



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 01:17 PM JST

PDB ID : 7XNY / pdb_00007xny
EMDB ID : EMD-33330
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 : 2.50 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

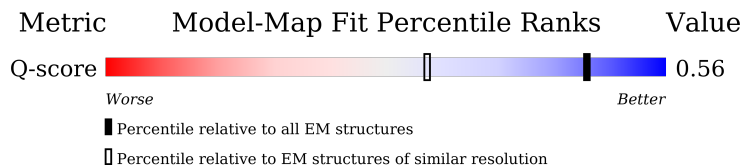
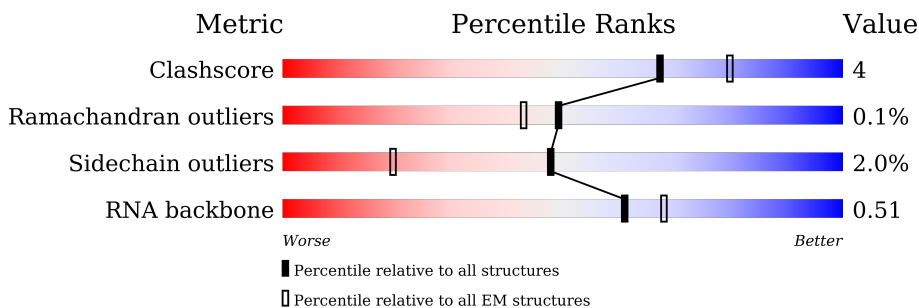
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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.



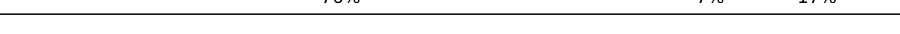
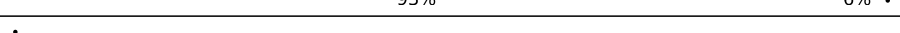
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	 6% 51% 20% 26%
2	L2	120	 80% 20%
3	L3	156	 5% 71% 25%

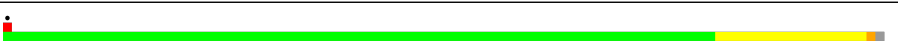
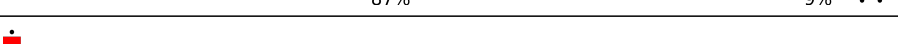
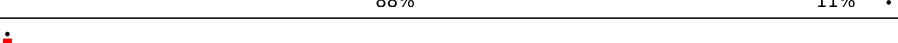
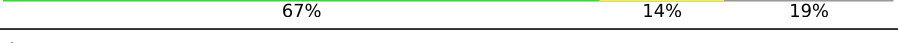
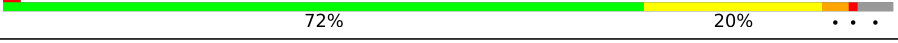
Continued on next page...

Continued from previous page...

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	135	

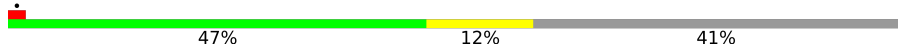
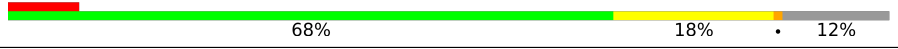
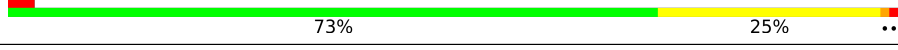
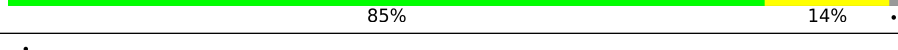
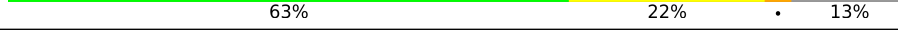
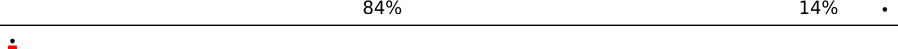
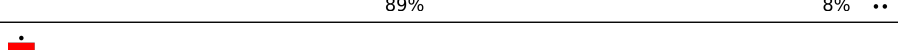
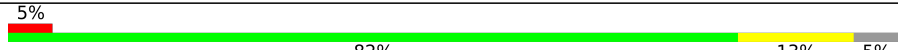
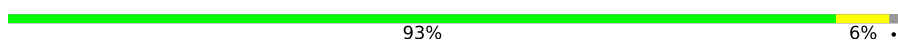
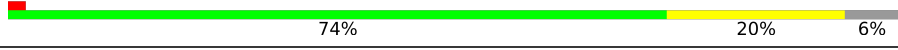
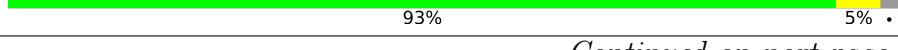
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	S2	1869	
47	SA	295	
48	SB	264	
49	SD	243	
50	SE	263	
51	SF	204	
52	SH	194	
53	SI	208	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Sf	156	31%8%61%

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 216242 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
			1107	714	208	182	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1740	Total	C	N	O	P	0	0
			36958	16514	6600	12105	1739		

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

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

- Molecule 48 is a protein called 40S ribosomal protein S3a.

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

- Molecule 49 is a protein called 40S ribosomal protein S3.

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

- Molecule 50 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S7.

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

- Molecule 53 is a protein called 40S ribosomal protein S8.

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

- Molecule 54 is a protein called 40S ribosomal protein S10.

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

- Molecule 55 is a protein called 40S ribosomal protein S11.

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

- Molecule 56 is a protein called 40S ribosomal protein S15.

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

- Molecule 57 is a protein called 40S ribosomal protein S16.

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

- Molecule 58 is a protein called 40S ribosomal protein S17.

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

- Molecule 59 is a protein called 40S ribosomal protein S18.

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

- Molecule 60 is a protein called 40S ribosomal protein S19.

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

- Molecule 61 is a protein called 40S ribosomal protein S20.

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

- Molecule 62 is a protein called 40S ribosomal protein S21.

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

- Molecule 63 is a protein called 40S ribosomal protein S23.

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

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

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

- Molecule 65 is a protein called 40S ribosomal protein S28.

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

- Molecule 66 is a protein called 40S ribosomal protein S29.

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

- Molecule 67 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 68 is a protein called 40S ribosomal protein S2.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called 40S ribosomal protein S9.

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

- Molecule 71 is a protein called 40S ribosomal protein S12.

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

- Molecule 72 is a protein called 40S ribosomal protein S13.

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

- Molecule 73 is a protein called 40S ribosomal protein S14.

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

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S24.

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

- Molecule 76 is a protein called 40S ribosomal protein S25.

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called 40S ribosomal protein S30.

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

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- 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	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	2	Total	Mg	0
			2	2	
80	Lf	1	Total	Mg	0
			1	1	
80	Lg	1	Total	Mg	0
			1	1	
80	Lo	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
80	S2	134	Total 134	Mg 134	0
80	ST	1	Total 1	Mg 1	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

- 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	767	Total O 767 767	0
83	L2	3	Total O 3 3	0
83	L3	6	Total O 6 6	0
83	LA	8	Total O 8 8	0
83	LB	2	Total O 2 2	0
83	LC	8	Total O 8 8	0
83	LD	1	Total O 1 1	0
83	LF	2	Total O 2 2	0
83	LI	1	Total O 1 1	0
83	LL	1	Total O 1 1	0
83	LN	2	Total O 2 2	0
83	LP	1	Total O 1 1	0
83	LR	1	Total O 1 1	0
83	LX	1	Total O 1 1	0
83	LY	1	Total O 1 1	0
83	La	5	Total O 5 5	0
83	Lb	1	Total O 1 1	0
83	Le	4	Total O 4 4	0
83	Lg	1	Total O 1 1	0
83	Lj	4	Total O 4 4	0
83	Ll	1	Total O 1 1	0
83	Lo	3	Total O 3 3	0

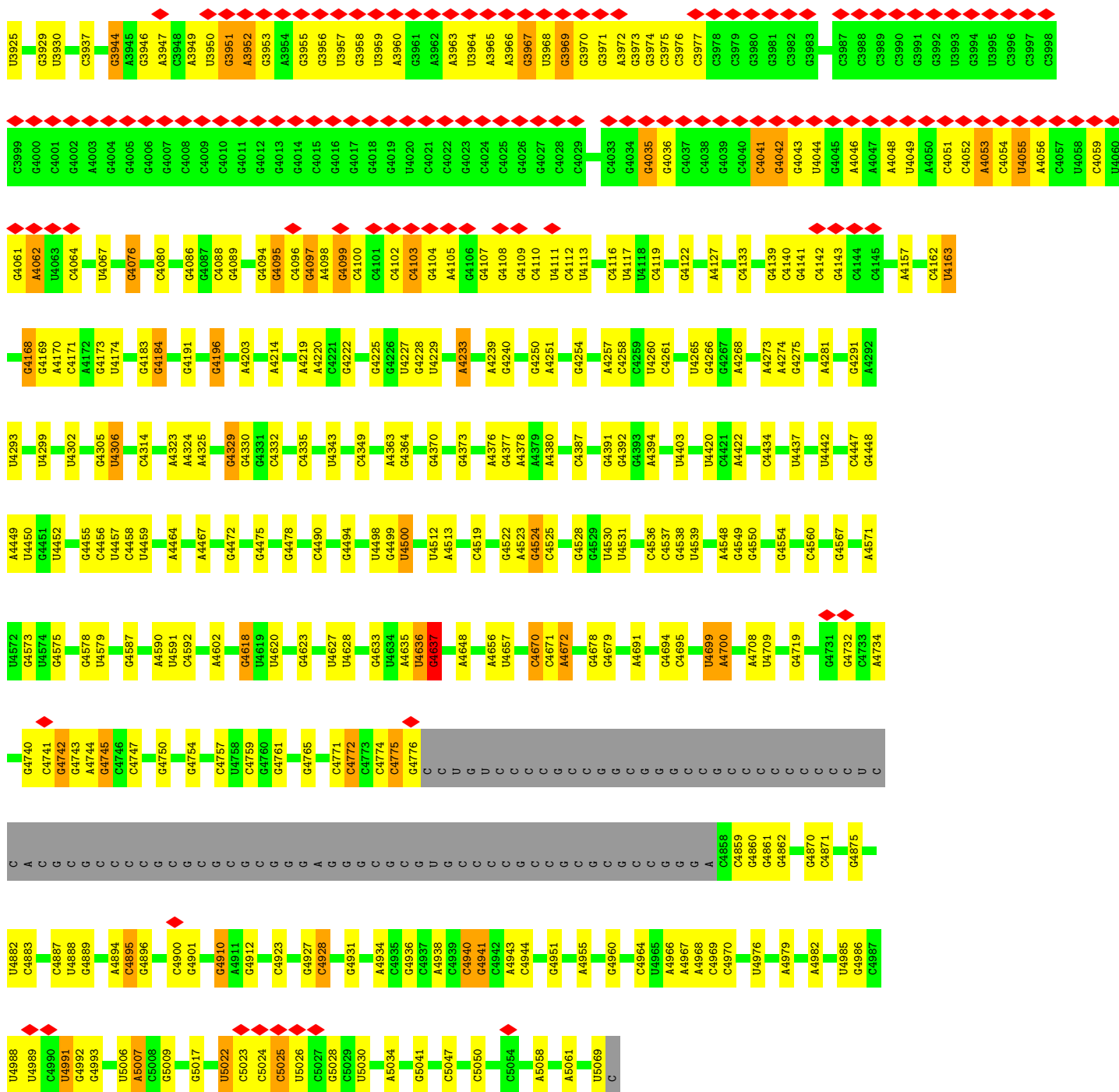
Continued on next page...

Continued from previous page...

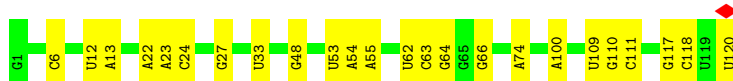
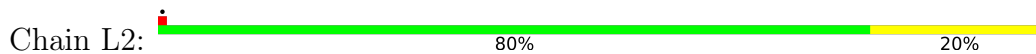
Mol	Chain	Residues	Atoms		AltConf
83	S2	9	Total 9	O 9	0
83	SQ	1	Total 1	O 1	0
83	SX	1	Total 1	O 1	0
83	Sd	1	Total 1	O 1	0



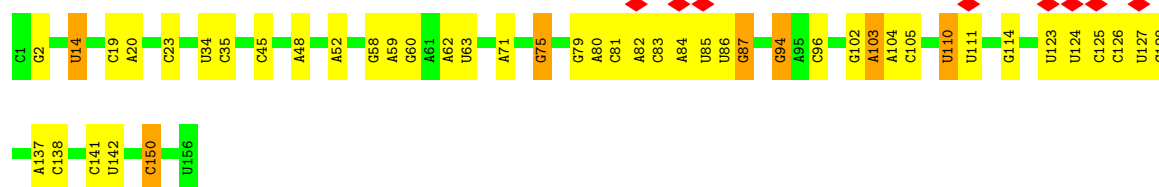
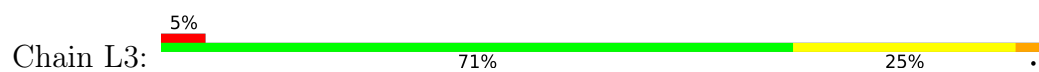




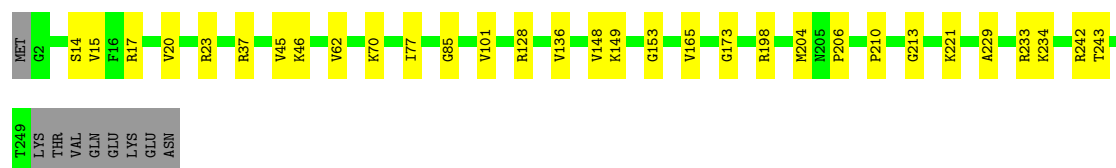
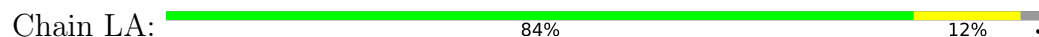
• Molecule 2: 5S rRNA



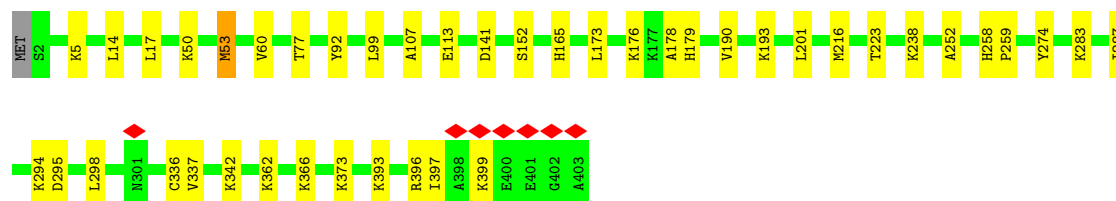
• Molecule 3: 5.8S rRNA



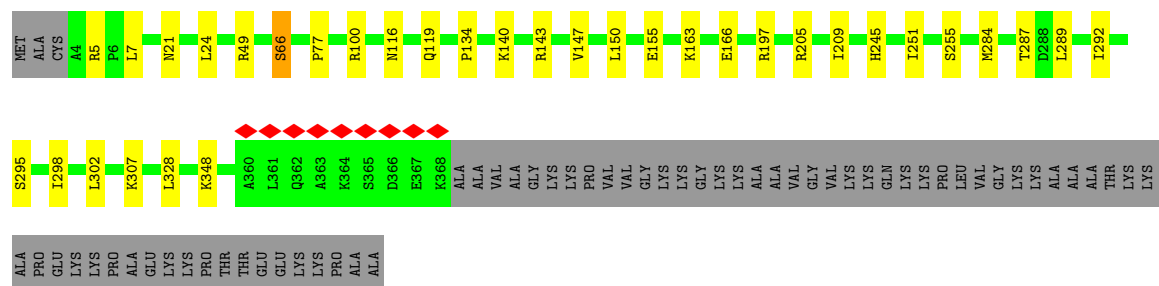
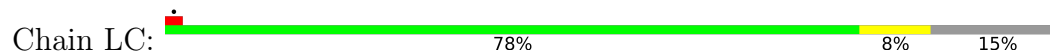
- Molecule 4: 60S ribosomal protein L8



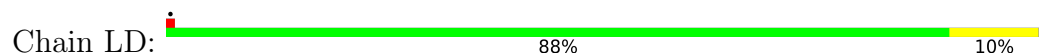
- Molecule 5: 60S ribosomal protein L3



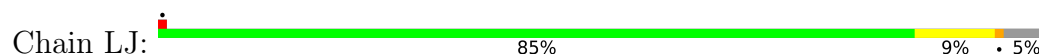
- Molecule 6: 60S ribosomal protein L4



- Molecule 7: 60S ribosomal protein L5



- Molecule 13: 60S ribosomal protein L11



- Molecule 14: 60S ribosomal protein L13



- Molecule 15: 60S ribosomal protein L14



- Molecule 16: 60S ribosomal protein L15



- Molecule 17: 60S ribosomal protein L13a

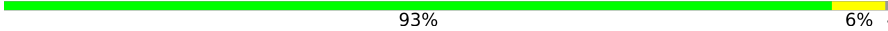


- Molecule 18: 60S ribosomal protein L17

Chain LP:  76% 7% 17%



- Molecule 19: 60S ribosomal protein L18

Chain LQ:  93% 6%



- Molecule 20: 60S ribosomal protein L19

Chain LR:  84% 12% 5%



- Molecule 21: 60S ribosomal protein L18a

Chain LS:  90% 10%



- Molecule 22: 60S ribosomal protein L21

Chain LT:  92% 7%



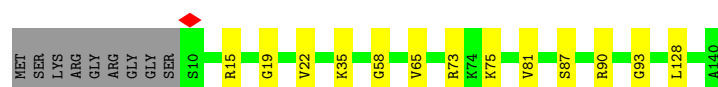
- Molecule 23: 60S ribosomal protein L22

Chain LU:  69% 9% 21%

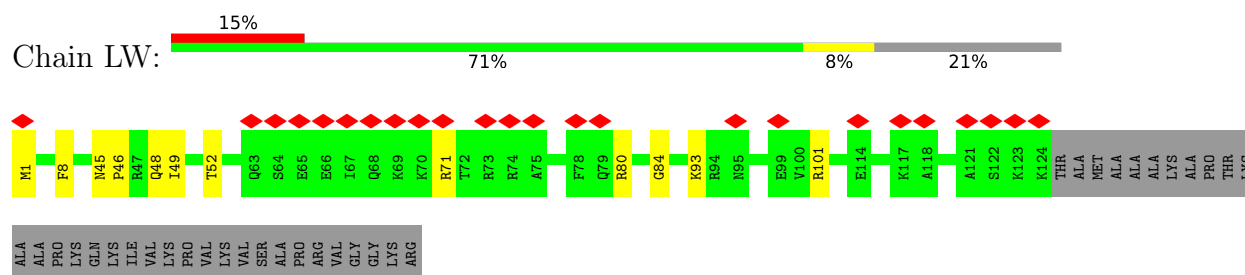


- Molecule 24: 60S ribosomal protein L23

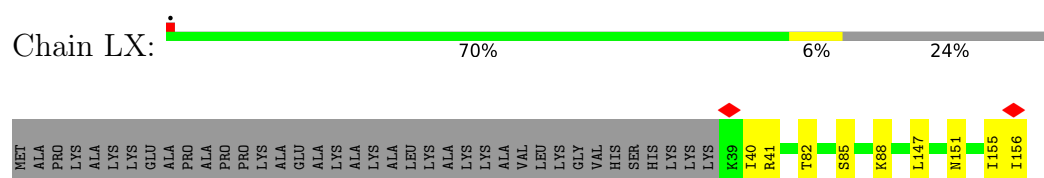
Chain LV:  84% 9% 6%



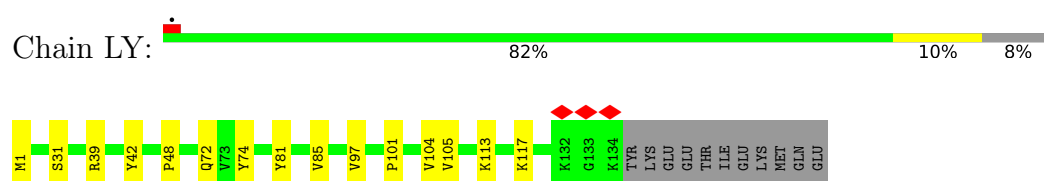
- Molecule 25: 60S ribosomal protein L24



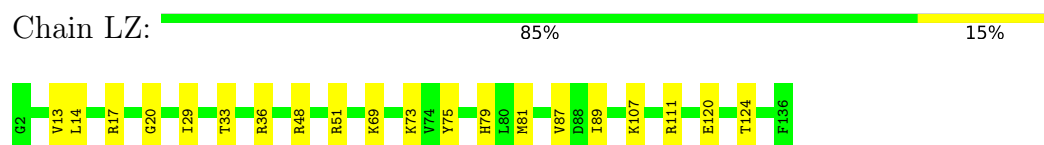
- Molecule 26: 60S ribosomal protein L23a



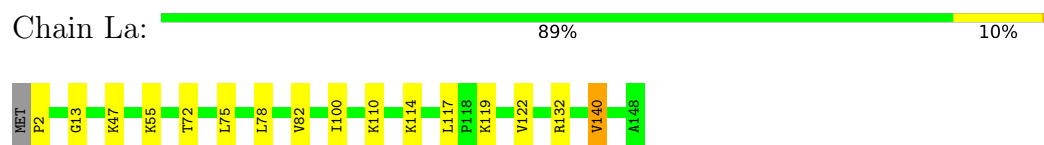
- Molecule 27: 60S ribosomal protein L26



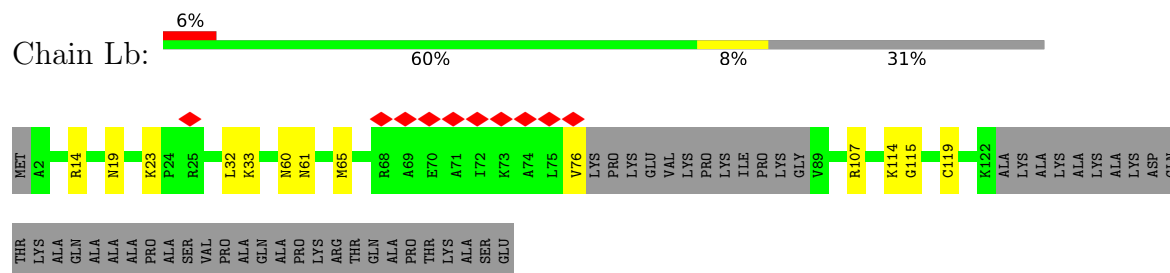
- Molecule 28: 60S ribosomal protein L27



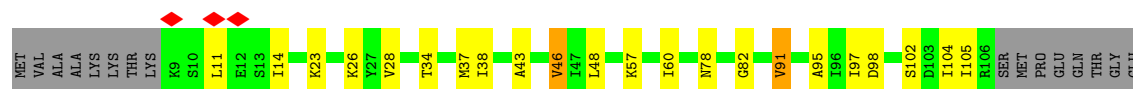
- Molecule 29: 60S ribosomal protein L27a



- Molecule 30: 60S ribosomal protein L29

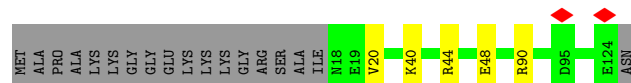
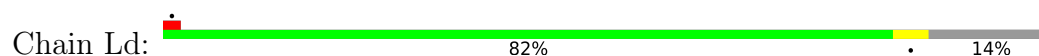


- Molecule 31: 60S ribosomal protein L30

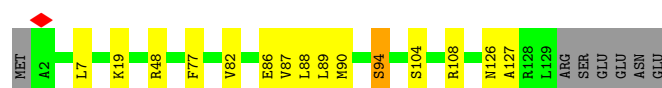
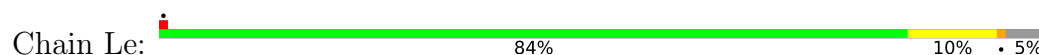


LYS

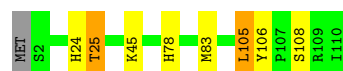
- Molecule 32: 60S ribosomal protein L31



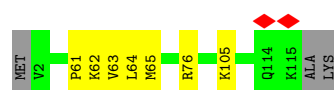
- Molecule 33: 60S ribosomal protein L32



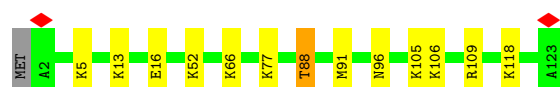
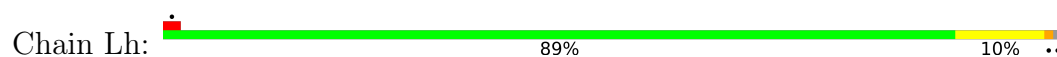
- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35

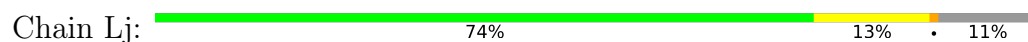


- Molecule 37: 60S ribosomal protein L36

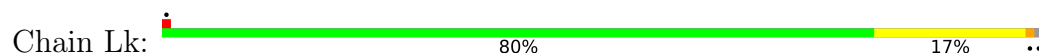




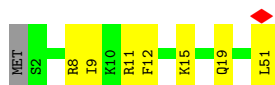
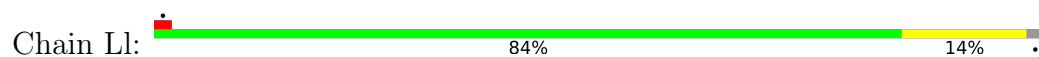
- Molecule 38: 60S ribosomal protein L37



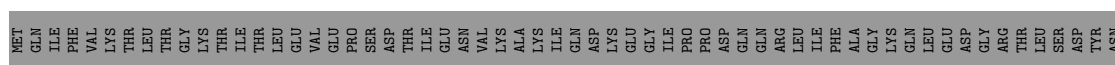
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



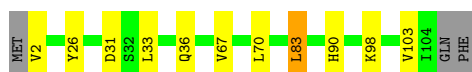
- Molecule 41: Ubiquitin-60S ribosomal protein L40



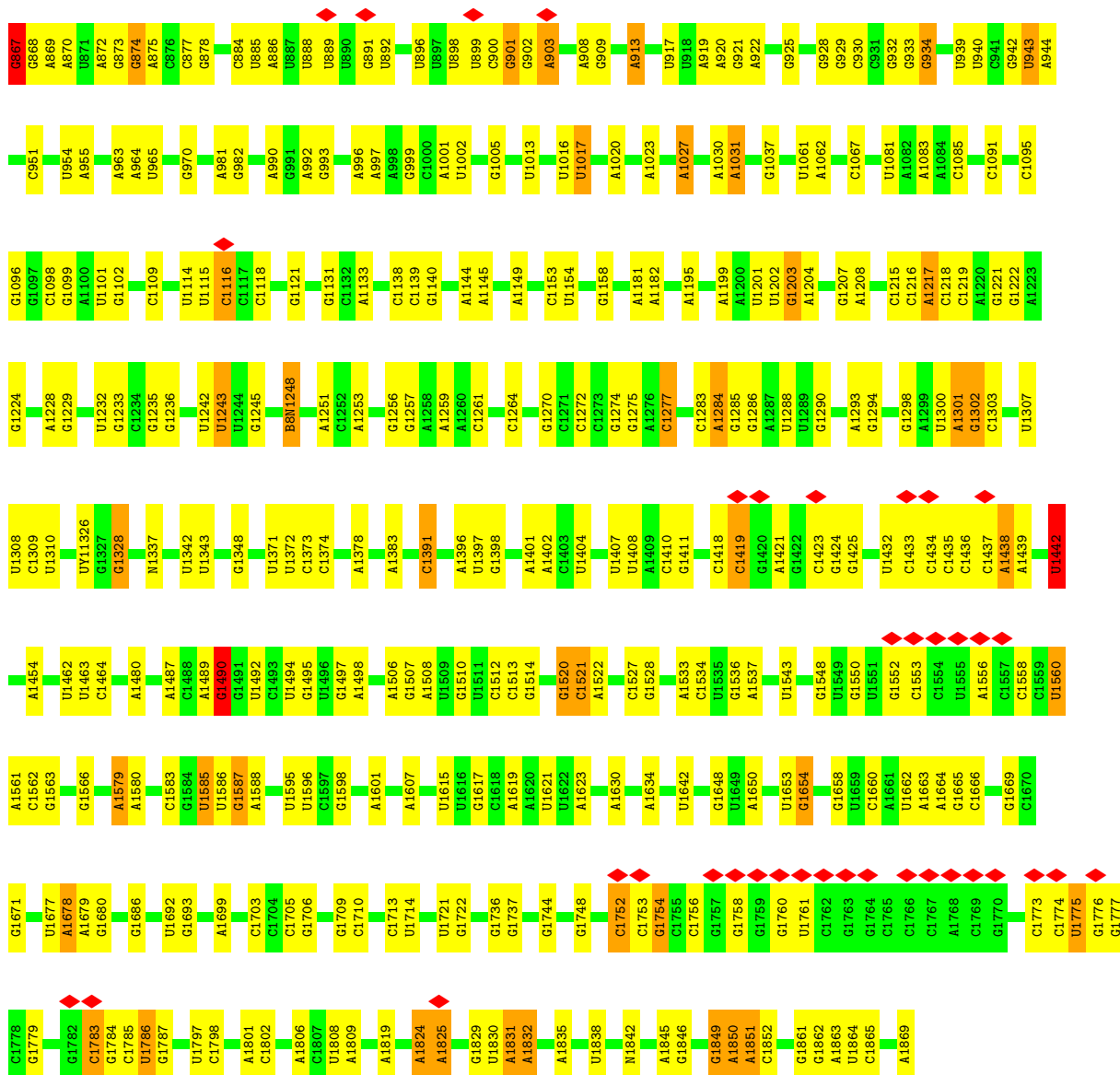
- Molecule 42: 60S ribosomal protein L41



- Molecule 43: 60S ribosomal protein L36a

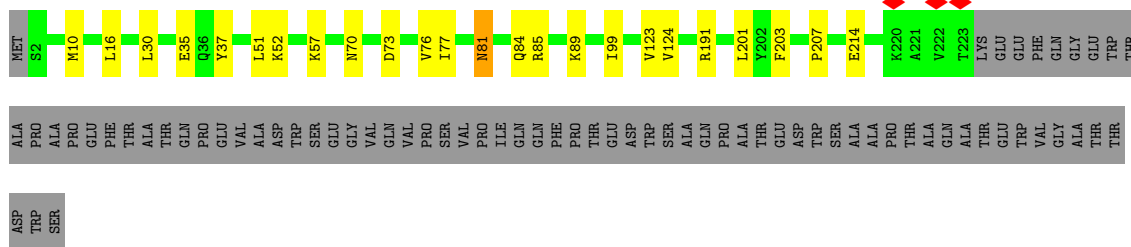


- Molecule 44: 60S ribosomal protein L37a



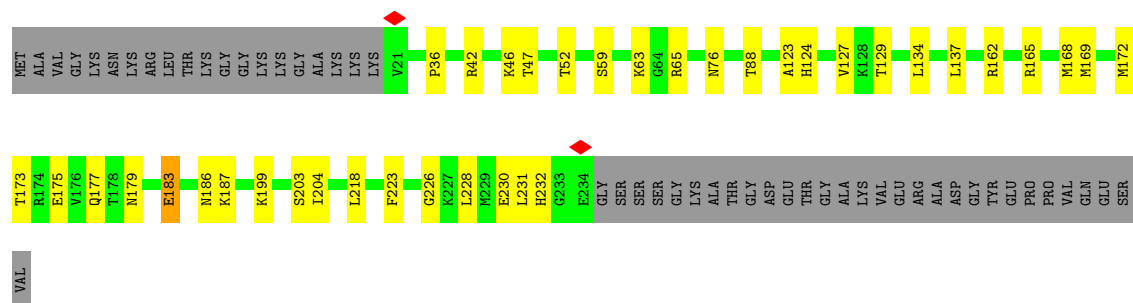
• Molecule 47: 40S ribosomal protein SA

Chain SA:



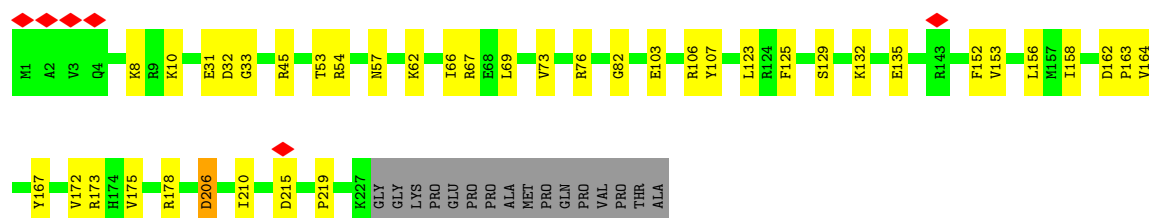
• Molecule 48: 40S ribosomal protein S3a

Chain SB:



- Molecule 49: 40S ribosomal protein S3

Chain SD: 77% 16% 7%



- Molecule 50: 40S ribosomal protein S4, X isoform

Chain SE: 89% 11%



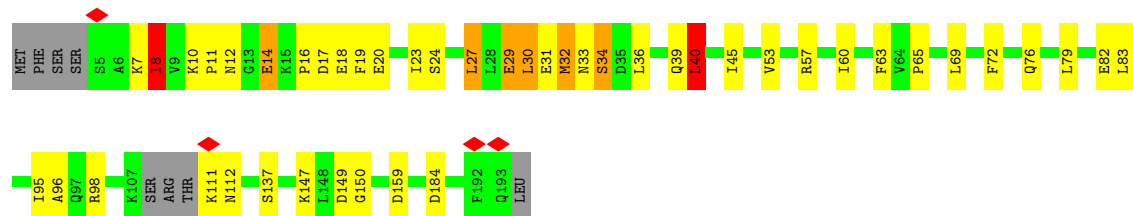
- Molecule 51: 40S ribosomal protein S5

Chain SF: 82% 7% 10%



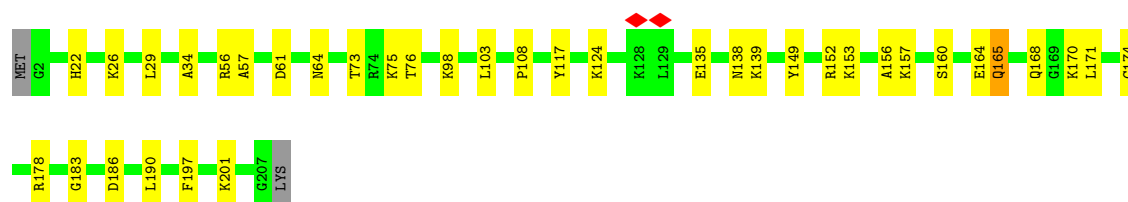
- Molecule 52: 40S ribosomal protein S7

Chain SH: 72% 20% ..

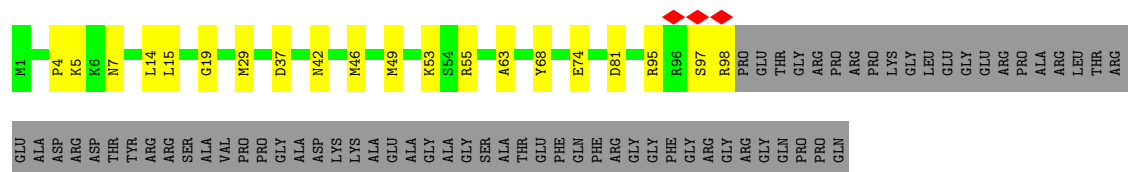


- Molecule 53: 40S ribosomal protein S8

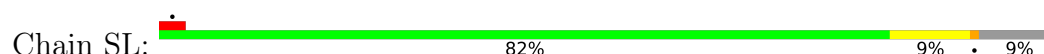
Chain SI: 81% 17%



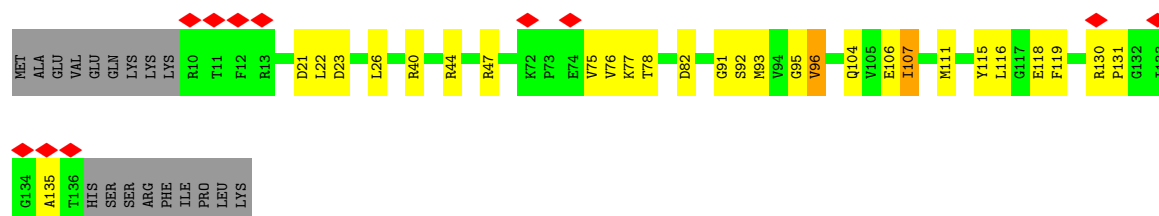
- Molecule 54: 40S ribosomal protein S10



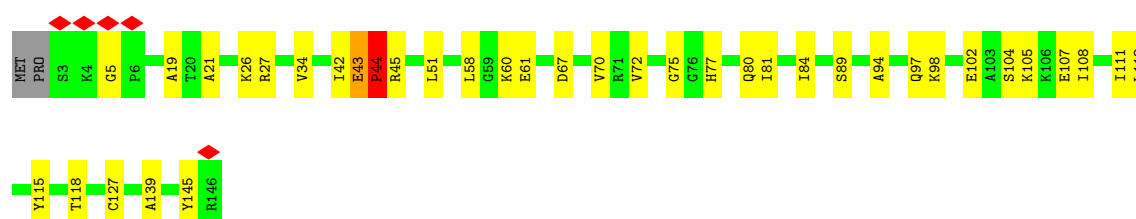
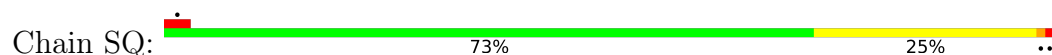
- Molecule 55: 40S ribosomal protein S11



- Molecule 56: 40S ribosomal protein S15

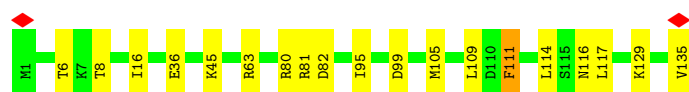


- Molecule 57: 40S ribosomal protein S16



- Molecule 58: 40S ribosomal protein S17





- Molecule 59: 40S ribosomal protein S18

Chain SS: 77% 18% 5%



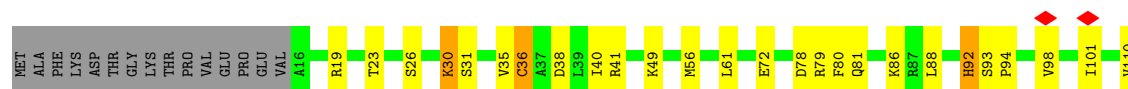
- Molecule 60: 40S ribosomal protein S19

Chain ST: 85% 14% .



- Molecule 61: 40S ribosomal protein S20

Chain SU: 63% 22% 13%



- Molecule 62: 40S ribosomal protein S21

Chain SV: 84% 14% .



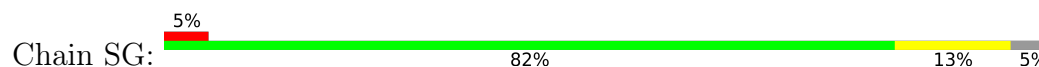
- Molecule 63: 40S ribosomal protein S23

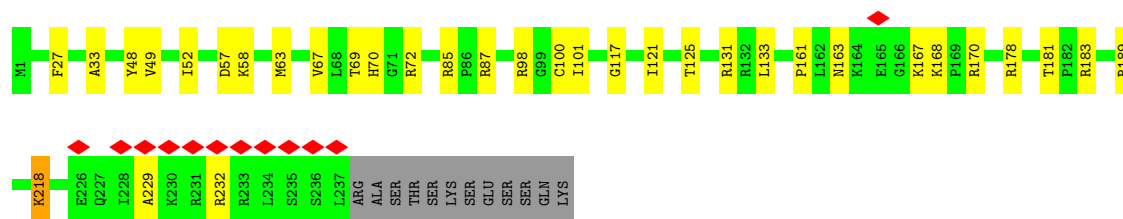
Chain SX: 89% 8% ..



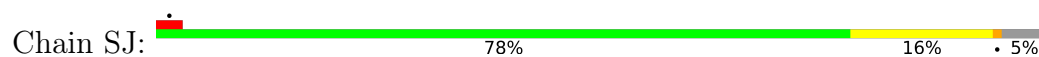
- Molecule 64: 40S ribosomal protein S26

Chain Sa: 77% 12% 11%

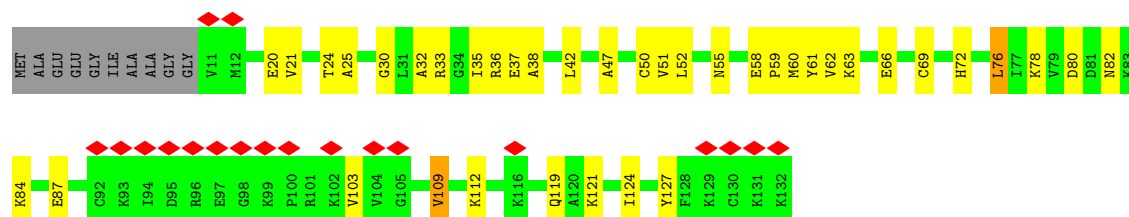




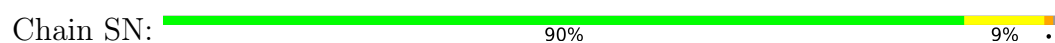
- Molecule 70: 40S ribosomal protein S9



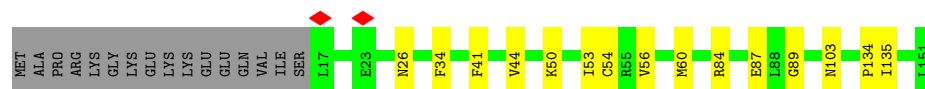
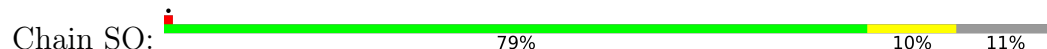
- Molecule 71: 40S ribosomal protein S12



- Molecule 72: 40S ribosomal protein S13



- Molecule 73: 40S ribosomal protein S14

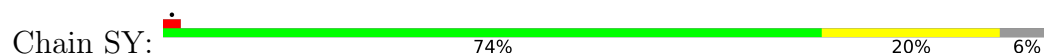


- Molecule 74: 40S ribosomal protein S15a

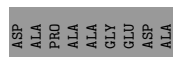
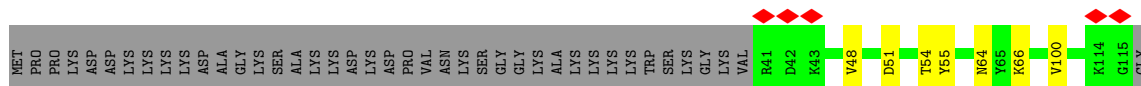




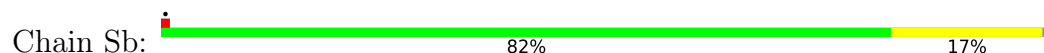
- Molecule 75: 40S ribosomal protein S24



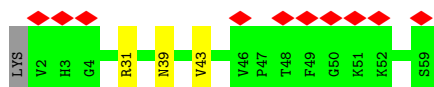
- Molecule 76: 40S ribosomal protein S25



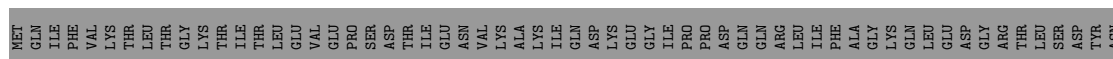
- Molecule 77: 40S ribosomal protein S27



- Molecule 78: 40S ribosomal protein S30



- Molecule 79: Ubiquitin-40S ribosomal protein S27a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114446	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	2.785	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: MG, B8T, OMC, 1MA, MA6, ZN, A2M, 5MU, K, 4AC, MLZ, 5MC, B8H, JMH, 6MZ, OMU, UY1, B8N, PSU, 2MG, OMG, M7A, UR3

