



Full wwPDB EM Validation Report ⓘ

Jul 16, 2026 – 11:35 am BST

PDB ID : 8QIE / pdb_00008qie
EMDB ID : EMD-18437
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
LM32Cs1C1 mutant snoRNA overexpression, class 4
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2023-09-12
Resolution : 2.43 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.dev133
Mogul : 1.8.4, 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) : 2.50

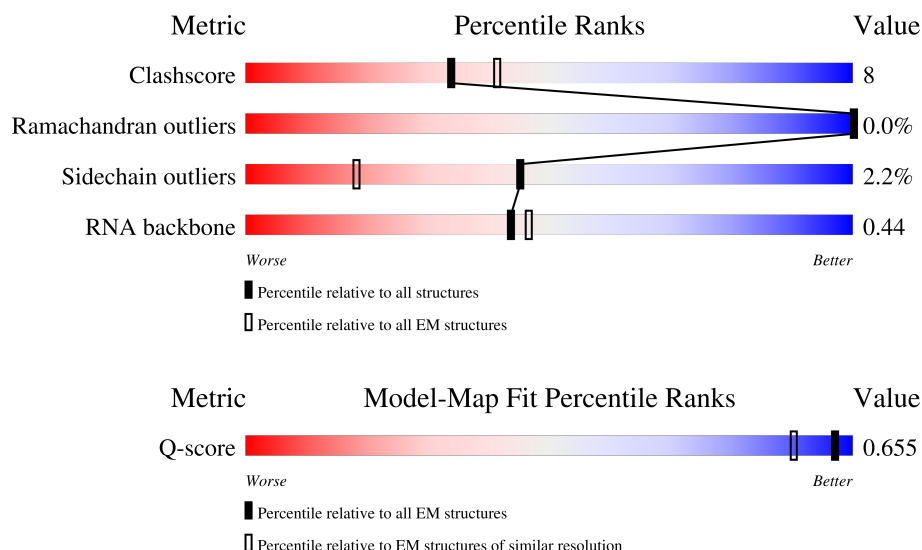
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 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.



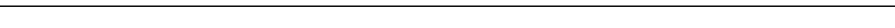
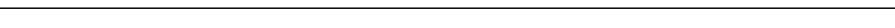
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5787 (1.94 - 2.93)

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	1	1782	
2	2	1526	
3	3	216	

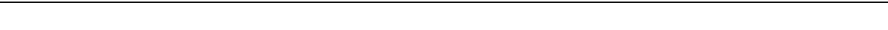
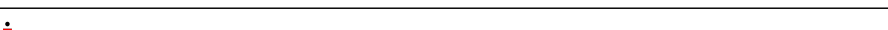
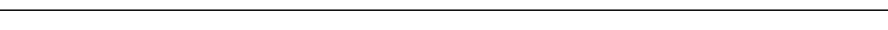
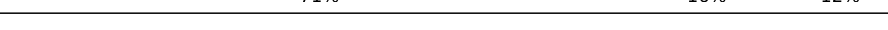
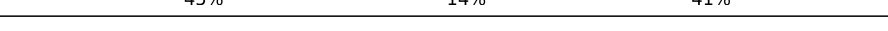
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	184	
5	5	135	
6	6	73	
7	7	171	
8	8	123	
9	A	260	
10	B	419	
11	C	373	
12	D	188	
13	E	190	
14	F	195	
15	G	264	
16	H	222	
17	I	220	
18	J	139	
19	K	175	
20	L	145	
21	M	204	
22	N	213	
23	O	305	
24	P	198	
25	Q	254	
26	R	179	
27	S	159	
28	S1	2204	

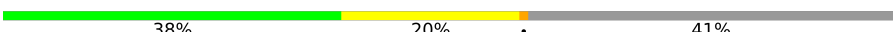
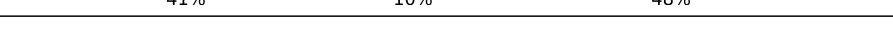
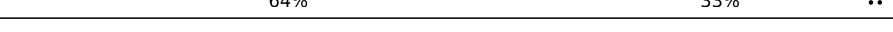
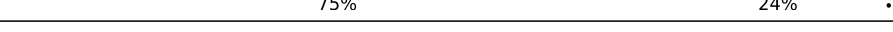
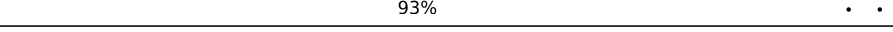
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	S4	76	
30	SA	264	
31	SB	246	
32	SC	219	
33	SD	190	
34	SE	273	
35	SF	265	
36	SG	249	
37	SH	190	
38	SI	200	
39	SJ	130	
40	SK	220	
41	SL	149	
42	SM	116	
43	SN	168	
44	SO	144	
45	SP	143	
46	SQ	141	
47	SR	153	
48	SS	57	
49	ST	151	
50	SU	173	
51	SV	143	
52	SW	152	
53	SX	161	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SY	164	
55	SZ	137	
56	Sa	120	
57	Sb	112	
58	Sc	86	
59	Sd	87	
60	Se	66	
61	Sf	152	
62	Sg	312	
63	Sh	235	
64	T	166	
65	U	129	
66	V	145	
67	W	143	
68	X	124	
69	Y	134	
70	Z	147	
71	a	127	
72	b	70	
73	c	252	
74	d	104	
75	e	188	
76	f	133	
77	g	144	
78	h	168	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	i	105	
80	j	83	
81	k	83	
82	l	51	
83	m	128	
84	n	34	
85	o	92	
86	p	106	

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 206527 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 LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1611	Total	C	N	O	P	0	0
			34568	15451	6340	11166	1611		

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1159	Total	C	N	O	P	0	0
			24802	11101	4482	8060	1159		

- Molecule 3 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	156	Total	C	N	O	P	0	0
			3312	1481	576	1099	156		

- Molecule 4 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	184	Total	C	N	O	P	0	0
			3937	1756	712	1285	184		

- Molecule 5 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	115	Total	C	N	O	P	0	0
			2453	1094	439	805	115		

- Molecule 6 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 7 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	164	Total	C	N	O	P	0	0
			3494	1566	621	1144	163		

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	255	Total	C	N	O	S	1	0
			1908	1189	390	319	10		

- Molecule 10 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	399	Total	C	N	O	S	0	0
			3051	1932	599	507	13		

- Molecule 11 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	366	Total	C	N	O	S	0	0
			2777	1740	556	466	15		

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	158	Total	C	N	O	S	0	0
			1008	629	203	170	6		

- Molecule 13 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	186	Total	C	N	O	S	0	0
			1395	889	267	233	6		

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	148	Total	C	N	O	S	0	0
			1067	686	203	176	2		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	226	Total	C	N	O	S	0	0
			1731	1097	344	283	7		

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	220	Total	C	N	O	S	0	0
			1734	1101	349	277	7		

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	208	Total	C	N	O	S	0	0
			1603	1001	326	269	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	137	Total	C	N	O	S	0	0
			999	631	190	172	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	170	Total	C	N	O	S	0	0
			1266	794	252	213	7		

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	203	Total	C	N	O	S	0	0
			1696	1071	361	256	8		

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	199	Total	C	N	O	S	0	0
			1607	1013	320	260	14		

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	276	Total	C	N	O	S	0	0
			1975	1260	379	333	3		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	197	Total	C	N	O	S	0	0
			1528	961	305	256	6		

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	187	Total	C	N	O	S	0	0
			1433	892	316	219	6		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	178	Total	C	N	O	S	0	0
			1413	904	273	231	5		

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	157	Total	C	N	O	S	0	0
			1234	784	240	206	4		

- Molecule 28 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S1	1787	Total	C	N	O	P	0	0
			38240	17106	6918	12429	1787		

- Molecule 29 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S4	50	Total	C	N	O	P	0	0
			1072	478	200	345	49		

- Molecule 30 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	225	Total	C	N	O	S	1	0
			1820	1141	346	321	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SB	208	Total	C	N	O	S	0	0
			1627	1034	297	284	12		

- Molecule 32 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SC	212	Total	C	N	O	S	1	0
			1624	1029	296	286	13		

- Molecule 33 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SD	167	Total	C	N	O	S	0	0
			1366	863	270	225	8		

- Molecule 34 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SE	260	Total	C	N	O	S	0	0
			2050	1299	393	349	9		

- Molecule 35 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SF	218	Total	C	N	O	S	0	0
			1662	1063	297	293	9		

- Molecule 36 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SG	231	Total	C	N	O	S	0	0
			1831	1144	374	310	3		

- Molecule 37 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SH	182	Total	C	N	O	S	0	0
			1436	892	278	259	7		

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SI	199	Total	C	N	O	S	0	0
			1619	1032	313	267	7		

- Molecule 39 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SK	182	Total	C	N	O	S	0	0
			1443	906	305	230	2		

- Molecule 41 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SL	143	Total	C	N	O	S	0	0
			1124	724	206	191	3		

- Molecule 42 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SM	102	Total	C	N	O	S	0	0
			796	498	145	151	2		

- Molecule 43 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SN	99	Total	C	N	O	S	0	0
			808	518	141	142	7		

- Molecule 44 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SO	135	Total	C	N	O	S	0	0
			1010	624	197	181	8		

- Molecule 45 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SP	141	Total	C	N	O	S	0	0
			1100	694	217	186	3		

- Molecule 46 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SQ	100	Total	C	N	O	S	0	0
			679	419	122	133	5		

- Molecule 47 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SR	130	Total	C	N	O	S	0	0
			1034	655	201	174	4		

- Molecule 48 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SS	56	Total	C	N	O	S	0	0
			452	279	94	73	6		

- Molecule 49 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	ST	142	Total	C	N	O	S	0	0
			1155	728	229	190	8		

- Molecule 50 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SU	156	Total	C	N	O	S	0	0
			1253	796	247	205	5		

- Molecule 51 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SV	71	Total	C	N	O	S	0	0
			577	368	110	97	2		

- Molecule 52 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SW	113	Total	C	N	O	S	0	0
			907	578	172	153	4		

- Molecule 53 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SX	152	Total	C	N	O	S	0	0
			1202	764	237	197	4		

- Molecule 54 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SY	84	Total	C	N	O	S	0	0
			616	381	115	116	4		

- Molecule 55 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SZ	127	Total	C	N	O	S	0	0
			1031	662	200	166	3		

- Molecule 56 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Sa	71	Total	C	N	O	S	0	0
			558	356	99	100	3		

- Molecule 57 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Sb	103	Total	C	N	O	S	0	0
			816	505	175	129	7		

- Molecule 58 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Sc	73	Total	C	N	O	S	0	0
			570	358	107	101	4		

- Molecule 59 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sd	66	Total	C	N	O	S	0	0
			483	295	97	87	4		

- Molecule 60 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Se	51	Total	C	N	O	S	0	0
			401	252	86	62	1		

- Molecule 61 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Sf	33	Total	C	N	O	S	0	0
			295	193	58	43	1		

- Molecule 62 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Sg	300	Total	C	N	O	S	0	0
			2284	1438	406	428	12		

- Molecule 63 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sh	134	Total	C	N	O	S	0	0
			948	603	179	164	2		

- Molecule 64 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	T	151	Total	C	N	O	S	0	0
			1211	757	240	203	11		

- Molecule 65 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	U	118	Total	C	N	O	S	0	0
			801	514	152	133	2		

- Molecule 66 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	V	118	Total	C	N	O	S	0	0
			926	587	178	159	2		

- Molecule 67 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	W	118	Total	C	N	O	S	0	0
			937	586	197	150	4		

- Molecule 68 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	X	64	Total	C	N	O	S	0	0
			548	359	105	80	4		

- Molecule 69 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Y	132	Total	C	N	O	S	0	0
			1027	661	206	157	3		

- Molecule 70 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Z	145	Total	C	N	O	S	0	0
			1095	671	234	185	5		

- Molecule 71 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	a	123	Total	C	N	O	S	0	0
			1006	630	211	161	4		

- Molecule 72 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	b	68	Total	C	N	O		0	0
			546	335	125	86			

- Molecule 73 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	c	229	Total	C	N	O	S	0	0
			1862	1185	358	308	11		

- Molecule 74 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	d	92	Total	C	N	O	S	0	0
			705	438	129	133	5		

- Molecule 75 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	e	180	Total	C	N	O	S	0	0
			1421	895	288	234	4		

- Molecule 76 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	f	125	Total	C	N	O	S	0	0
			1011	636	201	170	4		

- Molecule 77 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	g	142	Total	C	N	O	S	0	0
			1142	710	239	188	5		

- Molecule 78 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	h	127	Total	C	N	O	S	0	0
			1018	626	221	165	6		

- Molecule 79 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	i	88	Total	C	N	O	S	0	0
			689	438	143	106	2		

- Molecule 80 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	j	81	Total	C	N	O	S	0	0
			668	407	154	101	6		

- Molecule 81 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k	72	Total	C	N	O	S	0	0
			534	338	105	88	3		

- Molecule 82 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	l	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 83 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	m	51	Total	C	N	O	S	0	0
			378	238	74	59	7		

- Molecule 84 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	n	33	Total	C	N	O	S	0	0
			292	178	75	37	2		

- Molecule 85 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	o	88	Total	C	N	O	S	0	0
			688	428	142	112	6		

- Molecule 86 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	p	97	Total	C	N	O	S	0	0
			775	491	157	123	4		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	1	58	Total	Mg	0
			58	58	
87	2	66	Total	Mg	0
			66	66	
87	4	3	Total	Mg	0
			3	3	
87	5	3	Total	Mg	0
			3	3	
87	6	1	Total	Mg	0
			1	1	
87	7	2	Total	Mg	0
			2	2	
87	8	1	Total	Mg	0
			1	1	
87	A	2	Total	Mg	0
			2	2	
87	J	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	S	1	Total 1	Mg 1	0
87	S1	79	Total 79	Mg 79	0
87	SX	1	Total 1	Mg 1	0
87	Sb	1	Total 1	Mg 1	0

- Molecule 88 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
88	1	11	Total 11	Na 11	0
88	2	10	Total 10	Na 10	0
88	4	3	Total 3	Na 3	0
88	S1	9	Total 9	Na 9	0
88	S4	1	Total 1	Na 1	0

- Molecule 89 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
89	1	9	Total 9	K 9	0
89	2	3	Total 3	K 3	0
89	S1	4	Total 4	K 4	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	p	1	Total 1	Zn 1	0

- Molecule 91 is water.

