1	L1	209	U
1	L1	210	C
1	L1	216	C
1	L1	218	A
1	L1	219	G
1	L1	233	U
1	L1	234	G
1	L1	255	C
1	L1	256	G
1	L1	258	G
1	L1	259	C
1	L1	261	G
1	L1	265	C

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Mol	Chain	Res	Type
1	L1	269	G
1	L1	280	G
1	L1	297	U
1	L1	306	A
1	L1	315	G
1	L1	316	U
1	L1	322	C
1	L1	340	C
1	L1	350	C
1	L1	353	A
1	L1	373	G
1	L1	387	G
1	L1	388	A
1	L1	407	A
1	L1	408	A
1	L1	410	A
1	L1	412	G
1	L1	413	G
1	L1	414	C
1	L1	432	U
1	L1	449	C
1	L1	450	G
1	L1	452	A
1	L1	453	G
1	L1	454	U
1	L1	456	C
1	L1	457	G
1	L1	465	G
1	L1	467	U
1	L1	468	U
1	L1	484	U
1	L1	485	C
1	L1	486	C
1	L1	489	C
1	L1	493	G
1	L1	494	U
1	L1	497	G
1	L1	498	C
1	L1	500	G
1	L1	501	C
1	L1	502	C
1	L1	503	C

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Mol	Chain	Res	Type
1	L1	504	G
1	L1	505	G
1	L1	509	A
1	L1	510	U
1	L1	513	U
1	L1	514	U
1	L1	518	G
1	L1	643	C
1	L1	645	G
1	L1	646	G
1	L1	656	C
1	L1	657	C
1	L1	659	G
1	L1	665	C
1	L1	668	C
1	L1	685	C
1	L1	686	A
1	L1	687	U
1	L1	688	U
1	L1	696	C
1	L1	704	C
1	L1	731	G
1	L1	738	C
1	L1	739	G
1	L1	742	G
1	L1	749	G
1	L1	754	U
1	L1	759	G
1	L1	904	C
1	L1	905	C
1	L1	907	C
1	L1	913	U
1	L1	914	U
1	L1	915	A
1	L1	917	A
1	L1	918	G
1	L1	924	C
1	L1	925	C
1	L1	926	G
1	L1	932	A
1	L1	933	G
1	L1	934	C

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Mol	Chain	Res	Type
1	L1	935	A
1	L1	943	A
1	L1	944	A
1	L1	945	U
1	L1	946	C
1	L1	956	A
1	L1	959	G
1	L1	960	A
1	L1	962	C
1	L1	965	G
1	L1	966	A
1	L1	967	C
1	L1	968	C
1	L1	970	G
1	L1	982	U
1	L1	986	C
1	L1	989	U
1	L1	990	C
1	L1	991	C
1	L1	992	C
1	L1	993	G
1	L1	995	C
1	L1	1048	G
1	L1	1049	C
1	L1	1050	C
1	L1	1051	G
1	L1	1082	C
1	L1	1083	U
1	L1	1095	A
1	L1	1168	G
1	L1	1170	G
1	L1	1171	G
1	L1	1172	C
1	L1	1173	G
1	L1	1178	G
1	L1	1179	U
1	L1	1180	C
1	L1	1181	C
1	L1	1182	C
1	L1	1183	C
1	L1	1184	A
1	L1	1193	C

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Mol	Chain	Res	Type
1	L1	1200	G
1	L1	1202	C
1	L1	1203	G
1	L1	1210	C
1	L1	1211	G
1	L1	1214	C
1	L1	1215	C
1	L1	1218	G
1	L1	1219	G
1	L1	1220	G
1	L1	1221	G
1	L1	1222	A
1	L1	1241	C
1	L1	1246	G
1	L1	1254	A
1	L1	1255	A
1	L1	1258	G
1	L1	1266	G
1	L1	1269	G
1	L1	1270	A
1	L1	1271	G
1	L1	1273	G
1	L1	1275	G
1	L1	1280	C
1	L1	1284	G
1	L1	1285	U
1	L1	1287	G
1	L1	1293	G
1	L1	1294	A
1	L1	1295	C
1	L1	1296	G
1	L1	1301	C
1	L1	1302	U
1	L1	1303	A
1	L1	1313	C
1	L1	1326	A2M
1	L1	1337	A
1	L1	1340	OMC
1	L1	1354	A
1	L1	1358	G
1	L1	1359	G
1	L1	1365	C

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Mol	Chain	Res	Type
1	L1	1367	C
1	L1	1379	C
1	L1	1387	A
1	L1	1394	G
1	L1	1397	A
1	L1	1398	A
1	L1	1404	G
1	L1	1408	G
1	L1	1409	C
1	L1	1410	U
1	L1	1417	C
1	L1	1420	A
1	L1	1433	A
1	L1	1439	C
1	L1	1441	C
1	L1	1444	G
1	L1	1447	C
1	L1	1481	C
1	L1	1482	G
1	L1	1483	C
1	L1	1497	A
1	L1	1498	G
1	L1	1502	G
1	L1	1518	A
1	L1	1534	A2M
1	L1	1535	C
1	L1	1547	A
1	L1	1549	G
1	L1	1564	A
1	L1	1566	C
1	L1	1578	U
1	L1	1591	U
1	L1	1596	U
1	L1	1611	C
1	L1	1612	G
1	L1	1624	G
1	L1	1625	OMG
1	L1	1626	G
1	L1	1631	A
1	L1	1633	G
1	L1	1634	A
1	L1	1640	C

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Mol	Chain	Res	Type
1	L1	1642	A
1	L1	1654	G
1	L1	1661	C
1	L1	1676	C
1	L1	1677	PSU
1	L1	1678	C
1	L1	1681	G
1	L1	1694	C
1	L1	1697	G
1	L1	1699	A
1	L1	1700	G
1	L1	1701	A
1	L1	1702	C
1	L1	1704	C
1	L1	1705	G
1	L1	1707	C
1	L1	1726	U
1	L1	1731	C
1	L1	1734	G
1	L1	1735	U
1	L1	1742	A
1	L1	1755	C
1	L1	1756	U
1	L1	1757	U
1	L1	1758	G
1	L1	1760	G
1	L1	1761	G
1	L1	1762	C
1	L1	1763	C
1	L1	1765	A
1	L1	1766	A
1	L1	1767	A
1	L1	1768	C
1	L1	1769	G
1	L1	1770	A
1	L1	1775	A
1	L1	1785	C
1	L1	1787	A
1	L1	1797	G
1	L1	1804	A
1	L1	1806	G
1	L1	1810	G

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Mol	Chain	Res	Type
1	L1	1815	G
1	L1	1820	C
1	L1	1821	G
1	L1	1822	U
1	L1	1834	U
1	L1	1836	G
1	L1	1837	A
1	L1	1842	G
1	L1	1855	G
1	L1	1869	G
1	L1	1897	A
1	L1	1918	U
1	L1	1919	G
1	L1	1920	C
1	L1	1921	C
1	L1	1922	G
1	L1	1925	G
1	L1	1931	C
1	L1	1932	A
1	L1	1936	C
1	L1	1939	A
1	L1	1940	G
1	L1	1948	G
1	L1	1951	G
1	L1	1959	U
1	L1	1961	G
1	L1	1962	A
1	L1	1974	U
1	L1	1975	G
1	L1	1978	C
1	L1	1982	G
1	L1	1984	A
1	L1	1985	G
1	L1	1986	U
1	L1	1987	C
1	L1	1988	G
1	L1	1989	G
1	L1	1990	A
1	L1	1993	C
1	L1	1997	U
1	L1	1998	A
1	L1	2001	G

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Mol	Chain	Res	Type
1	L1	2002	A
1	L1	2003	G
1	L1	2004	U
1	L1	2011	C
1	L1	2017	A
1	L1	2018	C
1	L1	2026	A
1	L1	2046	G
1	L1	2048	U
1	L1	2052	G
1	L1	2055	G
1	L1	2056	G
1	L1	2069	A
1	L1	2084	C
1	L1	2085	G
1	L1	2090	U
1	L1	2092	G
1	L1	2093	A
1	L1	2094	G
1	L1	2095	A
1	L1	2097	U
1	L1	2098	G
1	L1	2100	A
1	L1	2101	C
1	L1	2102	G
1	L1	2110	C
1	L1	2112	G
1	L1	2252	G
1	L1	2253	A
1	L1	2256	C
1	L1	2258	C
1	L1	2289	C
1	L1	2300	A
1	L1	2301	G
1	L1	2313	A
1	L1	2316	G
1	L1	2333	G
1	L1	2348	G
1	L1	2351	OMC
1	L1	2357	G
1	L1	2360	A
1	L1	2382	A

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Mol	Chain	Res	Type
1	L1	2395	A
1	L1	2396	A
1	L1	2397	G
1	L1	2408	U
1	L1	2410	C
1	L1	2417	A
1	L1	2421	G
1	L1	2422	OMC
1	L1	2424	OMG
1	L1	2425	U
1	L1	2450	G
1	L1	2453	A
1	L1	2464	C
1	L1	2465	C
1	L1	2471	G
1	L1	2474	G
1	L1	2475	G
1	L1	2478	C
1	L1	2479	G
1	L1	2483	G
1	L1	2484	A
1	L1	2485	U
1	L1	2486	G
1	L1	2487	G
1	L1	2489	C
1	L1	2490	U
1	L1	2491	C
1	L1	2493	G
1	L1	2503	G
1	L1	2504	C
1	L1	2505	C
1	L1	2506	G
1	L1	2513	A
1	L1	2519	U
1	L1	2537	A
1	L1	2544	G
1	L1	2546	G
1	L1	2547	G
1	L1	2554	U
1	L1	2555	G
1	L1	2565	A
1	L1	2573	A

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Mol	Chain	Res	Type
1	L1	2583	C
1	L1	2587	A
1	L1	2589	C
1	L1	2601	A
1	L1	2618	G
1	L1	2627	C
1	L1	2638	G
1	L1	2653	C
1	L1	2662	G
1	L1	2669	C
1	L1	2670	C
1	L1	2687	U
1	L1	2694	G
1	L1	2695	A
1	L1	2696	A
1	L1	2710	C
1	L1	2711	G
1	L1	2725	A
1	L1	2726	G
1	L1	2739	C
1	L1	2743	A
1	L1	2754	G
1	L1	2756	G
1	L1	2761	U
1	L1	2763	U
1	L1	2764	A
1	L1	2769	U
1	L1	2770	C
1	L1	2788	U
1	L1	2790	U
1	L1	2794	C
1	L1	2814	C
1	L1	2825	A
1	L1	2826	U
1	L1	2827	G
1	L1	2838	G
1	L1	2855	G
1	L1	2867	C
1	L1	2892	C
1	L1	2899	C
1	L1	2900	U
1	L1	2902	G

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Mol	Chain	Res	Type
1	L1	2903	G
1	L1	2906	G
1	L1	2907	G
1	L1	2908	U
1	L1	2909	C
1	L1	2910	G
1	L1	3585	G
1	L1	3587	C
1	L1	3588	C
1	L1	3591	C
1	L1	3593	C
1	L1	3594	C
1	L1	3595	U
1	L1	3596	A
1	L1	3597	G
1	L1	3604	A
1	L1	3615	G
1	L1	3618	C
1	L1	3626	G
1	L1	3630	A
1	L1	3635	A
1	L1	3644	U
1	L1	3646	A
1	L1	3648	A
1	L1	3662	A
1	L1	3664	G
1	L1	3673	C
1	L1	3674	G
1	L1	3711	A
1	L1	3713	U
1	L1	3714	G
1	L1	3727	A
1	L1	3729	PSU
1	L1	3748	A
1	L1	3750	G
1	L1	3753	G
1	L1	3754	G
1	L1	3760	A
1	L1	3764	PSU
1	L1	3771	C
1	L1	3775	A
1	L1	3776	G

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Mol	Chain	Res	Type
1	L1	3777	G
1	L1	3784	A
1	L1	3785	A2M
1	L1	3786	U
1	L1	3802	U
1	L1	3808	OMC
1	L1	3811	G
1	L1	3814	U
1	L1	3817	A
1	L1	3818	UY1
1	L1	3819	G
1	L1	3838	U
1	L1	3840	U
1	L1	3867	A2M
1	L1	3868	G
1	L1	3876	A
1	L1	3877	A
1	L1	3878	C
1	L1	3879	G
1	L1	3897	G
1	L1	3898	G
1	L1	3900	G
1	L1	3901	A
1	L1	3906	A
1	L1	3907	G
1	L1	3908	A
1	L1	3915	U
1	L1	3930	U
1	L1	3944	OMG
1	L1	3947	A
1	L1	3949	A
1	L1	3950	U
1	L1	3951	G
1	L1	3952	A
1	L1	3955	G
1	L1	3956	G
1	L1	3957	U
1	L1	3958	G
1	L1	3959	U
1	L1	3960	A
1	L1	3963	A
1	L1	3964	U

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Mol	Chain	Res	Type
1	L1	3965	A
1	L1	3966	A
1	L1	3967	G
1	L1	3969	G
1	L1	3970	G
1	L1	3971	G
1	L1	3972	A
1	L1	3973	G
1	L1	3974	G
1	L1	3975	C
1	L1	3977	C
1	L1	4035	G
1	L1	4036	G
1	L1	4041	C
1	L1	4042	G
1	L1	4043	G
1	L1	4044	U
1	L1	4046	A
1	L1	4048	A
1	L1	4049	U
1	L1	4051	C
1	L1	4052	C
1	L1	4053	A
1	L1	4054	C
1	L1	4055	U
1	L1	4056	A
1	L1	4059	C
1	L1	4062	A
1	L1	4064	C
1	L1	4069	U
1	L1	4073	A
1	L1	4076	G
1	L1	4086	G
1	L1	4091	G
1	L1	4094	G
1	L1	4095	G
1	L1	4099	G
1	L1	4100	C
1	L1	4102	C
1	L1	4103	C
1	L1	4104	G
1	L1	4107	G

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Mol	Chain	Res	Type
1	L1	4112	C
1	L1	4113	U
1	L1	4114	C
1	L1	4115	G
1	L1	4116	C
1	L1	4117	U
1	L1	4119	C
1	L1	4122	G
1	L1	4127	A
1	L1	4133	C
1	L1	4139	G
1	L1	4140	C
1	L1	4141	G
1	L1	4142	C
1	L1	4143	G
1	L1	4160	C
1	L1	4162	C
1	L1	4163	U
1	L1	4168	G
1	L1	4170	A
1	L1	4183	G
1	L1	4184	G
1	L1	4191	G
1	L1	4203	A
1	L1	4222	G
1	L1	4229	U
1	L1	4233	A
1	L1	4251	A
1	L1	4254	G
1	L1	4265	U
1	L1	4266	G
1	L1	4268	A
1	L1	4273	A
1	L1	4281	A
1	L1	4291	G
1	L1	4304	A
1	L1	4305	G
1	L1	4329	G
1	L1	4330	G
1	L1	4332	C
1	L1	4339	A
1	L1	4349	C

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Mol	Chain	Res	Type
1	L1	4350	C
1	L1	4373	G
1	L1	4376	A
1	L1	4377	G
1	L1	4378	A
1	L1	4379	A
1	L1	4381	A
1	L1	4382	G
1	L1	4387	C
1	L1	4391	G
1	L1	4393	G
1	L1	4394	A
1	L1	4422	A
1	L1	4444	C
1	L1	4448	G
1	L1	4449	A
1	L1	4452	U
1	L1	4453	C
1	L1	4464	A
1	L1	4466	C
1	L1	4475	G
1	L1	4500	PSU
1	L1	4512	U
1	L1	4513	A
1	L1	4518	A
1	L1	4519	C
1	L1	4524	G
1	L1	4528	G
1	L1	4548	A
1	L1	4549	G
1	L1	4554	G
1	L1	4560	C
1	L1	4567	G
1	L1	4570	G
1	L1	4573	G
1	L1	4575	G
1	L1	4590	A
1	L1	4636	PSU
1	L1	4637	OMG
1	L1	4647	G
1	L1	4652	G
1	L1	4656	A

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Mol	Chain	Res	Type
1	L1	4657	U
1	L1	4670	C
1	L1	4672	A
1	L1	4679	G
1	L1	4687	A
1	L1	4695	C
1	L1	4700	A
1	L1	4708	A
1	L1	4709	U
1	L1	4719	G
1	L1	4720	C
1	L1	4732	G
1	L1	4734	A
1	L1	4741	C
1	L1	4742	G
1	L1	4745	G
1	L1	4747	C
1	L1	4754	G
1	L1	4757	C
1	L1	4759	C
1	L1	4761	G
1	L1	4765	G
1	L1	4772	C
1	L1	4773	C
1	L1	4775	C
1	L1	4776	G
1	L1	4859	C
1	L1	4870	G
1	L1	4871	C
1	L1	4875	G
1	L1	4882	U
1	L1	4883	C
1	L1	4889	G
1	L1	4895	C
1	L1	4896	G
1	L1	4900	C
1	L1	4901	G
1	L1	4910	G
1	L1	4912	G
1	L1	4923	C
1	L1	4926	C
1	L1	4928	C

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Mol	Chain	Res	Type
1	L1	4934	A
1	L1	4938	A
1	L1	4940	C
1	L1	4941	G
1	L1	4943	A
1	L1	4944	C
1	L1	4951	G
1	L1	4960	G
1	L1	4964	C
1	L1	4966	A
1	L1	4976	U
1	L1	4979	A
1	L1	4988	U
1	L1	4989	U
1	L1	4991	U
1	L1	5013	C
1	L1	5017	G
1	L1	5022	U
1	L1	5023	C
1	L1	5024	C
1	L1	5025	C
1	L1	5026	U
1	L1	5030	U
1	L1	5034	A
1	L1	5041	G
1	L1	5050	C
1	L1	5054	C
1	L1	5061	A
1	L1	5069	U
2	L2	22	A
2	L2	24	C
2	L2	33	U
2	L2	48	G
2	L2	53	U
2	L2	54	A
2	L2	63	C
2	L2	64	G
2	L2	97	G
2	L2	100	A
2	L2	111	C
3	L3	2	G
3	L3	23	C

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Mol	Chain	Res	Type
3	L3	34	U
3	L3	35	C
3	L3	38	U
3	L3	48	A
3	L3	52	A
3	L3	59	A
3	L3	60	G
3	L3	62	A
3	L3	63	U
3	L3	79	G
3	L3	80	A
3	L3	81	C
3	L3	82	A
3	L3	83	C
3	L3	84	A
3	L3	85	U
3	L3	86	U
3	L3	87	G
3	L3	94	G
3	L3	103	A
3	L3	105	C
3	L3	108	A
3	L3	110	U
3	L3	111	U
3	L3	112	G
3	L3	114	G
3	L3	123	U
3	L3	124	U
3	L3	125	C
3	L3	126	C
3	L3	127	U
3	L3	147	G
45	S2	4	C
45	S2	33	G
45	S2	41	G
45	S2	44	U
45	S2	46	A
45	S2	56	G
45	S2	58	C
45	S2	59	U
45	S2	62	G
45	S2	64	A

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Mol	Chain	Res	Type
45	S2	65	C
45	S2	67	C
45	S2	68	A
45	S2	72	C
45	S2	73	C
45	S2	74	G
45	S2	76	U
45	S2	99	A2M
45	S2	103	A
45	S2	113	G
45	S2	114	G
45	S2	115	U
45	S2	126	G
45	S2	130	G
45	S2	143	U
45	S2	149	A
45	S2	160	U
45	S2	162	C
45	S2	163	U
45	S2	171	A
45	S2	175	A
45	S2	184	G
45	S2	194	C
45	S2	196	C
45	S2	197	U
45	S2	198	U
45	S2	200	G
45	S2	203	G
45	S2	204	G
45	S2	311	C
45	S2	318	A
45	S2	319	C
45	S2	323	C
45	S2	324	C
45	S2	325	C
45	S2	326	C
45	S2	328	U
45	S2	329	G
45	S2	332	G
45	S2	351	G
45	S2	360	A
45	S2	362	C

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Mol	Chain	Res	Type
45	S2	364	A
45	S2	370	G
45	S2	385	G
45	S2	386	C
45	S2	407	G
45	S2	408	A
45	S2	409	C
45	S2	418	A
45	S2	420	G
45	S2	421	G
45	S2	438	G
45	S2	448	A
45	S2	449	A
45	S2	450	C
45	S2	452	G
45	S2	464	A
45	S2	471	G
45	S2	472	C
45	S2	473	A
45	S2	474	G
45	S2	476	A
45	S2	482	G
45	S2	487	U
45	S2	488	U
45	S2	492	C
45	S2	493	A
45	S2	500	A
45	S2	512	A2M
45	S2	516	A
45	S2	517	OMC
45	S2	525	A
45	S2	531	A
45	S2	532	C
45	S2	536	A
45	S2	537	C
45	S2	540	U
45	S2	544	G
45	S2	546	G
45	S2	547	G
45	S2	551	U
45	S2	554	A
45	S2	555	A

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Mol	Chain	Res	Type
45	S2	556	U
45	S2	557	U
45	S2	558	G
45	S2	559	G
45	S2	560	A
45	S2	563	G
45	S2	564	A
45	S2	576	A2M
45	S2	583	A
45	S2	587	A
45	S2	589	G
45	S2	590	A2M
45	S2	591	U
45	S2	594	A
45	S2	597	G
45	S2	598	G
45	S2	606	G
45	S2	607	U
45	S2	614	C
45	S2	617	G
45	S2	628	A
45	S2	629	A
45	S2	631	U
45	S2	643	A
45	S2	655	A
45	S2	660	C
45	S2	664	A
45	S2	668	A2M
45	S2	669	A
45	S2	671	A
45	S2	672	A
45	S2	673	G
45	S2	678	U
45	S2	683	OMG
45	S2	688	U
45	S2	689	U
45	S2	690	G
45	S2	692	G
45	S2	696	G
45	S2	698	G
45	S2	732	U
45	S2	733	C

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Mol	Chain	Res	Type
45	S2	735	C
45	S2	736	C
45	S2	738	C
45	S2	739	C
45	S2	748	C
45	S2	750	C
45	S2	751	G
45	S2	752	G
45	S2	753	C
45	S2	789	G
45	S2	791	C
45	S2	794	A
45	S2	797	C
45	S2	798	G
45	S2	799	U
45	S2	811	A
45	S2	821	G
45	S2	822	PSU
45	S2	830	A
45	S2	835	C
45	S2	836	G
45	S2	837	A
45	S2	838	G
45	S2	839	C
45	S2	840	C
45	S2	841	G
45	S2	842	C
45	S2	847	A
45	S2	867	OMG
45	S2	868	G
45	S2	869	A
45	S2	870	A
45	S2	872	A
45	S2	874	G
45	S2	877	C
45	S2	884	C
45	S2	888	U
45	S2	889	U
45	S2	891	G
45	S2	892	U
45	S2	896	U
45	S2	898	U

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Mol	Chain	Res	Type
45	S2	899	U
45	S2	900	C
45	S2	901	G
45	S2	903	A
45	S2	904	A
45	S2	909	G
45	S2	913	A
45	S2	917	U
45	S2	920	A
45	S2	922	A
45	S2	930	C
45	S2	933	G
45	S2	934	G
45	S2	943	U
45	S2	950	C
45	S2	955	A
45	S2	962	A
45	S2	963	A
45	S2	990	A
45	S2	992	A
45	S2	999	G
45	S2	1001	A
45	S2	1017	U
45	S2	1023	A
45	S2	1027	A
45	S2	1028	A
45	S2	1033	G
45	S2	1061	U
45	S2	1062	A
45	S2	1067	C
45	S2	1083	A
45	S2	1085	C
45	S2	1109	C
45	S2	1114	U
45	S2	1116	C
45	S2	1118	C
45	S2	1133	A
45	S2	1138	C
45	S2	1140	G
45	S2	1153	C
45	S2	1154	U
45	S2	1195	A

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Mol	Chain	Res	Type
45	S2	1207	G
45	S2	1208	A
45	S2	1215	C
45	S2	1216	C
45	S2	1217	A
45	S2	1224	G
45	S2	1242	U
45	S2	1243	PSU
45	S2	1248	B8N
45	S2	1251	A
45	S2	1253	A
45	S2	1256	G
45	S2	1257	G
45	S2	1259	A
45	S2	1264	C
45	S2	1265	A
45	S2	1274	G
45	S2	1275	G
45	S2	1284	A
45	S2	1285	G
45	S2	1286	G
45	S2	1300	U
45	S2	1301	A
45	S2	1302	G
45	S2	1303	C
45	S2	1308	U
45	S2	1313	A
45	S2	1322	G
45	S2	1342	U
45	S2	1343	U
45	S2	1348	G
45	S2	1371	U
45	S2	1372	U
45	S2	1373	C
45	S2	1378	A
45	S2	1382	A
45	S2	1397	U
45	S2	1402	A
45	S2	1404	U
45	S2	1406	G
45	S2	1421	A
45	S2	1423	C

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Mol	Chain	Res	Type
45	S2	1434	C
45	S2	1435	C
45	S2	1436	C
45	S2	1438	A
45	S2	1442	OMU
45	S2	1447	OMG
45	S2	1454	A
45	S2	1462	U
45	S2	1463	U
45	S2	1480	A
45	S2	1487	A
45	S2	1489	A
45	S2	1490	OMG
45	S2	1494	U
45	S2	1495	G
45	S2	1497	G
45	S2	1498	A
45	S2	1508	A
45	S2	1521	C
45	S2	1522	A
45	S2	1531	A
45	S2	1533	A
45	S2	1553	C
45	S2	1556	A
45	S2	1578	U
45	S2	1580	A
45	S2	1585	U
45	S2	1587	G
45	S2	1588	A
45	S2	1601	A
45	S2	1606	G
45	S2	1621	U
45	S2	1623	A
45	S2	1648	G
45	S2	1654	G
45	S2	1664	A
45	S2	1665	G
45	S2	1686	G
45	S2	1698	C
45	S2	1699	A
45	S2	1721	U
45	S2	1722	G

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Mol	Chain	Res	Type
45	S2	1742	C
45	S2	1744	G
45	S2	1752	C
45	S2	1753	C
45	S2	1754	G
45	S2	1758	G
45	S2	1760	G
45	S2	1761	U
45	S2	1773	C
45	S2	1774	C
45	S2	1775	U
45	S2	1777	G
45	S2	1781	A
45	S2	1782	G
45	S2	1783	C
45	S2	1784	G
45	S2	1786	U
45	S2	1824	A
45	S2	1825	A
45	S2	1829	G
45	S2	1831	A
45	S2	1835	A
45	S2	1838	U
45	S2	1849	G
45	S2	1851	MA6
45	S2	1852	C
45	S2	1861	G
45	S2	1862	G
45	S2	1863	A
45	S2	1864	U
45	S2	1865	C
79	CC	15	A
79	CC	16	C
79	CC	17	G
79	CC	18	G
79	CC	19	C
79	CC	20	U
79	CC	21	A
79	CC	28	C
79	CC	32	C
79	CC	33	U
79	CC	35	U