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	0.26	3/87525 (0.0%)	0.39	3/136449 (0.0%)
2	L2	0.22	0/2858	0.32	0/4455
3	L3	0.25	0/3653	0.34	0/5691
4	LA	0.35	0/1936	0.67	1/2596 (0.0%)
5	LB	0.29	0/3306	0.58	0/4424
6	LC	0.27	0/2962	0.56	3/3977 (0.1%)
7	LD	0.20	0/2428	0.44	0/3252
8	LE	0.24	0/1799	0.56	0/2414
9	LF	0.28	0/1905	0.53	0/2539
10	LG	0.22	0/1866	0.49	0/2511
11	LH	0.23	0/1537	0.47	0/2066
12	LI	0.28	0/1677	0.50	0/2237
13	LJ	0.20	0/1376	0.50	0/1840
14	LL	0.24	0/1732	0.51	0/2315
15	LM	0.30	0/1161	0.58	0/1554
16	LN	0.31	0/1746	0.59	1/2338 (0.0%)
17	LO	0.27	0/1682	0.53	1/2250 (0.0%)
18	LP	0.24	0/1268	0.51	0/1701
19	LQ	0.26	0/1537	0.51	0/2052
20	LR	0.27	0/1582	0.49	0/2091
21	LS	0.27	0/1501	0.50	0/2013
22	LT	0.25	0/1326	0.50	0/1770
23	LU	0.26	0/839	0.71	0/1126
24	LV	0.24	0/993	0.55	1/1332 (0.1%)
25	LW	0.23	0/1030	0.45	0/1364
26	LX	0.19	0/984	0.41	0/1323
27	LY	0.23	0/1132	0.49	0/1504
28	LZ	0.25	0/1130	0.54	0/1507
29	La	0.26	0/1191	0.52	0/1591
30	Lb	0.25	0/889	0.57	0/1175
31	Lc	0.23	0/774	0.48	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.23	0/903	0.46	0/1216
33	Le	0.26	0/1071	0.56	0/1429
34	Lf	0.27	0/895	0.57	0/1198
35	Lg	0.24	0/916	0.48	0/1220
36	Lh	0.22	0/1023	0.45	0/1351
37	Li	0.19	0/843	0.42	0/1115
38	Lj	0.33	0/720	0.65	0/952
39	Lk	0.20	0/575	0.53	0/761
40	Ll	0.30	0/454	0.61	0/599
41	Lm	0.19	0/435	0.47	0/575
42	Ln	0.24	0/231	0.43	0/294
43	Lo	0.19	0/845	0.42	0/1113
44	Lp	0.26	0/718	0.53	0/953
45	Lr	0.25	0/1017	0.52	1/1364 (0.1%)
46	S2	0.23	3/39987 (0.0%)	0.34	0/62288
47	SA	0.22	0/1784	0.49	1/2424 (0.0%)
48	SB	0.21	0/1765	0.50	0/2362
49	SD	0.25	0/1793	0.55	1/2414 (0.0%)
50	SE	0.22	0/2118	0.52	0/2849
51	SF	0.19	0/1481	0.49	0/1988
52	SH	0.43	0/1519	0.74	0/2033
53	SI	0.24	0/1715	0.53	0/2287
54	SK	0.31	0/851	0.71	0/1147
55	SL	0.22	0/1202	0.45	0/1606
56	SP	0.20	0/1065	0.61	2/1423 (0.1%)
57	SQ	0.32	0/1160	0.75	3/1553 (0.2%)
58	SR	0.24	0/1105	0.62	0/1484
59	SS	0.21	0/1216	0.57	0/1628
60	ST	0.21	0/1131	0.51	0/1515
61	SU	0.24	0/831	0.62	0/1115
62	SV	0.19	0/643	0.42	0/860
63	SX	0.24	0/1116	0.54	2/1490 (0.1%)
64	Sa	0.24	0/836	0.53	0/1121
65	Sc	0.19	0/508	0.51	0/680
66	Sd	0.30	0/470	0.73	0/623
67	Sg	0.19	0/2493	0.63	3/3394 (0.1%)
68	SC	0.24	0/1762	0.51	0/2381
69	SG	0.27	0/1946	0.54	0/2590
70	SJ	0.32	0/1550	0.59	0/2069
71	SM	0.25	0/950	0.68	1/1275 (0.1%)
72	SN	0.22	0/1232	0.43	0/1656
73	SO	0.23	0/1023	0.55	0/1372
74	SW	0.23	0/1051	0.50	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.22	0/1039	0.50	0/1381
76	SZ	0.18	0/604	0.49	0/810
77	Sb	0.19	0/665	0.46	0/891
78	Se	0.16	0/465	0.42	0/612
79	Sf	0.16	0/507	0.46	0/673
All	All	0.25	6/227554 (0.0%)	0.44	24/334035 (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
61	SU	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3785	A2M	O3'-P	5.46	1.61	1.56
46	S2	484	A2M	O3'-P	5.23	1.61	1.56
1	L1	1524	A2M	O3'-P	5.14	1.61	1.56
1	L1	3718	A2M	O3'-P	5.11	1.61	1.56
46	S2	1031	A2M	O3'-P	5.05	1.61	1.56
46	S2	1383	A2M	O3'-P	5.02	1.61	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Sg	8	ARG	CA-C-N	-9.58	115.57	122.18
67	Sg	8	ARG	C-N-CA	-9.58	115.57	122.18
57	SQ	44	PRO	N-CA-CB	-8.24	94.60	103.25
57	SQ	44	PRO	CA-N-CD	-8.22	100.49	112.00
49	SD	219	PRO	CA-N-CD	-8.04	100.75	112.00
56	SP	107	ILE	CA-C-N	7.74	137.26	121.48
56	SP	107	ILE	C-N-CA	7.74	137.26	121.48
47	SA	207	PRO	CA-N-CD	-6.43	103.00	112.00
57	SQ	44	PRO	CB-CA-C	6.33	122.00	111.56
6	LC	66	SER	N-CA-C	6.06	118.68	111.71
67	Sg	5	MET	CB-CG-SD	5.96	130.58	112.70
16	LN	124	ASP	N-CA-C	-5.86	101.25	109.69
24	LV	73	ARG	N-CA-C	5.70	117.17	111.07
45	Lr	125	MET	CB-CG-SD	5.49	129.17	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	SX	60	LYS	CA-C-N	5.47	127.80	120.58
63	SX	60	LYS	C-N-CA	5.47	127.80	120.58
1	L1	1082	C	O4'-C1'-N1	5.44	116.36	108.20
1	L1	417	G	O4'-C1'-N9	5.19	115.99	108.20
6	LC	49	ARG	CA-C-N	5.19	134.46	122.31
6	LC	49	ARG	C-N-CA	5.19	134.46	122.31
1	L1	456	C	O4'-C1'-N1	5.16	115.94	108.20
17	LO	110	PRO	N-CA-C	5.15	116.98	110.70
71	SM	66	GLU	CA-CB-CG	5.07	124.23	114.10
4	LA	153	GLY	N-CA-C	-5.05	108.35	114.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
61	SU	93	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	80211	0	40470	439	0
2	L2	2558	0	1296	10	0
3	L3	3316	0	1687	18	0
4	LA	1898	0	1993	18	0
5	LB	3238	0	3375	25	0
6	LC	2908	0	3082	19	0
7	LD	2382	0	2410	21	0
8	LE	1765	0	1917	19	0
9	LF	1870	0	1996	20	0
10	LG	1835	0	1976	13	0
11	LH	1518	0	1601	13	0
12	LI	1639	0	1687	15	0
13	LJ	1353	0	1393	9	0
14	LL	1701	0	1818	9	0
15	LM	1138	0	1204	11	0
16	LN	1701	0	1749	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	LO	1650	0	1794	9	0
18	LP	1242	0	1269	10	0
19	LQ	1513	0	1628	7	0
20	LR	1566	0	1729	14	0
21	LS	1461	0	1502	10	0
22	LT	1298	0	1366	8	0
23	LU	825	0	850	7	0
24	LV	979	0	1039	5	0
25	LW	1015	0	1079	8	0
26	LX	967	0	1040	4	0
27	LY	1115	0	1205	9	0
28	LZ	1107	0	1182	12	0
29	La	1162	0	1213	10	0
30	Lb	876	0	948	10	0
31	Lc	764	0	804	13	0
32	Ld	888	0	930	3	0
33	Le	1053	0	1147	11	0
34	Lf	876	0	912	5	0
35	Lg	906	0	998	6	0
36	Lh	1015	0	1148	12	0
37	Li	832	0	917	4	0
38	Lj	705	0	736	10	0
39	Lk	569	0	637	7	0
40	Ll	444	0	483	6	0
41	Lm	429	0	465	2	0
42	Ln	230	0	276	0	0
43	Lo	843	0	912	6	0
44	Lp	708	0	756	8	0
45	Lr	1002	0	1068	10	0
46	S2	36958	0	18650	236	0
47	SA	1747	0	1751	15	0
48	SB	1738	0	1809	20	0
49	SD	1765	0	1865	27	0
50	SE	2076	0	2177	14	0
51	SF	1461	0	1511	8	0
52	SH	1497	0	1590	29	0
53	SI	1686	0	1772	22	0
54	SK	827	0	854	17	0
55	SL	1182	0	1253	10	0
56	SP	1045	0	1095	23	0
57	SQ	1142	0	1213	27	0
58	SR	1090	0	1149	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	SS	1198	0	1261	21	0
60	ST	1112	0	1146	11	0
61	SU	821	0	883	17	0
62	SV	636	0	637	8	0
63	SX	1098	0	1167	10	0
64	Sa	821	0	870	7	0
65	Sc	506	0	536	3	0
66	Sd	459	0	448	7	0
67	Sg	2436	0	2393	44	0
68	SC	1725	0	1813	9	0
69	SG	1923	0	2089	23	0
70	SJ	1525	0	1640	22	0
71	SM	940	0	965	23	0
72	SN	1208	0	1294	10	0
73	SO	1010	0	1034	10	0
74	SW	1034	0	1080	6	0
75	SY	1022	0	1088	15	0
76	SZ	598	0	656	5	0
77	Sb	651	0	670	7	0
78	Se	459	0	503	2	0
79	Sf	497	0	495	8	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	LN	1	0	0	0	0
80	LP	1	0	0	0	0
80	LV	1	0	0	0	0
80	Le	2	0	0	0	0
80	Lf	1	0	0	0	0
80	Lg	1	0	0	0	0
80	Lo	1	0	0	0	0
80	S2	134	0	0	0	0
80	SG	1	0	0	0	0
80	SJ	1	0	0	0	0
80	ST	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	L1	767	0	0	4	0
83	L2	3	0	0	0	0
83	L3	6	0	0	0	0
83	LA	8	0	0	0	0
83	LB	2	0	0	0	0
83	LC	8	0	0	0	0
83	LD	1	0	0	0	0
83	LF	2	0	0	0	0
83	LI	1	0	0	0	0
83	LL	1	0	0	0	0
83	LN	2	0	0	0	0
83	LP	1	0	0	0	0
83	LR	1	0	0	0	0
83	LX	1	0	0	0	0
83	LY	1	0	0	0	0
83	La	5	0	0	0	0
83	Lb	1	0	0	0	0
83	Le	4	0	0	0	0
83	Lg	1	0	0	0	0
83	Lj	4	0	0	0	0
83	Ll	1	0	0	0	0
83	Lo	3	0	0	0	0
83	S2	9	0	0	0	0
83	SQ	1	0	0	0	0
83	SX	1	0	0	0	0
83	Sd	1	0	0	0	0
All	All	216242	0	159044	1398	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 (1398) 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)
46:S2:814:5MU:C4	46:S2:814:5MU:C5	1.79	1.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3762:B8H:C6	1:L1:3762:B8H:N1	1.67	1.54
1:L1:3762:B8H:C4	1:L1:3762:B8H:C5	1.84	1.53
1:L1:471:A:N6	1:L1:683:C:H42	1.50	1.08
1:L1:1176:C:H42	1:L1:1184:A:N6	1.52	1.07
1:L1:1176:C:N4	1:L1:1184:A:H61	1.52	1.07
1:L1:471:A:H61	1:L1:683:C:N4	1.51	1.07
1:L1:3951:G:N2	1:L1:4062:A:C6	2.29	1.01
1:L1:3951:G:C2	1:L1:4062:A:N6	2.29	1.01
46:S2:1756:C:N4	46:S2:1775:U:H3	1.58	0.99
52:SH:19:PHE:CZ	52:SH:60:ILE:HG23	1.96	0.99
1:L1:1175:A:H2	1:L1:1185:G:N1	1.63	0.97
1:L1:1761:G:N2	1:L1:1768:C:C2	2.34	0.96
1:L1:1175:A:C2	1:L1:1185:G:N1	2.33	0.95
52:SH:19:PHE:HZ	52:SH:60:ILE:CG2	1.81	0.94
46:S2:885:U:H3	46:S2:901:G:H1	1.03	0.93
46:S2:140:C:N4	46:S2:313:A:H61	1.66	0.93
1:L1:1094:G:H1	1:L1:1201:U:H3	1.03	0.92
1:L1:1174:G:H1	1:L1:1186:U:H3	1.16	0.92
46:S2:140:C:H42	46:S2:313:A:N6	1.67	0.91
1:L1:1764:G:C2	1:L1:1770:A:N6	2.39	0.91
64:Sa:21:ILE:O	64:Sa:29:CYS:HA	1.71	0.91
49:SD:163:PRO:O	49:SD:167:TYR:HB2	1.71	0.90
46:S2:886:A:N6	46:S2:901:G:C2	2.40	0.89
52:SH:19:PHE:CZ	52:SH:60:ILE:CG2	2.55	0.88
1:L1:1759:G:H1	1:L1:1773:U:H3	0.91	0.87
1:L1:1976:G:N1	1:L1:1991:A:C2	2.43	0.87
1:L1:1764:G:N2	1:L1:1770:A:C6	2.42	0.87
1:L1:1175:A:H2	1:L1:1185:G:H1	0.92	0.85
1:L1:3951:G:C2	1:L1:4062:A:C6	2.64	0.85
46:S2:533:A:H61	46:S2:550:C:N4	1.74	0.85
52:SH:72:PHE:O	52:SH:76:GLN:HB2	1.77	0.84
1:L1:2520:C:O2	1:L1:2640:G:N2	2.13	0.82
79:Sf:121:CYS:SG	79:Sf:126:CYS:HB2	2.21	0.81
1:L1:1095:A:H2	1:L1:1200:G:H1	1.28	0.80
1:L1:1764:G:C2	1:L1:1770:A:C6	2.69	0.80
46:S2:140:C:H42	46:S2:313:A:H61	0.84	0.79
1:L1:1761:G:C2	1:L1:1768:C:C2	2.70	0.79
46:S2:1709:G:H1	46:S2:1824:A:H2	1.30	0.79
1:L1:1761:G:C2	1:L1:1768:C:O2	2.36	0.78
1:L1:751:G:O6	1:L1:912:G:N2	2.16	0.78
1:L1:1443:A:H2	1:L1:2103:G:H1	1.27	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:27:G:H21	2:L2:55:A:N6	1.82	0.77
5:LB:223:THR:O	5:LB:274:TYR:HA	1.85	0.76
75:SY:82:ALA:O	75:SY:86:GLU:HB2	1.85	0.76
46:S2:928:G:H1	46:S2:1013:U:H3	1.30	0.76
52:SH:19:PHE:CE1	52:SH:60:ILE:HG23	2.20	0.75
1:L1:1095:A:C2	1:L1:1200:G:N1	2.53	0.75
1:L1:1764:G:N2	1:L1:1770:A:N6	2.35	0.74
1:L1:3951:G:N2	1:L1:4062:A:N6	2.32	0.74
1:L1:1976:G:C6	1:L1:1991:A:N1	2.57	0.73
52:SH:19:PHE:HZ	52:SH:60:ILE:HG21	1.53	0.72
46:S2:1756:C:H42	46:S2:1775:U:H3	0.79	0.72
52:SH:12:ASN:HD21	52:SH:14:GLU:HB2	1.53	0.71
22:LT:43:LYS:O	22:LT:58:HIS:ND1	2.24	0.70
46:S2:140:C:N3	46:S2:313:A:N1	2.39	0.70
1:L1:4982:A:OP1	18:LP:74:LYS:NZ	2.24	0.70
1:L1:5022:U:O2	1:L1:5025:C:N3	2.24	0.70
1:L1:4467:A:H61	1:L1:4490:C:H42	1.39	0.70
46:S2:1534:C:C2	46:S2:1598:G:N2	2.59	0.70
12:LI:42:LYS:HB2	12:LI:45:GLU:HG3	1.73	0.70
1:L1:1176:C:N3	1:L1:1184:A:N1	2.39	0.69
1:L1:471:A:N1	1:L1:683:C:N3	2.41	0.69
1:L1:3762:B8H:C6	1:L1:3762:B8H:CN1	2.70	0.69
1:L1:3951:G:N3	1:L1:4062:A:N1	2.41	0.69
38:Lj:8:PHE:HA	38:Lj:11:ARG:HD2	1.74	0.69
79:Sf:100:LEU:HB3	79:Sf:103:LEU:HB3	1.75	0.68
46:S2:925:G:H1	46:S2:1017:U:H3	1.41	0.68
1:L1:2486:G:C6	1:L1:2494:U:O2	2.47	0.68
1:L1:1940:G:H22	1:L1:4434:C:H5''	1.58	0.68
56:SP:91:GLY:HA2	56:SP:107:ILE:O	1.94	0.67
1:L1:2351:OMC:HM22	1:L1:2352:U:H5'	1.76	0.67
1:L1:3762:B8H:C6	1:L1:3762:B8H:C2	2.67	0.67
2:L2:27:G:N2	2:L2:55:A:N6	2.43	0.66
1:L1:169:G:N2	1:L1:266:C:O2	2.28	0.66
46:S2:70:G:H21	46:S2:79:A:H62	1.43	0.66
71:SM:60:MET:HE3	71:SM:60:MET:H	1.58	0.66
1:L1:2486:G:O6	1:L1:2494:U:O2	2.13	0.66
46:S2:1752:C:N3	46:S2:1779:G:N1	2.43	0.66
46:S2:533:A:N6	46:S2:550:C:H42	1.92	0.66
1:L1:1100:U:H3	1:L1:1195:G:H1	1.41	0.66
1:L1:1440:U:O2	1:L1:2106:G:C2	2.49	0.66
46:S2:1754:G:O6	46:S2:1779:G:N3	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4098:A:H3'	1:L1:4099:G:H4'	1.77	0.66
1:L1:5022:U:O2	1:L1:5025:C:C4	2.50	0.65
16:LN:124:ASP:OD1	16:LN:125:SER:N	2.29	0.65
46:S2:533:A:N6	46:S2:550:C:N4	2.45	0.65
46:S2:1543:U:H4'	57:SQ:43:GLU:HG2	1.78	0.65
1:L1:2469:C:H5	1:L1:2471:G:H1	1.43	0.65
1:L1:1824:G:H5''	22:LT:35:LYS:HE2	1.79	0.65
23:LU:65:ARG:HG2	23:LU:67:LYS:H	1.61	0.65
71:SM:58:GLU:HB3	71:SM:61:TYR:HB3	1.79	0.65
1:L1:1996:C:N4	1:L1:2000:G:H22	1.95	0.65
36:Lh:106:LYS:HG3	36:Lh:109:ARG:HH22	1.61	0.65
1:L1:1974:U:O4	1:L1:1993:C:N3	2.30	0.65
46:S2:1418:C:H2'	46:S2:1419:C:H2'	1.79	0.64
37:Li:51:ALA:HB3	37:Li:54:GLU:HG3	1.79	0.64
27:LY:31:SER:HA	27:LY:48:PRO:HA	1.80	0.64
57:SQ:112:LEU:O	57:SQ:115:TYR:O	2.16	0.64
36:Lh:13:LYS:NZ	36:Lh:16:GLU:OE1	2.30	0.64
1:L1:1996:C:H42	1:L1:2000:G:N2	1.97	0.63
1:L1:3823:G:OP2	1:L1:3823:G:N2	2.28	0.63
46:S2:377:G:H5'	53:SI:98:LYS:HB3	1.79	0.63
45:Lr:26:SER:OG	45:Lr:28:GLU:OE1	2.16	0.63
67:Sg:247:TRP:HB3	67:Sg:258:ILE:HD11	1.79	0.63
1:L1:1764:G:N3	1:L1:1770:A:N1	2.47	0.63
18:LP:138:PRO:HB3	18:LP:140:MET:HE3	1.80	0.63
25:LW:84:GLY:HA2	69:SG:161:PRO:HD3	1.80	0.63
1:L1:1095:A:N1	1:L1:1200:G:O6	2.31	0.63
52:SH:8:ILE:HD12	52:SH:16:PRO:HB3	1.80	0.63
18:LP:126:ARG:HG3	18:LP:140:MET:HE1	1.79	0.63
61:SU:80:PHE:HB3	66:Sd:52:PHE:HB3	1.79	0.63
1:L1:1700:G:H1	9:LF:177:ARG:HE	1.47	0.63
52:SH:27:LEU:HD11	52:SH:79:LEU:HD11	1.79	0.63
1:L1:2611:A:H5'	1:L1:2688:G:H4'	1.81	0.63
46:S2:1091:C:HO2'	74:SW:2:VAL:N	1.97	0.62
46:S2:1756:C:N4	46:S2:1775:U:N3	2.31	0.62
1:L1:1974:U:H3	1:L1:1993:C:N4	1.97	0.62
67:Sg:89:LEU:HB3	67:Sg:99:ARG:HB2	1.81	0.62
1:L1:1094:G:O6	1:L1:1201:U:O4	2.16	0.62
37:Li:2:ALA:N	37:Li:5:TYR:HH	1.97	0.62
52:SH:69:LEU:HG	52:SH:96:ALA:HB2	1.80	0.62
27:LY:39:ARG:O	27:LY:42:TYR:O	2.18	0.62
46:S2:818:A:OP1	70:SJ:80:ARG:NH1	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SB:173:THR:O	48:SB:177:GLN:HB2	2.00	0.62
53:SI:135:GLU:O	53:SI:139:LYS:HB3	1.99	0.62
46:S2:70:G:OP2	69:SG:167:LYS:NZ	2.32	0.62
1:L1:678:C:H4'	45:Lr:96:MET:HE2	1.82	0.62
1:L1:1175:A:N1	1:L1:1185:G:O6	2.33	0.62
1:L1:2601:A:N6	1:L1:2744:A:OP2	2.32	0.62
62:SV:32:ILE:HG12	62:SV:60:ARG:HD2	1.82	0.62
1:L1:4894:A:H5''	1:L1:4895:C:H2'	1.81	0.61
1:L1:2088:A:OP2	19:LQ:37:ARG:NH2	2.34	0.61
1:L1:1368:A:H1'	27:LY:1:MET:HE2	1.83	0.61
46:S2:121:OMU:HM23	50:SE:144:ALA:HB3	1.81	0.61
46:S2:1748:G:H1	46:S2:1786:U:H3	1.48	0.61
49:SD:67:ARG:HH11	54:SK:97:SER:H	1.48	0.61
1:L1:4041:C:H5'	1:L1:4042:G:H5''	1.82	0.61
66:Sd:15:GLY:H	66:Sd:19:ARG:HH12	1.48	0.61
26:LX:147:LEU:O	26:LX:151:ASN:ND2	2.34	0.61
46:S2:1490:OMG:N2	61:SU:72:GLU:OE1	2.33	0.61
57:SQ:97:GLN:OE1	67:Sg:60:ARG:NH1	2.34	0.61
1:L1:1095:A:H2	1:L1:1200:G:N1	1.95	0.60
1:L1:1870:C:H2'	1:L1:1871:A2M:H8	1.82	0.60
1:L1:2562:G:N2	1:L1:2565:A:OP2	2.34	0.60
1:L1:3967:G:O6	1:L1:4055:U:O4	2.18	0.60
49:SD:158:ILE:HG13	49:SD:164:VAL:HG12	1.81	0.60
1:L1:739:G:HO2'	1:L1:740:G:H8	1.49	0.60
1:L1:1759:G:O6	1:L1:1773:U:O4	2.19	0.60
56:SP:75:VAL:HG12	56:SP:93:MET:HG3	1.83	0.60
1:L1:3689:G:O2'	1:L1:3818:UY1:OP2	2.17	0.60
6:LC:140:LYS:HE3	6:LC:245:HIS:HB2	1.83	0.60
46:S2:1277:C:O2'	54:SK:55:ARG:NH1	2.34	0.60
8:LE:152:ILE:HD12	8:LE:189:THR:HG21	1.83	0.60
46:S2:1752:C:N4	46:S2:1779:G:N2	2.48	0.60
8:LE:46:ARG:O	8:LE:65:ARG:NH1	2.34	0.60
55:SL:88:ILE:HD11	55:SL:109:MET:HE3	1.83	0.60
1:L1:4095:G:H1	1:L1:4113:U:H3	1.48	0.60
52:SH:53:VAL:O	52:SH:57:ARG:HB3	2.02	0.60
52:SH:65:PRO:O	52:SH:69:LEU:N	2.34	0.60
69:SG:33:ALA:N	69:SG:52:ILE:O	2.35	0.60
1:L1:178:C:H2'	1:L1:179:G:H8	1.67	0.60
23:LU:105:ASN:HB3	23:LU:111:GLU:HG2	1.82	0.60
64:Sa:44:ILE:HG23	64:Sa:45:VAL:HG23	1.84	0.60
46:S2:533:A:H61	46:S2:550:C:H42	1.44	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4627:U:H5''	5:LB:373:LYS:HG2	1.84	0.59
10:LG:100:HIS:HA	10:LG:103:ARG:HG3	1.84	0.59
1:L1:3937:C:H1'	16:LN:125:SER:HB3	1.84	0.59
60:ST:104:LEU:HD13	60:ST:121:ARG:HE	1.66	0.59
1:L1:4888:U:O2	1:L1:4931:G:N2	2.35	0.59
60:ST:24:LYS:NZ	60:ST:25:SER:OG	2.35	0.59
1:L1:452:A:H4'	1:L1:453:G:H5'	1.85	0.59
57:SQ:43:GLU:HG3	57:SQ:44:PRO:HD2	1.85	0.59
61:SU:19:ARG:HH11	61:SU:92:HIS:HB3	1.68	0.59
61:SU:56:MET:HB2	61:SU:86:LYS:HB3	1.83	0.59
1:L1:2695:A:OP1	39:Lk:35:LYS:NZ	2.35	0.59
1:L1:3663:A:N6	1:L1:4168:G:O2'	2.36	0.59
1:L1:4694:G:O2'	11:LH:71:ARG:NH2	2.36	0.59
1:L1:1996:C:N4	1:L1:2000:G:N2	2.50	0.59
1:L1:3594:C:C2	1:L1:3597:G:C2	2.90	0.59
15:LM:123:ILE:HD13	17:LO:182:GLU:HG2	1.85	0.59
56:SP:91:GLY:CA	56:SP:107:ILE:O	2.51	0.59
71:SM:47:ALA:HA	71:SM:112:LYS:HA	1.85	0.59
1:L1:1459:A:OP1	19:LQ:65:ARG:NH1	2.36	0.59
1:L1:1687:U:OP2	30:Lb:19:ASN:ND2	2.36	0.59
46:S2:1396:A:O2'	46:S2:1398:G:N7	2.36	0.59
70:SJ:94:LEU:HA	70:SJ:97:ILE:HD12	1.85	0.59
54:SK:29:MET:SD	54:SK:42:ASN:ND2	2.73	0.59
1:L1:138:G:H2'	1:L1:139:G:C8	2.38	0.58
1:L1:1761:G:N2	1:L1:1768:C:O2	2.33	0.58
1:L1:234:G:O6	1:L1:2304:U:O2	2.21	0.58
1:L1:4250:G:O2'	13:LJ:129:ASP:OD1	2.20	0.58
46:S2:886:A:C6	46:S2:901:G:C2	2.91	0.58
67:Sg:272:GLN:NE2	67:Sg:284:PRO:O	2.36	0.58
70:SJ:65:GLU:HG3	70:SJ:66:LYS:HD3	1.85	0.58
34:Lf:78:HIS:O	34:Lf:83:MET:HB2	2.03	0.58
46:S2:508:A:H3'	46:S2:509:OMG:H8	1.69	0.58
46:S2:1158:G:H5''	74:SW:76:SER:HB3	1.85	0.58
67:Sg:176:VAL:HB	67:Sg:186:THR:HB	1.84	0.58
75:SY:4:THR:OG1	75:SY:32:LYS:NZ	2.37	0.58
46:S2:886:A:C6	46:S2:901:G:N2	2.71	0.58
46:S2:1020:A:N7	72:SN:70:LYS:NZ	2.51	0.58
46:S2:1754:G:O6	46:S2:1779:G:C2	2.57	0.58
70:SJ:182:GLN:O	70:SJ:185:ALA:C	2.47	0.58
1:L1:1591:U:OP2	1:L1:2856:C:O2'	2.21	0.58
45:Lr:82:ILE:HD11	45:Lr:96:MET:HE1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3711:A:C6	46:S2:970:G:C2	2.92	0.57
8:LE:152:ILE:O	8:LE:159:GLY:N	2.37	0.57
46:S2:303:C:H5''	53:SI:75:LYS:HE2	1.86	0.57
69:SG:98:ARG:NH1	69:SG:101:ILE:O	2.37	0.57
46:S2:329:G:H2'	46:S2:330:G:C8	2.39	0.57
1:L1:1480:C:O2'	1:L1:1482:G:OP2	2.22	0.57
1:L1:3920:U:OP1	83:L1:5401:HOH:O	2.17	0.57
46:S2:672:A:N6	46:S2:1027:A:OP1	2.37	0.57
56:SP:111:MET:HG3	59:SS:117:ILE:HD11	1.86	0.57
1:L1:1339:U:H2'	1:L1:1340:OMC:C6	2.40	0.57
1:L1:1976:G:C6	1:L1:1991:A:C2	2.92	0.57
46:S2:886:A:N6	46:S2:901:G:N1	2.52	0.57
1:L1:1718:C:OP2	9:LF:200:ARG:NH1	2.36	0.57
1:L1:2755:A:OP2	28:LZ:51:ARG:NH1	2.37	0.57
1:L1:4910:G:N2	17:LO:106:ASP:O	2.37	0.57
16:LN:200:LEU:HD22	16:LN:204:ARG:HD3	1.87	0.57
46:S2:326:C:O2	46:S2:327:G:N2	2.38	0.57
1:L1:2450:G:OP1	4:LA:17:ARG:NH2	2.38	0.57
1:L1:2520:C:H2'	1:L1:2521:G:H8	1.70	0.57
1:L1:4970:C:H5''	18:LP:71:ALA:HB1	1.86	0.57
71:SM:121:LYS:HA	71:SM:124:ILE:HD12	1.86	0.57
1:L1:1443:A:N1	1:L1:2104:G:C2	2.73	0.57
1:L1:1756:U:O2'	1:L1:1758:G:OP2	2.23	0.57
1:L1:4940:C:OP1	8:LE:156:ARG:NH1	2.34	0.57
26:LX:82:THR:HG22	26:LX:155:ILE:HG23	1.86	0.57
46:S2:878:G:H1	46:S2:908:A:H2	1.49	0.57
1:L1:1174:G:O6	1:L1:1186:U:O4	2.22	0.57
14:LL:46:ILE:HB	14:LL:49:ARG:HB2	1.86	0.57
1:L1:1684:A:OP1	29:La:47:LYS:NZ	2.35	0.56
57:SQ:44:PRO:HG2	57:SQ:77:HIS:HB3	1.86	0.56
7:LD:215:ASP:OD1	7:LD:216:GLU:N	2.35	0.56
46:S2:1824:A:O2'	46:S2:1825:A:N7	2.36	0.56
57:SQ:102:GLU:HA	57:SQ:105:LYS:HB3	1.86	0.56
1:L1:3968:U:O4	1:L1:3969:G:N2	2.38	0.56
13:LJ:112:HIS:HA	13:LJ:115:LEU:HB2	1.87	0.56
18:LP:39:MET:HG2	18:LP:43:LYS:HD3	1.87	0.56
46:S2:94:G:O2'	46:S2:508:A:O2'	2.22	0.56
46:S2:94:G:HO2'	46:S2:508:A:HO2'	1.54	0.56
67:Sg:256:ILE:HB	67:Sg:270:LEU:HB2	1.88	0.56
1:L1:757:G:H2'	1:L1:758:G:C8	2.41	0.56
1:L1:2578:G:N7	28:LZ:17:ARG:NH1	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4745:G:H1	1:L1:4955:A:H61	1.52	0.56
46:S2:355:G:OP2	55:SL:107:LYS:NZ	2.38	0.56
46:S2:1095:C:N3	46:S2:1149:A:N1	2.53	0.56
1:L1:3788:C:N4	1:L1:3812:C:OP2	2.39	0.56
12:LI:177:ASN:O	12:LI:181:PHE:HB2	2.05	0.56
53:SI:57:ALA:HB2	53:SI:183:GLY:HA2	1.85	0.56
67:Sg:87:LEU:HB2	67:Sg:101:PHE:HB2	1.88	0.56
1:L1:1443:A:C2	1:L1:2103:G:N1	2.62	0.56
20:LR:28:GLU:HG3	20:LR:49:LEU:HD22	1.87	0.56
12:LI:152:LEU:HB3	12:LI:165:ILE:HD12	1.88	0.56
14:LL:139:SER:OG	14:LL:142:GLU:OE1	2.23	0.56
46:S2:1228:A:H2'	46:S2:1229:G:C8	2.40	0.56
49:SD:206:ASP:OD2	49:SD:206:ASP:N	2.37	0.56
1:L1:3589:G:N2	1:L1:3590:G:N7	2.53	0.56
31:Lc:104:ILE:HG23	31:Lc:105:ILE:HG23	1.87	0.56
1:L1:495:C:N4	1:L1:496:G:O6	2.38	0.56
1:L1:1761:G:N1	1:L1:1768:C:N3	2.54	0.56
1:L1:3868:G:H22	1:L1:3900:G:H1'	1.71	0.56
21:LS:15:ARG:HB3	21:LS:27:LEU:HD23	1.87	0.56
46:S2:874:G:H2'	46:S2:875:A:H8	1.71	0.56
46:S2:922:A:OP1	74:SW:28:ARG:NH2	2.39	0.56
70:SJ:113:GLN:OE1	70:SJ:154:GLN:NE2	2.38	0.56
1:L1:1100:U:O2	1:L1:1195:G:N2	2.33	0.56
47:SA:89:LYS:HD3	47:SA:201:LEU:HG	1.87	0.56
67:Sg:261:LEU:HD23	67:Sg:264:LYS:HZ2	1.70	0.56
1:L1:2705:G:H22	1:L1:2710:C:H5	1.53	0.55
1:L1:3711:A:N1	46:S2:970:G:C2	2.74	0.55
6:LC:163:LYS:HB2	6:LC:166:GLU:HG3	1.88	0.55
59:SS:73:ASN:O	59:SS:76:GLN:NE2	2.39	0.55
46:S2:1017:U:H5'	72:SN:55:ARG:HD3	1.88	0.55
1:L1:4472:G:O2'	41:Lm:100:TYR:O	2.23	0.55
46:S2:1709:G:O6	46:S2:1824:A:N1	2.40	0.55
71:SM:69:CYS:O	71:SM:72:HIS:C	2.49	0.55
11:LH:140:GLN:HB2	11:LH:143:GLU:HG2	1.88	0.55
3:L3:87:G:OP2	36:Lh:5:LYS:NZ	2.40	0.55
62:SV:16:LYS:HA	62:SV:22:ARG:O	2.05	0.55
8:LE:119:GLU:HG3	33:Le:7:LEU:HD22	1.88	0.55
47:SA:30:LEU:HD21	47:SA:35:GLU:HG3	1.89	0.55
1:L1:992:C:N4	1:L1:994:G:O6	2.40	0.55
1:L1:1811:G:H4'	30:Lb:60:ASN:HD22	1.72	0.55
46:S2:1228:A:H2'	46:S2:1229:G:H8	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Sg:24:THR:HG23	67:Sg:27:PHE:H	1.72	0.55
1:L1:364:G:O6	38:Lj:55:ARG:NH2	2.36	0.55
1:L1:2800:G:H1'	38:Lj:9:GLY:HA3	1.89	0.55
1:L1:4467:A:N1	1:L1:4490:C:N3	2.55	0.55
24:LV:58:GLY:N	24:LV:81:VAL:O	2.37	0.55
34:Lf:45:LYS:HD2	34:Lf:105:LEU:HA	1.89	0.55
46:S2:656:G:O2'	68:SC:227:ARG:NH1	2.39	0.55
46:S2:1424:G:H2'	46:S2:1425:G:H8	1.72	0.55
46:S2:511:U:H2'	46:S2:512:A2M:H8	1.89	0.55
70:SJ:3:VAL:HB	70:SJ:5:ARG:HD3	1.88	0.55
70:SJ:114:VAL:HG12	70:SJ:157:ILE:HD11	1.89	0.55
1:L1:188:G:O2'	1:L1:190:G:OP2	2.25	0.54
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.89	0.54
8:LE:192:LYS:O	34:Lf:108:SER:OG	2.25	0.54
67:Sg:11:LEU:HB2	67:Sg:307:VAL:HB	1.90	0.54
72:SN:140:LYS:NZ	72:SN:141:TYR:O	2.40	0.54
79:Sf:132:MET:HG2	79:Sf:139:HIS:HB3	1.89	0.54
1:L1:1521:C:OP1	6:LC:100:ARG:NH2	2.33	0.54
1:L1:2101:C:N3	1:L1:2102:G:N2	2.47	0.54
1:L1:4088:C:OP1	4:LA:37:ARG:NH1	2.40	0.54
3:L3:110:U:H3'	40:Ll:8:ARG:HH12	1.72	0.54
33:Le:77:PHE:HB3	33:Le:88:LEU:HD11	1.89	0.54
36:Lh:88:THR:HG22	36:Lh:91:MET:H	1.71	0.54
52:SH:19:PHE:CE1	52:SH:60:ILE:CG2	2.88	0.54
1:L1:1699:A:OP1	1:L1:2085:G:O2'	2.26	0.54
1:L1:4299:U:OP1	30:Lb:33:LYS:NZ	2.40	0.54
12:LI:48:LEU:O	12:LI:139:ARG:HA	2.07	0.54
46:S2:1464:C:OP1	58:SR:63:ARG:NH2	2.40	0.54
53:SI:152:ARG:O	53:SI:156:ALA:HB2	2.07	0.54
70:SJ:138:ARG:NH2	70:SJ:152:ASP:OD2	2.40	0.54
77:Sb:49:HIS:ND1	77:Sb:69:GLY:O	2.40	0.54
1:L1:1095:A:N1	1:L1:1200:G:C6	2.76	0.54
1:L1:1419:G:O2'	1:L1:1501:C:N4	2.39	0.54
31:Lc:43:ALA:HA	31:Lc:97:ILE:HG22	1.89	0.54
59:SS:136:THR:O	59:SS:144:ARG:NH2	2.41	0.54
60:ST:22:LEU:HD12	60:ST:28:LEU:HD22	1.88	0.54
60:ST:42:HIS:HA	60:ST:83:GLN:HG3	1.89	0.54
29:La:72:THR:HG22	29:La:110:LYS:HB3	1.89	0.54
48:SB:124:HIS:HA	48:SB:137:LEU:O	2.07	0.54
1:L1:2906:G:N2	1:L1:3586:G:O6	2.41	0.54
1:L1:3717:A:H2'	1:L1:3718:A2M:H8	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LG:38:ASN:ND2	10:LG:43:GLN:OE1	2.41	0.54
45:Lr:66:ARG:NH2	45:Lr:68:SER:OG	2.40	0.54
67:Sg:163:PRO:HB2	67:Sg:179:LEU:HB3	1.89	0.54
1:L1:508:G:O2'	1:L1:510:U:OP2	2.21	0.54
1:L1:3946:G:O6	1:L1:4067:U:O4	2.25	0.54
1:L1:4103:C:C2	1:L1:4105:A:C6	2.95	0.54
1:L1:4184:G:H5'	4:LA:233:ARG:HB2	1.90	0.54
3:L3:58:G:O6	38:Lj:63:ARG:NH1	2.39	0.54
47:SA:214:GLU:OE1	58:SR:81:ARG:NH1	2.41	0.54
1:L1:3929:G:OP1	16:LN:72:LYS:NZ	2.41	0.54
45:Lr:7:TRP:O	45:Lr:11:ARG:HB2	2.07	0.54
46:S2:643:A:OP1	70:SJ:38:ARG:NH1	2.41	0.54
48:SB:76:ASN:OD1	48:SB:76:ASN:N	2.41	0.54
1:L1:184:U:O2	1:L1:254:G:O6	2.25	0.54
1:L1:1996:C:N3	1:L1:2000:G:N1	2.55	0.54
46:S2:1756:C:N4	46:S2:1775:U:C4	2.76	0.54
50:SE:87:MET:N	50:SE:101:LEU:O	2.41	0.54
1:L1:1789:C:OP1	12:LI:21:ARG:NH2	2.41	0.53
1:L1:4103:C:N3	1:L1:4105:A:C6	2.77	0.53
1:L1:4274:A:H2'	1:L1:4275:G:C8	2.43	0.53
1:L1:4771:C:H2'	1:L1:4772:C:C6	2.43	0.53
12:LI:177:ASN:HB2	12:LI:180:GLU:HG2	1.89	0.53
1:L1:2279:A:O2'	33:Le:48:ARG:NH2	2.41	0.53
1:L1:1443:A:C6	1:L1:2104:G:N1	2.77	0.53
1:L1:3762:B8H:C5	1:L1:3762:B8H:C2	2.85	0.53
22:LT:93:ILE:HA	22:LT:96:ILE:HG12	1.89	0.53
46:S2:913:A:N6	52:SH:98:ARG:O	2.39	0.53
46:S2:943:U:O2'	73:SO:135:ILE:O	2.25	0.53
44:Lp:85:ARG:NH1	46:S2:939:U:OP1	2.41	0.53
46:S2:951:C:O2'	73:SO:50:LYS:NZ	2.40	0.53
1:L1:3641:U:H5	1:L1:3646:A:N7	2.07	0.53
70:SJ:182:GLN:O	70:SJ:185:ALA:O	2.26	0.53
1:L1:2748:C:H4'	35:Lg:65:MET:HE2	1.89	0.53
1:L1:2758:G:O2'	1:L1:2765:A:N3	2.37	0.53
20:LR:178:GLN:HA	20:LR:181:LYS:HG2	1.91	0.53
46:S2:747:U:N3	46:S2:796:G:N1	2.57	0.53
57:SQ:94:ALA:HA	57:SQ:97:GLN:HG2	1.91	0.53
1:L1:233:U:H2'	1:L1:234:G:C8	2.43	0.53
8:LE:153:LEU:HD11	8:LE:195:ILE:HG13	1.89	0.53
49:SD:10:LYS:NZ	61:SU:111:GLU:OE1	2.38	0.53
50:SE:98:ASN:HB2	50:SE:114:ILE:HG13	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SH:33:ASN:O	52:SH:34:SER:HB2	2.07	0.53
1:L1:3717:A:H2'	1:L1:3718:A2M:C8	2.39	0.53
46:S2:466:G:O2'	69:SG:72:ARG:NH2	2.40	0.53
69:SG:48:TYR:HE1	69:SG:117:GLY:H	1.56	0.53
1:L1:5022:U:C2	1:L1:5025:C:N3	2.77	0.53
46:S2:1654:G:OP1	60:ST:90:SER:OG	2.26	0.53
46:S2:1662:U:O4	46:S2:1663:A:N6	2.42	0.53
53:SI:61:ASP:OD1	53:SI:61:ASP:N	2.40	0.53
1:L1:2903:G:H21	1:L1:3592:G:H22	1.57	0.53
3:L3:45:C:H4'	40:L1:11:ARG:HD3	1.91	0.53
6:LC:284:MET:HG2	6:LC:287:THR:HG22	1.90	0.53
23:LU:74:SER:OG	23:LU:76:VAL:O	2.26	0.53
46:S2:928:G:H2'	46:S2:929:G:C8	2.44	0.53
47:SA:76:VAL:HG12	47:SA:123:VAL:HB	1.91	0.53
7:LD:115:MET:HA	7:LD:118:ILE:HD12	1.91	0.52
1:L1:1443:A:N1	1:L1:2103:G:O6	2.41	0.52
31:Lc:48:LEU:HD21	31:Lc:60:ILE:HG21	1.91	0.52
46:S2:205:G:H2'	46:S2:206:G:C8	2.44	0.52
77:Sb:81:ARG:HD3	77:Sb:84:HIS:HA	1.90	0.52
1:L1:2486:G:O6	1:L1:2494:U:C2	2.62	0.52
1:L1:2583:C:OP2	35:Lg:76:ARG:NH1	2.41	0.52
47:SA:52:LYS:NZ	62:SV:83:PHE:O	2.42	0.52
52:SH:30:LEU:HD21	52:SH:82:GLU:HG2	1.92	0.52
1:L1:1764:G:N2	1:L1:1768:C:O2'	2.43	0.52
46:S2:1513:C:H2'	46:S2:1514:G:H8	1.73	0.52
52:SH:19:PHE:CZ	52:SH:60:ILE:HG21	2.34	0.52
61:SU:38:ASP:OD1	61:SU:41:ARG:NH2	2.42	0.52
67:Sg:227:LEU:HD13	67:Sg:228:TYR:HB2	1.91	0.52
1:L1:453:G:H4'	1:L1:454:U:H5'	1.91	0.52
1:L1:4258:C:H5'	13:LJ:68:ILE:HD11	1.90	0.52
33:Le:108:ARG:HD3	33:Le:127:ALA:HB3	1.91	0.52
46:S2:1236:G:O2'	56:SP:131:PRO:O	2.27	0.52
46:S2:1536:G:H2'	46:S2:1537:A:C8	2.45	0.52
2:L2:6:C:H4'	7:LD:52:ILE:HD13	1.92	0.52
11:LH:31:ARG:NH1	11:LH:149:ASN:OD1	2.42	0.52
32:Ld:44:ARG:O	32:Ld:48:GLU:HG2	2.10	0.52
53:SI:117:TYR:HD1	53:SI:152:ARG:HB3	1.74	0.52
56:SP:95:GLY:HA2	56:SP:104:GLN:HA	1.92	0.52
67:Sg:285:GLN:O	67:Sg:303:THR:OG1	2.27	0.52
1:L1:1405:C:N4	1:L1:1408:G:N3	2.50	0.52
1:L1:4992:G:H2'	1:L1:4993:G:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:71:A:N1	3:L3:81:C:O2'	2.40	0.52
15:LM:106:ASP:OD1	15:LM:109:ARG:NH2	2.42	0.52
59:SS:46:ARG:HH12	59:SS:52:LEU:HD22	1.75	0.52
46:S2:145:G:O6	69:SG:178:ARG:NH2	2.41	0.52
46:S2:1302:G:O6	46:S2:1307:U:O4	2.28	0.52
46:S2:1615:U:O4	56:SP:40:ARG:NH2	2.43	0.52
67:Sg:107:ASP:HB2	67:Sg:125:ARG:HD2	1.92	0.52
69:SG:85:ARG:O	69:SG:87:ARG:NH1	2.43	0.52
1:L1:2724:G:O2'	1:L1:2726:G:OP2	2.28	0.52
16:LN:138:PHE:HA	16:LN:143:ARG:HD2	1.92	0.52
17:LO:61:ARG:HA	17:LO:70:PRO:HD2	1.92	0.52
1:L1:1976:G:O6	1:L1:1991:A:N1	2.43	0.52
56:SP:92:SER:HB2	56:SP:107:ILE:HD13	1.92	0.52
18:LP:125:MET:HE3	18:LP:143:PRO:HG3	1.92	0.51
55:SL:126:VAL:HG12	55:SL:145:VAL:HG22	1.92	0.51
1:L1:138:G:H2'	1:L1:139:G:H8	1.74	0.51
5:LB:216:MET:HE2	5:LB:283:LYS:HD2	1.93	0.51
46:S2:587:A:H5'	46:S2:592:C:H41	1.75	0.51
46:S2:1096:G:OP1	74:SW:20:ARG:NH1	2.44	0.51
68:SC:187:ARG:HD3	68:SC:192:LEU:HD12	1.92	0.51
71:SM:80:ASP:OD2	71:SM:80:ASP:N	2.38	0.51
75:SY:83:LYS:HE3	75:SY:96:LEU:HD23	1.92	0.51
1:L1:4986:G:H5''	5:LB:176:LYS:HG3	1.92	0.51
28:LZ:48:ARG:HB2	28:LZ:69:LYS:HB3	1.92	0.51
46:S2:902:G:O2'	46:S2:903:A:O4'	2.29	0.51
57:SQ:21:ALA:HB2	57:SQ:72:VAL:HG13	1.92	0.51
57:SQ:112:LEU:O	57:SQ:115:TYR:C	2.54	0.51
59:SS:22:GLY:HA2	59:SS:56:ALA:HB3	1.91	0.51
1:L1:1750:G:H5'	12:LI:40:LYS:HZ2	1.76	0.51
1:L1:2672:C:OP1	44:Lp:44:LYS:NZ	2.42	0.51
1:L1:4774:C:O2'	1:L1:4775:C:O4'	2.27	0.51
1:L1:1974:U:N3	1:L1:1993:C:N4	2.58	0.51
61:SU:98:VAL:HA	61:SU:101:ILE:HG12	1.93	0.51
1:L1:2520:C:H2'	1:L1:2521:G:C8	2.46	0.51
5:LB:223:THR:O	5:LB:274:TYR:CA	2.57	0.51
14:LL:139:SER:O	14:LL:143:GLU:HB2	2.10	0.51
19:LQ:108:ARG:O	19:LQ:112:ARG:HG3	2.11	0.51
46:S2:10:G:H21	68:SC:114:LYS:HA	1.76	0.51
46:S2:1775:U:O2	46:S2:1776:G:N2	2.44	0.51
70:SJ:107:GLU:HA	70:SJ:112:THR:HG21	1.92	0.51
1:L1:1444:G:N2	1:L1:2102:G:O6	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:71:G:O6	69:SG:170:ARG:NH2	2.44	0.51
46:S2:940:U:H3	46:S2:1002:U:H3	1.58	0.51
46:S2:1005:G:OP2	48:SB:162:ARG:NH2	2.44	0.51
56:SP:115:TYR:HB2	56:SP:118:GLU:HG3	1.93	0.51
1:L1:4860:G:H2'	1:L1:4861:G:H8	1.76	0.51
8:LE:180:VAL:HG21	8:LE:258:LEU:HD11	1.92	0.51
54:SK:15:LEU:HD13	54:SK:49:MET:HE1	1.93	0.51
1:L1:3673:C:O2'	1:L1:4080:C:OP1	2.27	0.51
1:L1:4457:U:H1'	5:LB:252:ALA:HB3	1.93	0.51
6:LC:328:LEU:HD13	9:LF:187:MET:HE2	1.92	0.51
46:S2:84:A:N3	46:S2:150:A:O2'	2.42	0.51
46:S2:857:U:H2'	46:S2:858:A:C8	2.46	0.51
46:S2:878:G:O6	46:S2:908:A:N1	2.45	0.51
46:S2:1550:G:H3'	46:S2:1579:A:H61	1.75	0.51
67:Sg:39:THR:HG22	67:Sg:60:ARG:HG2	1.92	0.51
71:SM:69:CYS:O	71:SM:72:HIS:O	2.29	0.51
1:L1:1820:C:H2'	1:L1:1822:U:H5'	1.92	0.50
46:S2:533:A:H2'	46:S2:534:G:C8	2.47	0.50
46:S2:1669:G:OP1	61:SU:79:ARG:NH1	2.43	0.50
74:SW:3:ARG:HH12	74:SW:28:ARG:HH21	1.58	0.50
8:LE:193:PHE:HD1	34:Lf:106:TYR:HB2	1.76	0.50
20:LR:4:LEU:HD11	20:LR:29:THR:HG23	1.92	0.50
45:Lr:63:VAL:HG13	45:Lr:79:ARG:HG2	1.92	0.50
47:SA:85:ARG:NH1	47:SA:203:PHE:O	2.42	0.50
77:Sb:36:LYS:NZ	77:Sb:40:CYS:O	2.44	0.50
1:L1:1079:C:H2'	1:L1:1080:C:C6	2.46	0.50
1:L1:1270:A:O2'	1:L1:1439:C:O2	2.30	0.50
79:Sf:120:GLU:OE1	79:Sf:129:GLY:N	2.41	0.50
1:L1:2554:U:O2	1:L1:2764:A:N7	2.45	0.50
1:L1:4076:G:OP2	1:L1:4163:U:N3	2.37	0.50
28:LZ:87:VAL:HG12	28:LZ:89:ILE:HG13	1.94	0.50
46:S2:433:A:H5''	53:SI:22:HIS:HB3	1.93	0.50
46:S2:1520:G:O2'	46:S2:1521:C:OP1	2.28	0.50
1:L1:1238:A:O2'	9:LF:52:GLU:OE1	2.29	0.50
46:S2:552:G:OP2	46:S2:552:G:N2	2.33	0.50
46:S2:1785:C:O2'	46:S2:1786:U:O4'	2.28	0.50
1:L1:989:U:O2	1:L1:1064:G:O6	2.29	0.50
1:L1:3910:C:H2'	1:L1:3911:C:C6	2.47	0.50
33:Le:82:VAL:O	33:Le:86:GLU:HG2	2.12	0.50
46:S2:1562:C:H2'	46:S2:1563:G:H8	1.77	0.50
50:SE:11:ARG:HA	50:SE:28:ALA:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LG:99:ALA:HB1	10:LG:136:LEU:HD11	1.94	0.50
46:S2:885:U:O2	46:S2:901:G:N2	2.33	0.50
46:S2:1037:G:H4'	46:S2:1845:A:H4'	1.93	0.50
53:SI:149:TYR:O	53:SI:153:LYS:HG3	2.11	0.50
61:SU:61:LEU:O	61:SU:81:GLN:HA	2.12	0.50
1:L1:3976:C:N4	1:L1:4035:G:OP2	2.45	0.50
4:LA:206:PRO:HG3	4:LA:213:GLY:HA3	1.94	0.50
7:LD:156:GLY:HA2	7:LD:181:PRO:HG3	1.94	0.50
14:LL:145:LYS:HG3	14:LL:146:LEU:HG	1.94	0.50
22:LT:37:GLY:N	22:LT:64:VAL:O	2.36	0.50
46:S2:981:A:H2'	46:S2:982:G:C8	2.47	0.50
48:SB:175:GLU:HB3	48:SB:187:LYS:HE2	1.94	0.50
67:Sg:157:SER:HB2	67:Sg:164:ILE:HB	1.93	0.50
1:L1:137:G:H2'	1:L1:138:G:C8	2.46	0.50
1:L1:2257:C:O2'	1:L1:2259:G:OP2	2.23	0.50
1:L1:2362:U:H2'	1:L1:2363:A2M:H8	1.93	0.50
46:S2:1566:G:OP2	60:ST:102:ARG:NH2	2.45	0.50
47:SA:191:ARG:NH1	62:SV:44:GLY:O	2.45	0.50
51:SF:71:ARG:NH2	51:SF:148:ASN:OD1	2.44	0.50
71:SM:50:CYS:O	71:SM:76:LEU:HA	2.11	0.50
1:L1:2906:G:H2'	1:L1:2908:U:H1'	1.93	0.49
9:LF:182:TYR:HB3	9:LF:200:ARG:HG3	1.93	0.49
11:LH:150:ASP:HB3	11:LH:153:LEU:HB2	1.93	0.49
46:S2:1869:A:H3'	58:SR:135:VAL:HG21	1.94	0.49
50:SE:128:LYS:HB2	50:SE:140:VAL:HB	1.94	0.49
58:SR:6:THR:HG22	58:SR:8:THR:H	1.76	0.49
67:Sg:302:TYR:HD2	67:Sg:308:ARG:HD3	1.76	0.49
1:L1:3736:A:H2'	1:L1:3737:A:C8	2.46	0.49
1:L1:106:A:H1'	1:L1:336:A:N3	2.27	0.49
1:L1:1175:A:H2	1:L1:1185:G:C2	2.30	0.49
1:L1:1631:A:C2	4:LA:204:MET:HG2	2.47	0.49
1:L1:3880:G:H2'	1:L1:3881:G:C8	2.47	0.49
1:L1:4691:A:OP1	11:LH:71:ARG:NH1	2.38	0.49
4:LA:14:SER:OG	4:LA:15:VAL:N	2.44	0.49
25:LW:45:ASN:HB3	25:LW:48:GLN:HG2	1.94	0.49
27:LY:101:PRO:HA	27:LY:104:VAL:HG22	1.93	0.49
46:S2:1513:C:OP1	66:Sd:12:ARG:NH1	2.36	0.49
46:S2:1679:A:OP1	65:Sc:20:ARG:NH2	2.39	0.49
53:SI:26:LYS:HD2	53:SI:29:LEU:HD23	1.93	0.49
62:SV:17:CYS:O	62:SV:21:ASN:N	2.46	0.49
1:L1:1175:A:N1	1:L1:1185:G:C6	2.81	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4537:C:H2'	1:L1:4538:G:C8	2.47	0.49
5:LB:53:MET:HE1	5:LB:336:CYS:HB3	1.95	0.49
46:S2:528:A:H2'	46:S2:529:A:C8	2.48	0.49
46:S2:1521:C:O2'	59:SS:144:ARG:NH2	2.45	0.49
46:S2:1232:U:OP2	59:SS:135:HIS:ND1	2.45	0.49
46:S2:1705:C:H2'	46:S2:1706:G:C8	2.48	0.49
46:S2:1752:C:C4	46:S2:1779:G:N2	2.80	0.49
47:SA:70:ASN:HB3	47:SA:73:ASP:HB2	1.95	0.49
75:SY:39:GLU:HA	75:SY:42:GLU:HB2	1.94	0.49
20:LR:136:ARG:O	20:LR:140:GLU:HG2	2.12	0.49
46:S2:70:G:N2	46:S2:79:A:H62	2.09	0.49
51:SF:27:ASP:OD2	51:SF:107:ASN:ND2	2.46	0.49
51:SF:126:THR:OG1	65:Sc:26:GLN:NE2	2.42	0.49
1:L1:4587:G:OP1	17:LO:61:ARG:NH1	2.40	0.49
46:S2:964:A:H2'	46:S2:965:U:H6	1.78	0.49
48:SB:59:SER:O	48:SB:63:LYS:HB2	2.12	0.49
55:SL:49:GLU:HG3	55:SL:116:CYS:HA	1.95	0.49
1:L1:1698:C:O2'	1:L1:2086:G:OP1	2.30	0.49
1:L1:1857:C:H2'	1:L1:1858:A:H8	1.78	0.49
6:LC:66:SER:HA	6:LC:77:PRO:HA	1.94	0.49
11:LH:176:LEU:HB3	41:Lm:86:ALA:HB1	1.95	0.49
15:LM:40:GLY:HA3	15:LM:45:VAL:HG13	1.94	0.49
46:S2:1543:U:C4'	57:SQ:43:GLU:HG2	2.41	0.49
60:ST:35:ASP:OD2	60:ST:35:ASP:N	2.46	0.49
1:L1:92:C:C2	29:La:55:LYS:HE2	2.48	0.49
16:LN:159:ARG:HB3	16:LN:164:LEU:HB2	1.95	0.49
46:S2:396:U:OP2	55:SL:79:LYS:NZ	2.45	0.49
46:S2:1144:A:H2'	46:S2:1145:A:C8	2.48	0.49
46:S2:1677:U:H2'	46:S2:1678:A2M:H8	1.95	0.49
66:Sd:6:LEU:HA	66:Sd:9:SER:HB3	1.95	0.49
1:L1:3765:G:O2'	1:L1:3767:C:N4	2.46	0.49
40:Ll:9:ILE:HD13	40:Ll:51:LEU:HD21	1.94	0.49
46:S2:1560:U:O2'	46:S2:1583:C:O2'	2.31	0.49
56:SP:91:GLY:N	56:SP:107:ILE:O	2.46	0.49
5:LB:107:ALA:HB2	5:LB:201:LEU:HD22	1.94	0.48
6:LC:7:LEU:HD22	6:LC:21:ASN:HB3	1.94	0.48
46:S2:1217:A:H2'	46:S2:1218:C:H6	1.76	0.48
71:SM:84:LYS:HA	71:SM:87:GLU:HG2	1.95	0.48
4:LA:210:PRO:O	4:LA:221:LYS:NZ	2.46	0.48
5:LB:113:GLU:HB2	5:LB:178:ALA:HB2	1.95	0.48
12:LI:87:ILE:HG12	12:LI:138:ILE:HG12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:691:C:H2'	1:L1:692:A:C8	2.49	0.48
31:Lc:37:MET:HG2	31:Lc:97:ILE:HG21	1.94	0.48
46:S2:455:A:H2'	46:S2:456:C:C6	2.48	0.48
50:SE:162:ILE:HG22	50:SE:169:ILE:HA	1.96	0.48
54:SK:95:ARG:HH12	54:SK:98:ARG:HA	1.77	0.48
70:SJ:111:GLN:HE21	70:SJ:123:ILE:HG13	1.78	0.48
1:L1:1177:U:O2'	7:LD:286:SER:OG	2.21	0.48
1:L1:2083:C:OP2	19:LQ:14:ARG:NH2	2.41	0.48
1:L1:2745:A:H2'	1:L1:2746:A:C8	2.48	0.48
1:L1:3711:A:C6	46:S2:970:G:N1	2.81	0.48
10:LG:55:VAL:HG21	26:LX:41:ARG:HD3	1.94	0.48
58:SR:45:LYS:HE2	58:SR:45:LYS:HB3	1.60	0.48
68:SC:110:MET:HB3	68:SC:125:LYS:HB3	1.95	0.48
71:SM:52:LEU:HB3	71:SM:78:LYS:HZ2	1.78	0.48
1:L1:5025:C:H2'	1:L1:5028:G:H1'	1.94	0.48
54:SK:42:ASN:O	54:SK:46:MET:HG3	2.13	0.48
56:SP:130:ARG:HD2	56:SP:131:PRO:HD2	1.94	0.48
1:L1:3923:A:H2'	1:L1:3924:C:C6	2.48	0.48
1:L1:4455:G:H5''	5:LB:5:LYS:HE3	1.96	0.48
31:Lc:34:THR:HG23	31:Lc:95:ALA:HB2	1.95	0.48
46:S2:1432:U:O2'	46:S2:1437:C:O2'	2.31	0.48
75:SY:44:LEU:HB3	75:SY:55:ILE:HD13	1.95	0.48
1:L1:172:C:OP2	14:LL:130:LYS:NZ	2.47	0.48
1:L1:1097:C:H2'	1:L1:1098:G:H8	1.78	0.48
1:L1:1100:U:O3'	1:L1:1167:C:N4	2.47	0.48
13:LJ:146:ARG:HG2	13:LJ:147:ARG:HG2	1.95	0.48
46:S2:223:C:H2'	46:S2:224:A:C8	2.48	0.48
46:S2:1270:G:O2'	46:S2:1301:A:N7	2.46	0.48
49:SD:103:GLU:HA	49:SD:106:ARG:HG2	1.96	0.48
57:SQ:19:ALA:HB2	57:SQ:75:GLY:HA3	1.96	0.48
57:SQ:34:VAL:HG22	57:SQ:70:VAL:HB	1.94	0.48
59:SS:23:ARG:HB3	76:SZ:48:VAL:HG21	1.96	0.48
1:L1:1879:C:O2'	1:L1:1891:A:N3	2.47	0.48
1:L1:2864:A:H2'	1:L1:2865:U:C6	2.49	0.48
1:L1:3811:G:O2'	1:L1:3814:U:OP2	2.22	0.48
1:L1:4967:A:H2'	1:L1:4968:A:C8	2.49	0.48
16:LN:9:GLU:HB2	37:Li:44:ILE:HG13	1.95	0.48
1:L1:4670:C:O2'	1:L1:4672:A:OP2	2.32	0.48
2:L2:12:U:O3'	2:L2:109:U:O2'	2.27	0.48
6:LC:209:ILE:HD13	6:LC:251:ILE:HB	1.96	0.48
9:LF:43:ARG:HH21	9:LF:47:ARG:HD3	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LW:93:LYS:O	25:LW:101:ARG:NH2	2.46	0.48
28:LZ:73:LYS:HD3	28:LZ:75:TYR:CZ	2.49	0.48
46:S2:145:G:H2'	46:S2:146:G:C8	2.48	0.48
46:S2:944:A:H5''	73:SO:134:PRO:HB3	1.95	0.48
52:SH:12:ASN:ND2	52:SH:14:GLU:HB2	2.25	0.48
67:Sg:197:THR:HG21	67:Sg:238:ALA:HA	1.96	0.48
1:L1:502:C:H3'	1:L1:503:C:H3'	1.95	0.47
1:L1:1440:U:C2	1:L1:2106:G:C2	3.01	0.47
1:L1:3951:G:C2	1:L1:4062:A:N1	2.82	0.47
1:L1:4637:OMG:HM23	1:L1:4637:OMG:H1'	1.71	0.47
2:L2:120:U:H4'	7:LD:262:LYS:HG2	1.96	0.47
46:S2:1536:G:H2'	46:S2:1537:A:H8	1.79	0.47
47:SA:77:ILE:HG12	47:SA:99:ILE:HB	1.95	0.47
49:SD:135:GLU:HG3	49:SD:153:VAL:HG12	1.95	0.47
59:SS:16:LEU:HD13	59:SS:17:ASN:H	1.79	0.47
63:SX:74:LEU:O	63:SX:78:GLY:HA2	2.13	0.47
67:Sg:228:TYR:HD1	67:Sg:229:THR:H	1.61	0.47
71:SM:35:ILE:HD12	71:SM:35:ILE:H	1.79	0.47
1:L1:2253:A:N1	9:LF:24:ASN:N	2.62	0.47
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.49	0.47
30:Lb:114:LYS:HB2	30:Lb:114:LYS:HE2	1.66	0.47
67:Sg:174:VAL:HB	67:Sg:188:HIS:HB2	1.95	0.47
20:LR:105:LEU:HD23	20:LR:138:LEU:HD23	1.95	0.47
62:SV:70:LEU:HD21	62:SV:83:PHE:HZ	1.79	0.47
76:SZ:51:ASP:OD1	76:SZ:54:THR:OG1	2.31	0.47
1:L1:178:C:H2'	1:L1:179:G:C8	2.49	0.47
1:L1:3732:A:H2'	1:L1:3733:A:C8	2.50	0.47
1:L1:4743:G:H2'	1:L1:4744:A:C8	2.50	0.47
3:L3:110:U:H5'	40:Ll:8:ARG:HH22	1.79	0.47
5:LB:173:LEU:HD22	5:LB:342:LYS:HD3	1.97	0.47
47:SA:81:ASN:HA	47:SA:84:GLN:HB2	1.96	0.47
70:SJ:84:ILE:HD11	70:SJ:148:ILE:HG21	1.96	0.47
78:Se:39:ASN:HA	78:Se:43:VAL:HB	1.96	0.47
1:L1:1976:G:C2	1:L1:1991:A:C2	3.03	0.47
12:LI:76:MET:HE2	12:LI:76:MET:HA	1.95	0.47
57:SQ:107:GLU:O	57:SQ:111:ILE:HD12	2.15	0.47
65:Sc:21:THR:OG1	65:Sc:22:GLY:N	2.46	0.47
68:SC:76:LYS:HD3	68:SC:76:LYS:HA	1.64	0.47
7:LD:211:LEU:HD13	7:LD:219:TYR:HA	1.96	0.47
14:LL:164:GLU:HB3	29:La:100:ILE:HD13	1.97	0.47
15:LM:74:ARG:O	15:LM:78:GLN:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SP:92:SER:O	56:SP:106:GLU:HA	2.14	0.47
64:Sa:47:ALA:HA	64:Sa:50:VAL:HB	1.96	0.47
1:L1:136:C:N4	36:Lh:77:LYS:O	2.47	0.47
1:L1:262:G:H2'	1:L1:263:G:C8	2.49	0.47
1:L1:308:G:O6	16:LN:12:ARG:NH1	2.47	0.47
1:L1:407:A:O2'	1:L1:410:A:OP1	2.32	0.47
1:L1:963:G:N7	1:L1:964:A:N6	2.63	0.47
6:LC:134:PRO:HA	6:LC:150:LEU:HD22	1.96	0.47
25:LW:71:ARG:NH1	46:S2:1783:C:N3	2.59	0.47
27:LY:72:GLN:HB3	27:LY:81:TYR:HB2	1.96	0.47
48:SB:42:ARG:NH2	48:SB:232:HIS:O	2.48	0.47
59:SS:125:HIS:CD2	59:SS:131:VAL:HG11	2.50	0.47
1:L1:1468:C:OP1	29:La:132:ARG:NH2	2.48	0.47
1:L1:4478:G:O2'	1:L1:4602:A:N1	2.48	0.47
46:S2:495:U:O2'	50:SE:27:PHE:O	2.32	0.47
69:SG:33:ALA:CA	69:SG:52:ILE:O	2.63	0.47
69:SG:181:THR:HG22	69:SG:183:ARG:H	1.80	0.47
71:SM:21:VAL:HA	71:SM:24:THR:HG22	1.97	0.47
1:L1:469:C:H42	8:LE:105:ARG:HH21	1.63	0.47
1:L1:1727:U:OP1	9:LF:131:ASN:ND2	2.46	0.47
1:L1:2517:A:H5'	35:Lg:62:LYS:HE3	1.97	0.47
3:L3:75:OMG:HM23	3:L3:75:OMG:H1'	1.65	0.47
4:LA:173:GLY:O	44:Lp:69:TRP:NE1	2.46	0.47
31:Lc:38:ILE:HD11	31:Lc:46:VAL:HG11	1.96	0.47
39:Lk:14:THR:HA	39:Lk:17:ARG:HD3	1.96	0.47
58:SR:109:LEU:HD22	58:SR:111:PHE:HD2	1.80	0.47
71:SM:51:VAL:HB	71:SM:109:VAL:HG13	1.96	0.47
1:L1:1972:G:N1	1:L1:1995:G:O6	2.48	0.47
1:L1:3711:A:H2'	1:L1:3712:A:H8	1.80	0.47
1:L1:4936:G:C5	8:LE:183:ARG:HD2	2.50	0.47
1:L1:4969:C:O3'	18:LP:74:LYS:HE3	2.15	0.47
12:LI:36:LEU:HD22	12:LI:69:ARG:HD3	1.97	0.47
24:LV:35:LYS:HB3	24:LV:35:LYS:HE2	1.66	0.47
43:Lo:26:TYR:HB3	43:Lo:67:VAL:HB	1.97	0.47
46:S2:165:G:OP2	46:S2:165:G:N2	2.37	0.47
46:S2:508:A:H3'	46:S2:509:OMG:C8	2.50	0.47
46:S2:640:A:H2'	46:S2:641:A:C8	2.50	0.47
50:SE:19:MET:HE1	50:SE:108:ARG:HD2	1.96	0.47
60:ST:42:HIS:HB3	60:ST:93:SER:HB2	1.97	0.47
67:Sg:152:SER:H	67:Sg:169:GLY:HA2	1.80	0.47
1:L1:740:G:H21	1:L1:924:C:H41	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:292:ILE:O	6:LC:295:SER:OG	2.26	0.46
15:LM:36:ALA:HB2	15:LM:52:PHE:CE1	2.50	0.46
46:S2:57:U:OP1	46:S2:504:G:O2'	2.33	0.46
46:S2:72:C:O2'	46:S2:73:C:O4'	2.33	0.46
46:S2:1550:G:O2'	46:S2:1558:C:O2	2.32	0.46
51:SF:56:TYR:HD1	51:SF:62:ARG:HG2	1.80	0.46
57:SQ:104:SER:O	57:SQ:108:ILE:HG12	2.15	0.46
1:L1:93:G:H2'	1:L1:94:A:C8	2.50	0.46
1:L1:1624:G:OP1	1:L1:1626:G:O2'	2.31	0.46
1:L1:4097:G:H2'	1:L1:4098:A:H8	1.80	0.46
1:L1:4103:C:N3	1:L1:4105:A:N1	2.63	0.46
7:LD:204:VAL:HB	7:LD:236:MET:HE1	1.97	0.46
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.95	0.46
11:LH:92:MET:HE2	11:LH:179:ILE:HG22	1.95	0.46
18:LP:125:MET:HB2	18:LP:141:SER:HB2	1.98	0.46
46:S2:601:OMG:HM23	46:S2:601:OMG:H1'	1.67	0.46
52:SH:137:SER:OG	52:SH:159:ASP:OD1	2.30	0.46
13:LJ:35:ARG:HG2	13:LJ:123:ILE:HG22	1.97	0.46
48:SB:199:LYS:HE3	48:SB:199:LYS:HB3	1.73	0.46
52:SH:19:PHE:CZ	52:SH:23:ILE:HD11	2.51	0.46
56:SP:96:VAL:HG11	56:SP:116:LEU:HB3	1.97	0.46
1:L1:1443:A:C6	1:L1:2104:G:C2	3.04	0.46
4:LA:20:VAL:HA	4:LA:23:ARG:HG3	1.97	0.46
5:LB:362:LYS:HB2	5:LB:362:LYS:HE3	1.67	0.46
9:LF:94:ARG:O	9:LF:118:PHE:N	2.48	0.46
28:LZ:13:VAL:O	28:LZ:20:GLY:N	2.35	0.46
1:L1:4323:A:OP1	7:LD:179:ARG:NH1	2.42	0.46
15:LM:126:GLU:HB3	17:LO:181:ALA:HB1	1.96	0.46
46:S2:1585:U:O2'	46:S2:1587:G:OP2	2.34	0.46
49:SD:123:LEU:HD11	49:SD:152:PHE:HB3	1.98	0.46
51:SF:102:LEU:HD11	76:SZ:100:VAL:HG21	1.96	0.46
69:SG:63:MET:HE3	69:SG:100:CYS:HA	1.97	0.46
1:L1:3654:G:O2'	1:L1:3693:U:OP1	2.30	0.46
21:LS:142:VAL:HG12	21:LS:146:HIS:CE1	2.51	0.46
44:Lp:46:LYS:O	44:Lp:57:CYS:HA	2.15	0.46
47:SA:37:TYR:OH	47:SA:57:LYS:NZ	2.48	0.46
49:SD:76:ARG:HG3	54:SK:68:TYR:HE1	1.81	0.46
1:L1:1269:G:O2'	1:L1:1440:U:O3'	2.34	0.46
1:L1:3917:A:H2'	1:L1:3918:G:H8	1.79	0.46
1:L1:4169:G:H4'	1:L1:4171:C:C2	2.51	0.46
1:L1:4648:A:OP1	20:LR:62:ARG:NH2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:150:C:N4	10:LG:52:THR:O	2.49	0.46
6:LC:116:ASN:HB2	6:LC:119:GLN:HG3	1.98	0.46
6:LC:284:MET:HE2	6:LC:287:THR:HA	1.98	0.46
27:LY:39:ARG:O	27:LY:42:TYR:C	2.59	0.46
46:S2:1831:A:H2'	46:S2:1832:6MZ:H8	1.96	0.46
49:SD:45:ARG:NH1	49:SD:82:GLY:O	2.49	0.46
68:SC:116:THR:OG1	68:SC:119:GLY:O	2.29	0.46
75:SY:32:LYS:HE2	75:SY:32:LYS:HB2	1.70	0.46
1:L1:2640:G:H2'	1:L1:2641:A:C8	2.49	0.46
1:L1:2773:G:O2'	39:Lk:18:LYS:NZ	2.36	0.46
1:L1:4260:U:H2'	1:L1:4261:C:C6	2.51	0.46
3:L3:94:G:H21	38:Lj:82:THR:HG1	1.63	0.46
7:LD:64:ILE:HG13	7:LD:105:LEU:HD21	1.97	0.46
1:L1:2303:C:H5''	33:Le:104:SER:HB3	1.96	0.46
1:L1:3684:G:H2'	1:L1:3685:C:C6	2.51	0.46
8:LE:202:ASP:OD2	8:LE:204:SER:OG	2.33	0.46
20:LR:89:MET:HE3	20:LR:90:PRO:HD2	1.97	0.46
46:S2:1232:U:H3	46:S2:1527:C:N4	2.14	0.46
70:SJ:127:ARG:HD3	78:Se:31:ARG:HD3	1.98	0.46
73:SO:54:CYS:HB2	73:SO:84:ARG:HG2	1.98	0.46
1:L1:1662:C:H2'	1:L1:1663:C:C6	2.51	0.46
1:L1:1764:G:N3	1:L1:1770:A:C6	2.84	0.46
1:L1:2486:G:C6	1:L1:2495:U:C2	3.04	0.46
1:L1:2580:U:O2'	28:LZ:79:HIS:ND1	2.47	0.46
1:L1:3710:G:N3	1:L1:3711:A:N6	2.64	0.46
1:L1:3722:G:H2'	1:L1:3723:A2M:H8	1.98	0.46
1:L1:3808:OMC:H5''	1:L1:3809:G:N2	2.30	0.46
9:LF:26:ALA:HA	9:LF:29:LYS:HE2	1.98	0.46
46:S2:677:G:N1	46:S2:1027:A:OP2	2.34	0.46
46:S2:1115:U:H4'	46:S2:1116:C:H5'	1.97	0.46
54:SK:53:LYS:HB3	54:SK:53:LYS:HE3	1.84	0.46
57:SQ:98:LYS:O	67:Sg:57:ARG:NH2	2.48	0.46
1:L1:1988:G:H2'	1:L1:1989:G:C8	2.51	0.45
1:L1:2667:C:O4'	20:LR:96:MET:HG3	2.16	0.45
7:LD:79:TYR:O	7:LD:82:GLU:HG2	2.16	0.45
23:LU:89:LYS:HE3	23:LU:89:LYS:HB3	1.76	0.45
1:L1:746:A:H2'	1:L1:747:A:C8	2.51	0.45
1:L1:4699:U:H1'	1:L1:4700:A:H5''	1.98	0.45
14:LL:142:GLU:HA	14:LL:145:LYS:HG2	1.98	0.45
31:Lc:26:LYS:HB2	31:Lc:98:ASP:HB3	1.97	0.45
31:Lc:57:LYS:HE3	31:Lc:57:LYS:HB2	1.67	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:367:U:H4'	46:S2:371:A:C8	2.51	0.45
52:SH:147:LYS:O	52:SH:150:GLY:N	2.42	0.45
53:SI:98:LYS:HG3	53:SI:178:ARG:HG3	1.96	0.45
54:SK:7:ASN:OD1	54:SK:7:ASN:N	2.37	0.45
61:SU:115:THR:OG1	61:SU:116:ILE:N	2.50	0.45
77:Sb:54:VAL:HG22	77:Sb:64:CYS:HB2	1.98	0.45
1:L1:667:A:H5''	1:L1:668:C:H5''	1.98	0.45
1:L1:3688:U:OP2	4:LA:198:ARG:NH2	2.43	0.45
2:L2:74:A:O2'	21:LS:53:LYS:NZ	2.41	0.45
5:LB:396:ARG:HA	5:LB:399:LYS:HE2	1.98	0.45
6:LC:298:ILE:O	6:LC:302:LEU:HG	2.17	0.45
16:LN:140:LYS:HD3	16:LN:140:LYS:HA	1.81	0.45
21:LS:154:LEU:HB3	21:LS:157:ARG:HD3	1.98	0.45
46:S2:382:C:H2'	46:S2:383:G:H8	1.80	0.45
49:SD:210:ILE:HD13	58:SR:16:ILE:HG13	1.98	0.45
53:SI:138:ASN:OD1	53:SI:139:LYS:N	2.49	0.45
63:SX:74:LEU:O	63:SX:78:GLY:CA	2.64	0.45
63:SX:90:CYS:HA	63:SX:93:PHE:HD2	1.82	0.45
63:SX:101:LEU:HB3	63:SX:123:VAL:O	2.16	0.45
1:L1:1720:C:H5'	1:L1:1835:G:H21	1.80	0.45
31:Lc:28:VAL:HG11	31:Lc:37:MET:HE3	1.98	0.45
45:Lr:90:LEU:HG	45:Lr:111:ILE:HG23	1.99	0.45
48:SB:123:ALA:HB2	48:SB:165:ARG:HG3	1.99	0.45
53:SI:160:SER:O	53:SI:164:GLU:HG3	2.16	0.45
67:Sg:283:PRO:O	67:Sg:285:GLN:NE2	2.50	0.45
71:SM:20:GLU:OE2	71:SM:119:GLN:HB2	2.16	0.45
73:SO:34:PHE:HB3	73:SO:41:PHE:HB2	1.99	0.45
1:L1:1764:G:N2	1:L1:1770:A:C5	2.84	0.45
36:Lh:52:LYS:HA	36:Lh:52:LYS:HD3	1.77	0.45
44:Lp:74:THR:O	44:Lp:78:THR:HG22	2.17	0.45
46:S2:1512:C:H5''	66:Sd:8:TRP:HZ3	1.81	0.45
46:S2:1658:G:OP2	46:S2:1660:C:N4	2.48	0.45
69:SG:33:ALA:HA	69:SG:52:ILE:O	2.16	0.45
69:SG:168:LYS:HE3	69:SG:168:LYS:HB3	1.80	0.45
1:L1:155:C:OP1	36:Lh:109:ARG:NH2	2.41	0.45
20:LR:65:LYS:HE2	20:LR:65:LYS:HB3	1.87	0.45
46:S2:5:U:H2'	46:S2:6:G:H8	1.82	0.45
46:S2:932:G:O2'	46:S2:934:G:OP2	2.31	0.45
46:S2:1801:A:H2'	46:S2:1802:C:C6	2.51	0.45
48:SB:129:THR:OG1	48:SB:179:ASN:O	2.34	0.45
53:SI:34:ALA:HB2	53:SI:56:ARG:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Sg:230:LEU:HD21	67:Sg:264:LYS:HB3	1.98	0.45
1:L1:730:G:OP2	9:LF:76:ARG:NE	2.41	0.45
1:L1:1604:G:H2'	1:L1:1605:G:C8	2.52	0.45
3:L3:102:G:OP2	3:L3:104:A:O2'	2.35	0.45
30:Lb:61:ASN:O	30:Lb:65:MET:HG3	2.16	0.45
39:Lk:26:LYS:HD3	39:Lk:69:LEU:HD12	1.98	0.45
46:S2:1298:G:H4'	56:SP:78:THR:HA	1.98	0.45
1:L1:468:U:C4	1:L1:686:A:N1	2.85	0.45
1:L1:1077:C:H4'	1:L1:1215:C:C4	2.52	0.45
1:L1:1328:G:O2'	1:L1:2349:A:OP1	2.29	0.45
1:L1:4591:U:H2'	1:L1:4592:C:C6	2.52	0.45
49:SD:106:ARG:HB2	49:SD:175:VAL:HG22	1.98	0.45
72:SN:84:LEU:HD23	72:SN:89:TYR:HB2	1.99	0.45
1:L1:2706:G:H2'	1:L1:2708:U:H3	1.82	0.45
15:LM:100:ARG:HA	15:LM:103:LYS:HE2	1.98	0.45
46:S2:560:A:OP2	70:SJ:177:ASN:ND2	2.44	0.45
46:S2:1199:A:OP1	64:Sa:2:THR:N	2.50	0.45
46:S2:1678:A2M:HM'3	46:S2:1678:A2M:H1'	1.78	0.45
54:SK:46:MET:HE3	54:SK:46:MET:HB2	1.86	0.45
69:SG:67:VAL:HG12	69:SG:69:THR:HG22	1.98	0.45
75:SY:114:MET:O	75:SY:122:LYS:NZ	2.35	0.45
1:L1:2411:C:H2'	1:L1:2412:A:C8	2.51	0.45
1:L1:3792:OMG:H2'	1:L1:3793:U:C6	2.52	0.45
1:L1:3951:G:N2	1:L1:4062:A:C5	2.83	0.45
1:L1:4108:G:H2'	1:L1:4109:G:C8	2.52	0.45
1:L1:4233:A:H4'	43:Lo:98:LYS:HE2	1.99	0.45
17:LO:166:ILE:HG13	17:LO:169:ARG:HH21	1.82	0.45
39:Lk:36:VAL:HG13	39:Lk:43:TYR:HB2	1.99	0.45
46:S2:697:G:OP2	46:S2:733:C:N4	2.46	0.45
46:S2:1845:A:H2'	46:S2:1846:G:C8	2.52	0.45
47:SA:85:ARG:NH2	58:SR:82:ASP:O	2.38	0.45
59:SS:54:LYS:HD2	59:SS:58:GLU:HG2	1.98	0.45
61:SU:49:LYS:HE3	61:SU:49:LYS:HB3	1.77	0.45
68:SC:73:MET:HE2	68:SC:73:MET:HB2	1.91	0.45
71:SM:38:ALA:O	71:SM:42:LEU:HD22	2.16	0.45
1:L1:3786:U:OP1	1:L1:4550:G:O2'	2.30	0.44
3:L3:137:A:H2'	3:L3:138:C:C6	2.52	0.44
10:LG:212:LYS:HE3	10:LG:212:LYS:HB2	1.83	0.44
11:LH:50:LYS:HE3	11:LH:50:LYS:HB2	1.69	0.44
12:LI:76:MET:HG3	12:LI:87:ILE:HD11	1.98	0.44
46:S2:942:G:H2'	46:S2:943:U:C6	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SE:174:LYS:HB3	50:SE:174:LYS:HE3	1.76	0.44
52:SH:36:LEU:O	52:SH:40:LEU:HB2	2.18	0.44
63:SX:100:VAL:HG12	63:SX:125:VAL:HA	2.00	0.44
1:L1:513:U:H1'	1:L1:516:C:H5	1.81	0.44
1:L1:1365:C:H41	1:L1:1370:G:H22	1.65	0.44
17:LO:22:ILE:HD13	17:LO:120:VAL:HG11	1.99	0.44
1:L1:2411:C:H2'	1:L1:2412:A:H8	1.82	0.44
1:L1:2474:G:N2	1:L1:2502:G:O2'	2.51	0.44
5:LB:238:LYS:HB2	5:LB:238:LYS:HE2	1.72	0.44
7:LD:116:ASP:OD1	7:LD:116:ASP:N	2.50	0.44
28:LZ:107:LYS:HG2	28:LZ:111:ARG:HH11	1.81	0.44
44:Lp:90:LYS:O	44:Lp:92:GLN:NE2	2.50	0.44
46:S2:107:A:H2'	46:S2:108:G:C8	2.52	0.44
46:S2:694:G:H1	46:S2:737:G:H2'	1.81	0.44
49:SD:172:VAL:O	49:SD:173:ARG:NH1	2.40	0.44
52:SH:184:ASP:OD2	52:SH:184:ASP:N	2.50	0.44
67:Sg:251:ALA:HB1	67:Sg:286:CYS:HB3	1.99	0.44
75:SY:37:LYS:HA	75:SY:40:ILE:HB	1.98	0.44
1:L1:351:C:OP2	6:LC:197:ARG:NH1	2.43	0.44
1:L1:1332:C:H2'	1:L1:1333:A:H8	1.81	0.44
1:L1:3969:G:N2	1:L1:4053:A:O2'	2.51	0.44
3:L3:14:OMU:HM23	3:L3:14:OMU:H1'	1.65	0.44
5:LB:366:LYS:HB2	5:LB:366:LYS:HE2	1.61	0.44
47:SA:214:GLU:OE1	58:SR:80:ARG:NH2	2.49	0.44
54:SK:4:PRO:HG2	54:SK:7:ASN:HD21	1.83	0.44
54:SK:74:GLU:OE1	54:SK:74:GLU:N	2.49	0.44
64:Sa:23:CYS:HB3	64:Sa:28:ARG:H	1.83	0.44
67:Sg:33:SER:OG	67:Sg:43:TRP:NE1	2.41	0.44
67:Sg:148:SER:OG	67:Sg:149:GLU:OE1	2.34	0.44
69:SG:57:ASP:OD2	69:SG:58:LYS:N	2.44	0.44
1:L1:4329:G:N7	83:L1:5454:HOH:O	2.36	0.44
7:LD:232:THR:O	7:LD:236:MET:HG3	2.18	0.44
28:LZ:120:GLU:O	28:LZ:124:THR:HG23	2.18	0.44
46:S2:1808:U:H2'	46:S2:1809:A:C8	2.53	0.44
50:SE:104:ASP:HB3	50:SE:110:ALA:HB2	2.00	0.44
53:SI:124:LYS:HB3	53:SI:124:LYS:HE2	1.79	0.44
54:SK:5:LYS:HD3	54:SK:5:LYS:HA	1.84	0.44
69:SG:229:ALA:HA	69:SG:232:ARG:HG2	1.98	0.44
73:SO:26:ASN:OD1	73:SO:26:ASN:N	2.51	0.44
77:Sb:67:THR:OG1	77:Sb:70:LYS:O	2.24	0.44
1:L1:268:G:H2'	1:L1:269:G:H8	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1097:C:H2'	1:L1:1098:G:C8	2.52	0.44
1:L1:1509:C:H5''	29:La:2:PRO:HD2	2.00	0.44
1:L1:4467:A:N6	1:L1:4490:C:H42	2.10	0.44
45:Lr:57:GLY:C	45:Lr:58:LYS:HD2	2.43	0.44
46:S2:641:A:OP1	70:SJ:40:LYS:NZ	2.40	0.44
46:S2:1607:A:H5'	60:ST:87:VAL:HG21	2.00	0.44
56:SP:111:MET:HG2	56:SP:119:PHE:CE2	2.52	0.44
1:L1:907:C:H2'	1:L1:908:G:H8	1.82	0.44
1:L1:1660:U:H3'	29:La:13:GLY:HA2	2.00	0.44
1:L1:4888:U:O2	1:L1:4931:G:C2	2.70	0.44
3:L3:19:C:H2'	3:L3:20:A:C8	2.53	0.44
10:LG:44:ASP:OD2	10:LG:44:ASP:N	2.50	0.44
46:S2:71:G:H2'	46:S2:72:C:H4'	1.99	0.44
46:S2:1016:U:H5''	72:SN:14:SER:HB3	1.98	0.44
46:S2:1232:U:H2'	46:S2:1233:G:C8	2.53	0.44
75:SY:27:VAL:HB	75:SY:69:THR:HB	1.99	0.44
1:L1:751:G:O6	1:L1:912:G:C2	2.71	0.44
6:LC:150:LEU:HA	6:LC:150:LEU:HD12	1.75	0.44
13:LJ:39:VAL:HA	13:LJ:42:GLN:HG2	2.00	0.44
24:LV:90:ARG:O	24:LV:93:GLY:N	2.51	0.44
46:S2:509:OMG:HM23	46:S2:509:OMG:H1'	1.81	0.44
46:S2:1560:U:H2'	46:S2:1561:A:H8	1.82	0.44
48:SB:46:LYS:HB2	48:SB:46:LYS:HE2	1.75	0.44
48:SB:47:THR:OG1	48:SB:65:ARG:NH2	2.51	0.44
55:SL:80:MET:HE2	55:SL:80:MET:HB3	1.83	0.44
55:SL:128:VAL:HG12	55:SL:142:VAL:HA	1.99	0.44
1:L1:253:G:H2'	1:L1:254:G:C8	2.53	0.44
46:S2:1232:U:N3	46:S2:1527:C:N4	2.66	0.44
46:S2:1528:G:O2'	46:S2:1666:C:OP1	2.31	0.44
49:SD:125:PHE:O	49:SD:129:SER:OG	2.29	0.44
69:SG:218:LYS:HB3	69:SG:218:LYS:HE2	1.56	0.44
1:L1:2627:C:OP1	23:LU:92:LYS:NZ	2.51	0.43
5:LB:77:THR:HG21	5:LB:337:VAL:HG22	2.00	0.43
7:LD:152:ARG:HD2	7:LD:152:ARG:HA	1.81	0.43
11:LH:52:LYS:HD2	11:LH:52:LYS:HA	1.79	0.43
44:Lp:90:LYS:HE2	44:Lp:90:LYS:HB3	1.88	0.43
46:S2:49:C:H2'	46:S2:472:C:H41	1.83	0.43
46:S2:1284:A:C8	71:SM:33:ARG:HB2	2.53	0.43
67:Sg:4:GLN:HE22	67:Sg:314:ILE:HB	1.83	0.43
76:SZ:51:ASP:O	76:SZ:55:TYR:HB2	2.17	0.43
1:L1:2580:U:OP1	28:LZ:36:ARG:NH2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4302:U:H4'	22:LT:5:LYS:HD2	2.00	0.43
1:L1:4633:G:O2'	1:L1:4635:A:OP2	2.20	0.43
2:L2:117:G:OP1	7:LD:253:TYR:OH	2.31	0.43
3:L3:96:C:H5''	36:Lh:66:LYS:HG2	1.99	0.43
8:LE:268:GLN:H	8:LE:268:GLN:HG2	1.64	0.43
11:LH:23:ARG:HA	11:LH:45:LEU:HD12	2.00	0.43
12:LI:21:ARG:O	12:LI:24:ARG:NH1	2.52	0.43
22:LT:129:LYS:HB3	22:LT:129:LYS:HE2	1.89	0.43
46:S2:1261:C:O2	66:Sd:10:HIS:NE2	2.49	0.43
46:S2:1849:G:H3'	46:S2:1850:MA6:H8	2.01	0.43
52:SH:32:MET:O	52:SH:33:ASN:C	2.61	0.43
69:SG:121:ILE:N	69:SG:125:THR:OG1	2.50	0.43
70:SJ:93:LYS:HE2	70:SJ:93:LYS:HB2	1.87	0.43
1:L1:654:C:H2'	1:L1:655:C:C6	2.53	0.43
1:L1:906:C:H2'	1:L1:907:C:C6	2.53	0.43
1:L1:1443:A:N1	1:L1:2103:G:C6	2.86	0.43
1:L1:2664:G:H4'	1:L1:2677:G:H4'	2.00	0.43
2:L2:13:A:OP2	2:L2:66:G:N2	2.43	0.43
9:LF:35:LYS:HB3	9:LF:35:LYS:HE2	1.76	0.43
46:S2:116:OMU:H1'	46:S2:116:OMU:HM23	1.73	0.43
53:SI:64:ASN:O	53:SI:186:ASP:HA	2.18	0.43
70:SJ:106:LEU:HD23	70:SJ:109:ARG:HD2	2.00	0.43
1:L1:462:G:H2'	1:L1:463:A:C8	2.53	0.43
1:L1:1443:A:H2	1:L1:2103:G:N1	2.06	0.43
1:L1:1464:C:H5''	30:Lb:32:LEU:HD12	2.00	0.43
1:L1:4088:C:H2'	1:L1:4089:G:C8	2.54	0.43
7:LD:89:LYS:HE3	7:LD:89:LYS:HB3	1.76	0.43
9:LF:36:LYS:HB3	9:LF:36:LYS:HE3	1.67	0.43
9:LF:184:ILE:HG23	9:LF:189:ASP:HB3	2.00	0.43
14:LL:48:PRO:HG2	36:Lh:118:LYS:HD2	1.98	0.43
46:S2:1101:U:H2'	46:S2:1102:G:C8	2.53	0.43
46:S2:1181:A:H2'	46:S2:1182:A:C8	2.54	0.43
46:S2:1217:A:H2'	46:S2:1218:C:C6	2.52	0.43
48:SB:183:GLU:HA	48:SB:186:ASN:HB2	2.00	0.43
67:Sg:20:GLN:HG2	67:Sg:69:VAL:H	1.83	0.43
67:Sg:183:LYS:HA	67:Sg:183:LYS:HD3	1.86	0.43
75:SY:43:LYS:HB2	75:SY:43:LYS:HE2	1.87	0.43
1:L1:1241:C:O2	30:Lb:115:GLY:HA2	2.19	0.43
1:L1:1440:U:C2	1:L1:2106:G:N1	2.87	0.43
1:L1:3881:G:N7	83:L1:5459:HOH:O	2.36	0.43
38:Lj:83:THR:HA	38:Lj:84:PRO:HD3	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:851:C:H5''	46:S2:852:G:H5'	2.00	0.43
46:S2:1653:U:H2'	46:S2:1654:G:C8	2.53	0.43
55:SL:151:THR:OG1	55:SL:152:LYS:N	2.50	0.43
59:SS:121:ARG:HG3	59:SS:131:VAL:HB	1.99	0.43
1:L1:67:C:OP2	1:L1:312:G:N2	2.52	0.43
1:L1:184:U:O2	1:L1:254:G:C6	2.70	0.43
1:L1:2664:G:OP1	20:LR:110:ARG:NH1	2.51	0.43
7:LD:125:VAL:HG11	7:LD:199:ILE:HG21	1.99	0.43
19:LQ:49:LYS:HD2	19:LQ:50:ARG:HG3	2.00	0.43
22:LT:102:ARG:HE	22:LT:105:PHE:HD2	1.66	0.43
23:LU:64:GLU:HG2	23:LU:71:THR:HG23	2.00	0.43
30:Lb:107:ARG:HE	30:Lb:107:ARG:HB3	1.67	0.43
46:S2:921:G:C5	74:SW:28:ARG:HD2	2.54	0.43
46:S2:1619:A:OP2	56:SP:47:ARG:NH2	2.51	0.43
46:S2:1630:A:H5''	59:SS:37:GLY:N	2.33	0.43
51:SF:50:PRO:HG2	51:SF:90:VAL:HG22	2.01	0.43
57:SQ:26:LYS:O	57:SQ:67:ASP:N	2.41	0.43
1:L1:2543:A:H2	1:L1:2773:G:H22	1.66	0.43
46:S2:993:G:OP1	46:S2:1131:G:N2	2.48	0.43
53:SI:174:CYS:HB2	53:SI:190:LEU:HD21	2.01	0.43
1:L1:679:C:H2'	1:L1:680:G:H8	1.83	0.43
1:L1:2704:C:H2'	1:L1:2705:G:H8	1.83	0.43
1:L1:2748:C:O2'	35:Lg:61:PRO:O	2.32	0.43
15:LM:79:LYS:HE3	15:LM:79:LYS:HB3	1.74	0.43
43:Lo:2:VAL:N	43:Lo:90:HIS:O	2.52	0.43
46:S2:407:G:C6	63:SX:36:LEU:HD11	2.54	0.43
46:S2:867:OMG:H1'	46:S2:867:OMG:HM23	1.71	0.43
46:S2:1442:OMU:HM23	46:S2:1442:OMU:H1'	1.65	0.43
48:SB:226:GLY:O	48:SB:230:GLU:HG2	2.19	0.43
50:SE:232:ASN:O	50:SE:232:ASN:ND2	2.51	0.43
57:SQ:58:LEU:HD23	57:SQ:58:LEU:HA	1.90	0.43
57:SQ:60:LYS:HE3	57:SQ:60:LYS:HB3	1.75	0.43
70:SJ:140:GLN:NE2	75:SY:64:PHE:O	2.51	0.43
1:L1:1942:A:H2'	1:L1:1943:A:C8	2.54	0.43
1:L1:2744:A:H2'	1:L1:2745:A:C8	2.54	0.43
1:L1:3707:U:H2'	1:L1:3708:C:C6	2.53	0.43
1:L1:3902:A:N7	83:L1:5463:HOH:O	2.37	0.43
1:L1:4927:G:H5''	1:L1:4928:C:H5	1.84	0.43
4:LA:46:LYS:HE2	4:LA:62:VAL:HG21	2.00	0.43
4:LA:77:ILE:HD13	4:LA:128:ARG:HB3	2.01	0.43
16:LN:73:ARG:HB2	16:LN:92:LEU:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Lc:23:LYS:HE3	31:Lc:23:LYS:HB2	1.76	0.43
49:SD:62:LYS:HE3	49:SD:62:LYS:HB2	1.77	0.43
67:Sg:50:THR:OG1	67:Sg:51:ASN:N	2.51	0.43
73:SO:103:ASN:OD1	73:SO:103:ASN:N	2.44	0.43
75:SY:121:ALA:O	75:SY:125:VAL:HG12	2.19	0.43
1:L1:1332:C:H2'	1:L1:1333:A:C8	2.54	0.43
1:L1:3792:OMG:H1'	1:L1:3792:OMG:HM23	1.74	0.43
1:L1:4196:OMG:H1'	1:L1:4196:OMG:HM23	1.62	0.43
1:L1:4363:A:H5''	43:Lo:36:GLN:HG2	2.01	0.43
5:LB:50:LYS:O	5:LB:342:LYS:N	2.52	0.43
5:LB:190:VAL:HA	5:LB:193:LYS:HE2	2.01	0.43
10:LG:29:ASN:OD1	10:LG:29:ASN:N	2.51	0.43
25:LW:46:PRO:O	25:LW:52:THR:OG1	2.37	0.43
33:Le:90:MET:HE2	33:Le:90:MET:HA	2.00	0.43
38:Lj:34:CYS:HB3	38:Lj:39:TYR:H	1.83	0.43
46:S2:484:A2M:O5'	46:S2:484:A2M:H8	2.18	0.43
69:SG:69:THR:OG1	69:SG:70:HIS:N	2.52	0.43
1:L1:137:G:H2'	1:L1:138:G:H8	1.83	0.42
1:L1:1308:C:H2'	1:L1:1309:C:C6	2.54	0.42
1:L1:1415:G:H2'	1:L1:1416:G:H8	1.84	0.42
1:L1:2045:G:O6	1:L1:3870:C:O2'	2.37	0.42
1:L1:2498:C:H2'	1:L1:2499:C:H6	1.84	0.42
1:L1:3594:C:C2	1:L1:3597:G:N2	2.87	0.42
1:L1:3748:A:H5''	4:LA:243:THR:HB	2.01	0.42
12:LI:43:VAL:O	12:LI:171:TRP:NE1	2.37	0.42
31:Lc:11:LEU:HA	31:Lc:14:ILE:HG22	2.00	0.42
46:S2:115:U:H2'	46:S2:116:OMU:C6	2.49	0.42
46:S2:1328:OMG:HM23	46:S2:1328:OMG:H1'	1.62	0.42
46:S2:1642:U:O3'	57:SQ:145:TYR:OH	2.35	0.42
56:SP:21:ASP:OD2	56:SP:22:LEU:N	2.45	0.42
63:SX:90:CYS:HA	63:SX:93:PHE:CD2	2.53	0.42
64:Sa:53:ILE:HD13	64:Sa:53:ILE:HA	1.94	0.42
77:Sb:19:HIS:CD2	77:Sb:21:LYS:H	2.37	0.42
1:L1:21:G:H1'	3:L3:103:A:N3	2.34	0.42
1:L1:3744:OMG:HM23	1:L1:3744:OMG:H1'	1.68	0.42
1:L1:3952:A:H2'	1:L1:3953:G:C8	2.54	0.42
15:LM:11:ARG:NH1	15:LM:58:THR:O	2.52	0.42
46:S2:1310:U:H4'	79:Sf:143:LYS:HG3	2.01	0.42
73:SO:44:VAL:HG12	73:SO:53:ILE:HB	2.01	0.42
79:Sf:140:TYR:HA	79:Sf:146:LEU:O	2.19	0.42
1:L1:1535:C:H2'	1:L1:1536:U:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:141:C:H2'	3:L3:142:U:C6	2.55	0.42
5:LB:14:LEU:HD22	5:LB:17:LEU:HD13	2.01	0.42
40:L1:12:PHE:CD2	40:L1:51:LEU:HD23	2.54	0.42
46:S2:747:U:O4	46:S2:796:G:O6	2.38	0.42
46:S2:1235:G:H21	56:SP:135:ALA:HB1	1.85	0.42
64:Sa:7:ASN:O	64:Sa:9:GLY:N	2.45	0.42
72:SN:93:LYS:HB2	72:SN:150:VAL:HG21	2.01	0.42
1:L1:1645:C:H2'	1:L1:1646:A:C8	2.54	0.42
1:L1:1733:G:N3	1:L1:4214:A:H2'	2.34	0.42
1:L1:4274:A:H2'	1:L1:4275:G:H8	1.82	0.42
1:L1:4967:A:H2'	1:L1:4968:A:H8	1.84	0.42
4:LA:45:VAL:O	4:LA:85:GLY:N	2.51	0.42
7:LD:256:LYS:HD2	7:LD:257:PRO:HD2	2.01	0.42
10:LG:259:LYS:HE3	10:LG:259:LYS:HB3	1.74	0.42
21:LS:30:MET:HE2	21:LS:30:MET:HB3	1.85	0.42
25:LW:45:ASN:O	25:LW:49:ILE:HG12	2.20	0.42
57:SQ:43:GLU:CG	57:SQ:44:PRO:HD2	2.46	0.42
60:ST:127:GLY:O	60:ST:131:LEU:HB2	2.19	0.42
67:Sg:249:CYS:HB3	67:Sg:258:ILE:HD13	2.01	0.42
71:SM:60:MET:HA	71:SM:63:LYS:HE3	2.01	0.42
1:L1:717:U:H2'	1:L1:718:C:C6	2.54	0.42
1:L1:3711:A:N6	46:S2:970:G:N1	2.68	0.42
1:L1:4239:A:H2'	1:L1:4240:G:C8	2.54	0.42
8:LE:151:ILE:HA	8:LE:160:LYS:O	2.19	0.42
12:LI:52:MET:HE1	12:LI:155:ALA:HB3	2.02	0.42
20:LR:91:GLU:H	20:LR:91:GLU:HG3	1.63	0.42
31:Lc:82:GLY:HA2	31:Lc:91:VAL:HG13	2.02	0.42
46:S2:639:C:H2'	46:S2:640:A:C8	2.54	0.42
46:S2:695:C:H41	46:S2:736:C:H1'	1.83	0.42
46:S2:1797:U:H2'	46:S2:1798:C:C6	2.55	0.42
57:SQ:51:LEU:HD13	57:SQ:81:ILE:HB	2.01	0.42
67:Sg:238:ALA:HB3	67:Sg:251:ALA:HB3	2.01	0.42
1:L1:65:A:N6	1:L1:74:G:N2	2.68	0.42
1:L1:139:G:H2'	1:L1:140:G:C8	2.55	0.42
1:L1:964:A:H2'	1:L1:965:G:H4'	2.02	0.42
1:L1:2092:G:O2'	1:L1:2262:G:N7	2.47	0.42
1:L1:2112:G:H21	1:L1:2250:C:H41	1.67	0.42
1:L1:2112:G:H21	1:L1:2250:C:N4	2.17	0.42
1:L1:2293:U:H2'	1:L1:2294:G:C8	2.55	0.42
32:Ld:20:VAL:HA	32:Ld:90:ARG:O	2.19	0.42
39:Lk:8:ILE:HD13	39:Lk:45:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lp:86:LEU:HD23	44:Lp:86:LEU:HA	1.94	0.42
46:S2:331:C:H5''	69:SG:189:ARG:HD3	2.01	0.42
46:S2:838:G:N2	46:S2:840:C:O2'	2.53	0.42
46:S2:1203:G:H2'	46:S2:1204:A:C8	2.54	0.42
49:SD:178:ARG:HE	49:SD:178:ARG:HB2	1.62	0.42
59:SS:76:GLN:HE22	59:SS:77:TYR:HD2	1.67	0.42
1:L1:1786:A:H2'	1:L1:1789:C:C5	2.54	0.42
1:L1:1857:C:H2'	1:L1:1858:A:C8	2.54	0.42
1:L1:2804:OMC:HM23	1:L1:2804:OMC:H1'	1.89	0.42
1:L1:3827:G:O2'	1:L1:3829:G:OP2	2.30	0.42
1:L1:3871:A:H2'	1:L1:3872:A:C8	2.54	0.42
7:LD:211:LEU:HD23	7:LD:211:LEU:HA	1.89	0.42
11:LH:103:VAL:HA	11:LH:113:GLU:O	2.19	0.42
22:LT:102:ARG:HD2	22:LT:102:ARG:HA	1.80	0.42
49:SD:54:ARG:HB3	49:SD:57:ASN:HB2	2.02	0.42
52:SH:29:GLU:O	52:SH:33:ASN:OD1	2.37	0.42
53:SI:103:LEU:HD13	53:SI:170:LYS:HE3	2.02	0.42
61:SU:26:SER:HB2	61:SU:110:VAL:HG13	2.02	0.42
1:L1:444:G:H2'	1:L1:445:U:C6	2.55	0.42
1:L1:3726:A:H2'	1:L1:3727:A:C8	2.55	0.42
1:L1:4458:C:H2'	1:L1:4459:U:C6	2.55	0.42
1:L1:4618:OMG:H5''	24:LV:15:ARG:HB2	2.01	0.42
1:L1:4691:A:OP1	11:LH:75:SER:OG	2.34	0.42
1:L1:4742:G:H2'	1:L1:4743:G:H8	1.85	0.42
23:LU:80:LYS:HG2	23:LU:110:TYR:CE2	2.55	0.42
29:La:119:LYS:HA	29:La:140:VAL:HG22	2.02	0.42
40:Ll:15:LYS:O	40:Ll:19:GLN:HG2	2.19	0.42
46:S2:159:A2M:H8	46:S2:159:A2M:OP2	2.20	0.42
48:SB:165:ARG:O	48:SB:169:MET:HG3	2.19	0.42
50:SE:36:HIS:CG	50:SE:85:GLY:HA3	2.55	0.42
53:SI:165:GLN:HB3	53:SI:171:LEU:HD23	2.01	0.42
56:SP:23:ASP:HA	56:SP:26:LEU:HD12	2.01	0.42
70:SJ:81:LEU:HA	70:SJ:84:ILE:HG22	2.01	0.42
71:SM:32:ALA:HB1	71:SM:37:GLU:HB3	2.01	0.42
1:L1:135:G:H2'	36:Lh:96:ASN:HA	2.02	0.42
1:L1:158:A:H5''	1:L1:159:C:H2'	2.01	0.42
1:L1:729:2MG:N2	21:LS:66:GLN:O	2.28	0.42
1:L1:965:G:H21	1:L1:2092:G:H1'	1.85	0.42
1:L1:1759:G:N2	1:L1:1773:U:O2	2.41	0.42
4:LA:101:VAL:HG22	4:LA:165:VAL:HG22	2.01	0.42
5:LB:294:LYS:HE2	5:LB:298:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LE:190:HIS:HB3	8:LE:193:PHE:HD2	1.84	0.42
21:LS:173:ASN:ND2	21:LS:175:PHE:O	2.52	0.42
46:S2:494:C:N4	46:S2:509:OMG:HN22	2.17	0.42
46:S2:1030:A:H2'	46:S2:1031:A2M:H8	2.02	0.42
49:SD:31:GLU:HA	49:SD:107:TYR:CE1	2.54	0.42
59:SS:26:ILE:O	59:SS:30:ILE:HG12	2.20	0.42
61:SU:31:SER:O	61:SU:35:VAL:HG23	2.20	0.42
67:Sg:164:ILE:HG23	67:Sg:176:VAL:HG13	2.02	0.42
1:L1:1726:U:H5'	9:LF:135:ILE:HD11	2.02	0.42
1:L1:2382:A:N1	1:L1:2829:U:O2'	2.46	0.42
1:L1:2407:G:OP2	1:L1:2407:G:N2	2.46	0.42
2:L2:23:A:N3	2:L2:118:C:O2'	2.42	0.42
8:LE:119:GLU:OE2	33:Le:94:SER:OG	2.37	0.42
28:LZ:29:ILE:HG21	28:LZ:33:THR:HG23	2.02	0.42
43:Lo:70:LEU:HD11	43:Lo:83:LEU:HD12	2.02	0.42
46:S2:65:C:C2	69:SG:133:LEU:HD22	2.55	0.42
46:S2:436:OMG:HM22	46:S2:437:G:H5'	2.00	0.42
46:S2:874:G:H2'	46:S2:875:A:C8	2.52	0.42
46:S2:1432:U:H5''	46:S2:1433:C:H5''	2.01	0.42
68:SC:253:PRO:HA	68:SC:256:TRP:CG	2.54	0.42
1:L1:747:A:O2'	1:L1:749:G:OP2	2.38	0.41
1:L1:1979:A:N6	1:L1:1984:A:OP1	2.45	0.41
1:L1:2318:G:O6	33:Le:19:LYS:NZ	2.52	0.41
1:L1:4343:U:O2'	43:Lo:31:ASP:OD1	2.27	0.41
8:LE:72:LYS:HG3	30:Lb:119:CYS:HB3	2.02	0.41
9:LF:24:ASN:O	9:LF:28:LEU:HB2	2.19	0.41
9:LF:124:LYS:HB2	9:LF:124:LYS:HE3	1.93	0.41
18:LP:94:MET:HE3	18:LP:94:MET:HB2	1.82	0.41
26:LX:156:ILE:HD12	26:LX:156:ILE:HA	1.94	0.41
28:LZ:14:LEU:HD11	28:LZ:81:MET:HB2	2.01	0.41
33:Le:90:MET:HG3	45:Lr:33:LYS:HA	2.01	0.41
46:S2:996:A:H2'	46:S2:997:A:C8	2.55	0.41
46:S2:1410:C:H2'	46:S2:1411:G:H8	1.83	0.41
46:S2:1713:C:H2'	46:S2:1714:U:C6	2.54	0.41
49:SD:132:LYS:HB3	49:SD:132:LYS:HE3	1.87	0.41
56:SP:82:ASP:OD2	56:SP:82:ASP:N	2.50	0.41
59:SS:117:ILE:HD12	59:SS:117:ILE:HA	1.87	0.41
61:SU:36:CYS:O	61:SU:40:ILE:HG12	2.20	0.41
71:SM:25:ALA:O	71:SM:30:GLY:N	2.51	0.41
71:SM:36:ARG:HD2	79:Sf:102:VAL:HG13	2.01	0.41
75:SY:111:LYS:HB3	75:SY:111:LYS:HE3	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3917:A:H2'	1:L1:3918:G:C8	2.55	0.41
1:L1:4324:A:H2'	1:L1:4325:A:C8	2.55	0.41
1:L1:4522:G:O2'	1:L1:4525:C:OP2	2.31	0.41
20:LR:183:GLU:HA	20:LR:186:LYS:HG2	2.01	0.41
70:SJ:101:LYS:HB2	70:SJ:101:LYS:HE3	1.85	0.41
1:L1:655:C:H2'	1:L1:656:C:C6	2.56	0.41
1:L1:1345:A:H2'	1:L1:1346:C:C6	2.55	0.41
1:L1:1927:U:OP1	1:L1:1949:U:O2'	2.33	0.41
1:L1:1984:A:N7	1:L1:2010:A:O2'	2.53	0.41
1:L1:3723:A2M:HM'3	1:L1:3723:A2M:H1'	1.92	0.41
10:LG:170:LEU:HD23	10:LG:201:THR:HG21	2.02	0.41
13:LJ:114:ASP:OD1	13:LJ:114:ASP:N	2.54	0.41
46:S2:656:G:H5'	46:S2:662:G:N2	2.35	0.41
46:S2:919:A:OP2	72:SN:64:ARG:NH1	2.44	0.41
46:S2:1221:G:H2'	46:S2:1222:G:C8	2.55	0.41
46:S2:1293:A:H2'	46:S2:1294:G:H8	1.85	0.41
50:SE:44:LEU:HD11	50:SE:70:ILE:HG21	2.02	0.41
57:SQ:51:LEU:HD12	57:SQ:51:LEU:HA	1.87	0.41
67:Sg:65:PHE:C	67:Sg:82:SER:HG	2.29	0.41
72:SN:13:GLN:HG3	77:Sb:21:LYS:HE3	2.02	0.41
72:SN:76:LYS:HB3	72:SN:76:LYS:HE3	1.74	0.41
3:L3:94:G:N2	38:Lj:82:THR:OG1	2.41	0.41
20:LR:184:ILE:HD13	20:LR:184:ILE:HA	1.92	0.41
27:LY:113:LYS:O	27:LY:117:LYS:HG3	2.20	0.41
34:Lf:24:HIS:ND1	34:Lf:25:THR:HG22	2.35	0.41
46:S2:562:U:H2'	46:S2:563:G:C8	2.55	0.41
46:S2:873:G:O2'	55:SL:152:LYS:NZ	2.53	0.41
46:S2:901:G:H2'	46:S2:902:G:C8	2.55	0.41
57:SQ:5:GLY:H	57:SQ:27:ARG:NH1	2.19	0.41
58:SR:129:LYS:HE3	58:SR:129:LYS:HB2	1.95	0.41
63:SX:90:CYS:O	63:SX:94:ILE:HG13	2.20	0.41
1:L1:691:C:H2'	1:L1:692:A:H8	1.84	0.41
1:L1:3594:C:O2	1:L1:3597:G:C2	2.73	0.41
1:L1:3707:U:H2'	1:L1:3708:C:H6	1.84	0.41
1:L1:4860:G:H2'	1:L1:4861:G:C8	2.56	0.41
5:LB:92:TYR:HB3	5:LB:99:LEU:HG	2.03	0.41
11:LH:8:GLN:HE22	11:LH:71:ARG:HG2	1.86	0.41
21:LS:53:LYS:HB2	21:LS:53:LYS:HE3	1.84	0.41
46:S2:1121:G:O2'	48:SB:204:ILE:O	2.28	0.41
46:S2:1692:U:H2'	46:S2:1693:G:C8	2.56	0.41
47:SA:16:LEU:HD21	58:SR:114:LEU:HD21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SF:32:ASP:O	51:SF:36:GLN:HB2	2.20	0.41
52:SH:63:PHE:HA	52:SH:95:ILE:O	2.20	0.41
52:SH:111:LYS:HB3	52:SH:112:ASN:H	1.62	0.41
58:SR:114:LEU:HD11	58:SR:116:ASN:HB2	2.02	0.41
59:SS:116:LYS:HB2	59:SS:116:LYS:HE2	1.80	0.41
67:Sg:248:LEU:HB2	67:Sg:261:LEU:HD11	2.02	0.41
1:L1:1499:C:O2'	29:La:114:LYS:NZ	2.53	0.41
1:L1:1698:C:H5'	1:L1:1699:A:O4'	2.20	0.41
1:L1:1872:G:O2'	1:L1:4219:A:N3	2.50	0.41
1:L1:4742:G:H2'	1:L1:4743:G:C8	2.56	0.41
5:LB:393:LYS:O	5:LB:397:ILE:HG12	2.21	0.41
9:LF:171:ASP:HB3	9:LF:174:LEU:HG	2.02	0.41
10:LG:192:ARG:NH2	10:LG:196:ARG:O	2.53	0.41
46:S2:102:A:H4'	46:S2:104:A:C8	2.56	0.41
47:SA:10:MET:HE1	47:SA:51:LEU:HB3	2.02	0.41
53:SI:76:THR:HG22	53:SI:108:PRO:HG2	2.02	0.41
54:SK:15:LEU:O	54:SK:19:GLY:HA2	2.20	0.41
59:SS:5:ILE:HD12	59:SS:5:ILE:HA	1.97	0.41
61:SU:30:LYS:HD3	61:SU:30:LYS:HA	1.66	0.41
71:SM:55:ASN:HD21	71:SM:82:ASN:H	1.67	0.41
1:L1:156:G:OP2	36:Lh:109:ARG:NH2	2.53	0.41
1:L1:1875:C:H2'	1:L1:1876:U:C6	2.56	0.41
1:L1:2557:G:H1	1:L1:2570:U:H3	1.67	0.41
1:L1:4538:G:H2'	1:L1:4539:U:C6	2.56	0.41
2:L2:62:U:OP2	7:LD:276:LYS:NZ	2.52	0.41
3:L3:75:OMG:OP2	27:LY:74:TYR:OH	2.35	0.41
36:Lh:105:LYS:HE3	36:Lh:105:LYS:HB2	1.86	0.41
55:SL:111:VAL:HG12	55:SL:140:PHE:HB2	2.03	0.41
67:Sg:212:LYS:HA	67:Sg:235:ILE:HD12	2.01	0.41
73:SO:84:ARG:NH1	73:SO:87:GLU:OE1	2.53	0.41
1:L1:2046:G:C4	17:LO:60:LYS:HD2	2.56	0.41
1:L1:2730:U:H2'	1:L1:2731:C:C6	2.56	0.41
1:L1:3722:G:H2'	1:L1:3723:A2M:C8	2.51	0.41
6:LC:205:ARG:HD3	6:LC:205:ARG:HA	1.89	0.41
9:LF:57:TYR:OH	9:LF:189:ASP:OD2	2.30	0.41
10:LG:231:ASP:OD1	10:LG:234:ARG:NH2	2.53	0.41
46:S2:613:G:N2	46:S2:626:G:OP1	2.49	0.41
46:S2:1438:A:H2'	46:S2:1439:A:C8	2.55	0.41
48:SB:168:MET:O	48:SB:172:MET:HG3	2.21	0.41
52:SH:83:LEU:HD13	52:SH:83:LEU:HA	1.92	0.41
53:SI:197:PHE:O	53:SI:201:LYS:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Sg:190:GLY:HA3	67:Sg:217:MET:HE1	2.02	0.41
79:Sf:133:ALA:N	79:Sf:140:TYR:O	2.54	0.41
1:L1:1191:C:H2'	1:L1:1192:C:C6	2.55	0.41
1:L1:1279:A:O2'	1:L1:1281:G:N7	2.46	0.41
1:L1:1340:OMC:HM23	1:L1:1340:OMC:H1'	1.80	0.41
1:L1:1503:A:H4'	1:L1:1504:G:H5'	2.02	0.41
1:L1:1867:A:H2'	1:L1:1868:A:C8	2.56	0.41
1:L1:2497:C:H2'	1:L1:2498:C:H6	1.86	0.41
1:L1:3599:A:H2'	1:L1:3600:G:C8	2.56	0.41
1:L1:4578:G:H2'	1:L1:4579:U:C6	2.56	0.41
4:LA:136:VAL:HA	4:LA:148:VAL:HG12	2.02	0.41
8:LE:165:LEU:HD11	8:LE:176:THR:HG22	2.02	0.41
33:Le:104:SER:O	33:Le:108:ARG:HB2	2.21	0.41
46:S2:1277:C:H4'	54:SK:55:ARG:CZ	2.51	0.41
46:S2:1595:U:H2'	46:S2:1596:U:C6	2.56	0.41
46:S2:1617:G:H4'	66:Sd:14:PHE:CZ	2.55	0.41
46:S2:1786:U:H2'	46:S2:1787:G:H8	1.86	0.41
49:SD:8:LYS:HG2	61:SU:61:LEU:HD11	2.02	0.41
49:SD:66:ILE:HD12	49:SD:66:ILE:HA	1.96	0.41
49:SD:162:ASP:OD1	49:SD:162:ASP:N	2.47	0.41
50:SE:59:ASP:O	50:SE:62:LYS:HG3	2.21	0.41
57:SQ:43:GLU:CB	57:SQ:44:PRO:HD2	2.50	0.41
57:SQ:61:GLU:H	57:SQ:61:GLU:CD	2.28	0.41
59:SS:6:PRO:HD2	59:SS:9:PHE:HB2	2.03	0.41
59:SS:52:LEU:H	59:SS:52:LEU:HD23	1.86	0.41
62:SV:17:CYS:HB2	62:SV:56:CYS:HB3	2.03	0.41
67:Sg:188:HIS:HB3	67:Sg:219:TRP:CH2	2.56	0.41
71:SM:59:PRO:HA	71:SM:62:VAL:HG22	2.03	0.41
75:SY:92:ALA:HB2	75:SY:97:TYR:HD2	1.86	0.41
1:L1:4173:G:H2'	1:L1:4174:U:C6	2.56	0.41
1:L1:4524:G:C2	5:LB:252:ALA:HB1	2.56	0.41
4:LA:70:LYS:HB3	4:LA:70:LYS:HE3	1.91	0.41
32:Ld:40:LYS:O	32:Ld:44:ARG:HB2	2.21	0.41
46:S2:12:U:H2'	46:S2:13:C:C6	2.56	0.41
46:S2:1650:A:H5''	57:SQ:139:ALA:HB2	2.02	0.41
49:SD:32:ASP:OD1	49:SD:32:ASP:N	2.54	0.41
53:SI:157:LYS:HE2	53:SI:157:LYS:HA	2.03	0.41
56:SP:44:ARG:HH12	56:SP:82:ASP:HB2	1.86	0.41
61:SU:88:LEU:HD23	61:SU:88:LEU:HA	1.89	0.41
71:SM:60:MET:HA	71:SM:63:LYS:HG3	2.03	0.41
76:SZ:66:LYS:HE3	76:SZ:66:LYS:HB3	1.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:268:G:H2'	1:L1:269:G:C8	2.56	0.40
1:L1:325:U:H2'	1:L1:326:C:C6	2.56	0.40
1:L1:1443:A:C2	1:L1:2104:G:C2	3.10	0.40
1:L1:1617:G:H1'	1:L1:2513:A:N6	2.37	0.40
1:L1:1914:C:OP1	17:LO:25:LYS:NZ	2.43	0.40
1:L1:2267:U:OP1	45:Lr:37:SER:HB2	2.21	0.40
1:L1:2815:A2M:HM'3	1:L1:2815:A2M:H1'	1.91	0.40
1:L1:2846:G:O2'	24:LV:19:GLY:O	2.35	0.40
1:L1:4991:U:H2'	1:L1:4992:G:C8	2.56	0.40
1:L1:5006:U:H4'	1:L1:5007:A:H5'	2.03	0.40
4:LA:229:ALA:HB3	4:LA:234:LYS:HB3	2.03	0.40
5:LB:165:HIS:HA	5:LB:179:HIS:O	2.22	0.40
10:LG:96:LEU:HD23	10:LG:96:LEU:HA	1.92	0.40
15:LM:39:ASP:OD1	15:LM:47:ARG:HB2	2.22	0.40
21:LS:9:GLU:HG3	21:LS:33:PHE:CE2	2.55	0.40
46:S2:527:C:H2'	46:S2:528:A:C8	2.56	0.40
49:SD:33:GLY:HA3	49:SD:53:THR:HB	2.04	0.40
49:SD:173:ARG:HD3	49:SD:173:ARG:HA	1.82	0.40
56:SP:77:LYS:HA	56:SP:95:GLY:O	2.20	0.40
63:SX:74:LEU:O	63:SX:78:GLY:N	2.54	0.40
1:L1:732:A:H2'	1:L1:733:A:O4'	2.20	0.40
1:L1:1456:JMH:O2'	19:LQ:73:PRO:O	2.38	0.40
1:L1:4097:G:H2'	1:L1:4098:A:C8	2.56	0.40
6:LC:5:ARG:HD2	6:LC:24:LEU:O	2.21	0.40
6:LC:307:LYS:HE3	6:LC:307:LYS:HB2	1.81	0.40
14:LL:91:ALA:HB1	14:LL:96:ILE:HB	2.03	0.40
25:LW:8:PHE:HZ	25:LW:49:ILE:HG13	1.86	0.40
30:Lb:23:LYS:HE3	30:Lb:23:LYS:HB3	1.83	0.40
31:Lc:78:ASN:OD1	31:Lc:78:ASN:N	2.52	0.40
35:Lg:61:PRO:O	35:Lg:64:LEU:HB2	2.21	0.40
46:S2:674:C:H2'	46:S2:675:U:C6	2.56	0.40
46:S2:1630:A:H5''	59:SS:37:GLY:H	1.87	0.40
46:S2:1736:G:H2'	46:S2:1737:G:C8	2.57	0.40
52:SH:149:ASP:N	52:SH:149:ASP:OD2	2.54	0.40
60:ST:76:THR:HB	60:ST:94:ARG:HB3	2.02	0.40
67:Sg:86:THR:HG21	67:Sg:100:ARG:HH22	1.87	0.40
67:Sg:297:THR:HA	67:Sg:310:TRP:O	2.22	0.40
1:L1:2864:A:H2'	1:L1:2865:U:H6	1.85	0.40
1:L1:3911:C:H2'	1:L1:3912:U:H6	1.86	0.40
12:LI:31:ILE:HG22	12:LI:62:SER:HB2	2.04	0.40
13:LJ:151:ILE:HD11	13:LJ:156:ARG:HG2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LQ:29:VAL:O	19:LQ:33:ARG:HB2	2.21	0.40
21:LS:78:PHE:O	21:LS:96:GLU:HA	2.21	0.40
27:LY:85:VAL:HG12	27:LY:97:VAL:HB	2.03	0.40
29:La:75:LEU:HB3	29:La:117:LEU:HD21	2.01	0.40
46:S2:1098:C:H2'	46:S2:1099:G:C8	2.56	0.40
48:SB:36:PRO:HB3	48:SB:231:LEU:HD23	2.04	0.40
48:SB:134:LEU:HG	48:SB:218:LEU:HD12	2.03	0.40
48:SB:223:PHE:HE1	48:SB:228:LEU:HD22	1.86	0.40
51:SF:127:ARG:HB3	51:SF:136:ARG:HB3	2.04	0.40
57:SQ:80:GLN:O	57:SQ:84:ILE:HG13	2.21	0.40
70:SJ:136:ARG:HG2	70:SJ:160:SER:HA	2.03	0.40
72:SN:132:LYS:HD2	72:SN:132:LYS:HA	1.73	0.40
1:L1:1625:OMG:H4'	1:L1:1626:G:O5'	2.21	0.40
1:L1:2749:C:H5'	35:Lg:65:MET:HA	2.03	0.40
1:L1:4941:G:OP2	8:LE:188:ARG:NH2	2.36	0.40
6:LC:143:ARG:HD2	6:LC:143:ARG:HA	1.87	0.40
13:LJ:141:ILE:HA	13:LJ:144:LYS:HE2	2.02	0.40
38:Lj:65:ARG:O	38:Lj:69:ILE:HG13	2.21	0.40
46:S2:1201:U:H2'	46:S2:1202:U:C6	2.56	0.40
49:SD:69:LEU:O	49:SD:73:VAL:HG13	2.22	0.40
62:SV:27:LYS:HD3	62:SV:27:LYS:HA	1.88	0.40
67:Sg:68:ASP:HB3	67:Sg:111:VAL:HG22	2.03	0.40
67:Sg:109:LEU:HD23	67:Sg:109:LEU:HA	1.93	0.40
68:SC:196:ILE:HB	68:SC:223:TYR:HB2	2.03	0.40
73:SO:56:VAL:HG13	73:SO:60:MET:HE2	2.03	0.40
75:SY:62:THR:HA	75:SY:69:THR:HA	2.04	0.40
1:L1:188:G:N2	1:L1:191:G:N7	2.70	0.40
1:L1:1443:A:N6	1:L1:2104:G:N1	2.70	0.40
1:L1:2808:G:O3'	20:LR:60:ARG:NH1	2.54	0.40
5:LB:258:HIS:HA	5:LB:259:PRO:C	2.46	0.40
15:LM:24:LEU:HD11	15:LM:86:TRP:CG	2.57	0.40
25:LW:80:ARG:HH11	69:SG:131:ARG:HG2	1.86	0.40
37:Li:33:LEU:HD21	37:Li:38:LYS:HG3	2.03	0.40
38:Lj:3:LYS:H	38:Lj:3:LYS:HG2	1.68	0.40
39:Lk:11:PHE:HA	39:Lk:14:THR:HG22	2.03	0.40
46:S2:525:A:H2'	46:S2:526:A:H8	1.86	0.40
46:S2:1139:C:H2'	46:S2:1140:G:O4'	2.21	0.40
46:S2:1245:G:O2'	46:S2:1492:U:OP1	2.34	0.40
46:S2:1407:U:H2'	46:S2:1408:U:C6	2.57	0.40
49:SD:67:ARG:NH1	54:SK:97:SER:OG	2.54	0.40
54:SK:63:ALA:HB2	54:SK:68:TYR:HE2	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SP:107:ILE:HA	56:SP:111:MET:SD	2.61	0.40
63:SX:68:LYS:HB3	63:SX:91:LEU:HD13	2.02	0.40
67:Sg:155:ARG:HD3	67:Sg:155:ARG:HA	1.94	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%)	233 (95%)	13 (5%)	0	100	100
5	LB	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
6	LC	363/427 (85%)	355 (98%)	8 (2%)	0	100	100
7	LD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
8	LE	214/288 (74%)	208 (97%)	6 (3%)	0	100	100
9	LF	223/248 (90%)	215 (96%)	8 (4%)	0	100	100
10	LG	223/266 (84%)	220 (99%)	3 (1%)	0	100	100
11	LH	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	LI	198/214 (92%)	192 (97%)	6 (3%)	0	100	100
13	LJ	167/178 (94%)	163 (98%)	4 (2%)	0	100	100
14	LL	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
15	LM	137/215 (64%)	133 (97%)	4 (3%)	0	100	100
16	LN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
17	LO	199/203 (98%)	199 (100%)	0	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
20	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
22	LT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
23	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	122/157 (78%)	117 (96%)	5 (4%)	0	100	100
26	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
29	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
31	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
32	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
33	Le	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
34	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
39	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/128 (39%)	50 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
47	SA	220/295 (75%)	216 (98%)	4 (2%)	0	100	100
48	SB	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
49	SD	225/243 (93%)	218 (97%)	7 (3%)	0	100	100
50	SE	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
51	SF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
52	SH	182/194 (94%)	162 (89%)	16 (9%)	4 (2%)	5	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
54	SK	96/165 (58%)	92 (96%)	4 (4%)	0	100	100
55	SL	140/158 (89%)	132 (94%)	8 (6%)	0	100	100
56	SP	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
57	SQ	142/146 (97%)	130 (92%)	11 (8%)	1 (1%)	18	34
58	SR	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
59	SS	143/152 (94%)	137 (96%)	6 (4%)	0	100	100
60	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
61	SU	102/119 (86%)	96 (94%)	5 (5%)	1 (1%)	12	24
62	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
63	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
64	Sa	100/115 (87%)	97 (97%)	2 (2%)	1 (1%)	12	24
65	Sc	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
66	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
67	Sg	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
68	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
69	SG	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
70	SJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
71	SM	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
72	SN	148/151 (98%)	148 (100%)	0	0	100	100
73	SO	133/151 (88%)	124 (93%)	8 (6%)	1 (1%)	16	31
74	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
75	SY	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
76	SZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
77	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
78	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
79	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
All	All	11249/12687 (89%)	10882 (97%)	359 (3%)	8 (0%)	49	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	SH	34	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	SQ	44	PRO
52	SH	11	PRO
52	SH	40	LEU
61	SU	94	PRO
64	Sa	46	GLU
52	SH	8	ILE
73	SO	89	GLY