Mol	Chain	Residues	Atoms	AltConf
91	1	617	Total O 617 617	0
91	2	478	Total O 478 478	0
91	3	21	Total O 21 21	0
91	4	62	Total O 62 62	0
91	5	24	Total O 24 24	0
91	6	5	Total O 5 5	0
91	7	43	Total O 43 43	0
91	8	5	Total O 5 5	0
91	A	20	Total O 20 20	0
91	B	38	Total O 38 38	0
91	C	18	Total O 18 18	0
91	D	1	Total O 1 1	0
91	F	1	Total O 1 1	0
91	G	1	Total O 1 1	0
91	H	9	Total O 9 9	0
91	I	10	Total O 10 10	0
91	J	4	Total O 4 4	0
91	L	12	Total O 12 12	0
91	M	22	Total O 22 22	0
91	N	1	Total O 1 1	0
91	P	8	Total O 8 8	0
91	Q	2	Total O 2 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	R	1	Total 1	O 1	0
91	S	2	Total 2	O 2	0
91	S1	802	Total 802	O 802	0
91	S4	3	Total 3	O 3	0
91	SA	7	Total 7	O 7	0
91	SB	1	Total 1	O 1	0
91	SC	1	Total 1	O 1	0
91	SD	4	Total 4	O 4	0
91	SE	13	Total 13	O 13	0
91	SF	6	Total 6	O 6	0
91	SG	1	Total 1	O 1	0
91	SH	6	Total 6	O 6	0
91	SJ	12	Total 12	O 12	0
91	SK	13	Total 13	O 13	0
91	SL	3	Total 3	O 3	0
91	SM	6	Total 6	O 6	0
91	SN	2	Total 2	O 2	0
91	SO	7	Total 7	O 7	0
91	SP	12	Total 12	O 12	0
91	SR	4	Total 4	O 4	0
91	SS	1	Total 1	O 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	ST	19	Total 19	O 19	0
91	SU	5	Total 5	O 5	0
91	SX	5	Total 5	O 5	0
91	Sa	2	Total 2	O 2	0
91	Sb	23	Total 23	O 23	0
91	Sc	5	Total 5	O 5	0
91	T	9	Total 9	O 9	0
91	V	4	Total 4	O 4	0
91	W	2	Total 2	O 2	0
91	X	2	Total 2	O 2	0
91	Z	1	Total 1	O 1	0
91	b	3	Total 3	O 3	0
91	c	5	Total 5	O 5	0
91	e	3	Total 3	O 3	0
91	f	14	Total 14	O 14	0
91	g	11	Total 11	O 11	0
91	h	7	Total 7	O 7	0
91	i	1	Total 1	O 1	0
91	j	12	Total 12	O 12	0
91	l	5	Total 5	O 5	0
91	n	5	Total 5	O 5	0

Continued on next page...

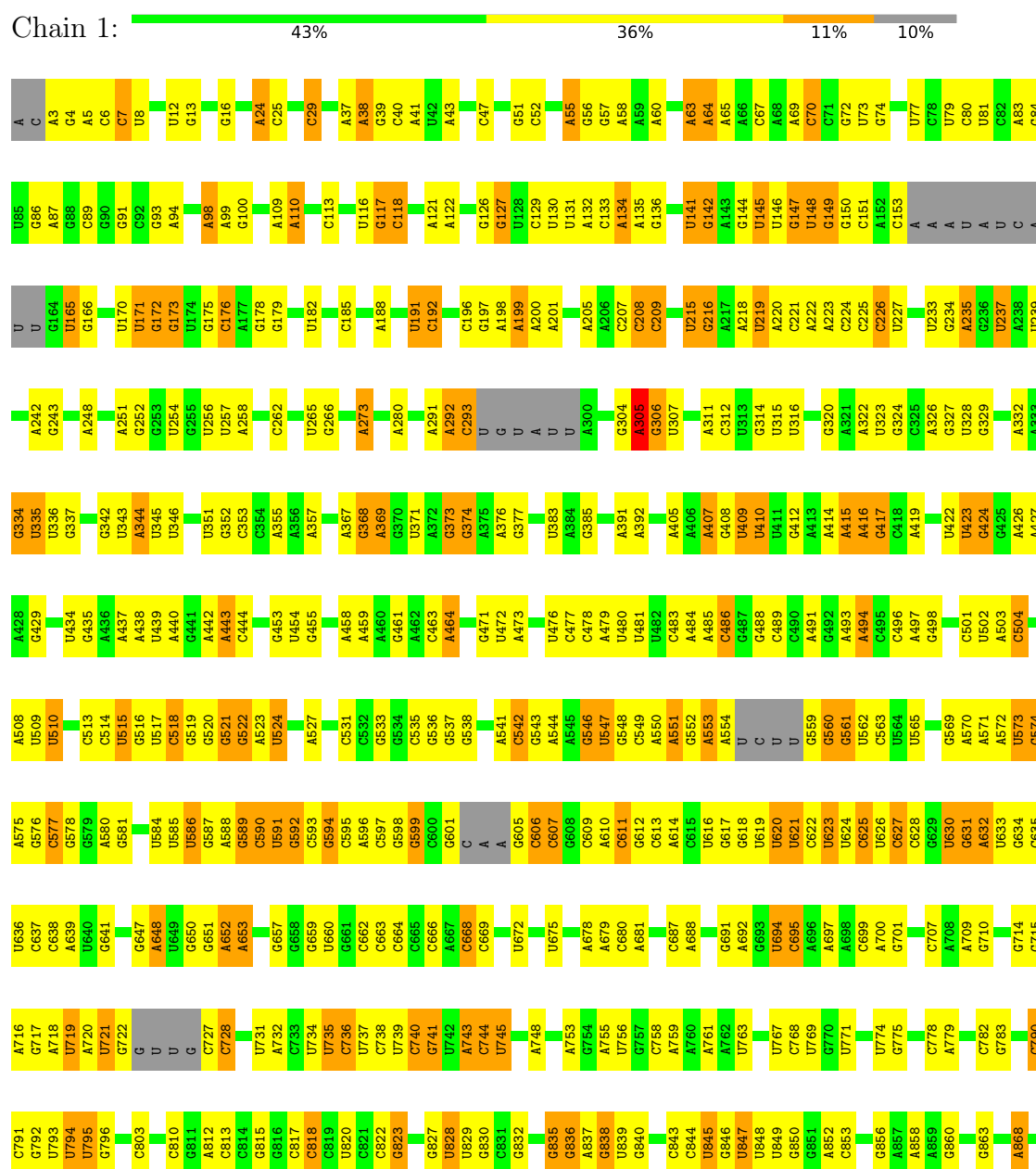
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	o	8	Total	O	0
			8	8	
91	p	5	Total	O	0
			5	5	

3 Residue-property plots

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

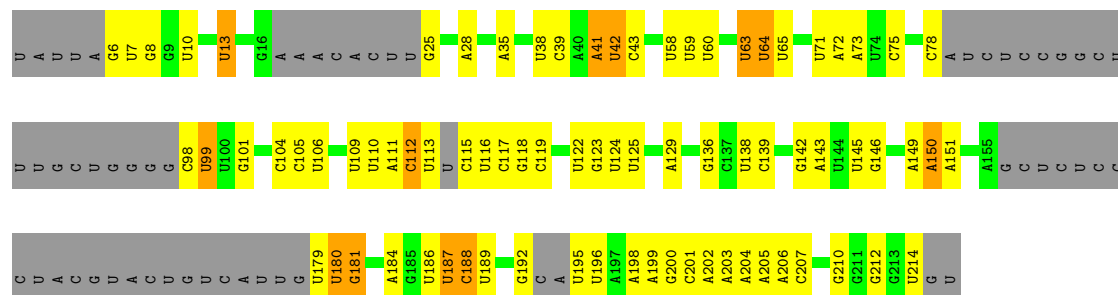
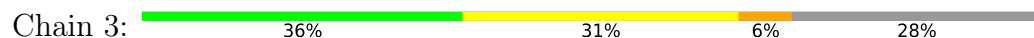
• Molecule 1: LSUa_rRNA_chain_1



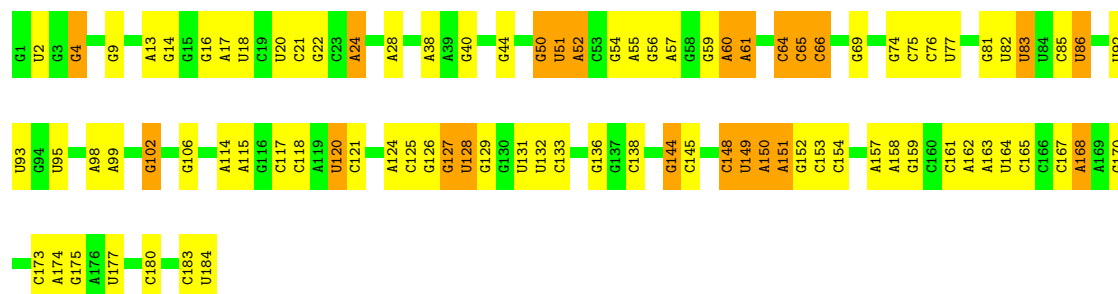


U1387	C1308	G1226	G1156	G1076	G	U	A720	A643	C554	G462	C351	C	U
G1388	G1309	G1229	U1157	U1077	G	A	G721	A644	A555	U463	G351	A	A
G1389	A1310	G1230	A1158	U1078	A	G787	G722	A645	U556	G464	C358	C	U
G1390	G1311	G1231	C1159	U1079	A	C788	G723	G646	G557	A465	G359	G	G
U1391	G1312	G1232	U1160	U1082	A	G789	G724	A647	A558	U471	C366	G	C
U1392	U1313	G1233	A1161	U1083	G	U790	A725	A648	A559	U472	G367	C	A
C1397	C1314	U1233	A1162	A1084	C	A791	A726	G649	U560	G477	G368	C	G
C1398	G1317	G1234	G1165	U1085	C	G792	U728	A650	G561	A478	A377	G	C
G1399	A1168	U1235	A1168	G1086	C	G799	G729	C652	U569	A479	A377	G	C
U1400	C1169	A1237	C1169	U1096	G	G800	A730	C653	A570	C478	A382	U	U
U1403	U1320	G1238	U1170	U1096	U	C801	A731	U654	G571	G480	U383	U	C
G1404	U1321	A1239	U1171	A1101	C	U802	U732	G665	A572	A488	U386	U	U
C1408	C1322	U1241	G1171	C	U	A803	U733	U656	C575	A489	U386	G	U
A1409	A1325	A1246	A1175	A	C	U804	A734	U657	A734	A490	U387	G	U
U1412	U1329	G1247	G1177	A	C	G805	C735	G658	U580	A491	U387	G	C
U1413	G1333	C1248	C1178	U1000	U	C806	C736	A659	C491	A388	A388	A	A
U1416	C1334	A1251	A1179	U1001	U	A807	A737	G660	A389	A389	A389	G	A
G1425	G1335	G1252	G1181	C1002	C	U808	C738	U661	U582	A390	A390	G	A
G1426	G1336	G1253	G1182	C1003	U	G809	C739	U662	C583	A391	A391	G	U
U1427	C1337	G1254	C1183	G1004	C	U810	A740	A665	U590	C392	C392	U	U
U1428	A1338	A1255	U1007	U1010	C	C812	U742	C666	A591	A393	A393	U	U
G1433	G1339	G1261	U1009	U1011	G	U813	G744	U667	C592	A404	A404	C	C
A1437	G1342	G1262	U1010	U1012	C	U819	G745	G683	U593	U415	U415	C	C
G1440	A1349	U1263	U1011	U1013	U	G820	A746	G686	U597	G416	G416	U	U
G1441	G1350	U1264	U1012	U1014	C	G821	U747	G687	A602	C427	C427	U	U
G1442	U1361	U1265	U1013	U1015	C	A822	G748	G688	A603	A428	A428	U	U
G1443	U1362	G1271	U1019	U1016	C	G824	U751	G691	A604	U437	U437	C	C
G1444	C1363	G1272	C1020	U1017	U	U825	G752	U692	C605	U443	U443	U	U
G1445	A1200	G1273	U1021	U1018	C	A	U756	C693	C608	A444	A444	C	A
A1446	G1201	G1274	U1022	U1019	C	U	A757	C694	C511	C445	C445	C	C
A1447	A1202	G1275	U1023	U1020	C	U	C758	G695	U512	C447	C447	C	C
A1448	A1203	G1276	U1024	U1021	C	U	U759	A696	C513	A434	A434	C	C
A1449	A1204	G1277	U1025	U1022	C	U	U760	G697	A613	U436	U436	G	G
G1450	A1205	G1278	U1026	U1023	C	A	U761	G698	A614	U437	U437	C	C
A1451	G1206	U1281	U1027	U1024	C	U	U762	U700	G700	A437	A437	C	C
U1452	U1284	G1282	U1028	U1025	C	G	U763	U701	G617	G519	G519	U	U
U1453	G1207	G1283	U1029	U1026	C	G	C763	A702	A618	C443	C443	U	U
U1454	A1208	U1284	U1030	U1027	C	C	A766	G703	C524	A444	A444	C	A
U1455	A1209	G1285	U1031	U1028	C	G	U767	U	A525	C445	C445	C	C
U1456	A1210	G1286	U1032	U1029	C	G	U768	A	A526	U446	U446	C	C
C1457	U1211	G1287	U1033	U1030	C	U	A769	U	A527	C447	C447	C	C
G1458	A1212	U1288	U1034	U1031	C	A	U770	A	U528	A447	A447	C	C
A1459	G1213	U1289	U1035	U1032	C	A	G771	G708	G529	C450	C450	C	C
U1462	U1214	G1290	U1036	U1033	C	C	U772	U709	C530	U451	U451	G	G
A1463	A1215	G1291	U1037	U1034	C	C	C775	U710	C531	A452	A452	C	U
A1464	C1216	G1292	U1038	U1035	C	C	G776	G711	U532	U342	U342	U	G
G1465	C1217	U1293	U1039	U1036	C	C	A777	G712	C533	U343	U343	C	A
	A1218	U1294	U1040	U1037	C	C	U778	A713	C534	U344	U344	A	U
	U1297	U1295	U1041	U1038	C	C	U779	A714	U535	C345	C345	C	A
	C1380	U1300	U1042	U1039	C	C	U780	G715	U544	U457	U457	U	C
	U1381	U1301	U1043	U1040	C	C	G781	C716	C458	A347	A347	C	C
	U1382	U1302	U1044	U1041	C	C	U782	G717	A459	A348	A348	U	G
	G1383	U1303	U1045	U1042	C	C	U783	C718	C552	A460	A460	U	G
	A1379	U1304	U1046	U1043	C	C	U784	G719	G553	U350	U350	C	C
	C1456	C1305	U1047	U1044	C	C							
	G1457	U1306	U1048	U1045	C	C							
	U1458	U1307	U1049	U1046	C	C							
	A1462	U1308	U1050	U1047	C	C							
	A1463	U1309	U1051	U1048	C	C							
	A1464	U1310	U1052	U1049	C	C							
	G1465	U1311	U1053	U1050	C	C							

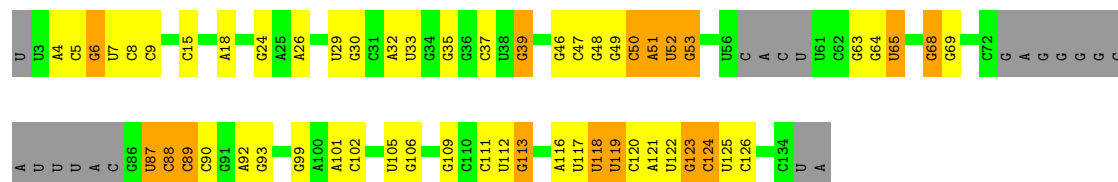
- Molecule 3: SR1 chain 3



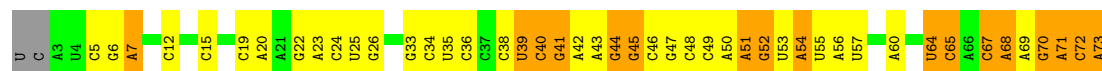
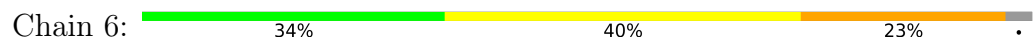
- Molecule 4: SR2 chain 4