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Mol	Chain	Res	Type
79	CC	36	C
79	CC	37	A
79	CC	39	C
79	CC	42	G
79	CC	45	G
79	CC	46	A
79	CC	47	C
79	CC	48	C
79	CC	57	A
79	CC	58	C
79	CC	72	G
79	CC	75	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	406	C
1	L1	914	U
1	L1	1082	C
1	L1	1590	C
1	L1	1613	A
1	L1	1625	OMG
1	L1	1633	G
1	L1	2760	G
1	L1	3614	G
1	L1	3673	C
1	L1	3878	C
1	L1	4699	U
45	S2	112	U
45	S2	563	G
45	S2	628	A
45	S2	688	U
45	S2	867	OMG
45	S2	954	U
45	S2	1434	C
45	S2	1446	A
45	S2	1520	G
79	CC	35	U
79	CC	74	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMG	L1	4196	1	23,26,27	2.36	9 (39%)	33,38,41	1.96	10 (30%)
45	OMU	S2	1442	45,80	19,22,23	2.94	7 (36%)	26,31,34	1.66	4 (15%)
1	OMU	L1	4498	1	19,22,23	2.85	7 (36%)	26,31,34	1.78	4 (15%)
45	OMC	S2	1391	45	19,22,23	3.02	8 (42%)	26,31,34	0.85	1 (3%)
1	5MC	L1	4335	1	18,22,23	3.51	7 (38%)	26,32,35	0.99	2 (7%)
45	OMU	S2	116	45	19,22,23	2.83	6 (31%)	26,31,34	1.71	5 (19%)
1	OMC	L1	3869	1	19,22,23	2.94	8 (42%)	26,31,34	0.74	0
45	OMU	S2	354	45	19,22,23	2.89	7 (36%)	26,31,34	1.80	5 (19%)
1	A2M	L1	3867	1	22,25,26	3.37	9 (40%)	31,36,39	2.73	10 (32%)
45	OMG	S2	436	45	23,26,27	2.42	8 (34%)	33,38,41	2.04	10 (30%)
45	OMG	S2	683	45	23,26,27	2.42	8 (34%)	33,38,41	2.09	10 (30%)
45	5MC	S2	1374	45	18,22,23	3.53	7 (38%)	26,32,35	1.02	2 (7%)
1	A2M	L1	1326	1	22,25,26	3.34	8 (36%)	31,36,39	2.58	9 (29%)
1	6MZ	L1	4220	1	22,25,26	2.64	3 (13%)	30,36,39	2.20	8 (26%)
1	OMC	L1	3808	1,80	19,22,23	2.94	8 (42%)	26,31,34	1.04	1 (3%)
1	PSU	L1	4450	1,80	18,21,22	1.11	1 (5%)	22,30,33	1.83	3 (13%)
45	A2M	S2	99	45,80	22,25,26	3.43	10 (45%)	31,36,39	2.59	9 (29%)
1	A2M	L1	2787	1	22,25,26	3.45	8 (36%)	31,36,39	2.63	9 (29%)
1	OMC	L1	4536	1	19,22,23	2.91	8 (42%)	26,31,34	0.75	0
1	OMG	L1	1522	1	23,26,27	2.42	9 (39%)	33,38,41	2.09	12 (36%)
1	OMC	L1	2824	1	19,22,23	2.93	8 (42%)	26,31,34	0.99	2 (7%)
1	OMG	L1	3627	1	23,26,27	2.42	8 (34%)	33,38,41	2.08	10 (30%)
1	OMG	L1	1625	1	23,26,27	1.32	3 (13%)	33,38,41	1.93	6 (18%)
45	PSU	S2	1081	45	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
1	A2M	L1	400	1	22,25,26	3.43	9 (40%)	31,36,39	2.66	8 (25%)
1	A2M	L1	398	1	22,25,26	3.44	9 (40%)	31,36,39	2.69	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L1	4637	1	23,26,27	2.37	7 (30%)	33,38,41	2.02	10 (30%)
1	OMG	L1	4618	1	23,26,27	2.40	7 (30%)	33,38,41	2.06	10 (30%)
45	A2M	S2	27	45,80	22,25,26	3.43	9 (40%)	31,36,39	2.68	9 (29%)
1	A2M	L1	1534	1,80	22,25,26	3.47	10 (45%)	31,36,39	2.65	8 (25%)
1	PSU	L1	1582	1	18,21,22	1.07	1 (5%)	22,30,33	1.57	4 (18%)
1	OMG	L1	3944	1	23,26,27	2.45	8 (34%)	33,38,41	2.02	10 (30%)
1	OMU	L1	4227	1	19,22,23	2.82	7 (36%)	26,31,34	1.72	4 (15%)
1	OMC	L1	1881	1,80	19,22,23	2.93	8 (42%)	26,31,34	0.95	0
1	OMC	L1	2861	1	19,22,23	2.93	8 (42%)	26,31,34	0.72	0
1	UR3	L1	4530	1	19,22,23	2.75	8 (42%)	26,32,35	1.44	3 (11%)
45	PSU	S2	119	45	18,21,22	0.97	1 (5%)	22,30,33	1.63	4 (18%)
1	OMG	L1	2424	1	23,26,27	2.41	9 (39%)	33,38,41	1.99	10 (30%)
1	OMG	L1	3899	1,80	23,26,27	2.41	9 (39%)	33,38,41	2.10	10 (30%)
45	OMC	S2	1272	45	19,22,23	3.06	8 (42%)	26,31,34	0.81	0
45	OMG	S2	1447	45	23,26,27	1.23	3 (13%)	33,38,41	2.17	9 (27%)
1	A2M	L1	3830	1	22,25,26	3.39	9 (40%)	31,36,39	2.78	10 (32%)
1	UY1	L1	3818	1,80,81	19,22,23	4.44	12 (63%)	22,31,34	2.02	4 (18%)
1	PSU	L1	4531	1	18,21,22	1.00	1 (5%)	22,30,33	1.70	4 (18%)
45	OMC	S2	1703	45	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
1	OMG	L1	4623	1	23,26,27	2.38	9 (39%)	33,38,41	2.08	10 (30%)
45	OMU	S2	172	45	19,22,23	2.88	6 (31%)	26,31,34	1.76	5 (19%)
1	OMG	L1	4494	1	23,26,27	2.36	8 (34%)	33,38,41	2.04	9 (27%)
45	6MZ	S2	1832	45,80	22,25,26	2.88	4 (18%)	30,36,39	2.24	10 (33%)
45	M7A	S2	1806	45	20,25,26	1.86	5 (25%)	28,37,40	3.94	8 (28%)
1	2MG	L1	729	1	23,26,27	2.60	9 (39%)	32,38,41	2.30	11 (34%)
45	PSU	S2	612	45	18,21,22	1.02	1 (5%)	22,30,33	1.81	5 (22%)
3	OMU	L3	14	3,1	19,22,23	2.88	6 (31%)	26,31,34	1.71	5 (19%)
45	4AC	S2	1842	45	21,24,25	3.40	10 (47%)	29,34,37	1.09	2 (6%)
45	OMG	S2	509	45,80	23,26,27	2.36	8 (34%)	33,38,41	1.95	9 (27%)
45	A2M	S2	484	45	22,25,26	3.40	9 (40%)	31,36,39	2.63	10 (32%)
1	A2M	L1	2363	1,80	22,25,26	3.46	9 (40%)	31,36,39	2.70	8 (25%)
1	PSU	L1	4403	1	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
45	A2M	S2	1383	45	22,25,26	3.38	8 (36%)	31,36,39	2.73	8 (25%)
1	PSU	L1	3729	1	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
45	OMC	S2	1710	45	19,22,23	3.04	8 (42%)	26,31,34	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	JMH	S2	1219	45,80	18,22,23	2.84	5 (27%)	21,32,35	1.74	4 (19%)
1	B8T	L1	4671	1	19,22,23	3.21	8 (42%)	26,31,34	0.98	1 (3%)
1	OMG	L1	2876	1	23,26,27	2.42	8 (34%)	33,38,41	2.12	8 (24%)
3	OMG	L3	75	3	23,26,27	2.42	8 (34%)	33,38,41	2.03	10 (30%)
1	A2M	L1	4523	1,80	22,25,26	3.37	9 (40%)	31,36,39	2.61	9 (29%)
45	5MU	S2	814	45	19,22,23	7.26	8 (42%)	28,32,35	3.30	12 (42%)
1	B8H	L1	3762	1	19,22,23	6.72	6 (31%)	22,32,35	2.39	5 (22%)
45	OMG	S2	601	45	23,26,27	2.39	8 (34%)	33,38,41	2.02	10 (30%)
1	OMG	L1	1316	1,80	23,26,27	2.41	7 (30%)	33,38,41	2.04	10 (30%)
45	OMG	S2	867	45	23,26,27	2.43	8 (34%)	33,38,41	2.01	9 (27%)
1	PSU	L1	3764	1	18,21,22	1.02	1 (5%)	22,30,33	1.65	4 (18%)
1	A2M	L1	3718	1	22,25,26	3.42	9 (40%)	31,36,39	2.51	10 (32%)
1	JMH	L1	1456	1	18,22,23	2.64	5 (27%)	21,32,35	0.91	1 (4%)
45	A2M	S2	468	45	22,25,26	3.41	10 (45%)	31,36,39	2.69	10 (32%)
45	A2M	S2	166	45	22,25,26	3.42	9 (40%)	31,36,39	2.72	8 (25%)
45	OMC	S2	462	45	19,22,23	2.97	8 (42%)	26,31,34	0.75	0
1	OMG	L1	4228	1	23,26,27	2.39	9 (39%)	33,38,41	2.05	10 (30%)
45	PSU	S2	823	45	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
45	OMU	S2	428	45	19,22,23	2.92	7 (36%)	26,31,34	1.71	4 (15%)
45	A2M	S2	1678	45	22,25,26	3.47	9 (40%)	31,36,39	2.73	11 (35%)
1	PSU	L1	1677	1,81	18,21,22	1.16	2 (11%)	22,30,33	1.94	5 (22%)
45	A2M	S2	159	45	22,25,26	3.43	9 (40%)	31,36,39	2.73	10 (32%)
1	A2M	L1	3723	1	22,25,26	3.43	9 (40%)	31,36,39	2.61	9 (29%)
1	OMU	L1	3925	1	19,22,23	2.85	6 (31%)	26,31,34	1.92	5 (19%)
45	OMU	S2	1288	45	19,22,23	2.94	8 (42%)	26,31,34	1.64	4 (15%)
1	PSU	L1	2508	1	18,21,22	1.04	1 (5%)	22,30,33	1.70	3 (13%)
1	A2M	L1	1524	1	22,25,26	3.41	10 (45%)	31,36,39	2.70	11 (35%)
1	OMC	L1	2365	1,80	19,22,23	2.90	8 (42%)	26,31,34	0.62	0
45	4AC	S2	1337	45	21,24,25	3.51	10 (47%)	29,34,37	1.07	2 (6%)
1	A2M	L1	4571	1	22,25,26	3.45	9 (40%)	31,36,39	2.59	8 (25%)
45	OMG	S2	1490	45,80	23,26,27	2.42	8 (34%)	33,38,41	1.92	9 (27%)
1	A2M	L1	2815	1	22,25,26	3.41	10 (45%)	31,36,39	2.65	8 (25%)
1	A2M	L1	1871	1,80	22,25,26	3.44	10 (45%)	31,36,39	2.72	11 (35%)
1	PSU	L1	4628	1	18,21,22	0.92	1 (5%)	22,30,33	1.69	3 (13%)
45	OMG	S2	1328	45	23,26,27	2.44	8 (34%)	33,38,41	2.01	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PSU	S2	1243	45	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
1	2MG	L1	978	1	23,26,27	2.65	9 (39%)	32,38,41	2.32	12 (37%)
1	OMU	L1	2837	1	19,22,23	2.84	6 (31%)	26,31,34	1.73	5 (19%)
45	OMG	S2	644	45	23,26,27	2.41	8 (34%)	33,38,41	2.00	10 (30%)
45	UY1	S2	1326	45,80	19,22,23	4.33	10 (52%)	22,31,34	1.84	3 (13%)
1	OMC	L1	3841	1	19,22,23	2.94	8 (42%)	26,31,34	0.91	1 (3%)
1	OMC	L1	3701	1,80	19,22,23	2.88	8 (42%)	26,31,34	0.84	0
1	OMU	L1	4306	1	19,22,23	2.79	6 (31%)	26,31,34	1.66	4 (15%)
1	5MC	L1	4447	1,80	18,22,23	3.41	7 (38%)	26,32,35	1.15	2 (7%)
42	MLZ	Lo	53	42	8,9,10	0.68	0	4,9,11	0.58	0
45	PSU	S2	822	45	18,21,22	1.05	1 (5%)	22,30,33	1.77	5 (22%)
45	A2M	S2	1031	45	22,25,26	3.38	10 (45%)	31,36,39	2.63	9 (29%)
1	OMG	L1	4499	1	23,26,27	2.41	8 (34%)	33,38,41	2.06	10 (30%)
45	MA6	S2	1851	45	23,26,27	1.31	4 (17%)	34,38,41	4.59	12 (35%)
1	OMG	L1	3792	1	23,26,27	2.40	8 (34%)	33,38,41	2.00	10 (30%)
1	A2M	L1	3825	1	22,25,26	3.41	9 (40%)	31,36,39	2.68	8 (25%)
1	PSU	L1	4636	1	18,21,22	1.09	1 (5%)	22,30,33	1.93	5 (22%)
1	OMG	L1	4370	1	23,26,27	2.37	8 (34%)	33,38,41	1.98	9 (27%)
1	OMU	L1	4620	1	19,22,23	2.80	7 (36%)	26,31,34	1.65	4 (15%)
1	OMC	L1	2804	1	19,22,23	2.89	7 (36%)	26,31,34	0.90	0
45	OMC	S2	174	45,80	19,22,23	3.01	8 (42%)	26,31,34	0.75	0
1	A2M	L1	2401	1	22,25,26	3.38	10 (45%)	31,36,39	2.69	9 (29%)
45	A2M	S2	590	45	22,25,26	3.39	9 (40%)	31,36,39	2.82	9 (29%)
1	1MA	L1	1322	1,80	21,25,26	2.66	6 (28%)	31,37,40	2.24	7 (22%)
1	PSU	L1	4500	1	18,21,22	0.98	1 (5%)	22,30,33	1.76	4 (18%)
45	OMU	S2	121	45	19,22,23	2.84	6 (31%)	26,31,34	1.58	4 (15%)
1	OMC	L1	2422	1,80	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
1	PSU	L1	3715	1	18,21,22	1.10	1 (5%)	22,30,33	1.84	5 (22%)
1	A2M	L1	3785	1	22,25,26	3.31	10 (45%)	31,36,39	2.90	10 (32%)
1	OMG	L1	3744	1	23,26,27	2.36	8 (34%)	33,38,41	2.02	10 (30%)
1	OMG	L1	2364	1,80	23,26,27	2.34	9 (39%)	33,38,41	2.06	13 (39%)
1	OMC	L1	4456	1	19,22,23	2.88	8 (42%)	26,31,34	0.86	0
45	A2M	S2	668	45,80	22,25,26	3.42	10 (45%)	31,36,39	2.73	12 (38%)
1	OMC	L1	2351	1	19,22,23	2.87	8 (42%)	26,31,34	1.25	3 (11%)
1	OMC	L1	3887	1	19,22,23	2.92	8 (42%)	26,31,34	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A2M	S2	576	45	22,25,26	3.40	9 (40%)	31,36,39	2.67	9 (29%)
45	B8N	S2	1248	45	24,29,30	3.11	7 (29%)	29,42,45	1.75	6 (20%)
1	5MC	L1	3782	1,80	18,22,23	3.37	7 (38%)	26,32,35	1.21	3 (11%)
1	2MG	L1	1517	1	23,26,27	2.61	10 (43%)	32,38,41	2.35	12 (37%)
45	A2M	S2	512	45	22,25,26	3.41	9 (40%)	31,36,39	2.75	9 (29%)
45	UR3	S2	1830	45	19,22,23	2.76	7 (36%)	26,32,35	1.61	4 (15%)
1	PSU	L1	1683	1,81	18,21,22	1.10	1 (5%)	22,30,33	1.67	3 (13%)
1	PSU	L1	4442	1	18,21,22	1.09	1 (5%)	22,30,33	1.78	5 (22%)
1	OMC	L1	1340	1	19,22,23	2.89	8 (42%)	26,31,34	0.85	0
45	MA6	S2	1850	45	23,26,27	1.36	4 (17%)	34,38,41	4.17	13 (38%)
1	OMG	L1	4392	1	23,26,27	2.43	7 (30%)	33,38,41	2.03	10 (30%)
1	PSU	L1	4293	1	18,21,22	1.00	1 (5%)	22,30,33	1.68	3 (13%)
45	OMC	S2	517	45	19,22,23	2.98	8 (42%)	26,31,34	0.78	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
1	OMG	L1	4196	1	-	1/9/27/28	0/3/3/3
45	OMU	S2	1442	45,80	-	3/9/27/28	0/2/2/2
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
45	OMC	S2	1391	45	-	2/9/27/28	0/2/2/2
1	5MC	L1	4335	1	-	0/7/25/26	0/2/2/2
45	OMU	S2	116	45	-	0/9/27/28	0/2/2/2
1	OMC	L1	3869	1	-	1/9/27/28	0/2/2/2
45	OMU	S2	354	45	-	0/9/27/28	0/2/2/2
1	A2M	L1	3867	1	-	2/9/27/28	0/3/3/3
45	OMG	S2	436	45	-	0/9/27/28	0/3/3/3
45	OMG	S2	683	45	-	2/9/27/28	0/3/3/3
45	5MC	S2	1374	45	-	0/7/25/26	0/2/2/2
1	A2M	L1	1326	1	-	1/9/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	3808	1,80	-	2/9/27/28	0/2/2/2
1	PSU	L1	4450	1,80	-	1/7/25/26	0/2/2/2
45	A2M	S2	99	45,80	-	2/9/27/28	0/3/3/3
1	A2M	L1	2787	1	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	L1	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	1522	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	2824	1	-	2/9/27/28	0/2/2/2
1	OMG	L1	3627	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	1625	1	-	0/9/27/28	0/3/3/3
45	PSU	S2	1081	45	-	1/7/25/26	0/2/2/2
1	A2M	L1	400	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	398	1	-	2/9/27/28	0/3/3/3
1	OMG	L1	4637	1	-	1/9/27/28	0/3/3/3
1	OMG	L1	4618	1	-	0/9/27/28	0/3/3/3
45	A2M	S2	27	45,80	-	0/9/27/28	0/3/3/3
1	A2M	L1	1534	1,80	-	3/9/27/28	0/3/3/3
1	PSU	L1	1582	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	3944	1	-	2/9/27/28	0/3/3/3
1	OMU	L1	4227	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	1881	1,80	-	0/9/27/28	0/2/2/2
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
45	PSU	S2	119	45	-	0/7/25/26	0/2/2/2
1	OMG	L1	2424	1	-	2/9/27/28	0/3/3/3
1	OMG	L1	3899	1,80	-	0/9/27/28	0/3/3/3
45	OMC	S2	1272	45	-	0/9/27/28	0/2/2/2
45	OMG	S2	1447	45	-	1/9/27/28	0/3/3/3
1	A2M	L1	3830	1	-	0/9/27/28	0/3/3/3
1	UY1	L1	3818	1,80,81	-	4/9/27/28	0/2/2/2
1	PSU	L1	4531	1	-	0/7/25/26	0/2/2/2
45	OMC	S2	1703	45	-	0/9/27/28	0/2/2/2
1	OMG	L1	4623	1	-	0/9/27/28	0/3/3/3
45	OMU	S2	172	45	-	0/9/27/28	0/2/2/2
1	OMG	L1	4494	1	-	0/9/27/28	0/3/3/3
45	6MZ	S2	1832	45,80	-	2/9/27/28	0/3/3/3
45	M7A	S2	1806	45	-	0/7/37/38	0/3/3/3
1	2MG	L1	729	1	-	1/9/27/28	0/3/3/3
45	PSU	S2	612	45	-	0/7/25/26	0/2/2/2
3	OMU	L3	14	3,1	-	1/9/27/28	0/2/2/2
45	4AC	S2	1842	45	-	0/11/29/30	0/2/2/2
45	OMG	S2	509	45,80	-	0/9/27/28	0/3/3/3
45	A2M	S2	484	45	-	0/9/27/28	0/3/3/3
1	A2M	L1	2363	1,80	-	1/9/27/28	0/3/3/3
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	1383	45	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	3729	1	-	2/7/25/26	0/2/2/2
45	OMC	S2	1710	45	-	0/9/27/28	0/2/2/2
45	JMH	S2	1219	45,80	-	2/7/25/26	0/2/2/2
1	B8T	L1	4671	1	-	1/7/27/28	0/2/2/2
1	OMG	L1	2876	1	-	0/9/27/28	0/3/3/3
3	OMG	L3	75	3	-	0/9/27/28	0/3/3/3
1	A2M	L1	4523	1,80	-	0/9/27/28	0/3/3/3
45	5MU	S2	814	45	-	0/7/25/26	0/2/2/2
1	B8H	L1	3762	1	-	0/7/25/26	0/2/2/2
45	OMG	S2	601	45	-	1/9/27/28	0/3/3/3
1	OMG	L1	1316	1,80	-	0/9/27/28	0/3/3/3
45	OMG	S2	867	45	-	3/9/27/28	0/3/3/3
1	PSU	L1	3764	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	3718	1	-	0/9/27/28	0/3/3/3
1	JMH	L1	1456	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	468	45	-	0/9/27/28	0/3/3/3
45	A2M	S2	166	45	-	0/9/27/28	0/3/3/3
45	OMC	S2	462	45	-	0/9/27/28	0/2/2/2
1	OMG	L1	4228	1	-	0/9/27/28	0/3/3/3
45	PSU	S2	823	45	-	0/7/25/26	0/2/2/2
45	OMU	S2	428	45	-	2/9/27/28	0/2/2/2
45	A2M	S2	1678	45	-	1/9/27/28	0/3/3/3
1	PSU	L1	1677	1,81	-	4/7/25/26	0/2/2/2
45	A2M	S2	159	45	-	2/9/27/28	0/3/3/3
1	A2M	L1	3723	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	3925	1	-	1/9/27/28	0/2/2/2
45	OMU	S2	1288	45	-	0/9/27/28	0/2/2/2
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1524	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	2365	1,80	-	0/9/27/28	0/2/2/2
45	4AC	S2	1337	45	-	0/11/29/30	0/2/2/2
1	A2M	L1	4571	1	-	0/9/27/28	0/3/3/3
45	OMG	S2	1490	45,80	-	1/9/27/28	0/3/3/3
1	A2M	L1	2815	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	1871	1,80	-	0/9/27/28	0/3/3/3
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
45	OMG	S2	1328	45	-	1/9/27/28	0/3/3/3
45	PSU	S2	1243	45	-	2/7/25/26	0/2/2/2
1	2MG	L1	978	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMG	S2	644	45	-	2/9/27/28	0/3/3/3
45	UY1	S2	1326	45,80	-	1/9/27/28	0/2/2/2
1	OMC	L1	3841	1	-	2/9/27/28	0/2/2/2
1	OMC	L1	3701	1,80	-	4/9/27/28	0/2/2/2
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
1	5MC	L1	4447	1,80	-	4/7/25/26	0/2/2/2
42	MLZ	Lo	53	42	-	2/7/8/10	-
45	PSU	S2	822	45	-	1/7/25/26	0/2/2/2
45	A2M	S2	1031	45	-	0/9/27/28	0/3/3/3
1	OMG	L1	4499	1	-	0/9/27/28	0/3/3/3
45	MA6	S2	1851	45	-	2/11/29/30	0/3/3/3
1	OMG	L1	3792	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4636	1	-	3/7/25/26	0/2/2/2
1	OMG	L1	4370	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	4620	1	-	1/9/27/28	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
45	OMC	S2	174	45,80	-	0/9/27/28	0/2/2/2
1	A2M	L1	2401	1	-	1/9/27/28	0/3/3/3
45	A2M	S2	590	45	-	4/9/27/28	0/3/3/3
1	1MA	L1	1322	1,80	-	2/7/25/26	0/3/3/3
1	PSU	L1	4500	1	-	3/7/25/26	0/2/2/2
45	OMU	S2	121	45	-	0/9/27/28	0/2/2/2
1	OMC	L1	2422	1,80	-	1/9/27/28	0/2/2/2
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	3785	1	-	2/9/27/28	0/3/3/3
1	OMG	L1	3744	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	2364	1,80	-	2/9/27/28	0/3/3/3
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
45	A2M	S2	668	45,80	-	3/9/27/28	0/3/3/3
1	OMC	L1	2351	1	-	3/9/27/28	0/2/2/2
1	OMC	L1	3887	1	-	0/9/27/28	0/2/2/2
45	A2M	S2	576	45	-	3/9/27/28	0/3/3/3
45	B8N	S2	1248	45	-	3/16/34/35	0/2/2/2
1	5MC	L1	3782	1,80	-	0/7/25/26	0/2/2/2
1	2MG	L1	1517	1	-	0/9/27/28	0/3/3/3
45	A2M	S2	512	45	-	2/9/27/28	0/3/3/3
45	UR3	S2	1830	45	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L1	1683	1,81	-	0/7/25/26	0/2/2/2
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1340	1	-	2/9/27/28	0/2/2/2
45	MA6	S2	1850	45	-	3/11/29/30	0/3/3/3
1	OMG	L1	4392	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4293	1	-	1/7/25/26	0/2/2/2
45	OMC	S2	517	45	-	2/9/27/28	0/2/2/2