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%)	188 (99%)	2 (1%)	65	84
5	LB	348/349 (100%)	342 (98%)	6 (2%)	53	78
6	LC	304/348 (87%)	299 (98%)	5 (2%)	55	79
7	LD	246/250 (98%)	242 (98%)	4 (2%)	55	79
8	LE	194/252 (77%)	191 (98%)	3 (2%)	57	80
9	LF	194/215 (90%)	189 (97%)	5 (3%)	40	68
10	LG	196/223 (88%)	195 (100%)	1 (0%)	81	92
11	LH	169/171 (99%)	167 (99%)	2 (1%)	63	83
12	LI	172/181 (95%)	171 (99%)	1 (1%)	78	91
13	LJ	142/149 (95%)	139 (98%)	3 (2%)	47	74
14	LL	176/177 (99%)	174 (99%)	2 (1%)	65	84
15	LM	118/161 (73%)	115 (98%)	3 (2%)	42	69
16	LN	171/172 (99%)	167 (98%)	4 (2%)	44	72
17	LO	173/174 (99%)	170 (98%)	3 (2%)	53	78
18	LP	134/163 (82%)	134 (100%)	0	100	100
19	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	83
20	LR	166/175 (95%)	164 (99%)	2 (1%)	63	83
21	LS	157/157 (100%)	154 (98%)	3 (2%)	50	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	89 (98%)	2 (2%)	45	73
24	LV	101/107 (94%)	96 (95%)	5 (5%)	22	44
25	LW	103/126 (82%)	102 (99%)	1 (1%)	68	86
26	LX	106/133 (80%)	103 (97%)	3 (3%)	38	66
27	LY	124/135 (92%)	123 (99%)	1 (1%)	73	88
28	LZ	117/117 (100%)	117 (100%)	0	100	100
29	La	120/121 (99%)	116 (97%)	4 (3%)	33	61
30	Lb	88/126 (70%)	86 (98%)	2 (2%)	44	72
31	Lc	83/97 (86%)	80 (96%)	3 (4%)	31	58
32	Ld	98/110 (89%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	110 (96%)	4 (4%)	32	58
34	Lf	88/89 (99%)	86 (98%)	2 (2%)	44	72
35	Lg	98/100 (98%)	96 (98%)	2 (2%)	48	75
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	87
37	Li	86/89 (97%)	85 (99%)	1 (1%)	63	83
38	Lj	73/80 (91%)	71 (97%)	2 (3%)	39	67
39	Lk	64/65 (98%)	61 (95%)	3 (5%)	23	47
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	48/116 (41%)	47 (98%)	1 (2%)	47	74
42	Ln	23/24 (96%)	21 (91%)	2 (9%)	9	21
43	Lo	90/93 (97%)	87 (97%)	3 (3%)	33	61
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
47	SA	184/243 (76%)	182 (99%)	2 (1%)	65	84
48	SB	195/231 (84%)	190 (97%)	5 (3%)	40	68
49	SD	190/202 (94%)	187 (98%)	3 (2%)	55	79
50	SE	224/225 (100%)	220 (98%)	4 (2%)	51	77
51	SF	156/170 (92%)	153 (98%)	3 (2%)	50	76
52	SH	166/174 (95%)	150 (90%)	16 (10%)	8	17
53	SI	178/180 (99%)	175 (98%)	3 (2%)	53	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	SK	89/136 (65%)	86 (97%)	3 (3%)	32	60
55	SL	130/142 (92%)	129 (99%)	1 (1%)	73	88
56	SP	113/130 (87%)	111 (98%)	2 (2%)	51	77
57	SQ	119/121 (98%)	112 (94%)	7 (6%)	18	37
58	SR	122/122 (100%)	116 (95%)	6 (5%)	22	45
59	SS	126/132 (96%)	123 (98%)	3 (2%)	43	70
60	ST	113/115 (98%)	110 (97%)	3 (3%)	39	67
61	SU	94/107 (88%)	89 (95%)	5 (5%)	20	42
62	SV	67/67 (100%)	64 (96%)	3 (4%)	24	49
63	SX	113/115 (98%)	110 (97%)	3 (3%)	39	67
64	Sa	89/98 (91%)	88 (99%)	1 (1%)	65	84
65	Sc	57/62 (92%)	57 (100%)	0	100	100
66	Sd	48/49 (98%)	48 (100%)	0	100	100
67	Sg	272/275 (99%)	265 (97%)	7 (3%)	40	68
68	SC	188/225 (84%)	188 (100%)	0	100	100
69	SG	207/218 (95%)	203 (98%)	4 (2%)	50	76
70	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	83
71	SM	102/108 (94%)	98 (96%)	4 (4%)	28	55
72	SN	130/131 (99%)	128 (98%)	2 (2%)	57	80
73	SO	105/119 (88%)	105 (100%)	0	100	100
74	SW	112/113 (99%)	109 (97%)	3 (3%)	39	67
75	SY	109/115 (95%)	107 (98%)	2 (2%)	51	77
76	SZ	66/103 (64%)	65 (98%)	1 (2%)	57	80
77	Sb	75/76 (99%)	73 (97%)	2 (3%)	39	67
78	Se	47/48 (98%)	47 (100%)	0	100	100
79	Sf	54/140 (39%)	53 (98%)	1 (2%)	50	76
All	All	9808/10799 (91%)	9614 (98%)	194 (2%)	48	75