- Molecule 5: SR4_chain_5

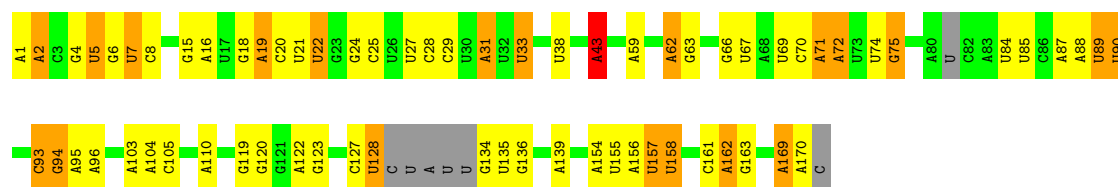


- Molecule 6: SR6 chain 6



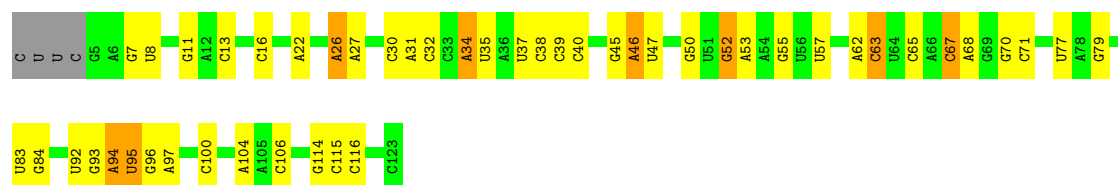
- Molecule 7: 5.8S_rRNA_chain_7

Chain 7: 



• Molecule 8: 5S_rRNA_chain_8

Chain 8: 



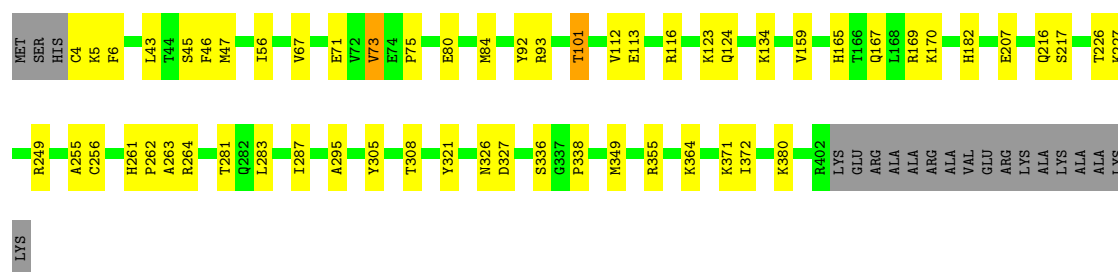
• Molecule 9: Putative 60S ribosomal protein L2

Chain A: 



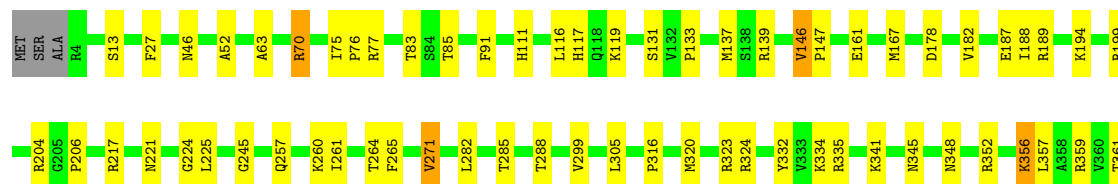
• Molecule 10: Putative ribosomal protein L3

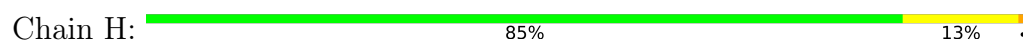
Chain B: 



• Molecule 11: Putative ribosomal protein L1a

Chain C: 

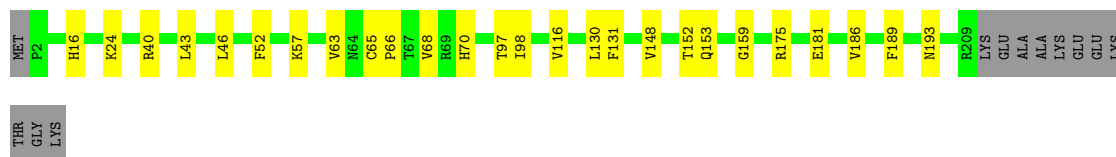






- Molecule 17: Putative 60S ribosomal protein L13

Chain I: 83% 12% 5%



- Molecule 18: Putative 60S ribosomal protein L23

Chain J: 82% 17% .



- Molecule 19: Putative 40S ribosomal protein L14

Chain K: 82% 15% .



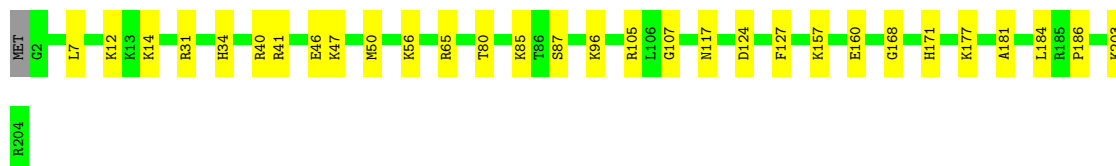
- Molecule 20: Putative 60S ribosomal protein L27A/L29

Chain L: 85% 14% .



- Molecule 21: Ribosomal protein L15

Chain M: 85% 15%



- Molecule 22: Putative 60S ribosomal protein L10

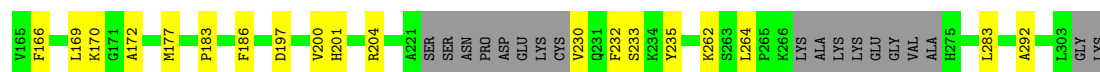
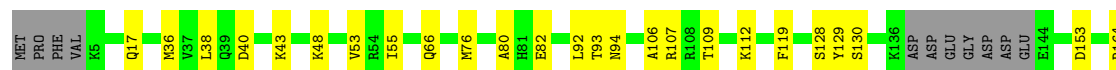
Chain N: 66% 26% 7%





• Molecule 23: Putative 60S ribosomal protein L5

Chain O: 76% 14% 10%



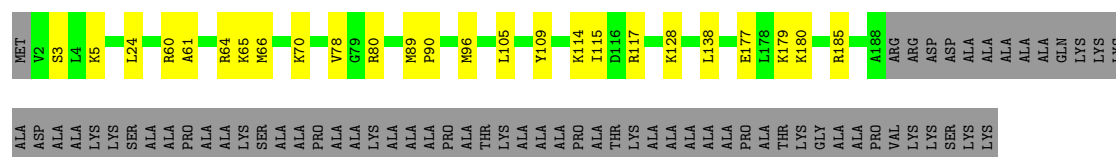
• Molecule 24: 60S ribosomal protein L18

Chain P: 85% 15%



• Molecule 25: Putative 60S ribosomal protein L19

Chain Q: 64% 10% 26%



• Molecule 26: 60S ribosomal protein L18a

Chain R: 85% 14% ..



• Molecule 27: Putative 60S ribosomal protein L21

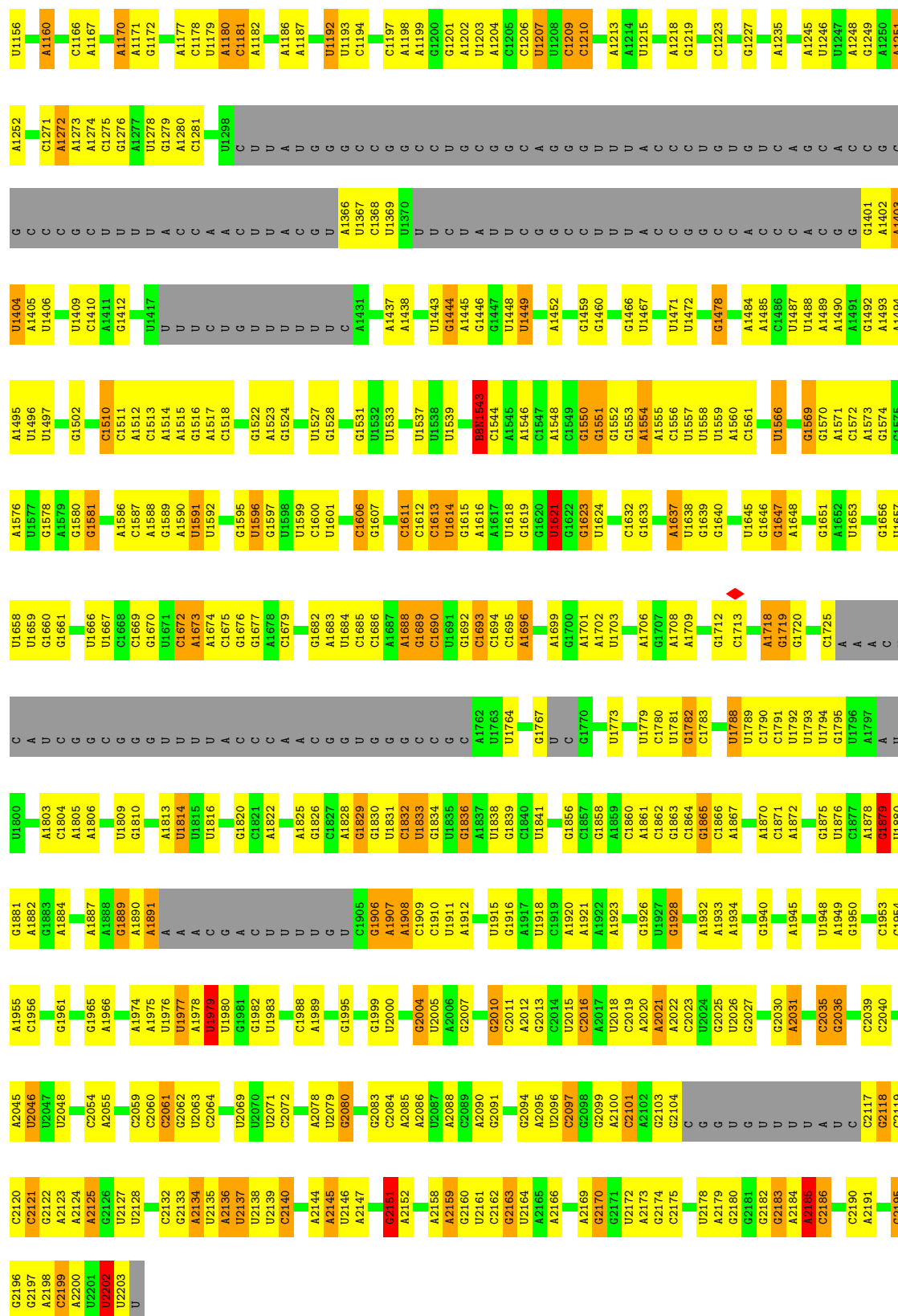
Chain S: 77% 19% ..



• Molecule 28: SSU_rRNA_chain_S1

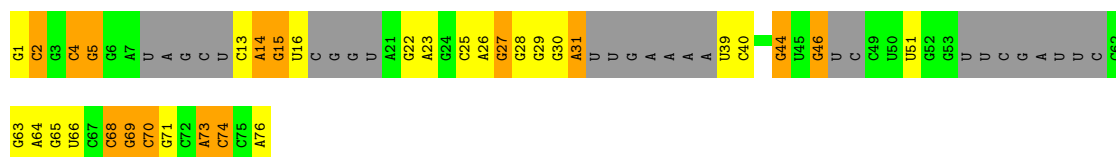
Chain S1: 40% 32% 9% 19%





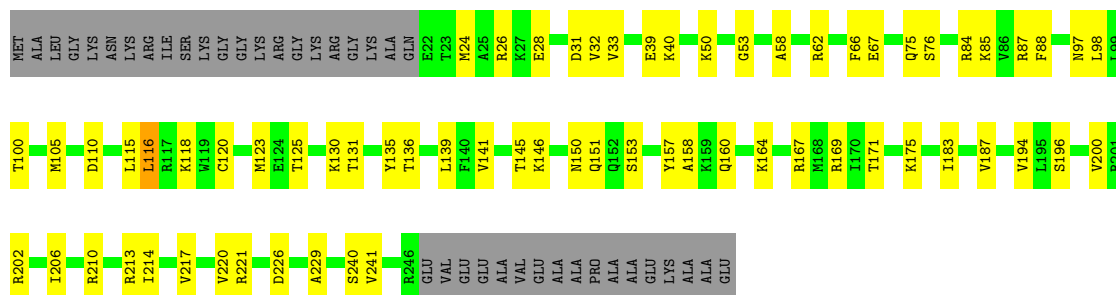
• Molecule 29: E-site_tRNA_chain_S4

Chain S4: 22% 25% 18% 34%



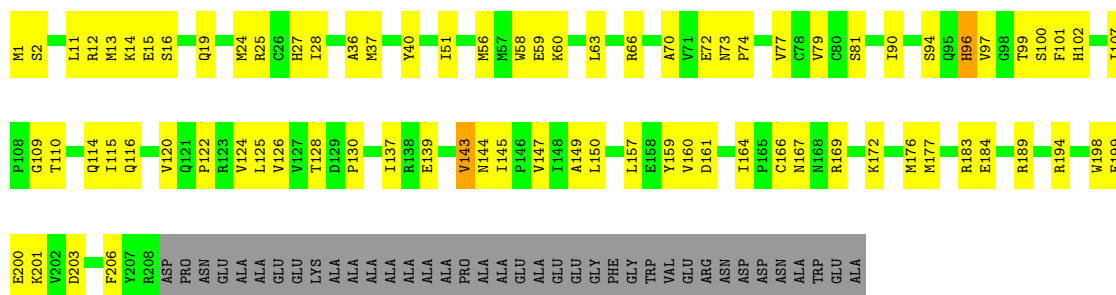
• Molecule 30: 40S ribosomal protein S3a

Chain SA:



• Molecule 31: 40S ribosomal protein SA

Chain SB:



• Molecule 32: Putative 40S ribosomal protein S3

Chain SC:



• Molecule 33: Putative 40S ribosomal protein S9

Chain SD:



MET	Q2	Q3	Q4	L5	R6		R9		K12		L19		F28		E31		H34		L37	R38	Q39	E40	P42	R43		V52	K63	V64	P55	R56	S57	K58	K59	T60	V61	L62		M72		R75	K76	V77		E84	R85	E86		P90	G91	C92	L93	V94	M95		D108		K119	L120
-----	----	----	----	----	----	--	----	--	-----	--	-----	--	-----	--	-----	--	-----	--	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	--	------	--	------	------



- Molecule 39: Putative 40S ribosomal protein S15A

Chain SJ: 85% 14% .