All (986) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	814	5MU	C4-C5	20.75	1.79	1.44
45	S2	814	5MU	C6-N1	16.52	1.66	1.38
1	L1	3762	B8H	C6-C5	-15.50	1.13	1.34
1	L1	3762	B8H	C4-N3	-14.86	1.11	1.38
1	L1	3762	B8H	C4-C5	14.15	1.84	1.44
1	L1	3762	B8H	C6-N1	12.60	1.67	1.36
45	S2	1832	6MZ	C6-N6	12.52	1.47	1.34
1	L1	3818	UY1	O4'-C1'	-11.74	1.27	1.43
1	L1	4220	6MZ	C6-N6	11.22	1.46	1.34
45	S2	1326	UY1	O4'-C1'	-11.19	1.28	1.43
45	S2	814	5MU	C4-N3	-11.07	1.18	1.38
45	S2	814	5MU	C6-C5	-10.71	1.17	1.34
1	L1	4335	5MC	C6-C5	9.06	1.49	1.34
1	L1	4447	5MC	C6-C5	8.98	1.49	1.34
45	S2	1374	5MC	C6-C5	8.98	1.49	1.34
1	L1	2363	A2M	C2'-C1'	-8.89	1.30	1.53
1	L1	398	A2M	O4'-C1'	8.78	1.62	1.42
1	L1	398	A2M	C2'-C1'	-8.73	1.30	1.53
1	L1	1534	A2M	C2'-C1'	-8.71	1.30	1.53
1	L1	2787	A2M	C2'-C1'	-8.71	1.30	1.53
1	L1	3867	A2M	C2'-C1'	-8.67	1.30	1.53
45	S2	512	A2M	O4'-C1'	8.66	1.62	1.42
45	S2	1383	A2M	O4'-C1'	8.66	1.62	1.42
45	S2	576	A2M	O4'-C1'	8.65	1.62	1.42
1	L1	4571	A2M	C2'-C1'	-8.65	1.30	1.53
45	S2	1678	A2M	C2'-C1'	-8.64	1.30	1.53
45	S2	166	A2M	O4'-C1'	8.64	1.62	1.42
45	S2	99	A2M	C2'-C1'	-8.64	1.30	1.53
1	L1	1326	A2M	C2'-C1'	-8.64	1.30	1.53
1	L1	3723	A2M	C2'-C1'	-8.64	1.30	1.53
45	S2	27	A2M	C2'-C1'	-8.63	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	159	A2M	C2'-C1'	-8.63	1.30	1.53
1	L1	3785	A2M	C2'-C1'	-8.62	1.30	1.53
1	L1	2815	A2M	C2'-C1'	-8.61	1.30	1.53
1	L1	1871	A2M	O4'-C1'	8.61	1.62	1.42
1	L1	400	A2M	O4'-C1'	8.60	1.62	1.42
1	L1	3782	5MC	C6-C5	8.59	1.48	1.34
1	L1	3723	A2M	O4'-C1'	8.59	1.62	1.42
45	S2	512	A2M	C2'-C1'	-8.58	1.31	1.53
1	L1	2401	A2M	O4'-C1'	8.58	1.62	1.42
45	S2	166	A2M	C2'-C1'	-8.57	1.31	1.53
1	L1	4571	A2M	O4'-C1'	8.57	1.62	1.42
1	L1	3718	A2M	O4'-C1'	8.57	1.62	1.42
45	S2	1678	A2M	O4'-C1'	8.56	1.62	1.42
1	L1	3825	A2M	C2'-C1'	-8.56	1.31	1.53
45	S2	468	A2M	C2'-C1'	-8.56	1.31	1.53
1	L1	3830	A2M	O4'-C1'	8.56	1.62	1.42
1	L1	3830	A2M	C2'-C1'	-8.55	1.31	1.53
1	L1	400	A2M	C2'-C1'	-8.54	1.31	1.53
45	S2	484	A2M	O4'-C1'	8.54	1.62	1.42
45	S2	576	A2M	C2'-C1'	-8.54	1.31	1.53
45	S2	159	A2M	O4'-C1'	8.53	1.62	1.42
1	L1	4523	A2M	O4'-C1'	8.53	1.62	1.42
45	S2	590	A2M	O4'-C1'	8.53	1.62	1.42
1	L1	1534	A2M	O4'-C1'	8.53	1.62	1.42
45	S2	99	A2M	O4'-C1'	8.53	1.62	1.42
1	L1	1871	A2M	C2'-C1'	-8.52	1.31	1.53
45	S2	27	A2M	O4'-C1'	8.51	1.62	1.42
1	L1	3825	A2M	O4'-C1'	8.51	1.62	1.42
1	L1	3718	A2M	C2'-C1'	-8.50	1.31	1.53
1	L1	2787	A2M	O4'-C1'	8.50	1.62	1.42
45	S2	468	A2M	O4'-C1'	8.50	1.62	1.42
45	S2	1383	A2M	C2'-C1'	-8.47	1.31	1.53
45	S2	484	A2M	C2'-C1'	-8.47	1.31	1.53
45	S2	1031	A2M	C2'-C1'	-8.44	1.31	1.53
1	L1	2815	A2M	O4'-C1'	8.42	1.61	1.42
45	S2	1031	A2M	O4'-C1'	8.41	1.61	1.42
1	L1	2363	A2M	O4'-C1'	8.40	1.61	1.42
45	S2	668	A2M	C2'-C1'	-8.40	1.31	1.53
1	L1	1524	A2M	O4'-C1'	8.34	1.61	1.42
1	L1	2401	A2M	C2'-C1'	-8.34	1.31	1.53
45	S2	1219	JMH	C2-N1	8.31	1.50	1.38
1	L1	4523	A2M	C2'-C1'	-8.31	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	590	A2M	C2'-C1'	-8.31	1.31	1.53
1	L1	1524	A2M	C2'-C1'	-8.28	1.31	1.53
1	L1	3867	A2M	O4'-C1'	8.16	1.61	1.42
1	L1	1326	A2M	O4'-C1'	8.06	1.61	1.42
45	S2	668	A2M	O4'-C1'	8.06	1.61	1.42
1	L1	3785	A2M	O4'-C1'	7.81	1.60	1.42
45	S2	1248	B8N	C6-N1	7.79	1.55	1.36
45	S2	1248	B8N	C4-N3	-7.49	1.26	1.40
1	L1	978	2MG	C2-N3	7.48	1.46	1.31
1	L1	1322	1MA	C2-N3	7.47	1.44	1.30
1	L1	729	2MG	C2-N3	7.40	1.46	1.31
45	S2	1830	UR3	C2-N1	7.38	1.49	1.38
1	L1	3818	UY1	C3'-C4'	-7.20	1.34	1.53
45	S2	1337	4AC	C4-N3	7.14	1.45	1.32
3	L3	14	OMU	C2-N1	7.13	1.49	1.38
45	S2	428	OMU	C2-N1	7.10	1.49	1.38
45	S2	1288	OMU	C2-N1	7.09	1.49	1.38
45	S2	1442	OMU	C2-N1	7.05	1.49	1.38
1	L1	1456	JMH	C2-N1	7.03	1.48	1.38
1	L1	4530	UR3	C2-N1	7.02	1.48	1.38
45	S2	1326	UY1	C3'-C4'	-7.01	1.35	1.53
1	L1	4671	B8T	C4-N3	7.00	1.45	1.32
45	S2	668	A2M	O4'-C4'	-6.99	1.29	1.45
45	S2	354	OMU	C2-N1	6.98	1.49	1.38
45	S2	172	OMU	C2-N1	6.96	1.49	1.38
1	L1	1517	2MG	C2-N3	6.93	1.45	1.31
1	L1	4498	OMU	C2-N1	6.91	1.49	1.38
1	L1	2837	OMU	C2-N1	6.90	1.49	1.38
45	S2	1842	4AC	C4-N3	6.83	1.44	1.32
1	L1	4227	OMU	C2-N1	6.81	1.49	1.38
1	L1	3925	OMU	C2-N1	6.74	1.49	1.38
45	S2	121	OMU	C2-N1	6.72	1.49	1.38
45	S2	116	OMU	C2-N1	6.69	1.49	1.38
45	S2	1442	OMU	C2-N3	6.68	1.49	1.38
1	L1	1524	A2M	O4'-C4'	-6.67	1.30	1.45
1	L1	4620	OMU	C2-N1	6.67	1.49	1.38
1	L1	1534	A2M	O4'-C4'	-6.63	1.30	1.45
45	S2	428	OMU	C2-N3	6.60	1.49	1.38
45	S2	1288	OMU	C2-N3	6.60	1.49	1.38
45	S2	1678	A2M	O4'-C4'	-6.60	1.30	1.45
45	S2	1248	B8N	C6-C5	6.55	1.44	1.34
1	L1	1322	1MA	C4-N3	6.54	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	172	OMU	C2-N3	6.53	1.49	1.38
1	L1	4571	A2M	O4'-C4'	-6.52	1.30	1.45
45	S2	590	A2M	O4'-C4'	-6.52	1.30	1.45
1	L1	4306	OMU	C2-N1	6.49	1.48	1.38
45	S2	1248	B8N	C2-N1	6.48	1.58	1.39
45	S2	436	OMG	C4-N3	6.48	1.49	1.34
45	S2	354	OMU	C2-N3	6.47	1.49	1.38
1	L1	3627	OMG	C4-N3	6.46	1.49	1.34
45	S2	683	OMG	C4-N3	6.45	1.49	1.34
1	L1	1871	A2M	O4'-C4'	-6.45	1.30	1.45
1	L1	3944	OMG	C4-N3	6.45	1.49	1.34
45	S2	1272	OMC	C2-N3	6.45	1.49	1.36
1	L1	400	A2M	O4'-C4'	-6.45	1.30	1.45
1	L1	2815	A2M	O4'-C4'	-6.44	1.30	1.45
1	L1	2363	A2M	O4'-C4'	-6.44	1.30	1.45
45	S2	121	OMU	C2-N3	6.43	1.49	1.38
45	S2	1710	OMC	C2-N3	6.43	1.49	1.36
45	S2	1374	5MC	C4-N3	6.42	1.45	1.34
1	L1	2876	OMG	C4-N3	6.42	1.49	1.34
45	S2	1328	OMG	C4-N3	6.41	1.49	1.34
45	S2	174	OMC	C2-N3	6.40	1.49	1.36
1	L1	3792	OMG	C4-N3	6.39	1.49	1.34
1	L1	3723	A2M	O4'-C4'	-6.38	1.30	1.45
45	S2	867	OMG	C4-N3	6.38	1.49	1.34
45	S2	1391	OMC	C2-N3	6.37	1.49	1.36
3	L3	75	OMG	C4-N3	6.37	1.49	1.34
1	L1	4618	OMG	C4-N3	6.37	1.49	1.34
45	S2	644	OMG	C4-N3	6.37	1.49	1.34
1	L1	2787	A2M	O4'-C4'	-6.36	1.30	1.45
45	S2	27	A2M	O4'-C4'	-6.36	1.30	1.45
45	S2	1337	4AC	C6-C5	6.36	1.49	1.35
45	S2	1490	OMG	C4-N3	6.36	1.49	1.34
45	S2	484	A2M	O4'-C4'	-6.35	1.30	1.45
1	L1	4392	OMG	C4-N3	6.34	1.49	1.34
1	L1	1522	OMG	C4-N3	6.33	1.49	1.34
45	S2	116	OMU	C2-N3	6.33	1.49	1.38
1	L1	4335	5MC	C4-N3	6.33	1.44	1.34
1	L1	1881	OMC	C2-N3	6.32	1.49	1.36
1	L1	1316	OMG	C4-N3	6.31	1.49	1.34
3	L3	14	OMU	C2-N3	6.31	1.49	1.38
45	S2	601	OMG	C4-N3	6.31	1.49	1.34
45	S2	468	A2M	O4'-C4'	-6.31	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	517	OMC	C2-N3	6.31	1.49	1.36
1	L1	4499	OMG	C4-N3	6.30	1.49	1.34
45	S2	99	A2M	O4'-C4'	-6.30	1.30	1.45
45	S2	1326	UY1	O4'-C4'	6.29	1.59	1.45
1	L1	3899	OMG	C4-N3	6.29	1.49	1.34
1	L1	2837	OMU	C2-N3	6.28	1.49	1.38
1	L1	4523	A2M	O4'-C4'	-6.27	1.31	1.45
45	S2	159	A2M	O4'-C4'	-6.27	1.31	1.45
45	S2	509	OMG	C4-N3	6.26	1.49	1.34
45	S2	166	A2M	O4'-C4'	-6.25	1.31	1.45
1	L1	1326	A2M	O4'-C4'	-6.25	1.31	1.45
1	L1	3925	OMU	C2-N3	6.25	1.49	1.38
1	L1	1340	OMC	C2-N3	6.24	1.49	1.36
1	L1	4370	OMG	C4-N3	6.24	1.49	1.34
45	S2	1031	A2M	O4'-C4'	-6.24	1.31	1.45
45	S2	462	OMC	C2-N3	6.24	1.49	1.36
1	L1	3718	A2M	O4'-C4'	-6.24	1.31	1.45
1	L1	4623	OMG	C4-N3	6.23	1.49	1.34
1	L1	3744	OMG	C4-N3	6.22	1.49	1.34
1	L1	4228	OMG	C4-N3	6.21	1.49	1.34
1	L1	3785	A2M	O4'-C4'	-6.21	1.31	1.45
1	L1	4637	OMG	C4-N3	6.20	1.49	1.34
1	L1	3825	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	3867	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	4227	OMU	C2-N3	6.18	1.49	1.38
45	S2	576	A2M	O4'-C4'	-6.17	1.31	1.45
1	L1	2424	OMG	C4-N3	6.17	1.48	1.34
45	S2	512	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	2401	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	2365	OMC	C2-N3	6.15	1.48	1.36
45	S2	1703	OMC	C2-N3	6.15	1.48	1.36
1	L1	398	A2M	O4'-C4'	-6.13	1.31	1.45
1	L1	4498	OMU	C2-N3	6.12	1.48	1.38
1	L1	4536	OMC	C2-N3	6.12	1.48	1.36
1	L1	4620	OMU	C2-N3	6.12	1.48	1.38
45	S2	1383	A2M	O4'-C4'	-6.12	1.31	1.45
45	S2	1337	4AC	C2-N3	6.11	1.48	1.36
1	L1	4306	OMU	C2-N3	6.11	1.48	1.38
1	L1	4456	OMC	C2-N3	6.10	1.48	1.36
45	S2	1842	4AC	C6-C5	6.09	1.49	1.35
45	S2	1374	5MC	C2-N3	6.09	1.48	1.36
1	L1	2861	OMC	C2-N3	6.08	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3808	OMC	C2-N3	6.08	1.48	1.36
1	L1	3887	OMC	C2-N3	6.08	1.48	1.36
1	L1	4494	OMG	C4-N3	6.07	1.48	1.34
1	L1	2824	OMC	C2-N3	6.03	1.48	1.36
1	L1	4196	OMG	C4-N3	6.03	1.48	1.34
45	S2	1272	OMC	C6-C5	6.01	1.49	1.35
1	L1	3830	A2M	O4'-C4'	-6.01	1.31	1.45
1	L1	4530	UR3	C6-C5	6.00	1.49	1.35
1	L1	4671	B8T	C6-C5	6.00	1.49	1.35
1	L1	4335	5MC	C2-N3	5.99	1.48	1.36
45	S2	1710	OMC	C6-C5	5.99	1.49	1.35
45	S2	174	OMC	C6-C5	5.98	1.49	1.35
1	L1	2364	OMG	C4-N3	5.98	1.48	1.34
45	S2	462	OMC	C6-C5	5.98	1.48	1.35
1	L1	2804	OMC	C2-N3	5.97	1.48	1.36
45	S2	1830	UR3	C6-C5	5.97	1.48	1.35
1	L1	3841	OMC	C2-N3	5.96	1.48	1.36
1	L1	3701	OMC	C6-C5	5.96	1.48	1.35
45	S2	1391	OMC	C6-C5	5.96	1.48	1.35
1	L1	3782	5MC	C4-N3	5.95	1.44	1.34
1	L1	2861	OMC	C6-C5	5.95	1.48	1.35
1	L1	4536	OMC	C6-C5	5.95	1.48	1.35
45	S2	1703	OMC	C6-C5	5.93	1.48	1.35
45	S2	517	OMC	C6-C5	5.92	1.48	1.35
1	L1	2422	OMC	C6-C5	5.91	1.48	1.35
1	L1	3808	OMC	C6-C5	5.90	1.48	1.35
45	S2	1337	4AC	C4-N4	5.90	1.48	1.39
1	L1	3701	OMC	C2-N3	5.89	1.48	1.36
45	S2	1288	OMU	C6-C5	5.89	1.48	1.35
1	L1	3818	UY1	O4'-C4'	5.88	1.58	1.45
1	L1	1456	JMH	C6-C5	5.86	1.48	1.35
1	L1	3869	OMC	C2-N3	5.86	1.48	1.36
45	S2	1842	4AC	C2-N3	5.83	1.48	1.36
1	L1	3869	OMC	C6-C5	5.83	1.48	1.35
45	S2	1442	OMU	C6-C5	5.83	1.48	1.35
1	L1	2422	OMC	C2-N3	5.82	1.48	1.36
1	L1	2365	OMC	C6-C5	5.81	1.48	1.35
1	L1	2351	OMC	C6-C5	5.80	1.48	1.35
45	S2	1337	4AC	C7-N4	5.79	1.47	1.37
1	L1	3841	OMC	C6-C5	5.76	1.48	1.35
45	S2	1219	JMH	C6-C5	5.76	1.48	1.35
1	L1	3782	5MC	C2-N3	5.75	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3887	OMC	C6-C5	5.74	1.48	1.35
45	S2	428	OMU	C6-C5	5.74	1.48	1.35
1	L1	4447	5MC	C4-N3	5.74	1.43	1.34
45	S2	121	OMU	C6-C5	5.73	1.48	1.35
1	L1	2824	OMC	C6-C5	5.73	1.48	1.35
45	S2	116	OMU	C6-C5	5.72	1.48	1.35
45	S2	172	OMU	C6-C5	5.71	1.48	1.35
1	L1	2804	OMC	C6-C5	5.69	1.48	1.35
1	L1	1881	OMC	C6-C5	5.69	1.48	1.35
1	L1	4620	OMU	C6-C5	5.67	1.48	1.35
1	L1	4671	B8T	C2-N3	5.66	1.47	1.36
1	L1	4498	OMU	C6-C5	5.66	1.48	1.35
1	L1	4456	OMC	C6-C5	5.65	1.48	1.35
45	S2	354	OMU	C6-C5	5.63	1.48	1.35
1	L1	4306	OMU	C6-C5	5.62	1.48	1.35
45	S2	1842	4AC	C7-N4	5.61	1.47	1.37
1	L1	2837	OMU	C6-C5	5.58	1.48	1.35
1	L1	4447	5MC	C2-N3	5.57	1.47	1.36
1	L1	1316	OMG	C2-N3	5.57	1.46	1.33
1	L1	4227	OMU	C6-C5	5.56	1.48	1.35
1	L1	3944	OMG	C2-N3	5.56	1.46	1.33
45	S2	1842	4AC	C4-N4	5.55	1.47	1.39
1	L1	1340	OMC	C6-C5	5.54	1.47	1.35
1	L1	2351	OMC	C2-N3	5.52	1.47	1.36
45	S2	1328	OMG	C2-N3	5.52	1.46	1.33
1	L1	3925	OMU	C6-C5	5.50	1.47	1.35
45	S2	683	OMG	C2-N3	5.48	1.46	1.33
3	L3	14	OMU	C6-C5	5.48	1.47	1.35
45	S2	867	OMG	C2-N3	5.46	1.46	1.33
1	L1	2876	OMG	C2-N3	5.45	1.46	1.33
1	L1	3627	OMG	C2-N3	5.45	1.46	1.33
1	L1	1522	OMG	C2-N3	5.44	1.46	1.33
1	L1	3818	UY1	O4-C4	-5.43	1.13	1.23
45	S2	509	OMG	C2-N3	5.43	1.46	1.33
3	L3	75	OMG	C2-N3	5.41	1.46	1.33
45	S2	1490	OMG	C2-N3	5.40	1.46	1.33
1	L1	4618	OMG	C2-N3	5.40	1.46	1.33
1	L1	4392	OMG	C2-N3	5.40	1.46	1.33
1	L1	3818	UY1	O2-C2	-5.40	1.12	1.23
45	S2	644	OMG	C2-N3	5.39	1.46	1.33
45	S2	601	OMG	C2-N3	5.39	1.46	1.33
45	S2	436	OMG	C2-N3	5.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4637	OMG	C2-N3	5.37	1.46	1.33
1	L1	4499	OMG	C2-N3	5.35	1.46	1.33
45	S2	1326	UY1	O4-C4	-5.31	1.13	1.23
1	L1	4530	UR3	C2-N3	5.31	1.49	1.39
1	L1	4370	OMG	C2-N3	5.29	1.45	1.33
1	L1	4623	OMG	C2-N3	5.29	1.45	1.33
1	L1	2424	OMG	C2-N3	5.27	1.45	1.33
45	S2	1272	OMC	C4-N3	5.26	1.45	1.34
1	L1	978	2MG	C2-N2	5.26	1.45	1.33
1	L1	3792	OMG	C2-N3	5.25	1.45	1.33
1	L1	1517	2MG	C2-N2	5.21	1.45	1.33
1	L1	729	2MG	C4-N3	5.20	1.46	1.34
1	L1	4196	OMG	C2-N3	5.19	1.45	1.33
1	L1	4494	OMG	C2-N3	5.18	1.45	1.33
1	L1	1517	2MG	C4-N3	5.17	1.46	1.34
1	L1	978	2MG	C4-N3	5.16	1.46	1.34
1	L1	3744	OMG	C2-N3	5.16	1.45	1.33
1	L1	729	2MG	C2-N2	5.16	1.44	1.33
45	S2	814	5MU	C2-N3	5.16	1.47	1.38
45	S2	174	OMC	C4-N3	5.12	1.44	1.34
1	L1	3899	OMG	C2-N3	5.10	1.45	1.33
45	S2	1710	OMC	C4-N3	5.09	1.44	1.34
45	S2	1391	OMC	C4-N3	5.09	1.44	1.34
1	L1	4228	OMG	C2-N3	5.08	1.45	1.33
45	S2	517	OMC	C4-N3	5.06	1.44	1.34
1	L1	1881	OMC	C4-N3	5.05	1.44	1.34
45	S2	1272	OMC	C4-N4	5.01	1.45	1.33
1	L1	1340	OMC	C4-N3	5.00	1.44	1.34
1	L1	3841	OMC	C4-N3	4.99	1.44	1.34
1	L1	2351	OMC	C2-N1	4.98	1.50	1.40
45	S2	462	OMC	C4-N3	4.94	1.44	1.34
45	S2	1710	OMC	C4-N4	4.93	1.45	1.33
1	L1	3762	B8H	C2-N3	4.92	1.46	1.38
45	S2	1703	OMC	C4-N3	4.92	1.44	1.34
45	S2	1326	UY1	O2-C2	-4.91	1.13	1.23
1	L1	3869	OMC	C4-N3	4.91	1.44	1.34
1	L1	2364	OMG	C2-N3	4.89	1.44	1.33
45	S2	1391	OMC	C4-N4	4.88	1.45	1.33
45	S2	462	OMC	C4-N4	4.87	1.45	1.33
45	S2	174	OMC	C4-N4	4.87	1.45	1.33
1	L1	3887	OMC	C4-N3	4.86	1.44	1.34
1	L1	4671	B8T	C4-N4	4.85	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2804	OMC	C4-N3	4.85	1.44	1.34
45	S2	1326	UY1	C1'-C5	4.84	1.61	1.50
1	L1	2861	OMC	C4-N3	4.83	1.44	1.34
45	S2	1830	UR3	C2-N3	4.82	1.48	1.39
45	S2	1703	OMC	C4-N4	4.82	1.45	1.33
45	S2	1219	JMH	C2-N3	4.80	1.48	1.39
1	L1	3944	OMG	C2-N2	4.78	1.45	1.34
1	L1	2365	OMC	C4-N4	4.78	1.45	1.33
1	L1	2861	OMC	C4-N4	4.77	1.45	1.33
1	L1	1881	OMC	C4-N4	4.77	1.45	1.33
1	L1	2365	OMC	C4-N3	4.77	1.44	1.34
1	L1	2824	OMC	C4-N3	4.77	1.44	1.34
45	S2	1328	OMG	C2-N2	4.76	1.45	1.34
1	L1	2422	OMC	C4-N4	4.74	1.45	1.33
1	L1	2824	OMC	C4-N4	4.74	1.45	1.33
1	L1	3887	OMC	C4-N4	4.73	1.45	1.33
45	S2	517	OMC	C4-N4	4.73	1.45	1.33
45	S2	1272	OMC	C2-N1	4.72	1.50	1.40
1	L1	4456	OMC	C4-N3	4.71	1.44	1.34
1	L1	3808	OMC	C2-N1	4.71	1.50	1.40
45	S2	1490	OMG	C2-N2	4.71	1.45	1.34
1	L1	1340	OMC	C4-N4	4.70	1.45	1.33
1	L1	2804	OMC	C4-N4	4.69	1.45	1.33
1	L1	3701	OMC	C4-N3	4.69	1.44	1.34
1	L1	4536	OMC	C4-N3	4.68	1.43	1.34
1	L1	3869	OMC	C4-N4	4.68	1.44	1.33
45	S2	1391	OMC	C2-N1	4.68	1.50	1.40
1	L1	2424	OMG	C2-N2	4.67	1.45	1.34
1	L1	4456	OMC	C2-N1	4.67	1.50	1.40
45	S2	1710	OMC	C2-N1	4.66	1.50	1.40
1	L1	4499	OMG	C2-N2	4.66	1.45	1.34
45	S2	867	OMG	C2-N2	4.65	1.45	1.34
3	L3	75	OMG	C2-N2	4.64	1.45	1.34
1	L1	3792	OMG	C2-N2	4.64	1.45	1.34
45	S2	683	OMG	C2-N2	4.64	1.45	1.34
45	S2	436	OMG	C2-N2	4.64	1.45	1.34
1	L1	2422	OMC	C4-N3	4.61	1.43	1.34
45	S2	517	OMC	C2-N1	4.61	1.50	1.40
1	L1	3808	OMC	C4-N3	4.61	1.43	1.34
1	L1	3841	OMC	C2-N1	4.60	1.50	1.40
1	L1	3869	OMC	C2-N1	4.59	1.50	1.40
45	S2	601	OMG	C2-N2	4.59	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3808	OMC	C4-N4	4.58	1.44	1.33
1	L1	3841	OMC	C4-N4	4.58	1.44	1.33
1	L1	2824	OMC	C2-N1	4.57	1.49	1.40
1	L1	4618	OMG	C2-N2	4.56	1.45	1.34
1	L1	4456	OMC	C4-N4	4.55	1.44	1.33
45	S2	644	OMG	C2-N2	4.55	1.45	1.34
45	S2	1678	A2M	C6-N6	4.54	1.45	1.34
1	L1	4370	OMG	C2-N2	4.53	1.45	1.34
1	L1	2364	OMG	C2-N2	4.53	1.45	1.34
1	L1	4536	OMC	C4-N4	4.52	1.44	1.33
1	L1	4196	OMG	C2-N2	4.52	1.44	1.34
1	L1	1316	OMG	C2-N2	4.52	1.44	1.34
45	S2	1806	M7A	C6-N6	4.51	1.45	1.34
45	S2	590	A2M	C6-N6	4.51	1.45	1.34
1	L1	3701	OMC	C4-N4	4.51	1.44	1.33
45	S2	166	A2M	C6-N6	4.50	1.45	1.34
1	L1	4671	B8T	C2-N1	4.50	1.49	1.40
45	S2	159	A2M	C6-N6	4.50	1.45	1.34
45	S2	174	OMC	C2-N1	4.50	1.49	1.40
45	S2	1374	5MC	C6-N1	4.50	1.45	1.38
1	L1	2351	OMC	C4-N4	4.49	1.44	1.33
1	L1	2804	OMC	C2-N1	4.49	1.49	1.40
1	L1	4228	OMG	C2-N2	4.49	1.44	1.34
45	S2	1703	OMC	C2-N1	4.47	1.49	1.40
45	S2	668	A2M	C6-N6	4.47	1.45	1.34
1	L1	3899	OMG	C2-N2	4.47	1.44	1.34
1	L1	4623	OMG	C2-N2	4.46	1.44	1.34
45	S2	576	A2M	C6-N6	4.46	1.45	1.34
45	S2	468	A2M	C6-N6	4.46	1.45	1.34
1	L1	398	A2M	C6-N6	4.46	1.45	1.34
1	L1	3627	OMG	C2-N2	4.46	1.44	1.34
1	L1	400	A2M	C6-N6	4.46	1.45	1.34
45	S2	462	OMC	C2-N1	4.45	1.49	1.40
1	L1	1456	JMH	C2-N3	4.45	1.47	1.39
1	L1	1524	A2M	C6-N6	4.45	1.45	1.34
1	L1	4494	OMG	C2-N2	4.44	1.44	1.34
45	S2	27	A2M	C6-N6	4.43	1.45	1.34
1	L1	2876	OMG	C2-N2	4.43	1.44	1.34
1	L1	4335	5MC	C6-N1	4.43	1.45	1.38
1	L1	3744	OMG	C2-N2	4.42	1.44	1.34
45	S2	484	A2M	C6-N6	4.41	1.45	1.34
1	L1	3887	OMC	C2-N1	4.41	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3818	UY1	C1'-C5	4.41	1.60	1.50
1	L1	4392	OMG	C2-N2	4.40	1.44	1.34
45	S2	512	A2M	C6-N6	4.39	1.45	1.34
1	L1	3867	A2M	C6-N6	4.39	1.45	1.34
1	L1	2401	A2M	C6-N6	4.39	1.45	1.34
45	S2	509	OMG	C2-N2	4.38	1.44	1.34
1	L1	3723	A2M	C6-N6	4.37	1.45	1.34
1	L1	3718	A2M	C6-N6	4.36	1.45	1.34
45	S2	1383	A2M	C6-N6	4.36	1.45	1.34
45	S2	1374	5MC	C4-N4	4.36	1.45	1.34
1	L1	4637	OMG	C2-N2	4.36	1.44	1.34
1	L1	2351	OMC	C4-N3	4.36	1.43	1.34
1	L1	4571	A2M	C6-N6	4.36	1.45	1.34
1	L1	1881	OMC	C2-N1	4.33	1.49	1.40
45	S2	99	A2M	C6-N6	4.33	1.45	1.34
1	L1	2422	OMC	C2-N1	4.32	1.49	1.40
1	L1	4447	5MC	C6-N1	4.31	1.45	1.38
1	L1	1871	A2M	C6-N6	4.30	1.44	1.34
1	L1	4447	5MC	C4-N4	4.30	1.45	1.34
1	L1	1522	OMG	C2-N2	4.30	1.44	1.34
1	L1	1534	A2M	C6-N6	4.29	1.44	1.34
1	L1	2861	OMC	C2-N1	4.29	1.49	1.40
45	S2	1337	4AC	C5-C4	4.28	1.49	1.40
1	L1	4335	5MC	C4-N4	4.27	1.45	1.34
1	L1	3782	5MC	C6-N1	4.26	1.45	1.38
45	S2	1031	A2M	C6-N6	4.25	1.44	1.34
1	L1	4523	A2M	C6-N6	4.24	1.44	1.34
45	S2	1326	UY1	C6-C5	4.22	1.40	1.35
1	L1	3825	A2M	C6-N6	4.21	1.44	1.34
1	L1	2815	A2M	C6-N6	4.21	1.44	1.34
1	L1	4536	OMC	C2-N1	4.20	1.49	1.40
1	L1	2787	A2M	C6-N6	4.20	1.44	1.34
45	S2	1842	4AC	C5-C4	4.19	1.49	1.40
1	L1	3830	A2M	C6-N6	4.19	1.44	1.34
1	L1	1340	OMC	C2-N1	4.17	1.49	1.40
1	L1	2363	A2M	C6-N6	4.14	1.44	1.34
1	L1	3782	5MC	C2-N1	4.13	1.49	1.40
45	S2	814	5MU	C2-N1	4.13	1.45	1.38
45	S2	1374	5MC	C2-N1	4.12	1.48	1.40
1	L1	3701	OMC	C2-N1	4.08	1.48	1.40
45	S2	1337	4AC	C2-N1	4.07	1.48	1.40
1	L1	1322	1MA	C2-N1	4.05	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3782	5MC	C4-N4	4.04	1.44	1.34
1	L1	1326	A2M	C6-N6	4.00	1.44	1.34
1	L1	2365	OMC	C2-N1	3.97	1.48	1.40
1	L1	4335	5MC	C2-N1	3.93	1.48	1.40
1	L1	3785	A2M	C6-N6	3.90	1.43	1.34
1	L1	3818	UY1	C6-C5	3.90	1.39	1.35
45	S2	1842	4AC	C2-N1	3.89	1.48	1.40
1	L1	3818	UY1	C2-N3	-3.81	1.31	1.37
1	L1	4447	5MC	C2-N1	3.79	1.48	1.40
1	L1	4392	OMG	C5-N7	-3.79	1.31	1.39
45	S2	1326	UY1	C2-N3	-3.70	1.31	1.37
45	S2	1243	PSU	C6-C5	3.59	1.39	1.35
1	L1	1322	1MA	C5-C6	3.58	1.53	1.43
45	S2	1806	M7A	C2-N1	3.53	1.40	1.33
1	L1	3818	UY1	C2-N1	-3.53	1.32	1.36
45	S2	1288	OMU	C4-N3	3.53	1.44	1.38
1	L1	1683	PSU	C6-C5	3.51	1.39	1.35
1	L1	2876	OMG	C5-N7	-3.49	1.32	1.39
1	L1	1582	PSU	C6-C5	3.49	1.39	1.35
1	L1	4196	OMG	C5-N7	-3.48	1.32	1.39
45	S2	1442	OMU	C4-N3	3.46	1.44	1.38
1	L1	1316	OMG	C5-N7	-3.46	1.32	1.39
1	L1	4450	PSU	C6-C5	3.46	1.39	1.35
1	L1	2351	OMC	C6-N1	3.45	1.46	1.38
1	L1	978	2MG	C2-N1	3.44	1.42	1.36
1	L1	3899	OMG	C5-N7	-3.44	1.32	1.39
1	L1	4494	OMG	C5-N7	-3.44	1.32	1.39
45	S2	1806	M7A	C71-N7	-3.44	1.40	1.46
1	L1	4442	PSU	C6-C5	3.43	1.39	1.35
1	L1	2364	OMG	C5-N7	-3.43	1.32	1.39
1	L1	4228	OMG	C5-N7	-3.43	1.32	1.39
1	L1	4671	B8T	C5-C4	3.41	1.48	1.40
1	L1	3792	OMG	C5-N7	-3.41	1.32	1.39
1	L1	3744	OMG	C5-N7	-3.40	1.32	1.39
1	L1	4637	OMG	C5-N7	-3.40	1.32	1.39
1	L1	1517	2MG	C2-N1	3.39	1.42	1.36
1	L1	4671	B8T	C6-N1	3.38	1.46	1.38
1	L1	3869	OMC	C6-N1	3.37	1.46	1.38
45	S2	644	OMG	C5-N7	-3.36	1.32	1.39
1	L1	2365	OMC	C6-N1	3.35	1.46	1.38
1	L1	2424	OMG	C5-N7	-3.34	1.32	1.39
1	L1	4499	OMG	C5-N7	-3.33	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2508	PSU	C6-C5	3.33	1.39	1.35
45	S2	172	OMU	C4-N3	3.33	1.44	1.38
1	L1	4370	OMG	C5-N7	-3.33	1.32	1.39
45	S2	428	OMU	C4-N3	3.31	1.44	1.38
45	S2	436	OMG	C5-N7	-3.31	1.32	1.39
1	L1	3715	PSU	C6-C5	3.30	1.39	1.35
1	L1	3925	OMU	O2-C2	-3.30	1.17	1.23
1	L1	4671	B8T	O2-C2	-3.30	1.17	1.23
1	L1	4536	OMC	C6-N1	3.30	1.46	1.38
1	L1	2787	A2M	O3'-C3'	-3.29	1.35	1.43
1	L1	2422	OMC	C6-N1	3.29	1.45	1.38
1	L1	3785	A2M	C5-C4	-3.29	1.32	1.39
1	L1	3729	PSU	C6-C5	3.29	1.39	1.35
45	S2	683	OMG	C5-N7	-3.29	1.32	1.39
45	S2	1806	M7A	C4-N9	3.28	1.44	1.38
3	L3	75	OMG	C5-N7	-3.28	1.32	1.39
1	L1	3830	A2M	C5-C4	-3.28	1.32	1.39
1	L1	3887	OMC	C6-N1	3.27	1.45	1.38
45	S2	822	PSU	C6-C5	3.27	1.39	1.35
1	L1	2787	A2M	C5-C4	-3.27	1.32	1.39
45	S2	823	PSU	C6-C5	3.27	1.39	1.35
45	S2	1081	PSU	C6-C5	3.26	1.39	1.35
45	S2	1490	OMG	C5-N7	-3.26	1.32	1.39
1	L1	3825	A2M	C5-C4	-3.25	1.32	1.39
1	L1	3764	PSU	C6-C5	3.25	1.39	1.35
1	L1	4636	PSU	C6-C5	3.25	1.39	1.35
45	S2	509	OMG	C5-N7	-3.24	1.32	1.39
1	L1	729	2MG	C2-N1	3.24	1.41	1.36
45	S2	1842	4AC	C6-N1	3.24	1.45	1.38
45	S2	1391	OMC	C6-N1	3.24	1.45	1.38
1	L1	3627	OMG	C5-N7	-3.23	1.32	1.39
45	S2	1219	JMH	C6-N1	3.23	1.45	1.38
1	L1	1456	JMH	C6-N1	3.22	1.45	1.38
1	L1	4623	OMG	C5-N7	-3.22	1.32	1.39
1	L1	1522	OMG	C5-N7	-3.22	1.32	1.39
45	S2	601	OMG	C5-N7	-3.22	1.32	1.39
45	S2	867	OMG	C5-N7	-3.22	1.32	1.39
45	S2	1248	B8N	O4-C4	-3.22	1.16	1.23
3	L3	14	OMU	C4-N3	3.21	1.44	1.38
45	S2	1710	OMC	C6-N1	3.21	1.45	1.38
1	L1	3701	OMC	C6-N1	3.21	1.45	1.38
1	L1	4403	PSU	C6-C5	3.21	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3808	OMC	C6-N1	3.21	1.45	1.38
45	S2	1272	OMC	C6-N1	3.20	1.45	1.38
1	L1	2363	A2M	C5-N7	-3.20	1.33	1.39
1	L1	3925	OMU	O4-C4	-3.20	1.18	1.24
45	S2	1703	OMC	C6-N1	3.20	1.45	1.38
1	L1	4392	OMG	O6-C6	-3.20	1.17	1.23
45	S2	159	A2M	O3'-C3'	-3.19	1.35	1.43
1	L1	4618	OMG	C5-N7	-3.19	1.32	1.39
45	S2	121	OMU	C4-N3	3.19	1.44	1.38
45	S2	1851	MA6	C6-N6	3.19	1.46	1.36
1	L1	2824	OMC	C6-N1	3.19	1.45	1.38
45	S2	116	OMU	C4-N3	3.19	1.44	1.38
45	S2	174	OMC	C6-N1	3.18	1.45	1.38
45	S2	1337	4AC	C6-N1	3.18	1.45	1.38
1	L1	4523	A2M	C5-C4	-3.17	1.33	1.39
45	S2	462	OMC	C6-N1	3.17	1.45	1.38
1	L1	3944	OMG	C5-N7	-3.17	1.32	1.39
1	L1	2815	A2M	O3'-C3'	-3.17	1.35	1.43
45	S2	119	PSU	C6-C5	3.17	1.39	1.35
1	L1	4306	OMU	O2-C2	-3.17	1.17	1.23
1	L1	3841	OMC	C6-N1	3.17	1.45	1.38
45	S2	1678	A2M	O3'-C3'	-3.16	1.35	1.43
1	L1	2363	A2M	C5-C4	-3.16	1.33	1.39
1	L1	1871	A2M	O3'-C3'	-3.16	1.35	1.43
1	L1	3701	OMC	O2-C2	-3.16	1.17	1.23
1	L1	4498	OMU	C4-N3	3.15	1.44	1.38
45	S2	354	OMU	C4-N3	3.15	1.44	1.38
1	L1	1677	PSU	C6-C5	3.15	1.39	1.35
45	S2	1326	UY1	C2-N1	-3.15	1.32	1.36
45	S2	99	A2M	O3'-C3'	-3.14	1.35	1.43
45	S2	612	PSU	C6-C5	3.14	1.39	1.35
1	L1	2837	OMU	O4-C4	-3.13	1.18	1.24
1	L1	2804	OMC	O2-C2	-3.12	1.17	1.23
1	L1	4498	OMU	O4-C4	-3.12	1.18	1.24
45	S2	468	A2M	O3'-C3'	-3.12	1.35	1.43
1	L1	4293	PSU	C6-C5	3.12	1.39	1.35
45	S2	517	OMC	C6-N1	3.11	1.45	1.38
45	S2	1031	A2M	C5-C4	-3.11	1.33	1.39
45	S2	1850	MA6	C6-N6	3.11	1.46	1.36
1	L1	2861	OMC	C6-N1	3.11	1.45	1.38
1	L1	4536	OMC	O2-C2	-3.11	1.18	1.23
45	S2	1328	OMG	C5-N7	-3.10	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3830	A2M	O3'-C3'	-3.10	1.35	1.43
1	L1	2787	A2M	C5-N7	-3.09	1.33	1.39
1	L1	1625	OMG	C5-C4	3.09	1.47	1.38
1	L1	4531	PSU	C6-C5	3.09	1.38	1.35
1	L1	4227	OMU	C4-N3	3.08	1.44	1.38
1	L1	3925	OMU	C4-N3	3.08	1.44	1.38
45	S2	1842	4AC	O2-C2	-3.07	1.18	1.23
45	S2	166	A2M	O3'-C3'	-3.07	1.35	1.43
1	L1	1522	OMG	O6-C6	-3.06	1.17	1.23
1	L1	2861	OMC	O2-C2	-3.06	1.18	1.23
1	L1	398	A2M	O3'-C3'	-3.05	1.35	1.43
3	L3	14	OMU	O4-C4	-3.04	1.18	1.24
1	L1	3627	OMG	O6-C6	-3.04	1.17	1.23
45	S2	1383	A2M	O3'-C3'	-3.04	1.35	1.43
45	S2	27	A2M	O3'-C3'	-3.04	1.35	1.43
1	L1	2837	OMU	C4-N3	3.03	1.44	1.38
1	L1	1517	2MG	O6-C6	-3.03	1.17	1.23
45	S2	590	A2M	O3'-C3'	-3.03	1.35	1.43
1	L1	1524	A2M	C5-N7	-3.02	1.33	1.39
1	L1	1326	A2M	O2'-C2'	3.01	1.50	1.42
45	S2	576	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	4571	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	2422	OMC	O2-C2	-3.01	1.18	1.23
1	L1	3899	OMG	O6-C6	-3.01	1.17	1.23
45	S2	1447	OMG	C5-C4	3.01	1.47	1.38
1	L1	4456	OMC	O2-C2	-3.01	1.18	1.23
45	S2	99	A2M	C5-C4	-3.00	1.33	1.39
1	L1	1322	1MA	C5-N7	-3.00	1.33	1.39
1	L1	3808	OMC	O2-C2	-3.00	1.18	1.23
1	L1	1326	A2M	C5-N7	-2.99	1.33	1.39
1	L1	3841	OMC	O2-C2	-2.99	1.18	1.23
45	S2	354	OMU	O4-C4	-2.99	1.18	1.24
1	L1	4523	A2M	C5-N7	-2.99	1.33	1.39
1	L1	4306	OMU	C4-N3	2.98	1.43	1.38
1	L1	3869	OMC	O2-C2	-2.98	1.18	1.23
1	L1	2804	OMC	C6-N1	2.98	1.45	1.38
45	S2	512	A2M	O3'-C3'	-2.98	1.36	1.43
1	L1	1340	OMC	O2-C2	-2.98	1.18	1.23
1	L1	400	A2M	O3'-C3'	-2.98	1.36	1.43
45	S2	1678	A2M	O2'-C2'	2.98	1.50	1.42
1	L1	2815	A2M	O2'-C2'	2.97	1.50	1.42
1	L1	3718	A2M	C5-N7	-2.97	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	14	OMU	O2-C2	-2.96	1.17	1.23
1	L1	3718	A2M	O2'-C2'	2.96	1.50	1.42
1	L1	2401	A2M	C5-C4	-2.95	1.33	1.39
45	S2	1703	OMC	O2-C2	-2.94	1.18	1.23
1	L1	3718	A2M	O3'-C3'	-2.94	1.36	1.43
1	L1	4447	5MC	O2-C2	-2.94	1.18	1.23
45	S2	1830	UR3	C6-N1	2.94	1.45	1.38
1	L1	4620	OMU	C4-N3	2.94	1.43	1.38
1	L1	2351	OMC	O2-C2	-2.94	1.18	1.23
1	L1	4494	OMG	O6-C6	-2.93	1.18	1.23
1	L1	2365	OMC	O2-C2	-2.93	1.18	1.23
1	L1	2824	OMC	O2-C2	-2.93	1.18	1.23
1	L1	2363	A2M	O3'-C3'	-2.93	1.36	1.43
1	L1	1534	A2M	C5-C4	-2.93	1.33	1.39
1	L1	3825	A2M	O3'-C3'	-2.93	1.36	1.43
45	S2	1850	MA6	C5-C4	-2.93	1.33	1.39
45	S2	1031	A2M	O2'-C2'	2.93	1.50	1.42
45	S2	27	A2M	C5-C4	-2.93	1.33	1.39
1	L1	2401	A2M	C5-N7	-2.92	1.33	1.39
1	L1	3723	A2M	O3'-C3'	-2.92	1.36	1.43
1	L1	1524	A2M	O3'-C3'	-2.92	1.36	1.43
1	L1	3887	OMC	O2-C2	-2.92	1.18	1.23
1	L1	2876	OMG	O6-C6	-2.92	1.18	1.23
1	L1	4227	OMU	O4-C4	-2.91	1.18	1.24
1	L1	1871	A2M	C5-N7	-2.91	1.33	1.39
1	L1	3867	A2M	O2'-C2'	2.91	1.50	1.42
45	S2	668	A2M	C5-C4	-2.91	1.33	1.39
1	L1	4306	OMU	O4-C4	-2.91	1.18	1.24
45	S2	1383	A2M	C5-C4	-2.91	1.33	1.39
45	S2	1851	MA6	C5-N7	-2.91	1.33	1.39
1	L1	1871	A2M	O2'-C2'	2.90	1.50	1.42
1	L1	729	2MG	C5-N7	-2.90	1.33	1.39
1	L1	4456	OMC	C6-N1	2.90	1.45	1.38
1	L1	3867	A2M	C5-N7	-2.90	1.33	1.39
1	L1	4637	OMG	O6-C6	-2.90	1.18	1.23
1	L1	3782	5MC	O2-C2	-2.89	1.18	1.23
1	L1	3723	A2M	C5-C4	-2.89	1.33	1.39
1	L1	1326	A2M	C5-C4	-2.89	1.33	1.39
1	L1	3867	A2M	C5-C4	-2.89	1.33	1.39
1	L1	4227	OMU	O2-C2	-2.89	1.17	1.23
1	L1	1871	A2M	C5-C4	-2.88	1.33	1.39
1	L1	4620	OMU	O2-C2	-2.88	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1524	A2M	C5-C4	-2.88	1.33	1.39
1	L1	400	A2M	C5-C4	-2.87	1.33	1.39
45	S2	484	A2M	C5-N7	-2.87	1.33	1.39
45	S2	1850	MA6	C5-N7	-2.87	1.33	1.39
1	L1	3718	A2M	C5-C4	-2.87	1.33	1.39
45	S2	512	A2M	C5-N7	-2.86	1.33	1.39
45	S2	159	A2M	O2'-C2'	2.86	1.50	1.42
45	S2	1031	A2M	O3'-C3'	-2.86	1.36	1.43
1	L1	3785	A2M	C5-N7	-2.85	1.33	1.39
45	S2	1337	4AC	O2-C2	-2.85	1.18	1.23
1	L1	1881	OMC	O2-C2	-2.84	1.18	1.23
45	S2	99	A2M	C5-N7	-2.84	1.33	1.39
45	S2	166	A2M	C5-C4	-2.84	1.33	1.39
45	S2	468	A2M	C5-C4	-2.83	1.33	1.39
45	S2	1678	A2M	C5-C4	-2.83	1.33	1.39
1	L1	3825	A2M	C5-N7	-2.83	1.33	1.39
45	S2	683	OMG	O6-C6	-2.83	1.18	1.23
1	L1	4618	OMG	O6-C6	-2.82	1.18	1.23
1	L1	4571	A2M	C5-C4	-2.82	1.33	1.39
1	L1	3867	A2M	O3'-C3'	-2.82	1.36	1.43
1	L1	1625	OMG	C6-N1	-2.82	1.33	1.38
1	L1	4228	OMG	O6-C6	-2.82	1.18	1.23
45	S2	484	A2M	O2'-C2'	2.82	1.49	1.42
45	S2	590	A2M	O2'-C2'	2.82	1.49	1.42
1	L1	2401	A2M	O3'-C3'	-2.82	1.36	1.43
1	L1	4571	A2M	C5-N7	-2.82	1.33	1.39
1	L1	1340	OMC	C6-N1	2.82	1.44	1.38
1	L1	4620	OMU	O4-C4	-2.82	1.19	1.24
45	S2	27	A2M	O2'-C2'	2.82	1.49	1.42
45	S2	668	A2M	C5-N7	-2.81	1.33	1.39
45	S2	1031	A2M	C5-N7	-2.81	1.33	1.39
45	S2	576	A2M	O2'-C2'	2.81	1.49	1.42
1	L1	1524	A2M	O2'-C2'	2.81	1.49	1.42
1	L1	1534	A2M	O3'-C3'	-2.81	1.36	1.43
1	L1	4335	5MC	O2-C2	-2.81	1.18	1.23
1	L1	4623	OMG	O6-C6	-2.81	1.18	1.23
45	S2	116	OMU	O2-C2	-2.81	1.17	1.23
1	L1	3744	OMG	O6-C6	-2.81	1.18	1.23
1	L1	2815	A2M	C5-C4	-2.80	1.33	1.39
1	L1	1517	2MG	CM2-N2	2.80	1.50	1.45
45	S2	1806	M7A	C5-N7	2.80	1.46	1.39
1	L1	3723	A2M	O2'-C2'	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	978	2MG	O6-C6	-2.80	1.18	1.23
1	L1	1881	OMC	C6-N1	2.79	1.44	1.38
45	S2	116	OMU	O4-C4	-2.79	1.19	1.24
45	S2	166	A2M	O2'-C2'	2.79	1.49	1.42
1	L1	4498	OMU	O2-C2	-2.79	1.17	1.23
1	L1	4370	OMG	O6-C6	-2.79	1.18	1.23
1	L1	398	A2M	C5-C4	-2.79	1.33	1.39
1	L1	3825	A2M	O2'-C2'	2.78	1.49	1.42
45	S2	668	A2M	O3'-C3'	-2.78	1.36	1.43
45	S2	512	A2M	C5-C4	-2.78	1.33	1.39
45	S2	517	OMC	O2-C2	-2.78	1.18	1.23
45	S2	159	A2M	C5-C4	-2.78	1.33	1.39
45	S2	462	OMC	O2-C2	-2.78	1.18	1.23
1	L1	1326	A2M	O3'-C3'	-2.78	1.36	1.43
45	S2	428	OMU	O4-C4	-2.77	1.19	1.24
1	L1	1534	A2M	C5-N7	-2.77	1.33	1.39
45	S2	1383	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	400	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	2401	A2M	O2'-C2'	2.77	1.49	1.42
45	S2	668	A2M	O2'-C2'	2.77	1.49	1.42
45	S2	590	A2M	C5-N7	-2.77	1.33	1.39
1	L1	4196	OMG	O6-C6	-2.77	1.18	1.23
45	S2	484	A2M	O3'-C3'	-2.77	1.36	1.43
45	S2	1851	MA6	C5-C4	-2.77	1.33	1.39
1	L1	3792	OMG	O6-C6	-2.77	1.18	1.23
45	S2	1710	OMC	O2-C2	-2.76	1.18	1.23
45	S2	121	OMU	O2-C2	-2.76	1.18	1.23
1	L1	4530	UR3	C6-N1	2.76	1.44	1.38
1	L1	2363	A2M	O2'-C2'	2.74	1.49	1.42
1	L1	2837	OMU	O2-C2	-2.74	1.18	1.23
45	S2	99	A2M	O2'-C2'	2.74	1.49	1.42
45	S2	1374	5MC	O2-C2	-2.73	1.18	1.23
45	S2	428	OMU	O2-C2	-2.73	1.18	1.23
1	L1	1316	OMG	O6-C6	-2.73	1.18	1.23
1	L1	2424	OMG	O6-C6	-2.73	1.18	1.23
45	S2	1391	OMC	O2-C2	-2.73	1.18	1.23
1	L1	1517	2MG	C5-N7	-2.72	1.33	1.39
1	L1	4571	A2M	O2'-C2'	2.72	1.49	1.42
45	S2	354	OMU	O2-C2	-2.72	1.18	1.23
1	L1	3785	A2M	O2'-C2'	2.72	1.49	1.42
45	S2	174	OMC	O2-C2	-2.72	1.18	1.23
45	S2	121	OMU	O4-C4	-2.72	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	576	A2M	C5-N7	-2.72	1.33	1.39
1	L1	398	A2M	O2'-C2'	2.71	1.49	1.42
1	L1	4523	A2M	O3'-C3'	-2.71	1.36	1.43
45	S2	484	A2M	C5-C4	-2.71	1.33	1.39
1	L1	3830	A2M	O2'-C2'	2.71	1.49	1.42
1	L1	978	2MG	C5-N7	-2.71	1.33	1.39
45	S2	1272	OMC	O2-C2	-2.71	1.18	1.23
1	L1	4499	OMG	O6-C6	-2.71	1.18	1.23
45	S2	27	A2M	C5-N7	-2.71	1.33	1.39
1	L1	4499	OMG	C2-N1	2.71	1.44	1.37
45	S2	172	OMU	O4-C4	-2.70	1.19	1.24
1	L1	398	A2M	C5-N7	-2.69	1.33	1.39
45	S2	576	A2M	C5-C4	-2.69	1.34	1.39
45	S2	512	A2M	O2'-C2'	2.69	1.49	1.42
1	L1	400	A2M	C5-N7	-2.68	1.34	1.39
1	L1	3723	A2M	C5-N7	-2.67	1.34	1.39
1	L1	1534	A2M	O2'-C2'	2.67	1.49	1.42
45	S2	1328	OMG	C2-N1	2.67	1.44	1.37
45	S2	436	OMG	O6-C6	-2.66	1.18	1.23
45	S2	814	5MU	O4-C4	-2.66	1.18	1.23
3	L3	75	OMG	O6-C6	-2.66	1.18	1.23
45	S2	1678	A2M	C5-N7	-2.66	1.34	1.39
1	L1	729	2MG	O6-C6	-2.65	1.18	1.23
1	L1	2364	OMG	O6-C6	-2.65	1.18	1.23
45	S2	172	OMU	O2-C2	-2.65	1.18	1.23
45	S2	468	A2M	O2'-C2'	2.65	1.49	1.42
1	L1	3830	A2M	C5-N7	-2.65	1.34	1.39
1	L1	3944	OMG	C2-N1	2.64	1.44	1.37
1	L1	4628	PSU	C6-C5	2.64	1.38	1.35
45	S2	1442	OMU	O4-C4	-2.64	1.19	1.24
1	L1	4523	A2M	O2'-C2'	2.64	1.49	1.42
1	L1	4500	PSU	C6-C5	2.63	1.38	1.35
45	S2	1288	OMU	O4-C4	-2.63	1.19	1.24
1	L1	1322	1MA	C4-N9	-2.63	1.31	1.38
1	L1	2787	A2M	O2'-C2'	2.63	1.49	1.42
1	L1	3944	OMG	O6-C6	-2.63	1.18	1.23
45	S2	468	A2M	C5-N7	-2.62	1.34	1.39
45	S2	601	OMG	O6-C6	-2.62	1.18	1.23
45	S2	867	OMG	C2-N1	2.62	1.44	1.37
45	S2	590	A2M	C5-C4	-2.62	1.34	1.39
45	S2	1442	OMU	O2-C2	-2.61	1.18	1.23
45	S2	159	A2M	C5-N7	-2.61	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2815	A2M	C5-N7	-2.60	1.34	1.39
45	S2	509	OMG	O6-C6	-2.60	1.18	1.23
45	S2	814	5MU	O2-C2	-2.60	1.18	1.23
1	L1	1625	OMG	C5-N7	-2.60	1.34	1.39
45	S2	1383	A2M	C5-N7	-2.59	1.34	1.39
45	S2	644	OMG	O6-C6	-2.59	1.18	1.23
45	S2	166	A2M	C5-N7	-2.59	1.34	1.39
1	L1	2424	OMG	C2-N1	2.59	1.44	1.37
45	S2	1490	OMG	O6-C6	-2.58	1.18	1.23
45	S2	1328	OMG	O6-C6	-2.57	1.18	1.23
45	S2	1830	UR3	O2-C2	-2.56	1.17	1.22
45	S2	1703	OMC	C5-C4	2.56	1.48	1.42
1	L1	4220	6MZ	C5-C4	-2.56	1.34	1.39
3	L3	75	OMG	C2-N1	2.56	1.44	1.37
45	S2	867	OMG	O6-C6	-2.55	1.18	1.23
1	L1	1534	A2M	C8-N9	-2.55	1.32	1.37
1	L1	3899	OMG	C2-N1	2.55	1.44	1.37
1	L1	4228	OMG	C2-N1	2.54	1.44	1.37
1	L1	4530	UR3	O4-C4	-2.53	1.18	1.23
1	L1	2364	OMG	C2-N1	2.51	1.43	1.37
45	S2	1490	OMG	C2-N1	2.51	1.43	1.37
1	L1	978	2MG	CM2-N2	2.51	1.50	1.45
45	S2	601	OMG	C2-N1	2.51	1.43	1.37
1	L1	1522	OMG	C5-C6	2.50	1.53	1.44
45	S2	174	OMC	C5-C4	2.50	1.48	1.42
45	S2	1710	OMC	C5-C4	2.50	1.48	1.42
45	S2	1447	OMG	C6-N1	-2.50	1.34	1.38
1	L1	4637	OMG	C5-C6	2.50	1.53	1.44
45	S2	436	OMG	C2-N1	2.49	1.43	1.37
45	S2	1288	OMU	O2-C2	-2.49	1.18	1.23
1	L1	3701	OMC	C5-C4	2.48	1.48	1.42
45	S2	1850	MA6	C8-N9	-2.48	1.33	1.37
1	L1	3762	B8H	O2-C2	-2.48	1.18	1.23
1	L1	2364	OMG	C5-C6	2.47	1.53	1.44
1	L1	3869	OMC	C5-C4	2.46	1.48	1.42
1	L1	4392	OMG	C5-C6	2.46	1.53	1.44
45	S2	462	OMC	C5-C4	2.45	1.48	1.42
45	S2	644	OMG	C2-N1	2.45	1.43	1.37
1	L1	3944	OMG	C5-C6	2.45	1.53	1.44
1	L1	3744	OMG	C2-N1	2.45	1.43	1.37
1	L1	2876	OMG	C2-N1	2.45	1.43	1.37
1	L1	4494	OMG	C2-N1	2.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	1272	OMC	C5-C4	2.45	1.48	1.42
1	L1	4618	OMG	C2-N1	2.45	1.43	1.37
1	L1	1456	JMH	C5-C4	2.44	1.48	1.42
1	L1	3818	UY1	C4-C5	-2.44	1.37	1.44
1	L1	1517	2MG	C4-N9	-2.44	1.31	1.38
1	L1	3627	OMG	C5-C6	2.44	1.53	1.44
1	L1	4220	6MZ	C5-N7	-2.44	1.34	1.39
45	S2	1328	OMG	C5-C6	2.44	1.53	1.44
1	L1	2363	A2M	C8-N9	-2.44	1.33	1.37
1	L1	3744	OMG	C5-C6	2.44	1.53	1.44
45	S2	683	OMG	C2-N1	2.43	1.43	1.37
45	S2	509	OMG	C5-C6	2.43	1.53	1.44
1	L1	4392	OMG	C2-N1	2.43	1.43	1.37
1	L1	2876	OMG	C5-C6	2.43	1.53	1.44
45	S2	1851	MA6	C8-N9	-2.42	1.33	1.37
1	L1	4370	OMG	C2-N1	2.41	1.43	1.37
45	S2	867	OMG	C6-N1	2.41	1.43	1.38
45	S2	509	OMG	C2-N1	2.41	1.43	1.37
1	L1	1517	2MG	C6-N1	2.40	1.43	1.38
1	L1	4196	OMG	C2-N1	2.40	1.43	1.37
1	L1	4623	OMG	C5-C6	2.39	1.53	1.44
45	S2	517	OMC	C5-C4	2.39	1.48	1.42
3	L3	75	OMG	C5-C6	2.39	1.53	1.44
1	L1	4530	UR3	O2-C2	-2.38	1.18	1.22
1	L1	4623	OMG	C2-N1	2.38	1.43	1.37
45	S2	668	A2M	O5'-C5'	-2.38	1.38	1.44
1	L1	4618	OMG	C5-C6	2.38	1.53	1.44
1	L1	2422	OMC	C5-C4	2.37	1.48	1.42
1	L1	978	2MG	C6-N1	2.37	1.43	1.38
1	L1	2365	OMC	C5-C4	2.37	1.48	1.42
45	S2	1328	OMG	C6-N1	2.37	1.43	1.38
45	S2	436	OMG	C5-C6	2.37	1.53	1.44
45	S2	1842	4AC	O7-C7	-2.36	1.17	1.23
45	S2	644	OMG	C5-C6	2.36	1.53	1.44
1	L1	4228	OMG	C5-C6	2.36	1.53	1.44
45	S2	1490	OMG	C5-C6	2.36	1.53	1.44
1	L1	3792	OMG	C5-C6	2.36	1.53	1.44
1	L1	1316	OMG	C2-N1	2.36	1.43	1.37
45	S2	1391	OMC	C5-C4	2.35	1.48	1.42
1	L1	4536	OMC	C5-C4	2.35	1.48	1.42
45	S2	683	OMG	C5-C6	2.35	1.53	1.44
1	L1	4494	OMG	C5-C6	2.34	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1881	OMC	C5-C4	2.34	1.48	1.42
1	L1	4196	OMG	C5-C6	2.34	1.53	1.44
1	L1	4499	OMG	C5-C6	2.33	1.53	1.44
1	L1	4228	OMG	C4-N9	-2.33	1.32	1.38
45	S2	867	OMG	C5-C6	2.33	1.53	1.44
1	L1	3944	OMG	C6-N1	2.33	1.43	1.38
45	S2	1830	UR3	O4-C4	-2.33	1.18	1.23
1	L1	3808	OMC	C5-C4	2.33	1.48	1.42
1	L1	1316	OMG	C5-C6	2.32	1.53	1.44
1	L1	1677	PSU	O4'-C1'	-2.32	1.40	1.43
45	S2	601	OMG	C5-C6	2.32	1.53	1.44
1	L1	3792	OMG	C2-N1	2.31	1.43	1.37
1	L1	978	2MG	C4-N9	-2.31	1.32	1.38
1	L1	3899	OMG	C4-N9	-2.31	1.32	1.38
1	L1	3899	OMG	C5-C6	2.30	1.53	1.44
1	L1	729	2MG	C4-N9	-2.30	1.32	1.38
1	L1	2861	OMC	C5-C4	2.30	1.48	1.42
1	L1	2364	OMG	C6-N1	2.30	1.43	1.38
1	L1	3867	A2M	C8-N9	-2.30	1.33	1.37
1	L1	3841	OMC	C5-C4	2.30	1.48	1.42
45	S2	1326	UY1	C4-C5	-2.30	1.37	1.44
45	S2	512	A2M	C8-N9	-2.29	1.33	1.37
45	S2	1832	6MZ	C5-C4	-2.28	1.34	1.39
45	S2	1832	6MZ	C8-N9	-2.28	1.33	1.37
1	L1	1522	OMG	C2-N1	2.27	1.43	1.37
1	L1	1524	A2M	C8-N9	-2.27	1.33	1.37
45	S2	644	OMG	C6-N1	2.27	1.43	1.38
45	S2	1490	OMG	C6-N1	2.26	1.43	1.38
45	S2	1678	A2M	C8-N9	-2.26	1.33	1.37
1	L1	2351	OMC	C5-C4	2.26	1.48	1.42
1	L1	4637	OMG	C2-N1	2.25	1.43	1.37
45	S2	484	A2M	C8-N9	-2.25	1.33	1.37
3	L3	75	OMG	C6-N1	2.24	1.43	1.38
1	L1	2424	OMG	C4-N9	-2.24	1.32	1.38
1	L1	4370	OMG	C5-C6	2.24	1.52	1.44
1	L1	3887	OMC	C5-C4	2.23	1.48	1.42
1	L1	2824	OMC	C5-C4	2.23	1.48	1.42
1	L1	3627	OMG	C2-N1	2.23	1.43	1.37
45	S2	601	OMG	C6-N1	2.22	1.43	1.38
1	L1	2424	OMG	C6-N1	2.22	1.43	1.38
45	S2	159	A2M	C8-N9	-2.22	1.33	1.37
1	L1	3785	A2M	O3'-C3'	-2.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	668	A2M	C8-N9	-2.20	1.33	1.37
1	L1	2424	OMG	C5-C6	2.20	1.52	1.44
45	S2	1832	6MZ	C5-N7	-2.19	1.34	1.39
45	S2	1447	OMG	C5-N7	-2.18	1.34	1.39
1	L1	3718	A2M	C8-N9	-2.18	1.33	1.37
1	L1	3785	A2M	O5'-C5'	-2.18	1.39	1.44
1	L1	2364	OMG	C4-N9	-2.18	1.32	1.38
1	L1	4571	A2M	C8-N9	-2.18	1.33	1.37
1	L1	3818	UY1	O2'-C2'	-2.18	1.37	1.42
1	L1	2401	A2M	C8-N9	-2.17	1.33	1.37
45	S2	1219	JMH	C5-C4	2.17	1.47	1.42
45	S2	683	OMG	C6-N1	2.16	1.42	1.38
1	L1	2815	A2M	C8-N9	-2.16	1.33	1.37
1	L1	2815	A2M	O5'-C5'	-2.15	1.39	1.44
45	S2	590	A2M	C8-N9	-2.15	1.33	1.37
1	L1	3818	UY1	O3'-C3'	2.15	1.48	1.43
1	L1	729	2MG	CM2-N2	2.15	1.49	1.45
45	S2	436	OMG	C6-N1	2.14	1.42	1.38
45	S2	27	A2M	C8-N9	-2.14	1.33	1.37
1	L1	4499	OMG	C6-N1	2.14	1.42	1.38
1	L1	2876	OMG	C6-N1	2.14	1.42	1.38
1	L1	3627	OMG	C6-N1	2.13	1.42	1.38
1	L1	1524	A2M	O5'-C5'	-2.13	1.39	1.44
1	L1	3825	A2M	C8-N9	-2.13	1.33	1.37
1	L1	4196	OMG	C6-N1	2.13	1.42	1.38
1	L1	4620	OMU	C6-N1	2.12	1.43	1.38
1	L1	3723	A2M	C8-N9	-2.12	1.33	1.37
45	S2	1288	OMU	C5-C4	2.12	1.48	1.43
1	L1	1522	OMG	C6-N1	2.11	1.42	1.38
1	L1	4498	OMU	C6-N1	2.11	1.43	1.38
45	S2	99	A2M	C8-N9	-2.11	1.33	1.37
45	S2	1031	A2M	C8-N9	-2.11	1.33	1.37
45	S2	1248	B8N	O4'-C1'	-2.11	1.40	1.43
1	L1	1871	A2M	O5'-C5'	-2.11	1.39	1.44
45	S2	576	A2M	C8-N9	-2.10	1.33	1.37
45	S2	1442	OMU	C6-N1	2.10	1.43	1.38
45	S2	1337	4AC	O7-C7	-2.10	1.18	1.23
1	L1	400	A2M	C8-N9	-2.10	1.33	1.37
1	L1	4456	OMC	C5-C4	2.10	1.47	1.42
45	S2	1830	UR3	C5-C4	2.10	1.49	1.43
45	S2	1288	OMU	C6-N1	2.09	1.43	1.38
1	L1	4228	OMG	C6-N1	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4623	OMG	C6-N1	2.09	1.42	1.38
1	L1	3899	OMG	C6-N1	2.09	1.42	1.38
1	L1	3785	A2M	C8-N9	-2.08	1.33	1.37
1	L1	1871	A2M	C8-N9	-2.08	1.33	1.37
45	S2	166	A2M	C8-N9	-2.08	1.33	1.37
45	S2	468	A2M	O5'-C5'	-2.08	1.39	1.44
1	L1	1340	OMC	C5-C4	2.07	1.47	1.42
1	L1	398	A2M	C8-N9	-2.07	1.33	1.37
1	L1	1522	OMG	C4-N9	-2.06	1.32	1.38
45	S2	99	A2M	O5'-C5'	-2.05	1.39	1.44
1	L1	4530	UR3	C5-C4	2.05	1.49	1.43
45	S2	468	A2M	C8-N9	-2.05	1.33	1.37
1	L1	4494	OMG	C6-N1	2.05	1.42	1.38
1	L1	4227	OMU	C6-N1	2.05	1.42	1.38
1	L1	2401	A2M	O5'-C5'	-2.05	1.39	1.44
1	L1	4623	OMG	C4-N9	-2.05	1.32	1.38
1	L1	4196	OMG	C4-N9	-2.04	1.32	1.38
1	L1	3792	OMG	C6-N1	2.04	1.42	1.38
1	L1	1534	A2M	O5'-C5'	-2.03	1.39	1.44
45	S2	1031	A2M	O5'-C5'	-2.03	1.39	1.44
1	L1	4523	A2M	O5'-C5'	-2.03	1.39	1.44
45	S2	509	OMG	C6-N1	2.03	1.42	1.38
45	S2	354	OMU	C5-C4	2.03	1.48	1.43
1	L1	3830	A2M	O5'-C5'	-2.03	1.39	1.44
1	L1	4370	OMG	C4-N9	-2.03	1.32	1.38
1	L1	729	2MG	C6-N1	2.02	1.42	1.38
45	S2	1248	B8N	C32-C33	2.02	1.57	1.53
1	L1	4530	UR3	C4-N3	2.02	1.45	1.40
1	L1	1517	2MG	C5-C6	2.02	1.51	1.44
45	S2	428	OMU	C6-N1	2.01	1.42	1.38
1	L1	3744	OMG	C4-N9	-2.01	1.32	1.38