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	149	LYS
4	LA	242	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	LB	53	MET
5	LB	60	VAL
5	LB	141	ASP
5	LB	152	SER
5	LB	287	ILE
5	LB	295	ASP
6	LC	147	VAL
6	LC	155	GLU
6	LC	255	SER
6	LC	289	LEU
6	LC	348	LYS
7	LD	7	VAL
7	LD	194	VAL
7	LD	213	GLU
7	LD	232	THR
8	LE	51	VAL
8	LE	203	ILE
8	LE	206	VAL
9	LF	68	GLU
9	LF	102	SER
9	LF	221	LYS
9	LF	222	LYS
9	LF	223	LYS
10	LG	202	VAL
11	LH	137	SER
11	LH	143	GLU
12	LI	35	ASP
13	LJ	28	GLU
13	LJ	102	THR
13	LJ	115	LEU
14	LL	52	SER
14	LL	144	LEU
15	LM	7	VAL
15	LM	28	VAL
15	LM	45	VAL
16	LN	10	LEU
16	LN	18	VAL
16	LN	126	THR
16	LN	166	SER
17	LO	5	GLN
17	LO	129	LEU
17	LO	171	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	LQ	66	MET
19	LQ	130	SER
20	LR	43	LYS
20	LR	122	SER
21	LS	49	SER
21	LS	88	SER
21	LS	135	SER
23	LU	23	LEU
23	LU	71	THR
24	LV	22	VAL
24	LV	65	VAL
24	LV	75	LYS
24	LV	87	SER
24	LV	128	LEU
25	LW	1	MET
26	LX	40	ILE
26	LX	85	SER
26	LX	88	LYS
27	LY	105	VAL
29	La	78	LEU
29	La	82	VAL
29	La	122	VAL
29	La	140	VAL
30	Lb	14	ARG
30	Lb	76	VAL
31	Lc	46	VAL
31	Lc	91	VAL
31	Lc	102	SER
33	Le	87	VAL
33	Le	89	LEU
33	Le	94	SER
33	Le	126	ASN
34	Lf	25	THR
34	Lf	105	LEU
35	Lg	63	VAL
35	Lg	105	LYS
36	Lh	88	THR
37	Li	11	LEU
38	Lj	32	SER
38	Lj	83	THR
39	Lk	22	SER
39	Lk	36	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	Lk	46	VAL
41	Lm	87	GLN
42	Ln	16	LYS
42	Ln	24	SER
43	Lo	33	LEU
43	Lo	83	LEU
43	Lo	103	VAL
47	SA	81	ASN
47	SA	124	VAL
48	SB	52	THR
48	SB	88	THR
48	SB	127	VAL
48	SB	183	GLU
48	SB	203	SER
49	SD	156	LEU
49	SD	206	ASP
49	SD	215	ASP
50	SE	126	VAL
50	SE	143	ASP
50	SE	156	VAL
50	SE	208	VAL
51	SF	78	MET
51	SF	83	ASN
51	SF	136	ARG
52	SH	7	LYS
52	SH	8	ILE
52	SH	10	LYS
52	SH	14	GLU
52	SH	17	ASP
52	SH	18	GLU
52	SH	20	GLU
52	SH	24	SER
52	SH	27	LEU
52	SH	29	GLU
52	SH	30	LEU
52	SH	31	GLU
52	SH	32	MET
52	SH	39	GLN
52	SH	40	LEU
52	SH	45	ILE
53	SI	73	THR
53	SI	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	SI	168	GLN
54	SK	14	LEU
54	SK	37	ASP
54	SK	81	ASP
55	SL	152	LYS
56	SP	76	VAL
56	SP	96	VAL
57	SQ	42	ILE
57	SQ	43	GLU
57	SQ	44	PRO
57	SQ	45	ARG
57	SQ	89	SER
57	SQ	118	THR
57	SQ	127	CYS
58	SR	36	GLU
58	SR	95	ILE
58	SR	99	ASP
58	SR	105	MET
58	SR	111	PHE
58	SR	117	LEU
59	SS	16	LEU
59	SS	68	ILE
59	SS	111	LEU
60	ST	7	LYS
60	ST	8	ASP
60	ST	39	LEU
61	SU	23	THR
61	SU	30	LYS
61	SU	36	CYS
61	SU	78	ASP
61	SU	92	HIS
62	SV	52	THR
62	SV	79	VAL
62	SV	83	PHE
63	SX	34	THR
63	SX	36	LEU
63	SX	125	VAL
64	Sa	30	VAL
67	Sg	49	GLU
67	Sg	70	VAL
67	Sg	113	PHE
67	Sg	166	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	Sg	235	ILE
67	Sg	266	ILE
67	Sg	297	THR
69	SG	27	PHE
69	SG	49	VAL
69	SG	163	ASN
69	SG	218	LYS
70	SJ	152	ASP
70	SJ	157	ILE
71	SM	76	LEU
71	SM	103	VAL
71	SM	109	VAL
71	SM	127	TYR
72	SN	117	LEU
72	SN	150	VAL
74	SW	30	CYS
74	SW	104	LEU
74	SW	105	THR
75	SY	24	VAL
75	SY	85	ASN
76	SZ	64	ASN
77	Sb	44	THR
77	Sb	77	CYS
79	Sf	102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	22	HIS
4	LA	95	GLN
4	LA	140	ASN
5	LB	184	GLN
5	LB	258	HIS
6	LC	21	ASN
6	LC	89	GLN
6	LC	112	HIS
6	LC	119	GLN
6	LC	282	HIS
8	LE	182	ASN
8	LE	245	GLN
9	LF	24	ASN
9	LF	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	LG	38	ASN
10	LG	108	GLN
10	LG	195	HIS
11	LH	7	ASN
11	LH	116	ASN
12	LI	73	ASN
13	LJ	42	GLN
13	LJ	98	ASN
13	LJ	104	ASN
14	LL	87	HIS
14	LL	115	GLN
15	LM	20	HIS
15	LM	75	GLN
16	LN	15	GLN
16	LN	32	GLN
17	LO	42	ASN
17	LO	180	GLN
18	LP	34	GLN
18	LP	75	GLN
20	LR	39	GLN
20	LR	40	GLN
20	LR	66	ASN
21	LS	173	ASN
22	LT	131	GLN
27	LY	96	HIS
29	La	60	HIS
30	Lb	6	ASN
33	Le	81	ASN
33	Le	117	GLN
33	Le	126	ASN
35	Lg	100	GLN
37	Li	12	ASN
38	Lj	13	ASN
38	Lj	66	HIS
41	Lm	109	ASN
45	Lr	30	ASN
45	Lr	121	GLN
47	SA	9	GLN
47	SA	132	GLN
47	SA	215	GLN
48	SB	92	GLN
49	SD	145	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	SD	174	HIS
50	SE	138	HIS
50	SE	142	HIS
51	SF	31	ASN
51	SF	36	GLN
51	SF	79	HIS
51	SF	83	ASN
51	SF	101	HIS
51	SF	118	ASN
52	SH	12	ASN
52	SH	33	ASN
52	SH	44	ASN
52	SH	164	ASN
53	SI	146	GLN
54	SK	44	HIS
54	SK	66	HIS
55	SL	19	ASN
55	SL	94	HIS
57	SQ	77	HIS
57	SQ	114	GLN
58	SR	62	GLN
58	SR	116	ASN
59	SS	101	ASN
59	SS	125	HIS
61	SU	47	ASN
63	SX	127	ASN
64	Sa	7	ASN
67	Sg	133	ASN
67	Sg	296	GLN
68	SC	115	GLN
68	SC	277	HIS
69	SG	197	GLN
70	SJ	140	GLN
71	SM	46	GLN
71	SM	119	GLN
72	SN	105	ASN
74	SW	24	GLN
75	SY	106	GLN
75	SY	112	ASN
77	Sb	65	GLN
78	Se	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3705/5070 (73%)	721 (19%)	11 (0%)
2	L2	119/120 (99%)	11 (9%)	0
3	L3	155/156 (99%)	31 (20%)	0
46	S2	1715/1869 (91%)	329 (19%)	9 (0%)
All	All	5694/7215 (78%)	1092 (19%)	20 (0%)

All (1092) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	15	A
1	L1	39	A
1	L1	42	A
1	L1	48	G
1	L1	56	A
1	L1	58	G
1	L1	59	A
1	L1	64	A
1	L1	65	A
1	L1	69	A
1	L1	73	A
1	L1	85	G
1	L1	91	G
1	L1	98	A
1	L1	108	A
1	L1	109	G
1	L1	110	C
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	157	U
1	L1	159	C
1	L1	169	G
1	L1	170	C
1	L1	172	C
1	L1	178	C
1	L1	183	C
1	L1	184	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	185	C
1	L1	188	G
1	L1	200	U
1	L1	210	C
1	L1	216	C
1	L1	218	A
1	L1	219	G
1	L1	220	C
1	L1	233	U
1	L1	234	G
1	L1	254	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
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	340	C
1	L1	350	C
1	L1	373	G
1	L1	387	G
1	L1	388	A
1	L1	398	A2M
1	L1	407	A
1	L1	410	A
1	L1	412	G
1	L1	413	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	L1	504	G
1	L1	505	G
1	L1	509	A
1	L1	510	U
1	L1	512	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	667	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	758	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
1	L1	935	A
1	L1	941	C
1	L1	944	A
1	L1	945	U
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	971	U
1	L1	982	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	1220	G
1	L1	1221	G
1	L1	1222	A
1	L1	1241	C
1	L1	1246	G
1	L1	1253	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	1272	C
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1295	C
1	L1	1296	G
1	L1	1301	C
1	L1	1302	U
1	L1	1313	C
1	L1	1326	A2M
1	L1	1337	A
1	L1	1340	OMC
1	L1	1344	C
1	L1	1354	A
1	L1	1358	G
1	L1	1359	G
1	L1	1365	C
1	L1	1367	C
1	L1	1371	A
1	L1	1387	A
1	L1	1394	G
1	L1	1397	A
1	L1	1398	A
1	L1	1404	G
1	L1	1407	C
1	L1	1409	C
1	L1	1410	U
1	L1	1414	C
1	L1	1417	C
1	L1	1420	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	1534	A2M
1	L1	1547	A
1	L1	1549	G
1	L1	1564	A
1	L1	1566	C
1	L1	1578	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1591	U
1	L1	1596	U
1	L1	1624	G
1	L1	1625	OMG
1	L1	1631	A
1	L1	1633	G
1	L1	1634	A
1	L1	1638	A
1	L1	1640	C
1	L1	1642	A
1	L1	1654	G
1	L1	1661	C
1	L1	1670	G
1	L1	1676	C
1	L1	1677	PSU
1	L1	1678	C
1	L1	1681	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	1724	G
1	L1	1726	U
1	L1	1734	G
1	L1	1741	G
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	1764	G
1	L1	1765	A
1	L1	1766	A
1	L1	1767	A
1	L1	1768	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1769	G
1	L1	1770	A
1	L1	1775	A
1	L1	1781	U
1	L1	1787	A
1	L1	1804	A
1	L1	1810	G
1	L1	1820	C
1	L1	1821	G
1	L1	1822	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	1940	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1997	U
1	L1	1998	A
1	L1	2001	G
1	L1	2002	A
1	L1	2011	C
1	L1	2017	A
1	L1	2018	C
1	L1	2026	A
1	L1	2044	U
1	L1	2046	G
1	L1	2048	U
1	L1	2055	G
1	L1	2056	G
1	L1	2069	A
1	L1	2084	C
1	L1	2085	G
1	L1	2092	G
1	L1	2093	A
1	L1	2095	A
1	L1	2097	U
1	L1	2098	G
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	2261	G
1	L1	2289	C
1	L1	2300	A
1	L1	2301	G
1	L1	2313	A
1	L1	2333	G
1	L1	2348	G
1	L1	2351	OMC
1	L1	2360	A
1	L1	2395	A
1	L1	2397	G
1	L1	2417	A
1	L1	2421	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	2422	OMC
1	L1	2424	OMG
1	L1	2425	U
1	L1	2447	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	2494	U
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	2544	G
1	L1	2546	G
1	L1	2547	G
1	L1	2554	U
1	L1	2565	A
1	L1	2573	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2703	G
1	L1	2710	C
1	L1	2711	G
1	L1	2712	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	2803	U
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	2902	G
1	L1	2903	G
1	L1	2906	G
1	L1	2907	G
1	L1	2908	U
1	L1	2909	C
1	L1	3585	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	3601	C
1	L1	3604	A
1	L1	3606	U
1	L1	3615	G
1	L1	3618	C
1	L1	3626	G
1	L1	3635	A
1	L1	3644	U
1	L1	3646	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	3736	A
1	L1	3748	A
1	L1	3750	G
1	L1	3753	G
1	L1	3754	G
1	L1	3760	A
1	L1	3771	C
1	L1	3775	A
1	L1	3776	G
1	L1	3777	G
1	L1	3783	A
1	L1	3784	A
1	L1	3785	A2M
1	L1	3786	U
1	L1	3802	U
1	L1	3808	OMC
1	L1	3811	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	3812	C
1	L1	3814	U
1	L1	3817	A
1	L1	3818	UY1
1	L1	3819	G
1	L1	3838	U
1	L1	3839	G
1	L1	3840	U
1	L1	3841	OMC
1	L1	3867	A2M
1	L1	3877	A
1	L1	3878	C
1	L1	3879	G
1	L1	3897	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	4061	G
1	L1	4062	A
1	L1	4064	C
1	L1	4076	G
1	L1	4086	G
1	L1	4094	G
1	L1	4095	G
1	L1	4096	C
1	L1	4097	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
1	L1	4110	C
1	L1	4111	U
1	L1	4112	C
1	L1	4116	C
1	L1	4117	U
1	L1	4119	C
1	L1	4122	G
1	L1	4127	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	4157	A
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	4225	G
1	L1	4229	U
1	L1	4233	A
1	L1	4251	A
1	L1	4254	G
1	L1	4257	A
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	4305	G
1	L1	4306	OMU
1	L1	4314	C
1	L1	4329	G
1	L1	4330	G
1	L1	4332	C
1	L1	4349	C
1	L1	4364	G
1	L1	4373	G
1	L1	4376	A
1	L1	4377	G
1	L1	4378	A
1	L1	4380	A
1	L1	4387	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	4391	G
1	L1	4394	A
1	L1	4420	U
1	L1	4422	A
1	L1	4437	U
1	L1	4448	G
1	L1	4449	A
1	L1	4452	U
1	L1	4464	A
1	L1	4475	G
1	L1	4500	PSU
1	L1	4512	U
1	L1	4513	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	4573	G
1	L1	4575	G
1	L1	4590	A
1	L1	4636	PSU
1	L1	4637	OMG
1	L1	4656	A
1	L1	4657	U
1	L1	4670	C
1	L1	4672	A
1	L1	4679	G
1	L1	4695	C
1	L1	4700	A
1	L1	4708	A
1	L1	4709	U
1	L1	4719	G
1	L1	4732	G
1	L1	4734	A
1	L1	4740	G
1	L1	4741	C
1	L1	4742	G
1	L1	4745	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	4747	C
1	L1	4750	G
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	4775	C
1	L1	4776	G
1	L1	4859	C
1	L1	4862	G
1	L1	4870	G
1	L1	4871	C
1	L1	4875	G
1	L1	4882	U
1	L1	4883	C
1	L1	4887	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	4928	C
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	4985	U
1	L1	4988	U
1	L1	4989	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	4991	U
1	L1	5007	A
1	L1	5009	G
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	5047	C
1	L1	5050	C
1	L1	5058	A
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	100	A
2	L2	110	G
2	L2	111	C
3	L3	2	G
3	L3	23	C
3	L3	34	U
3	L3	35	C
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	82	A
3	L3	83	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	110	U
3	L3	111	U
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	128	C
3	L3	150	C
46	S2	17	C
46	S2	23	G
46	S2	33	G
46	S2	41	G
46	S2	46	A
46	S2	56	G
46	S2	58	C
46	S2	59	U
46	S2	64	A
46	S2	65	C
46	S2	67	C
46	S2	68	A
46	S2	71	G
46	S2	72	C
46	S2	73	C
46	S2	74	G
46	S2	76	U
46	S2	99	A2M
46	S2	103	A
46	S2	113	G
46	S2	114	G
46	S2	115	U
46	S2	126	G
46	S2	130	G
46	S2	143	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	149	A
46	S2	155	G
46	S2	159	A2M
46	S2	160	U
46	S2	162	C
46	S2	175	A
46	S2	184	G
46	S2	194	C
46	S2	196	C
46	S2	197	U
46	S2	198	U
46	S2	200	G
46	S2	203	G
46	S2	204	G
46	S2	311	C
46	S2	318	A
46	S2	319	C
46	S2	323	C
46	S2	324	C
46	S2	325	C
46	S2	326	C
46	S2	328	U
46	S2	329	G
46	S2	332	G
46	S2	351	G
46	S2	360	A
46	S2	362	C
46	S2	364	A
46	S2	369	C
46	S2	370	G
46	S2	385	G
46	S2	386	C
46	S2	408	A
46	S2	409	C
46	S2	421	G
46	S2	438	G
46	S2	448	A
46	S2	449	A
46	S2	450	C
46	S2	452	G
46	S2	464	A
46	S2	471	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	472	C
46	S2	473	A
46	S2	474	G
46	S2	476	A
46	S2	482	G
46	S2	487	U
46	S2	488	U
46	S2	492	C
46	S2	493	A
46	S2	500	A
46	S2	516	A
46	S2	525	A
46	S2	530	U
46	S2	531	A
46	S2	532	C
46	S2	536	A
46	S2	537	C
46	S2	540	U
46	S2	544	G
46	S2	546	G
46	S2	547	G
46	S2	551	U
46	S2	554	A
46	S2	555	A
46	S2	556	U
46	S2	557	U
46	S2	558	G
46	S2	559	G
46	S2	560	A
46	S2	563	G
46	S2	564	A
46	S2	576	A2M
46	S2	583	A
46	S2	587	A
46	S2	589	G
46	S2	590	A2M
46	S2	591	U
46	S2	594	A
46	S2	597	G
46	S2	598	G
46	S2	604	A
46	S2	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	614	C
46	S2	628	A
46	S2	629	A
46	S2	631	U
46	S2	643	A
46	S2	655	A
46	S2	660	C
46	S2	664	A
46	S2	668	A2M
46	S2	669	A
46	S2	671	A
46	S2	672	A
46	S2	673	G
46	S2	688	U
46	S2	689	U
46	S2	690	G
46	S2	692	G
46	S2	696	G
46	S2	698	G
46	S2	732	U
46	S2	733	C
46	S2	736	C
46	S2	738	C
46	S2	739	C
46	S2	748	C
46	S2	751	G
46	S2	752	G
46	S2	753	C
46	S2	789	G
46	S2	791	C
46	S2	794	A
46	S2	797	C
46	S2	798	G
46	S2	799	U
46	S2	811	A
46	S2	821	G
46	S2	822	PSU
46	S2	823	PSU
46	S2	830	A
46	S2	834	C
46	S2	835	C
46	S2	836	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	837	A
46	S2	838	G
46	S2	839	C
46	S2	840	C
46	S2	841	G
46	S2	842	C
46	S2	847	A
46	S2	867	OMG
46	S2	868	G
46	S2	869	A
46	S2	870	A
46	S2	872	A
46	S2	874	G
46	S2	877	C
46	S2	884	C
46	S2	888	U
46	S2	889	U
46	S2	891	G
46	S2	892	U
46	S2	896	U
46	S2	898	U
46	S2	899	U
46	S2	900	C
46	S2	901	G
46	S2	903	A
46	S2	909	G
46	S2	913	A
46	S2	917	U
46	S2	920	A
46	S2	930	C
46	S2	933	G
46	S2	934	G
46	S2	943	U
46	S2	955	A
46	S2	963	A
46	S2	990	A
46	S2	992	A
46	S2	999	G
46	S2	1001	A
46	S2	1017	U
46	S2	1023	A
46	S2	1027	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	1061	U
46	S2	1062	A
46	S2	1067	C
46	S2	1083	A
46	S2	1085	C
46	S2	1109	C
46	S2	1114	U
46	S2	1116	C
46	S2	1118	C
46	S2	1133	A
46	S2	1138	C
46	S2	1153	C
46	S2	1154	U
46	S2	1195	A
46	S2	1203	G
46	S2	1207	G
46	S2	1208	A
46	S2	1215	C
46	S2	1216	C
46	S2	1217	A
46	S2	1224	G
46	S2	1242	U
46	S2	1243	PSU
46	S2	1248	B8N
46	S2	1251	A
46	S2	1253	A
46	S2	1256	G
46	S2	1257	G
46	S2	1259	A
46	S2	1264	C
46	S2	1274	G
46	S2	1275	G
46	S2	1277	C
46	S2	1283	C
46	S2	1284	A
46	S2	1285	G
46	S2	1286	G
46	S2	1290	G
46	S2	1300	U
46	S2	1301	A
46	S2	1302	G
46	S2	1303	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	1308	U
46	S2	1309	C
46	S2	1342	U
46	S2	1343	U
46	S2	1348	G
46	S2	1371	U
46	S2	1372	U
46	S2	1373	C
46	S2	1378	A
46	S2	1391	OMC
46	S2	1397	U
46	S2	1401	A
46	S2	1402	A
46	S2	1404	U
46	S2	1419	C
46	S2	1421	A
46	S2	1423	C
46	S2	1435	C
46	S2	1436	C
46	S2	1438	A
46	S2	1442	OMU
46	S2	1454	A
46	S2	1462	U
46	S2	1463	U
46	S2	1480	A
46	S2	1487	A
46	S2	1489	A
46	S2	1490	OMG
46	S2	1494	U
46	S2	1495	G
46	S2	1497	G
46	S2	1498	A
46	S2	1506	A
46	S2	1507	G
46	S2	1508	A
46	S2	1510	G
46	S2	1520	G
46	S2	1521	C
46	S2	1522	A
46	S2	1533	A
46	S2	1548	G
46	S2	1552	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	1553	C
46	S2	1556	A
46	S2	1560	U
46	S2	1579	A
46	S2	1580	A
46	S2	1585	U
46	S2	1586	U
46	S2	1587	G
46	S2	1588	A
46	S2	1601	A
46	S2	1621	U
46	S2	1623	A
46	S2	1634	A
46	S2	1648	G
46	S2	1654	G
46	S2	1664	A
46	S2	1665	G
46	S2	1671	G
46	S2	1680	G
46	S2	1686	G
46	S2	1699	A
46	S2	1721	U
46	S2	1722	G
46	S2	1744	G
46	S2	1752	C
46	S2	1753	C
46	S2	1754	G
46	S2	1758	G
46	S2	1760	G
46	S2	1761	U
46	S2	1773	C
46	S2	1774	C
46	S2	1775	U
46	S2	1777	G
46	S2	1783	C
46	S2	1784	G
46	S2	1786	U
46	S2	1819	A
46	S2	1824	A
46	S2	1825	A
46	S2	1829	G
46	S2	1831	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	S2	1835	A
46	S2	1838	U
46	S2	1849	G
46	S2	1851	MA6
46	S2	1852	C
46	S2	1861	G
46	S2	1862	G
46	S2	1863	A
46	S2	1864	U
46	S2	1865	C

All (20) 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	1633	G
1	L1	2760	G
1	L1	3614	G
1	L1	3673	C
1	L1	4678	G
1	L1	4699	U
46	S2	112	U
46	S2	563	G
46	S2	628	A
46	S2	688	U
46	S2	867	OMG
46	S2	954	U
46	S2	1434	C
46	S2	1497	G
46	S2	1520	G