- Molecule 40: 40S ribosomal protein S8

Chain SK: 69% 14% 17%



- Molecule 41: Putative 40S ribosomal protein S16

Chain SL: 82% 14% .



- Molecule 42: Putative ribosomal protein S20

Chain SM: 71% 16% 12%



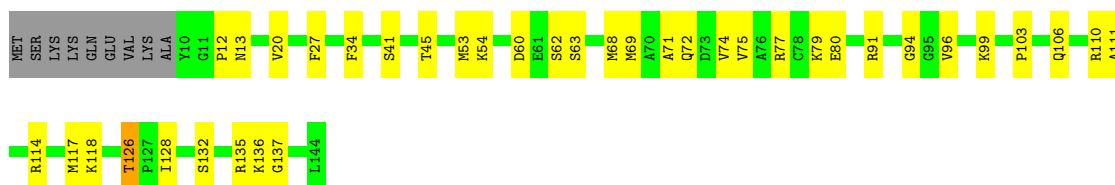
- Molecule 43: Putative 40S ribosomal protein S10

Chain SN: 45% 14% 41%



- Molecule 44: 40S ribosomal protein S14

Chain SO: 67% 26% 6%



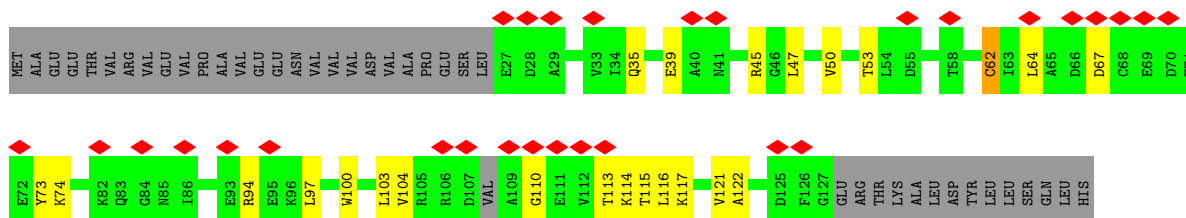
- Molecule 45: Putative 40S ribosomal protein S23

Chain SP: 82% 17% .



- Molecule 46: 40S ribosomal protein S12

Chain SQ: 21% 54% 16% 29% .



- Molecule 47: Putative 40S ribosomal protein S18

Chain SR: 70% 14% 15% .



- Molecule 48: Putative ribosomal protein S29

Chain SS: 81% 18% .



- Molecule 49: Putative 40S ribosomal protein S13

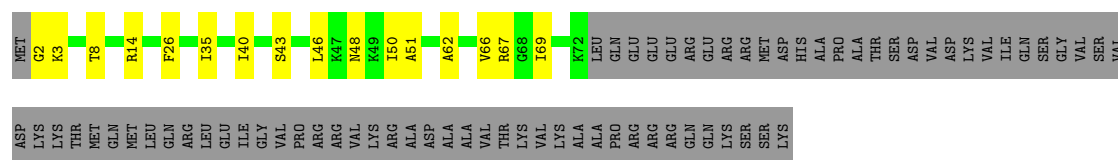
Chain ST: 75% 19% 6% .

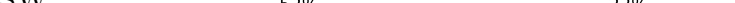


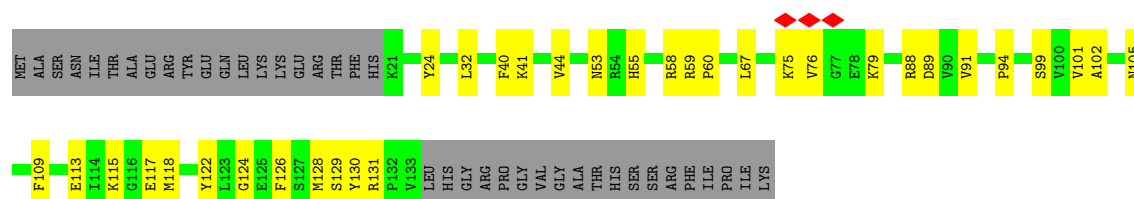
- Molecule 50: Putative 40S ribosomal protein S11

MT1	PRO	V3	Y7	V13	D14	Q18	H19	E20	K21	A28	M33	P36	K39	H40	V41	N42	H46	N65	V89	M95	T98	K110	Q113	Q116	K148	V158	SER	LYS	SER	SER	ALA	ALA	ASP	LYS	LYS	MET	GLY	LYS	LYS	PHE	ALA	LYS	ASN
-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

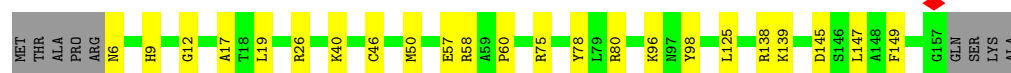
- Chain SV:

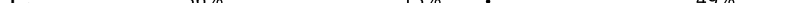


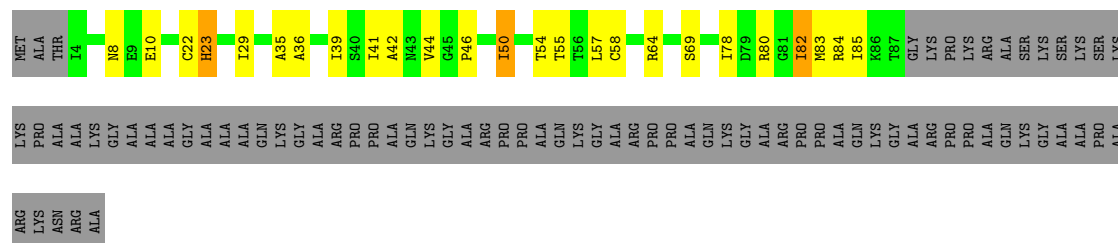
- Chain SW: 



- Chain SX: 80% 14% 6%



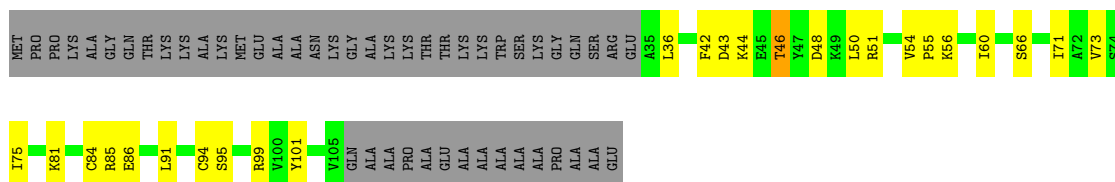
- Chain SY: 



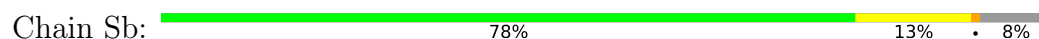
- Chain SZ: 



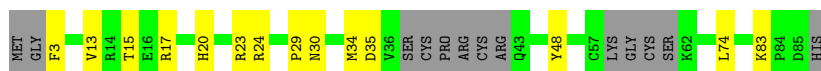
- Molecule 56: 40S ribosomal protein S25



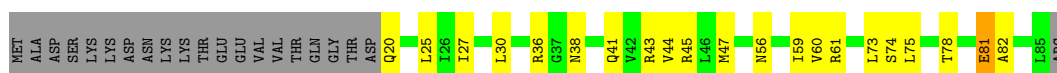
- Molecule 57: 40S ribosomal protein S26



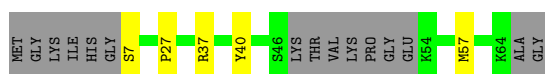
- Molecule 58: Putative 40S ribosomal protein S27-1



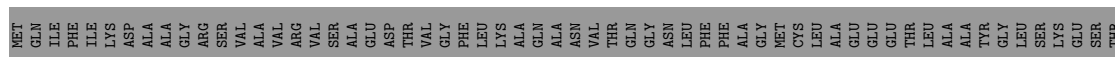
- Molecule 59: Putative 40S ribosomal protein S33

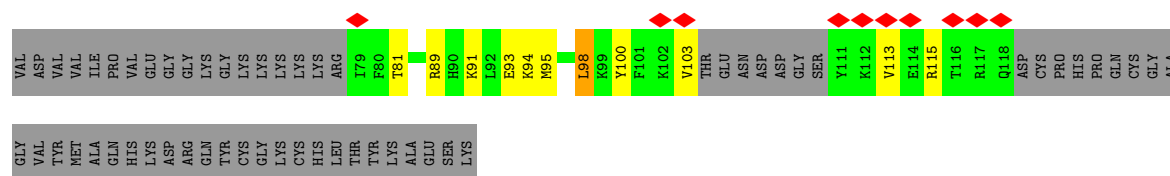


- Molecule 60: 40S ribosomal protein S30

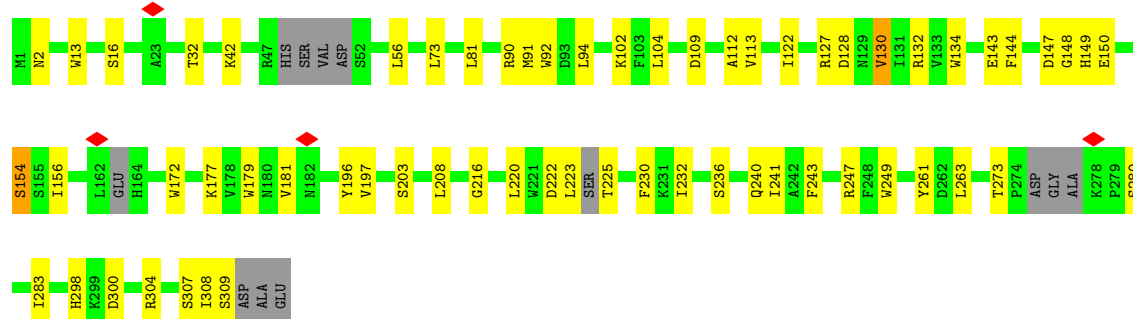
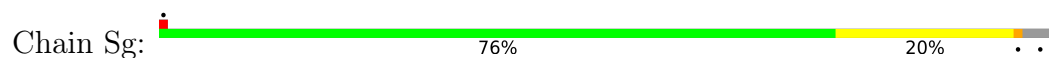


- Molecule 61: Ubiquitin-60S ribosomal protein L40

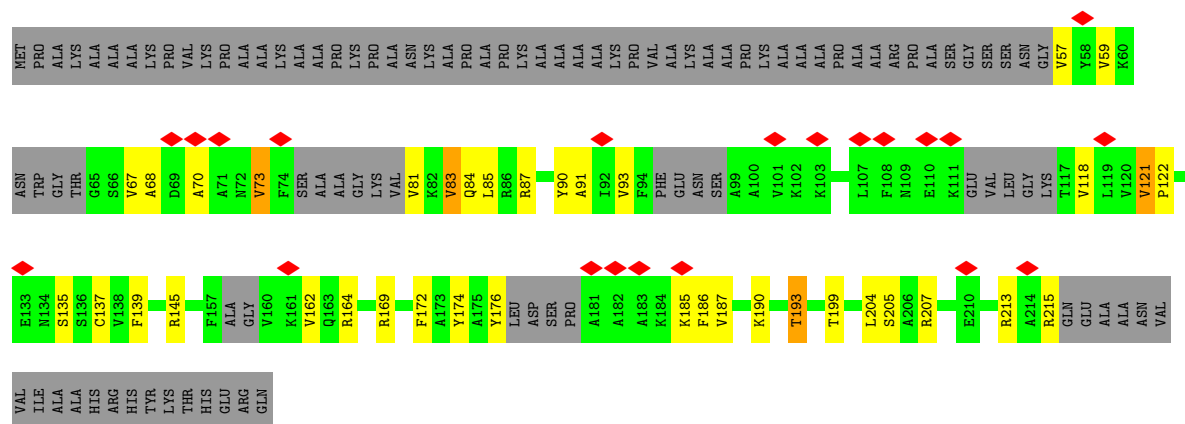
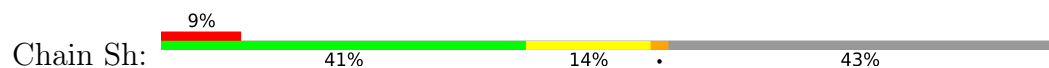




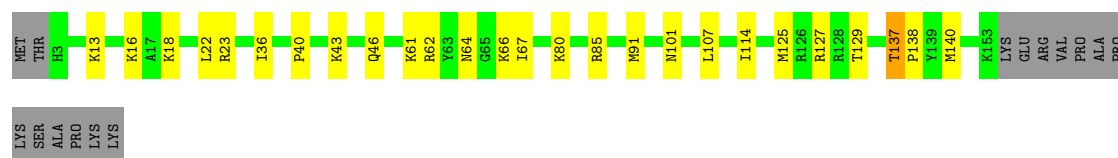
• Molecule 62: Guanine nucleotide-binding protein subunit beta-like protein



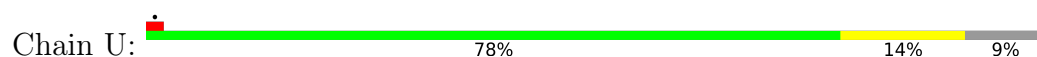
• Molecule 63: Putative RNA binding protein



• Molecule 64: Putative 60S ribosomal protein L17

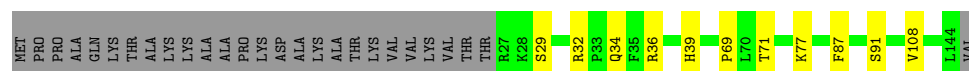


• Molecule 65: Putative 60S ribosomal protein L22

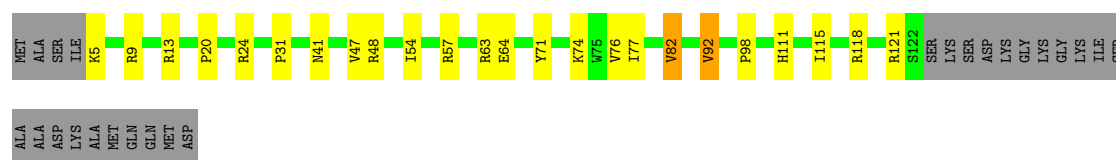




- Molecule 66: Putative 60S ribosomal protein L23a



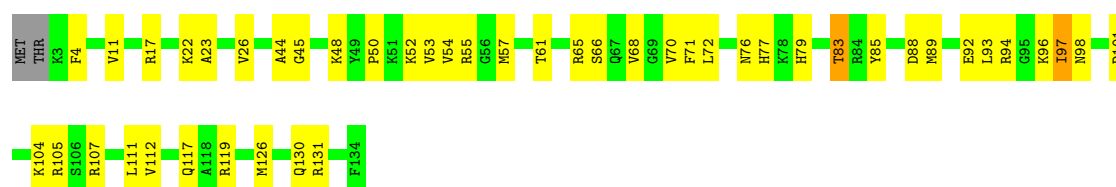
- Molecule 67: Putative 60S ribosomal protein L26



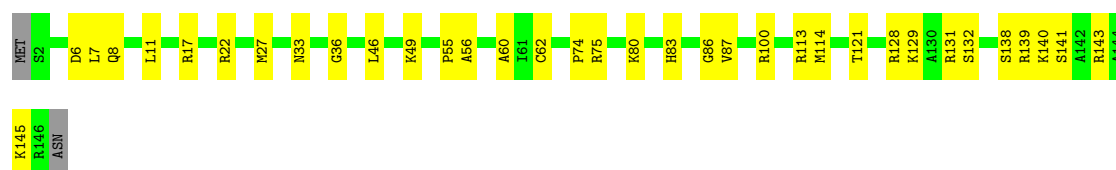
- Molecule 68: Putative ribosomal protein L24



- Molecule 69: 60S ribosomal protein L27

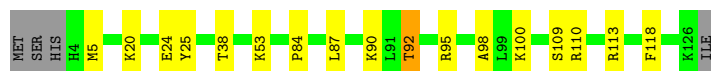


- Molecule 70: Putative 60S ribosomal protein L28



- Molecule 71: Putative 60S ribosomal protein L35

Chain a:  83% 13% ..