All (888) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	1851	MA6	N1-C6-N6	-18.31	97.06	117.08
45	S2	1850	MA6	N1-C6-N6	-15.79	99.82	117.08
45	S2	1806	M7A	C5-C6-N6	13.72	147.18	123.74
45	S2	1806	M7A	N6-C6-N1	-11.74	92.64	118.35
45	S2	1851	MA6	C5-C6-N6	10.50	143.58	125.30
45	S2	814	5MU	C5-C4-N3	9.82	123.69	115.31
45	S2	1850	MA6	C5-C6-N6	9.01	141.00	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	814	5MU	C5-C6-N1	-7.87	115.24	123.34
1	L1	3785	A2M	N6-C6-N1	-7.33	102.29	118.35
45	S2	1850	MA6	C4-N9-C1'	-7.32	109.16	126.59
1	L1	1534	A2M	N6-C6-N1	-7.30	102.37	118.35
1	L1	3830	A2M	N6-C6-N1	-7.29	102.39	118.35
1	L1	3867	A2M	N6-C6-N1	-7.20	102.59	118.35
45	S2	512	A2M	N6-C6-N1	-7.18	102.63	118.35
1	L1	2363	A2M	N6-C6-N1	-7.15	102.69	118.35
1	L1	2815	A2M	N6-C6-N1	-7.11	102.78	118.35
1	L1	3825	A2M	N6-C6-N1	-7.08	102.84	118.35
1	L1	1871	A2M	N6-C6-N1	-7.07	102.88	118.35
45	S2	27	A2M	N6-C6-N1	-7.05	102.92	118.35
45	S2	166	A2M	N6-C6-N1	-7.04	102.93	118.35
1	L1	400	A2M	N6-C6-N1	-7.02	102.97	118.35
45	S2	576	A2M	N6-C6-N1	-6.96	103.11	118.35
45	S2	159	A2M	N6-C6-N1	-6.96	103.11	118.35
45	S2	668	A2M	N6-C6-N1	-6.95	103.14	118.35
45	S2	468	A2M	N6-C6-N1	-6.93	103.17	118.35
1	L1	398	A2M	N6-C6-N1	-6.93	103.18	118.35
45	S2	1383	A2M	N6-C6-N1	-6.92	103.20	118.35
1	L1	2401	A2M	N6-C6-N1	-6.91	103.21	118.35
1	L1	1517	2MG	C2-N3-C4	6.90	120.59	112.04
45	S2	484	A2M	N6-C6-N1	-6.89	103.26	118.35
45	S2	1678	A2M	N6-C6-N1	-6.88	103.28	118.35
45	S2	590	A2M	N6-C6-N1	-6.88	103.29	118.35
1	L1	3718	A2M	N6-C6-N1	-6.86	103.32	118.35
1	L1	3762	B8H	C4-N3-C2	-6.86	118.47	127.35
1	L1	4571	A2M	N6-C6-N1	-6.82	103.42	118.35
1	L1	3723	A2M	N6-C6-N1	-6.81	103.44	118.35
45	S2	1851	MA6	C5-C4-N3	-6.75	117.95	126.75
45	S2	99	A2M	N6-C6-N1	-6.70	103.68	118.35
1	L1	1871	A2M	C5-C6-N6	6.67	137.94	123.43
45	S2	1031	A2M	N6-C6-N1	-6.65	103.79	118.35
1	L1	1326	A2M	N6-C6-N1	-6.64	103.80	118.35
1	L1	2876	OMG	C5-C4-N3	-6.62	117.72	128.46
45	S2	1850	MA6	C1'-N9-C8	6.60	142.03	127.14
1	L1	2787	A2M	N6-C6-N1	-6.54	104.02	118.35
45	S2	814	5MU	C4-N3-C2	-6.53	118.90	127.35
45	S2	512	A2M	C5-C6-N6	6.51	137.60	123.43
1	L1	1534	A2M	C5-C6-N6	6.49	137.55	123.43
1	L1	4523	A2M	N6-C6-N1	-6.46	104.21	118.35
1	L1	978	2MG	C2-N3-C4	6.45	120.04	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	590	A2M	C5-C4-N3	-6.44	118.35	126.75
1	L1	1524	A2M	N6-C6-N1	-6.43	104.26	118.35
1	L1	1625	OMG	C5-C4-N3	-6.35	118.16	128.46
45	S2	668	A2M	C5-C6-N6	6.34	137.23	123.43
1	L1	2401	A2M	C5-C6-N6	6.32	137.17	123.43
1	L1	2363	A2M	C5-C6-N6	6.29	137.11	123.43
1	L1	400	A2M	C5-C6-N6	6.27	137.08	123.43
1	L1	3867	A2M	C5-C6-N6	6.25	137.02	123.43
45	S2	166	A2M	C5-C6-N6	6.23	136.98	123.43
1	L1	3818	UY1	N1-C2-N3	6.19	122.14	115.13
1	L1	3825	A2M	C5-C6-N6	6.18	136.89	123.43
1	L1	3830	A2M	C5-C6-N6	6.18	136.87	123.43
45	S2	576	A2M	C5-C6-N6	6.18	136.87	123.43
45	S2	27	A2M	C5-C6-N6	6.18	136.87	123.43
1	L1	3718	A2M	C5-C6-N6	6.17	136.85	123.43
45	S2	468	A2M	C5-C6-N6	6.16	136.83	123.43
45	S2	159	A2M	C5-C6-N6	6.15	136.81	123.43
45	S2	1447	OMG	C5-C4-N3	-6.14	118.49	128.46
45	S2	1678	A2M	C5-C6-N6	6.13	136.78	123.43
1	L1	4571	A2M	C5-C6-N6	6.13	136.76	123.43
1	L1	398	A2M	C5-C6-N6	6.12	136.75	123.43
1	L1	2815	A2M	C5-C6-N6	6.12	136.75	123.43
45	S2	484	A2M	C5-C6-N6	6.10	136.71	123.43
1	L1	4392	OMG	C5-C4-N3	-6.09	118.58	128.46
1	L1	1322	1MA	C1'-N9-C8	-6.09	109.36	126.70
45	S2	512	A2M	N3-C2-N1	-6.09	119.08	128.60
45	S2	1851	MA6	C4-N9-C1'	-6.05	112.17	126.59
1	L1	3825	A2M	N3-C2-N1	-6.05	119.14	128.60
1	L1	3785	A2M	C5-C6-N6	6.04	136.58	123.43
45	S2	1031	A2M	C5-C6-N6	6.02	136.54	123.43
1	L1	3830	A2M	N3-C2-N1	-6.01	119.20	128.60
1	L1	729	2MG	C2-N3-C4	5.99	119.46	112.04
45	S2	1383	A2M	C5-C6-N6	5.98	136.45	123.43
45	S2	1031	A2M	N3-C2-N1	-5.97	119.27	128.60
1	L1	1326	A2M	C5-C6-N6	5.96	136.40	123.43
1	L1	3925	OMU	C4-N3-C2	-5.95	118.73	126.58
1	L1	3723	A2M	C5-C6-N6	5.95	136.38	123.43
1	L1	4220	6MZ	N1-C2-N3	-5.95	119.30	128.60
45	S2	1851	MA6	N1-C2-N3	-5.91	119.35	128.60
45	S2	99	A2M	C5-C6-N6	5.91	136.29	123.43
45	S2	590	A2M	C5-C6-N6	5.90	136.28	123.43
1	L1	3762	B8H	N3-C2-N1	5.90	121.51	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	166	A2M	N3-C2-N1	-5.85	119.44	128.60
1	L1	2401	A2M	N3-C2-N1	-5.85	119.46	128.60
45	S2	683	OMG	C5-C4-N3	-5.84	118.98	128.46
1	L1	4637	OMG	C5-C4-N3	-5.83	119.01	128.46
1	L1	398	A2M	C5-C4-N3	-5.82	119.16	126.75
1	L1	2363	A2M	N3-C2-N1	-5.81	119.52	128.60
1	L1	2815	A2M	N3-C2-N1	-5.80	119.52	128.60
1	L1	3867	A2M	C5-C4-N3	-5.79	119.19	126.75
1	L1	1524	A2M	N3-C2-N1	-5.79	119.54	128.60
1	L1	1871	A2M	N3-C2-N1	-5.78	119.56	128.60
45	S2	468	A2M	N3-C2-N1	-5.76	119.60	128.60
45	S2	576	A2M	C5-C4-N3	-5.74	119.26	126.75
45	S2	1851	MA6	C1'-N9-C8	5.71	140.02	127.14
1	L1	1524	A2M	C5-C6-N6	5.70	135.84	123.43
45	S2	1383	A2M	N3-C2-N1	-5.69	119.70	128.60
1	L1	3723	A2M	N3-C2-N1	-5.69	119.70	128.60
1	L1	2787	A2M	C5-C6-N6	5.69	135.80	123.43
1	L1	400	A2M	N3-C2-N1	-5.67	119.74	128.60
1	L1	4571	A2M	N3-C2-N1	-5.66	119.75	128.60
45	S2	1678	A2M	N3-C2-N1	-5.65	119.76	128.60
45	S2	436	OMG	C5-C4-N3	-5.65	119.29	128.46
1	L1	4523	A2M	C5-C6-N6	5.65	135.72	123.43
1	L1	3792	OMG	C5-C4-N3	-5.65	119.30	128.46
1	L1	1316	OMG	C5-C4-N3	-5.65	119.30	128.46
45	S2	159	A2M	N3-C2-N1	-5.65	119.77	128.60
1	L1	1534	A2M	N3-C2-N1	-5.64	119.78	128.60
1	L1	4498	OMU	C4-N3-C2	-5.63	119.15	126.58
1	L1	1524	A2M	C5-C4-N3	-5.63	119.41	126.75
1	L1	2787	A2M	N3-C2-N1	-5.62	119.81	128.60
45	S2	590	A2M	N3-C2-N1	-5.62	119.81	128.60
45	S2	27	A2M	N3-C2-N1	-5.61	119.82	128.60
1	L1	4523	A2M	N3-C2-N1	-5.61	119.83	128.60
1	L1	4494	OMG	C5-C4-N3	-5.60	119.38	128.46
45	S2	99	A2M	N3-C2-N1	-5.60	119.85	128.60
45	S2	644	OMG	C5-C4-N3	-5.58	119.41	128.46
1	L1	4499	OMG	C5-C4-N3	-5.57	119.42	128.46
45	S2	512	A2M	C5-C4-N3	-5.57	119.49	126.75
45	S2	1832	6MZ	N1-C2-N3	-5.55	119.92	128.60
1	L1	2787	A2M	C5-C4-N3	-5.53	119.53	126.75
1	L1	4523	A2M	C5-C4-N3	-5.53	119.53	126.75
45	S2	1383	A2M	C5-C4-N3	-5.52	119.55	126.75
45	S2	354	OMU	C4-N3-C2	-5.51	119.31	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	159	A2M	C5-C4-N3	-5.51	119.56	126.75
1	L1	1326	A2M	N3-C2-N1	-5.51	119.99	128.60
45	S2	668	A2M	N3-C2-N1	-5.49	120.01	128.60
1	L1	398	A2M	N3-C2-N1	-5.49	120.02	128.60
1	L1	4618	OMG	C5-C4-N3	-5.48	119.57	128.46
1	L1	3944	OMG	C5-C4-N3	-5.48	119.57	128.46
45	S2	484	A2M	N3-C2-N1	-5.48	120.04	128.60
1	L1	3830	A2M	C5-C4-N3	-5.47	119.61	126.75
45	S2	166	A2M	C5-C4-N3	-5.47	119.61	126.75
1	L1	1322	1MA	C1'-N9-C4	5.47	142.75	126.50
3	L3	75	OMG	C5-C4-N3	-5.47	119.59	128.46
45	S2	509	OMG	C5-C4-N3	-5.45	119.61	128.46
45	S2	27	A2M	C5-C4-N3	-5.45	119.64	126.75
45	S2	1678	A2M	C5-C4-N3	-5.45	119.64	126.75
45	S2	601	OMG	C5-C4-N3	-5.43	119.65	128.46
45	S2	484	A2M	C5-C4-N3	-5.43	119.67	126.75
1	L1	3785	A2M	C5-C4-N3	-5.43	119.67	126.75
45	S2	576	A2M	N3-C2-N1	-5.42	120.12	128.60
45	S2	1326	UY1	N1-C2-N3	5.41	121.25	115.13
1	L1	3627	OMG	C5-C4-N3	-5.40	119.70	128.46
1	L1	3785	A2M	N3-C2-N1	-5.37	120.19	128.60
1	L1	2401	A2M	C5-C4-N3	-5.37	119.74	126.75
1	L1	3744	OMG	C5-C4-N3	-5.36	119.76	128.46
45	S2	99	A2M	C5-C4-N3	-5.35	119.77	126.75
45	S2	1850	MA6	C5-C4-N3	-5.35	119.77	126.75
1	L1	3718	A2M	C5-C4-N3	-5.35	119.77	126.75
1	L1	2363	A2M	C5-C4-N3	-5.35	119.78	126.75
45	S2	1850	MA6	N1-C2-N3	-5.34	120.25	128.60
45	S2	172	OMU	C4-N3-C2	-5.33	119.55	126.58
45	S2	1328	OMG	C5-C4-N3	-5.33	119.82	128.46
45	S2	867	OMG	C5-C4-N3	-5.32	119.84	128.46
1	L1	2815	A2M	C5-C4-N3	-5.31	119.82	126.75
1	L1	1322	1MA	N1-C2-N3	-5.31	119.69	126.00
45	S2	1806	M7A	N3-C2-N1	-5.29	120.32	128.60
1	L1	4227	OMU	C4-N3-C2	-5.29	119.60	126.58
1	L1	1326	A2M	C5-C4-N3	-5.28	119.86	126.75
45	S2	1219	JMH	C1'-N1-C2	5.28	125.90	116.99
45	S2	468	A2M	C5-C4-N3	-5.26	119.88	126.75
1	L1	4196	OMG	C5-C4-N3	-5.26	119.93	128.46
1	L1	3723	A2M	C5-C4-N3	-5.22	119.94	126.75
3	L3	14	OMU	C4-N3-C2	-5.21	119.71	126.58
1	L1	3825	A2M	C5-C4-N3	-5.21	119.95	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	1031	A2M	C5-C4-N3	-5.21	119.96	126.75
1	L1	400	A2M	C5-C4-N3	-5.20	119.97	126.75
1	L1	2364	OMG	C5-C4-N3	-5.19	120.04	128.46
45	S2	428	OMU	C4-N3-C2	-5.19	119.73	126.58
1	L1	4370	OMG	C5-C4-N3	-5.19	120.04	128.46
1	L1	2837	OMU	C4-N3-C2	-5.19	119.74	126.58
1	L1	1677	PSU	N1-C2-N3	5.17	120.99	115.13
45	S2	1490	OMG	C5-C4-N3	-5.17	120.07	128.46
1	L1	1522	OMG	C5-C4-N3	-5.16	120.08	128.46
1	L1	4530	UR3	C4-N3-C2	-5.16	119.70	124.56
1	L1	4623	OMG	C5-C4-N3	-5.15	120.11	128.46
1	L1	2876	OMG	C2-N3-C4	5.14	121.46	112.30
1	L1	4306	OMU	C4-N3-C2	-5.13	119.81	126.58
45	S2	668	A2M	C5-C4-N3	-5.12	120.07	126.75
1	L1	3867	A2M	N3-C2-N1	-5.11	120.61	128.60
1	L1	1871	A2M	C5-C4-N3	-5.11	120.09	126.75
1	L1	4571	A2M	C5-C4-N3	-5.10	120.09	126.75
45	S2	1442	OMU	C4-N3-C2	-5.08	119.87	126.58
1	L1	3718	A2M	N3-C2-N1	-5.08	120.65	128.60
45	S2	1806	M7A	N3-C4-N9	5.06	133.26	126.87
45	S2	1288	OMU	C4-N3-C2	-5.04	119.93	126.58
1	L1	4636	PSU	C4-N3-C2	-5.01	119.12	126.34
45	S2	116	OMU	C4-N3-C2	-5.01	119.97	126.58
45	S2	1447	OMG	C2-N3-C4	5.00	121.21	112.30
45	S2	1248	B8N	C5-C4-N3	4.96	125.36	116.17
1	L1	3899	OMG	C5-C4-N3	-4.95	120.43	128.46
1	L1	2424	OMG	C5-C4-N3	-4.94	120.44	128.46
1	L1	1625	OMG	N9-C4-N3	4.93	135.83	125.94
1	L1	4220	6MZ	C5-C4-N3	-4.93	120.32	126.75
45	S2	1832	6MZ	C5-C4-N3	-4.92	120.33	126.75
1	L1	2364	OMG	C2-N3-C4	4.91	121.04	112.30
1	L1	1677	PSU	C4-N3-C2	-4.86	119.34	126.34
1	L1	1625	OMG	C2-N3-C4	4.85	120.95	112.30
1	L1	729	2MG	C5-C4-N3	-4.85	120.60	128.46
1	L1	4620	OMU	C4-N3-C2	-4.82	120.22	126.58
1	L1	978	2MG	C5-C4-N3	-4.80	120.68	128.46
1	L1	1534	A2M	C5-C4-N3	-4.78	120.51	126.75
1	L1	4450	PSU	C4-N3-C2	-4.78	119.45	126.34
1	L1	4636	PSU	N1-C2-N3	4.75	120.52	115.13
1	L1	3715	PSU	N1-C2-N3	4.74	120.50	115.13
1	L1	4450	PSU	N1-C2-N3	4.72	120.48	115.13
1	L1	4403	PSU	C4-N3-C2	-4.71	119.55	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	683	OMG	C2-N3-C4	4.71	120.69	112.30
1	L1	4228	OMG	C5-C4-N3	-4.70	120.83	128.46
1	L1	1517	2MG	C5-C4-N3	-4.70	120.84	128.46
45	S2	814	5MU	N3-C2-N1	4.70	121.12	114.89
1	L1	729	2MG	C1'-N9-C8	-4.69	113.35	126.70
1	L1	3792	OMG	C2-N3-C4	4.68	120.64	112.30
3	L3	75	OMG	C2-N3-C4	4.68	120.63	112.30
1	L1	3627	OMG	C2-N3-C4	4.67	120.63	112.30
45	S2	1851	MA6	N3-C4-N9	4.67	134.77	127.08
1	L1	4618	OMG	C2-N3-C4	4.66	120.61	112.30
45	S2	1081	PSU	C4-N3-C2	-4.66	119.62	126.34
1	L1	4499	OMG	C2-N3-C4	4.66	120.60	112.30
45	S2	612	PSU	N1-C2-N3	4.63	120.38	115.13
1	L1	4228	OMG	C1'-N9-C4	-4.63	112.76	126.50
45	S2	121	OMU	C4-N3-C2	-4.60	120.51	126.58
45	S2	1081	PSU	N1-C2-N3	4.60	120.34	115.13
1	L1	3715	PSU	C4-N3-C2	-4.59	119.73	126.34
45	S2	823	PSU	C4-N3-C2	-4.58	119.73	126.34
1	L1	4494	OMG	C2-N3-C4	4.58	120.47	112.30
45	S2	436	OMG	C2-N3-C4	4.58	120.45	112.30
1	L1	3944	OMG	C2-N3-C4	4.58	120.45	112.30
45	S2	822	PSU	N1-C2-N3	4.57	120.31	115.13
45	S2	1851	MA6	C4-C5-C6	4.57	120.99	115.88
1	L1	1683	PSU	N1-C2-N3	4.56	120.30	115.13
45	S2	601	OMG	C2-N3-C4	4.55	120.41	112.30
1	L1	4442	PSU	C4-N3-C2	-4.55	119.79	126.34
1	L1	4403	PSU	N1-C2-N3	4.54	120.28	115.13
1	L1	4623	OMG	C2-N3-C4	4.52	120.36	112.30
1	L1	3925	OMU	N3-C2-N1	4.51	120.87	114.89
1	L1	4196	OMG	C2-N3-C4	4.50	120.32	112.30
1	L1	4637	OMG	C2-N3-C4	4.50	120.32	112.30
1	L1	3744	OMG	C2-N3-C4	4.50	120.31	112.30
1	L1	4531	PSU	C4-N3-C2	-4.48	119.88	126.34
1	L1	4442	PSU	N1-C2-N3	4.46	120.18	115.13
45	S2	1447	OMG	N9-C4-N3	4.46	134.89	125.94
45	S2	644	OMG	C2-N3-C4	4.45	120.23	112.30
1	L1	1522	OMG	C2-N3-C4	4.45	120.22	112.30
45	S2	1850	MA6	C4-C5-C6	4.45	120.86	115.88
45	S2	822	PSU	C4-N3-C2	-4.44	119.94	126.34
45	S2	1328	OMG	C2-N3-C4	4.44	120.20	112.30
1	L1	4392	OMG	C2-N3-C4	4.43	120.20	112.30
1	L1	2508	PSU	C4-N3-C2	-4.43	119.95	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	867	OMG	C2-N3-C4	4.43	120.19	112.30
1	L1	4293	PSU	C4-N3-C2	-4.43	119.96	126.34
45	S2	1678	A2M	N9-C8-N7	-4.41	107.88	113.91
1	L1	4628	PSU	C4-N3-C2	-4.41	119.98	126.34
1	L1	2508	PSU	N1-C2-N3	4.41	120.13	115.13
1	L1	4500	PSU	C4-N3-C2	-4.41	119.98	126.34
45	S2	1243	PSU	N1-C2-N3	4.41	120.12	115.13
45	S2	1830	UR3	C4-N3-C2	-4.40	120.42	124.56
45	S2	612	PSU	C4-N3-C2	-4.39	120.02	126.34
1	L1	3899	OMG	C2-N3-C4	4.38	120.10	112.30
1	L1	4228	OMG	C1'-N9-C8	4.37	139.15	126.70
1	L1	2424	OMG	C2-N3-C4	4.37	120.08	112.30
1	L1	978	2MG	C2-N1-C6	-4.36	119.46	124.48
45	S2	823	PSU	N1-C2-N3	4.35	120.06	115.13
45	S2	590	A2M	N3-C4-N9	4.34	134.24	127.08
1	L1	1316	OMG	C2-N3-C4	4.34	120.02	112.30
1	L1	2876	OMG	N9-C4-N3	4.32	134.62	125.94
1	L1	4293	PSU	N1-C2-N3	4.32	120.03	115.13
45	S2	1243	PSU	C4-N3-C2	-4.32	120.12	126.34
1	L1	4500	PSU	N1-C2-N3	4.32	120.02	115.13
45	S2	119	PSU	N1-C2-N3	4.32	120.02	115.13
45	S2	1490	OMG	C2-N3-C4	4.31	119.98	112.30
45	S2	1850	MA6	N9-C8-N7	-4.29	108.05	113.91
1	L1	3785	A2M	O4'-C1'-N9	4.29	116.51	108.06
45	S2	1830	UR3	C1'-N1-C2	4.28	124.22	116.99
45	S2	668	A2M	N9-C8-N7	-4.28	108.06	113.91
1	L1	4531	PSU	N1-C2-N3	4.28	119.98	115.13
45	S2	1248	B8N	C4-N3-C2	-4.27	120.06	125.46
1	L1	3764	PSU	N1-C2-N3	4.26	119.96	115.13
1	L1	3729	PSU	C4-N3-C2	-4.23	120.24	126.34
1	L1	1683	PSU	C4-N3-C2	-4.23	120.25	126.34
1	L1	4628	PSU	N1-C2-N3	4.23	119.92	115.13
45	S2	1806	M7A	C4-N9-C1'	-4.22	116.58	126.60
45	S2	468	A2M	N9-C8-N7	-4.22	108.14	113.91
45	S2	1832	6MZ	N9-C8-N7	-4.22	108.15	113.91
1	L1	4370	OMG	C2-N3-C4	4.21	119.80	112.30
45	S2	1851	MA6	C2-N3-C4	4.21	121.70	111.75
1	L1	3818	UY1	C4-N3-C2	-4.21	120.27	126.34
1	L1	729	2MG	C2-N1-C6	-4.21	119.64	124.48
45	S2	814	5MU	C5M-C5-C6	-4.20	117.24	122.85
1	L1	3899	OMG	C1'-N9-C4	-4.19	114.07	126.50
45	S2	509	OMG	C2-N3-C4	4.18	119.75	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3764	PSU	C4-N3-C2	-4.17	120.33	126.34
1	L1	1582	PSU	N1-C2-N3	4.17	119.85	115.13
45	S2	119	PSU	C4-N3-C2	-4.17	120.33	126.34
1	L1	1517	2MG	C2-N1-C6	-4.17	119.69	124.48
1	L1	3825	A2M	N9-C8-N7	-4.16	108.22	113.91
45	S2	27	A2M	N9-C8-N7	-4.16	108.22	113.91
1	L1	2401	A2M	N9-C8-N7	-4.14	108.25	113.91
1	L1	3729	PSU	N1-C2-N3	4.14	119.81	115.13
1	L1	3830	A2M	N9-C8-N7	-4.13	108.26	113.91
1	L1	3723	A2M	N9-C8-N7	-4.12	108.27	113.91
1	L1	1522	OMG	C1'-N9-C4	-4.12	114.26	126.50
45	S2	166	A2M	N9-C8-N7	-4.11	108.30	113.91
1	L1	4623	OMG	C1'-N9-C4	-4.08	114.38	126.50
1	L1	3785	A2M	N9-C8-N7	-4.07	108.34	113.91
45	S2	1850	MA6	N3-C4-N9	4.07	133.79	127.08
45	S2	1383	A2M	N9-C8-N7	-4.07	108.35	113.91
1	L1	4228	OMG	C2-N3-C4	4.07	119.55	112.30
45	S2	159	A2M	N9-C8-N7	-4.05	108.38	113.91
45	S2	1851	MA6	N9-C8-N7	-4.04	108.39	113.91
1	L1	978	2MG	C1'-N9-C8	-4.04	115.21	126.70
1	L1	4523	A2M	N9-C8-N7	-4.03	108.40	113.91
1	L1	4220	6MZ	C9-N6-C6	-4.03	119.41	122.87
1	L1	1871	A2M	N9-C8-N7	-4.01	108.43	113.91
1	L1	400	A2M	N9-C8-N7	-4.01	108.43	113.91
1	L1	2363	A2M	N9-C8-N7	-4.00	108.44	113.91
1	L1	2787	A2M	N9-C8-N7	-4.00	108.44	113.91
45	S2	590	A2M	C2-N3-C4	4.00	121.20	111.75
1	L1	2351	OMC	O2-C2-N3	-3.98	115.86	122.33
45	S2	1031	A2M	N9-C8-N7	-3.98	108.47	113.91
45	S2	116	OMU	N3-C2-N1	3.98	120.17	114.89
45	S2	1219	JMH	C6-N1-C2	-3.97	118.23	121.79
1	L1	4498	OMU	N3-C2-N1	3.96	120.15	114.89
45	S2	1326	UY1	C4-N3-C2	-3.96	120.63	126.34
45	S2	99	A2M	N9-C8-N7	-3.94	108.52	113.91
1	L1	1522	OMG	C1'-N9-C8	3.93	137.87	126.70
1	L1	2424	OMG	C1'-N9-C4	-3.92	114.86	126.50
1	L1	4370	OMG	C1'-N9-C4	-3.89	114.95	126.50
45	S2	354	OMU	N3-C2-N1	3.88	120.04	114.89
1	L1	3825	A2M	C2-N3-C4	3.88	120.91	111.75
1	L1	1582	PSU	C4-N3-C2	-3.88	120.75	126.34
1	L1	3830	A2M	C2-N3-C4	3.87	120.89	111.75
1	L1	398	A2M	N9-C8-N7	-3.87	108.62	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4571	A2M	N9-C8-N7	-3.86	108.63	113.91
1	L1	4447	5MC	C5-C6-N1	-3.86	119.37	123.34
1	L1	4623	OMG	C1'-N9-C8	3.85	137.65	126.70
1	L1	3867	A2M	N9-C8-N7	-3.83	108.67	113.91
1	L1	4498	OMU	C5-C4-N3	3.83	120.58	114.84
1	L1	1524	A2M	N9-C8-N7	-3.82	108.69	113.91
1	L1	4306	OMU	N3-C2-N1	3.81	119.94	114.89
1	L1	2815	A2M	N9-C8-N7	-3.80	108.71	113.91
45	S2	512	A2M	C2-N3-C4	3.80	120.73	111.75
1	L1	4392	OMG	N9-C4-N3	3.80	133.57	125.94
45	S2	172	OMU	N3-C2-N1	3.80	119.93	114.89
45	S2	166	A2M	C2-N3-C4	3.80	120.72	111.75
45	S2	1851	MA6	C2-N1-C6	3.78	120.69	111.75
1	L1	729	2MG	C1'-N9-C4	3.78	137.74	126.50
1	L1	1326	A2M	N9-C8-N7	-3.78	108.75	113.91
45	S2	590	A2M	N9-C8-N7	-3.77	108.76	113.91
45	S2	867	OMG	C1'-N9-C4	-3.76	115.32	126.50
1	L1	3818	UY1	O2-C2-N1	-3.75	118.66	122.79
1	L1	2424	OMG	C1'-N9-C8	3.75	137.38	126.70
1	L1	2815	A2M	C2-N3-C4	3.75	120.61	111.75
1	L1	1524	A2M	N3-C4-N9	3.75	133.26	127.08
1	L1	1524	A2M	C2-N3-C4	3.75	120.60	111.75
1	L1	4620	OMU	N3-C2-N1	3.74	119.86	114.89
45	S2	576	A2M	N9-C8-N7	-3.74	108.80	113.91
1	L1	2363	A2M	C2-N3-C4	3.74	120.58	111.75
1	L1	2787	A2M	C2-N3-C4	3.73	120.56	111.75
45	S2	428	OMU	N3-C2-N1	3.72	119.83	114.89
45	S2	1328	OMG	C1'-N9-C4	-3.72	115.44	126.50
1	L1	1534	A2M	N9-C8-N7	-3.72	108.82	113.91
1	L1	1517	2MG	C1'-N9-C8	-3.72	116.11	126.70
1	L1	398	A2M	C2-N3-C4	3.71	120.52	111.75
45	S2	512	A2M	N9-C8-N7	-3.71	108.84	113.91
1	L1	3627	OMG	C1'-N9-C4	-3.70	115.50	126.50
1	L1	3744	OMG	C1'-N9-C4	-3.70	115.50	126.50
45	S2	159	A2M	C2-N3-C4	3.70	120.50	111.75
45	S2	1383	A2M	C2-N3-C4	3.69	120.47	111.75
45	S2	1678	A2M	C2-N3-C4	3.69	120.47	111.75
45	S2	512	A2M	N3-C4-N9	3.69	133.16	127.08
1	L1	2401	A2M	C2-N3-C4	3.69	120.46	111.75
45	S2	576	A2M	C2-N3-C4	3.68	120.45	111.75
45	S2	27	A2M	C2-N3-C4	3.68	120.45	111.75
1	L1	3899	OMG	C1'-N9-C8	3.68	137.17	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	867	OMG	C1'-N9-C8	3.67	137.14	126.70
1	L1	4523	A2M	C2-N3-C4	3.66	120.40	111.75
1	L1	4220	6MZ	N9-C8-N7	-3.66	108.91	113.91
1	L1	4227	OMU	C5-C4-N3	3.65	120.30	114.84
45	S2	484	A2M	N9-C8-N7	-3.64	108.93	113.91
1	L1	3867	A2M	C2-N3-C4	3.64	120.35	111.75
1	L1	1316	OMG	N9-C4-N3	3.64	133.25	125.94
45	S2	468	A2M	C2-N3-C4	3.64	120.35	111.75
1	L1	4370	OMG	C1'-N9-C8	3.64	137.05	126.70
45	S2	683	OMG	N9-C4-N3	3.63	133.23	125.94
1	L1	1517	2MG	N9-C8-N7	-3.63	106.56	113.39
1	L1	3785	A2M	C2-N3-C4	3.62	120.30	111.75
45	S2	1442	OMU	N3-C2-N1	3.61	119.69	114.89
1	L1	4227	OMU	N3-C2-N1	3.61	119.68	114.89
45	S2	1031	A2M	C2-N3-C4	3.60	120.27	111.75
1	L1	3723	A2M	C2-N3-C4	3.59	120.24	111.75
1	L1	400	A2M	C2-N3-C4	3.59	120.23	111.75
45	S2	99	A2M	C2-N3-C4	3.59	120.23	111.75
1	L1	3744	OMG	C1'-N9-C8	3.59	136.91	126.70
1	L1	2364	OMG	C1'-N9-C4	-3.59	115.85	126.50
1	L1	4618	OMG	C1'-N9-C4	-3.59	115.85	126.50
1	L1	4220	6MZ	C2-N3-C4	3.58	120.21	111.75
45	S2	1832	6MZ	C5-N7-C8	3.58	108.59	103.51
45	S2	1850	MA6	C2-N1-C6	3.57	120.20	111.75
1	L1	2876	OMG	C2-N1-C6	-3.57	118.58	125.10
45	S2	576	A2M	N3-C4-N9	3.57	132.96	127.08
45	S2	354	OMU	C5-C4-N3	3.57	120.18	114.84
1	L1	2837	OMU	N3-C2-N1	3.56	119.62	114.89
3	L3	14	OMU	C5-C4-N3	3.55	120.16	114.84
45	S2	484	A2M	C2-N3-C4	3.55	120.14	111.75
45	S2	1288	OMU	N3-C2-N1	3.55	119.60	114.89
1	L1	1326	A2M	C2-N3-C4	3.55	120.13	111.75
1	L1	3792	OMG	N9-C4-N3	3.55	133.06	125.94
45	S2	1490	OMG	C1'-N9-C4	-3.54	115.98	126.50
1	L1	3762	B8H	O2-C2-N1	-3.53	118.90	122.87
1	L1	2364	OMG	C1'-N9-C8	3.53	136.74	126.70
1	L1	4637	OMG	N9-C4-N3	3.52	133.00	125.94
45	S2	1832	6MZ	C4-C5-C6	3.52	119.53	116.81
1	L1	4499	OMG	C1'-N9-C4	-3.52	116.06	126.50
1	L1	4571	A2M	C2-N3-C4	3.52	120.06	111.75
3	L3	14	OMU	N3-C2-N1	3.51	119.55	114.89
45	S2	601	OMG	C1'-N9-C4	-3.51	116.09	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	814	5MU	O4-C4-C5	-3.50	120.84	124.90
1	L1	2815	A2M	N3-C4-N9	3.50	132.85	127.08
45	S2	1374	5MC	C5-C6-N1	-3.48	119.75	123.34
45	S2	436	OMG	N9-C4-N3	3.48	132.93	125.94
1	L1	4494	OMG	C1'-N9-C8	3.48	136.60	126.70
1	L1	1534	A2M	C2-N3-C4	3.48	119.97	111.75
45	S2	814	5MU	C6-C5-C4	3.47	120.94	118.03
3	L3	75	OMG	C1'-N9-C4	-3.47	116.20	126.50
45	S2	644	OMG	N9-C4-N3	3.47	132.90	125.94
45	S2	1328	OMG	C1'-N9-C8	3.46	136.56	126.70
1	L1	3925	OMU	C5-C4-N3	3.46	120.01	114.84
1	L1	1871	A2M	C2-N3-C4	3.46	119.91	111.75
45	S2	1832	6MZ	C2-N3-C4	3.46	119.91	111.75
1	L1	2837	OMU	C5-C4-N3	3.45	120.01	114.84
45	S2	121	OMU	N3-C2-N1	3.45	119.47	114.89
1	L1	1322	1MA	C2-N3-C4	3.44	119.18	112.41
1	L1	3944	OMG	C1'-N9-C4	-3.44	116.27	126.50
1	L1	3627	OMG	N9-C4-N3	3.44	132.85	125.94
45	S2	509	OMG	C1'-N9-C4	-3.44	116.28	126.50
1	L1	4618	OMG	N9-C4-N3	3.44	132.84	125.94
1	L1	1316	OMG	C1'-N9-C4	-3.43	116.31	126.50
45	S2	509	OMG	C1'-N9-C8	3.42	136.42	126.70
1	L1	3867	A2M	N3-C4-N9	3.42	132.71	127.08
45	S2	668	A2M	C2-N3-C4	3.41	119.81	111.75
1	L1	4196	OMG	C1'-N9-C4	-3.41	116.38	126.50
1	L1	398	A2M	N3-C4-N9	3.40	132.69	127.08
1	L1	4494	OMG	C1'-N9-C4	-3.40	116.40	126.50
1	L1	4523	A2M	N3-C4-N9	3.40	132.68	127.08
45	S2	1678	A2M	N3-C4-N9	3.39	132.66	127.08
45	S2	1490	OMG	C1'-N9-C8	3.39	136.34	126.70
45	S2	159	A2M	N3-C4-N9	3.39	132.66	127.08
45	S2	1850	MA6	C2-N3-C4	3.38	119.75	111.75
1	L1	4499	OMG	N9-C4-N3	3.38	132.74	125.94
1	L1	3762	B8H	C5-C4-N3	3.38	124.23	116.58
45	S2	1678	A2M	C5-N7-C8	3.38	108.31	103.51
1	L1	4220	6MZ	C4-C5-C6	3.38	119.42	116.81
45	S2	1851	MA6	C5-N7-C8	3.37	108.30	103.51
45	S2	683	OMG	C2-N1-C6	-3.37	118.95	125.10
3	L3	75	OMG	N9-C4-N3	3.37	132.70	125.94
1	L1	1871	A2M	N3-C4-N9	3.36	132.62	127.08
1	L1	3627	OMG	C1'-N9-C8	3.36	136.25	126.70
1	L1	2401	A2M	N3-C4-N9	3.35	132.60	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	1383	A2M	N3-C4-N9	3.35	132.60	127.08
1	L1	4335	5MC	C5-C6-N1	-3.34	119.90	123.34
45	S2	172	OMU	C5-C4-N3	3.34	119.84	114.84
1	L1	4499	OMG	C1'-N9-C8	3.34	136.20	126.70
1	L1	4392	OMG	C2-N1-C6	-3.34	119.02	125.10
1	L1	2363	A2M	N3-C4-N9	3.33	132.58	127.08
45	S2	1442	OMU	C5-C4-N3	3.33	119.82	114.84
1	L1	3944	OMG	N9-C4-N3	3.33	132.62	125.94
45	S2	644	OMG	C1'-N9-C4	-3.33	116.62	126.50
45	S2	436	OMG	C1'-N9-C4	-3.32	116.64	126.50
45	S2	166	A2M	N3-C4-N9	3.31	132.54	127.08
1	L1	3718	A2M	C2-N3-C4	3.31	119.58	111.75
45	S2	428	OMU	C5-C4-N3	3.31	119.79	114.84
1	L1	4620	OMU	C5-C4-N3	3.30	119.78	114.84
45	S2	601	OMG	N9-C4-N3	3.30	132.56	125.94
45	S2	1031	A2M	N3-C4-N9	3.29	132.50	127.08
1	L1	978	2MG	N9-C8-N7	-3.29	107.20	113.39
45	S2	1288	OMU	C5-C4-N3	3.29	119.75	114.84
1	L1	4494	OMG	C2-N1-C6	-3.28	119.11	125.10
3	L3	75	OMG	C1'-N9-C8	3.28	136.03	126.70
1	L1	4306	OMU	C5-C4-N3	3.28	119.75	114.84
1	L1	729	2MG	N9-C8-N7	-3.28	107.22	113.39
1	L1	2787	A2M	N3-C4-N9	3.27	132.47	127.08
45	S2	601	OMG	C1'-N9-C8	3.27	136.01	126.70
45	S2	1248	B8N	N3-C2-N1	3.27	121.38	116.76
1	L1	3944	OMG	C1'-N9-C8	3.26	135.99	126.70
1	L1	4618	OMG	C1'-N9-C8	3.26	135.99	126.70
45	S2	683	OMG	C1'-N9-C4	-3.26	116.81	126.50
45	S2	1806	M7A	C2-N3-C4	3.26	119.45	111.75
45	S2	1447	OMG	C6-C5-N7	3.25	136.29	130.25
1	L1	1326	A2M	N3-C4-N9	3.25	132.44	127.08
45	S2	509	OMG	N9-C4-N3	3.25	132.46	125.94
45	S2	116	OMU	C5-C4-N3	3.24	119.69	114.84
1	L1	4196	OMG	C1'-N9-C8	3.23	135.90	126.70
1	L1	4370	OMG	N9-C4-N3	3.23	132.42	125.94
45	S2	99	A2M	N3-C4-N9	3.23	132.40	127.08
45	S2	1326	UY1	O2-C2-N1	-3.23	119.24	122.79
1	L1	3723	A2M	N3-C4-N9	3.22	132.40	127.08
1	L1	3785	A2M	N3-C4-N9	3.22	132.39	127.08
1	L1	3899	OMG	N9-C4-N3	3.22	132.40	125.94
45	S2	484	A2M	N3-C4-N9	3.22	132.38	127.08
45	S2	601	OMG	C2-N1-C6	-3.21	119.24	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3830	A2M	N3-C4-N9	3.21	132.38	127.08
1	L1	978	2MG	C1'-N9-C4	3.21	136.04	126.50
45	S2	27	A2M	N3-C4-N9	3.21	132.37	127.08
1	L1	3782	5MC	C5-C6-N1	-3.21	120.04	123.34
1	L1	1316	OMG	C1'-N9-C8	3.20	135.80	126.70
1	L1	4637	OMG	C1'-N9-C4	-3.19	117.02	126.50
45	S2	509	OMG	C2-N1-C6	-3.19	119.28	125.10
45	S2	1328	OMG	N9-C4-N3	3.19	132.34	125.94
45	S2	668	A2M	C5-N7-C8	3.19	108.04	103.51
45	S2	1219	JMH	O2-C2-N3	-3.18	116.86	121.34
1	L1	4637	OMG	C2-N1-C6	-3.17	119.31	125.10
1	L1	2363	A2M	C5-N7-C8	3.17	108.01	103.51
45	S2	468	A2M	N3-C4-N9	3.17	132.30	127.08
1	L1	1322	1MA	C5-C4-N3	-3.16	122.54	127.26
45	S2	1832	6MZ	C9-N6-C6	3.16	125.59	122.87
45	S2	27	A2M	C5-N7-C8	3.16	107.99	103.51
1	L1	4494	OMG	N9-C4-N3	3.15	132.26	125.94
1	L1	3899	OMG	C2-N1-C6	-3.14	119.37	125.10
45	S2	683	OMG	C1'-N9-C8	3.14	135.64	126.70
1	L1	3867	A2M	C5-N7-C8	3.14	107.97	103.51
45	S2	436	OMG	C1'-N9-C8	3.14	135.63	126.70
45	S2	121	OMU	C5-C4-N3	3.14	119.53	114.84
1	L1	2401	A2M	C5-N7-C8	3.13	107.96	103.51
1	L1	4499	OMG	C2-N1-C6	-3.13	119.38	125.10
45	S2	867	OMG	N9-C4-N3	3.13	132.23	125.94
45	S2	436	OMG	C2-N1-C6	-3.13	119.39	125.10
45	S2	644	OMG	C2-N1-C6	-3.13	119.39	125.10
1	L1	3785	A2M	C2'-C1'-N9	-3.13	108.27	113.53
45	S2	468	A2M	C5-N7-C8	3.13	107.95	103.51
1	L1	3944	OMG	C2-N1-C6	-3.12	119.41	125.10
1	L1	4196	OMG	N9-C4-N3	3.11	132.18	125.94
1	L1	3825	A2M	N3-C4-N9	3.11	132.20	127.08
45	S2	644	OMG	C1'-N9-C8	3.10	135.53	126.70
1	L1	398	A2M	C5-N7-C8	3.10	107.91	103.51
3	L3	75	OMG	C2-N1-C6	-3.09	119.46	125.10
1	L1	400	A2M	N3-C4-N9	3.09	132.18	127.08
45	S2	1447	OMG	C2'-C1'-N9	-3.09	108.22	114.22
45	S2	1328	OMG	C2-N1-C6	-3.09	119.47	125.10
1	L1	4571	A2M	N3-C4-N9	3.08	132.16	127.08
45	S2	1806	M7A	C71-N7-C5	-3.08	112.18	124.01
1	L1	4637	OMG	C1'-N9-C8	3.07	135.44	126.70
1	L1	2424	OMG	C2-N1-C6	-3.07	119.50	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	166	A2M	C5-N7-C8	3.07	107.86	103.51
1	L1	3792	OMG	C1'-N9-C4	-3.06	117.42	126.50
45	S2	1490	OMG	N9-C4-N3	3.06	132.08	125.94
1	L1	3792	OMG	C2-N1-C6	-3.06	119.53	125.10
1	L1	4370	OMG	C2-N1-C6	-3.05	119.54	125.10
45	S2	590	A2M	C5-N7-C8	3.04	107.83	103.51
1	L1	4618	OMG	C2-N1-C6	-3.04	119.56	125.10
45	S2	159	A2M	C5-N7-C8	3.04	107.82	103.51
1	L1	3830	A2M	C5-N7-C8	3.03	107.82	103.51
1	L1	2351	OMC	O2-C2-N1	3.03	125.14	118.89
1	L1	3825	A2M	C5-N7-C8	3.03	107.81	103.51
1	L1	4628	PSU	O2-C2-N1	-3.03	119.46	122.79
1	L1	3744	OMG	N9-C4-N3	3.02	132.01	125.94
1	L1	4196	OMG	C2-N1-C6	-3.01	119.60	125.10
1	L1	3899	OMG	N9-C8-N7	-3.01	107.72	113.39
1	L1	4500	PSU	O2-C2-N1	-3.01	119.48	122.79
45	S2	668	A2M	N3-C4-N9	3.01	132.04	127.08
1	L1	4228	OMG	N9-C8-N7	-3.00	107.75	113.39
1	L1	4623	OMG	N9-C4-N3	2.99	131.95	125.94
45	S2	1383	A2M	C5-N7-C8	2.99	107.76	103.51
1	L1	4623	OMG	C2-N1-C6	-2.99	119.65	125.10
1	L1	3744	OMG	C2-N1-C6	-2.99	119.65	125.10
1	L1	4523	A2M	C5-N7-C8	2.99	107.75	103.51
1	L1	4671	B8T	C6-C5-C4	2.99	120.62	116.96
1	L1	1316	OMG	C2-N1-C6	-2.99	119.65	125.10
45	S2	867	OMG	C2-N1-C6	-2.98	119.67	125.10
1	L1	3627	OMG	C2-N1-C6	-2.98	119.67	125.10
1	L1	4227	OMU	O4-C4-C5	-2.97	119.93	125.16
1	L1	1322	1MA	N9-C8-N7	-2.97	107.80	113.39
1	L1	2787	A2M	C5-N7-C8	2.96	107.72	103.51
1	L1	3718	A2M	N9-C8-N7	-2.96	109.86	113.91
1	L1	1677	PSU	C6-C5-C4	2.96	120.27	118.20
1	L1	3718	A2M	N3-C4-N9	2.95	131.94	127.08
45	S2	1850	MA6	C5-N7-C8	2.95	107.70	103.51
1	L1	3782	5MC	CM5-C5-C6	-2.94	118.92	122.85
1	L1	400	A2M	C5-N7-C8	2.94	107.69	103.51
1	L1	729	2MG	N9-C4-N3	2.94	131.85	125.94
1	L1	3925	OMU	O4-C4-C5	-2.94	119.99	125.16
45	S2	428	OMU	O4-C4-C5	-2.93	120.00	125.16
45	S2	683	OMG	C5-C6-N1	2.93	120.63	113.19
1	L1	1871	A2M	C5-N7-C8	2.92	107.66	103.51
45	S2	484	A2M	C5-N7-C8	2.92	107.65	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4392	OMG	C1'-N9-C4	-2.91	117.85	126.50
1	L1	3723	A2M	C5-N7-C8	2.91	107.64	103.51
45	S2	99	A2M	C5-N7-C8	2.90	107.63	103.51
1	L1	2424	OMG	N9-C4-N3	2.89	131.75	125.94
1	L1	3627	OMG	C5-C6-N1	2.88	120.51	113.19
45	S2	1442	OMU	O4-C4-C5	-2.88	120.09	125.16
1	L1	2876	OMG	C5-C6-N1	2.87	120.47	113.19
1	L1	3715	PSU	O2-C2-N1	-2.87	119.64	122.79
45	S2	354	OMU	O4-C4-C5	-2.86	120.12	125.16
45	S2	576	A2M	C5-N7-C8	2.86	107.58	103.51
1	L1	3899	OMG	C5-C6-N1	2.86	120.46	113.19
1	L1	4392	OMG	C1'-N9-C8	2.86	134.84	126.70
1	L1	3627	OMG	N9-C8-N7	-2.86	108.00	113.39
1	L1	1522	OMG	N9-C4-N3	2.86	131.67	125.94
1	L1	4618	OMG	C5-C6-N1	2.85	120.44	113.19
1	L1	1524	A2M	C5-N7-C8	2.85	107.56	103.51
45	S2	116	OMU	O4-C4-C5	-2.85	120.15	125.16
1	L1	3792	OMG	C1'-N9-C8	2.84	134.79	126.70
45	S2	612	PSU	O2-C2-N1	-2.84	119.66	122.79
45	S2	601	OMG	C5-C6-N1	2.84	120.40	113.19
1	L1	2364	OMG	C2-N1-C6	-2.84	119.92	125.10
45	S2	1850	MA6	C4-N9-C8	2.84	108.80	105.73
45	S2	1830	UR3	C6-N1-C2	-2.84	119.25	121.79
1	L1	3785	A2M	C5-N7-C8	2.84	107.54	103.51
1	L1	1326	A2M	C5-N7-C8	2.84	107.54	103.51
45	S2	512	A2M	C5-N7-C8	2.83	107.53	103.51
1	L1	4618	OMG	N9-C8-N7	-2.83	108.07	113.39
1	L1	4228	OMG	C2-N1-C6	-2.82	119.95	125.10
1	L1	2815	A2M	C5-N7-C8	2.82	107.52	103.51
45	S2	814	5MU	O2-C2-N3	-2.81	116.26	121.50
45	S2	1288	OMU	O4-C4-C5	-2.81	120.21	125.16
1	L1	2424	OMG	C5-C6-N1	2.81	120.32	113.19
3	L3	75	OMG	C5-C6-N1	2.81	120.32	113.19
1	L1	3808	OMC	O2-C2-N3	-2.80	117.77	122.33
1	L1	4623	OMG	C5-C6-N1	2.80	120.31	113.19
45	S2	1842	4AC	C6-C5-C4	2.80	120.39	116.96
45	S2	1031	A2M	C5-N7-C8	2.80	107.48	103.51
1	L1	1517	2MG	C5-C6-N1	2.79	120.28	113.19
1	L1	3944	OMG	C5-C6-N1	2.79	120.27	113.19
1	L1	4623	OMG	N9-C8-N7	-2.79	108.14	113.39
45	S2	172	OMU	O4-C4-C5	-2.78	120.27	125.16
1	L1	1517	2MG	C1'-N9-C4	2.78	134.76	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	814	5MU	C5M-C5-C4	2.78	121.82	118.77
1	L1	1522	OMG	C2-N1-C6	-2.78	120.04	125.10
45	S2	814	5MU	C1'-N1-C2	2.77	122.59	117.57
1	L1	1517	2MG	N1-C2-N3	-2.77	119.67	123.95
45	S2	436	OMG	C5-C6-N1	2.76	120.21	113.19
1	L1	978	2MG	C5-C6-N1	2.76	120.21	113.19
1	L1	3792	OMG	C5-C6-N1	2.76	120.20	113.19
1	L1	1534	A2M	N3-C4-N9	2.76	131.63	127.08
1	L1	4571	A2M	C5-N7-C8	2.75	107.41	103.51
45	S2	1832	6MZ	C4-C5-N7	-2.75	107.27	110.62
45	S2	1832	6MZ	N3-C4-N9	2.74	131.60	127.08
1	L1	4499	OMG	C5-C6-N1	2.74	120.15	113.19
45	S2	1490	OMG	C2-N1-C6	-2.74	120.10	125.10
1	L1	4220	6MZ	N3-C4-N9	2.74	131.60	127.08
1	L1	1522	OMG	N9-C8-N7	-2.74	108.24	113.39
1	L1	4370	OMG	C5-C6-N1	2.73	120.11	113.19
45	S2	1328	OMG	N9-C8-N7	-2.73	108.26	113.39
45	S2	121	OMU	O4-C4-C5	-2.73	120.37	125.16
45	S2	1328	OMG	C5-C6-N1	2.72	120.09	113.19
1	L1	978	2MG	N9-C4-N3	2.71	131.37	125.94
1	L1	2424	OMG	O6-C6-C5	-2.70	119.43	126.60
45	S2	1337	4AC	C6-C5-C4	2.70	120.27	116.96
1	L1	4494	OMG	C5-C6-N1	2.70	120.05	113.19
45	S2	601	OMG	N9-C8-N7	-2.69	108.32	113.39
1	L1	1534	A2M	C5-N7-C8	2.69	107.33	103.51
1	L1	2364	OMG	N9-C8-N7	-2.69	108.32	113.39
1	L1	3744	OMG	N9-C8-N7	-2.69	108.33	113.39
1	L1	3762	B8H	O4-C4-N3	-2.68	114.98	120.12
1	L1	1677	PSU	O2-C2-N1	-2.68	119.84	122.79
45	S2	1447	OMG	C4-C5-N7	-2.68	106.48	110.72
1	L1	4450	PSU	C6-C5-C4	2.67	120.07	118.20
1	L1	4499	OMG	O6-C6-C5	-2.67	119.51	126.60
1	L1	4392	OMG	C5-C6-N1	2.67	119.97	113.19
1	L1	4531	PSU	O2-C2-N1	-2.67	119.85	122.79
1	L1	4637	OMG	C5-C6-N1	2.67	119.96	113.19
1	L1	1625	OMG	C6-C5-N7	2.66	135.20	130.25
1	L1	3744	OMG	C5-C6-N1	2.65	119.93	113.19
45	S2	867	OMG	C5-C6-N1	2.65	119.93	113.19
1	L1	2837	OMU	O4-C4-C5	-2.65	120.50	125.16
3	L3	75	OMG	N9-C8-N7	-2.65	108.41	113.39
1	L1	2364	OMG	N9-C4-N3	2.64	131.25	125.94
1	L1	1522	OMG	C5-C6-N1	2.64	119.90	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	644	OMG	N9-C8-N7	-2.64	108.41	113.39
45	S2	683	OMG	O6-C6-C5	-2.64	119.59	126.60
45	S2	644	OMG	C5-C6-N1	2.64	119.89	113.19
1	L1	4494	OMG	O6-C6-C5	-2.64	119.60	126.60
45	S2	822	PSU	O2-C2-N1	-2.64	119.89	122.79
45	S2	509	OMG	C5-C6-N1	2.64	119.89	113.19
1	L1	4370	OMG	N9-C8-N7	-2.64	108.43	113.39
1	L1	4636	PSU	C6-C5-C4	2.64	120.04	118.20
1	L1	4196	OMG	C5-C6-N1	2.63	119.88	113.19
1	L1	1316	OMG	C5-C6-N1	2.63	119.87	113.19
45	S2	436	OMG	N9-C8-N7	-2.62	108.45	113.39
1	L1	4196	OMG	N9-C8-N7	-2.62	108.45	113.39
1	L1	4498	OMU	O4-C4-C5	-2.62	120.55	125.16
45	S2	601	OMG	O6-C6-C5	-2.62	119.65	126.60
1	L1	3944	OMG	N9-C8-N7	-2.62	108.46	113.39
1	L1	3792	OMG	N9-C8-N7	-2.61	108.47	113.39
1	L1	4403	PSU	O2-C2-N1	-2.61	119.91	122.79
1	L1	4499	OMG	N9-C8-N7	-2.61	108.47	113.39
1	L1	729	2MG	C5-C6-N1	2.61	119.81	113.19
1	L1	3764	PSU	O2-C2-N1	-2.60	119.93	122.79
1	L1	2364	OMG	C5-C6-N1	2.60	119.79	113.19
3	L3	14	OMU	O4-C4-C5	-2.59	120.60	125.16
1	L1	1316	OMG	N9-C8-N7	-2.59	108.50	113.39
45	S2	1447	OMG	O4'-C1'-N9	2.59	114.29	108.36
3	L3	75	OMG	O6-C6-C5	-2.59	119.74	126.60
45	S2	1806	M7A	C5-C4-N3	-2.58	120.56	126.62
1	L1	4220	6MZ	C5-N7-C8	2.58	107.17	103.51
45	S2	683	OMG	N9-C8-N7	-2.58	108.54	113.39
1	L1	4228	OMG	C5-C6-N1	2.57	119.71	113.19
1	L1	3899	OMG	O6-C6-C5	-2.57	119.79	126.60
1	L1	4637	OMG	N9-C8-N7	-2.56	108.57	113.39
45	S2	1243	PSU	O2-C2-N1	-2.55	119.98	122.79
45	S2	867	OMG	O6-C6-C5	-2.55	119.83	126.60
1	L1	1517	2MG	N9-C4-N3	2.54	131.04	125.94
45	S2	612	PSU	C6-N1-C2	-2.53	120.09	122.68
1	L1	4500	PSU	C6-N1-C2	-2.53	120.09	122.68
45	S2	1490	OMG	C5-C6-N1	2.53	119.60	113.19
1	L1	4530	UR3	C1'-N1-C2	2.52	121.25	116.99
1	L1	2824	OMC	O2-C2-N3	-2.52	118.23	122.33
45	S2	590	A2M	C6-C5-C4	2.52	120.57	117.18
1	L1	3944	OMG	O6-C6-C5	-2.52	119.91	126.60
1	L1	1517	2MG	C8-N7-C5	2.52	108.80	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1456	JMH	C6-N1-C2	-2.51	119.54	121.79
1	L1	1316	OMG	O6-C6-C5	-2.51	119.94	126.60
45	S2	1328	OMG	O6-C6-C5	-2.51	119.95	126.60
45	S2	823	PSU	O2-C2-N1	-2.51	120.03	122.79
45	S2	436	OMG	O6-C6-C5	-2.50	119.97	126.60
1	L1	3841	OMC	O2-C2-N3	-2.50	118.27	122.33
45	S2	1490	OMG	N9-C8-N7	-2.50	108.69	113.39
1	L1	4306	OMU	O4-C4-C5	-2.49	120.78	125.16
1	L1	2364	OMG	N2-C2-N1	2.49	122.01	116.71
1	L1	3792	OMG	O6-C6-C5	-2.49	120.00	126.60
1	L1	2876	OMG	O6-C6-C5	-2.48	120.01	126.60
1	L1	4618	OMG	O6-C6-C5	-2.48	120.01	126.60
1	L1	2424	OMG	N9-C8-N7	-2.48	108.72	113.39
45	S2	867	OMG	N9-C8-N7	-2.47	108.74	113.39
45	S2	1337	4AC	C5-C4-N3	-2.46	118.64	122.59
45	S2	814	5MU	O4-C4-N3	-2.46	115.41	120.12
1	L1	978	2MG	N1-C2-N3	-2.45	120.16	123.95
45	S2	119	PSU	O2-C2-N1	-2.45	120.09	122.79
1	L1	978	2MG	O6-C6-C5	-2.45	120.11	126.60
1	L1	4293	PSU	O2-C2-N1	-2.44	120.10	122.79
45	S2	644	OMG	O6-C6-C5	-2.44	120.13	126.60
1	L1	1517	2MG	O6-C6-C5	-2.44	120.14	126.60
1	L1	3764	PSU	C6-N1-C2	-2.43	120.19	122.68
1	L1	3729	PSU	O2-C2-N1	-2.43	120.11	122.79
45	S2	1490	OMG	O6-C6-C5	-2.43	120.16	126.60
3	L3	14	OMU	C1'-N1-C2	2.43	121.96	117.57
45	S2	1830	UR3	O2-C2-N3	-2.42	117.93	121.34
1	L1	3925	OMU	O2-C2-N1	-2.41	119.58	122.79
1	L1	4370	OMG	O6-C6-C5	-2.41	120.20	126.60
1	L1	4228	OMG	N9-C4-N3	2.41	130.78	125.94
1	L1	4620	OMU	O4-C4-C5	-2.41	120.93	125.16
1	L1	1582	PSU	O2-C2-N1	-2.41	120.14	122.79
1	L1	4623	OMG	O6-C6-C5	-2.40	120.22	126.60
45	S2	1243	PSU	C6-N1-C2	-2.40	120.23	122.68
1	L1	4392	OMG	N9-C8-N7	-2.40	108.88	113.39
45	S2	668	A2M	C3'-C2'-C1'	2.39	107.38	102.89
45	S2	822	PSU	C6-N1-C2	-2.38	120.25	122.68
45	S2	509	OMG	O6-C6-C5	-2.38	120.28	126.60
1	L1	978	2MG	CM2-N2-C2	-2.38	118.61	123.86
1	L1	1683	PSU	C6-N1-C2	-2.38	120.25	122.68
1	L1	1677	PSU	C6-N1-C2	-2.37	120.26	122.68
1	L1	3718	A2M	C6-C5-C4	2.36	120.36	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4636	PSU	O2-C2-N1	-2.36	120.19	122.79
1	L1	1524	A2M	O4'-C1'-N9	2.35	112.69	108.06
1	L1	4196	OMG	O6-C6-C5	-2.35	120.36	126.60
1	L1	3627	OMG	O6-C6-C5	-2.35	120.37	126.60
45	S2	116	OMU	O2-C2-N1	-2.35	119.67	122.79
1	L1	3715	PSU	C6-N1-C2	-2.35	120.28	122.68
45	S2	1842	4AC	C5-C4-N3	-2.34	118.82	122.59
1	L1	3744	OMG	O6-C6-C5	-2.34	120.40	126.60
1	L1	4494	OMG	N9-C8-N7	-2.33	109.00	113.39
1	L1	3718	A2M	C5-N7-C8	2.33	106.82	103.51
1	L1	1524	A2M	C6-C5-C4	2.32	120.30	117.18
1	L1	4530	UR3	C6-N1-C2	-2.31	119.72	121.79
1	L1	729	2MG	O6-C6-C5	-2.31	120.46	126.60
45	S2	1248	B8N	O4'-C1'-C2'	2.31	108.41	105.14
1	L1	398	A2M	C6-C5-C4	2.31	120.29	117.18
1	L1	978	2MG	C8-N7-C5	2.30	108.41	104.24
1	L1	4523	A2M	C6-C5-C4	2.30	120.27	117.18
1	L1	4228	OMG	O6-C6-C5	-2.30	120.50	126.60
45	S2	509	OMG	N9-C8-N7	-2.29	109.08	113.39
45	S2	1219	JMH	C1'-N1-C6	-2.29	115.86	120.84
1	L1	4392	OMG	O6-C6-C5	-2.28	120.54	126.60
45	S2	814	5MU	C1'-N1-C6	-2.28	117.32	121.12
1	L1	729	2MG	C8-N7-C5	2.28	108.36	104.24
45	S2	1678	A2M	C4-N9-C8	2.28	108.19	105.73
45	S2	576	A2M	C6-C5-C4	2.27	120.24	117.18
45	S2	612	PSU	O4'-C1'-C2'	2.27	108.34	105.14
45	S2	1248	B8N	C31-N3-C4	2.26	120.64	117.31
1	L1	1522	OMG	O6-C6-C5	-2.25	120.63	126.60
1	L1	4447	5MC	C5-C4-N3	-2.23	119.27	121.67
1	L1	2364	OMG	C8-N7-C5	2.23	108.28	104.24
1	L1	2824	OMC	C1'-N1-C2	2.23	123.39	118.42
45	S2	1447	OMG	O4'-C4'-C3'	-2.22	100.71	105.11
45	S2	822	PSU	O4'-C1'-C2'	2.22	108.28	105.14
1	L1	3818	UY1	C5-C6-N1	-2.22	118.78	122.11
1	L1	4442	PSU	C6-C5-C4	2.22	119.75	118.20
1	L1	4442	PSU	O4'-C1'-C2'	2.22	108.27	105.14
45	S2	119	PSU	C6-N1-C2	-2.22	120.42	122.68
45	S2	1678	A2M	C4-C5-N7	-2.22	107.92	110.62
1	L1	4531	PSU	C6-N1-C2	-2.22	120.42	122.68
1	L1	3830	A2M	C2'-C1'-N9	-2.21	109.81	113.53
1	L1	3830	A2M	O4'-C1'-N9	2.21	112.42	108.06
1	L1	2364	OMG	O6-C6-C5	-2.21	120.74	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1625	OMG	C4-C5-N7	-2.21	107.22	110.72
1	L1	2787	A2M	C6-C5-C4	2.21	120.15	117.18
1	L1	3867	A2M	C4-C5-N7	-2.20	107.94	110.62
1	L1	729	2MG	N1-C2-N3	-2.19	120.57	123.95
1	L1	4636	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	L1	1322	1MA	C2'-C1'-N9	2.18	119.40	113.22
1	L1	1522	OMG	C8-N7-C5	2.18	108.19	104.24
1	L1	1522	OMG	C2'-C1'-N9	-2.18	109.99	114.22
45	S2	1248	B8N	O4-C4-N3	-2.17	116.29	119.98
1	L1	2351	OMC	C1'-N1-C2	2.17	123.26	118.42
1	L1	2508	PSU	O2-C2-N1	-2.17	120.41	122.79
1	L1	398	A2M	C4-C5-N7	-2.16	107.99	110.62
1	L1	2837	OMU	C2'-C1'-N1	-2.15	110.04	114.22
1	L1	2364	OMG	C4-C5-N7	-2.15	107.31	110.72
1	L1	3867	A2M	C6-C5-C4	2.15	120.07	117.18
1	L1	3718	A2M	C5-C4-N9	2.15	108.28	105.78
1	L1	3729	PSU	C6-N1-C2	-2.15	120.49	122.68
1	L1	1625	OMG	O6-C6-C5	-2.15	120.91	126.60
45	S2	1447	OMG	O6-C6-C5	-2.15	120.91	126.60
1	L1	2876	OMG	C8-N7-C5	2.14	108.11	104.24
45	S2	484	A2M	C6-C5-C4	2.14	120.06	117.18
1	L1	4228	OMG	C8-N7-C5	2.14	108.11	104.24
45	S2	27	A2M	C4-C5-N7	-2.13	108.02	110.62
1	L1	3744	OMG	C8-N7-C5	2.13	108.10	104.24
45	S2	1081	PSU	O2-C2-N1	-2.13	120.44	122.79
45	S2	1081	PSU	O4'-C1'-C2'	2.13	108.15	105.14
45	S2	1710	OMC	O2-C2-N3	-2.13	118.88	122.33
1	L1	3899	OMG	C8-N7-C5	2.12	108.09	104.24
1	L1	1582	PSU	C6-N1-C2	-2.12	120.51	122.68
45	S2	668	A2M	C4-C5-N7	-2.12	108.03	110.62
1	L1	1871	A2M	C2'-C1'-N9	-2.12	109.95	113.53
1	L1	2876	OMG	N9-C8-N7	-2.12	109.39	113.39
1	L1	3782	5MC	O2-C2-N3	-2.12	118.88	122.33
45	S2	1678	A2M	C6-C5-C4	2.12	120.03	117.18
1	L1	3627	OMG	C8-N7-C5	2.11	108.06	104.24
45	S2	99	A2M	C6-C5-C4	2.11	120.02	117.18
1	L1	1871	A2M	C6-C5-C4	2.10	120.01	117.18
1	L1	4392	OMG	C8-N7-C5	2.10	108.04	104.24
1	L1	3723	A2M	C4-N9-C8	2.09	107.99	105.73
1	L1	2364	OMG	N1-C2-N3	-2.09	119.43	123.32
45	S2	512	A2M	C6-C5-C4	2.09	119.99	117.18
1	L1	1316	OMG	C8-N7-C5	2.09	108.01	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4442	PSU	O2-C2-N1	-2.08	120.50	122.79
45	S2	172	OMU	O2-C2-N1	-2.08	120.03	122.79
45	S2	668	A2M	C4-N9-C8	2.07	107.97	105.73
45	S2	436	OMG	C8-N7-C5	2.07	107.99	104.24
1	L1	4637	OMG	C8-N7-C5	2.07	107.99	104.24
45	S2	668	A2M	C6-C5-C4	2.07	119.97	117.18
1	L1	1326	A2M	C6-C5-C4	2.07	119.96	117.18
45	S2	1391	OMC	O2-C2-N3	-2.07	118.97	122.33
1	L1	4618	OMG	C8-N7-C5	2.06	107.98	104.24
45	S2	159	A2M	C6-C5-C4	2.06	119.96	117.18
45	S2	1031	A2M	C6-C5-C4	2.06	119.95	117.18
1	L1	1524	A2M	C4'-O4'-C1'	-2.06	104.93	109.47
1	L1	1517	2MG	C4-C5-N7	-2.05	107.47	110.72
1	L1	4403	PSU	O4'-C1'-C2'	2.05	108.04	105.14
45	S2	354	OMU	O2-C2-N1	-2.05	120.06	122.79
1	L1	1871	A2M	C4-N9-C8	2.04	107.94	105.73
45	S2	644	OMG	C8-N7-C5	2.04	107.94	104.24
45	S2	1374	5MC	CM5-C5-C6	-2.04	120.12	122.85
1	L1	4637	OMG	O6-C6-C5	-2.04	121.19	126.60
45	S2	1081	PSU	C6-N1-C2	-2.04	120.60	122.68
45	S2	468	A2M	C4-N9-C8	2.04	107.94	105.73
1	L1	398	A2M	C5-C4-N9	2.03	108.15	105.78
45	S2	484	A2M	C4-C5-N7	-2.03	108.15	110.62
1	L1	3715	PSU	C6-C5-C4	2.03	119.62	118.20
1	L1	2424	OMG	N2-C2-N1	2.03	121.03	116.71
45	S2	468	A2M	C4-C5-N7	-2.02	108.15	110.62
1	L1	3944	OMG	C8-N7-C5	2.02	107.91	104.24
45	S2	823	PSU	C6-N1-C2	-2.02	120.61	122.68
1	L1	4499	OMG	C8-N7-C5	2.02	107.90	104.24
45	S2	159	A2M	C4-C5-N7	-2.02	108.16	110.62
1	L1	4623	OMG	C8-N7-C5	2.02	107.90	104.24
45	S2	1832	6MZ	C4-N9-C8	2.02	107.92	105.73
1	L1	4196	OMG	C8-N7-C5	2.02	107.89	104.24
1	L1	1522	OMG	C4-C5-N7	-2.01	107.53	110.72
1	L1	3792	OMG	C8-N7-C5	2.01	107.88	104.24
1	L1	2401	A2M	C6-C5-C4	2.01	119.89	117.18
45	S2	1328	OMG	C8-N7-C5	2.01	107.88	104.24
45	S2	683	OMG	C8-N7-C5	2.01	107.88	104.24
1	L1	4335	5MC	CM5-C5-C6	-2.01	120.17	122.85
3	L3	75	OMG	C8-N7-C5	2.00	107.87	104.24
45	S2	601	OMG	C8-N7-C5	2.00	107.86	104.24