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

143 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
46	A2M	S2	576	46	22,25,26	3.40	9 (40%)	31,36,39	2.68	10 (32%)
1	2MG	L1	1517	1	23,26,27	2.50	9 (39%)	32,38,41	2.31	12 (37%)
46	UY1	S2	1326	46,80	19,22,23	4.34	12 (63%)	22,31,34	1.85	3 (13%)
1	PSU	L1	4628	1	18,21,22	0.99	1 (5%)	22,30,33	1.78	5 (22%)
1	PSU	L1	4636	1	18,21,22	1.10	1 (5%)	22,30,33	1.96	5 (22%)
1	5MC	L1	4447	1,80	18,22,23	3.51	7 (38%)	26,32,35	1.26	2 (7%)
1	B8H	L1	3762	1	19,22,23	6.72	6 (31%)	22,32,35	2.35	5 (22%)
1	1MA	L1	1322	1,80	21,25,26	2.67	6 (28%)	31,37,40	2.31	8 (25%)
1	OMG	L1	1625	1	23,26,27	2.43	7 (30%)	33,38,41	2.06	9 (27%)
46	A2M	S2	512	46	22,25,26	3.41	9 (40%)	31,36,39	2.68	9 (29%)
46	A2M	S2	166	46	22,25,26	3.42	9 (40%)	31,36,39	2.75	9 (29%)
1	OMG	L1	3899	1,80	23,26,27	2.42	9 (39%)	33,38,41	2.13	11 (33%)
46	6MZ	S2	1832	46,80	22,25,26	2.90	3 (13%)	30,36,39	2.38	11 (36%)
1	OMC	L1	3701	1,80	19,22,23	2.87	8 (42%)	26,31,34	0.86	0
46	A2M	S2	668	46,80	22,25,26	3.41	10 (45%)	31,36,39	2.76	10 (32%)
46	A2M	S2	484	46	22,25,26	3.36	9 (40%)	31,36,39	2.70	11 (35%)
1	A2M	L1	2815	1	22,25,26	3.40	8 (36%)	31,36,39	2.68	9 (29%)
1	OMU	L1	4306	1	19,22,23	2.82	6 (31%)	26,31,34	1.71	5 (19%)
46	A2M	S2	1678	46	22,25,26	3.47	9 (40%)	31,36,39	2.72	11 (35%)
1	OMG	L1	3627	1	23,26,27	2.39	8 (34%)	33,38,41	2.08	10 (30%)
1	6MZ	L1	4220	1	22,25,26	2.73	3 (13%)	30,36,39	2.27	11 (36%)
1	OMC	L1	4456	1	19,22,23	2.87	8 (42%)	26,31,34	0.82	1 (3%)
46	OMG	S2	601	46	23,26,27	2.41	8 (34%)	33,38,41	1.96	10 (30%)
46	OMC	S2	1703	46	19,22,23	2.97	8 (42%)	26,31,34	0.72	0
46	OMC	S2	517	46	19,22,23	2.97	8 (42%)	26,31,34	0.80	1 (3%)
1	A2M	L1	3785	1	22,25,26	3.23	9 (40%)	31,36,39	3.05	12 (38%)
1	OMU	L1	4620	1	19,22,23	2.83	7 (36%)	26,31,34	1.70	4 (15%)
1	OMC	L1	1881	1,80	19,22,23	2.93	8 (42%)	26,31,34	0.92	0
46	OMU	S2	428	46	19,22,23	2.88	6 (31%)	26,31,34	1.68	4 (15%)
46	OMC	S2	1272	46	19,22,23	3.06	8 (42%)	26,31,34	0.82	0
43	MLZ	Lo	53	43	8,9,10	0.71	0	4,9,11	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L1	4571	1	22,25,26	3.43	9 (40%)	31,36,39	2.70	9 (29%)
46	B8N	S2	1248	46	24,29,30	3.10	6 (25%)	29,42,45	1.72	6 (20%)
1	OMC	L1	2824	1	19,22,23	2.97	8 (42%)	26,31,34	0.97	2 (7%)
1	OMU	L1	3925	1	19,22,23	2.92	7 (36%)	26,31,34	1.77	4 (15%)
1	OMG	L1	4228	1	23,26,27	2.42	9 (39%)	33,38,41	2.06	10 (30%)
1	A2M	L1	2401	1	22,25,26	3.39	10 (45%)	31,36,39	2.78	10 (32%)
1	OMC	L1	3841	1	19,22,23	2.99	8 (42%)	26,31,34	0.95	1 (3%)
46	OMU	S2	172	46	19,22,23	2.89	6 (31%)	26,31,34	1.76	5 (19%)
1	OMG	L1	4370	1	23,26,27	2.41	9 (39%)	33,38,41	2.04	10 (30%)
1	OMG	L1	2364	1,80	23,26,27	2.39	7 (30%)	33,38,41	2.06	10 (30%)
46	PSU	S2	823	46	18,21,22	1.76	6 (33%)	22,30,33	2.06	4 (18%)
1	A2M	L1	1871	1,80	22,25,26	3.43	9 (40%)	31,36,39	2.79	12 (38%)
1	PSU	L1	4500	1	18,21,22	0.95	1 (5%)	22,30,33	1.76	5 (22%)
46	OMU	S2	121	46	19,22,23	2.86	6 (31%)	26,31,34	1.75	5 (19%)
1	OMG	L1	2424	1	23,26,27	2.42	9 (39%)	33,38,41	1.98	9 (27%)
1	OMC	L1	3887	1	19,22,23	2.93	8 (42%)	26,31,34	0.81	0
1	A2M	L1	3830	1	22,25,26	3.38	9 (40%)	31,36,39	2.65	8 (25%)
1	PSU	L1	1683	1,81	18,21,22	1.11	1 (5%)	22,30,33	1.91	5 (22%)
1	PSU	L1	4442	1	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
46	OMG	S2	509	46	23,26,27	2.36	9 (39%)	33,38,41	2.00	9 (27%)
46	OMG	S2	436	46	23,26,27	2.42	8 (34%)	33,38,41	2.02	9 (27%)
1	OMC	L1	2351	1,80	19,22,23	2.95	8 (42%)	26,31,34	1.16	3 (11%)
1	5MC	L1	4335	1	18,22,23	3.50	7 (38%)	26,32,35	1.06	2 (7%)
1	A2M	L1	1524	1	22,25,26	3.35	10 (45%)	31,36,39	2.74	10 (32%)
1	OMC	L1	3808	1	19,22,23	2.94	8 (42%)	26,31,34	0.98	1 (3%)
46	4AC	S2	1337	46	21,24,25	3.45	10 (47%)	29,34,37	1.06	2 (6%)
1	OMG	L1	4392	1	23,26,27	2.38	8 (34%)	33,38,41	2.05	10 (30%)
1	B8T	L1	4671	1	19,22,23	3.19	8 (42%)	26,31,34	0.91	1 (3%)
1	OMC	L1	2861	1	19,22,23	2.96	8 (42%)	26,31,34	0.75	0
46	OMG	S2	683	46	23,26,27	2.41	8 (34%)	33,38,41	2.06	10 (30%)
1	PSU	L1	4450	1,80	18,21,22	1.03	1 (5%)	22,30,33	1.78	5 (22%)
1	OMG	L1	4637	1	23,26,27	2.37	7 (30%)	33,38,41	1.99	10 (30%)
1	A2M	L1	3718	1	22,25,26	3.42	9 (40%)	31,36,39	2.50	10 (32%)
1	OMG	L1	2876	1	23,26,27	2.45	8 (34%)	33,38,41	2.08	10 (30%)
1	A2M	L1	3825	1	22,25,26	3.42	10 (45%)	31,36,39	2.70	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	4531	1	18,21,22	1.12	1 (5%)	22,30,33	1.79	5 (22%)
1	PSU	L1	3729	1	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
1	OMC	L1	2804	1	19,22,23	2.92	8 (42%)	26,31,34	0.81	0
46	A2M	S2	99	46,80	22,25,26	3.41	9 (40%)	31,36,39	2.63	9 (29%)
46	OMU	S2	1442	46,80	19,22,23	2.91	8 (42%)	26,31,34	1.67	5 (19%)
46	4AC	S2	1842	46	21,24,25	3.32	10 (47%)	29,34,37	1.06	3 (10%)
1	OMG	L1	4618	1	23,26,27	2.41	8 (34%)	33,38,41	2.05	10 (30%)
1	A2M	L1	400	1	22,25,26	3.41	9 (40%)	31,36,39	2.61	9 (29%)
1	A2M	L1	2363	1,80	22,25,26	3.44	10 (45%)	31,36,39	2.59	9 (29%)
1	OMU	L1	4498	1	19,22,23	2.86	6 (31%)	26,31,34	1.77	4 (15%)
46	5MC	S2	1374	46	18,22,23	3.56	7 (38%)	26,32,35	1.05	2 (7%)
46	OMC	S2	1710	46	19,22,23	2.99	8 (42%)	26,31,34	0.88	1 (3%)
46	MA6	S2	1850	46	23,26,27	1.43	4 (17%)	34,38,41	4.09	14 (41%)
46	PSU	S2	119	46	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
1	PSU	L1	2508	1	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
1	5MC	L1	3782	1,80	18,22,23	3.37	7 (38%)	26,32,35	1.10	2 (7%)
46	OMU	S2	116	46	19,22,23	2.86	6 (31%)	26,31,34	1.69	5 (19%)
1	A2M	L1	4523	1,80	22,25,26	3.39	10 (45%)	31,36,39	2.74	10 (32%)
1	A2M	L1	3723	1	22,25,26	3.43	9 (40%)	31,36,39	2.60	8 (25%)
1	OMG	L1	4494	1	23,26,27	2.42	7 (30%)	33,38,41	2.03	9 (27%)
1	UR3	L1	4530	1	19,22,23	2.71	7 (36%)	26,32,35	1.33	3 (11%)
46	JMH	S2	1219	46,80	18,22,23	2.78	5 (27%)	21,32,35	1.60	4 (19%)
46	PSU	S2	1081	46	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
46	OMG	S2	1328	46	23,26,27	2.44	8 (34%)	33,38,41	2.01	10 (30%)
1	OMC	L1	1340	1	19,22,23	2.83	8 (42%)	26,31,34	0.82	0
1	PSU	L1	4293	1	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
3	OMU	L3	14	1,3	19,22,23	2.85	7 (36%)	26,31,34	1.79	4 (15%)
46	A2M	S2	27	46,80	22,25,26	3.43	9 (40%)	31,36,39	2.66	8 (25%)
1	PSU	L1	1677	1,81	18,21,22	1.12	2 (11%)	22,30,33	1.69	4 (18%)
1	OMG	L1	4196	1	23,26,27	2.41	8 (34%)	33,38,41	2.03	10 (30%)
3	OMG	L3	75	3	23,26,27	2.41	8 (34%)	33,38,41	2.07	10 (30%)
46	A2M	S2	468	46	22,25,26	3.43	10 (45%)	31,36,39	2.67	9 (29%)
46	5MU	S2	814	46	19,22,23	7.24	8 (42%)	28,32,35	3.31	12 (42%)
1	A2M	L1	1534	1,80	22,25,26	3.45	10 (45%)	31,36,39	2.75	10 (32%)
46	A2M	S2	1031	46	22,25,26	3.40	9 (40%)	31,36,39	2.62	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	159	46	22,25,26	3.43	9 (40%)	31,36,39	2.70	10 (32%)
46	OMG	S2	1490	46,80	23,26,27	2.40	8 (34%)	33,38,41	1.94	9 (27%)
1	A2M	L1	398	1	22,25,26	3.42	9 (40%)	31,36,39	2.64	10 (32%)
46	M7A	S2	1806	46	20,25,26	1.88	5 (25%)	28,37,40	3.87	8 (28%)
46	A2M	S2	590	46	22,25,26	3.39	9 (40%)	31,36,39	2.83	10 (32%)
46	UR3	S2	1830	46	19,22,23	2.78	7 (36%)	26,32,35	1.54	4 (15%)
1	JMH	L1	1456	1	18,22,23	2.64	5 (27%)	21,32,35	0.89	1 (4%)
46	OMC	S2	174	46,80	19,22,23	2.99	8 (42%)	26,31,34	0.75	0
1	OMC	L1	4536	1	19,22,23	2.84	8 (42%)	26,31,34	0.79	0
46	OMG	S2	644	46	23,26,27	2.40	8 (34%)	33,38,41	1.97	10 (30%)
1	OMG	L1	4623	1	23,26,27	2.39	8 (34%)	33,38,41	2.01	10 (30%)
1	UY1	L1	3818	1,80,81	19,22,23	4.44	12 (63%)	22,31,34	1.92	4 (18%)
46	OMC	S2	462	46	19,22,23	2.99	8 (42%)	26,31,34	0.76	0
1	A2M	L1	1326	1	22,25,26	3.39	9 (40%)	31,36,39	2.68	10 (32%)
46	OMU	S2	354	46	19,22,23	2.82	6 (31%)	26,31,34	1.73	5 (19%)
1	PSU	L1	4403	1	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
1	OMG	L1	3944	1	23,26,27	2.43	8 (34%)	33,38,41	2.04	10 (30%)
46	OMC	S2	1391	46	19,22,23	2.98	8 (42%)	26,31,34	0.90	1 (3%)
46	PSU	S2	1243	46,80	18,21,22	1.07	1 (5%)	22,30,33	1.67	4 (18%)
1	A2M	L1	2787	1	22,25,26	3.36	8 (36%)	31,36,39	2.80	12 (38%)
46	PSU	S2	612	46	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
1	OMG	L1	1316	1,80	23,26,27	2.43	8 (34%)	33,38,41	2.13	11 (33%)
1	OMU	L1	4227	1	19,22,23	2.89	8 (42%)	26,31,34	1.74	4 (15%)
1	A2M	L1	3867	1	22,25,26	3.42	10 (45%)	31,36,39	2.74	11 (35%)
46	OMU	S2	1288	46	19,22,23	2.98	8 (42%)	26,31,34	1.69	5 (19%)
46	MA6	S2	1851	46	23,26,27	1.32	4 (17%)	34,38,41	4.37	13 (38%)
1	OMG	L1	4499	1	23,26,27	2.42	8 (34%)	33,38,41	2.01	10 (30%)
46	A2M	S2	1383	46	22,25,26	3.40	9 (40%)	31,36,39	2.72	10 (32%)
1	OMC	L1	2365	1,80	19,22,23	2.85	8 (42%)	26,31,34	0.70	0
1	OMG	L1	3744	1	23,26,27	2.45	8 (34%)	33,38,41	2.02	10 (30%)
1	PSU	L1	3715	1	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
1	OMU	L1	2837	1	19,22,23	2.84	6 (31%)	26,31,34	1.74	6 (23%)
46	OMG	S2	867	46	23,26,27	2.44	8 (34%)	33,38,41	2.05	9 (27%)
1	OMC	L1	3869	1	19,22,23	2.96	8 (42%)	26,31,34	0.94	1 (3%)
1	OMG	L1	1522	1	23,26,27	2.40	8 (34%)	33,38,41	2.19	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	3764	1	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
1	2MG	L1	978	1	23,26,27	2.63	9 (39%)	32,38,41	2.31	12 (37%)
1	OMC	L1	2422	1,80	19,22,23	2.89	8 (42%)	26,31,34	0.77	1 (3%)
1	OMG	L1	3792	1	23,26,27	2.39	7 (30%)	33,38,41	1.97	10 (30%)
1	PSU	L1	1582	1	18,21,22	1.07	1 (5%)	22,30,33	1.59	4 (18%)
46	PSU	S2	822	46	18,21,22	1.06	1 (5%)	22,30,33	1.82	5 (22%)
1	2MG	L1	729	1	23,26,27	2.59	9 (39%)	32,38,41	2.29	10 (31%)

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
46	A2M	S2	576	46	-	2/9/27/28	0/3/3/3
1	2MG	L1	1517	1	-	0/9/27/28	0/3/3/3
46	UY1	S2	1326	46,80	-	2/9/27/28	0/2/2/2
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4636	1	-	3/7/25/26	0/2/2/2
1	5MC	L1	4447	1,80	-	4/7/25/26	0/2/2/2
1	B8H	L1	3762	1	-	0/7/25/26	0/2/2/2
1	1MA	L1	1322	1,80	-	0/7/25/26	0/3/3/3
1	OMG	L1	1625	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	512	46	-	2/9/27/28	0/3/3/3
46	A2M	S2	166	46	-	0/9/27/28	0/3/3/3
1	OMG	L1	3899	1,80	-	0/9/27/28	0/3/3/3
46	6MZ	S2	1832	46,80	-	0/9/27/28	0/3/3/3
1	OMC	L1	3701	1,80	-	4/9/27/28	0/2/2/2
46	A2M	S2	668	46,80	-	3/9/27/28	0/3/3/3
46	A2M	S2	484	46	-	0/9/27/28	0/3/3/3
1	A2M	L1	2815	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
46	A2M	S2	1678	46	-	1/9/27/28	0/3/3/3
1	OMG	L1	3627	1	-	0/9/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	601	46	-	1/9/27/28	0/3/3/3
46	OMC	S2	1703	46	-	0/9/27/28	0/2/2/2
46	OMC	S2	517	46	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	L1	3785	1	-	2/9/27/28	0/3/3/3
1	OMU	L1	4620	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	1881	1,80	-	0/9/27/28	0/2/2/2
46	OMU	S2	428	46	-	5/9/27/28	0/2/2/2
46	OMC	S2	1272	46	-	0/9/27/28	0/2/2/2
43	MLZ	Lo	53	43	-	3/7/8/10	-
1	A2M	L1	4571	1	-	0/9/27/28	0/3/3/3
46	B8N	S2	1248	46	-	2/16/34/35	0/2/2/2
1	OMC	L1	2824	1	-	1/9/27/28	0/2/2/2
1	OMU	L1	3925	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	4228	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	2401	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	3841	1	-	2/9/27/28	0/2/2/2
46	OMU	S2	172	46	-	0/9/27/28	0/2/2/2
1	OMG	L1	4370	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	2364	1,80	-	2/9/27/28	0/3/3/3
46	PSU	S2	823	46	-	2/7/25/26	0/2/2/2
1	A2M	L1	1871	1,80	-	0/9/27/28	0/3/3/3
1	PSU	L1	4500	1	-	3/7/25/26	0/2/2/2
46	OMU	S2	121	46	-	0/9/27/28	0/2/2/2
1	OMG	L1	2424	1	-	2/9/27/28	0/3/3/3
1	OMC	L1	3887	1	-	1/9/27/28	0/2/2/2
1	A2M	L1	3830	1	-	0/9/27/28	0/3/3/3
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
46	OMG	S2	509	46	-	0/9/27/28	0/3/3/3
46	OMG	S2	436	46	-	0/9/27/28	0/3/3/3
1	OMC	L1	2351	1,80	-	2/9/27/28	0/2/2/2
1	5MC	L1	4335	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1524	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	3808	1	-	2/9/27/28	0/2/2/2
46	4AC	S2	1337	46	-	0/11/29/30	0/2/2/2
1	OMG	L1	4392	1	-	0/9/27/28	0/3/3/3
1	B8T	L1	4671	1	-	0/7/27/28	0/2/2/2
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	683	46	-	1/9/27/28	0/3/3/3
1	PSU	L1	4450	1,80	-	2/7/25/26	0/2/2/2
1	OMG	L1	4637	1	-	1/9/27/28	0/3/3/3
1	A2M	L1	3718	1	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	2876	1	-	1/9/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4531	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3729	1	-	2/7/25/26	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
46	A2M	S2	99	46,80	-	2/9/27/28	0/3/3/3
46	OMU	S2	1442	46,80	-	3/9/27/28	0/2/2/2
46	4AC	S2	1842	46	-	0/11/29/30	0/2/2/2
1	OMG	L1	4618	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	400	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	2363	1,80	-	2/9/27/28	0/3/3/3
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
46	5MC	S2	1374	46	-	0/7/25/26	0/2/2/2
46	OMC	S2	1710	46	-	0/9/27/28	0/2/2/2
46	MA6	S2	1850	46	-	0/11/29/30	0/3/3/3
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
1	5MC	L1	3782	1,80	-	0/7/25/26	0/2/2/2
46	OMU	S2	116	46	-	1/9/27/28	0/2/2/2
1	A2M	L1	4523	1,80	-	0/9/27/28	0/3/3/3
1	A2M	L1	3723	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	4494	1	-	0/9/27/28	0/3/3/3
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
46	JMH	S2	1219	46,80	-	1/7/25/26	0/2/2/2
46	PSU	S2	1081	46	-	1/7/25/26	0/2/2/2
46	OMG	S2	1328	46	-	1/9/27/28	0/3/3/3
1	OMC	L1	1340	1	-	2/9/27/28	0/2/2/2
1	PSU	L1	4293	1	-	0/7/25/26	0/2/2/2
3	OMU	L3	14	1,3	-	1/9/27/28	0/2/2/2
46	A2M	S2	27	46,80	-	0/9/27/28	0/3/3/3
1	PSU	L1	1677	1,81	-	3/7/25/26	0/2/2/2
1	OMG	L1	4196	1	-	1/9/27/28	0/3/3/3
3	OMG	L3	75	3	-	1/9/27/28	0/3/3/3
46	A2M	S2	468	46	-	0/9/27/28	0/3/3/3
46	5MU	S2	814	46	-	0/7/25/26	0/2/2/2
1	A2M	L1	1534	1,80	-	3/9/27/28	0/3/3/3
46	A2M	S2	1031	46	-	0/9/27/28	0/3/3/3
46	A2M	S2	159	46	-	2/9/27/28	0/3/3/3
46	OMG	S2	1490	46,80	-	1/9/27/28	0/3/3/3
1	A2M	L1	398	1	-	2/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	M7A	S2	1806	46	-	0/7/37/38	0/3/3/3
46	A2M	S2	590	46	-	4/9/27/28	0/3/3/3
46	UR3	S2	1830	46	-	2/7/25/26	0/2/2/2
1	JMH	L1	1456	1	-	0/7/25/26	0/2/2/2
46	OMC	S2	174	46,80	-	0/9/27/28	0/2/2/2
1	OMC	L1	4536	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	644	46	-	1/9/27/28	0/3/3/3
1	OMG	L1	4623	1	-	0/9/27/28	0/3/3/3
1	UY1	L1	3818	1,80,81	-	6/9/27/28	0/2/2/2
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
1	A2M	L1	1326	1	-	1/9/27/28	0/3/3/3
46	OMU	S2	354	46	-	0/9/27/28	0/2/2/2
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	3944	1	-	2/9/27/28	0/3/3/3
46	OMC	S2	1391	46	-	2/9/27/28	0/2/2/2
46	PSU	S2	1243	46,80	-	2/7/25/26	0/2/2/2
1	A2M	L1	2787	1	-	5/9/27/28	0/3/3/3
46	PSU	S2	612	46	-	0/7/25/26	0/2/2/2
1	OMG	L1	1316	1,80	-	0/9/27/28	0/3/3/3
1	OMU	L1	4227	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	3867	1	-	2/9/27/28	0/3/3/3
46	OMU	S2	1288	46	-	1/9/27/28	0/2/2/2
46	MA6	S2	1851	46	-	2/11/29/30	0/3/3/3
1	OMG	L1	4499	1	-	2/9/27/28	0/3/3/3
46	A2M	S2	1383	46	-	0/9/27/28	0/3/3/3
1	OMC	L1	2365	1,80	-	0/9/27/28	0/2/2/2
1	OMG	L1	3744	1	-	1/9/27/28	0/3/3/3
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	867	46	-	3/9/27/28	0/3/3/3
1	OMC	L1	3869	1	-	1/9/27/28	0/2/2/2
1	OMG	L1	1522	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	3764	1	-	2/7/25/26	0/2/2/2
1	2MG	L1	978	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	2422	1,80	-	1/9/27/28	0/2/2/2
1	OMG	L1	3792	1	-	3/9/27/28	0/3/3/3
1	PSU	L1	1582	1	-	1/7/25/26	0/2/2/2
46	PSU	S2	822	46	-	1/7/25/26	0/2/2/2
1	2MG	L1	729	1	-	1/9/27/28	0/3/3/3