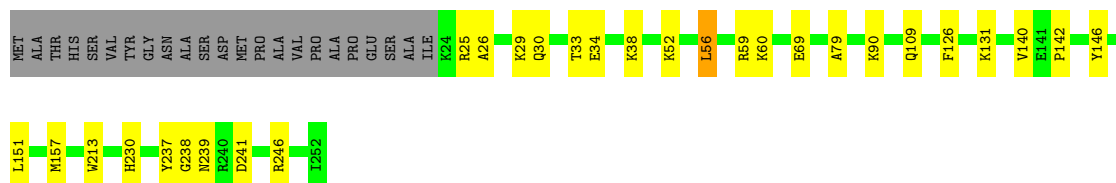
- Molecule 72: 60S ribosomal protein L29

Chain b:  93% ..



- Molecule 73: Putative 60S ribosomal protein L7

Chain c:  79% 11% 9%



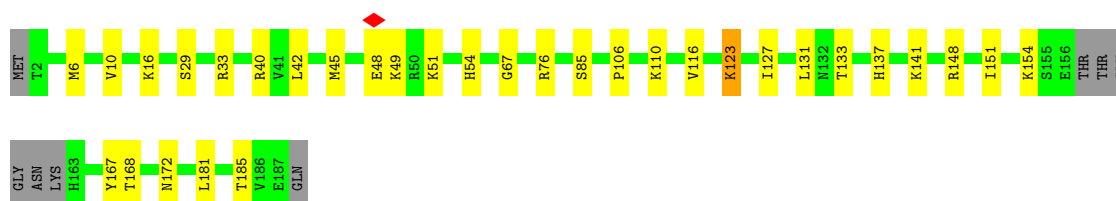
- Molecule 74: 60S ribosomal protein L30

Chain d:  63% 22% 12%



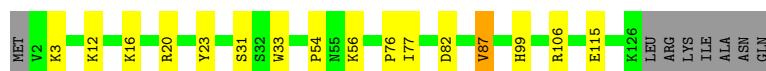
- Molecule 75: Putative 60S ribosomal subunit protein L31

Chain e:  79% 16% ..



- Molecule 76: 60S ribosomal protein L32

Chain f:  82% 11% 6%

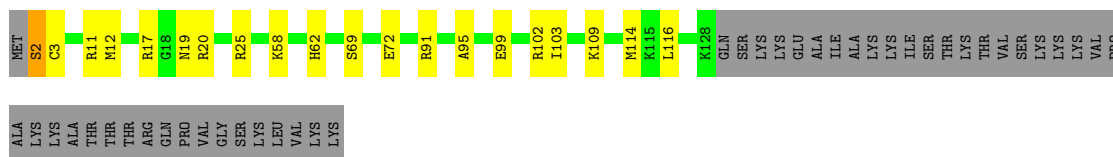


- Molecule 77: Putative ribosomal protein l35a

Chain g:  86% 12% ..



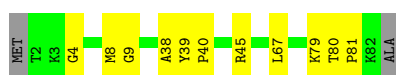
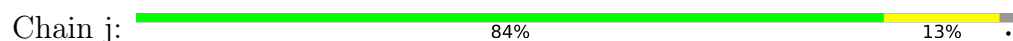
- Molecule 78: Putative 60S ribosomal protein L34



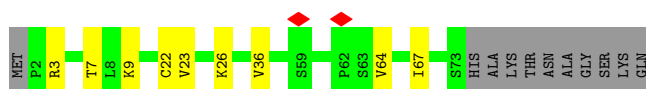
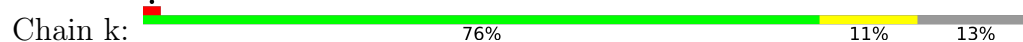
- Molecule 79: Putative 60S Ribosomal protein L36



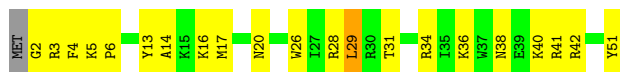
- Molecule 80: Ribosomal protein L37



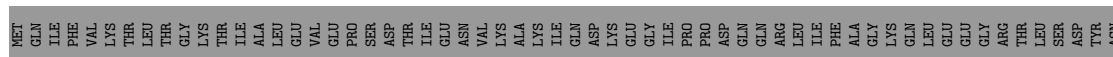
- Molecule 81: Putative ribosomal protein L38

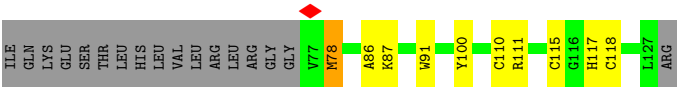


- Molecule 82: Putative 60S ribosomal protein L39



- Molecule 83: Ubiquitin-60S ribosomal protein L40





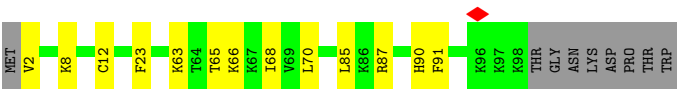
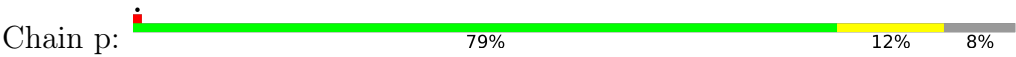
• Molecule 84: 60S ribosomal protein L41



• Molecule 85: 60S ribosomal protein L37a



• Molecule 86: Putative 60S ribosomal protein L44



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.94	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, ZN, OMC, 5MC, 7MG, NA, OMU, MA6, 1MA, OMG, K, PSU, MG, A2M

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	1	0.24	0/37788	0.44	0/58914
2	2	0.25	5/26311 (0.0%)	0.44	0/40996
3	3	0.20	0/3671	0.41	0/5704
4	4	0.20	0/4376	0.41	0/6822
5	5	0.21	0/2739	0.46	0/4263
6	6	0.19	0/1683	0.48	0/2618
7	7	0.24	0/3758	0.42	0/5847
8	8	0.17	0/2829	0.35	0/4405
9	A	0.19	0/1950	0.44	0/2622
10	B	0.18	0/3117	0.40	0/4212
11	C	0.18	0/2827	0.43	0/3808
12	D	0.16	0/1026	0.40	0/1395
13	E	0.20	0/1415	0.49	2/1914 (0.1%)
14	F	0.18	0/1089	0.40	0/1486
15	G	0.17	0/1755	0.38	0/2370
16	H	0.18	0/1769	0.40	0/2381
17	I	0.28	0/1636	0.50	0/2202
18	J	0.19	0/1016	0.45	0/1375
19	K	0.17	0/1285	0.36	0/1736
20	L	0.20	0/1151	0.46	0/1538
21	M	0.22	0/1736	0.42	0/2320
22	N	0.19	0/1639	0.46	0/2194
23	O	0.18	0/2012	0.41	0/2724
24	P	0.18	0/1553	0.40	0/2080
25	Q	0.18	0/1452	0.37	0/1939
26	R	0.18	0/1447	0.35	0/1957
27	S	0.19	0/1263	0.42	0/1705
28	S1	0.20	3/41642 (0.0%)	0.39	0/64864
29	S4	0.17	0/1194	0.39	0/1850
30	SA	0.17	0/1848	0.43	0/2487
31	SB	0.18	0/1660	0.42	0/2246
32	SC	0.13	0/1652	0.34	0/2212

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SD	0.15	0/1393	0.32	0/1874
34	SE	0.16	0/2088	0.40	0/2814
35	SF	0.18	0/1698	0.37	0/2301
36	SG	0.16	0/1853	0.40	1/2475 (0.0%)
37	SH	0.13	0/1458	0.32	0/1955
38	SI	0.16	0/1649	0.38	0/2220
39	SJ	0.16	0/1038	0.37	0/1391
40	SK	0.17	0/1465	0.37	0/1964
41	SL	0.14	0/1145	0.34	0/1540
42	SM	0.15	0/806	0.36	0/1093
43	SN	0.14	0/831	0.34	0/1127
44	SO	0.19	0/1025	0.43	0/1377
45	SP	0.14	0/1120	0.39	0/1500
46	SQ	0.14	0/682	0.34	0/927
47	SR	0.13	0/1052	0.34	0/1414
48	SS	0.13	0/458	0.34	0/607
49	ST	0.24	0/1178	0.43	0/1580
50	SU	0.16	0/1283	0.39	0/1729
51	SV	0.14	0/584	0.31	0/777
52	SW	0.14	0/926	0.35	0/1245
53	SX	0.13	0/1233	0.34	0/1656
54	SY	0.50	1/625 (0.2%)	0.84	3/851 (0.4%)
55	SZ	0.13	0/1051	0.35	0/1399
56	Sa	0.16	0/563	0.45	0/757
57	Sb	0.32	0/833	0.47	0/1116
58	Sc	0.14	0/580	0.35	0/780
59	Sd	0.16	0/485	0.37	0/652
60	Se	1.53	1/407 (0.2%)	0.69	1/540 (0.2%)
61	Sf	0.13	0/301	0.38	0/396
62	Sg	0.14	0/2339	0.36	0/3183
63	Sh	0.17	0/957	0.42	0/1291
64	T	0.21	0/1235	0.44	0/1656
65	U	0.18	0/810	0.47	0/1086
66	V	0.17	0/941	0.38	0/1269
67	W	0.17	0/951	0.40	0/1270
68	X	0.17	0/569	0.38	0/767
69	Y	0.17	0/1048	0.41	0/1409
70	Z	0.20	0/1111	0.39	0/1492
71	a	0.18	0/1016	0.36	0/1351
72	b	0.18	0/557	0.42	0/743
73	c	0.22	0/1896	0.43	0/2540
74	d	0.20	0/715	0.40	0/968
75	e	0.17	0/1439	0.39	0/1912

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	f	0.25	0/1031	0.46	0/1380
77	g	0.18	0/1165	0.37	0/1563
78	h	0.19	0/1034	0.44	0/1378
79	i	0.17	0/699	0.36	0/929
80	j	0.19	0/682	0.45	0/910
81	k	0.15	0/542	0.39	0/733
82	l	0.20	0/463	0.42	0/617
83	m	0.25	0/384	0.55	1/518 (0.2%)
84	n	0.28	0/296	0.51	0/386
85	o	0.22	0/700	0.51	0/933
86	p	0.18	0/788	0.39	0/1043
All	All	0.22	10/215467 (0.0%)	0.42	8/316570 (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
42	SM	0	1
49	ST	0	1
57	Sb	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Se	27	PRO	N-CD	-30.53	1.05	1.47
54	SY	46	PRO	CG-CD	-10.67	1.14	1.50
2	2	1419	OMU	O3'-P	5.40	1.61	1.56
2	2	527	A2M	O3'-P	5.25	1.61	1.56
28	S1	479	A2M	O3'-P	5.19	1.61	1.56
28	S1	512	A2M	O3'-P	5.12	1.61	1.56
28	S1	2021	A2M	O3'-P	5.11	1.61	1.56
2	2	1384	A2M	O3'-P	5.08	1.61	1.56
2	2	572	A2M	O3'-P	5.04	1.61	1.56
2	2	604	A2M	O3'-P	5.04	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SY	46	PRO	N-CD-CG	-14.37	81.64	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Se	27	PRO	N-CD-CG	12.94	122.61	103.20
54	SY	46	PRO	CA-CB-CG	-12.91	79.96	104.50
83	m	78	MET	CG-SD-CE	7.05	116.41	100.90
13	E	95	TYR	CA-C-N	-6.40	112.50	122.42
13	E	95	TYR	C-N-CA	-6.40	112.50	122.42
54	SY	46	PRO	CA-N-CD	-6.03	103.56	112.00
36	SG	121	ASP	CB-CA-C	-5.74	109.97	116.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	SM	65	THR	Peptide
49	ST	124	ARG	Sidechain
57	Sb	10	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	34568	0	17433	571	0
2	2	24802	0	12569	392	0
3	3	3312	0	1680	54	0
4	4	3937	0	1989	70	0
5	5	2453	0	1244	51	0
6	6	1506	0	768	36	0
7	7	3494	0	1774	48	0
8	8	2531	0	1283	34	0
9	A	1908	0	1940	21	0
10	B	3051	0	3080	54	0
11	C	2777	0	2856	61	0
12	D	1008	0	775	9	0
13	E	1395	0	1410	27	0
14	F	1067	0	1077	12	0
15	G	1731	0	1818	27	0
16	H	1734	0	1819	21	0
17	I	1603	0	1623	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	999	0	1023	15	0
19	K	1266	0	1270	27	0
20	L	1124	0	1151	16	0
21	M	1696	0	1770	26	0
22	N	1607	0	1663	43	0
23	O	1975	0	1873	30	0
24	P	1528	0	1618	20	0
25	Q	1433	0	1440	17	0
26	R	1413	0	1433	18	0
27	S	1234	0	1254	26	0
28	S1	38240	0	19316	566	0
29	S4	1072	0	551	15	0
30	SA	1820	0	1904	46	0
31	SB	1627	0	1649	62	0
32	SC	1624	0	1677	19	0
33	SD	1366	0	1406	26	0
34	SE	2050	0	2144	29	0
35	SF	1662	0	1708	28	0
36	SG	1831	0	1955	27	0
37	SH	1436	0	1467	15	0
38	SI	1619	0	1697	46	0
39	SJ	1021	0	1050	14	0
40	SK	1443	0	1524	23	0
41	SL	1124	0	1179	13	0
42	SM	796	0	838	14	0
43	SN	808	0	786	17	0
44	SO	1010	0	1034	27	0
45	SP	1100	0	1146	15	0
46	SQ	679	0	609	17	0
47	SR	1034	0	1073	13	0
48	SS	452	0	463	8	0
49	ST	1155	0	1220	27	0
50	SU	1253	0	1281	16	0
51	SV	577	0	626	13	0
52	SW	907	0	935	22	0
53	SX	1202	0	1227	16	0
54	SY	616	0	601	20	0
55	SZ	1031	0	1105	17	0
56	Sa	558	0	606	16	0
57	Sb	816	0	847	13	0
58	Sc	570	0	557	10	0
59	Sd	483	0	494	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Se	401	0	436	6	0
61	Sf	295	0	324	9	0
62	Sg	2284	0	2172	40	0
63	Sh	948	0	881	23	0
64	T	1211	0	1247	20	0
65	U	801	0	724	14	0
66	V	926	0	973	9	0
67	W	937	0	1009	18	0
68	X	548	0	553	13	0
69	Y	1027	0	1059	34	0
70	Z	1095	0	1117	30	0
71	a	1006	0	1098	13	0
72	b	546	0	575	4	0
73	c	1862	0	1959	27	0
74	d	705	0	719	17	0
75	e	1421	0	1552	23	0
76	f	1011	0	1054	15	0
77	g	1142	0	1196	14	0
78	h	1018	0	1058	16	0
79	i	689	0	751	10	0
80	j	668	0	684	7	0
81	k	534	0	534	6	0
82	l	450	0	483	18	0
83	m	378	0	377	10	0
84	n	292	0	331	9	0
85	o	688	0	711	21	0
86	p	775	0	824	8	0
87	1	58	0	0	0	0
87	2	66	0	0	0	0
87	4	3	0	0	0	0
87	5	3	0	0	0	0
87	6	1	0	0	0	0
87	7	2	0	0	0	0
87	8	1	0	0	0	0
87	A	2	0	0	0	0
87	J	1	0	0	0	0
87	S	1	0	0	0	0
87	S1	79	0	0	2	0
87	SX	1	0	0	0	0
87	Sb	1	0	0	0	0
88	1	11	0	0	0	0
88	2	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	4	3	0	0	0	0
88	S1	9	0	0	0	0
88	S4	1	0	0	0	0
89	1	9	0	0	0	0
89	2	3	0	0	0	0
89	S1	4	0	0	0	0
90	p	1	0	0	0	0
91	1	617	0	0	24	0
91	2	478	0	0	9	0
91	3	21	0	0	1	0
91	4	62	0	0	2	0
91	5	24	0	0	0	0
91	6	5	0	0	0	0
91	7	43	0	0	1	0
91	8	5	0	0	0	0
91	A	20	0	0	2	0
91	B	38	0	0	2	0
91	C	18	0	0	2	0
91	D	1	0	0	0	0
91	F	1	0	0	0	0
91	G	1	0	0	0	0
91	H	9	0	0	0	0
91	I	10	0	0	0	0
91	J	4	0	0	0	0
91	L	12	0	0	0	0
91	M	22	0	0	0	0
91	N	1	0	0	0	0
91	P	8	0	0	0	0
91	Q	2	0	0	0	0
91	R	1	0	0	0	0
91	S	2	0	0	0	0
91	S1	802	0	0	16	0
91	S4	3	0	0	0	0
91	SA	7	0	0	0	0
91	SB	1	0	0	0	0
91	SC	1	0	0	0	0
91	SD	4	0	0	0	0
91	SE	13	0	0	0	0
91	SF	6	0	0	0	0
91	SG	1	0	0	0	0
91	SH	6	0	0	0	0
91	SJ	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	SK	13	0	0	1	0
91	SL	3	0	0	0	0
91	SM	6	0	0	0	0
91	SN	2	0	0	2	0
91	SO	7	0	0	1	0
91	SP	12	0	0	0	0
91	SR	4	0	0	0	0
91	SS	1	0	0	0	0
91	ST	19	0	0	0	0
91	SU	5	0	0	0	0
91	SX	5	0	0	0	0
91	Sa	2	0	0	0	0
91	Sb	23	0	0	0	0
91	Sc	5	0	0	0	0
91	T	9	0	0	0	0
91	V	4	0	0	0	0
91	W	2	0	0	1	0
91	X	2	0	0	1	0
91	Z	1	0	0	0	0
91	b	3	0	0	0	0
91	c	5	0	0	1	0
91	e	3	0	0	0	0
91	f	14	0	0	2	0
91	g	11	0	0	0	0
91	h	7	0	0	1	0
91	i	1	0	0	0	0
91	j	12	0	0	0	0
91	l	5	0	0	0	0
91	n	5	0	0	0	0
91	o	8	0	0	0	0
91	p	5	0	0	0	0
All	All	206527	0	148709	2875	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 8.