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L1	1340	OMC	C3'-C4'-C5'-O5'
1	L1	1340	OMC	O4'-C4'-C5'-O5'
1	L1	1677	PSU	C2'-C1'-C5-C6
1	L1	2424	OMG	O4'-C4'-C5'-O5'
1	L1	2424	OMG	C3'-C4'-C5'-O5'
1	L1	3701	OMC	C2'-C1'-N1-C6
1	L1	3764	PSU	C3'-C4'-C5'-O5'
1	L1	3764	PSU	O4'-C4'-C5'-O5'
1	L1	3808	OMC	C3'-C4'-C5'-O5'
1	L1	3818	UY1	O4'-C4'-C5'-O5'
1	L1	3841	OMC	C3'-C4'-C5'-O5'
1	L1	3867	A2M	C3'-C4'-C5'-O5'
1	L1	3925	OMU	C1'-C2'-O2'-CM2
1	L1	3944	OMG	C3'-C4'-C5'-O5'
1	L1	4196	OMG	C1'-C2'-O2'-CM2
1	L1	4500	PSU	C3'-C4'-C5'-O5'
1	L1	4636	PSU	C3'-C4'-C5'-O5'
1	L1	4637	OMG	C1'-C2'-O2'-CM2
3	L3	14	OMU	C1'-C2'-O2'-CM2
45	S2	512	A2M	O4'-C4'-C5'-O5'
45	S2	576	A2M	O4'-C4'-C5'-O5'
45	S2	576	A2M	C3'-C4'-C5'-O5'
45	S2	590	A2M	O4'-C4'-C5'-O5'
45	S2	601	OMG	C1'-C2'-O2'-CM2
45	S2	644	OMG	C1'-C2'-O2'-CM2
45	S2	668	A2M	O4'-C4'-C5'-O5'
45	S2	668	A2M	C3'-C4'-C5'-O5'
45	S2	867	OMG	C3'-C4'-C5'-O5'
45	S2	867	OMG	C1'-C2'-O2'-CM2
45	S2	1248	B8N	O4'-C4'-C5'-O5'
45	S2	1248	B8N	C3'-C4'-C5'-O5'
45	S2	1328	OMG	C1'-C2'-O2'-CM2
45	S2	1391	OMC	C3'-C4'-C5'-O5'
45	S2	1442	OMU	C1'-C2'-O2'-CM2
45	S2	1442	OMU	O4'-C4'-C5'-O5'
45	S2	1447	OMG	C1'-C2'-O2'-CM2
45	S2	1678	A2M	C1'-C2'-O2'-CM'
45	S2	1830	UR3	O4'-C1'-N1-C2
45	S2	1832	6MZ	N1-C6-N6-C9
1	L1	3701	OMC	C2'-C1'-N1-C2
1	L1	3729	PSU	O4'-C4'-C5'-O5'
1	L1	3785	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L1	3785	A2M	C3'-C4'-C5'-O5'
1	L1	3841	OMC	O4'-C4'-C5'-O5'
1	L1	3867	A2M	O4'-C4'-C5'-O5'
1	L1	4500	PSU	O4'-C4'-C5'-O5'
45	S2	512	A2M	C3'-C4'-C5'-O5'
45	S2	590	A2M	C3'-C4'-C5'-O5'
45	S2	683	OMG	O4'-C4'-C5'-O5'
45	S2	683	OMG	C3'-C4'-C5'-O5'
45	S2	1243	PSU	O4'-C4'-C5'-O5'
45	S2	1391	OMC	O4'-C4'-C5'-O5'
45	S2	1851	MA6	O4'-C4'-C5'-O5'
1	L1	3808	OMC	O4'-C4'-C5'-O5'
1	L1	3818	UY1	C3'-C4'-C5'-O5'
1	L1	3944	OMG	O4'-C4'-C5'-O5'
1	L1	4636	PSU	O4'-C4'-C5'-O5'
45	S2	99	A2M	O4'-C4'-C5'-O5'
45	S2	867	OMG	O4'-C4'-C5'-O5'
45	S2	1442	OMU	C3'-C4'-C5'-O5'
45	S2	1851	MA6	C3'-C4'-C5'-O5'
45	S2	1830	UR3	O4'-C1'-N1-C6
1	L1	1534	A2M	C3'-C2'-O2'-CM'
1	L1	4447	5MC	C2'-C1'-N1-C6
1	L1	3729	PSU	C3'-C4'-C5'-O5'
45	S2	1243	PSU	C3'-C4'-C5'-O5'
42	Lo	53	MLZ	CE-CD-CG-CB
1	L1	398	A2M	O4'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C4'-C5'-O5'
1	L1	2364	OMG	O4'-C4'-C5'-O5'
45	S2	159	A2M	C3'-C4'-C5'-O5'
1	L1	2787	A2M	C2'-C1'-N9-C8
1	L1	2787	A2M	C2'-C1'-N9-C4
45	S2	1850	MA6	C5-C6-N6-C10
1	L1	1677	PSU	C3'-C4'-C5'-O5'
1	L1	4447	5MC	O4'-C1'-N1-C6
45	S2	517	OMC	O4'-C4'-C5'-O5'
1	L1	4620	OMU	C1'-C2'-O2'-CM2
1	L1	4447	5MC	C2'-C1'-N1-C2
1	L1	1534	A2M	C4'-C5'-O5'-P
1	L1	3818	UY1	C4'-C5'-O5'-P
45	S2	517	OMC	C3'-C4'-C5'-O5'
1	L1	4500	PSU	C4'-C5'-O5'-P
1	L1	2824	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
45	S2	1248	B8N	N3-C31-C32-C33
1	L1	3701	OMC	O4'-C1'-N1-C6
1	L1	4447	5MC	O4'-C1'-N1-C2
45	S2	590	A2M	C4'-C5'-O5'-P
45	S2	1490	OMG	C4'-C5'-O5'-P
45	S2	159	A2M	O4'-C4'-C5'-O5'
1	L1	3701	OMC	O4'-C1'-N1-C2
1	L1	1524	A2M	C3'-C2'-O2'-CM'
1	L1	1322	1MA	C2'-C1'-N9-C8
1	L1	2364	OMG	C3'-C4'-C5'-O5'
45	S2	668	A2M	C2'-C1'-N9-C8
1	L1	1322	1MA	C2'-C1'-N9-C4
42	Lo	53	MLZ	CG-CD-CE-NZ
45	S2	1219	JMH	C2'-C1'-N1-C6
1	L1	3818	UY1	O4'-C1'-C5-C4
1	L1	4450	PSU	O4'-C1'-C5-C4
45	S2	1326	UY1	O4'-C1'-C5-C4
1	L1	2351	OMC	C3'-C2'-O2'-CM2
1	L1	2363	A2M	C3'-C2'-O2'-CM'
1	L1	2401	A2M	C3'-C2'-O2'-CM'
45	S2	644	OMG	C4'-C5'-O5'-P
45	S2	428	OMU	C2'-C1'-N1-C6
1	L1	4293	PSU	O4'-C4'-C5'-O5'
45	S2	1832	6MZ	C5-C6-N6-C9
45	S2	590	A2M	O4'-C1'-N9-C8
1	L1	2824	OMC	O4'-C4'-C5'-O5'
45	S2	99	A2M	C3'-C4'-C5'-O5'
45	S2	428	OMU	O4'-C1'-N1-C6
1	L1	2787	A2M	O4'-C1'-N9-C8
1	L1	1534	A2M	O4'-C4'-C5'-O5'
1	L1	2787	A2M	C3'-C4'-C5'-O5'
45	S2	1850	MA6	O4'-C4'-C5'-O5'
45	S2	1850	MA6	C3'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C1'-C5-C6
1	L1	4636	PSU	O4'-C1'-C5-C6
1	L1	2351	OMC	C2'-C1'-N1-C2
45	S2	1219	JMH	C2'-C1'-N1-C2
1	L1	729	2MG	O4'-C4'-C5'-O5'
1	L1	2351	OMC	O4'-C4'-C5'-O5'
1	L1	2422	OMC	O4'-C4'-C5'-O5'
45	S2	822	PSU	C3'-C4'-C5'-O5'
1	L1	3869	OMC	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	L1	398	A2M	C3'-C4'-C5'-O5'
1	L1	1326	A2M	C4'-C5'-O5'-P
1	L1	4671	B8T	C4'-C5'-O5'-P
45	S2	576	A2M	C4'-C5'-O5'-P
45	S2	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