All (990) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	814	5MU	C4-C5	20.67	1.79	1.44
46	S2	814	5MU	C6-N1	16.38	1.66	1.38
1	L1	3762	B8H	C6-C5	-15.56	1.13	1.34
1	L1	3762	B8H	C4-N3	-14.87	1.11	1.38
1	L1	3762	B8H	C4-C5	14.06	1.84	1.44
46	S2	1832	6MZ	C6-N6	12.70	1.47	1.34
1	L1	3762	B8H	C6-N1	12.59	1.67	1.36
1	L1	4220	6MZ	C6-N6	11.61	1.46	1.34
1	L1	3818	UY1	O4'-C1'	-11.54	1.28	1.43
46	S2	1326	UY1	O4'-C1'	-11.21	1.28	1.43
46	S2	814	5MU	C4-N3	-11.12	1.18	1.38
46	S2	814	5MU	C6-C5	-10.71	1.17	1.34
1	L1	4447	5MC	C6-C5	9.30	1.49	1.34
46	S2	1374	5MC	C6-C5	9.07	1.49	1.34
1	L1	4335	5MC	C6-C5	8.88	1.49	1.34
1	L1	1871	A2M	C2'-C1'	-8.85	1.30	1.53
1	L1	3782	5MC	C6-C5	8.80	1.49	1.34
46	S2	27	A2M	C2'-C1'	-8.79	1.30	1.53
46	S2	166	A2M	O4'-C1'	8.74	1.62	1.42
46	S2	1383	A2M	O4'-C1'	8.73	1.62	1.42
1	L1	2363	A2M	C2'-C1'	-8.72	1.30	1.53
46	S2	1678	A2M	C2'-C1'	-8.70	1.30	1.53
1	L1	1534	A2M	O4'-C1'	8.68	1.62	1.42
1	L1	4571	A2M	O4'-C1'	8.66	1.62	1.42
1	L1	3723	A2M	O4'-C1'	8.64	1.62	1.42
1	L1	398	A2M	C2'-C1'	-8.63	1.30	1.53
1	L1	1326	A2M	C2'-C1'	-8.62	1.30	1.53
46	S2	468	A2M	C2'-C1'	-8.62	1.30	1.53
1	L1	3718	A2M	C2'-C1'	-8.59	1.31	1.53
46	S2	1031	A2M	C2'-C1'	-8.58	1.31	1.53
1	L1	1871	A2M	O4'-C1'	8.58	1.62	1.42
1	L1	398	A2M	O4'-C1'	8.58	1.62	1.42
1	L1	2815	A2M	O4'-C1'	8.58	1.62	1.42
46	S2	99	A2M	O4'-C1'	8.58	1.62	1.42
46	S2	468	A2M	O4'-C1'	8.58	1.62	1.42
1	L1	3867	A2M	C2'-C1'	-8.58	1.31	1.53
46	S2	1678	A2M	O4'-C1'	8.58	1.62	1.42
46	S2	166	A2M	C2'-C1'	-8.58	1.31	1.53
1	L1	4523	A2M	O4'-C1'	8.57	1.62	1.42
46	S2	159	A2M	C2'-C1'	-8.57	1.31	1.53
46	S2	159	A2M	O4'-C1'	8.56	1.62	1.42
1	L1	3723	A2M	C2'-C1'	-8.56	1.31	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	99	A2M	C2'-C1'	-8.55	1.31	1.53
46	S2	576	A2M	O4'-C1'	8.55	1.62	1.42
1	L1	400	A2M	C2'-C1'	-8.55	1.31	1.53
1	L1	2401	A2M	C2'-C1'	-8.55	1.31	1.53
1	L1	3718	A2M	O4'-C1'	8.55	1.62	1.42
1	L1	1534	A2M	C2'-C1'	-8.54	1.31	1.53
46	S2	590	A2M	O4'-C1'	8.54	1.62	1.42
1	L1	3825	A2M	O4'-C1'	8.53	1.62	1.42
46	S2	512	A2M	C2'-C1'	-8.53	1.31	1.53
46	S2	512	A2M	O4'-C1'	8.53	1.62	1.42
1	L1	400	A2M	O4'-C1'	8.52	1.62	1.42
46	S2	27	A2M	O4'-C1'	8.51	1.62	1.42
1	L1	4571	A2M	C2'-C1'	-8.50	1.31	1.53
1	L1	3825	A2M	C2'-C1'	-8.50	1.31	1.53
1	L1	2401	A2M	O4'-C1'	8.49	1.62	1.42
46	S2	576	A2M	C2'-C1'	-8.48	1.31	1.53
1	L1	3830	A2M	O4'-C1'	8.48	1.62	1.42
46	S2	484	A2M	O4'-C1'	8.47	1.62	1.42
1	L1	2363	A2M	O4'-C1'	8.47	1.62	1.42
1	L1	2815	A2M	C2'-C1'	-8.47	1.31	1.53
46	S2	1031	A2M	O4'-C1'	8.46	1.62	1.42
1	L1	2787	A2M	O4'-C1'	8.45	1.62	1.42
1	L1	3830	A2M	C2'-C1'	-8.44	1.31	1.53
1	L1	4523	A2M	C2'-C1'	-8.40	1.31	1.53
46	S2	1383	A2M	C2'-C1'	-8.39	1.31	1.53
1	L1	1326	A2M	O4'-C1'	8.38	1.61	1.42
46	S2	590	A2M	C2'-C1'	-8.34	1.31	1.53
46	S2	668	A2M	C2'-C1'	-8.32	1.31	1.53
1	L1	3867	A2M	O4'-C1'	8.27	1.61	1.42
46	S2	484	A2M	C2'-C1'	-8.26	1.31	1.53
1	L1	3785	A2M	C2'-C1'	-8.26	1.31	1.53
1	L1	2787	A2M	C2'-C1'	-8.24	1.31	1.53
46	S2	668	A2M	O4'-C1'	8.16	1.61	1.42
1	L1	1524	A2M	C2'-C1'	-8.11	1.32	1.53
1	L1	1524	A2M	O4'-C1'	8.11	1.61	1.42
46	S2	1219	JMH	C2-N1	8.01	1.50	1.38
1	L1	3785	A2M	O4'-C1'	7.82	1.60	1.42
46	S2	1248	B8N	C6-N1	7.80	1.55	1.36
46	S2	1288	OMU	C2-N1	7.44	1.50	1.38
46	S2	1830	UR3	C2-N1	7.43	1.49	1.38
1	L1	729	2MG	C2-N3	7.41	1.46	1.31
46	S2	1248	B8N	C4-N3	-7.38	1.26	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	978	2MG	C2-N3	7.29	1.45	1.31
1	L1	3925	OMU	C2-N1	7.25	1.50	1.38
1	L1	1322	1MA	C2-N3	7.23	1.44	1.30
1	L1	4671	B8T	C4-N3	7.18	1.45	1.32
1	L1	3818	UY1	C3'-C4'	-7.13	1.34	1.53
1	L1	4498	OMU	C2-N1	7.13	1.49	1.38
3	L3	14	OMU	C2-N1	7.11	1.49	1.38
1	L1	4227	OMU	C2-N1	7.03	1.49	1.38
46	S2	1326	UY1	C3'-C4'	-7.03	1.35	1.53
46	S2	1442	OMU	C2-N1	6.97	1.49	1.38
46	S2	172	OMU	C2-N1	6.95	1.49	1.38
1	L1	1456	JMH	C2-N1	6.95	1.48	1.38
46	S2	1337	4AC	C4-N3	6.92	1.44	1.32
1	L1	2837	OMU	C2-N1	6.91	1.49	1.38
1	L1	4530	UR3	C2-N1	6.88	1.48	1.38
46	S2	116	OMU	C2-N1	6.86	1.49	1.38
1	L1	1524	A2M	O4'-C4'	-6.86	1.29	1.45
46	S2	428	OMU	C2-N1	6.83	1.49	1.38
46	S2	121	OMU	C2-N1	6.82	1.49	1.38
46	S2	668	A2M	O4'-C4'	-6.82	1.29	1.45
46	S2	1248	B8N	C6-C5	6.68	1.44	1.34
46	S2	354	OMU	C2-N1	6.67	1.49	1.38
1	L1	4306	OMU	C2-N1	6.66	1.49	1.38
1	L1	1517	2MG	C2-N3	6.66	1.44	1.31
46	S2	1288	OMU	C2-N3	6.65	1.49	1.38
1	L1	4620	OMU	C2-N1	6.64	1.49	1.38
46	S2	1842	4AC	C4-N3	6.64	1.44	1.32
1	L1	1534	A2M	O4'-C4'	-6.60	1.30	1.45
1	L1	1322	1MA	C4-N3	6.59	1.49	1.35
46	S2	1442	OMU	C2-N3	6.58	1.49	1.38
1	L1	3867	A2M	O4'-C4'	-6.58	1.30	1.45
46	S2	172	OMU	C2-N3	6.57	1.49	1.38
46	S2	590	A2M	O4'-C4'	-6.57	1.30	1.45
1	L1	3744	OMG	C4-N3	6.55	1.49	1.34
46	S2	1678	A2M	O4'-C4'	-6.51	1.30	1.45
46	S2	116	OMU	C2-N3	6.50	1.49	1.38
46	S2	428	OMU	C2-N3	6.49	1.49	1.38
46	S2	1272	OMC	C2-N3	6.48	1.49	1.36
46	S2	1248	B8N	C2-N1	6.48	1.58	1.39
46	S2	121	OMU	C2-N3	6.46	1.49	1.38
46	S2	1374	5MC	C4-N3	6.45	1.45	1.34
46	S2	436	OMG	C4-N3	6.44	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4618	OMG	C4-N3	6.42	1.49	1.34
1	L1	2876	OMG	C4-N3	6.40	1.49	1.34
1	L1	4370	OMG	C4-N3	6.39	1.49	1.34
1	L1	3944	OMG	C4-N3	6.39	1.49	1.34
1	L1	3792	OMG	C4-N3	6.39	1.49	1.34
1	L1	400	A2M	O4'-C4'	-6.38	1.30	1.45
46	S2	1490	OMG	C4-N3	6.38	1.49	1.34
46	S2	468	A2M	O4'-C4'	-6.38	1.30	1.45
1	L1	4571	A2M	O4'-C4'	-6.38	1.30	1.45
46	S2	867	OMG	C4-N3	6.38	1.49	1.34
46	S2	683	OMG	C4-N3	6.38	1.49	1.34
46	S2	159	A2M	O4'-C4'	-6.38	1.30	1.45
46	S2	1328	OMG	C4-N3	6.38	1.49	1.34
1	L1	1522	OMG	C4-N3	6.36	1.49	1.34
1	L1	4523	A2M	O4'-C4'	-6.36	1.30	1.45
1	L1	4228	OMG	C4-N3	6.35	1.49	1.34
3	L3	75	OMG	C4-N3	6.35	1.49	1.34
46	S2	1710	OMC	C2-N3	6.35	1.49	1.36
46	S2	27	A2M	O4'-C4'	-6.34	1.30	1.45
46	S2	601	OMG	C4-N3	6.34	1.49	1.34
1	L1	2815	A2M	O4'-C4'	-6.33	1.30	1.45
1	L1	1625	OMG	C4-N3	6.33	1.49	1.34
1	L1	4498	OMU	C2-N3	6.32	1.49	1.38
46	S2	1337	4AC	C6-C5	6.32	1.49	1.35
1	L1	4494	OMG	C4-N3	6.32	1.49	1.34
1	L1	2363	A2M	O4'-C4'	-6.31	1.30	1.45
1	L1	1316	OMG	C4-N3	6.31	1.49	1.34
1	L1	398	A2M	O4'-C4'	-6.31	1.30	1.45
1	L1	3723	A2M	O4'-C4'	-6.31	1.30	1.45
46	S2	462	OMC	C2-N3	6.30	1.49	1.36
46	S2	1326	UY1	O4'-C4'	6.29	1.59	1.45
46	S2	512	A2M	O4'-C4'	-6.27	1.31	1.45
46	S2	1391	OMC	C2-N3	6.26	1.49	1.36
1	L1	2861	OMC	C2-N3	6.26	1.49	1.36
46	S2	576	A2M	O4'-C4'	-6.26	1.31	1.45
46	S2	517	OMC	C2-N3	6.25	1.49	1.36
46	S2	174	OMC	C2-N3	6.25	1.49	1.36
1	L1	4335	5MC	C4-N3	6.25	1.44	1.34
1	L1	4227	OMU	C2-N3	6.25	1.49	1.38
46	S2	484	A2M	O4'-C4'	-6.25	1.31	1.45
1	L1	3899	OMG	C4-N3	6.24	1.49	1.34
1	L1	2424	OMG	C4-N3	6.24	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	99	A2M	O4'-C4'	-6.23	1.31	1.45
1	L1	3925	OMU	C2-N3	6.23	1.49	1.38
1	L1	4306	OMU	C2-N3	6.23	1.49	1.38
46	S2	1703	OMC	C2-N3	6.23	1.49	1.36
1	L1	4499	OMG	C4-N3	6.22	1.49	1.34
1	L1	3825	A2M	O4'-C4'	-6.22	1.31	1.45
1	L1	4620	OMU	C2-N3	6.21	1.49	1.38
1	L1	2364	OMG	C4-N3	6.21	1.49	1.34
46	S2	166	A2M	O4'-C4'	-6.21	1.31	1.45
46	S2	644	OMG	C4-N3	6.20	1.49	1.34
46	S2	354	OMU	C2-N3	6.19	1.49	1.38
1	L1	4392	OMG	C4-N3	6.19	1.49	1.34
1	L1	3830	A2M	O4'-C4'	-6.18	1.31	1.45
46	S2	1031	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	3627	OMG	C4-N3	6.17	1.48	1.34
1	L1	4196	OMG	C4-N3	6.17	1.48	1.34
1	L1	2837	OMU	C2-N3	6.16	1.48	1.38
46	S2	1383	A2M	O4'-C4'	-6.16	1.31	1.45
1	L1	1326	A2M	O4'-C4'	-6.15	1.31	1.45
1	L1	4335	5MC	C2-N3	6.13	1.48	1.36
1	L1	4637	OMG	C4-N3	6.13	1.48	1.34
1	L1	3818	UY1	O4'-C4'	6.12	1.58	1.45
1	L1	2401	A2M	O4'-C4'	-6.11	1.31	1.45
1	L1	3718	A2M	O4'-C4'	-6.11	1.31	1.45
1	L1	2824	OMC	C2-N3	6.11	1.48	1.36
1	L1	3701	OMC	C6-C5	6.11	1.49	1.35
1	L1	2787	A2M	O4'-C4'	-6.10	1.31	1.45
46	S2	509	OMG	C4-N3	6.10	1.48	1.34
3	L3	14	OMU	C2-N3	6.09	1.48	1.38
1	L1	4623	OMG	C4-N3	6.09	1.48	1.34
1	L1	2351	OMC	C6-C5	6.08	1.49	1.35
1	L1	3841	OMC	C2-N3	6.08	1.48	1.36
46	S2	1337	4AC	C2-N3	6.07	1.48	1.36
1	L1	2804	OMC	C2-N3	6.06	1.48	1.36
46	S2	1830	UR3	C6-C5	6.04	1.49	1.35
46	S2	1842	4AC	C6-C5	6.04	1.49	1.35
1	L1	1881	OMC	C2-N3	6.03	1.48	1.36
46	S2	1374	5MC	C2-N3	6.03	1.48	1.36
1	L1	3869	OMC	C6-C5	6.03	1.49	1.35
1	L1	2422	OMC	C6-C5	6.01	1.49	1.35
46	S2	462	OMC	C6-C5	6.01	1.49	1.35
46	S2	1272	OMC	C6-C5	5.98	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3808	OMC	C6-C5	5.97	1.48	1.35
46	S2	174	OMC	C6-C5	5.97	1.48	1.35
1	L1	3808	OMC	C2-N3	5.96	1.48	1.36
1	L1	1340	OMC	C2-N3	5.95	1.48	1.36
1	L1	1871	A2M	O4'-C4'	-5.95	1.31	1.45
46	S2	517	OMC	C6-C5	5.95	1.48	1.35
1	L1	4447	5MC	C4-N3	5.95	1.44	1.34
46	S2	1710	OMC	C6-C5	5.94	1.48	1.35
46	S2	1391	OMC	C6-C5	5.91	1.48	1.35
1	L1	2861	OMC	C6-C5	5.91	1.48	1.35
1	L1	4671	B8T	C6-C5	5.91	1.48	1.35
1	L1	2351	OMC	C2-N3	5.90	1.48	1.36
1	L1	3887	OMC	C6-C5	5.90	1.48	1.35
1	L1	3869	OMC	C2-N3	5.90	1.48	1.36
1	L1	3785	A2M	O4'-C4'	-5.90	1.31	1.45
1	L1	4530	UR3	C6-C5	5.90	1.48	1.35
1	L1	3841	OMC	C6-C5	5.89	1.48	1.35
1	L1	3887	OMC	C2-N3	5.88	1.48	1.36
46	S2	1703	OMC	C6-C5	5.88	1.48	1.35
1	L1	1456	JMH	C6-C5	5.87	1.48	1.35
1	L1	4456	OMC	C6-C5	5.87	1.48	1.35
1	L1	3782	5MC	C4-N3	5.86	1.44	1.34
1	L1	2804	OMC	C6-C5	5.85	1.48	1.35
1	L1	2365	OMC	C6-C5	5.84	1.48	1.35
1	L1	4536	OMC	C6-C5	5.83	1.48	1.35
46	S2	1288	OMU	C6-C5	5.81	1.48	1.35
1	L1	2422	OMC	C2-N3	5.81	1.48	1.36
1	L1	4447	5MC	C2-N3	5.79	1.48	1.36
46	S2	172	OMU	C6-C5	5.79	1.48	1.35
46	S2	1442	OMU	C6-C5	5.79	1.48	1.35
1	L1	4536	OMC	C2-N3	5.79	1.48	1.36
1	L1	3701	OMC	C2-N3	5.77	1.48	1.36
1	L1	1881	OMC	C6-C5	5.77	1.48	1.35
1	L1	3925	OMU	C6-C5	5.77	1.48	1.35
46	S2	428	OMU	C6-C5	5.76	1.48	1.35
1	L1	1340	OMC	C6-C5	5.75	1.48	1.35
1	L1	3782	5MC	C2-N3	5.74	1.48	1.36
46	S2	1842	4AC	C2-N3	5.74	1.48	1.36
1	L1	2837	OMU	C6-C5	5.74	1.48	1.35
46	S2	354	OMU	C6-C5	5.74	1.48	1.35
1	L1	4456	OMC	C2-N3	5.74	1.48	1.36
46	S2	1219	JMH	C6-C5	5.74	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2824	OMC	C6-C5	5.73	1.48	1.35
46	S2	1337	4AC	C7-N4	5.71	1.47	1.37
1	L1	4227	OMU	C6-C5	5.71	1.48	1.35
1	L1	4620	OMU	C6-C5	5.70	1.48	1.35
46	S2	121	OMU	C6-C5	5.69	1.48	1.35
1	L1	2365	OMC	C2-N3	5.67	1.47	1.36
1	L1	4306	OMU	C6-C5	5.66	1.48	1.35
3	L3	14	OMU	C6-C5	5.65	1.48	1.35
46	S2	116	OMU	C6-C5	5.60	1.48	1.35
1	L1	4671	B8T	C2-N3	5.59	1.47	1.36
46	S2	1337	4AC	C4-N4	5.58	1.47	1.39
1	L1	4499	OMG	C2-N3	5.56	1.46	1.33
46	S2	1328	OMG	C2-N3	5.54	1.46	1.33
1	L1	2876	OMG	C2-N3	5.52	1.46	1.33
1	L1	4498	OMU	C6-C5	5.51	1.47	1.35
1	L1	1625	OMG	C2-N3	5.50	1.46	1.33
1	L1	4637	OMG	C2-N3	5.50	1.46	1.33
1	L1	4494	OMG	C2-N3	5.49	1.46	1.33
46	S2	867	OMG	C2-N3	5.47	1.46	1.33
1	L1	3744	OMG	C2-N3	5.45	1.46	1.33
1	L1	3818	UY1	O2-C2	-5.44	1.12	1.23
1	L1	3944	OMG	C2-N3	5.43	1.46	1.33
46	S2	601	OMG	C2-N3	5.42	1.46	1.33
1	L1	3818	UY1	O4-C4	-5.42	1.13	1.23
1	L1	4228	OMG	C2-N3	5.41	1.46	1.33
1	L1	1522	OMG	C2-N3	5.39	1.46	1.33
1	L1	4370	OMG	C2-N3	5.39	1.46	1.33
1	L1	3792	OMG	C2-N3	5.38	1.46	1.33
1	L1	4196	OMG	C2-N3	5.37	1.46	1.33
46	S2	644	OMG	C2-N3	5.36	1.46	1.33
46	S2	1490	OMG	C2-N3	5.36	1.46	1.33
46	S2	1842	4AC	C7-N4	5.35	1.47	1.37
1	L1	2364	OMG	C2-N3	5.35	1.46	1.33
46	S2	436	OMG	C2-N3	5.35	1.46	1.33
1	L1	4392	OMG	C2-N3	5.35	1.46	1.33
46	S2	1326	UY1	O4-C4	-5.34	1.13	1.23
46	S2	509	OMG	C2-N3	5.34	1.46	1.33
46	S2	683	OMG	C2-N3	5.33	1.46	1.33
1	L1	4618	OMG	C2-N3	5.33	1.46	1.33
3	L3	75	OMG	C2-N3	5.31	1.46	1.33
1	L1	1316	OMG	C2-N3	5.31	1.46	1.33
1	L1	2424	OMG	C2-N3	5.30	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3899	OMG	C2-N3	5.26	1.45	1.33
1	L1	3627	OMG	C2-N3	5.23	1.45	1.33
46	S2	1272	OMC	C4-N3	5.22	1.45	1.34
1	L1	4623	OMG	C2-N3	5.18	1.45	1.33
46	S2	814	5MU	C2-N3	5.17	1.47	1.38
1	L1	978	2MG	C2-N2	5.17	1.44	1.33
1	L1	729	2MG	C4-N3	5.17	1.46	1.34
46	S2	1842	4AC	C4-N4	5.14	1.47	1.39
46	S2	1703	OMC	C4-N3	5.12	1.44	1.34
1	L1	4530	UR3	C2-N3	5.12	1.48	1.39
46	S2	174	OMC	C4-N3	5.06	1.44	1.34
46	S2	462	OMC	C4-N3	5.03	1.44	1.34
1	L1	978	2MG	C4-N3	4.98	1.46	1.34
1	L1	2824	OMC	C4-N3	4.97	1.44	1.34
1	L1	729	2MG	C2-N2	4.95	1.44	1.33
46	S2	1272	OMC	C4-N4	4.95	1.45	1.33
46	S2	1710	OMC	C4-N3	4.94	1.44	1.34
46	S2	517	OMC	C4-N3	4.94	1.44	1.34
46	S2	1326	UY1	O2-C2	-4.93	1.13	1.23
1	L1	1517	2MG	C2-N2	4.93	1.44	1.33
1	L1	1340	OMC	C4-N3	4.91	1.44	1.34
46	S2	1391	OMC	C4-N3	4.90	1.44	1.34
46	S2	462	OMC	C4-N4	4.88	1.45	1.33
46	S2	1391	OMC	C4-N4	4.88	1.45	1.33
46	S2	174	OMC	C4-N4	4.87	1.45	1.33
1	L1	2861	OMC	C4-N3	4.87	1.44	1.34
1	L1	3841	OMC	C4-N3	4.86	1.44	1.34
1	L1	1517	2MG	C4-N3	4.85	1.45	1.34
1	L1	3762	B8H	C2-N3	4.85	1.46	1.38
46	S2	1219	JMH	C2-N3	4.85	1.48	1.39
46	S2	1326	UY1	C1'-C5	4.84	1.61	1.50
1	L1	2351	OMC	C4-N4	4.83	1.45	1.33
46	S2	1710	OMC	C4-N4	4.83	1.45	1.33
1	L1	1881	OMC	C4-N3	4.81	1.44	1.34
1	L1	3869	OMC	C4-N3	4.81	1.44	1.34
46	S2	867	OMG	C2-N2	4.81	1.45	1.34
46	S2	1830	UR3	C2-N3	4.80	1.48	1.39
1	L1	2424	OMG	C2-N2	4.79	1.45	1.34
1	L1	3841	OMC	C2-N1	4.78	1.50	1.40
1	L1	3887	OMC	C4-N3	4.78	1.44	1.34
46	S2	1703	OMC	C4-N4	4.76	1.45	1.33
1	L1	2861	OMC	C4-N4	4.76	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1328	OMG	C2-N2	4.75	1.45	1.34
1	L1	3808	OMC	C4-N4	4.74	1.45	1.33
1	L1	2365	OMC	C4-N3	4.74	1.44	1.34
46	S2	517	OMC	C4-N4	4.73	1.45	1.33
1	L1	4499	OMG	C2-N2	4.73	1.45	1.34
1	L1	2804	OMC	C4-N3	4.73	1.44	1.34
1	L1	3944	OMG	C2-N2	4.72	1.45	1.34
46	S2	1272	OMC	C2-N1	4.71	1.50	1.40
1	L1	3887	OMC	C4-N4	4.70	1.45	1.33
1	L1	3869	OMC	C4-N4	4.68	1.44	1.33
1	L1	4671	B8T	C4-N4	4.68	1.45	1.35
46	S2	1391	OMC	C2-N1	4.67	1.50	1.40
46	S2	1710	OMC	C2-N1	4.67	1.50	1.40
1	L1	2824	OMC	C4-N4	4.67	1.44	1.33
46	S2	601	OMG	C2-N2	4.67	1.45	1.34
1	L1	2422	OMC	C4-N4	4.66	1.44	1.33
1	L1	3899	OMG	C2-N2	4.65	1.45	1.34
46	S2	1806	M7A	C6-N6	4.64	1.45	1.34
1	L1	1625	OMG	C2-N2	4.63	1.45	1.34
1	L1	2804	OMC	C4-N4	4.63	1.44	1.33
1	L1	2824	OMC	C2-N1	4.62	1.50	1.40
1	L1	4447	5MC	C6-N1	4.62	1.45	1.38
46	S2	1374	5MC	C6-N1	4.61	1.45	1.38
1	L1	3818	UY1	C1'-C5	4.60	1.60	1.50
1	L1	2351	OMC	C2-N1	4.60	1.50	1.40
1	L1	3808	OMC	C4-N3	4.60	1.43	1.34
46	S2	683	OMG	C2-N2	4.59	1.45	1.34
46	S2	644	OMG	C2-N2	4.58	1.45	1.34
46	S2	436	OMG	C2-N2	4.58	1.45	1.34
46	S2	1490	OMG	C2-N2	4.58	1.45	1.34
1	L1	3841	OMC	C4-N4	4.58	1.44	1.33
1	L1	1316	OMG	C2-N2	4.58	1.45	1.34
1	L1	4618	OMG	C2-N2	4.57	1.45	1.34
1	L1	4494	OMG	C2-N2	4.57	1.45	1.34
1	L1	3869	OMC	C2-N1	4.57	1.49	1.40
1	L1	3701	OMC	C4-N4	4.56	1.44	1.33
1	L1	4456	OMC	C4-N4	4.56	1.44	1.33
1	L1	2351	OMC	C4-N3	4.56	1.43	1.34
1	L1	2365	OMC	C4-N4	4.54	1.44	1.33
1	L1	4196	OMG	C2-N2	4.54	1.45	1.34
1	L1	4228	OMG	C2-N2	4.53	1.45	1.34
1	L1	3808	OMC	C2-N1	4.52	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	75	OMG	C2-N2	4.52	1.44	1.34
1	L1	3744	OMG	C2-N2	4.52	1.44	1.34
1	L1	3701	OMC	C4-N3	4.51	1.43	1.34
1	L1	1340	OMC	C4-N4	4.51	1.44	1.33
1	L1	2861	OMC	C2-N1	4.51	1.49	1.40
1	L1	4571	A2M	C6-N6	4.51	1.45	1.34
46	S2	1678	A2M	C6-N6	4.50	1.45	1.34
1	L1	2364	OMG	C2-N2	4.50	1.44	1.34
1	L1	4536	OMC	C4-N4	4.50	1.44	1.33
1	L1	4370	OMG	C2-N2	4.50	1.44	1.34
1	L1	1881	OMC	C4-N4	4.49	1.44	1.33
46	S2	590	A2M	C6-N6	4.49	1.45	1.34
1	L1	3627	OMG	C2-N2	4.48	1.44	1.34
46	S2	166	A2M	C6-N6	4.48	1.45	1.34
1	L1	4623	OMG	C2-N2	4.48	1.44	1.34
1	L1	3792	OMG	C2-N2	4.47	1.44	1.34
1	L1	4456	OMC	C4-N3	4.47	1.43	1.34
46	S2	517	OMC	C2-N1	4.47	1.49	1.40
46	S2	1031	A2M	C6-N6	4.47	1.45	1.34
1	L1	3723	A2M	C6-N6	4.46	1.45	1.34
1	L1	1456	JMH	C2-N3	4.46	1.47	1.39
46	S2	159	A2M	C6-N6	4.46	1.45	1.34
1	L1	2815	A2M	C6-N6	4.46	1.45	1.34
46	S2	509	OMG	C2-N2	4.46	1.44	1.34
1	L1	2876	OMG	C2-N2	4.45	1.44	1.34
46	S2	462	OMC	C2-N1	4.45	1.49	1.40
1	L1	2422	OMC	C4-N3	4.45	1.43	1.34
46	S2	174	OMC	C2-N1	4.45	1.49	1.40
46	S2	484	A2M	C6-N6	4.45	1.45	1.34
46	S2	576	A2M	C6-N6	4.45	1.45	1.34
1	L1	4637	OMG	C2-N2	4.44	1.44	1.34
1	L1	4392	OMG	C2-N2	4.44	1.44	1.34
46	S2	1383	A2M	C6-N6	4.44	1.45	1.34
1	L1	4536	OMC	C4-N3	4.44	1.43	1.34
1	L1	3718	A2M	C6-N6	4.40	1.45	1.34
46	S2	468	A2M	C6-N6	4.40	1.45	1.34
46	S2	512	A2M	C6-N6	4.39	1.45	1.34
1	L1	1881	OMC	C2-N1	4.39	1.49	1.40
1	L1	3867	A2M	C6-N6	4.39	1.45	1.34
1	L1	2804	OMC	C2-N1	4.37	1.49	1.40
1	L1	1522	OMG	C2-N2	4.35	1.44	1.34
1	L1	3830	A2M	C6-N6	4.35	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	400	A2M	C6-N6	4.34	1.45	1.34
46	S2	27	A2M	C6-N6	4.34	1.45	1.34
1	L1	1524	A2M	C6-N6	4.33	1.45	1.34
1	L1	2401	A2M	C6-N6	4.31	1.44	1.34
1	L1	4456	OMC	C2-N1	4.31	1.49	1.40
46	S2	1374	5MC	C4-N4	4.30	1.45	1.34
1	L1	398	A2M	C6-N6	4.30	1.44	1.34
1	L1	1326	A2M	C6-N6	4.29	1.44	1.34
1	L1	4335	5MC	C6-N1	4.29	1.45	1.38
46	S2	668	A2M	C6-N6	4.27	1.44	1.34
1	L1	1871	A2M	C6-N6	4.27	1.44	1.34
1	L1	4335	5MC	C4-N4	4.27	1.45	1.34
46	S2	1703	OMC	C2-N1	4.26	1.49	1.40
1	L1	2787	A2M	C6-N6	4.26	1.44	1.34
1	L1	4536	OMC	C2-N1	4.25	1.49	1.40
1	L1	3825	A2M	C6-N6	4.25	1.44	1.34
1	L1	2422	OMC	C2-N1	4.25	1.49	1.40
1	L1	4335	5MC	C2-N1	4.24	1.49	1.40
46	S2	99	A2M	C6-N6	4.24	1.44	1.34
1	L1	3887	OMC	C2-N1	4.24	1.49	1.40
1	L1	2363	A2M	C6-N6	4.23	1.44	1.34
1	L1	1534	A2M	C6-N6	4.23	1.44	1.34
46	S2	1374	5MC	C2-N1	4.23	1.49	1.40
46	S2	1337	4AC	C5-C4	4.21	1.49	1.40
1	L1	4523	A2M	C6-N6	4.20	1.44	1.34
1	L1	2365	OMC	C2-N1	4.20	1.49	1.40
46	S2	1326	UY1	C6-C5	4.19	1.40	1.35
1	L1	4671	B8T	C2-N1	4.19	1.49	1.40
1	L1	4447	5MC	C4-N4	4.19	1.45	1.34
1	L1	1322	1MA	C2-N1	4.17	1.43	1.35
46	S2	1842	4AC	C5-C4	4.16	1.49	1.40
1	L1	3782	5MC	C6-N1	4.06	1.45	1.38
1	L1	3818	UY1	C6-C5	4.03	1.40	1.35
1	L1	3701	OMC	C2-N1	4.02	1.48	1.40
1	L1	3782	5MC	C4-N4	4.01	1.44	1.34
46	S2	814	5MU	C2-N1	3.99	1.44	1.38
1	L1	1340	OMC	C2-N1	3.99	1.48	1.40
1	L1	3782	5MC	C2-N1	3.96	1.48	1.40
1	L1	3818	UY1	C2-N3	-3.95	1.30	1.37
46	S2	1337	4AC	C2-N1	3.94	1.48	1.40
1	L1	1322	1MA	C5-C6	3.94	1.54	1.43
46	S2	1842	4AC	C2-N1	3.87	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3785	A2M	C6-N6	3.74	1.43	1.34
1	L1	2876	OMG	C5-N7	-3.74	1.31	1.39
1	L1	3887	OMC	C6-N1	3.70	1.46	1.38
46	S2	1326	UY1	C2-N3	-3.64	1.31	1.37
1	L1	4531	PSU	C6-C5	3.63	1.39	1.35
1	L1	1625	OMG	C5-N7	-3.62	1.32	1.39
1	L1	4447	5MC	C2-N1	3.60	1.47	1.40
46	S2	1806	M7A	C2-N1	3.59	1.40	1.33
1	L1	4494	OMG	C5-N7	-3.55	1.32	1.39
1	L1	2787	A2M	C5-N7	-3.55	1.32	1.39
1	L1	4671	B8T	C5-C4	3.55	1.48	1.40
46	S2	1243	PSU	C6-C5	3.54	1.39	1.35
1	L1	4637	OMG	C5-N7	-3.53	1.32	1.39
46	S2	1806	M7A	C71-N7	-3.53	1.40	1.46
1	L1	2351	OMC	C6-N1	3.52	1.46	1.38
46	S2	1288	OMU	C4-N3	3.52	1.44	1.38
1	L1	1683	PSU	C6-C5	3.50	1.39	1.35
46	S2	1442	OMU	C4-N3	3.47	1.44	1.38
46	S2	1081	PSU	C6-C5	3.46	1.39	1.35
1	L1	3792	OMG	C5-N7	-3.45	1.32	1.39
1	L1	978	2MG	C2-N1	3.45	1.42	1.36
1	L1	4392	OMG	C5-N7	-3.44	1.32	1.39
1	L1	4636	PSU	C6-C5	3.44	1.39	1.35
1	L1	3764	PSU	C6-C5	3.44	1.39	1.35
1	L1	4623	OMG	C5-N7	-3.43	1.32	1.39
1	L1	3744	OMG	C5-N7	-3.42	1.32	1.39
46	S2	116	OMU	C4-N3	3.42	1.44	1.38
1	L1	1582	PSU	C6-C5	3.42	1.39	1.35
1	L1	3869	OMC	C6-N1	3.42	1.46	1.38
1	L1	4196	OMG	C5-N7	-3.41	1.32	1.39
1	L1	3627	OMG	C5-N7	-3.41	1.32	1.39
1	L1	2364	OMG	C5-N7	-3.40	1.32	1.39
1	L1	4671	B8T	C6-N1	3.39	1.46	1.38
1	L1	3899	OMG	C5-N7	-3.39	1.32	1.39
1	L1	1881	OMC	O2-C2	-3.38	1.17	1.23
46	S2	822	PSU	C6-C5	3.37	1.39	1.35
1	L1	4403	PSU	C6-C5	3.36	1.39	1.35
1	L1	3825	A2M	C5-C4	-3.36	1.32	1.39
46	S2	172	OMU	C4-N3	3.35	1.44	1.38
46	S2	428	OMU	C4-N3	3.35	1.44	1.38
46	S2	119	PSU	C6-C5	3.34	1.39	1.35
46	S2	1490	OMG	C5-N7	-3.34	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4536	OMC	C6-N1	3.33	1.46	1.38
46	S2	601	OMG	C5-N7	-3.33	1.32	1.39
1	L1	2424	OMG	C5-N7	-3.33	1.32	1.39
1	L1	1456	JMH	C6-N1	3.33	1.46	1.38
1	L1	4442	PSU	C6-C5	3.32	1.39	1.35
46	S2	436	OMG	C5-N7	-3.32	1.32	1.39
1	L1	2508	PSU	C6-C5	3.31	1.39	1.35
46	S2	823	PSU	C4-N3	-3.31	1.32	1.38
1	L1	2365	OMC	C6-N1	3.30	1.46	1.38
46	S2	644	OMG	C5-N7	-3.30	1.32	1.39
1	L1	3841	OMC	O2-C2	-3.30	1.17	1.23
1	L1	1316	OMG	C5-N7	-3.30	1.32	1.39
46	S2	683	OMG	C5-N7	-3.30	1.32	1.39
1	L1	4456	OMC	O2-C2	-3.30	1.17	1.23
46	S2	1842	4AC	O2-C2	-3.30	1.17	1.23
1	L1	2422	OMC	C6-N1	3.27	1.45	1.38
1	L1	1517	2MG	C2-N1	3.26	1.41	1.36
1	L1	3808	OMC	C6-N1	3.26	1.45	1.38
46	S2	159	A2M	O3'-C3'	-3.26	1.35	1.43
1	L1	2804	OMC	C6-N1	3.25	1.45	1.38
1	L1	4447	5MC	O2-C2	-3.25	1.17	1.23
1	L1	4499	OMG	C5-N7	-3.24	1.32	1.39
1	L1	3785	A2M	C5-C4	-3.24	1.33	1.39
1	L1	4370	OMG	C5-N7	-3.24	1.32	1.39
1	L1	3701	OMC	C6-N1	3.24	1.45	1.38
46	S2	612	PSU	C6-C5	3.24	1.39	1.35
46	S2	174	OMC	C6-N1	3.24	1.45	1.38
1	L1	3729	PSU	C6-C5	3.24	1.39	1.35
1	L1	4293	PSU	C6-C5	3.24	1.39	1.35
1	L1	1316	OMG	O6-C6	-3.23	1.17	1.23
1	L1	3715	PSU	C6-C5	3.23	1.39	1.35
1	L1	4227	OMU	C4-N3	3.23	1.44	1.38
46	S2	1337	4AC	C6-N1	3.22	1.45	1.38
1	L1	3925	OMU	O2-C2	-3.22	1.17	1.23
46	S2	509	OMG	C5-N7	-3.22	1.32	1.39
46	S2	867	OMG	C5-N7	-3.22	1.32	1.39
46	S2	462	OMC	C6-N1	3.21	1.45	1.38
1	L1	729	2MG	C2-N1	3.21	1.41	1.36
46	S2	1272	OMC	C6-N1	3.21	1.45	1.38
46	S2	517	OMC	C6-N1	3.21	1.45	1.38
1	L1	1677	PSU	C6-C5	3.20	1.39	1.35
1	L1	4671	B8T	O2-C2	-3.20	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1851	MA6	C6-N6	3.20	1.46	1.36
1	L1	4456	OMC	C6-N1	3.19	1.45	1.38
1	L1	4228	OMG	C5-N7	-3.19	1.32	1.39
46	S2	121	OMU	C4-N3	3.19	1.44	1.38
1	L1	2363	A2M	C5-N7	-3.18	1.33	1.39
1	L1	3841	OMC	C6-N1	3.18	1.45	1.38
46	S2	668	A2M	C5-C4	-3.18	1.33	1.39
46	S2	1391	OMC	C6-N1	3.18	1.45	1.38
46	S2	1248	B8N	O4-C4	-3.18	1.16	1.23
1	L1	3818	UY1	C2-N1	-3.18	1.32	1.36
46	S2	1703	OMC	C6-N1	3.17	1.45	1.38
1	L1	2861	OMC	C6-N1	3.17	1.45	1.38
46	S2	1850	MA6	C6-N6	3.16	1.46	1.36
46	S2	1328	OMG	C5-N7	-3.16	1.32	1.39
1	L1	3867	A2M	O3'-C3'	-3.16	1.35	1.43
1	L1	3701	OMC	O2-C2	-3.16	1.17	1.23
1	L1	4450	PSU	C6-C5	3.15	1.39	1.35
46	S2	354	OMU	C4-N3	3.15	1.44	1.38
46	S2	1326	UY1	C2-N1	-3.15	1.32	1.36
1	L1	1881	OMC	C6-N1	3.14	1.45	1.38
3	L3	75	OMG	C5-N7	-3.14	1.33	1.39
1	L1	3718	A2M	C5-N7	-3.13	1.33	1.39
1	L1	2824	OMC	C6-N1	3.13	1.45	1.38
1	L1	2422	OMC	O2-C2	-3.13	1.17	1.23
46	S2	1710	OMC	C6-N1	3.13	1.45	1.38
1	L1	4618	OMG	C5-N7	-3.13	1.33	1.39
1	L1	3944	OMG	C5-N7	-3.13	1.33	1.39
46	S2	1703	OMC	O2-C2	-3.12	1.17	1.23
46	S2	1219	JMH	C6-N1	3.12	1.45	1.38
1	L1	3825	A2M	O3'-C3'	-3.12	1.35	1.43
46	S2	512	A2M	O3'-C3'	-3.12	1.35	1.43
1	L1	4536	OMC	O2-C2	-3.12	1.17	1.23
1	L1	3830	A2M	O3'-C3'	-3.11	1.35	1.43
1	L1	2815	A2M	O3'-C3'	-3.11	1.35	1.43
46	S2	1842	4AC	C6-N1	3.11	1.45	1.38
46	S2	823	PSU	C2'-C1'	-3.11	1.49	1.53
3	L3	14	OMU	O4-C4	-3.11	1.18	1.24
1	L1	2824	OMC	O2-C2	-3.10	1.18	1.23
46	S2	99	A2M	O3'-C3'	-3.10	1.35	1.43
1	L1	1517	2MG	O6-C6	-3.09	1.17	1.23
1	L1	1522	OMG	O6-C6	-3.09	1.17	1.23
46	S2	1678	A2M	O3'-C3'	-3.09	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1850	MA6	C5-C4	-3.08	1.33	1.39
1	L1	2804	OMC	O2-C2	-3.08	1.18	1.23
46	S2	1806	M7A	C4-N9	3.08	1.43	1.38
1	L1	4306	OMU	C4-N3	3.07	1.44	1.38
1	L1	4523	A2M	C5-N7	-3.06	1.33	1.39
46	S2	468	A2M	O3'-C3'	-3.06	1.35	1.43
1	L1	4620	OMU	O2-C2	-3.06	1.17	1.23
46	S2	166	A2M	O3'-C3'	-3.06	1.35	1.43
1	L1	400	A2M	O3'-C3'	-3.05	1.35	1.43
1	L1	4571	A2M	O3'-C3'	-3.05	1.35	1.43
1	L1	4498	OMU	C4-N3	3.05	1.44	1.38
1	L1	4620	OMU	O4-C4	-3.05	1.18	1.24
1	L1	4628	PSU	C6-C5	3.05	1.38	1.35
46	S2	668	A2M	O3'-C3'	-3.04	1.35	1.43
1	L1	4306	OMU	O4-C4	-3.04	1.18	1.24
1	L1	1326	A2M	C5-N7	-3.04	1.33	1.39
1	L1	3925	OMU	C4-N3	3.04	1.44	1.38
46	S2	590	A2M	O3'-C3'	-3.03	1.35	1.43
46	S2	27	A2M	O3'-C3'	-3.03	1.35	1.43
1	L1	2787	A2M	O3'-C3'	-3.03	1.35	1.43
1	L1	2837	OMU	C4-N3	3.03	1.44	1.38
46	S2	99	A2M	C5-C4	-3.03	1.33	1.39
1	L1	398	A2M	C5-C4	-3.03	1.33	1.39
46	S2	1830	UR3	C6-N1	3.02	1.45	1.38
46	S2	576	A2M	O3'-C3'	-3.02	1.35	1.43
1	L1	1871	A2M	C5-N7	-3.02	1.33	1.39
1	L1	2365	OMC	O2-C2	-3.02	1.18	1.23
1	L1	2364	OMG	O6-C6	-3.01	1.17	1.23
1	L1	1326	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	1522	OMG	C5-N7	-3.01	1.33	1.39
1	L1	2401	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	1625	OMG	O6-C6	-3.00	1.17	1.23
46	S2	1850	MA6	C5-N7	-3.00	1.33	1.39
46	S2	1678	A2M	O2'-C2'	2.99	1.50	1.42
1	L1	4623	OMG	O6-C6	-2.99	1.17	1.23
1	L1	3782	5MC	O2-C2	-2.99	1.18	1.23
46	S2	484	A2M	O2'-C2'	2.99	1.50	1.42
1	L1	4530	UR3	C6-N1	2.99	1.45	1.38
1	L1	2363	A2M	C5-C4	-2.98	1.33	1.39
1	L1	3723	A2M	O3'-C3'	-2.98	1.36	1.43
1	L1	3887	OMC	O2-C2	-2.98	1.18	1.23
1	L1	2815	A2M	O2'-C2'	2.98	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	14	OMU	O2-C2	-2.98	1.17	1.23
1	L1	3723	A2M	C5-C4	-2.98	1.33	1.39
1	L1	1871	A2M	O3'-C3'	-2.98	1.36	1.43
46	S2	468	A2M	C5-C4	-2.97	1.33	1.39
1	L1	3869	OMC	O2-C2	-2.97	1.18	1.23
1	L1	3627	OMG	O6-C6	-2.96	1.18	1.23
46	S2	1678	A2M	C5-C4	-2.95	1.33	1.39
1	L1	2876	OMG	O6-C6	-2.95	1.18	1.23
46	S2	121	OMU	O2-C2	-2.94	1.17	1.23
1	L1	4228	OMG	O6-C6	-2.94	1.18	1.23
1	L1	729	2MG	C5-N7	-2.94	1.33	1.39
1	L1	3718	A2M	O2'-C2'	2.94	1.50	1.42
46	S2	1031	A2M	O2'-C2'	2.94	1.50	1.42
46	S2	683	OMG	O6-C6	-2.94	1.18	1.23
46	S2	27	A2M	C5-C4	-2.93	1.33	1.39
1	L1	4227	OMU	O2-C2	-2.93	1.17	1.23
1	L1	398	A2M	O3'-C3'	-2.93	1.36	1.43
1	L1	3899	OMG	O6-C6	-2.93	1.18	1.23
1	L1	4571	A2M	C5-C4	-2.92	1.33	1.39
1	L1	3808	OMC	O2-C2	-2.92	1.18	1.23
46	S2	1383	A2M	O3'-C3'	-2.92	1.36	1.43
1	L1	2401	A2M	C5-N7	-2.92	1.33	1.39
46	S2	668	A2M	O2'-C2'	2.92	1.50	1.42
1	L1	1871	A2M	C5-C4	-2.92	1.33	1.39
1	L1	1534	A2M	O3'-C3'	-2.91	1.36	1.43
1	L1	1534	A2M	C5-N7	-2.91	1.33	1.39
1	L1	4620	OMU	C4-N3	2.91	1.43	1.38
1	L1	1340	OMC	O2-C2	-2.91	1.18	1.23
1	L1	2861	OMC	O2-C2	-2.91	1.18	1.23
1	L1	1326	A2M	C5-C4	-2.90	1.33	1.39
46	S2	1383	A2M	C5-C4	-2.90	1.33	1.39
1	L1	2837	OMU	O2-C2	-2.90	1.17	1.23
1	L1	4196	OMG	O6-C6	-2.89	1.18	1.23
1	L1	3867	A2M	O2'-C2'	2.89	1.50	1.42
1	L1	1534	A2M	C5-C4	-2.89	1.33	1.39
46	S2	1851	MA6	C5-N7	-2.89	1.33	1.39
1	L1	3825	A2M	C5-N7	-2.89	1.33	1.39
1	L1	4571	A2M	O2'-C2'	2.88	1.50	1.42
1	L1	400	A2M	C5-N7	-2.88	1.33	1.39
46	S2	484	A2M	C5-N7	-2.88	1.33	1.39
1	L1	4498	OMU	O4-C4	-2.87	1.18	1.24
46	S2	354	OMU	O4-C4	-2.87	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2837	OMU	O4-C4	-2.87	1.18	1.24
1	L1	1524	A2M	O2'-C2'	2.87	1.50	1.42
1	L1	2401	A2M	C5-C4	-2.87	1.33	1.39
46	S2	428	OMU	O4-C4	-2.87	1.18	1.24
1	L1	4227	OMU	O4-C4	-2.87	1.18	1.24
46	S2	517	OMC	O2-C2	-2.87	1.18	1.23
1	L1	3925	OMU	O4-C4	-2.86	1.18	1.24
46	S2	1851	MA6	C5-C4	-2.86	1.33	1.39
1	L1	1524	A2M	C5-N7	-2.86	1.33	1.39
1	L1	3830	A2M	C5-C4	-2.86	1.33	1.39
1	L1	400	A2M	C5-C4	-2.85	1.33	1.39
1	L1	3825	A2M	O2'-C2'	2.85	1.49	1.42
46	S2	1383	A2M	O2'-C2'	2.85	1.49	1.42
46	S2	512	A2M	C5-N7	-2.84	1.33	1.39
46	S2	576	A2M	C5-C4	-2.84	1.33	1.39
1	L1	3867	A2M	C5-N7	-2.84	1.33	1.39
46	S2	1337	4AC	O2-C2	-2.84	1.18	1.23
1	L1	2815	A2M	C5-C4	-2.84	1.33	1.39
1	L1	4498	OMU	O2-C2	-2.84	1.17	1.23
1	L1	3718	A2M	C5-C4	-2.84	1.33	1.39
1	L1	3785	A2M	C5-N7	-2.83	1.33	1.39
46	S2	1031	A2M	C5-N7	-2.83	1.33	1.39
1	L1	4306	OMU	O2-C2	-2.83	1.17	1.23
46	S2	512	A2M	O2'-C2'	2.82	1.49	1.42
46	S2	1806	M7A	C5-N7	2.82	1.46	1.39
1	L1	4494	OMG	O6-C6	-2.82	1.18	1.23
1	L1	3723	A2M	O2'-C2'	2.82	1.49	1.42
46	S2	512	A2M	C5-C4	-2.81	1.33	1.39
46	S2	1374	5MC	O2-C2	-2.81	1.18	1.23
46	S2	99	A2M	C5-N7	-2.81	1.33	1.39
46	S2	166	A2M	O2'-C2'	2.81	1.49	1.42
46	S2	436	OMG	O6-C6	-2.81	1.18	1.23
46	S2	1850	MA6	C8-N9	-2.81	1.32	1.37
1	L1	2351	OMC	O2-C2	-2.81	1.18	1.23
1	L1	2363	A2M	O2'-C2'	2.80	1.49	1.42
46	S2	166	A2M	C5-C4	-2.80	1.33	1.39
46	S2	159	A2M	O2'-C2'	2.79	1.49	1.42
46	S2	484	A2M	C5-C4	-2.79	1.33	1.39
1	L1	4523	A2M	O3'-C3'	-2.79	1.36	1.43
46	S2	174	OMC	O2-C2	-2.79	1.18	1.23
46	S2	576	A2M	O2'-C2'	2.79	1.49	1.42
1	L1	978	2MG	C5-N7	-2.79	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3744	OMG	O6-C6	-2.79	1.18	1.23
46	S2	590	A2M	O2'-C2'	2.79	1.49	1.42
46	S2	462	OMC	O2-C2	-2.78	1.18	1.23
1	L1	2363	A2M	O3'-C3'	-2.78	1.36	1.43
1	L1	1534	A2M	O2'-C2'	2.78	1.49	1.42
46	S2	99	A2M	O2'-C2'	2.78	1.49	1.42
46	S2	354	OMU	O2-C2	-2.78	1.18	1.23
1	L1	3867	A2M	C5-C4	-2.78	1.33	1.39
46	S2	159	A2M	C5-C4	-2.78	1.33	1.39
46	S2	1031	A2M	C5-C4	-2.77	1.33	1.39
1	L1	4370	OMG	O6-C6	-2.77	1.18	1.23
1	L1	1340	OMC	C6-N1	2.77	1.44	1.38
1	L1	3830	A2M	O2'-C2'	2.77	1.49	1.42
46	S2	27	A2M	C5-N7	-2.77	1.33	1.39
1	L1	1326	A2M	O2'-C2'	2.77	1.49	1.42
1	L1	2787	A2M	O2'-C2'	2.76	1.49	1.42
1	L1	3718	A2M	O3'-C3'	-2.76	1.36	1.43
1	L1	1517	2MG	C5-N7	-2.76	1.33	1.39
46	S2	1031	A2M	O3'-C3'	-2.75	1.36	1.43
1	L1	978	2MG	O6-C6	-2.75	1.18	1.23
1	L1	3792	OMG	O6-C6	-2.75	1.18	1.23
1	L1	1871	A2M	O2'-C2'	2.75	1.49	1.42
1	L1	2787	A2M	C5-C4	-2.75	1.33	1.39
1	L1	398	A2M	O2'-C2'	2.75	1.49	1.42
1	L1	4618	OMG	O6-C6	-2.75	1.18	1.23
46	S2	1391	OMC	O2-C2	-2.74	1.18	1.23
46	S2	1710	OMC	O2-C2	-2.74	1.18	1.23
1	L1	3785	A2M	O2'-C2'	2.74	1.49	1.42
3	L3	75	OMG	O6-C6	-2.74	1.18	1.23
1	L1	4220	6MZ	C5-C4	-2.74	1.33	1.39
46	S2	121	OMU	O4-C4	-2.74	1.19	1.24
1	L1	4523	A2M	C5-C4	-2.74	1.33	1.39
1	L1	1524	A2M	O3'-C3'	-2.74	1.36	1.43
1	L1	2401	A2M	O2'-C2'	2.73	1.49	1.42
46	S2	668	A2M	C5-N7	-2.73	1.33	1.39
46	S2	814	5MU	O4-C4	-2.73	1.18	1.23
46	S2	484	A2M	O3'-C3'	-2.73	1.36	1.43
1	L1	4571	A2M	C5-N7	-2.73	1.33	1.39
46	S2	468	A2M	O2'-C2'	2.73	1.49	1.42
46	S2	116	OMU	O4-C4	-2.73	1.19	1.24
46	S2	116	OMU	O2-C2	-2.73	1.18	1.23
1	L1	398	A2M	C5-N7	-2.72	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4523	A2M	O2'-C2'	2.71	1.49	1.42
1	L1	1524	A2M	C5-C4	-2.71	1.33	1.39
46	S2	428	OMU	O2-C2	-2.71	1.18	1.23
1	L1	1322	1MA	C4-N9	-2.71	1.31	1.38
46	S2	576	A2M	C5-N7	-2.71	1.33	1.39
1	L1	4196	OMG	C2-N1	2.70	1.44	1.37
1	L1	4637	OMG	O6-C6	-2.69	1.18	1.23
1	L1	400	A2M	O2'-C2'	2.69	1.49	1.42
1	L1	3830	A2M	C5-N7	-2.68	1.34	1.39
3	L3	14	OMU	C4-N3	2.68	1.43	1.38
46	S2	1272	OMC	O2-C2	-2.68	1.18	1.23
1	L1	1322	1MA	C5-N7	-2.68	1.33	1.39
1	L1	4335	5MC	O2-C2	-2.68	1.18	1.23
1	L1	4499	OMG	O6-C6	-2.68	1.18	1.23
46	S2	172	OMU	O2-C2	-2.68	1.18	1.23
46	S2	814	5MU	O2-C2	-2.67	1.18	1.23
1	L1	729	2MG	O6-C6	-2.67	1.18	1.23
46	S2	867	OMG	C2-N1	2.67	1.44	1.37
46	S2	159	A2M	C5-N7	-2.67	1.34	1.39
46	S2	1383	A2M	C5-N7	-2.67	1.34	1.39
46	S2	644	OMG	O6-C6	-2.67	1.18	1.23
1	L1	2815	A2M	C5-N7	-2.66	1.34	1.39
46	S2	468	A2M	C5-N7	-2.66	1.34	1.39
46	S2	1328	OMG	C2-N1	2.66	1.44	1.37
46	S2	27	A2M	O2'-C2'	2.66	1.49	1.42
46	S2	1442	OMU	O4-C4	-2.66	1.19	1.24
1	L1	4392	OMG	O6-C6	-2.65	1.18	1.23
46	S2	590	A2M	C5-C4	-2.65	1.34	1.39
46	S2	590	A2M	C5-N7	-2.65	1.34	1.39
46	S2	509	OMG	O6-C6	-2.65	1.18	1.23
46	S2	601	OMG	O6-C6	-2.64	1.18	1.23
1	L1	1316	OMG	C5-C6	2.64	1.54	1.44
1	L1	2424	OMG	C2-N1	2.64	1.44	1.37
46	S2	172	OMU	O4-C4	-2.64	1.19	1.24
1	L1	1517	2MG	C4-N9	-2.64	1.31	1.38
1	L1	2424	OMG	O6-C6	-2.63	1.18	1.23
46	S2	1490	OMG	O6-C6	-2.61	1.18	1.23
1	L1	3869	OMC	C5-C4	2.61	1.48	1.42
1	L1	3944	OMG	C2-N1	2.61	1.44	1.37
1	L1	1316	OMG	C2-N1	2.61	1.44	1.37
1	L1	3723	A2M	C5-N7	-2.61	1.34	1.39
3	L3	75	OMG	C2-N1	2.60	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1288	OMU	O4-C4	-2.60	1.19	1.24
1	L1	4456	OMC	C5-C4	2.60	1.48	1.42
1	L1	4500	PSU	C6-C5	2.59	1.38	1.35
1	L1	978	2MG	CM2-N2	2.59	1.50	1.45
46	S2	1288	OMU	O2-C2	-2.57	1.18	1.23
1	L1	4623	OMG	C2-N1	2.57	1.44	1.37
1	L1	3944	OMG	O6-C6	-2.57	1.18	1.23
46	S2	1442	OMU	O2-C2	-2.57	1.18	1.23
1	L1	4228	OMG	C2-N1	2.57	1.44	1.37
46	S2	823	PSU	C2-N1	-2.57	1.33	1.36
46	S2	823	PSU	C2-N3	-2.57	1.33	1.37
1	L1	4499	OMG	C2-N1	2.57	1.44	1.37
46	S2	1678	A2M	C5-N7	-2.56	1.34	1.39
1	L1	2364	OMG	C2-N1	2.56	1.44	1.37
46	S2	867	OMG	O6-C6	-2.56	1.18	1.23
1	L1	4392	OMG	C5-C6	2.56	1.53	1.44
1	L1	3701	OMC	C5-C4	2.55	1.48	1.42
46	S2	1272	OMC	C5-C4	2.55	1.48	1.42
46	S2	436	OMG	C2-N1	2.55	1.44	1.37
46	S2	644	OMG	C2-N1	2.55	1.44	1.37
1	L1	978	2MG	C4-N9	-2.55	1.31	1.38
1	L1	2422	OMC	C5-C4	2.54	1.48	1.42
1	L1	1881	OMC	C5-C4	2.54	1.48	1.42
46	S2	1328	OMG	O6-C6	-2.54	1.18	1.23
46	S2	1851	MA6	C8-N9	-2.54	1.33	1.37
1	L1	3762	B8H	O2-C2	-2.54	1.18	1.23
46	S2	166	A2M	C5-N7	-2.54	1.34	1.39
1	L1	3818	UY1	C4-C5	-2.54	1.36	1.44
46	S2	601	OMG	C2-N1	2.54	1.43	1.37
1	L1	3744	OMG	C2-N1	2.52	1.43	1.37
46	S2	174	OMC	C5-C4	2.51	1.48	1.42
1	L1	3627	OMG	C2-N1	2.51	1.43	1.37
46	S2	1830	UR3	O2-C2	-2.51	1.18	1.22
1	L1	4623	OMG	C5-C6	2.50	1.53	1.44
1	L1	3627	OMG	C5-C6	2.49	1.53	1.44
1	L1	1522	OMG	C2-N1	2.49	1.43	1.37
1	L1	978	2MG	C6-N1	2.49	1.43	1.38
3	L3	75	OMG	C5-C6	2.49	1.53	1.44
1	L1	2804	OMC	C5-C4	2.49	1.48	1.42
1	L1	4196	OMG	C5-C6	2.48	1.53	1.44
46	S2	509	OMG	C2-N1	2.47	1.43	1.37
46	S2	1328	OMG	C5-C6	2.47	1.53	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3744	OMG	C5-C6	2.47	1.53	1.44
1	L1	4618	OMG	C2-N1	2.46	1.43	1.37
1	L1	4618	OMG	C5-C6	2.46	1.53	1.44
1	L1	2861	OMC	C5-C4	2.45	1.48	1.42
1	L1	1534	A2M	C8-N9	-2.45	1.33	1.37
1	L1	4494	OMG	C5-C6	2.45	1.53	1.44
1	L1	4370	OMG	C5-C6	2.44	1.53	1.44
1	L1	2363	A2M	C8-N9	-2.44	1.33	1.37
46	S2	683	OMG	C2-N1	2.44	1.43	1.37
46	S2	867	OMG	C5-C6	2.44	1.53	1.44
46	S2	601	OMG	C5-C6	2.43	1.53	1.44
1	L1	4370	OMG	C2-N1	2.43	1.43	1.37
1	L1	3887	OMC	C5-C4	2.43	1.48	1.42
46	S2	644	OMG	C5-C6	2.42	1.53	1.44
1	L1	3944	OMG	C5-C6	2.42	1.53	1.44
1	L1	3899	OMG	C2-N1	2.42	1.43	1.37
1	L1	4637	OMG	C5-C6	2.42	1.53	1.44
1	L1	4392	OMG	C2-N1	2.42	1.43	1.37
1	L1	1522	OMG	C5-C6	2.41	1.53	1.44
1	L1	4494	OMG	C2-N1	2.40	1.43	1.37
1	L1	1456	JMH	C5-C4	2.40	1.48	1.42
46	S2	517	OMC	C5-C4	2.40	1.48	1.42
1	L1	3944	OMG	C6-N1	2.40	1.43	1.38
1	L1	1625	OMG	C5-C6	2.39	1.53	1.44
46	S2	462	OMC	C5-C4	2.39	1.48	1.42
1	L1	3792	OMG	C5-C6	2.39	1.53	1.44
1	L1	729	2MG	C4-N9	-2.39	1.31	1.38
1	L1	4499	OMG	C5-C6	2.38	1.53	1.44
46	S2	1830	UR3	O4-C4	-2.38	1.18	1.23
1	L1	4637	OMG	C2-N1	2.38	1.43	1.37
1	L1	1517	2MG	C6-N1	2.38	1.43	1.38
1	L1	2364	OMG	C5-C6	2.38	1.53	1.44
46	S2	823	PSU	C6-C5	2.38	1.38	1.35
46	S2	509	OMG	C5-C6	2.37	1.53	1.44
1	L1	1625	OMG	C2-N1	2.36	1.43	1.37
1	L1	3867	A2M	C8-N9	-2.36	1.33	1.37
1	L1	4220	6MZ	C5-N7	-2.36	1.34	1.39
1	L1	4228	OMG	C5-C6	2.36	1.53	1.44
1	L1	3792	OMG	C2-N1	2.36	1.43	1.37
1	L1	2351	OMC	C5-C4	2.36	1.48	1.42
46	S2	867	OMG	C6-N1	2.36	1.43	1.38
46	S2	1391	OMC	C5-C4	2.35	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1871	A2M	C8-N9	-2.35	1.33	1.37
1	L1	2365	OMC	C5-C4	2.35	1.48	1.42
46	S2	1703	OMC	C5-C4	2.35	1.48	1.42
3	L3	75	OMG	C6-N1	2.35	1.43	1.38
46	S2	1710	OMC	C5-C4	2.35	1.48	1.42
1	L1	2424	OMG	C6-N1	2.34	1.43	1.38
46	S2	1326	UY1	C4-C5	-2.34	1.37	1.44
46	S2	1490	OMG	C2-N1	2.34	1.43	1.37
46	S2	1328	OMG	C6-N1	2.34	1.43	1.38
46	S2	1490	OMG	C5-C6	2.33	1.53	1.44
1	L1	3785	A2M	O5'-C5'	-2.33	1.39	1.44
1	L1	2876	OMG	C5-C6	2.33	1.53	1.44
46	S2	436	OMG	C5-C6	2.32	1.53	1.44
1	L1	3808	OMC	C5-C4	2.32	1.48	1.42
1	L1	3841	OMC	C5-C4	2.32	1.48	1.42
1	L1	3899	OMG	C5-C6	2.30	1.52	1.44
46	S2	1832	6MZ	C5-C4	-2.30	1.34	1.39
1	L1	2424	OMG	C5-C6	2.29	1.52	1.44
46	S2	683	OMG	C5-C6	2.29	1.52	1.44
1	L1	4536	OMC	C5-C4	2.29	1.48	1.42
1	L1	1524	A2M	C8-N9	-2.29	1.33	1.37
1	L1	4530	UR3	O4-C4	-2.28	1.18	1.23
1	L1	4530	UR3	O2-C2	-2.28	1.18	1.22
46	S2	1678	A2M	C8-N9	-2.28	1.33	1.37
1	L1	3899	OMG	C4-N9	-2.27	1.32	1.38
1	L1	2876	OMG	C2-N1	2.27	1.43	1.37
46	S2	1842	4AC	O7-C7	-2.26	1.18	1.23
46	S2	683	OMG	C6-N1	2.26	1.43	1.38
1	L1	4618	OMG	C6-N1	2.23	1.43	1.38
1	L1	2401	A2M	O5'-C5'	-2.23	1.39	1.44
1	L1	4530	UR3	C4-N3	2.23	1.45	1.40
1	L1	1517	2MG	CM2-N2	2.22	1.49	1.45
1	L1	2824	OMC	C5-C4	2.21	1.48	1.42
1	L1	4623	OMG	C4-N9	-2.21	1.32	1.38
1	L1	3718	A2M	C8-N9	-2.21	1.33	1.37
46	S2	668	A2M	C8-N9	-2.21	1.33	1.37
1	L1	4392	OMG	C6-N1	2.20	1.42	1.38
1	L1	4227	OMU	C5-C4	2.20	1.48	1.43
46	S2	1832	6MZ	C8-N9	-2.18	1.33	1.37
1	L1	3785	A2M	O3'-C3'	-2.18	1.37	1.43
1	L1	4499	OMG	C6-N1	2.18	1.42	1.38
1	L1	3899	OMG	C6-N1	2.18	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	576	A2M	C8-N9	-2.18	1.33	1.37
1	L1	3744	OMG	C6-N1	2.18	1.42	1.38
1	L1	4228	OMG	C6-N1	2.18	1.42	1.38
46	S2	1830	UR3	C5-C4	2.17	1.49	1.43
46	S2	159	A2M	C8-N9	-2.16	1.33	1.37
46	S2	436	OMG	C6-N1	2.16	1.42	1.38
1	L1	4370	OMG	C6-N1	2.16	1.42	1.38
1	L1	3723	A2M	C8-N9	-2.16	1.33	1.37
1	L1	3818	UY1	O3'-C3'	2.16	1.48	1.43
46	S2	1031	A2M	O5'-C5'	-2.16	1.39	1.44
1	L1	1522	OMG	C6-N1	2.15	1.42	1.38
46	S2	590	A2M	C8-N9	-2.15	1.33	1.37
1	L1	398	A2M	C8-N9	-2.15	1.33	1.37
1	L1	3818	UY1	O2'-C2'	-2.15	1.37	1.42
1	L1	2363	A2M	O5'-C5'	-2.15	1.39	1.44
1	L1	3867	A2M	O5'-C5'	-2.14	1.39	1.44
3	L3	14	OMU	C5-C4	2.14	1.48	1.43
46	S2	484	A2M	C8-N9	-2.14	1.33	1.37
46	S2	99	A2M	C8-N9	-2.14	1.33	1.37
46	S2	1490	OMG	C6-N1	2.13	1.42	1.38
1	L1	1326	A2M	C8-N9	-2.13	1.33	1.37
46	S2	1288	OMU	C6-N1	2.13	1.43	1.38
1	L1	4523	A2M	O5'-C5'	-2.13	1.39	1.44
46	S2	1337	4AC	O7-C7	-2.12	1.18	1.23
1	L1	729	2MG	C6-N1	2.12	1.42	1.38
1	L1	729	2MG	CM2-N2	2.11	1.49	1.45
46	S2	644	OMG	C6-N1	2.11	1.42	1.38
46	S2	512	A2M	C8-N9	-2.10	1.33	1.37
1	L1	1524	A2M	O5'-C5'	-2.09	1.39	1.44
46	S2	509	OMG	C4-N9	-2.09	1.32	1.38
46	S2	601	OMG	C6-N1	2.09	1.42	1.38
1	L1	1677	PSU	O4'-C1'	-2.09	1.40	1.43
46	S2	1383	A2M	C8-N9	-2.08	1.33	1.37
1	L1	3830	A2M	O5'-C5'	-2.08	1.39	1.44
1	L1	3627	OMG	C6-N1	2.08	1.42	1.38
1	L1	2401	A2M	C8-N9	-2.08	1.33	1.37
46	S2	166	A2M	C8-N9	-2.08	1.33	1.37
1	L1	4370	OMG	C4-N9	-2.07	1.32	1.38
1	L1	1534	A2M	O5'-C5'	-2.07	1.39	1.44
1	L1	4228	OMG	C4-N9	-2.07	1.32	1.38
1	L1	3825	A2M	O5'-C5'	-2.06	1.39	1.44
1	L1	3925	OMU	C6-N1	2.06	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3825	A2M	C8-N9	-2.06	1.33	1.37
1	L1	2424	OMG	C4-N9	-2.06	1.32	1.38
46	S2	1326	UY1	O3'-C3'	2.05	1.47	1.43
46	S2	1326	UY1	O2'-C2'	-2.05	1.37	1.42
1	L1	2876	OMG	C6-N1	2.05	1.42	1.38
1	L1	400	A2M	O5'-C5'	-2.05	1.39	1.44
46	S2	468	A2M	C8-N9	-2.05	1.33	1.37
1	L1	1340	OMC	C5-C4	2.04	1.47	1.42
1	L1	4523	A2M	C8-N9	-2.04	1.33	1.37
46	S2	823	PSU	C6-N1	-2.04	1.32	1.36
46	S2	468	A2M	O5'-C5'	-2.04	1.39	1.44
1	L1	1316	OMG	C6-N1	2.03	1.42	1.38
46	S2	668	A2M	O5'-C5'	-2.03	1.39	1.44
46	S2	1442	OMU	C6-N1	2.03	1.42	1.38
46	S2	1219	JMH	C5-C4	2.03	1.47	1.42
46	S2	1288	OMU	C5-C4	2.03	1.48	1.43
46	S2	509	OMG	C6-N1	2.02	1.42	1.38
1	L1	4571	A2M	C8-N9	-2.02	1.33	1.37
1	L1	4196	OMG	C6-N1	2.02	1.42	1.38
1	L1	4620	OMU	C5-C4	2.01	1.48	1.43
46	S2	1442	OMU	C5-C4	2.01	1.48	1.43
46	S2	1248	B8N	C32-C33	2.01	1.57	1.53
1	L1	4227	OMU	C6-N1	2.01	1.42	1.38
46	S2	27	A2M	O5'-C5'	-2.00	1.39	1.44