All (2875) 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)
87:S1:2327:MG:MG	91:S1:2537:HOH:O	0.77	1.25
87:S1:2329:MG:MG	91:S1:3183:HOH:O	0.88	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:955:A:N6	28:S1:980:G:H1	1.47	1.13
29:S4:26:A:H62	29:S4:44:G:N2	1.56	1.02
3:3:101:G:H1	3:3:139:C:H5	1.09	1.00
4:4:129:G:H1	4:4:161:C:H5	1.03	1.00
27:S:109:GLU:O	27:S:113:GLN:OE1	1.81	0.99
1:1:374:G:H1	7:7:28:C:H5	1.09	0.97
28:S1:486:C:H5	28:S1:509:G:H1	1.13	0.96
29:S4:26:A:N6	29:S4:44:G:H21	1.63	0.96
1:1:1419:C:H5	1:1:1440:G:H1	1.09	0.95
1:1:200:A:OP1	70:Z:139:ARG:NH1	1.98	0.94
2:2:1441:C:H5	6:6:6:G:H1	1.14	0.94
1:1:1472:G:H1	1:1:1514:C:H5	1.16	0.94
2:2:44:C:H5	2:2:52:G:H1	1.15	0.94
29:S4:26:A:H62	29:S4:44:G:H21	0.98	0.94
28:S1:354:C:H5	28:S1:400:G:H1	1.12	0.94
28:S1:953:U:H3	28:S1:982:G:H1	0.94	0.93
28:S1:1104:A:H61	38:SI:72:MET:HE3	1.33	0.93
1:1:668:C:H5	2:2:621:G:H1	1.12	0.93
28:S1:1114:G:H1	28:S1:1207:U:H3	1.12	0.93
7:7:1:A:HO2'	7:7:2:A:H8	1.00	0.93
30:SA:84:ARG:HD2	30:SA:105:MET:HE3	1.48	0.93
5:5:35:G:H1	5:5:111:C:H5	1.15	0.92
5:5:65:U:H3	5:5:93:G:H1	1.11	0.92
2:2:974:G:HO2'	2:2:975:A:H8	0.92	0.92
28:S1:484:G:H1	28:S1:511:C:H5	1.10	0.92
1:1:118:C:H5	1:1:150:G:H1	1.05	0.92
28:S1:1718:A:N6	56:Sa:84:CYS:SG	2.42	0.92
1:1:63:A:OP1	21:M:177:LYS:NZ	2.03	0.92
1:1:853:C:H5	1:1:992:G:H1	1.16	0.91
28:S1:559:G:H1	28:S1:592:C:H5	1.17	0.91
52:SW:79:LYS:HE2	52:SW:113:GLU:OE1	1.70	0.91
4:4:138:C:H5	4:4:152:G:H1	1.17	0.91
73:c:25:ARG:HE	73:c:29:LYS:HB3	1.35	0.90
28:S1:991:G:H21	38:SI:43:ARG:HH21	1.19	0.90
2:2:1261:G:H1	2:2:1305:C:H5	1.16	0.90
5:5:30:G:H1	5:5:124:C:H5	1.16	0.90
1:1:890:C:H5	1:1:905:G:H1	1.16	0.89
1:1:700:A:N1	1:1:845:OMU:H5	1.87	0.89
13:E:95:TYR:O	83:m:78:MET:HE3	1.72	0.89
40:SK:214:ARG:NH1	50:SU:21:LYS:HA	1.86	0.89
49:ST:4:MET:HE3	49:ST:5:HIS:CE1	2.08	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:104:C:H5	3:3:136:G:H1	1.12	0.89
2:2:453:A:HO2'	2:2:455:U:H3	1.20	0.89
1:1:586:U:H5''	11:C:335:ARG:HD2	1.55	0.88
1:1:1051:C:H5	1:1:1097:A:H62	1.20	0.88
28:S1:257:A:H8	28:S1:965:G:H22	1.21	0.88
1:1:1675:A:H61	1:1:1724:C:H42	1.17	0.88
28:S1:1589:G:H1	28:S1:1600:C:H5	1.18	0.88
1:1:1205:G:H1	1:1:1212:C:H5	1.15	0.88
28:S1:2136:A:O2'	28:S1:2137:U:O2	1.92	0.88
4:4:4:G:H1	4:4:20:U:H3	1.17	0.88
31:SB:24:MET:HG3	31:SB:176:MET:HG2	1.56	0.88
7:7:128:U:H3	7:7:134:G:H1	0.90	0.87
34:SE:117:GLN:HG2	34:SE:162:LYS:HD2	1.57	0.87
5:5:68:G:H1	5:5:90:C:H5	1.23	0.87
1:1:373:G:H1	7:7:29:C:H5	1.19	0.86
57:Sb:47:LEU:HD12	57:Sb:68:MET:HE1	1.55	0.86
4:4:44:G:H1	4:4:66:C:H5	1.24	0.86
28:S1:340:G:H5''	34:SE:137:VAL:HG11	1.56	0.85
71:a:92:THR:HG22	71:a:95:ARG:H	1.41	0.85
11:C:167:MET:HA	11:C:167:MET:HE3	1.57	0.85
7:7:4:G:H2'	7:7:5:U:H5''	1.59	0.85
33:SD:57:LEU:HD21	33:SD:67:ARG:HH22	1.42	0.85
28:S1:788:A:H61	28:S1:832:C:H41	1.23	0.85
8:8:77:U:O2	8:8:106:C:N4	2.09	0.85
2:2:844:C:H5'	2:2:845:C:H5''	1.59	0.84
1:1:594:G:H1	1:1:613:C:H5	1.23	0.84
1:1:514:C:H5	1:1:537:G:H1	1.25	0.84
4:4:65:C:O2'	4:4:66:C:O2	1.96	0.84
1:1:117:G:O2'	1:1:118:C:O2	1.95	0.83
1:1:1266:A:H61	1:1:1361:C:H42	1.25	0.82
49:ST:2:VAL:HG23	49:ST:3:ARG:H	1.44	0.82
2:2:695:G:H2'	2:2:696:A:C8	2.14	0.82
2:2:134:C:H5	2:2:344:G:H1	1.27	0.82
1:1:790:C:H5	11:C:305:LEU:H	1.28	0.81
49:ST:4:MET:CE	49:ST:5:HIS:CE1	2.62	0.81
73:c:52:LYS:HE2	73:c:56:LEU:HD21	1.60	0.81
2:2:781:G:H1	2:2:808:C:H5	1.24	0.81
2:2:1510:A:N6	10:B:327:ASP:H	1.78	0.81
1:1:1242:U:OP1	19:K:17:ARG:NH2	2.13	0.81
63:Sh:135:SER:HB2	63:Sh:204:LEU:HD12	1.60	0.81
1:1:1063:G:H1	1:1:1089:C:H5	1.24	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SQ:45:ARG:HD2	46:SQ:103:LEU:HD21	1.60	0.81
4:4:120:U:O2'	18:J:14:ARG:NH2	2.14	0.81
28:S1:2059:C:H5	28:S1:2166:A:H61	1.29	0.81
41:SL:32:GLN:NE2	53:SX:12:GLY:O	2.14	0.80
1:1:1571:C:H5	64:T:85:ARG:HH21	1.29	0.80
1:1:1775:U:H3	2:2:7:C:H41	1.26	0.80
64:T:40:PRO:HD2	64:T:43:LYS:HD2	1.64	0.80
2:2:683:G:H1	2:2:756:C:H5	1.30	0.79
28:S1:291:G:H1	28:S1:298:C:H5	1.30	0.79
31:SB:11:LEU:HD23	31:SB:194:ARG:HH22	1.48	0.79
42:SM:48:HIS:HB2	42:SM:87:ASP:HB2	1.65	0.79
1:1:1731:G:OP1	66:V:36:ARG:NH1	2.16	0.79
3:3:115:C:N3	74:d:86:HIS:NE2	2.29	0.78
28:S1:1645:U:H3	28:S1:1674:A:H62	1.32	0.78
33:SD:76:MET:HE3	33:SD:92:LEU:HA	1.62	0.78
30:SA:84:ARG:CD	30:SA:105:MET:HE3	2.14	0.78
1:1:518:C:H5	1:1:533:G:H1	1.29	0.78
3:3:43:C:N4	3:3:186:U:O2	2.15	0.78
31:SB:166:CYS:HB2	31:SB:177:MET:HE3	1.63	0.78
2:2:984:G:O6	2:2:1000:U:O4	2.02	0.78
28:S1:753:A:H3'	28:S1:754:G:H21	1.49	0.78
5:5:123:G:O2'	5:5:124:C:O2	2.01	0.78
38:SI:86:GLU:HG3	38:SI:94:VAL:HG12	1.63	0.78
5:5:63:G:H3'	5:5:64:G:H21	1.48	0.78
22:N:36:ILE:HG22	22:N:87:MET:HB3	1.66	0.78
38:SI:174:TYR:O	38:SI:178:GLN:NE2	2.17	0.77
28:S1:1145:A:H5''	44:SO:53:MET:HE3	1.66	0.77
2:2:708:G:OP2	2:2:740:A:N6	2.17	0.77
3:3:41:A:O2'	3:3:188:C:N4	2.16	0.77
7:7:93:C:H2'	7:7:94:G:H5''	1.66	0.77
28:S1:1788:U:H5'	51:SV:48:ASN:HB3	1.67	0.77
18:J:91:ASP:HB2	68:X:1:MET:HE1	1.65	0.77
52:SW:117:GLU:OE2	52:SW:117:GLU:N	2.15	0.77
28:S1:955:A:N1	28:S1:980:G:N2	2.30	0.77
74:d:48:ASN:ND2	74:d:73:SER:O	2.18	0.77
2:2:1456:C:H5	2:2:1468:G:H1	1.30	0.77
31:SB:120:VAL:HG13	31:SB:122:PRO:HD3	1.67	0.77
78:h:95:ALA:O	78:h:99:GLU:HG3	1.84	0.77
1:1:1730:A:OP2	66:V:32:ARG:NH1	2.19	0.76
28:S1:951:U:H3	28:S1:984:G:H1	0.80	0.76
28:S1:1978:A:H4'	28:S1:1979:OMU:H5''	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SF:249:ARG:NH1	35:SF:254:GLU:HG3	2.01	0.76
34:SE:92:THR:OG1	34:SE:94:ASP:OD1	2.04	0.76
40:SK:214:ARG:HH11	50:SU:21:LYS:HA	1.48	0.76
2:2:975:A:OP1	78:h:91:ARG:NH2	2.18	0.76
41:SL:56:GLU:OE2	41:SL:88:ARG:NH1	2.18	0.75
7:7:31:A:O2'	7:7:33:U:OP2	2.04	0.75
28:S1:254:A:H61	28:S1:974:G:H21	1.33	0.75
28:S1:1878:A:O2'	53:SX:60:PRO:O	2.03	0.75
19:K:25:GLY:HA2	19:K:40:ASN:HB2	1.69	0.75
28:S1:2134:A:H3'	28:S1:2135:U:O2	1.87	0.75
34:SE:48:ARG:NH2	34:SE:106:PHE:O	2.20	0.75
70:Z:22:ARG:HB3	76:f:76:PRO:HG2	1.67	0.75
28:S1:991:G:N2	38:SI:40:GLU:OE2	2.19	0.75
38:SI:164:ARG:NH1	38:SI:165:ILE:HB	2.02	0.74
44:SO:137:GLY:O	91:SO:201:HOH:O	2.06	0.74
8:8:55:G:H21	12:D:11:MET:HE2	1.49	0.74
78:h:17:ARG:HA	78:h:20:ARG:HE	1.53	0.74
1:1:549:C:OP2	73:c:246:ARG:NH2	2.16	0.74
2:2:741:C:H2'	2:2:742:U:C6	2.22	0.74
28:S1:40:A:OP1	33:SD:1:MET:N	2.21	0.74
38:SI:144:ARG:HD2	39:SJ:49:GLU:OE1	1.88	0.74
1:1:483:C:H5	1:1:650:G:H1	1.31	0.74
28:S1:2161:U:O4	91:S1:2402:HOH:O	2.06	0.74
1:1:493:A:H2'	1:1:494:A:H5''	1.70	0.73
7:7:70:C:OP2	67:W:111:HIS:NE2	2.18	0.73
36:SG:149:ASN:O	36:SG:149:ASN:ND2	2.19	0.73
2:2:813:U:O2	2:2:965:C:N4	2.20	0.73
1:1:846:G:H2'	1:1:847:OMU:H6	1.70	0.73
28:S1:1856:G:O6	91:S1:2401:HOH:O	2.05	0.73
20:L:39:HIS:O	20:L:40:HIS:ND1	2.22	0.73
2:2:741:C:H2'	2:2:742:U:H6	1.53	0.73
1:1:586:U:O4	1:1:623:U:N3	2.16	0.73
2:2:124:G:OP1	25:Q:80:ARG:NH1	2.21	0.73
1:1:1206:A:N7	91:1:1913:HOH:O	2.21	0.73
2:2:1214:G:H1	2:2:1222:C:H5	1.36	0.73
3:3:25:G:O6	3:3:212:G:N2	2.19	0.73
1:1:1260:G:H4'	1:1:1261:U:H5'	1.71	0.73
28:S1:1980:U:H4'	28:S1:2019:C:H4'	1.70	0.73
1:1:547:U:HO2'	1:1:548:G:H8	1.35	0.73
1:1:599:G:OP1	27:S:139:ARG:NH1	2.22	0.73
2:2:1510:A:H61	10:B:327:ASP:H	1.34	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:36:GLU:HG3	9:A:91:GLY:HA2	1.71	0.72