48 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	4196	OMG	1	0
1	L1	1326	A2M	1	0
1	L1	4220	6MZ	1	0
1	L1	398	A2M	1	0
1	L1	4637	OMG	1	0
1	L1	4618	OMG	1	0
1	L1	2861	OMC	1	0
45	S2	1447	OMG	1	0
1	L1	3818	UY1	1	0
1	L1	4623	OMG	1	0
45	S2	1832	6MZ	1	0
1	L1	729	2MG	1	0
45	S2	612	PSU	1	0
45	S2	509	OMG	3	0
45	S2	484	A2M	1	0
1	L1	2363	A2M	1	0
3	L3	75	OMG	1	0
45	S2	814	5MU	1	0
1	L1	3762	B8H	6	0
45	S2	601	OMG	1	0
45	S2	867	OMG	1	0
1	L1	3718	A2M	3	0
1	L1	1456	JMH	1	0
45	S2	166	A2M	2	0
45	S2	823	PSU	1	0
45	S2	428	OMU	1	0
45	S2	1678	A2M	2	0
1	L1	3723	A2M	1	0
1	L1	3925	OMU	1	0
45	S2	1288	OMU	2	0
45	S2	1490	OMG	2	0
1	L1	1871	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	S2	1328	OMG	1	0
45	S2	644	OMG	1	0
1	L1	4447	5MC	1	0
45	S2	1031	A2M	1	0
1	L1	3792	OMG	1	0
1	L1	4370	OMG	2	0
1	L1	2804	OMC	1	0
45	S2	121	OMU	1	0
1	L1	2422	OMC	1	0
1	L1	3744	OMG	1	0
1	L1	2351	OMC	2	0
45	S2	576	A2M	1	0
45	S2	512	A2M	1	0
45	S2	1830	UR3	1	0
1	L1	1340	OMC	1	0
1	L1	4392	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 442 ligands modelled in this entry, 442 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