All (914) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1851	MA6	N1-C6-N6	-16.93	98.57	117.08
46	S2	1850	MA6	N1-C6-N6	-15.09	100.58	117.08
46	S2	1806	M7A	C5-C6-N6	13.64	147.03	123.74
46	S2	1806	M7A	N6-C6-N1	-11.50	93.16	118.35
46	S2	814	5MU	C5-C4-N3	10.06	123.90	115.31
46	S2	1851	MA6	C5-C6-N6	9.64	142.10	125.30
46	S2	1850	MA6	C5-C6-N6	8.64	140.36	125.30
46	S2	814	5MU	C5-C6-N1	-8.00	115.11	123.34
1	L1	1534	A2M	N6-C6-N1	-7.31	102.35	118.35
1	L1	2401	A2M	N6-C6-N1	-7.20	102.59	118.35
1	L1	4571	A2M	N6-C6-N1	-7.19	102.61	118.35
1	L1	3785	A2M	N6-C6-N1	-7.17	102.64	118.35
46	S2	668	A2M	N6-C6-N1	-7.16	102.67	118.35
46	S2	484	A2M	N6-C6-N1	-7.15	102.69	118.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	166	A2M	N6-C6-N1	-7.13	102.74	118.35
46	S2	1383	A2M	N6-C6-N1	-7.04	102.94	118.35
1	L1	1524	A2M	N6-C6-N1	-7.02	102.98	118.35
46	S2	590	A2M	N6-C6-N1	-6.97	103.08	118.35
46	S2	468	A2M	N6-C6-N1	-6.95	103.13	118.35
46	S2	27	A2M	N6-C6-N1	-6.94	103.15	118.35
46	S2	1678	A2M	N6-C6-N1	-6.93	103.17	118.35
1	L1	4523	A2M	N6-C6-N1	-6.92	103.19	118.35
1	L1	3830	A2M	N6-C6-N1	-6.92	103.20	118.35
46	S2	159	A2M	N6-C6-N1	-6.92	103.21	118.35
46	S2	576	A2M	N6-C6-N1	-6.92	103.21	118.35
46	S2	512	A2M	N6-C6-N1	-6.88	103.28	118.35
46	S2	1850	MA6	C4-N9-C1'	-6.85	110.26	126.59
1	L1	1517	2MG	C2-N3-C4	6.85	120.54	112.04
46	S2	99	A2M	N6-C6-N1	-6.84	103.38	118.35
1	L1	3723	A2M	N6-C6-N1	-6.83	103.39	118.35
1	L1	3718	A2M	N6-C6-N1	-6.77	103.53	118.35
1	L1	3762	B8H	C4-N3-C2	-6.75	118.61	127.35
1	L1	2815	A2M	N6-C6-N1	-6.75	103.57	118.35
1	L1	400	A2M	N6-C6-N1	-6.75	103.57	118.35
1	L1	3867	A2M	N6-C6-N1	-6.73	103.62	118.35
46	S2	1031	A2M	N6-C6-N1	-6.72	103.64	118.35
1	L1	398	A2M	N6-C6-N1	-6.71	103.66	118.35
46	S2	1851	MA6	C5-C4-N3	-6.70	118.01	126.75
1	L1	1326	A2M	N6-C6-N1	-6.70	103.68	118.35
46	S2	814	5MU	C4-N3-C2	-6.67	118.72	127.35
1	L1	3825	A2M	N6-C6-N1	-6.66	103.76	118.35
1	L1	1871	A2M	N6-C6-N1	-6.61	103.88	118.35
1	L1	2787	A2M	N6-C6-N1	-6.60	103.90	118.35
1	L1	1534	A2M	C5-C6-N6	6.53	137.63	123.43
46	S2	823	PSU	N1-C2-N3	6.53	122.52	115.13
1	L1	1322	1MA	N1-C2-N3	-6.49	118.28	126.00
1	L1	2787	A2M	C5-C4-N3	-6.48	118.29	126.75
46	S2	668	A2M	C5-C6-N6	6.39	137.34	123.43
1	L1	2363	A2M	N6-C6-N1	-6.38	104.38	118.35
1	L1	1625	OMG	C5-C4-N3	-6.36	118.14	128.46
46	S2	590	A2M	C5-C4-N3	-6.35	118.46	126.75
1	L1	4571	A2M	C5-C6-N6	6.35	137.25	123.43
1	L1	978	2MG	C2-N3-C4	6.34	119.90	112.04
46	S2	484	A2M	C5-C6-N6	6.34	137.22	123.43
46	S2	1383	A2M	C5-C6-N6	6.32	137.18	123.43
1	L1	2876	OMG	C5-C4-N3	-6.30	118.23	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	2401	A2M	C5-C6-N6	6.28	137.09	123.43
46	S2	166	A2M	C5-C6-N6	6.27	137.07	123.43
1	L1	1524	A2M	C5-C6-N6	6.26	137.05	123.43
1	L1	1326	A2M	C5-C6-N6	6.26	137.05	123.43
1	L1	4523	A2M	C5-C6-N6	6.24	137.02	123.43
46	S2	512	A2M	C5-C6-N6	6.24	137.02	123.43
1	L1	1871	A2M	N3-C2-N1	-6.22	118.87	128.60
1	L1	3718	A2M	C5-C6-N6	6.19	136.91	123.43
1	L1	3830	A2M	C5-C6-N6	6.16	136.84	123.43
46	S2	1031	A2M	C5-C6-N6	6.16	136.82	123.43
46	S2	576	A2M	C5-C6-N6	6.14	136.78	123.43
46	S2	1678	A2M	C5-C6-N6	6.13	136.78	123.43
46	S2	668	A2M	N3-C2-N1	-6.13	119.01	128.60
46	S2	1031	A2M	N3-C2-N1	-6.12	119.03	128.60
46	S2	159	A2M	C5-C6-N6	6.10	136.70	123.43
46	S2	468	A2M	C5-C6-N6	6.09	136.69	123.43
1	L1	1871	A2M	C5-C6-N6	6.09	136.68	123.43
46	S2	512	A2M	N3-C2-N1	-6.06	119.12	128.60
46	S2	27	A2M	C5-C6-N6	6.06	136.62	123.43
1	L1	2815	A2M	C5-C6-N6	6.04	136.57	123.43
46	S2	1832	6MZ	N1-C2-N3	-6.03	119.17	128.60
1	L1	3723	A2M	C5-C6-N6	6.02	136.53	123.43
46	S2	590	A2M	C5-C6-N6	6.02	136.52	123.43
46	S2	1851	MA6	C4-N9-C1'	-6.00	112.30	126.59
1	L1	3785	A2M	C5-C6-N6	5.99	136.47	123.43
1	L1	2787	A2M	C5-C6-N6	5.97	136.42	123.43
1	L1	3867	A2M	C5-C6-N6	5.97	136.42	123.43
46	S2	99	A2M	C5-C6-N6	5.96	136.41	123.43
1	L1	3762	B8H	N3-C2-N1	5.96	121.58	115.14
1	L1	1326	A2M	N3-C2-N1	-5.95	119.29	128.60
46	S2	1850	MA6	C1'-N9-C8	5.94	140.54	127.14
1	L1	400	A2M	C5-C6-N6	5.93	136.33	123.43
1	L1	3825	A2M	C5-C6-N6	5.90	136.26	123.43
1	L1	4220	6MZ	N1-C2-N3	-5.88	119.41	128.60
1	L1	2401	A2M	C5-C4-N3	-5.87	119.10	126.75
1	L1	2364	OMG	C5-C4-N3	-5.85	118.97	128.46
1	L1	398	A2M	C5-C6-N6	5.84	136.15	123.43
1	L1	3818	UY1	N1-C2-N3	5.81	121.72	115.13
1	L1	4392	OMG	C5-C4-N3	-5.81	119.03	128.46
1	L1	2363	A2M	C5-C6-N6	5.81	136.08	123.43
1	L1	729	2MG	C2-N3-C4	5.81	119.24	112.04
46	S2	27	A2M	N3-C2-N1	-5.80	119.53	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1322	1MA	C1'-N9-C8	-5.78	110.25	126.70
1	L1	1871	A2M	C5-C4-N3	-5.78	119.21	126.75
1	L1	4637	OMG	C5-C4-N3	-5.77	119.10	128.46
1	L1	2815	A2M	N3-C2-N1	-5.77	119.58	128.60
46	S2	1850	MA6	C5-C4-N3	-5.75	119.25	126.75
1	L1	3825	A2M	N3-C2-N1	-5.75	119.61	128.60
1	L1	3867	A2M	N3-C2-N1	-5.73	119.64	128.60
1	L1	4494	OMG	C5-C4-N3	-5.72	119.18	128.46
1	L1	1316	OMG	C5-C4-N3	-5.72	119.19	128.46
1	L1	3627	OMG	C5-C4-N3	-5.70	119.21	128.46
46	S2	1678	A2M	N3-C2-N1	-5.70	119.69	128.60
1	L1	2401	A2M	N3-C2-N1	-5.69	119.69	128.60
1	L1	3792	OMG	C5-C4-N3	-5.68	119.24	128.46
46	S2	590	A2M	N3-C2-N1	-5.68	119.71	128.60
1	L1	3830	A2M	N3-C2-N1	-5.68	119.72	128.60
46	S2	166	A2M	N3-C2-N1	-5.67	119.72	128.60
1	L1	4571	A2M	N3-C2-N1	-5.67	119.73	128.60
46	S2	1383	A2M	N3-C2-N1	-5.67	119.74	128.60
46	S2	484	A2M	C5-C4-N3	-5.66	119.37	126.75
1	L1	4196	OMG	C5-C4-N3	-5.66	119.28	128.46
46	S2	1851	MA6	N1-C2-N3	-5.65	119.77	128.60
46	S2	436	OMG	C5-C4-N3	-5.65	119.30	128.46
1	L1	2363	A2M	C5-C4-N3	-5.62	119.42	126.75
1	L1	4523	A2M	N3-C2-N1	-5.62	119.81	128.60
46	S2	468	A2M	N3-C2-N1	-5.62	119.81	128.60
3	L3	14	OMU	C4-N3-C2	-5.62	119.17	126.58
1	L1	4498	OMU	C4-N3-C2	-5.61	119.17	126.58
1	L1	398	A2M	N3-C2-N1	-5.59	119.85	128.60
1	L1	1534	A2M	C5-C4-N3	-5.59	119.45	126.75
1	L1	3723	A2M	N3-C2-N1	-5.59	119.86	128.60
46	S2	99	A2M	N3-C2-N1	-5.58	119.87	128.60
1	L1	1524	A2M	N3-C2-N1	-5.58	119.87	128.60
1	L1	1534	A2M	N3-C2-N1	-5.58	119.88	128.60
46	S2	683	OMG	C5-C4-N3	-5.57	119.43	128.46
1	L1	2815	A2M	C5-C4-N3	-5.56	119.50	126.75
46	S2	159	A2M	C5-C4-N3	-5.53	119.53	126.75
46	S2	159	A2M	N3-C2-N1	-5.53	119.96	128.60
1	L1	3867	A2M	C5-C4-N3	-5.52	119.55	126.75
1	L1	1524	A2M	C5-C4-N3	-5.52	119.55	126.75
46	S2	166	A2M	C5-C4-N3	-5.51	119.56	126.75
1	L1	398	A2M	C5-C4-N3	-5.51	119.56	126.75
1	L1	3744	OMG	C5-C4-N3	-5.51	119.53	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3825	A2M	C5-C4-N3	-5.49	119.59	126.75
46	S2	576	A2M	C5-C4-N3	-5.49	119.59	126.75
46	S2	484	A2M	N3-C2-N1	-5.48	120.03	128.60
1	L1	400	A2M	C5-C4-N3	-5.48	119.60	126.75
46	S2	512	A2M	C5-C4-N3	-5.48	119.60	126.75
46	S2	576	A2M	N3-C2-N1	-5.47	120.05	128.60
1	L1	1522	OMG	C5-C4-N3	-5.47	119.59	128.46
46	S2	1850	MA6	N1-C2-N3	-5.46	120.06	128.60
46	S2	1851	MA6	C1'-N9-C8	5.45	139.44	127.14
46	S2	867	OMG	C5-C4-N3	-5.45	119.62	128.46
1	L1	3785	A2M	O4'-C1'-N9	5.45	118.79	108.06
46	S2	1383	A2M	C5-C4-N3	-5.44	119.66	126.75
1	L1	4227	OMU	C4-N3-C2	-5.43	119.42	126.58
1	L1	3785	A2M	N3-C2-N1	-5.42	120.12	128.60
46	S2	601	OMG	C5-C4-N3	-5.41	119.68	128.46
46	S2	27	A2M	C5-C4-N3	-5.41	119.70	126.75
46	S2	99	A2M	C5-C4-N3	-5.41	119.70	126.75
1	L1	400	A2M	N3-C2-N1	-5.39	120.17	128.60
1	L1	2787	A2M	N3-C2-N1	-5.39	120.17	128.60
46	S2	1326	UY1	N1-C2-N3	5.39	121.23	115.13
1	L1	4523	A2M	C5-C4-N3	-5.38	119.74	126.75
1	L1	3944	OMG	C5-C4-N3	-5.36	119.77	128.46
46	S2	1806	M7A	N3-C2-N1	-5.35	120.23	128.60
46	S2	1490	OMG	C5-C4-N3	-5.35	119.79	128.46
1	L1	3925	OMU	C4-N3-C2	-5.34	119.54	126.58
46	S2	1678	A2M	C5-C4-N3	-5.33	119.80	126.75
1	L1	1683	PSU	N1-C2-N3	5.32	121.16	115.13
46	S2	509	OMG	C5-C4-N3	-5.32	119.83	128.46
1	L1	3785	A2M	C5-C4-N3	-5.32	119.81	126.75
1	L1	2363	A2M	N3-C2-N1	-5.31	120.29	128.60
1	L1	4571	A2M	C5-C4-N3	-5.31	119.82	126.75
1	L1	3830	A2M	C5-C4-N3	-5.31	119.83	126.75
1	L1	4499	OMG	C5-C4-N3	-5.30	119.86	128.46
46	S2	172	OMU	C4-N3-C2	-5.29	119.60	126.58
46	S2	468	A2M	C5-C4-N3	-5.29	119.84	126.75
1	L1	4306	OMU	C4-N3-C2	-5.27	119.63	126.58
46	S2	1328	OMG	C5-C4-N3	-5.26	119.92	128.46
46	S2	644	OMG	C5-C4-N3	-5.26	119.93	128.46
46	S2	354	OMU	C4-N3-C2	-5.25	119.65	126.58
1	L1	4618	OMG	C5-C4-N3	-5.23	119.97	128.46
1	L1	4636	PSU	C4-N3-C2	-5.20	118.85	126.34
1	L1	3723	A2M	C5-C4-N3	-5.20	119.97	126.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3718	A2M	C5-C4-N3	-5.20	119.97	126.75
1	L1	1326	A2M	C5-C4-N3	-5.19	119.98	126.75
46	S2	121	OMU	C4-N3-C2	-5.17	119.77	126.58
46	S2	428	OMU	C4-N3-C2	-5.13	119.81	126.58
1	L1	3899	OMG	C5-C4-N3	-5.13	120.14	128.46
46	S2	1031	A2M	C5-C4-N3	-5.12	120.07	126.75
1	L1	2837	OMU	C4-N3-C2	-5.12	119.82	126.58
3	L3	75	OMG	C5-C4-N3	-5.12	120.15	128.46
46	S2	1442	OMU	C4-N3-C2	-5.12	119.83	126.58
1	L1	4623	OMG	C5-C4-N3	-5.09	120.21	128.46
1	L1	4228	OMG	C5-C4-N3	-5.07	120.24	128.46
1	L1	3718	A2M	N3-C2-N1	-5.06	120.69	128.60
1	L1	4370	OMG	C5-C4-N3	-5.05	120.27	128.46
1	L1	4620	OMU	C4-N3-C2	-5.00	119.98	126.58
46	S2	1806	M7A	N3-C4-N9	4.99	133.17	126.87
1	L1	4392	OMG	C2-N3-C4	4.99	121.18	112.30
1	L1	1322	1MA	C1'-N9-C4	4.99	141.31	126.50
46	S2	1288	OMU	C4-N3-C2	-4.99	120.00	126.58
46	S2	1850	MA6	C4-C5-C6	4.98	121.45	115.88
46	S2	116	OMU	C4-N3-C2	-4.97	120.02	126.58
46	S2	668	A2M	C5-C4-N3	-4.95	120.29	126.75
46	S2	1248	B8N	C5-C4-N3	4.95	125.33	116.17
46	S2	1219	JMH	C1'-N1-C2	4.94	125.33	116.99
1	L1	2876	OMG	C2-N3-C4	4.93	121.09	112.30
46	S2	1851	MA6	N3-C4-N9	4.93	135.20	127.08
1	L1	4636	PSU	N1-C2-N3	4.92	120.71	115.13
1	L1	1316	OMG	C2-N3-C4	4.89	121.01	112.30
1	L1	2424	OMG	C5-C4-N3	-4.89	120.53	128.46
46	S2	1832	6MZ	C5-C4-N3	-4.85	120.43	126.75
1	L1	729	2MG	C5-C4-N3	-4.84	120.61	128.46
1	L1	1522	OMG	C2-N3-C4	4.80	120.85	112.30
1	L1	3627	OMG	C2-N3-C4	4.79	120.83	112.30
1	L1	2364	OMG	C2-N3-C4	4.79	120.83	112.30
1	L1	1625	OMG	C2-N3-C4	4.76	120.78	112.30
46	S2	1832	6MZ	N9-C8-N7	-4.75	107.42	113.91
1	L1	3899	OMG	C2-N3-C4	4.74	120.75	112.30
1	L1	4628	PSU	N1-C2-N3	4.73	120.49	115.13
46	S2	1851	MA6	C4-C5-C6	4.73	121.17	115.88
46	S2	683	OMG	C2-N3-C4	4.71	120.70	112.30
46	S2	822	PSU	N1-C2-N3	4.71	120.46	115.13
1	L1	4618	OMG	C2-N3-C4	4.68	120.63	112.30
1	L1	4220	6MZ	N9-C8-N7	-4.68	107.52	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4494	OMG	C2-N3-C4	4.67	120.63	112.30
1	L1	2508	PSU	N1-C2-N3	4.67	120.42	115.13
1	L1	729	2MG	C1'-N9-C8	-4.67	113.40	126.70
1	L1	4220	6MZ	C5-C4-N3	-4.65	120.68	126.75
46	S2	1850	MA6	N3-C4-N9	4.65	134.74	127.08
1	L1	4450	PSU	C4-N3-C2	-4.63	119.66	126.34
46	S2	814	5MU	N3-C2-N1	4.62	121.02	114.89
46	S2	436	OMG	C2-N3-C4	4.61	120.51	112.30
3	L3	75	OMG	C2-N3-C4	4.61	120.51	112.30
46	S2	867	OMG	C2-N3-C4	4.60	120.49	112.30
1	L1	4450	PSU	N1-C2-N3	4.59	120.33	115.13
46	S2	1081	PSU	N1-C2-N3	4.59	120.33	115.13
1	L1	978	2MG	C5-C4-N3	-4.59	121.02	128.46
1	L1	3792	OMG	C2-N3-C4	4.59	120.47	112.30
1	L1	4531	PSU	N1-C2-N3	4.58	120.32	115.13
1	L1	3715	PSU	N1-C2-N3	4.57	120.31	115.13
1	L1	3825	A2M	N9-C8-N7	-4.56	107.67	113.91
46	S2	612	PSU	N1-C2-N3	4.56	120.29	115.13
1	L1	4499	OMG	C2-N3-C4	4.55	120.41	112.30
1	L1	2508	PSU	C4-N3-C2	-4.54	119.79	126.34
1	L1	4442	PSU	N1-C2-N3	4.54	120.28	115.13
1	L1	1677	PSU	C4-N3-C2	-4.53	119.82	126.34
1	L1	4531	PSU	C4-N3-C2	-4.51	119.84	126.34
1	L1	4196	OMG	C2-N3-C4	4.50	120.33	112.30
1	L1	3785	A2M	C2'-C1'-N9	-4.50	105.95	113.53
1	L1	3944	OMG	C2-N3-C4	4.50	120.32	112.30
46	S2	1490	OMG	C2-N3-C4	4.49	120.30	112.30
1	L1	1677	PSU	N1-C2-N3	4.49	120.22	115.13
1	L1	3744	OMG	C2-N3-C4	4.48	120.28	112.30
1	L1	4442	PSU	C4-N3-C2	-4.48	119.89	126.34
46	S2	1678	A2M	N9-C8-N7	-4.47	107.80	113.91
1	L1	4293	PSU	N1-C2-N3	4.47	120.20	115.13
1	L1	1683	PSU	C4-N3-C2	-4.46	119.91	126.34
1	L1	4628	PSU	C4-N3-C2	-4.46	119.91	126.34
1	L1	1517	2MG	C5-C4-N3	-4.45	121.24	128.46
1	L1	4500	PSU	N1-C2-N3	4.45	120.17	115.13
46	S2	612	PSU	C4-N3-C2	-4.43	119.95	126.34
46	S2	1328	OMG	C2-N3-C4	4.43	120.19	112.30
1	L1	4293	PSU	C4-N3-C2	-4.42	119.96	126.34
46	S2	668	A2M	N9-C8-N7	-4.42	107.87	113.91
1	L1	978	2MG	C2-N1-C6	-4.41	119.41	124.48
46	S2	1850	MA6	N9-C8-N7	-4.40	107.90	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3729	PSU	C4-N3-C2	-4.40	120.00	126.34
46	S2	119	PSU	N1-C2-N3	4.39	120.11	115.13
1	L1	4637	OMG	C2-N3-C4	4.39	120.12	112.30
46	S2	822	PSU	C4-N3-C2	-4.38	120.03	126.34
46	S2	1830	UR3	C4-N3-C2	-4.37	120.45	124.56
1	L1	4623	OMG	C2-N3-C4	4.37	120.08	112.30
1	L1	3715	PSU	C4-N3-C2	-4.37	120.05	126.34
1	L1	3785	A2M	N9-C8-N7	-4.36	107.95	113.91
1	L1	4228	OMG	C2-N3-C4	4.36	120.07	112.30
1	L1	729	2MG	C2-N1-C6	-4.35	119.47	124.48
1	L1	3729	PSU	N1-C2-N3	4.35	120.06	115.13
46	S2	1243	PSU	N1-C2-N3	4.35	120.06	115.13
1	L1	4370	OMG	C2-N3-C4	4.35	120.04	112.30
46	S2	601	OMG	C2-N3-C4	4.34	120.04	112.30
3	L3	14	OMU	N3-C2-N1	4.30	120.59	114.89
46	S2	509	OMG	C2-N3-C4	4.29	119.95	112.30
1	L1	4403	PSU	C4-N3-C2	-4.29	120.16	126.34
46	S2	644	OMG	C2-N3-C4	4.27	119.90	112.30
1	L1	3764	PSU	N1-C2-N3	4.26	119.96	115.13
46	S2	1243	PSU	C4-N3-C2	-4.26	120.20	126.34
1	L1	4500	PSU	C4-N3-C2	-4.26	120.20	126.34
46	S2	119	PSU	C4-N3-C2	-4.23	120.24	126.34
1	L1	4228	OMG	C1'-N9-C4	-4.23	113.94	126.50
46	S2	590	A2M	N3-C4-N9	4.23	134.05	127.08
1	L1	2876	OMG	N9-C4-N3	4.22	134.42	125.94
1	L1	3899	OMG	C1'-N9-C4	-4.22	113.97	126.50
46	S2	468	A2M	N9-C8-N7	-4.22	108.15	113.91
1	L1	1326	A2M	N9-C8-N7	-4.21	108.16	113.91
1	L1	1582	PSU	N1-C2-N3	4.20	119.89	115.13
1	L1	3925	OMU	N3-C2-N1	4.20	120.47	114.89
1	L1	4523	A2M	N9-C8-N7	-4.20	108.17	113.91
1	L1	398	A2M	N9-C8-N7	-4.19	108.18	113.91
46	S2	1081	PSU	C4-N3-C2	-4.19	120.30	126.34
1	L1	4370	OMG	C1'-N9-C4	-4.17	114.10	126.50
1	L1	4227	OMU	N3-C2-N1	4.17	120.43	114.89
46	S2	166	A2M	N9-C8-N7	-4.17	108.21	113.91
1	L1	2815	A2M	N9-C8-N7	-4.16	108.22	113.91
1	L1	3867	A2M	N9-C8-N7	-4.16	108.22	113.91
1	L1	4403	PSU	N1-C2-N3	4.16	119.84	115.13
1	L1	2424	OMG	C2-N3-C4	4.14	119.68	112.30
1	L1	1625	OMG	N9-C4-N3	4.14	134.26	125.94
1	L1	4571	A2M	N9-C8-N7	-4.14	108.25	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1851	MA6	N9-C8-N7	-4.12	108.27	113.91
1	L1	1522	OMG	C1'-N9-C4	-4.11	114.30	126.50
1	L1	4620	OMU	N3-C2-N1	4.11	120.34	114.89
46	S2	1851	MA6	C2-N3-C4	4.10	121.43	111.75
1	L1	3764	PSU	C4-N3-C2	-4.10	120.44	126.34
46	S2	159	A2M	N9-C8-N7	-4.09	108.31	113.91
46	S2	1248	B8N	C4-N3-C2	-4.09	120.29	125.46
46	S2	27	A2M	N9-C8-N7	-4.07	108.35	113.91
1	L1	4530	UR3	C4-N3-C2	-4.07	120.73	124.56
3	L3	75	OMG	C1'-N9-C4	-4.05	114.47	126.50
46	S2	99	A2M	N9-C8-N7	-4.04	108.39	113.91
46	S2	590	A2M	C2-N3-C4	4.03	121.28	111.75
46	S2	576	A2M	N9-C8-N7	-4.03	108.40	113.91
46	S2	1383	A2M	N9-C8-N7	-4.02	108.42	113.91
46	S2	121	OMU	N3-C2-N1	4.01	120.21	114.89
46	S2	814	5MU	C5M-C5-C6	-4.01	117.50	122.85
46	S2	1832	6MZ	C5-N7-C8	4.01	109.20	103.51
1	L1	2424	OMG	C1'-N9-C4	-4.00	114.62	126.50
1	L1	2401	A2M	N9-C8-N7	-4.00	108.44	113.91
1	L1	4306	OMU	N3-C2-N1	4.00	120.20	114.89
1	L1	3723	A2M	N9-C8-N7	-3.99	108.45	113.91
1	L1	400	A2M	N9-C8-N7	-3.99	108.46	113.91
1	L1	3830	A2M	N9-C8-N7	-3.99	108.46	113.91
1	L1	1582	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L1	3818	UY1	C4-N3-C2	-3.97	120.62	126.34
46	S2	1326	UY1	C4-N3-C2	-3.97	120.62	126.34
1	L1	1517	2MG	C2-N1-C6	-3.95	119.94	124.48
46	S2	814	5MU	O4-C4-C5	-3.95	120.33	124.90
1	L1	2363	A2M	N9-C8-N7	-3.94	108.52	113.91
46	S2	823	PSU	O2-C2-N1	-3.94	118.46	122.79
1	L1	978	2MG	C1'-N9-C8	-3.91	115.57	126.70
46	S2	172	OMU	N3-C2-N1	3.91	120.08	114.89
1	L1	2424	OMG	C1'-N9-C8	3.89	137.77	126.70
1	L1	1871	A2M	C2-N3-C4	3.89	120.93	111.75
1	L1	4228	OMG	C1'-N9-C8	3.89	137.76	126.70
1	L1	4498	OMU	N3-C2-N1	3.86	120.02	114.89
1	L1	2837	OMU	N3-C2-N1	3.86	120.01	114.89
1	L1	4623	OMG	C1'-N9-C4	-3.86	115.05	126.50
46	S2	354	OMU	N3-C2-N1	3.85	119.99	114.89
1	L1	3899	OMG	C1'-N9-C8	3.83	137.60	126.70
1	L1	4447	5MC	C5-C6-N1	-3.83	119.40	123.34
1	L1	1871	A2M	N9-C8-N7	-3.83	108.68	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	2401	A2M	C2-N3-C4	3.82	120.78	111.75
46	S2	1806	M7A	C4-N9-C1'	-3.82	117.53	126.60
1	L1	4618	OMG	C1'-N9-C4	-3.82	115.17	126.50
1	L1	2787	A2M	C2-N3-C4	3.81	120.76	111.75
1	L1	4370	OMG	C1'-N9-C8	3.79	137.48	126.70
1	L1	3825	A2M	C2-N3-C4	3.79	120.69	111.75
46	S2	509	OMG	C1'-N9-C4	-3.78	115.27	126.50
1	L1	2787	A2M	N3-C4-N9	3.78	133.31	127.08
1	L1	3867	A2M	C2-N3-C4	3.77	120.67	111.75
1	L1	729	2MG	C1'-N9-C4	3.75	137.65	126.50
1	L1	2815	A2M	C2-N3-C4	3.75	120.61	111.75
46	S2	668	A2M	C2-N3-C4	3.74	120.59	111.75
1	L1	1524	A2M	N9-C8-N7	-3.74	108.80	113.91
1	L1	1534	A2M	C2-N3-C4	3.74	120.59	111.75
1	L1	1534	A2M	N9-C8-N7	-3.74	108.80	113.91
46	S2	166	A2M	C2-N3-C4	3.74	120.58	111.75
46	S2	1328	OMG	C1'-N9-C4	-3.73	115.41	126.50
46	S2	27	A2M	C2-N3-C4	3.73	120.56	111.75
46	S2	590	A2M	N9-C8-N7	-3.73	108.81	113.91
1	L1	4623	OMG	C1'-N9-C8	3.72	137.29	126.70
1	L1	3792	OMG	N9-C4-N3	3.72	133.41	125.94
46	S2	1219	JMH	C6-N1-C2	-3.72	118.46	121.79
1	L1	4571	A2M	C2-N3-C4	3.72	120.53	111.75
1	L1	2363	A2M	N3-C4-N9	3.71	133.20	127.08
46	S2	484	A2M	C2-N3-C4	3.70	120.50	111.75
46	S2	1031	A2M	N9-C8-N7	-3.70	108.85	113.91
46	S2	512	A2M	C2-N3-C4	3.70	120.50	111.75
1	L1	1522	OMG	C1'-N9-C8	3.70	137.23	126.70
46	S2	1830	UR3	C1'-N1-C2	3.70	123.23	116.99
46	S2	1442	OMU	N3-C2-N1	3.69	119.79	114.89
46	S2	512	A2M	N3-C4-N9	3.69	133.17	127.08
46	S2	512	A2M	N9-C8-N7	-3.69	108.86	113.91
1	L1	4618	OMG	C1'-N9-C8	3.69	137.20	126.70
46	S2	159	A2M	C2-N3-C4	3.69	120.46	111.75
1	L1	3944	OMG	C1'-N9-C4	-3.69	115.56	126.50
1	L1	1524	A2M	N3-C4-N9	3.68	133.15	127.08
46	S2	1383	A2M	C2-N3-C4	3.68	120.45	111.75
3	L3	75	OMG	C1'-N9-C8	3.68	137.16	126.70
46	S2	509	OMG	C1'-N9-C8	3.68	137.16	126.70
46	S2	867	OMG	C1'-N9-C4	-3.67	115.59	126.50
1	L1	398	A2M	C2-N3-C4	3.67	120.42	111.75
46	S2	1678	A2M	C2-N3-C4	3.67	120.41	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1832	6MZ	C2-N3-C4	3.66	120.40	111.75
1	L1	1322	1MA	C2-N3-C4	3.66	119.61	112.41
46	S2	1288	OMU	N3-C2-N1	3.65	119.74	114.89
1	L1	3830	A2M	C2-N3-C4	3.65	120.38	111.75
46	S2	823	PSU	C4-N3-C2	-3.65	121.08	126.34
46	S2	116	OMU	N3-C2-N1	3.65	119.73	114.89
46	S2	576	A2M	C2-N3-C4	3.64	120.36	111.75
46	S2	99	A2M	C2-N3-C4	3.64	120.36	111.75
46	S2	1031	A2M	C2-N3-C4	3.63	120.34	111.75
1	L1	4498	OMU	C5-C4-N3	3.63	120.28	114.84
1	L1	4523	A2M	C2-N3-C4	3.63	120.34	111.75
46	S2	1851	MA6	C2-N1-C6	3.63	120.33	111.75
1	L1	2787	A2M	N9-C8-N7	-3.63	108.95	113.91
46	S2	683	OMG	N9-C4-N3	3.63	133.23	125.94
1	L1	2364	OMG	N9-C4-N3	3.63	133.22	125.94
46	S2	644	OMG	C1'-N9-C4	-3.63	115.73	126.50
1	L1	1326	A2M	N3-C4-N9	3.63	133.06	127.08
1	L1	1524	A2M	C2-N3-C4	3.62	120.31	111.75
1	L1	3785	A2M	N3-C4-N9	3.62	133.04	127.08
1	L1	1871	A2M	N3-C4-N9	3.60	133.02	127.08
1	L1	3867	A2M	N3-C4-N9	3.60	133.01	127.08
46	S2	1850	MA6	C2-N1-C6	3.60	120.25	111.75
46	S2	484	A2M	N9-C8-N7	-3.60	109.00	113.91
46	S2	468	A2M	C2-N3-C4	3.59	120.24	111.75
46	S2	867	OMG	C1'-N9-C8	3.59	136.93	126.70
46	S2	436	OMG	N9-C4-N3	3.59	133.15	125.94
1	L1	2815	A2M	N3-C4-N9	3.59	133.00	127.08
1	L1	2401	A2M	N3-C4-N9	3.58	132.98	127.08
1	L1	1517	2MG	N9-C8-N7	-3.57	106.67	113.39
1	L1	3723	A2M	C2-N3-C4	3.57	120.17	111.75
46	S2	428	OMU	N3-C2-N1	3.55	119.60	114.89
1	L1	400	A2M	C2-N3-C4	3.54	120.12	111.75
1	L1	1517	2MG	C1'-N9-C8	-3.53	116.64	126.70
1	L1	1326	A2M	C2-N3-C4	3.53	120.08	111.75
1	L1	3825	A2M	C5-N7-C8	3.53	108.52	103.51
1	L1	4220	6MZ	C2-N3-C4	3.52	120.07	111.75
1	L1	3785	A2M	C2-N3-C4	3.51	120.04	111.75
1	L1	2787	A2M	C5-N7-C8	3.51	108.49	103.51
1	L1	4499	OMG	C1'-N9-C4	-3.50	116.10	126.50
1	L1	3944	OMG	C1'-N9-C8	3.50	136.65	126.70
1	L1	3744	OMG	N9-C4-N3	3.49	132.95	125.94
46	S2	1328	OMG	C1'-N9-C8	3.49	136.62	126.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4196	OMG	N9-C4-N3	3.47	132.90	125.94
46	S2	1850	MA6	C2-N3-C4	3.46	119.94	111.75
46	S2	601	OMG	C1'-N9-C4	-3.46	116.24	126.50
1	L1	1316	OMG	N9-C4-N3	3.45	132.87	125.94
1	L1	2363	A2M	C2-N3-C4	3.45	119.90	111.75
1	L1	4530	UR3	C6-N1-C2	-3.44	118.71	121.79
1	L1	400	A2M	N3-C4-N9	3.43	132.74	127.08
46	S2	644	OMG	C1'-N9-C8	3.43	136.45	126.70
1	L1	3744	OMG	C1'-N9-C4	-3.42	116.33	126.50
46	S2	683	OMG	C1'-N9-C4	-3.42	116.35	126.50
3	L3	14	OMU	C5-C4-N3	3.41	119.94	114.84
46	S2	814	5MU	C6-C5-C4	3.41	120.88	118.03
1	L1	1522	OMG	C2-N1-C6	-3.40	118.90	125.10
46	S2	354	OMU	C5-C4-N3	3.39	119.92	114.84
1	L1	4494	OMG	N9-C4-N3	3.39	132.75	125.94
1	L1	2364	OMG	C2-N1-C6	-3.39	118.91	125.10
1	L1	4227	OMU	C5-C4-N3	3.39	119.92	114.84
1	L1	4637	OMG	N9-C4-N3	3.38	132.73	125.94
1	L1	3627	OMG	C1'-N9-C4	-3.37	116.48	126.50
1	L1	4220	6MZ	C5-N7-C8	3.37	108.30	103.51
46	S2	99	A2M	N3-C4-N9	3.37	132.64	127.08
1	L1	1522	OMG	N9-C4-N3	3.37	132.71	125.94
1	L1	978	2MG	N9-C8-N7	-3.37	107.04	113.39
46	S2	1832	6MZ	C9-N6-C6	3.37	125.77	122.87
1	L1	3825	A2M	N3-C4-N9	3.36	132.62	127.08
1	L1	1316	OMG	C1'-N9-C4	-3.36	116.52	126.50
1	L1	4499	OMG	N9-C4-N3	3.36	132.68	125.94
46	S2	576	A2M	N3-C4-N9	3.35	132.61	127.08
46	S2	159	A2M	N3-C4-N9	3.35	132.61	127.08
1	L1	4392	OMG	C1'-N9-C8	3.35	136.22	126.70
1	L1	4523	A2M	C5-N7-C8	3.34	108.26	103.51
46	S2	116	OMU	C5-C4-N3	3.34	119.84	114.84
1	L1	3762	B8H	C5-C4-N3	3.34	124.13	116.58
46	S2	1490	OMG	C1'-N9-C4	-3.33	116.60	126.50
1	L1	4306	OMU	C5-C4-N3	3.33	119.83	114.84
46	S2	428	OMU	C5-C4-N3	3.33	119.81	114.84
1	L1	4196	OMG	C2-N1-C6	-3.33	119.04	125.10
1	L1	398	A2M	N3-C4-N9	3.32	132.56	127.08
1	L1	1625	OMG	C2-N1-C6	-3.31	119.07	125.10
46	S2	1678	A2M	N3-C4-N9	3.30	132.53	127.08
1	L1	3627	OMG	N9-C4-N3	3.30	132.57	125.94
46	S2	27	A2M	N3-C4-N9	3.30	132.52	127.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1678	A2M	C5-N7-C8	3.30	108.20	103.51
46	S2	601	OMG	C1'-N9-C8	3.30	136.09	126.70
1	L1	3627	OMG	C1'-N9-C8	3.30	136.08	126.70
46	S2	1851	MA6	C5-N7-C8	3.29	108.19	103.51
1	L1	1534	A2M	N3-C4-N9	3.29	132.50	127.08
46	S2	166	A2M	N3-C4-N9	3.28	132.48	127.08
1	L1	4392	OMG	N9-C4-N3	3.28	132.52	125.94
46	S2	1442	OMU	C5-C4-N3	3.27	119.73	114.84
1	L1	3762	B8H	O2-C2-N1	-3.26	119.20	122.87
1	L1	2837	OMU	C5-C4-N3	3.25	119.71	114.84
46	S2	1288	OMU	C5-C4-N3	3.25	119.71	114.84
1	L1	1316	OMG	C2-N1-C6	-3.25	119.17	125.10
46	S2	121	OMU	C5-C4-N3	3.25	119.70	114.84
1	L1	4196	OMG	C1'-N9-C4	-3.24	116.86	126.50
46	S2	1374	5MC	C5-C6-N1	-3.24	120.00	123.34
1	L1	729	2MG	N9-C8-N7	-3.23	107.30	113.39
1	L1	4220	6MZ	C9-N6-C6	-3.23	120.09	122.87
46	S2	1490	OMG	N9-C4-N3	3.23	132.42	125.94
46	S2	1490	OMG	C1'-N9-C8	3.23	135.88	126.70
1	L1	2876	OMG	C2-N1-C6	-3.22	119.23	125.10
46	S2	468	A2M	N3-C4-N9	3.22	132.38	127.08
1	L1	3627	OMG	C2-N1-C6	-3.21	119.24	125.10
46	S2	172	OMU	C5-C4-N3	3.21	119.65	114.84
1	L1	1322	1MA	N9-C8-N7	-3.21	107.34	113.39
1	L1	3718	A2M	C2-N3-C4	3.21	119.33	111.75
1	L1	4392	OMG	C1'-N9-C4	-3.20	116.99	126.50
1	L1	4637	OMG	C1'-N9-C8	3.20	135.81	126.70
1	L1	2401	A2M	C5-N7-C8	3.20	108.05	103.51
46	S2	166	A2M	C5-N7-C8	3.18	108.03	103.51
1	L1	3782	5MC	C5-C6-N1	-3.18	120.07	123.34
46	S2	1326	UY1	O2-C2-N1	-3.18	119.29	122.79
1	L1	2815	A2M	C5-N7-C8	3.17	108.02	103.51
1	L1	4499	OMG	C1'-N9-C8	3.17	135.73	126.70
1	L1	4494	OMG	C1'-N9-C8	3.17	135.72	126.70
46	S2	1832	6MZ	C4-C5-C6	3.17	119.27	116.81
46	S2	1248	B8N	N3-C2-N1	3.17	121.24	116.76
46	S2	601	OMG	N9-C4-N3	3.17	132.29	125.94
46	S2	1850	MA6	C4-N9-C8	3.16	109.16	105.73
1	L1	3744	OMG	C1'-N9-C8	3.16	135.69	126.70
1	L1	3944	OMG	N9-C4-N3	3.15	132.27	125.94
46	S2	159	A2M	C5-N7-C8	3.15	107.99	103.51
46	S2	1832	6MZ	C4-C5-N7	-3.15	106.78	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1326	A2M	C5-N7-C8	3.15	107.98	103.51
46	S2	1830	UR3	C6-N1-C2	-3.15	118.97	121.79
46	S2	436	OMG	C2-N1-C6	-3.15	119.36	125.10
46	S2	683	OMG	C1'-N9-C8	3.14	135.64	126.70
1	L1	4637	OMG	C1'-N9-C4	-3.14	117.17	126.50
46	S2	509	OMG	C2-N1-C6	-3.14	119.38	125.10
1	L1	4523	A2M	N3-C4-N9	3.14	132.25	127.08
1	L1	4571	A2M	N3-C4-N9	3.14	132.25	127.08
46	S2	1383	A2M	N3-C4-N9	3.14	132.25	127.08
1	L1	3925	OMU	C5-C4-N3	3.14	119.53	114.84
46	S2	436	OMG	C1'-N9-C4	-3.13	117.19	126.50
1	L1	3944	OMG	C2-N1-C6	-3.13	119.39	125.10
1	L1	4494	OMG	C1'-N9-C4	-3.13	117.21	126.50
1	L1	3830	A2M	N3-C4-N9	3.13	132.24	127.08
1	L1	4494	OMG	C2-N1-C6	-3.13	119.40	125.10
1	L1	4220	6MZ	C4-C5-C6	3.12	119.23	116.81
1	L1	3867	A2M	C5-N7-C8	3.12	107.94	103.51
46	S2	867	OMG	N9-C4-N3	3.12	132.21	125.94
1	L1	3744	OMG	C2-N1-C6	-3.12	119.41	125.10
46	S2	1806	M7A	C2-N3-C4	3.12	119.12	111.75
1	L1	398	A2M	C5-N7-C8	3.12	107.94	103.51
1	L1	2363	A2M	C5-N7-C8	3.11	107.93	103.51
1	L1	4620	OMU	C5-C4-N3	3.11	119.50	114.84
1	L1	1522	OMG	C5-C6-N1	3.11	121.09	113.19
1	L1	1871	A2M	C5-N7-C8	3.11	107.93	103.51
1	L1	3723	A2M	N3-C4-N9	3.11	132.21	127.08
46	S2	484	A2M	N3-C4-N9	3.11	132.20	127.08
1	L1	1534	A2M	C5-N7-C8	3.11	107.92	103.51
46	S2	1328	OMG	N9-C4-N3	3.10	132.16	125.94
1	L1	4571	A2M	C5-N7-C8	3.10	107.91	103.51
1	L1	3818	UY1	O2-C2-N1	-3.10	119.38	122.79
1	L1	1683	PSU	C6-N1-C2	-3.10	119.52	122.68
1	L1	1316	OMG	C1'-N9-C8	3.10	135.51	126.70
1	L1	4370	OMG	N9-C4-N3	3.10	132.16	125.94
46	S2	867	OMG	C2-N1-C6	-3.10	119.45	125.10
46	S2	1328	OMG	C2-N1-C6	-3.10	119.45	125.10
1	L1	4442	PSU	O2-C2-N1	-3.09	119.39	122.79
46	S2	683	OMG	C2-N1-C6	-3.09	119.47	125.10
46	S2	1850	MA6	C5-N7-C8	3.08	107.89	103.51
1	L1	4228	OMG	N9-C4-N3	3.08	132.13	125.94
46	S2	1031	A2M	N3-C4-N9	3.08	132.15	127.08
3	L3	75	OMG	N9-C4-N3	3.08	132.12	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1383	A2M	C5-N7-C8	3.07	107.88	103.51
1	L1	3785	A2M	C5-N7-C8	3.07	107.88	103.51
1	L1	4637	OMG	C2-N1-C6	-3.07	119.50	125.10
46	S2	644	OMG	C2-N1-C6	-3.07	119.51	125.10
46	S2	428	OMU	O4-C4-C5	-3.07	119.77	125.16
46	S2	27	A2M	C5-N7-C8	3.06	107.85	103.51
46	S2	509	OMG	N9-C4-N3	3.06	132.07	125.94
1	L1	4447	5MC	C1'-N1-C6	3.05	126.20	121.12
46	S2	668	A2M	C5-N7-C8	3.05	107.84	103.51
1	L1	2787	A2M	C6-C5-C4	3.05	121.28	117.18
46	S2	644	OMG	N9-C4-N3	3.05	132.06	125.94
1	L1	3899	OMG	N9-C8-N7	-3.05	107.65	113.39
46	S2	468	A2M	C5-N7-C8	3.05	107.84	103.51
1	L1	3718	A2M	N9-C8-N7	-3.05	109.75	113.91
1	L1	978	2MG	C1'-N9-C4	3.04	135.54	126.50
1	L1	3899	OMG	N9-C4-N3	3.04	132.05	125.94
46	S2	484	A2M	C5-N7-C8	3.03	107.82	103.51
1	L1	4196	OMG	C1'-N9-C8	3.03	135.32	126.70
46	S2	1806	M7A	C71-N7-C5	-3.03	112.37	124.01
3	L3	75	OMG	C2-N1-C6	-3.02	119.60	125.10
1	L1	4228	OMG	C2-N1-C6	-3.01	119.60	125.10
1	L1	2424	OMG	C2-N1-C6	-3.01	119.61	125.10
1	L1	2351	OMC	O2-C2-N3	-3.00	117.45	122.33
46	S2	99	A2M	C5-N7-C8	2.99	107.76	103.51
46	S2	116	OMU	O4-C4-C5	-2.99	119.91	125.16
1	L1	4618	OMG	N9-C4-N3	2.99	131.94	125.94
1	L1	1524	A2M	C4'-O4'-C1'	-2.99	102.88	109.47
3	L3	75	OMG	N9-C8-N7	-2.99	107.77	113.39
1	L1	4392	OMG	C2-N1-C6	-2.98	119.66	125.10
1	L1	4370	OMG	N9-C8-N7	-2.98	107.78	113.39
1	L1	3830	A2M	C5-N7-C8	2.98	107.74	103.51
46	S2	576	A2M	C5-N7-C8	2.98	107.74	103.51
1	L1	4335	5MC	C5-C6-N1	-2.97	120.28	123.34
46	S2	601	OMG	C2-N1-C6	-2.97	119.69	125.10
46	S2	590	A2M	C5-N7-C8	2.97	107.72	103.51
46	S2	436	OMG	C1'-N9-C8	2.96	135.12	126.70
1	L1	4500	PSU	C6-N1-C2	-2.95	119.66	122.68
1	L1	729	2MG	N9-C4-N3	2.95	131.87	125.94
1	L1	4499	OMG	C2-N1-C6	-2.95	119.73	125.10
1	L1	400	A2M	C5-N7-C8	2.94	107.69	103.51
1	L1	4623	OMG	C2-N1-C6	-2.94	119.73	125.10
1	L1	1316	OMG	N9-C8-N7	-2.93	107.88	113.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	2364	OMG	C1'-N9-C4	-2.92	117.84	126.50
46	S2	121	OMU	O4-C4-C5	-2.91	120.04	125.16
1	L1	1522	OMG	N9-C8-N7	-2.90	107.93	113.39
1	L1	4228	OMG	N9-C8-N7	-2.90	107.93	113.39
46	S2	1442	OMU	O4-C4-C5	-2.90	120.06	125.16
1	L1	3723	A2M	C5-N7-C8	2.89	107.62	103.51
1	L1	3792	OMG	C1'-N9-C4	-2.89	117.92	126.50
1	L1	1524	A2M	C5-N7-C8	2.89	107.61	103.51
1	L1	3792	OMG	C2-N1-C6	-2.89	119.84	125.10
1	L1	978	2MG	CM2-N2-C2	-2.89	117.49	123.86
1	L1	3782	5MC	CM5-C5-C6	-2.88	119.00	122.85
1	L1	3899	OMG	C2-N1-C6	-2.87	119.86	125.10
1	L1	1517	2MG	N1-C2-N3	-2.87	119.51	123.95
1	L1	4370	OMG	C2-N1-C6	-2.87	119.86	125.10
1	L1	4618	OMG	C2-N1-C6	-2.86	119.88	125.10
46	S2	172	OMU	O4-C4-C5	-2.86	120.14	125.16
1	L1	4293	PSU	O2-C2-N1	-2.85	119.65	122.79
1	L1	2364	OMG	C5-C6-N1	2.85	120.43	113.19
1	L1	1316	OMG	C5-C6-N1	2.85	120.43	113.19
1	L1	3718	A2M	N3-C4-N9	2.85	131.78	127.08
1	L1	3899	OMG	C5-C6-N1	2.84	120.41	113.19
1	L1	4531	PSU	C6-C5-C4	2.83	120.18	118.20
46	S2	683	OMG	C5-C6-N1	2.81	120.33	113.19
46	S2	1288	OMU	O4-C4-C5	-2.81	120.22	125.16
1	L1	4498	OMU	O4-C4-C5	-2.80	120.23	125.16
46	S2	1490	OMG	C2-N1-C6	-2.80	120.00	125.10
1	L1	4494	OMG	C5-C6-N1	2.79	120.28	113.19
3	L3	75	OMG	C5-C6-N1	2.79	120.27	113.19
1	L1	4228	OMG	C5-C6-N1	2.79	120.27	113.19
46	S2	436	OMG	C5-C6-N1	2.78	120.24	113.19
46	S2	1328	OMG	N9-C8-N7	-2.77	108.17	113.39
1	L1	4618	OMG	C5-C6-N1	2.77	120.22	113.19
1	L1	3744	OMG	C5-C6-N1	2.76	120.21	113.19
46	S2	668	A2M	N3-C4-N9	2.76	131.63	127.08
1	L1	4623	OMG	N9-C4-N3	2.76	131.48	125.94
1	L1	2364	OMG	C1'-N9-C8	2.76	134.55	126.70
1	L1	4628	PSU	O2-C2-N1	-2.75	119.76	122.79
46	S2	1031	A2M	C5-N7-C8	2.75	107.42	103.51
1	L1	2424	OMG	N9-C4-N3	2.75	131.46	125.94
1	L1	2876	OMG	C5-C6-N1	2.75	120.17	113.19
1	L1	3944	OMG	C5-C6-N1	2.75	120.16	113.19
1	L1	2424	OMG	O6-C6-C5	-2.75	119.32	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4228	OMG	O6-C6-C5	-2.74	119.33	126.60
46	S2	1328	OMG	C5-C6-N1	2.74	120.14	113.19
1	L1	3627	OMG	C5-C6-N1	2.73	120.13	113.19
46	S2	867	OMG	C5-C6-N1	2.73	120.12	113.19
1	L1	4499	OMG	N9-C8-N7	-2.73	108.25	113.39
1	L1	4623	OMG	N9-C8-N7	-2.73	108.25	113.39
46	S2	644	OMG	N9-C8-N7	-2.72	108.26	113.39
1	L1	3744	OMG	N9-C8-N7	-2.72	108.28	113.39
46	S2	1830	UR3	O2-C2-N3	-2.71	117.52	121.34
1	L1	3944	OMG	N9-C8-N7	-2.71	108.29	113.39
1	L1	4370	OMG	C5-C6-N1	2.70	120.06	113.19
1	L1	4499	OMG	C5-C6-N1	2.70	120.06	113.19
46	S2	512	A2M	C5-N7-C8	2.70	107.35	103.51
1	L1	4196	OMG	N9-C8-N7	-2.70	108.30	113.39
1	L1	2363	A2M	C6-C5-C4	2.69	120.81	117.18
46	S2	1337	4AC	C6-C5-C4	2.69	120.26	116.96
1	L1	1677	PSU	O2-C2-N1	-2.69	119.83	122.79
1	L1	978	2MG	C5-C6-N1	2.69	120.03	113.19
1	L1	1517	2MG	C5-C6-N1	2.69	120.01	113.19
1	L1	1625	OMG	C5-C6-N1	2.68	120.00	113.19
46	S2	683	OMG	N9-C8-N7	-2.68	108.35	113.39
1	L1	4335	5MC	CM5-C5-C6	-2.67	119.28	122.85
1	L1	4618	OMG	N9-C8-N7	-2.67	108.36	113.39
1	L1	1625	OMG	O6-C6-C5	-2.66	119.53	126.60
1	L1	3792	OMG	C5-C6-N1	2.66	119.95	113.19
1	L1	2364	OMG	N9-C8-N7	-2.66	108.38	113.39
1	L1	1522	OMG	O6-C6-C5	-2.66	119.55	126.60
46	S2	1490	OMG	C5-C6-N1	2.66	119.94	113.19
1	L1	3729	PSU	O2-C2-N1	-2.65	119.87	122.79
1	L1	4403	PSU	O2-C2-N1	-2.65	119.87	122.79
46	S2	1832	6MZ	N3-C4-N9	2.65	131.45	127.08
1	L1	4196	OMG	C5-C6-N1	2.65	119.92	113.19
46	S2	354	OMU	O4-C4-C5	-2.65	120.50	125.16
46	S2	436	OMG	O6-C6-C5	-2.65	119.58	126.60
1	L1	1871	A2M	C2'-C1'-N9	-2.64	109.09	113.53
46	S2	509	OMG	C5-C6-N1	2.63	119.88	113.19
1	L1	4392	OMG	C5-C6-N1	2.63	119.87	113.19
46	S2	822	PSU	O2-C2-N1	-2.63	119.90	122.79
1	L1	3925	OMU	O4-C4-C5	-2.63	120.54	125.16
1	L1	3792	OMG	C1'-N9-C8	2.63	134.17	126.70
1	L1	1517	2MG	CM2-N2-C2	-2.62	118.08	123.86
1	L1	2424	OMG	C5-C6-N1	2.62	119.83	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3627	OMG	N9-C8-N7	-2.61	108.47	113.39
1	L1	1522	OMG	C2'-C1'-N9	-2.61	109.16	114.22
1	L1	3899	OMG	O6-C6-C5	-2.61	119.67	126.60
1	L1	2508	PSU	O2-C2-N1	-2.61	119.92	122.79
1	L1	3792	OMG	N9-C8-N7	-2.61	108.48	113.39
1	L1	4499	OMG	O6-C6-C5	-2.60	119.69	126.60
1	L1	4671	B8T	C6-C5-C4	2.60	120.14	116.96
1	L1	1517	2MG	C1'-N9-C4	2.60	134.22	126.50
46	S2	644	OMG	C5-C6-N1	2.60	119.79	113.19
46	S2	814	5MU	C5M-C5-C4	2.59	121.62	118.77
1	L1	4456	OMC	O2-C2-N3	-2.59	118.12	122.33
46	S2	867	OMG	O6-C6-C5	-2.59	119.73	126.60
46	S2	601	OMG	C5-C6-N1	2.59	119.76	113.19
1	L1	4227	OMU	O4-C4-C5	-2.58	120.62	125.16
1	L1	4500	PSU	O2-C2-N1	-2.58	119.95	122.79
1	L1	1456	JMH	C6-N1-C2	-2.58	119.48	121.79
1	L1	2424	OMG	N9-C8-N7	-2.58	108.53	113.39
46	S2	1219	JMH	O2-C2-N3	-2.58	117.71	121.34
1	L1	4442	PSU	C6-N1-C2	-2.57	120.05	122.68
46	S2	612	PSU	O2-C2-N1	-2.57	119.96	122.79
1	L1	4623	OMG	C5-C6-N1	2.57	119.72	113.19
46	S2	1288	OMU	C1'-N1-C2	2.57	122.22	117.57
1	L1	729	2MG	C5-C6-N1	2.56	119.68	113.19
1	L1	4196	OMG	O6-C6-C5	-2.55	119.83	126.60
46	S2	683	OMG	O6-C6-C5	-2.55	119.83	126.60
1	L1	1322	1MA	CM1-N1-C2	-2.55	115.18	120.55
1	L1	4306	OMU	O2-C2-N1	-2.55	119.40	122.79
1	L1	978	2MG	O6-C6-C5	-2.55	119.85	126.60
1	L1	2876	OMG	O6-C6-C5	-2.55	119.85	126.60
1	L1	3744	OMG	O6-C6-C5	-2.54	119.85	126.60
46	S2	601	OMG	N9-C8-N7	-2.54	108.60	113.39
1	L1	2364	OMG	O6-C6-C5	-2.54	119.86	126.60
46	S2	867	OMG	N9-C8-N7	-2.54	108.61	113.39
1	L1	3762	B8H	O4-C4-N3	-2.54	115.25	120.12
1	L1	1517	2MG	O6-C6-C5	-2.54	119.87	126.60
1	L1	3715	PSU	C6-N1-C2	-2.54	120.09	122.68
46	S2	436	OMG	N9-C8-N7	-2.54	108.61	113.39
1	L1	4636	PSU	O2-C2-N1	-2.53	120.00	122.79
46	S2	1832	6MZ	C4-N9-C8	2.53	108.47	105.73
3	L3	14	OMU	O4-C4-C5	-2.52	120.72	125.16
46	S2	1328	OMG	O6-C6-C5	-2.52	119.91	126.60
1	L1	1582	PSU	C6-N1-C2	-2.52	120.11	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1081	PSU	C6-N1-C2	-2.51	120.11	122.68
1	L1	3808	OMC	O2-C2-N3	-2.51	118.25	122.33
46	S2	1490	OMG	O6-C6-C5	-2.51	119.95	126.60
1	L1	4637	OMG	C5-C6-N1	2.50	119.55	113.19
46	S2	822	PSU	C6-N1-C2	-2.50	120.12	122.68
1	L1	978	2MG	N9-C4-N3	2.50	130.96	125.94
1	L1	4618	OMG	O6-C6-C5	-2.49	119.99	126.60
1	L1	3944	OMG	O6-C6-C5	-2.48	120.01	126.60
46	S2	612	PSU	C6-N1-C2	-2.48	120.14	122.68
46	S2	814	5MU	O2-C2-N3	-2.48	116.88	121.50
1	L1	1871	A2M	O4'-C1'-N9	2.48	112.95	108.06
46	S2	1243	PSU	O2-C2-N1	-2.47	120.07	122.79
1	L1	3718	A2M	C6-C5-C4	2.47	120.51	117.18
46	S2	509	OMG	N9-C8-N7	-2.47	108.74	113.39
46	S2	509	OMG	O6-C6-C5	-2.47	120.05	126.60
3	L3	75	OMG	O6-C6-C5	-2.47	120.06	126.60
1	L1	4494	OMG	O6-C6-C5	-2.47	120.06	126.60
1	L1	1316	OMG	C8-N7-C5	2.46	108.69	104.24
46	S2	1806	M7A	C5-C4-N3	-2.44	120.89	126.62
1	L1	3764	PSU	C6-N1-C2	-2.44	120.19	122.68
46	S2	1842	4AC	C5-C4-N3	-2.44	118.67	122.59
1	L1	3718	A2M	C5-N7-C8	2.43	106.97	103.51
1	L1	4220	6MZ	C4-C5-N7	-2.42	107.67	110.62
1	L1	4306	OMU	O4-C4-C5	-2.42	120.91	125.16
1	L1	1677	PSU	C6-N1-C2	-2.41	120.21	122.68
1	L1	2876	OMG	N9-C8-N7	-2.41	108.86	113.39
46	S2	1248	B8N	C31-N3-C4	2.41	120.86	117.31
46	S2	119	PSU	C6-N1-C2	-2.40	120.23	122.68
46	S2	1678	A2M	C4-N9-C8	2.40	108.33	105.73
1	L1	1871	A2M	C6-C5-C4	2.40	120.41	117.18
1	L1	4494	OMG	N9-C8-N7	-2.40	108.88	113.39
1	L1	4637	OMG	N9-C8-N7	-2.40	108.88	113.39
46	S2	814	5MU	C1'-N1-C2	2.40	121.91	117.57
46	S2	822	PSU	O4'-C1'-C2'	2.40	108.52	105.14
46	S2	1490	OMG	N9-C8-N7	-2.39	108.88	113.39
1	L1	4628	PSU	C6-N1-C2	-2.39	120.24	122.68
46	S2	1842	4AC	C6-C5-C4	2.39	119.89	116.96
46	S2	644	OMG	O6-C6-C5	-2.39	120.25	126.60
1	L1	2876	OMG	C1'-N9-C4	-2.39	119.42	126.50
1	L1	3869	OMC	O2-C2-N3	-2.39	118.45	122.33
1	L1	1517	2MG	C8-N7-C5	2.38	108.55	104.24
1	L1	2824	OMC	O2-C2-N3	-2.38	118.46	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	978	2MG	N1-C2-N3	-2.38	120.28	123.95
1	L1	1517	2MG	N9-C4-N3	2.37	130.71	125.94
1	L1	3715	PSU	O2-C2-N1	-2.37	120.19	122.79
1	L1	3792	OMG	O6-C6-C5	-2.36	120.33	126.60
46	S2	590	A2M	C6-C5-C4	2.36	120.36	117.18
1	L1	3867	A2M	C2'-C1'-N9	2.36	117.50	113.53
1	L1	2837	OMU	O4-C4-C5	-2.35	121.02	125.16
46	S2	1337	4AC	C5-C4-N3	-2.35	118.81	122.59
1	L1	4392	OMG	O6-C6-C5	-2.35	120.37	126.60
1	L1	729	2MG	O6-C6-C5	-2.34	120.39	126.60
1	L1	4293	PSU	C6-N1-C2	-2.34	120.29	122.68
46	S2	1243	PSU	C6-N1-C2	-2.33	120.30	122.68
1	L1	4530	UR3	C1'-N1-C2	2.32	120.91	116.99
1	L1	4220	6MZ	N3-C4-N9	2.32	130.91	127.08
1	L1	4450	PSU	O2-C2-N1	-2.32	120.24	122.79
46	S2	1710	OMC	O2-C2-N3	-2.32	118.56	122.33
1	L1	3729	PSU	C6-N1-C2	-2.32	120.31	122.68
1	L1	3785	A2M	C4-N9-C8	2.31	108.23	105.73
46	S2	1851	MA6	C4-N9-C8	2.31	108.23	105.73
1	L1	1316	OMG	O6-C6-C5	-2.31	120.48	126.60
1	L1	1322	1MA	C5-C4-N3	-2.31	123.82	127.26
46	S2	601	OMG	O6-C6-C5	-2.30	120.49	126.60
1	L1	4620	OMU	O4-C4-C5	-2.30	121.11	125.16
1	L1	4450	PSU	C6-C5-C4	2.30	119.81	118.20
1	L1	4392	OMG	N9-C8-N7	-2.30	109.06	113.39
46	S2	1248	B8N	O4'-C1'-C2'	2.29	108.38	105.14
1	L1	1326	A2M	C4-N9-C8	2.29	108.21	105.73
1	L1	1625	OMG	C1'-N9-C4	-2.29	119.70	126.50
46	S2	814	5MU	O4-C4-N3	-2.29	115.73	120.12
46	S2	119	PSU	O2-C2-N1	-2.29	120.27	122.79
46	S2	590	A2M	C4'-O4'-C1'	-2.29	104.43	109.47
1	L1	978	2MG	C8-N7-C5	2.29	108.38	104.24
1	L1	3627	OMG	O6-C6-C5	-2.29	120.53	126.60
1	L1	1625	OMG	N9-C8-N7	-2.29	109.08	113.39
46	S2	484	A2M	C5-C4-N9	2.27	108.43	105.78
1	L1	1625	OMG	C1'-N9-C8	2.27	133.16	126.70
1	L1	2837	OMU	C2'-C1'-N1	-2.26	109.83	114.22
1	L1	3764	PSU	O2-C2-N1	-2.26	120.30	122.79
1	L1	4370	OMG	O6-C6-C5	-2.26	120.60	126.60
46	S2	354	OMU	O2-C2-N1	-2.26	119.78	122.79
1	L1	3825	A2M	C6-C5-C4	2.26	120.22	117.18
1	L1	4220	6MZ	C5-C4-N9	2.26	108.41	105.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1850	MA6	C6-C5-N7	-2.25	129.51	133.28
1	L1	729	2MG	C8-N7-C5	2.25	108.31	104.24
1	L1	2787	A2M	C5-C4-N9	2.25	108.40	105.78
46	S2	484	A2M	C4-C5-N7	-2.24	107.88	110.62
1	L1	2876	OMG	C1'-N9-C8	2.24	133.08	126.70
46	S2	612	PSU	O4'-C1'-C2'	2.24	108.31	105.14
1	L1	2876	OMG	C8-N7-C5	2.24	108.30	104.24
1	L1	2824	OMC	C1'-N1-C2	2.24	123.41	118.42
1	L1	3841	OMC	O2-C2-N3	-2.23	118.70	122.33
1	L1	2787	A2M	C4-C5-N7	-2.23	107.90	110.62
1	L1	1534	A2M	C4-C5-N7	-2.23	107.91	110.62
1	L1	4623	OMG	O6-C6-C5	-2.22	120.70	126.60
1	L1	4531	PSU	O2-C2-N1	-2.22	120.35	122.79
1	L1	4523	A2M	C4-C5-N7	-2.22	107.92	110.62
46	S2	1081	PSU	O4'-C1'-C2'	2.22	108.27	105.14
3	L3	75	OMG	C8-N7-C5	2.22	108.25	104.24
1	L1	1326	A2M	C6-C5-C4	2.21	120.16	117.18
46	S2	116	OMU	C1'-N1-C2	2.21	121.58	117.57
1	L1	400	A2M	C6-C5-C4	2.21	120.16	117.18
1	L1	2351	OMC	O2-C2-N1	2.21	123.45	118.89
46	S2	1374	5MC	CM5-C5-C6	-2.20	119.91	122.85
46	S2	484	A2M	C6-C5-C4	2.20	120.14	117.18
1	L1	3867	A2M	C4-N9-C8	2.20	108.11	105.73
1	L1	3899	OMG	C8-N7-C5	2.19	108.21	104.24
46	S2	668	A2M	C4-N9-C8	2.19	108.11	105.73
1	L1	4196	OMG	C8-N7-C5	2.19	108.21	104.24
1	L1	4220	6MZ	C4-N9-C8	2.19	108.10	105.73
46	S2	1842	4AC	O2-C2-N3	-2.19	118.77	122.33
1	L1	1582	PSU	O2-C2-N1	-2.19	120.38	122.79
1	L1	3899	OMG	N1-C2-N3	-2.18	119.25	123.32
1	L1	1534	A2M	C6-C5-C4	2.18	120.11	117.18
1	L1	2364	OMG	C8-N7-C5	2.18	108.18	104.24
1	L1	4370	OMG	C8-N7-C5	2.18	108.18	104.24
46	S2	1391	OMC	O2-C2-N3	-2.17	118.80	122.33
46	S2	166	A2M	C4-C5-N7	-2.17	107.98	110.62
1	L1	4500	PSU	O4'-C1'-C2'	2.16	108.19	105.14
1	L1	3627	OMG	C8-N7-C5	2.16	108.15	104.24
46	S2	1248	B8N	O4-C4-N3	-2.16	116.31	119.98
1	L1	4450	PSU	C6-N1-C2	-2.16	120.47	122.68
1	L1	4637	OMG	O6-C6-C5	-2.16	120.87	126.60
46	S2	1678	A2M	C4-C5-N7	-2.16	107.99	110.62
1	L1	4636	PSU	O4'-C1'-C2'	2.15	108.18	105.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	2401	A2M	C6-C5-C4	2.15	120.07	117.18
1	L1	1524	A2M	C6-C5-C4	2.14	120.06	117.18
1	L1	4636	PSU	C6-C5-C4	2.14	119.69	118.20
1	L1	1322	1MA	C2'-C1'-N9	2.14	119.27	113.22
46	S2	159	A2M	C6-C5-C4	2.13	120.05	117.18
1	L1	2351	OMC	C1'-N1-C2	2.13	123.18	118.42
46	S2	823	PSU	C5-C6-N1	-2.13	118.91	122.11
1	L1	4523	A2M	C6-C5-C4	2.13	120.05	117.18
46	S2	517	OMC	O2-C2-N3	-2.13	118.87	122.33
46	S2	1219	JMH	C1'-N1-C6	-2.13	116.20	120.84
1	L1	2815	A2M	C6-C5-C4	2.13	120.04	117.18
46	S2	576	A2M	C2'-C1'-N9	-2.12	109.95	113.53
1	L1	4531	PSU	C6-N1-C2	-2.12	120.52	122.68
1	L1	2422	OMC	O2-C2-N3	-2.12	118.88	122.33
1	L1	3718	A2M	C5-C4-N9	2.12	108.25	105.78
1	L1	3825	A2M	C4-C5-N7	-2.12	108.04	110.62
1	L1	3744	OMG	C8-N7-C5	2.11	108.07	104.24
1	L1	3867	A2M	C6-C5-C4	2.11	120.02	117.18
1	L1	4623	OMG	C8-N7-C5	2.11	108.06	104.24
46	S2	576	A2M	C6-C5-C4	2.10	120.01	117.18
1	L1	2508	PSU	C6-N1-C2	-2.10	120.53	122.68
1	L1	4637	OMG	C8-N7-C5	2.10	108.05	104.24
1	L1	398	A2M	C6-C5-C4	2.10	120.00	117.18
46	S2	121	OMU	O2-C2-N1	-2.10	120.00	122.79
46	S2	159	A2M	C4-C5-N7	-2.10	108.07	110.62
46	S2	1383	A2M	C4-C5-N7	-2.10	108.07	110.62
46	S2	172	OMU	O2-C2-N1	-2.09	120.01	122.79
46	S2	512	A2M	C6-C5-C4	2.08	119.98	117.18
1	L1	3825	A2M	C4-N9-C8	2.07	107.97	105.73
46	S2	668	A2M	C4-C5-N7	-2.07	108.10	110.62
46	S2	644	OMG	C8-N7-C5	2.07	107.98	104.24
46	S2	1328	OMG	C8-N7-C5	2.07	107.98	104.24
1	L1	1683	PSU	O2-C2-N1	-2.06	120.52	122.79
1	L1	3944	OMG	C8-N7-C5	2.06	107.97	104.24
1	L1	2787	A2M	C5'-C4'-C3'	-2.05	107.49	115.18
46	S2	1383	A2M	C6-C5-C4	2.05	119.94	117.18
46	S2	468	A2M	C4-N9-C8	2.04	107.94	105.73
46	S2	814	5MU	C1'-N1-C6	-2.04	117.73	121.12
1	L1	4618	OMG	N1-C2-N3	-2.04	119.52	123.32
1	L1	4499	OMG	C8-N7-C5	2.04	107.93	104.24
46	S2	1678	A2M	C6-C5-C4	2.04	119.92	117.18
1	L1	398	A2M	C4-C5-N7	-2.03	108.14	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3785	A2M	C4'-O4'-C1'	-2.03	105.00	109.47
1	L1	3792	OMG	C8-N7-C5	2.03	107.91	104.24
1	L1	4571	A2M	C4-C5-N7	-2.02	108.15	110.62
46	S2	601	OMG	C8-N7-C5	2.02	107.90	104.24
1	L1	4392	OMG	C8-N7-C5	2.02	107.90	104.24
46	S2	99	A2M	C6-C5-C4	2.02	119.90	117.18
1	L1	3818	UY1	C5-C6-N1	-2.02	119.08	122.11
1	L1	1683	PSU	C6-C5-C4	2.02	119.61	118.20
46	S2	683	OMG	C8-N7-C5	2.02	107.89	104.24
1	L1	1316	OMG	C4-C5-N7	-2.01	107.53	110.72
1	L1	1871	A2M	C4-C5-N7	-2.01	108.17	110.62
46	S2	1832	6MZ	C5-C4-N9	2.01	108.12	105.78
1	L1	2837	OMU	O2-C2-N1	-2.01	120.11	122.79
46	S2	1442	OMU	O2-C2-N1	-2.01	120.12	122.79
1	L1	2401	A2M	C4-C5-N7	-2.01	108.17	110.62
1	L1	4628	PSU	O4'-C1'-C2'	2.01	107.97	105.14
1	L1	4228	OMG	C8-N7-C5	2.01	107.87	104.24
1	L1	4403	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