2:2:974:G:O2'	2:2:975:A:H8	1.68	0.72
81:k:23:VAL:HG22	81:k:36:VAL:HG22	1.71	0.72
1:1:40:C:OP2	91:1:1901:HOH:O	2.08	0.72
1:1:897:A:N6	28:S1:1218:A:N1	2.38	0.72
30:SA:33:VAL:O	30:SA:100:THR:OG1	2.07	0.72
62:Sg:2:ASN:ND2	62:Sg:309:SER:OG	2.22	0.72
26:R:70:LYS:O	26:R:74:ARG:NH2	2.22	0.72
28:S1:2010:G:H1	28:S1:2026:U:H3	1.36	0.72
35:SF:238:THR:HG22	35:SF:240:ASP:H	1.55	0.72
61:Sf:103:VAL:HG23	61:Sf:113:VAL:HG22	1.69	0.72
2:2:1336:G:OP2	13:E:172:ARG:NH1	2.21	0.72
28:S1:951:U:O4	28:S1:984:G:O6	2.07	0.71
31:SB:172:LYS:HA	31:SB:206:PHE:CE1	2.25	0.71
74:d:46:ILE:HD11	74:d:58:VAL:HG11	1.70	0.71
2:2:97:A:O2'	2:2:366:C:O2	2.09	0.71
2:2:974:G:O6	78:h:102:ARG:NH2	2.24	0.71
2:2:1020:C:HO2'	2:2:1021:A:H8	1.38	0.71
5:5:88:C:O2'	5:5:89:C:O5'	2.07	0.71
1:1:77:U:H5''	21:M:186:PRO:HG3	1.71	0.71
1:1:1264:A:H1'	2:2:1294:G:OP1	1.89	0.71
74:d:16:LEU:O	74:d:20:MET:HG2	1.91	0.71
28:S1:1223:C:OP1	49:ST:109:ARG:NH1	2.23	0.71
59:Sd:59:ILE:HG13	59:Sd:81:GLU:HG2	1.72	0.70
46:SQ:39:GLU:N	46:SQ:39:GLU:OE2	2.24	0.70
28:S1:1138:G:H2'	28:S1:1139:G:C8	2.26	0.70
4:4:163:A:OP1	16:H:167:LYS:NZ	2.24	0.70
8:8:52:G:H5''	23:O:235:TYR:HE2	1.57	0.70
11:C:70:ARG:O	91:C:401:HOH:O	2.08	0.70
27:S:24:VAL:HG13	27:S:25:PRO:HD2	1.74	0.70
77:g:35:MET:HE2	77:g:70:TYR:OH	1.90	0.70
2:2:54:U:OP1	91:2:4301:HOH:O	2.09	0.70
2:2:846:G:H22	2:2:952:G:H22	1.40	0.70
6:6:39:U:H4'	19:K:91:ARG:HH22	1.57	0.70
2:2:716:C:H2'	2:2:717:G:C8	2.26	0.70
31:SB:114:GLN:HG2	31:SB:115:ILE:HG23	1.72	0.70
1:1:130:U:H2'	1:1:132:A:H62	1.55	0.70
1:1:304:G:OP2	91:1:1902:HOH:O	2.10	0.70
2:2:1045:G:OP1	22:N:116:ARG:NH1	2.25	0.70
28:S1:322:C:N3	28:S1:327:U:O4	2.25	0.70
3:3:78:C:O2	3:3:143:A:N6	2.17	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:1578:G:N7	46:SQ:114:LYS:NZ	2.33	0.70
28:S1:2088:A:N1	28:S1:2135:U:H5	1.90	0.70
56:Sa:55:PRO:O	56:Sa:56:LYS:HG2	1.92	0.70
76:f:99:HIS:NE2	91:f:201:HOH:O	2.25	0.70
68:X:44:TYR:CD1	68:X:45:MET:HE3	2.27	0.69
70:Z:55:PRO:HD3	70:Z:114:MET:HE3	1.73	0.69
78:h:58:LYS:HG3	78:h:72:GLU:HG3	1.73	0.69
1:1:39:G:OP1	91:1:1901:HOH:O	2.09	0.69
1:1:1675:A:H61	1:1:1724:C:N4	1.89	0.69
28:S1:1557:U:OP2	91:S1:2401:HOH:O	2.08	0.69
40:SK:119:ILE:HD11	40:SK:166:ARG:HD3	1.74	0.69
28:S1:171:C:OP1	36:SG:134:ARG:NE	2.25	0.69
28:S1:2086:A:N1	28:S1:2137:U:H5	1.91	0.69
1:1:216:G:OP2	70:Z:132:SER:OG	2.11	0.69
1:1:1046:U:H5	1:1:1105:A:N7	1.90	0.69
28:S1:1908:A:H5''	28:S1:1909:C:H5	1.57	0.69
4:4:2:U:H3	4:4:22:G:H1	1.40	0.69
46:SQ:97:LEU:HD11	46:SQ:121:VAL:HG23	1.74	0.69
26:R:50:LYS:NZ	27:S:147:ALA:O	2.26	0.69
28:S1:1659:U:H3	28:S1:1670:G:H22	1.38	0.69
28:S1:952:U:O4	28:S1:983:C:N3	2.26	0.69
28:S1:1974:A:O2'	52:SW:89:ASP:OD1	2.10	0.69
35:SF:149:VAL:HG21	35:SF:231:ARG:HG3	1.74	0.69
1:1:344:A:N1	2:2:1221:U:H5	1.91	0.68
1:1:1247:U:OP1	1:1:1272:U:O2'	2.10	0.68
28:S1:232:C:H2'	28:S1:233:G:H8	1.58	0.68
50:SU:42:ASN:HD21	50:SU:46:HIS:HB2	1.58	0.68
28:S1:1132:G:H2'	28:S1:1133:U:C6	2.27	0.68
52:SW:24:TYR:HB3	52:SW:32:LEU:HD11	1.76	0.68
1:1:305:A2M:HM'3	21:M:12:LYS:HG3	1.75	0.68
74:d:55:ARG:O	74:d:59:GLU:HG2	1.93	0.68
36:SG:143:LYS:HA	36:SG:146:LYS:HB2	1.74	0.68
15:G:179:ALA:HB2	15:G:219:VAL:HG22	1.76	0.68
1:1:927:A2M:HM'2	1:1:928:C:H5'	1.76	0.68
1:1:997:C:HO2'	1:1:998:A:H8	1.40	0.68
1:1:1392:G:O6	19:K:45:LYS:NZ	2.22	0.68
10:B:71:GLU:OE2	68:X:1:MET:HG2	1.94	0.68
75:e:29:SER:OG	75:e:33:ARG:NH2	2.26	0.68
28:S1:1858:G:O2'	28:S1:1978:A:N6	2.24	0.68
2:2:133:G:H1	2:2:345:C:H5	1.43	0.67
2:2:1020:C:O2'	2:2:1021:A:H8	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:51:ARG:HA	24:P:54:LYS:HD2	1.77	0.67
28:S1:1121:C:H2'	28:S1:1122:G:C8	2.29	0.67
6:6:68:A:H5'	14:F:47:ARG:CZ	2.24	0.67
28:S1:558:U:H2'	28:S1:559:G:C8	2.30	0.67
70:Z:113:ARG:NH1	76:f:87:VAL:O	2.27	0.67
73:c:69:GLU:OE1	73:c:69:GLU:HA	1.93	0.67
2:2:558:A:OP1	2:2:560:OMU:H5	1.95	0.67
7:7:38:U:O2'	71:a:90:LYS:NZ	2.28	0.67
28:S1:1459:G:N7	91:S1:2419:HOH:O	2.26	0.67
2:2:1376:G:N7	91:2:4308:HOH:O	2.26	0.67
28:S1:356:A:N7	91:S1:2420:HOH:O	2.27	0.67
28:S1:260:A:H2'	28:S1:261:A:C8	2.30	0.67
28:S1:1569:G:O6	48:SS:8:ARG:NH1	2.28	0.67
1:1:385:G:OP2	91:1:1904:HOH:O	2.13	0.67
4:4:163:A:N7	91:4:302:HOH:O	2.27	0.67
29:S4:29:G:H2'	29:S4:30:G:C8	2.29	0.67
36:SG:80:ARG:HG2	36:SG:87:THR:HA	1.77	0.67
2:2:712:G:H3'	2:2:713:A:H8	1.59	0.67
14:F:42:LEU:HD11	14:F:85:ILE:HG13	1.76	0.67
28:S1:1117:A:H2'	28:S1:1118:G:C8	2.30	0.67
1:1:226:C:H2'	1:1:227:U:H6	1.59	0.67
1:1:882:A:N1	1:1:914:U:H5	1.92	0.67
3:3:187:U:O2'	3:3:188:C:O2	2.12	0.67
6:6:40:C:OP1	6:6:41:G:N2	2.28	0.67
10:B:43:LEU:O	91:B:501:HOH:O	2.13	0.67
38:SI:60:THR:HG1	38:SI:92:CYS:HG	1.42	0.67
1:1:226:C:H2'	1:1:227:U:C6	2.31	0.66
2:2:851:C:N3	2:2:947:U:O4	2.28	0.66
28:S1:45:U:O2'	28:S1:46:U:H2'	1.94	0.66
28:S1:1510:C:H5	28:S1:1515:A:H61	1.42	0.66
1:1:868:A:OP2	91:1:1903:HOH:O	2.12	0.66
1:1:1363:A:H4'	1:1:1364:A:H5''	1.77	0.66
1:1:1728:A:O2'	1:1:1729:A:O5'	2.12	0.66
1:1:1574:C:H2'	1:1:1575:G:C8	2.30	0.66
2:2:392:C:OP2	91:2:4302:HOH:O	2.14	0.66
2:2:1143:U:H5	2:2:1168:A:N1	1.93	0.66
28:S1:321:G:O6	36:SG:186:ARG:NH2	2.27	0.66
31:SB:167:ASN:OD1	31:SB:169:ARG:NH1	2.28	0.66
1:1:368:G:OP1	17:I:24:LYS:NZ	2.24	0.66
2:2:460:A:HO2'	2:2:461:C:H6	1.44	0.66
35:SF:249:ARG:HH12	35:SF:254:GLU:HG3	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:h:25:ARG:O	91:h:201:HOH:O	2.12	0.66
1:1:417:G:O2'	1:1:442:A:N6	2.28	0.66
25:Q:89:MET:HE3	25:Q:90:PRO:HD2	1.78	0.66
44:SO:110:ARG:HD2	57:Sb:51:SER:HA	1.78	0.66
1:1:109:A:H4'	1:1:110:A:H5'	1.76	0.66
1:1:251:A:N7	67:W:5:LYS:N	2.44	0.66
1:1:1583:C:OP2	91:2:4301:HOH:O	2.14	0.66
4:4:138:C:H5	4:4:152:G:N1	1.93	0.66
28:S1:1278:U:H5	28:S1:1445:A:N7	1.93	0.66
43:SN:25:CYS:SG	91:SN:202:HOH:O	2.54	0.66
2:2:1151:U:H5	2:2:1161:A:N1	1.94	0.66
28:S1:512:A2M:OP1	91:S1:2403:HOH:O	2.15	0.66
65:U:67:LYS:HD2	65:U:83:MET:HE3	1.78	0.66
21:M:65:ARG:HD3	21:M:127:PHE:CD1	2.30	0.65
34:SE:155:ASP:OD1	34:SE:171:LYS:HA	1.95	0.65
67:W:71:TYR:O	91:W:201:HOH:O	2.13	0.65
4:4:51:U:O2'	4:4:52:A:H8	1.80	0.65
22:N:93:PRO:HB2	22:N:125:VAL:HG13	1.78	0.65
7:7:15:G:N7	91:7:301:HOH:O	2.29	0.65
1:1:237:U:OP1	67:W:57:ARG:NH1	2.30	0.65
1:1:626:U:HO2'	1:1:627:C:H6	1.45	0.65
4:4:92:U:H2'	4:4:93:U:C6	2.31	0.65
5:5:118:U:O2'	5:5:119:U:O2	2.14	0.65
9:A:32:LEU:HD13	9:A:163:ARG:HD3	1.77	0.65
28:S1:694:U:H3	28:S1:751:G:H22	1.43	0.65
57:Sb:47:LEU:HB3	57:Sb:51:SER:HB2	1.77	0.65
4:4:24:A:H5''	16:H:7:LYS:HB2	1.78	0.65
28:S1:2016:C:OP1	48:SS:17:LYS:NZ	2.28	0.65
3:3:98:C:O2'	3:3:99:U:OP2	2.14	0.65
9:A:213:GLY:O	91:A:401:HOH:O	2.15	0.65
10:B:167:GLN:NE2	10:B:207:GLU:OE2	2.27	0.65
3:3:72:A:OP2	91:3:301:HOH:O	2.15	0.65
3:3:105:C:H2'	3:3:106:U:C6	2.31	0.65
23:O:76:MET:CE	23:O:112:LYS:HD3	2.26	0.65
10:B:227:LYS:HD2	10:B:338:PRO:HB3	1.78	0.65
28:S1:1207:U:H5'	49:ST:55:ARG:HD3	1.78	0.65
28:S1:1276:G:O2'	28:S1:1278:U:O2	2.15	0.65
47:SR:88:GLN:HA	47:SR:96:THR:HG23	1.79	0.65
62:Sg:42:LYS:HZ2	62:Sg:56:LEU:HB2	1.62	0.65
77:g:61:VAL:HG13	77:g:66:ASP:HB2	1.79	0.65
2:2:459:A:O2'	2:2:460:A:H5'	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:65:U:O2	5:5:93:G:N2	2.24	0.64
1:1:215:U:H4'	1:1:216:G:OP1	1.97	0.64
1:1:830:G:OP1	24:P:192:ARG:NH2	2.30	0.64