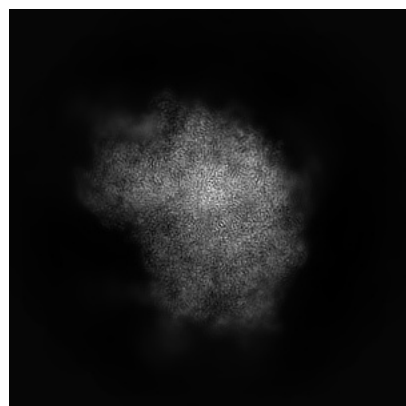
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33329. These allow visual inspection of the internal detail of the map and identification of artifacts.

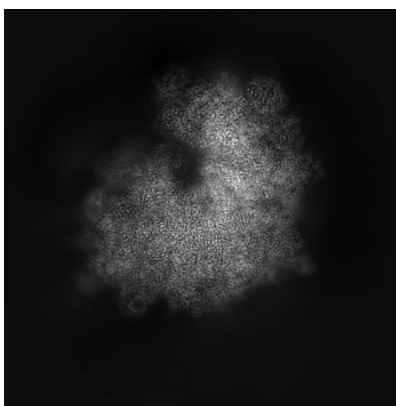
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

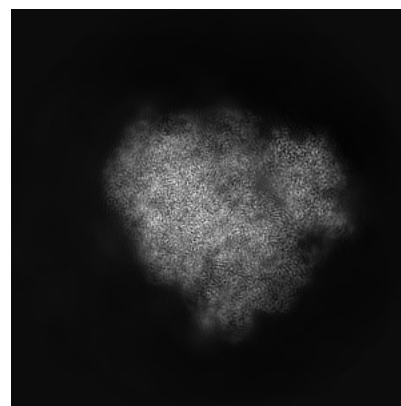
6.1.1 Primary map



X

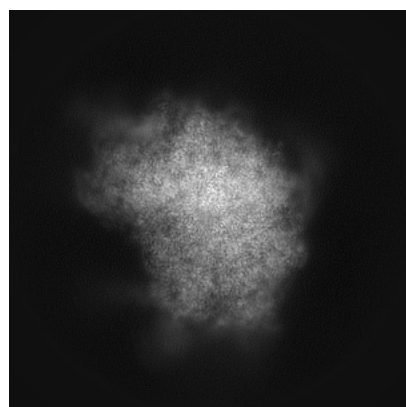


Y

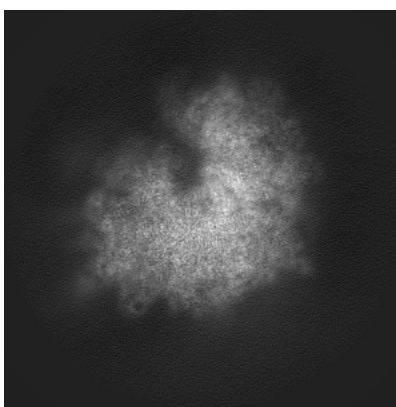


Z

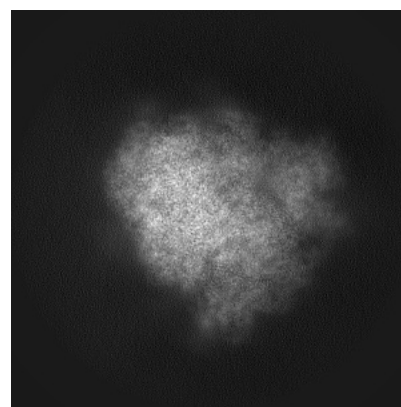
6.1.2 Raw map



X



Y

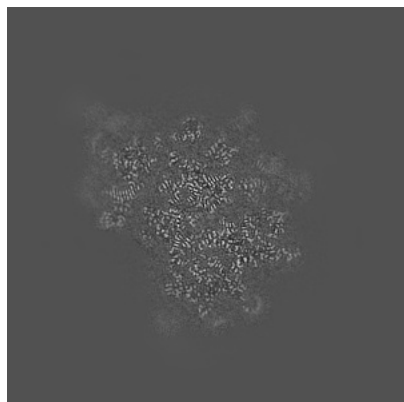


Z

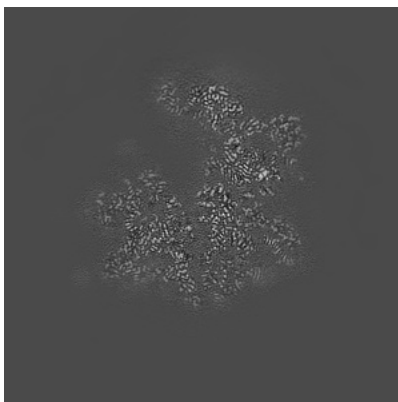
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

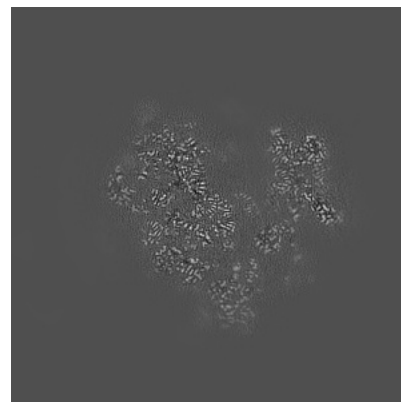
6.2.1 Primary map



X Index: 210

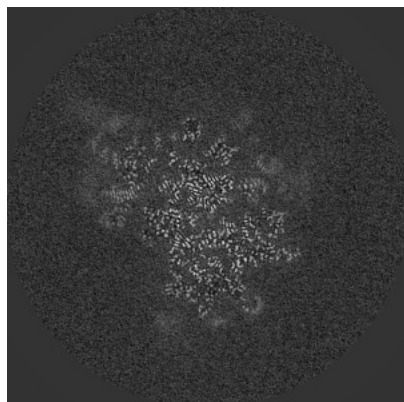


Y Index: 210

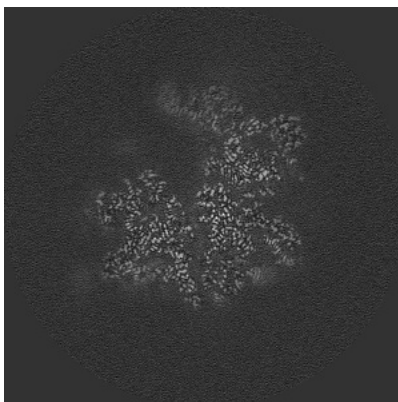


Z Index: 210

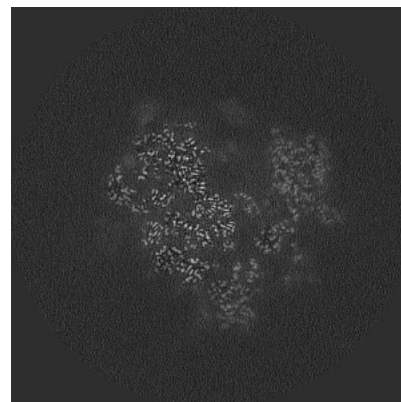
6.2.2 Raw map



X Index: 210



Y Index: 210

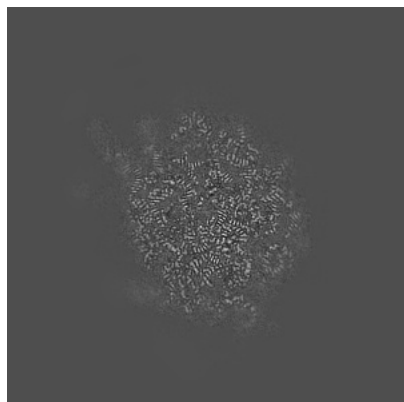


Z Index: 210

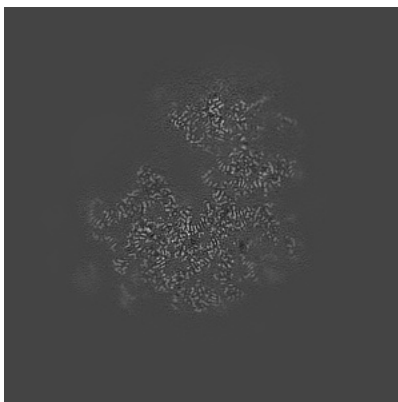
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

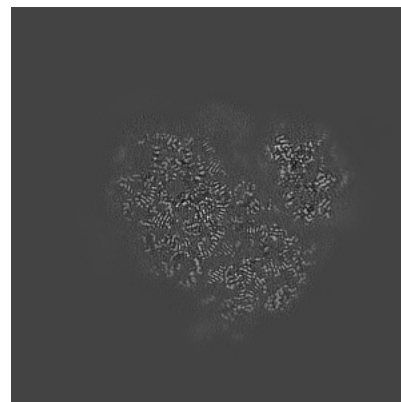
6.3.1 Primary map



X Index: 188

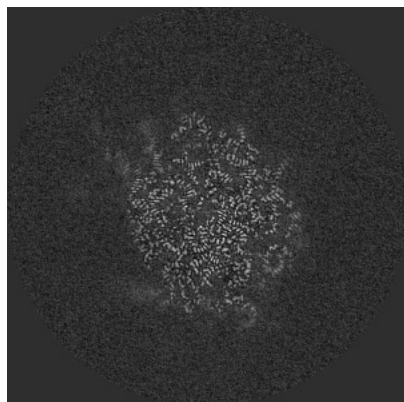


Y Index: 223

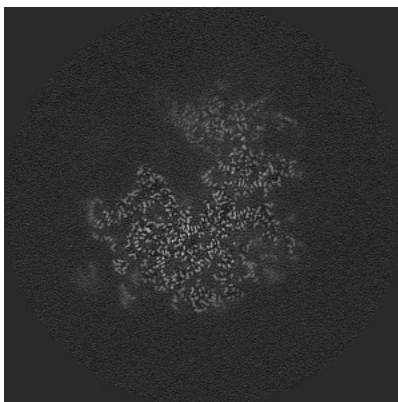


Z Index: 231

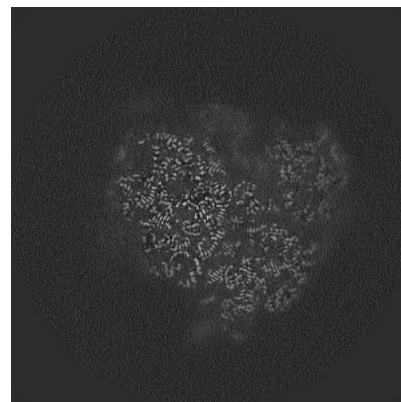
6.3.2 Raw map



X Index: 188



Y Index: 223

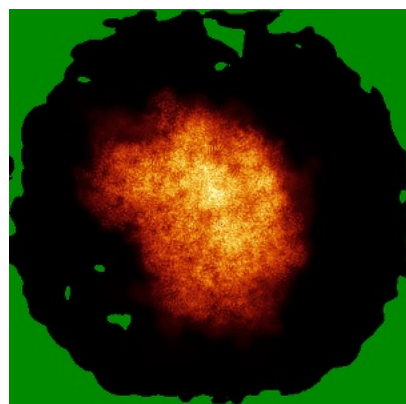


Z Index: 231

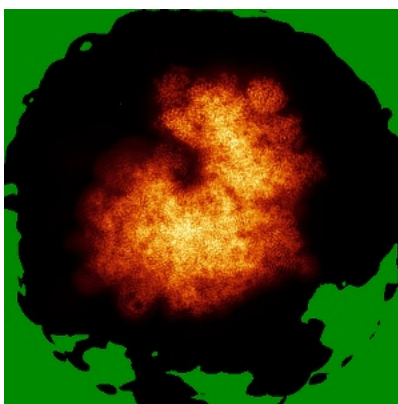
The images above show the largest variance slices of the map in three orthogonal directions.