All (132) 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	1534	A2M	C3'-C2'-O2'-CM'
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	3744	OMG	C1'-C2'-O2'-CM2
1	L1	3792	OMG	C1'-C2'-O2'-CM2
1	L1	3808	OMC	C3'-C4'-C5'-O5'
1	L1	3818	UY1	C2'-C1'-C5-C4
1	L1	3818	UY1	O4'-C4'-C5'-O5'
1	L1	3841	OMC	C3'-C4'-C5'-O5'
1	L1	3841	OMC	O4'-C4'-C5'-O5'
1	L1	3867	A2M	O4'-C4'-C5'-O5'
1	L1	3867	A2M	C3'-C4'-C5'-O5'
1	L1	3944	OMG	C3'-C4'-C5'-O5'
1	L1	4196	OMG	C1'-C2'-O2'-CM2
1	L1	4450	PSU	C2'-C1'-C5-C4
1	L1	4636	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	L1	4637	OMG	C1'-C2'-O2'-CM2
3	L3	14	OMU	C1'-C2'-O2'-CM2
3	L3	75	OMG	C1'-C2'-O2'-CM2
46	S2	116	OMU	C1'-C2'-O2'-CM2
46	S2	159	A2M	C3'-C4'-C5'-O5'
46	S2	576	A2M	O4'-C4'-C5'-O5'
46	S2	576	A2M	C3'-C4'-C5'-O5'
46	S2	601	OMG	C1'-C2'-O2'-CM2
46	S2	668	A2M	C3'-C4'-C5'-O5'
46	S2	867	OMG	C3'-C4'-C5'-O5'
46	S2	867	OMG	C1'-C2'-O2'-CM2
46	S2	1248	B8N	O4'-C4'-C5'-O5'
46	S2	1248	B8N	C3'-C4'-C5'-O5'
46	S2	1326	UY1	C2'-C1'-C5'-C4
46	S2	1328	OMG	C1'-C2'-O2'-CM2
46	S2	1391	OMC	C3'-C4'-C5'-O5'
46	S2	1391	OMC	O4'-C4'-C5'-O5'
46	S2	1442	OMU	C1'-C2'-O2'-CM2
46	S2	1442	OMU	O4'-C4'-C5'-O5'
46	S2	1678	A2M	C1'-C2'-O2'-CM'
46	S2	1851	MA6	O4'-C4'-C5'-O5'
46	S2	1830	UR3	O4'-C1'-N1-C2
1	L1	3701	OMC	C2'-C1'-N1-C2
1	L1	398	A2M	O4'-C4'-C5'-O5'
1	L1	1677	PSU	C3'-C4'-C5'-O5'
1	L1	3785	A2M	O4'-C4'-C5'-O5'
1	L1	3785	A2M	C3'-C4'-C5'-O5'
1	L1	4500	PSU	C3'-C4'-C5'-O5'
1	L1	4500	PSU	O4'-C4'-C5'-O5'
46	S2	159	A2M	O4'-C4'-C5'-O5'
46	S2	590	A2M	O4'-C4'-C5'-O5'
46	S2	590	A2M	C3'-C4'-C5'-O5'
46	S2	668	A2M	O4'-C4'-C5'-O5'
46	S2	823	PSU	C3'-C4'-C5'-O5'
46	S2	1851	MA6	C3'-C4'-C5'-O5'
1	L1	1677	PSU	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'
46	S2	99	A2M	O4'-C4'-C5'-O5'
46	S2	512	A2M	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	S2	867	OMG	O4'-C4'-C5'-O5'
46	S2	1442	OMU	C3'-C4'-C5'-O5'
46	S2	1830	UR3	O4'-C1'-N1-C6
46	S2	428	OMU	C2'-C1'-N1-C6
1	L1	398	A2M	C3'-C4'-C5'-O5'
1	L1	3764	PSU	C3'-C4'-C5'-O5'
46	S2	823	PSU	O4'-C4'-C5'-O5'
1	L1	4447	5MC	C2'-C1'-N1-C6
43	Lo	53	MLZ	CE-CD-CG-CB
1	L1	2364	OMG	O4'-C4'-C5'-O5'
1	L1	3764	PSU	O4'-C4'-C5'-O5'
46	S2	512	A2M	C3'-C4'-C5'-O5'
1	L1	2787	A2M	C2'-C1'-N9-C8
1	L1	2787	A2M	C2'-C1'-N9-C4
46	S2	428	OMU	C2'-C1'-N1-C2
1	L1	3729	PSU	O4'-C4'-C5'-O5'
46	S2	99	A2M	C3'-C4'-C5'-O5'
46	S2	1243	PSU	O4'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C1'-N1-C6
1	L1	4499	OMG	O4'-C4'-C5'-O5'
1	L1	1326	A2M	C4'-C5'-O5'-P
1	L1	2787	A2M	C3'-C4'-C5'-O5'
1	L1	3701	OMC	O4'-C1'-N1-C2
1	L1	4447	5MC	C2'-C1'-N1-C2
1	L1	3869	OMC	C3'-C2'-O2'-CM2
1	L1	3701	OMC	O4'-C1'-N1-C6
1	L1	4447	5MC	O4'-C1'-N1-C6
1	L1	1534	A2M	C4'-C5'-O5'-P
46	S2	590	A2M	C4'-C5'-O5'-P
1	L1	1582	PSU	C3'-C4'-C5'-O5'
1	L1	2364	OMG	C3'-C4'-C5'-O5'
1	L1	3818	UY1	C4'-C5'-O5'-P
1	L1	4447	5MC	O4'-C1'-N1-C2
46	S2	428	OMU	O4'-C1'-N1-C2
1	L1	2363	A2M	C3'-C2'-O2'-CM'
46	S2	644	OMG	C4'-C5'-O5'-P
46	S2	1490	OMG	C4'-C5'-O5'-P
1	L1	2824	OMC	C3'-C4'-C5'-O5'
1	L1	4499	OMG	C3'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C1'-C5-C4
1	L1	3818	UY1	O4'-C1'-C5-C4
1	L1	4450	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	S2	1326	UY1	O4'-C1'-C5-C4
1	L1	3792	OMG	O4'-C4'-C5'-O5'
1	L1	2787	A2M	O4'-C1'-N9-C8
43	Lo	53	MLZ	CD-CE-NZ-CM
1	L1	4500	PSU	C4'-C5'-O5'-P
1	L1	729	2MG	O4'-C4'-C5'-O5'
1	L1	2422	OMC	O4'-C4'-C5'-O5'
1	L1	2876	OMG	C3'-C4'-C5'-O5'
43	Lo	53	MLZ	CA-CB-CG-CD
46	S2	683	OMG	O4'-C4'-C5'-O5'
46	S2	822	PSU	C3'-C4'-C5'-O5'
46	S2	1243	PSU	C3'-C4'-C5'-O5'
1	L1	2363	A2M	C1'-C2'-O2'-CM'
1	L1	2351	OMC	C2'-C1'-N1-C2
46	S2	1219	JMH	C2'-C1'-N1-C2
46	S2	1288	OMU	C2'-C1'-N1-C2
46	S2	590	A2M	O4'-C1'-N9-C8
1	L1	2787	A2M	O4'-C4'-C5'-O5'
1	L1	3729	PSU	C3'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C4'-C5'-O5'
1	L1	3818	UY1	O4'-C1'-C5-C6
1	L1	4636	PSU	O4'-C1'-C5-C6
1	L1	1534	A2M	O4'-C4'-C5'-O5'
46	S2	1081	PSU	C4'-C5'-O5'-P
1	L1	2401	A2M	C3'-C2'-O2'-CM'
1	L1	2351	OMC	O4'-C4'-C5'-O5'
46	S2	668	A2M	C2'-C1'-N9-C8
1	L1	3887	OMC	C4'-C5'-O5'-P
1	L1	3792	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	3762	B8H	5	0
1	L1	1625	OMG	1	0
46	S2	512	A2M	1	0
46	S2	1832	6MZ	1	0
46	S2	484	A2M	1	0
1	L1	2815	A2M	1	0
46	S2	1678	A2M	2	0
46	S2	601	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	1871	A2M	1	0
46	S2	121	OMU	1	0
46	S2	509	OMG	4	0
46	S2	436	OMG	1	0
1	L1	2351	OMC	1	0
1	L1	3808	OMC	1	0
1	L1	4637	OMG	1	0
1	L1	3718	A2M	2	0
1	L1	2804	OMC	1	0
46	S2	1442	OMU	1	0
1	L1	4618	OMG	1	0
1	L1	2363	A2M	1	0
46	S2	1850	MA6	1	0
46	S2	116	OMU	2	0
1	L1	3723	A2M	3	0
46	S2	1328	OMG	1	0
1	L1	1340	OMC	2	0
3	L3	14	OMU	1	0
1	L1	4196	OMG	1	0
3	L3	75	OMG	2	0
46	S2	814	5MU	1	0
46	S2	1031	A2M	1	0
46	S2	159	A2M	1	0
46	S2	1490	OMG	1	0
1	L1	1456	JMH	1	0
1	L1	3818	UY1	1	0
1	L1	3744	OMG	1	0
46	S2	867	OMG	1	0
1	L1	3792	OMG	2	0
1	L1	729	2MG	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

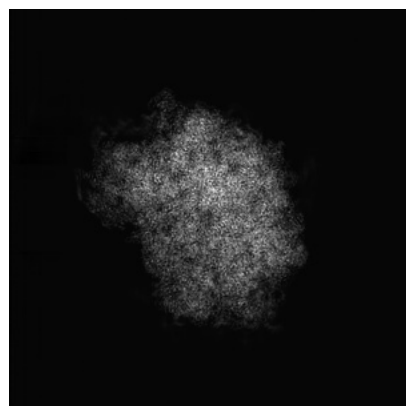
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33330. These allow visual inspection of the internal detail of the map and identification of artifacts.

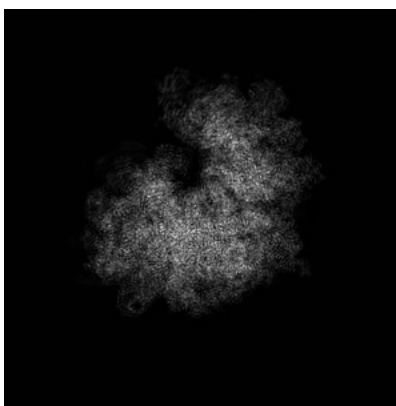
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

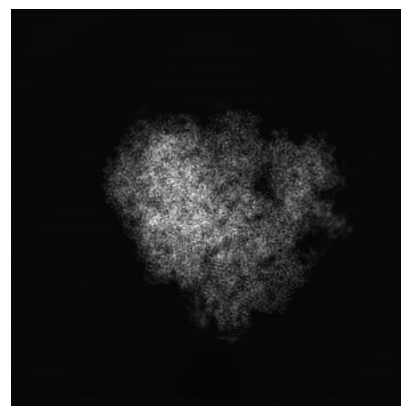
6.1.1 Primary map



X

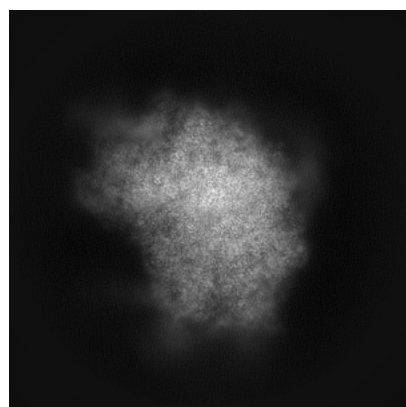


Y

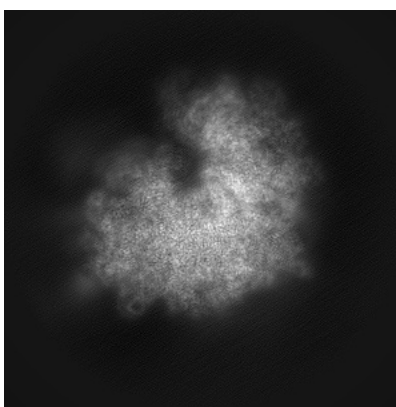


Z

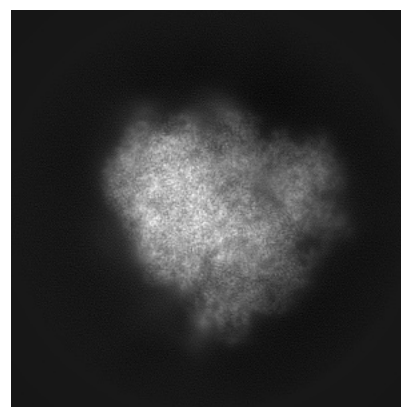
6.1.2 Raw map



X



Y

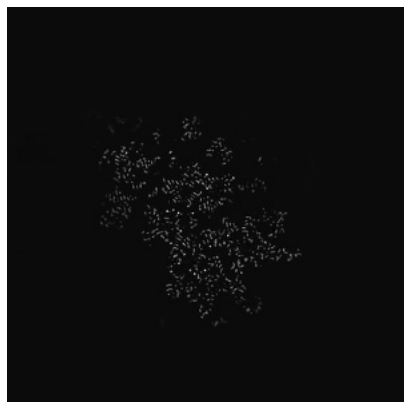


Z

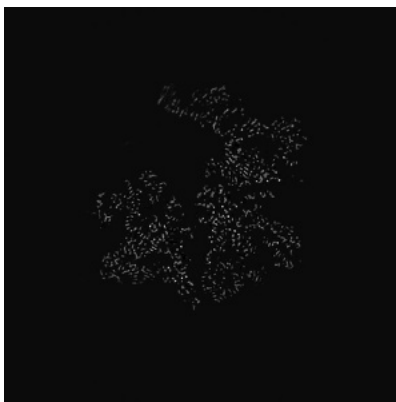
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210

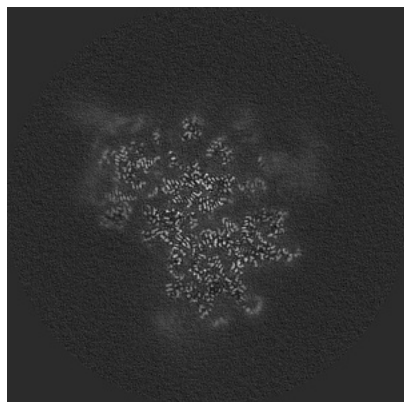


Y Index: 210

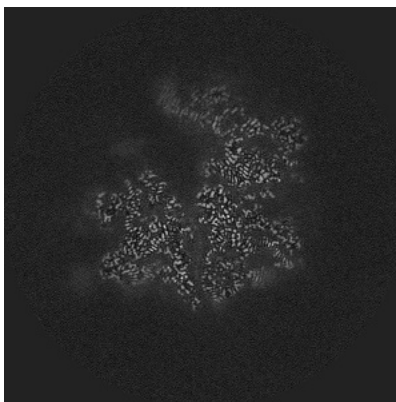


Z Index: 210

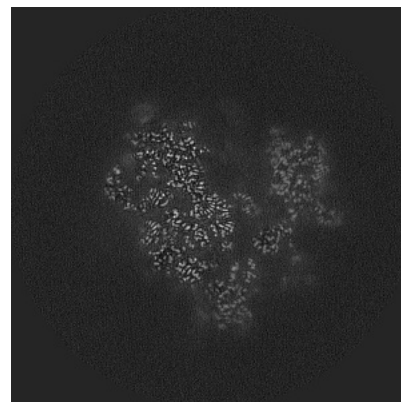
6.2.2 Raw map



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: 170

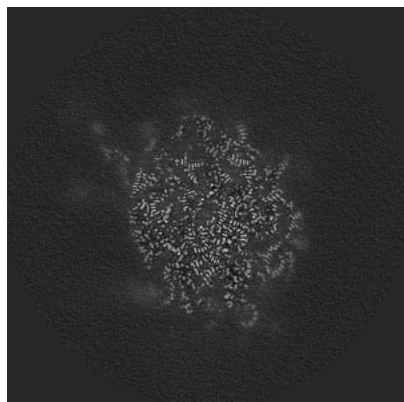


Y Index: 203

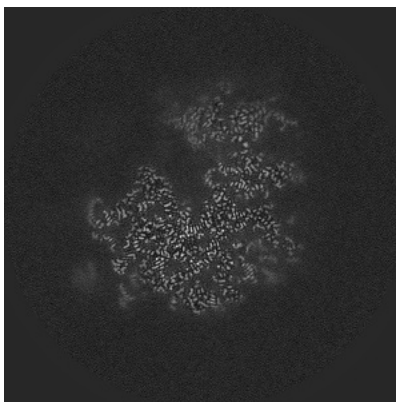


Z Index: 232

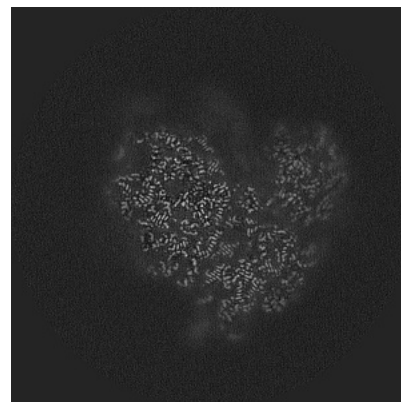
6.3.2 Raw map



X Index: 187



Y Index: 224

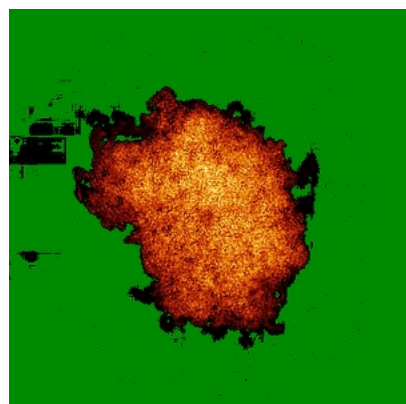


Z Index: 230

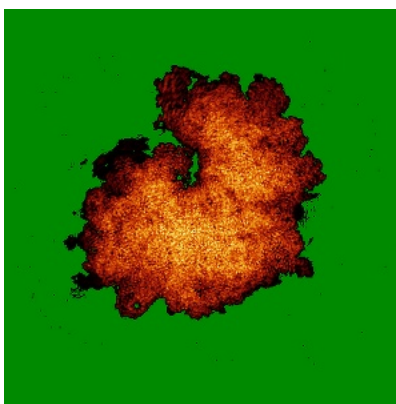
The images above show the largest variance slices of the map in three orthogonal directions.

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

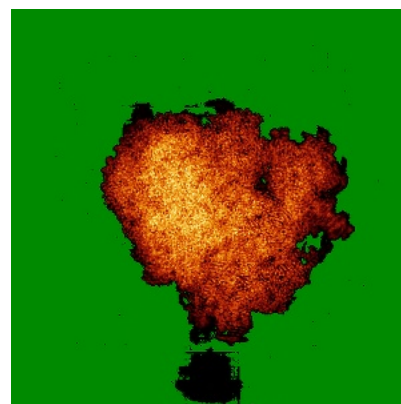
6.4.1 Primary map



X

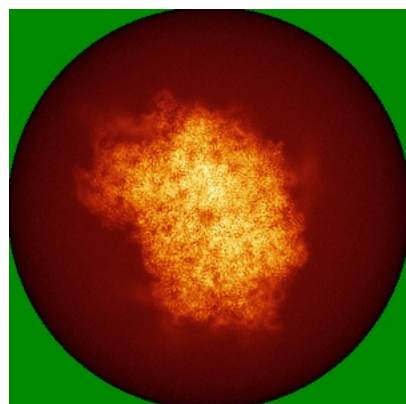


Y

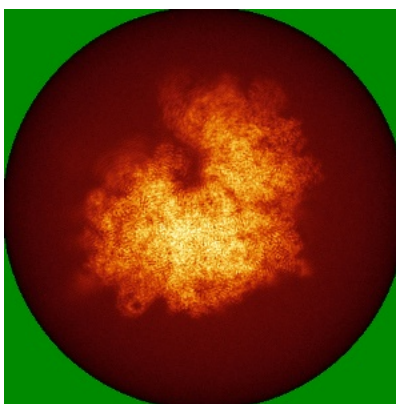


Z

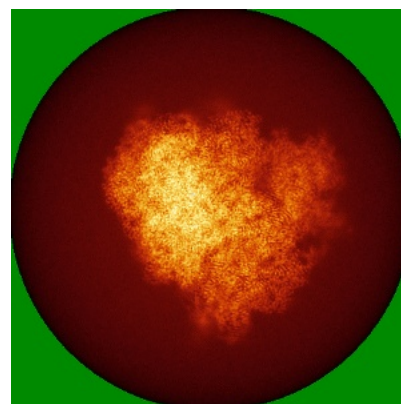
6.4.2 Raw map



X



Y

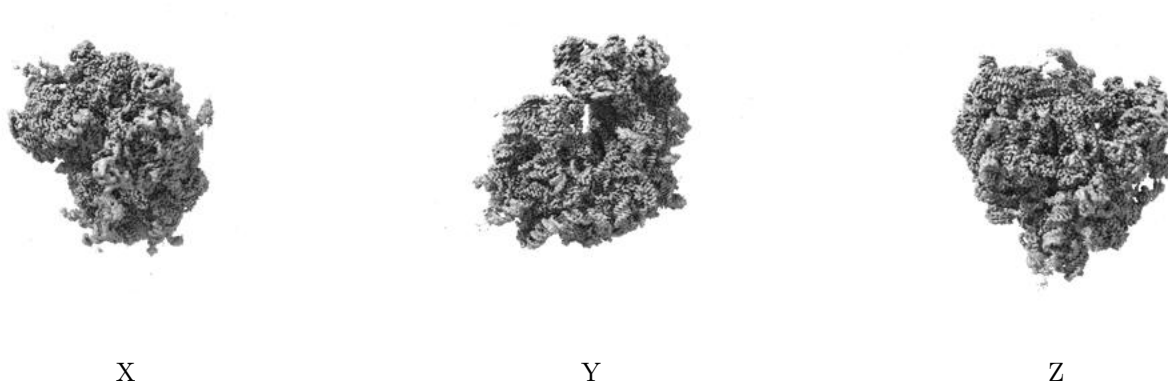


Z

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

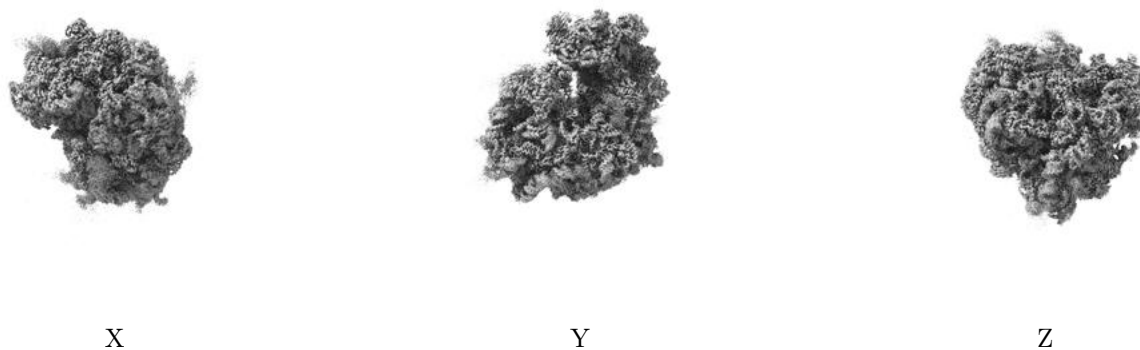
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

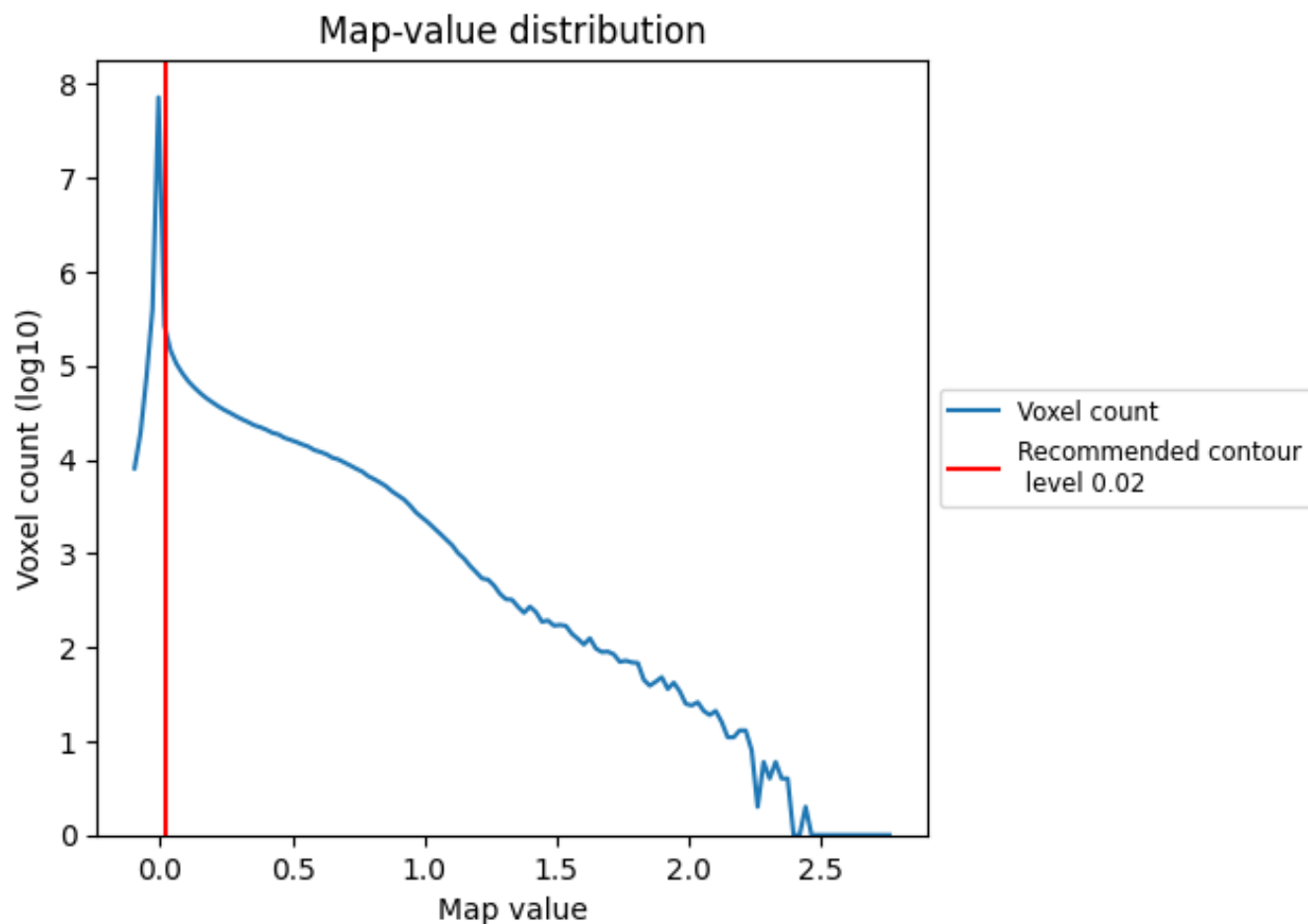
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

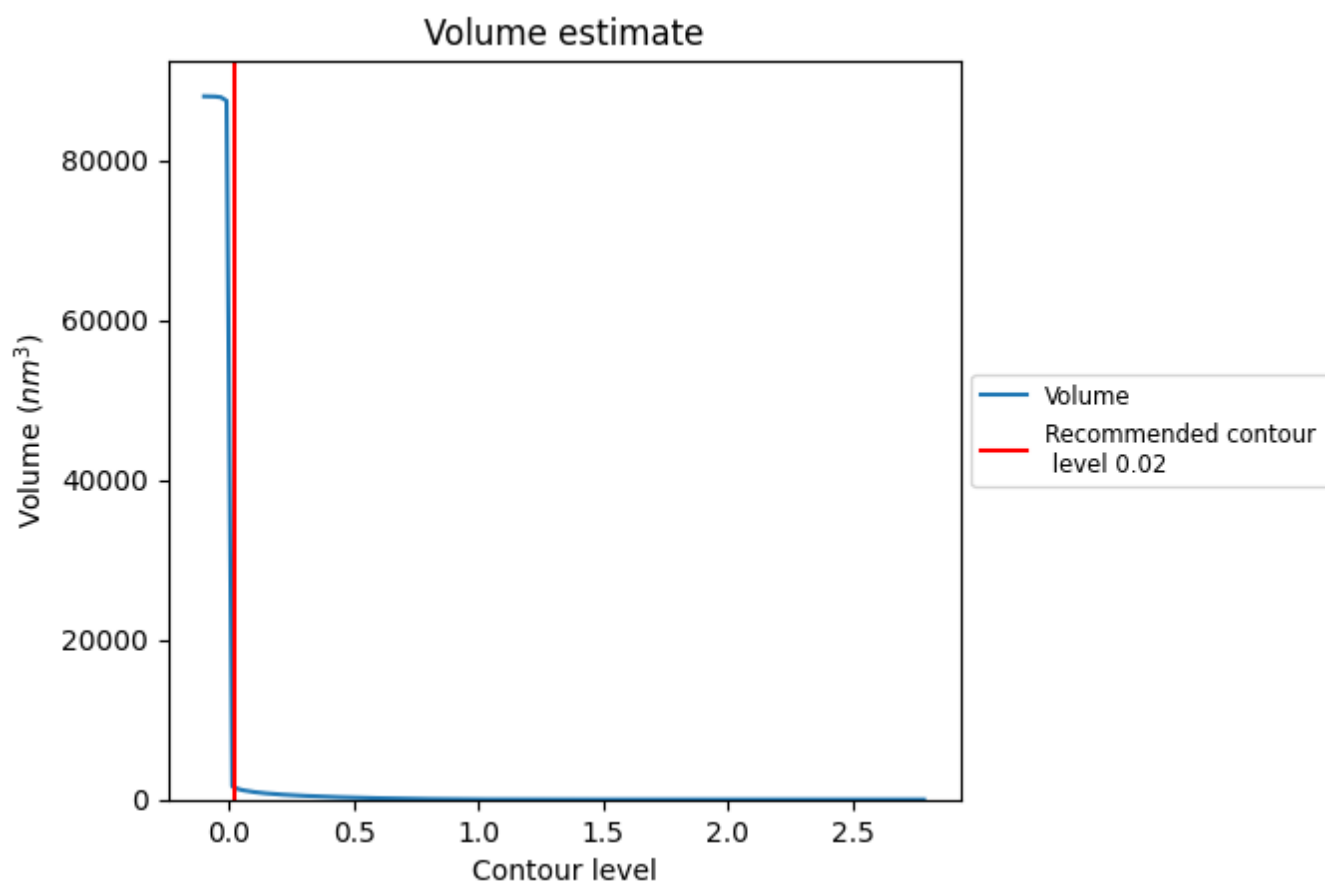
This section contains the results of statistical analysis of the map.

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.

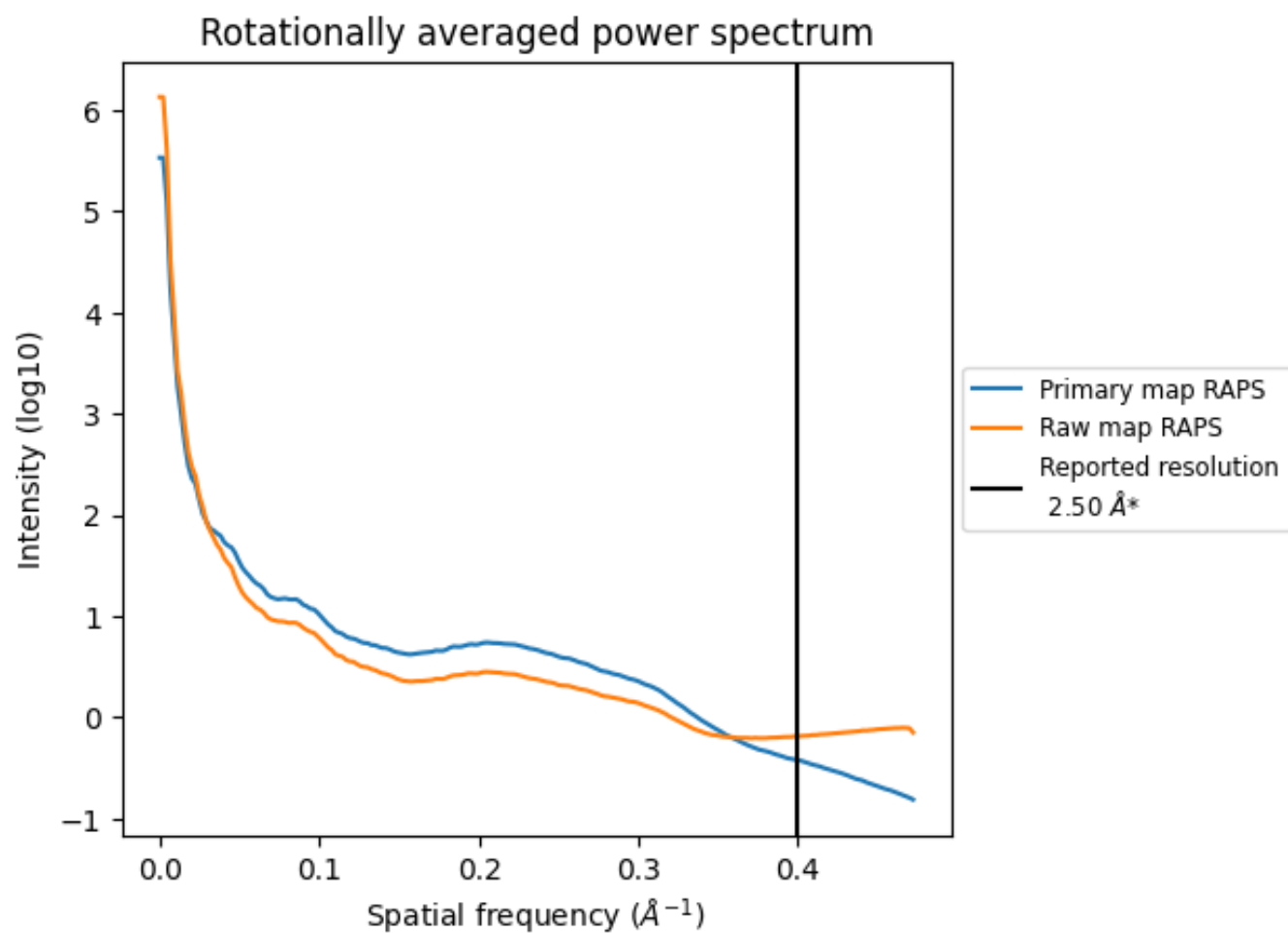
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1583 nm^3 ; this corresponds to an approximate mass of 1430 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 ⓘ

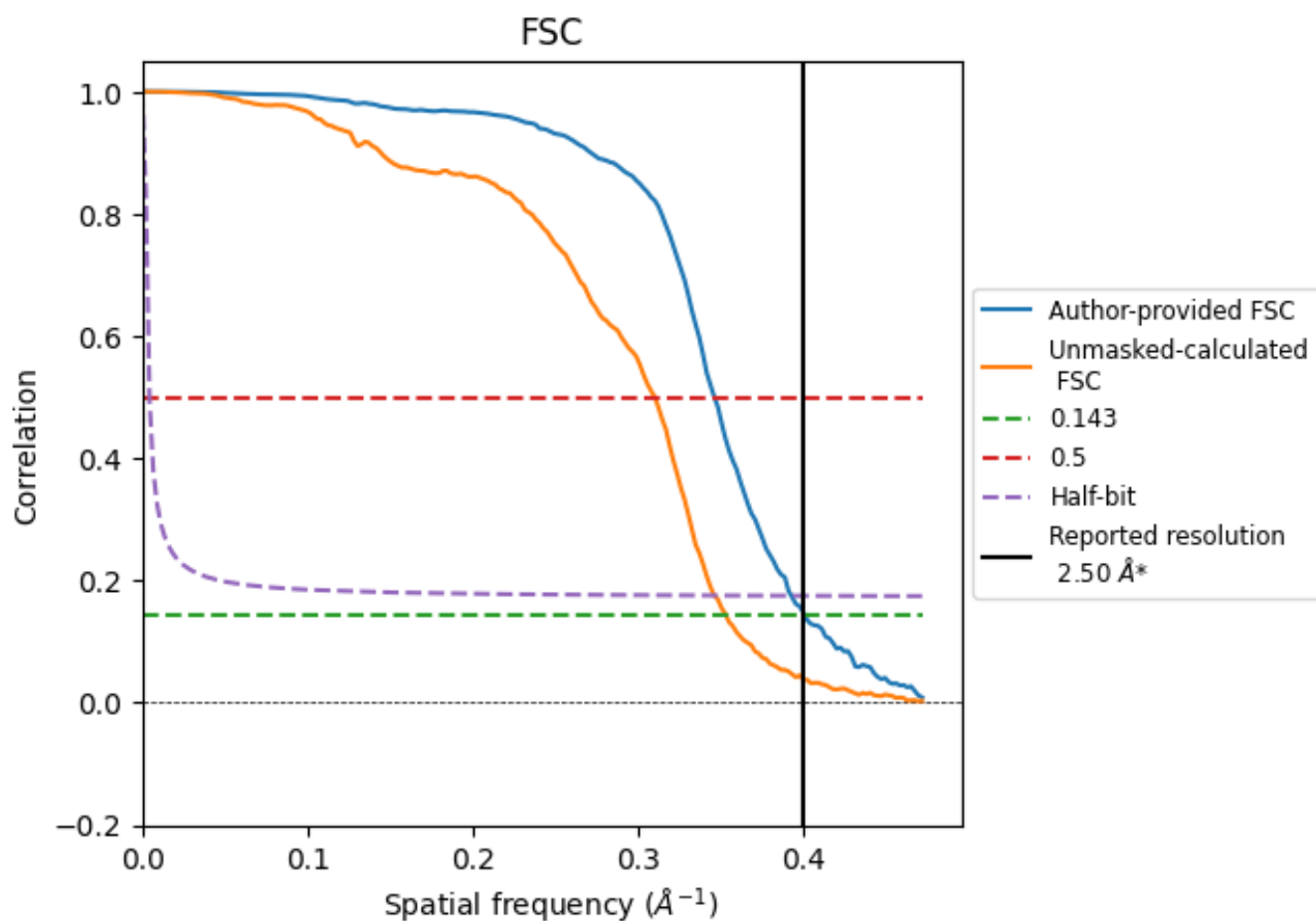


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

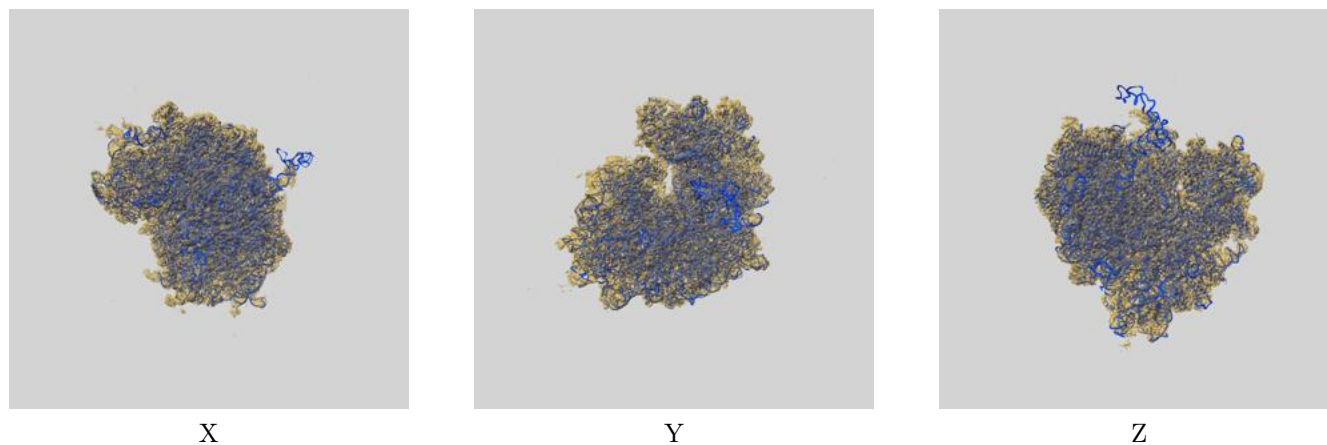
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.89	2.55
Unmasked-calculated*	2.83	3.22	2.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.83 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

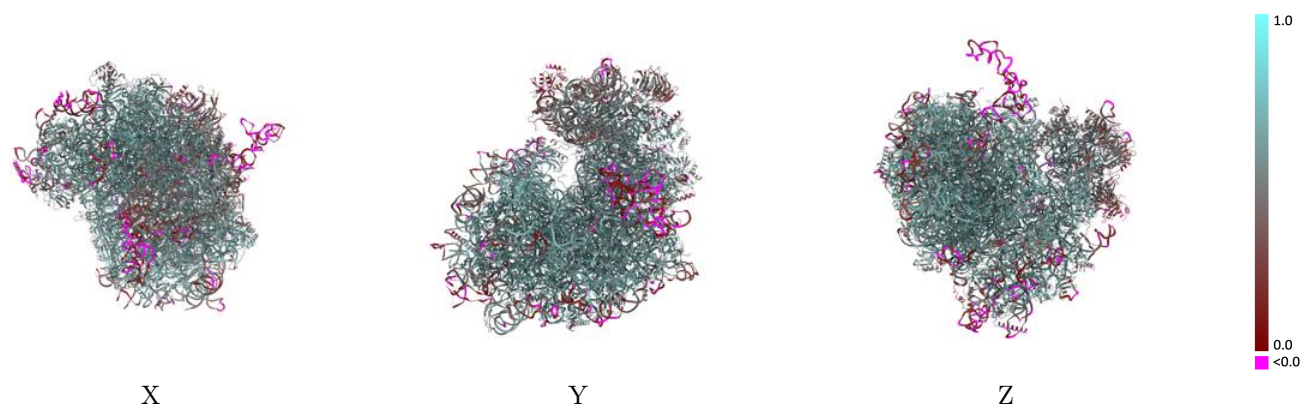
This section contains information regarding the fit between EMDB map EMD-33330 and PDB model 7XNY. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



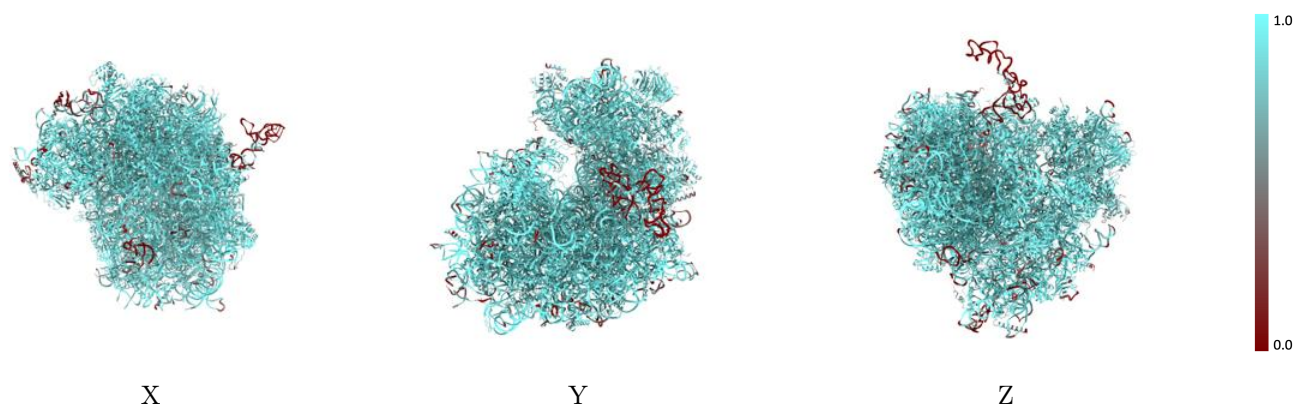
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



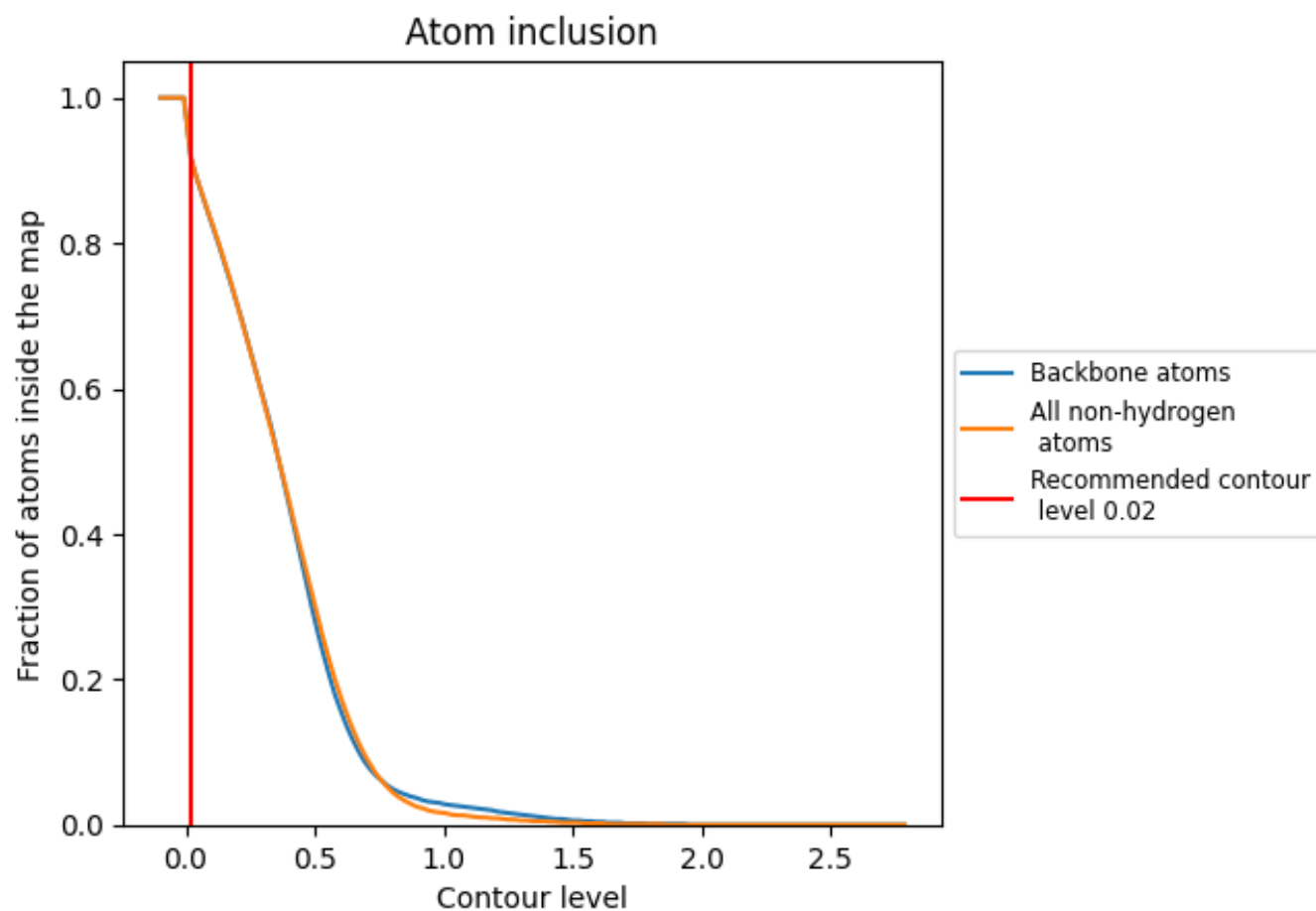
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.5600
L1	 0.9070	 0.5570
L2	 0.9920	 0.6420
L3	 0.9310	 0.5930
LA	 0.9800	 0.6660
LB	 0.9490	 0.6340
LC	 0.9560	 0.6380
LD	 0.9370	 0.5890
LE	 0.9480	 0.5930
LF	 0.9620	 0.6540
LG	 0.9210	 0.5740
LH	 0.9450	 0.6000
LI	 0.9560	 0.6220
LJ	 0.9160	 0.5370
LL	 0.9180	 0.5870
LM	 0.9490	 0.6120
LN	 0.9820	 0.6700
LO	 0.9520	 0.6360
LP	 0.9490	 0.6450
LQ	 0.9660	 0.6550
LR	 0.9090	 0.5840
LS	 0.9790	 0.6550
LT	 0.9380	 0.6080
LU	 0.8760	 0.4830
LV	 0.9560	 0.6440
LW	 0.7220	 0.3800
LX	 0.9370	 0.6200
LY	 0.9310	 0.6040
LZ	 0.9550	 0.6050
La	 0.9690	 0.6530
Lb	 0.8680	 0.5420
Lc	 0.9370	 0.6280
Ld	 0.9320	 0.6100
Le	 0.9670	 0.6480
Lf	 0.9750	 0.6590



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lg	 0.9450	 0.6200
Lh	 0.9220	 0.5900
Li	 0.9390	 0.5890
Lj	 0.9720	 0.6370
Lk	 0.8890	 0.5310
Ll	 0.9360	 0.6000
Lm	 0.9420	 0.6180
Ln	 0.9380	 0.6130
Lo	 0.9390	 0.6240
Lp	 0.9350	 0.6340
Lr	 0.9670	 0.6430
S2	 0.9320	 0.5450
SA	 0.9460	 0.5840
SB	 0.9410	 0.5860
SC	 0.9530	 0.6080
SD	 0.8840	 0.4580
SE	 0.9500	 0.5920
SF	 0.9170	 0.4870
SG	 0.8720	 0.4700
SH	 0.8820	 0.4870
SI	 0.9210	 0.5630
SJ	 0.9190	 0.5490
SK	 0.8600	 0.3830
SL	 0.9390	 0.6210
SM	 0.6410	 0.1100
SN	 0.9620	 0.6210
SO	 0.9470	 0.5980
SP	 0.7840	 0.3350
SQ	 0.8900	 0.4770
SR	 0.8900	 0.4920
SS	 0.8610	 0.3910
ST	 0.8780	 0.4270
SU	 0.8750	 0.4150
SV	 0.9570	 0.5940
SW	 0.9680	 0.6410
SX	 0.9490	 0.6160
SY	 0.9190	 0.5260
SZ	 0.7940	 0.3540
Sa	 0.9300	 0.5740
Sb	 0.9170	 0.5400
Sc	 0.8520	 0.4740
Sd	 0.9190	 0.5200

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Se	 0.7720	 0.4650
Sf	 0.7400	 0.1880
Sg	 0.8670	 0.3790