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

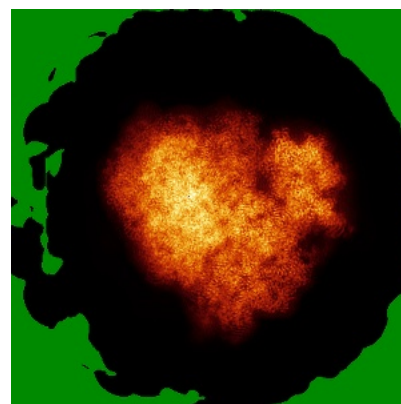
6.4.1 Primary map



X

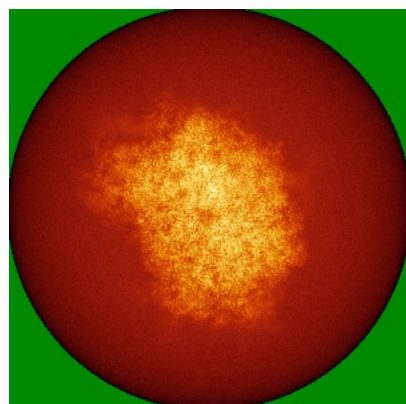


Y

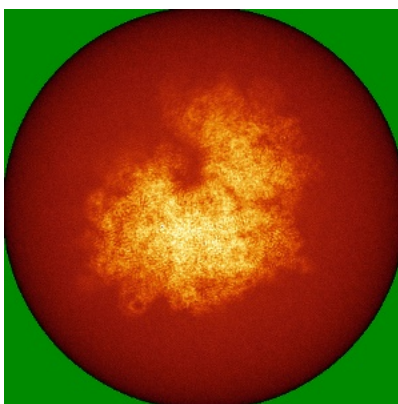


Z

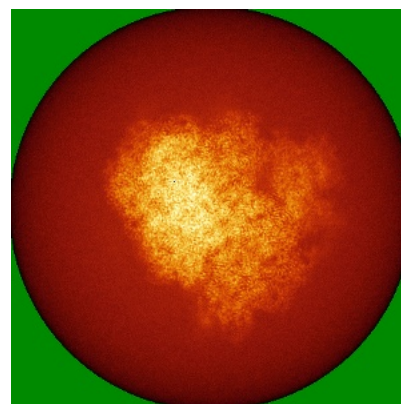
6.4.2 Raw map



X



Y

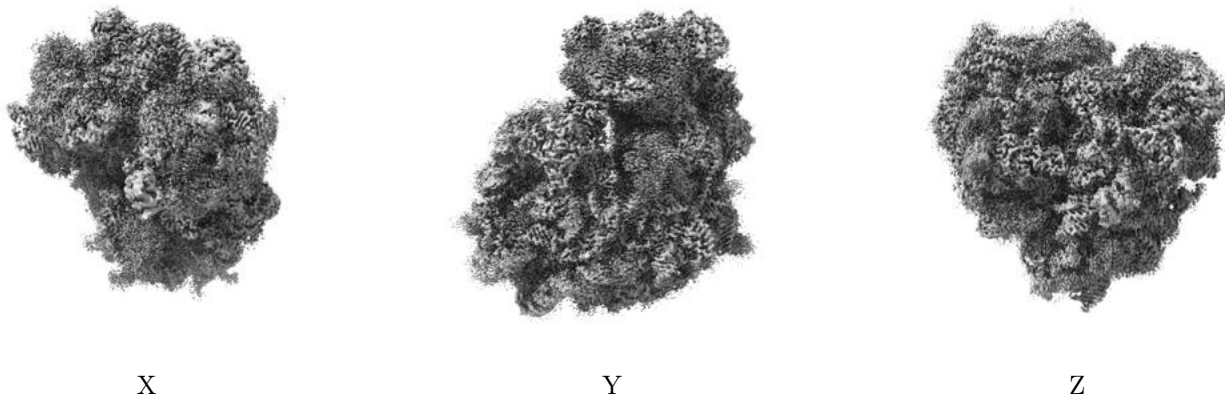


Z

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.

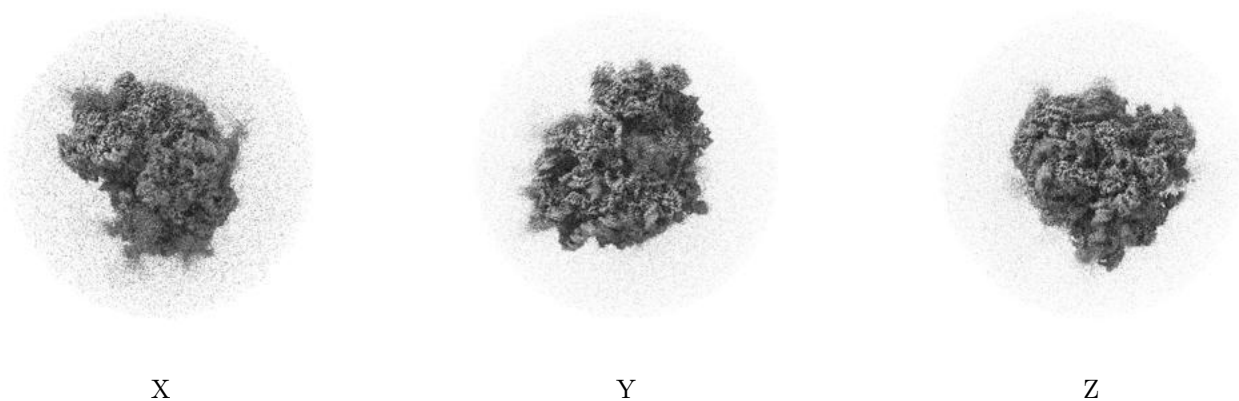
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

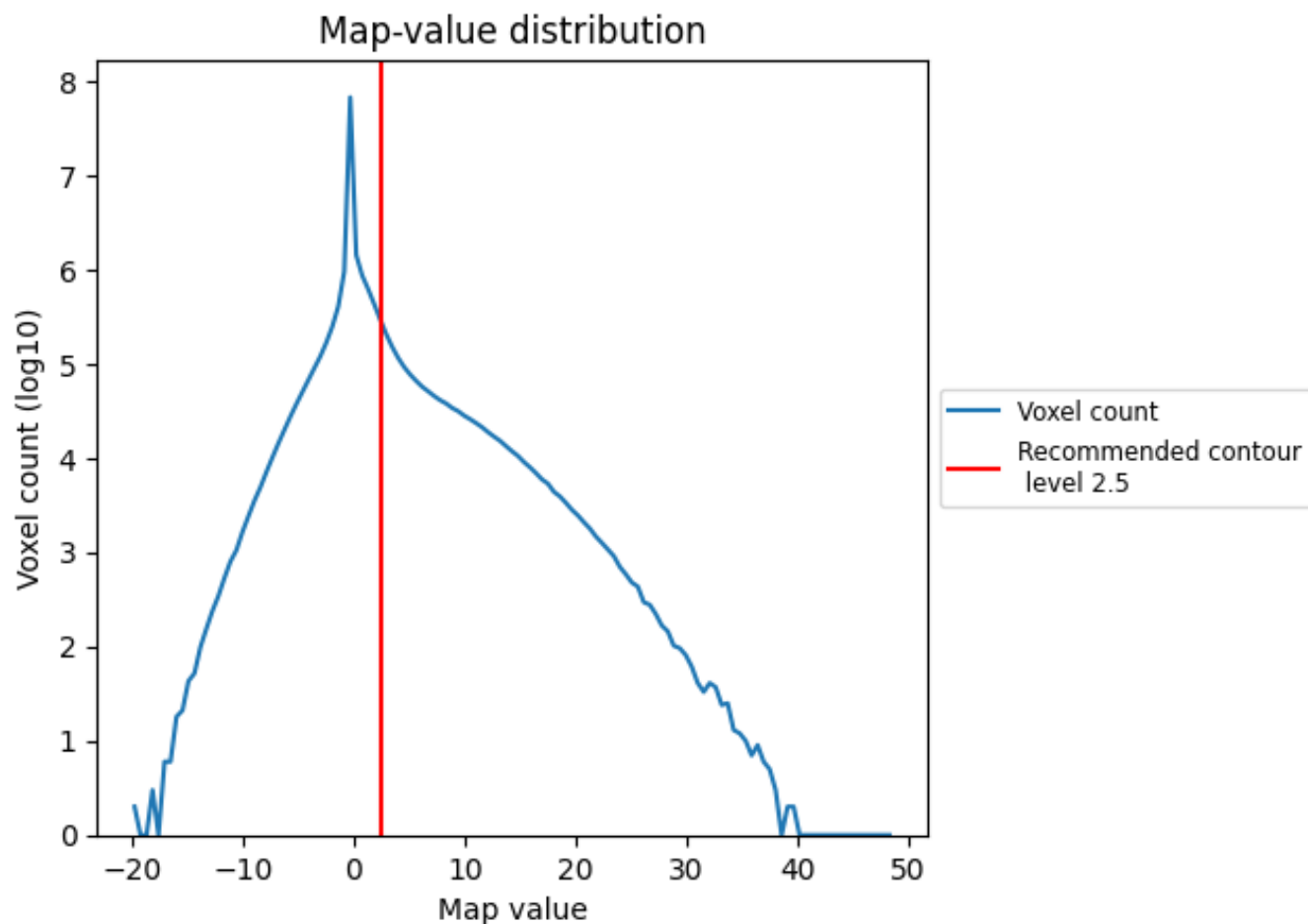
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

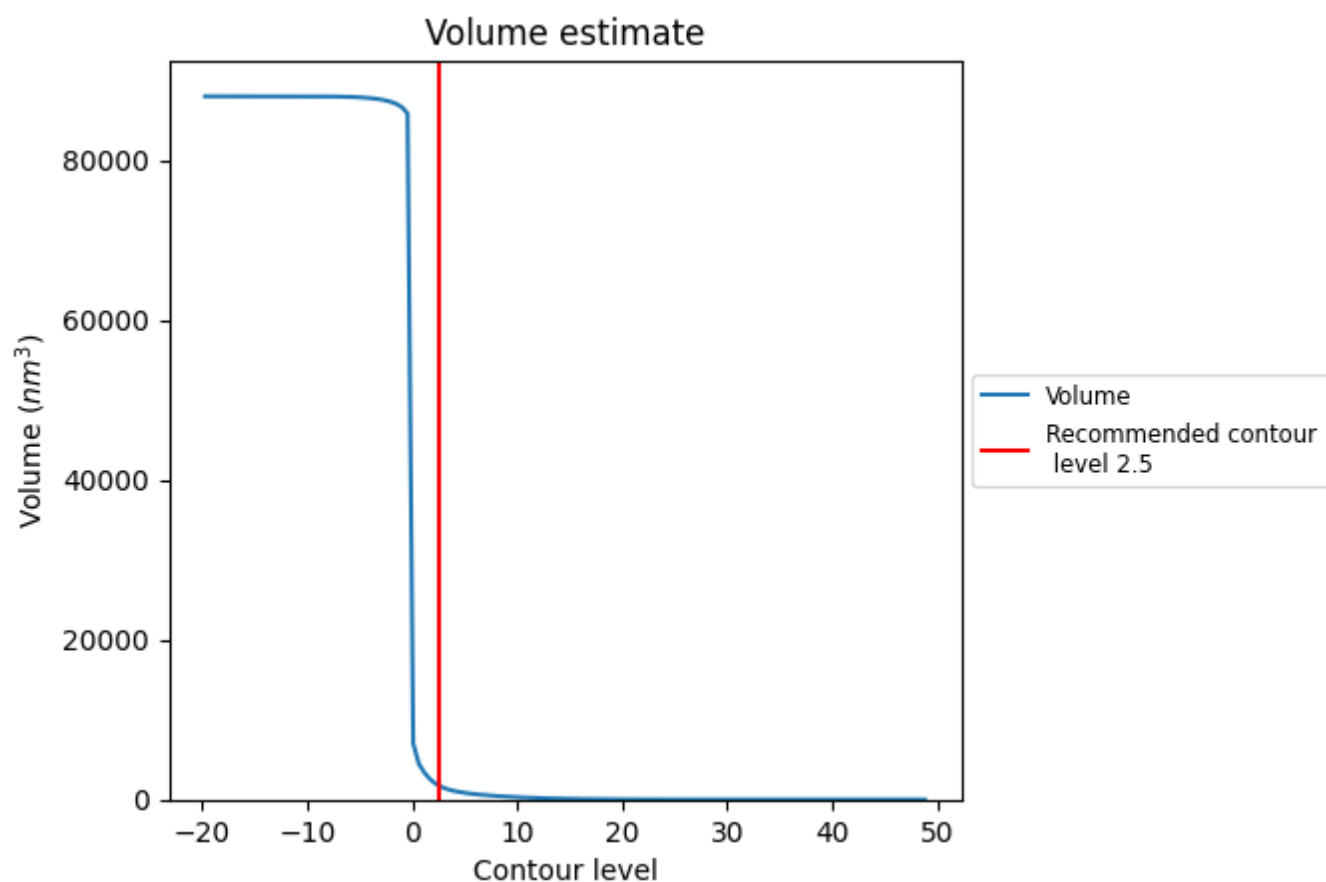
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

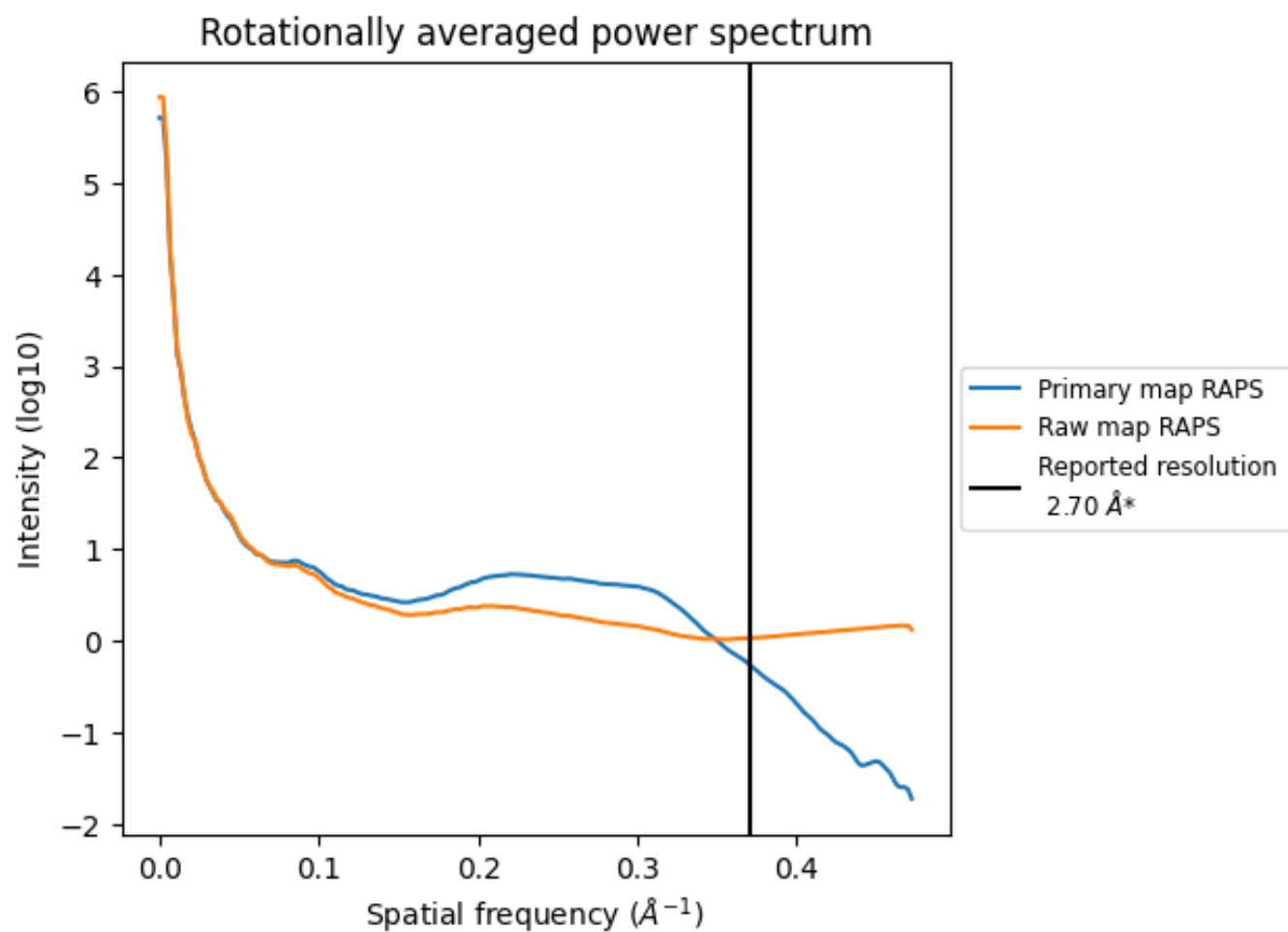
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1791 nm^3 ; this corresponds to an approximate mass of 1617 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

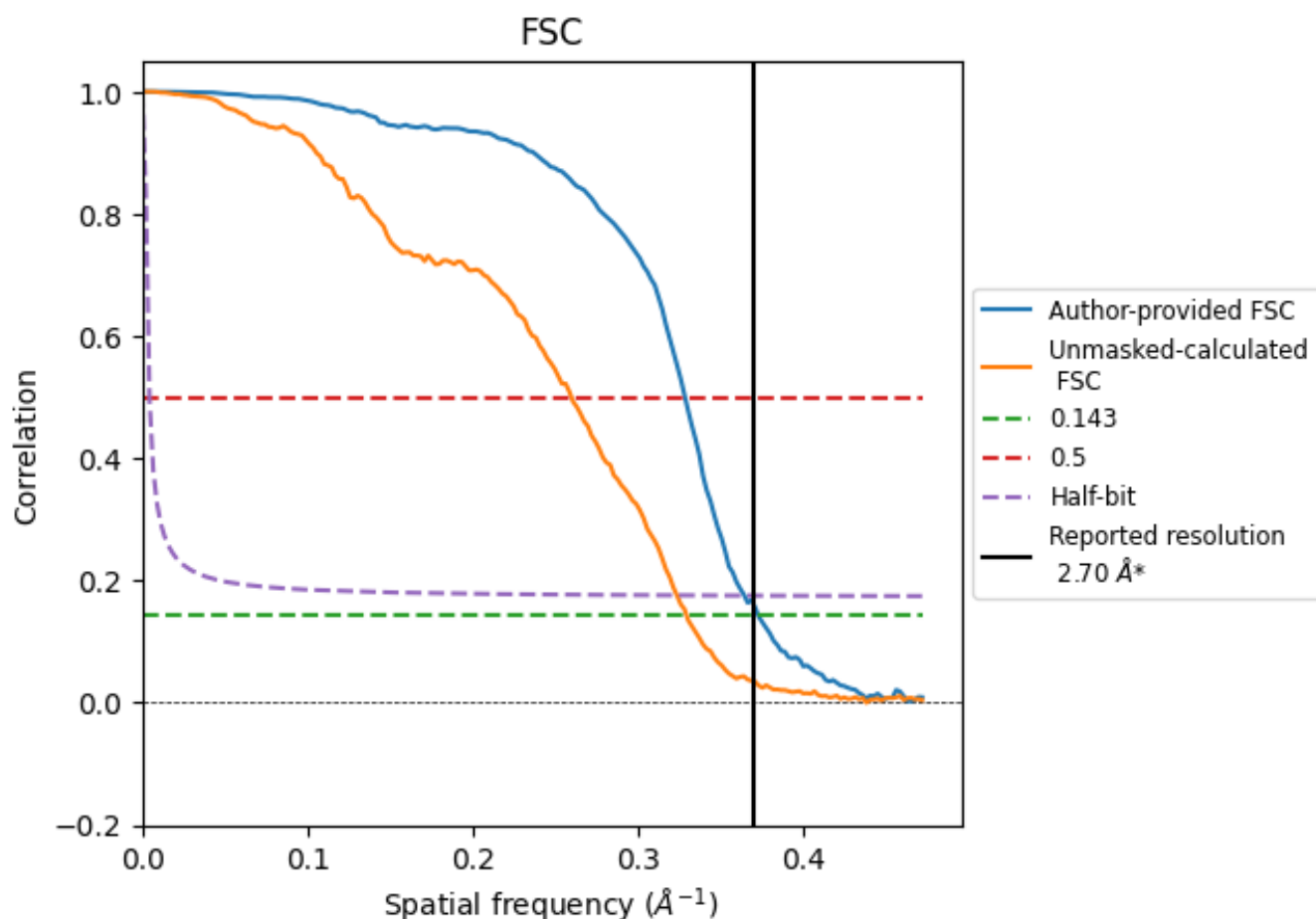


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

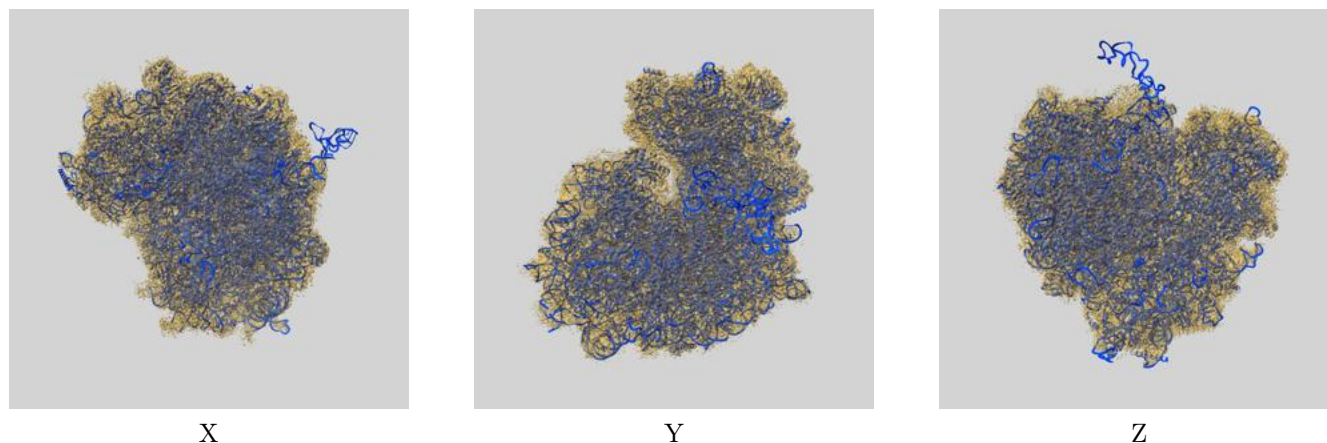
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.04	2.74
Unmasked-calculated*	3.03	3.85	3.09

*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 3.03 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

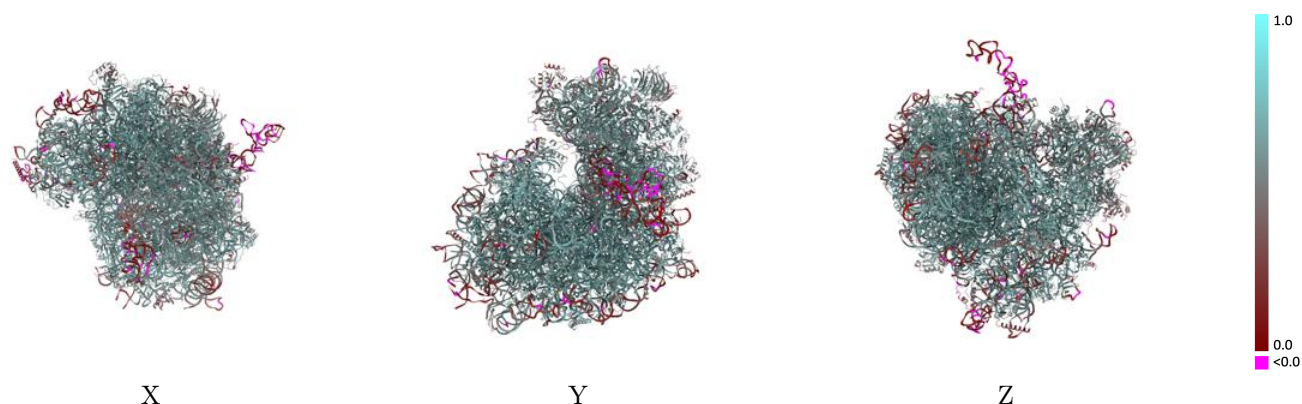
This section contains information regarding the fit between EMDB map EMD-33329 and PDB model 7XNX. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



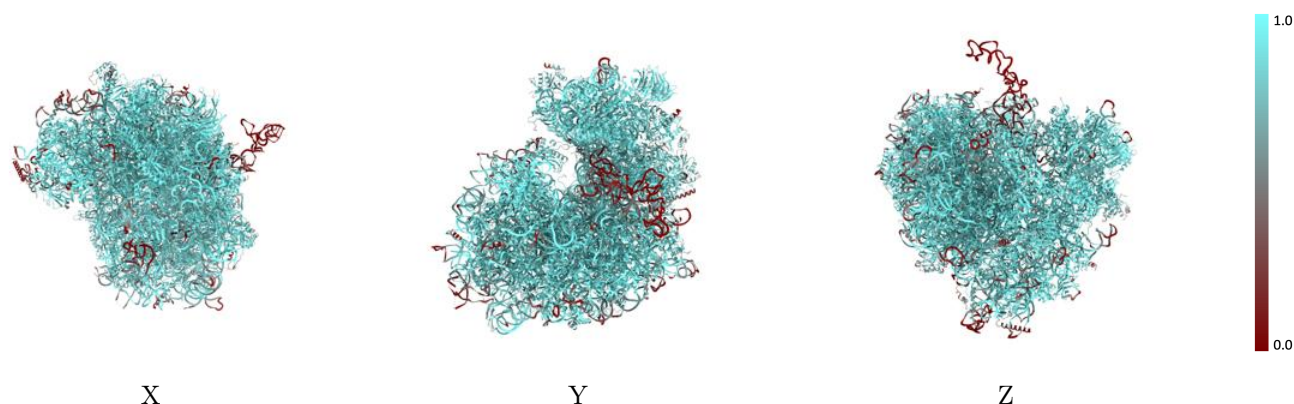
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



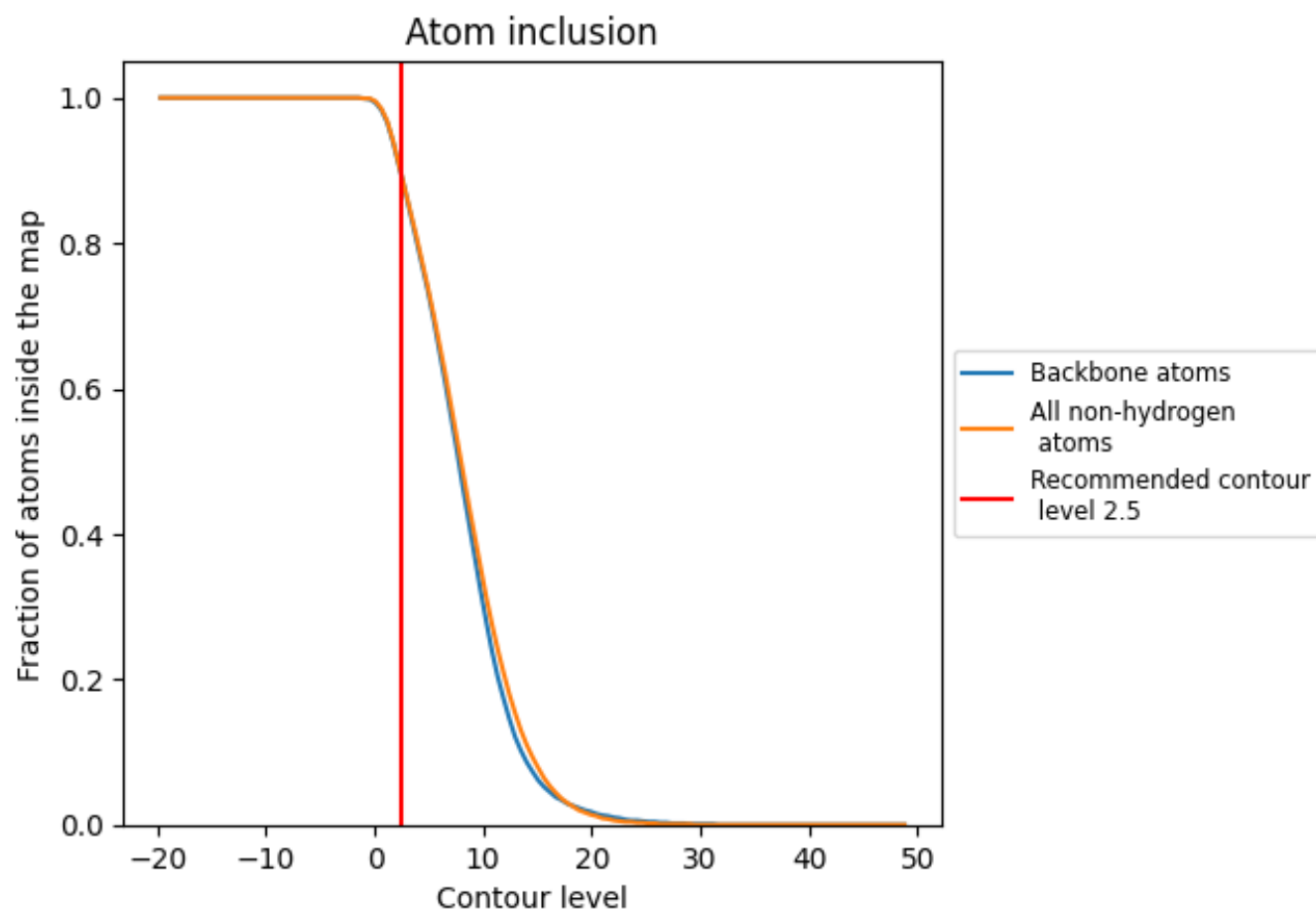
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.5800
CC	 0.3530	 0.3020
CE	 0.7000	 0.5000
L1	 0.8790	 0.5720
L2	 0.9870	 0.6430
L3	 0.9340	 0.6070
LA	 0.9810	 0.6740
LB	 0.9310	 0.6390
LC	 0.9360	 0.6380
LD	 0.8840	 0.6010
LE	 0.8790	 0.5910
LF	 0.9550	 0.6530
LG	 0.8360	 0.5730
LH	 0.9080	 0.6100
LI	 0.9420	 0.6350
LJ	 0.8190	 0.5520
LL	 0.8790	 0.5920
LM	 0.9120	 0.6020
LN	 0.9890	 0.6800
LO	 0.9470	 0.6490
LP	 0.9380	 0.6510
LQ	 0.9700	 0.6660
LR	 0.8510	 0.6000
LS	 0.9670	 0.6540
LT	 0.9200	 0.6230
LU	 0.7080	 0.5060
LV	 0.9570	 0.6520
LW	 0.5960	 0.4410
LX	 0.9300	 0.6350
LY	 0.8990	 0.6060
LZ	 0.9040	 0.6110
La	 0.9530	 0.6540
Lb	 0.7910	 0.5400
Lc	 0.9370	 0.6250
Ld	 0.8950	 0.6190



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Chain	Atom inclusion	Q-score
Le	 0.9620	 0.6530
Lf	 0.9700	 0.6590
Lg	 0.9140	 0.6220
Lh	 0.8900	 0.5990
Li	 0.9070	 0.5990
Lj	 0.9720	 0.6580
Lk	 0.7500	 0.5510
Ll	 0.9480	 0.6340
Lm	 0.9280	 0.6340
Ln	 0.9620	 0.6230
Lo	 0.9350	 0.6420
Lp	 0.9650	 0.6600
Lr	 0.9410	 0.6320
S2	 0.9120	 0.5780
SA	 0.9090	 0.5950
SB	 0.9140	 0.5880
SC	 0.9630	 0.6240
SD	 0.9350	 0.5380
SE	 0.9460	 0.5990
SF	 0.9370	 0.5560
SG	 0.8420	 0.5110
SH	 0.8060	 0.4950
SI	 0.8870	 0.5720
SJ	 0.9030	 0.5730
SK	 0.9080	 0.5160
SL	 0.9360	 0.6330
SM	 0.6560	 0.2980
SN	 0.9570	 0.6340
SO	 0.9470	 0.6090
SP	 0.8680	 0.4790
SQ	 0.9150	 0.5290
SR	 0.7960	 0.5340
SS	 0.8830	 0.4890
ST	 0.9140	 0.5330
SU	 0.8790	 0.4870
SV	 0.9260	 0.6000
SW	 0.9720	 0.6430
SX	 0.9580	 0.6240
SY	 0.9080	 0.5570
SZ	 0.8830	 0.5120
Sa	 0.9250	 0.6030
Sb	 0.8980	 0.5840

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Chain	Atom inclusion	Q-score
Sc	 0.8890	 0.5170
Sd	 0.9500	 0.5660
Se	 0.7810	 0.5200
Sf	 0.8140	 0.4610
Sg	 0.9100	 0.5050