1:1:1675:A:N6	1:1:1724:C:H42	1.93	0.64
28:S1:148:G:H2'	28:S1:149:G:C8	2.32	0.64
38:SI:95:MET:HE3	38:SI:132:MET:HG2	1.78	0.64
53:SX:46:CYS:SG	53:SX:50:MET:HE2	2.37	0.64
7:7:4:G:C2'	7:7:5:U:H5''	2.27	0.64
28:S1:1523:A:H2'	28:S1:1524:G:C8	2.31	0.64
54:SY:35:ALA:O	54:SY:64:ARG:NH1	2.30	0.64
10:B:92:TYR:HB2	10:B:159:VAL:HB	1.80	0.64
5:5:53:G:H22	5:5:63:G:H22	1.43	0.64
1:1:73:U:H5''	17:I:63:VAL:HB	1.80	0.64
28:S1:1492:G:N7	91:S1:2424:HOH:O	2.29	0.64
3:3:75:C:O2'	81:k:3:ARG:NH1	2.31	0.64
28:S1:527:A:OP1	33:SD:120:SER:OG	2.15	0.64
28:S1:949:U:H3	28:S1:986:C:H42	1.45	0.64
40:SK:162:TRP:HB3	40:SK:166:ARG:HH21	1.62	0.64
62:Sg:223:LEU:O	62:Sg:225:THR:N	2.31	0.64
2:2:1058:PSU:H6	2:2:1058:PSU:H5'	1.63	0.64
30:SA:146:LYS:HB3	30:SA:210:ARG:HB2	1.79	0.64
1:1:423:U:O2'	1:1:424:G:O5'	2.16	0.64
3:3:200:G:N1	85:o:50:LYS:O	2.31	0.64
4:4:54:G:N2	4:4:57:A:OP2	2.31	0.64
71:a:98:ALA:O	71:a:100:LYS:NZ	2.30	0.64
74:d:24:LYS:HB2	74:d:96:ASN:HB3	1.80	0.64
36:SG:157:ARG:HD2	36:SG:182:LEU:HD21	1.80	0.64
1:1:836:G:OP2	24:P:98:ARG:NH2	2.30	0.63
13:E:84:THR:HG22	13:E:85:LYS:HG3	1.79	0.63
28:S1:553:U:O2'	28:S1:554:U:O5'	2.15	0.63
1:1:334:G:H4'	1:1:335:U:OP1	1.96	0.63
50:SU:95:MET:HE3	50:SU:98:THR:HB	1.80	0.63
1:1:407:A2M:HM'2	1:1:408:G:H5''	1.78	0.63
1:1:1598:A:N1	82:l:5:LYS:HE2	2.14	0.63
28:S1:2195:G:H5''	57:Sb:3:THR:HA	1.79	0.63
63:Sh:137:CYS:SG	63:Sh:205:SER:OG	2.54	0.63
2:2:652:C:H2'	2:2:653:C:C6	2.34	0.63
6:6:64:U:OP2	14:F:78:ARG:NE	2.24	0.63
1:1:1171:PSU:H5'	1:1:1171:PSU:H6	1.64	0.63
6:6:60:A:C5	14:F:69:MET:HE1	2.33	0.63
28:S1:395:U:OP2	45:SP:15:ARG:NH2	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:ST:46:MET:HE3	49:ST:86:GLU:HG3	1.78	0.63
28:S1:640:A:H2'	28:S1:641:A:C8	2.33	0.63
54:SY:41:ILE:HG23	54:SY:55:THR:HB	1.80	0.63
63:Sh:185:LYS:HD2	63:Sh:186:PHE:N	2.14	0.63
1:1:443:A:N3	82:1:36:LYS:NZ	2.42	0.63
1:1:593:C:H42	1:1:614:A:H61	1.46	0.63
16:H:204:ALA:O	16:H:208:MET:HG2	1.99	0.63
28:S1:1219:G:O6	91:S1:2404:HOH:O	2.15	0.63
1:1:734:U:O2'	1:1:735:U:H5'	1.98	0.63
23:O:197:ASP:OD1	23:O:200:VAL:HG23	1.99	0.63
28:S1:955:A:H61	28:S1:980:G:H1	0.73	0.63
28:S1:1881:G:H2'	28:S1:1882:A:C8	2.34	0.63
47:SR:118:MET:HE2	52:SW:117:GLU:O	1.99	0.63
23:O:232:PHE:HD1	23:O:235:TYR:CD2	2.17	0.62
28:S1:1543:B8N:O3'	41:SL:148:TYR:O	2.17	0.62
33:SD:69:LEU:O	33:SD:73:SER:OG	2.12	0.62
35:SF:92:MET:SD	35:SF:114:ASN:ND2	2.69	0.62
43:SN:5:VAL:HG22	43:SN:48:GLN:HG2	1.80	0.62
1:1:605:G:O2'	1:1:606:C:O2	2.15	0.62
1:1:1727:A:H2'	1:1:1728:A:H5'	1.80	0.62
2:2:525:A:N7	2:2:532:U:H5	1.98	0.62
3:3:119:C:OP1	25:Q:117:ARG:NH1	2.32	0.62
28:S1:773:A:H2'	28:S1:774:A:C8	2.34	0.62
5:5:112:U:H5	5:5:121:A:N7	1.96	0.62
49:ST:49:GLN:O	49:ST:53:GLU:HG2	1.99	0.62
49:ST:49:GLN:NE2	49:ST:53:GLU:OE2	2.31	0.62
1:1:1090:U:H2'	1:1:1091:A:C8	2.34	0.62
2:2:602:A:OP1	64:T:140:MET:N	2.27	0.62
2:2:1294:G:OP1	2:2:1294:G:H4'	1.97	0.62
10:B:113:GLU:OE1	10:B:169:ARG:HG3	2.00	0.62
11:C:257:GLN:HG2	11:C:260:LYS:HE3	1.81	0.62
21:M:31:ARG:NH1	21:M:124:ASP:OD1	2.32	0.62
36:SG:33:LEU:HD11	36:SG:64:MET:HB2	1.82	0.62
63:Sh:186:PHE:CE1	63:Sh:190:LYS:HG3	2.35	0.62
5:5:68:G:H5'	40:SK:92:ARG:HG2	1.81	0.62
34:SE:104:GLY:O	34:SE:186:ARG:NH1	2.32	0.62
1:1:6:C:O2'	1:1:7:C:H6	1.83	0.62
1:1:38:A:H5''	20:L:35:ALA:HB1	1.81	0.62
2:2:655:OMG:HM21	2:2:657:U:H5''	1.82	0.62
28:S1:965:G:H5'	28:S1:966:G:H5''	1.82	0.62
41:SL:101:LYS:HD3	41:SL:102:TYR:CZ	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SO:12:PRO:HG3	44:SO:20:VAL:HG11	1.81	0.62
1:1:151:C:OP1	71:a:113:ARG:NH2	2.20	0.62
2:2:478:A:H2'	2:2:479:C:O2	1.99	0.62
23:O:170:LYS:HD3	23:O:201:HIS:HE1	1.63	0.62
28:S1:450:A:H2'	28:S1:451:C:C6	2.35	0.62
28:S1:2182:G:O6	84:n:21:ARG:NH1	2.33	0.62
31:SB:77:VAL:HG22	31:SB:124:VAL:HB	1.81	0.62
69:Y:88:ASP:O	69:Y:119:ARG:NH1	2.32	0.62
1:1:148:U:O2'	1:1:149:G:O5'	2.18	0.62
1:1:1527:OMC:HM22	1:1:1528:PSU:H5''	1.82	0.62
8:8:31:A:H2'	8:8:32:C:C6	2.35	0.62
28:S1:1412:G:N7	91:S1:2428:HOH:O	2.31	0.62
46:SQ:97:LEU:HD11	46:SQ:121:VAL:CG2	2.29	0.62
69:Y:54:VAL:H	69:Y:57:MET:HE2	1.65	0.62
1:1:904:G:O2'	1:1:905:G:O4'	2.17	0.62
28:S1:263:G:H5'	63:Sh:169:ARG:HB2	1.79	0.62
50:SU:110:LYS:O	50:SU:113:GLN:NE2	2.31	0.62
61:Sf:95:MET:HE3	61:Sf:98:LEU:HD12	1.82	0.62
1:1:997:C:O2'	1:1:998:A:H8	1.82	0.61
43:SN:84:ARG:NH1	43:SN:93:ALA:O	2.33	0.61
2:2:825:U:O2	2:2:846:G:N2	2.33	0.61
23:O:170:LYS:HD3	23:O:201:HIS:CE1	2.35	0.61
28:S1:1409:U:H2'	28:S1:1410:C:C6	2.34	0.61
28:S1:1684:U:H3	28:S1:1820:G:H22	1.48	0.61
69:Y:83:THR:HG23	69:Y:85:TYR:HD1	1.65	0.61
1:1:913:C:H2'	1:1:914:U:O2	2.00	0.61
1:1:1019:G:H2'	1:1:1020:C:C6	2.35	0.61
2:2:1141:G:H5''	2:2:1143:U:C2	2.36	0.61
13:E:75:HIS:O	13:E:79:MET:HG3	2.01	0.61
28:S1:1621:OMU:H6	28:S1:1621:OMU:H5''	1.82	0.61
55:SZ:44:GLN:OE1	55:SZ:44:GLN:N	2.26	0.61
2:2:972:C:O2	85:o:62:LYS:NZ	2.33	0.61
2:2:1510:A:H61	10:B:326:ASN:HB3	1.66	0.61
12:D:145:ARG:HG2	12:D:146:LYS:HG3	1.83	0.61
1:1:149:G:OP1	21:M:56:LYS:NZ	2.26	0.61
1:1:1093:U:H5''	22:N:196:HIS:NE2	2.15	0.61
1:1:1453:G:N7	91:1:1931:HOH:O	2.31	0.61
28:S1:878:C:N4	55:SZ:15:SER:OG	2.33	0.61
1:1:844:C:H2'	1:1:845:OMU:O2	2.01	0.61
2:2:1404:G:H5''	9:A:220:GLY:HA3	1.83	0.61
11:C:257:GLN:HG2	11:C:260:LYS:NZ	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:547:U:H4'	26:R:65:VAL:HG21	1.83	0.61
6:6:73:A:H5'	77:g:29:LYS:HD2	1.83	0.61
8:8:93:G:H2'	8:8:94:A:C8	2.36	0.61
27:S:102:GLN:O	27:S:106:LYS:HG2	2.00	0.61
28:S1:771:G:O2'	28:S1:772:A:H5'	2.00	0.61
1:1:929:G:OP2	91:1:1906:HOH:O	2.16	0.61
2:2:708:G:O6	2:2:739:C:O2'	2.17	0.61
62:Sg:149:HIS:CE1	62:Sg:177:LYS:HD2	2.36	0.61
1:1:625:C:OP2	11:C:341:LYS:HE3	2.01	0.61
1:1:700:A:C2	1:1:845:OMU:H5	2.35	0.61
1:1:1352:C:H2'	1:1:1353:A:C8	2.36	0.61
1:1:1510:C:N4	11:C:187:GLU:OE2	2.28	0.61
2:2:453:A:N6	2:2:454:A:N3	2.48	0.61
6:6:67:C:OP1	77:g:96:ARG:NH2	2.32	0.61
23:O:55:ILE:HG21	23:O:164:ARG:HH21	1.65	0.61
28:S1:1804:C:OP1	51:SV:2:GLY:N	2.34	0.61
3:3:112:C:H5'	3:3:117:C:H1'	1.83	0.60
5:5:53:G:H22	5:5:63:G:N2	1.98	0.60
43:SN:94:MET:HE2	43:SN:94:MET:HA	1.83	0.60
62:Sg:147:ASP:OD1	62:Sg:177:LYS:NZ	2.34	0.60
1:1:454:U:H2'	1:1:455:G:C8	2.36	0.60
1:1:1523:A:OP1	76:f:20:ARG:NH2	2.33	0.60
2:2:406:G:H2'	2:2:407:C:C6	2.36	0.60
2:2:716:C:H2'	2:2:717:G:H8	1.67	0.60
28:S1:193:G:H3'	28:S1:194:U:H4'	1.82	0.60
28:S1:301:U:H2'	28:S1:302:U:O2	2.01	0.60
28:S1:2135:U:O2'	28:S1:2136:A:H5'	2.01	0.60
32:SC:63:ARG:HG3	43:SN:98:GLN:OE1	2.01	0.60
42:SM:77:PHE:HB3	48:SS:53:PHE:HB3	1.82	0.60
1:1:820:U:H6	1:1:823:G:H1	1.48	0.60
2:2:749:G:HO2'	2:2:750:U:H6	1.49	0.60
2:2:1157:U:H5	2:2:1237:A:N1	1.98	0.60
28:S1:1686:C:H4'	48:SS:56:LEU:HD13	1.81	0.60
44:SO:106:GLN:HG2	57:Sb:47:LEU:HD23	1.82	0.60
47:SR:15:ARG:NH1	47:SR:20:ASN:OD1	2.33	0.60
1:1:434:U:H5	1:1:438:A:N7	2.00	0.60
1:1:1092:U:H1'	22:N:193:ARG:HH22	1.66	0.60
28:S1:245:A:N1	28:S1:302:U:H5	2.00	0.60
28:S1:277:U:OP2	36:SG:228:HIS:ND1	2.35	0.60
28:S1:1794:U:H2'	28:S1:1795:G:C8	2.37	0.60
68:X:44:TYR:HD1	68:X:45:MET:HE3	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Z:128:ARG:NH1	76:f:115:GLU:OE1	2.25	0.60
2:2:1506:G:N2	75:e:40:ARG:HE	1.98	0.60
4:4:180:C:O2'	5:5:4:A:N3	2.28	0.60
13:E:62:SER:O	13:E:66:ILE:HG12	2.01	0.60
28:S1:1369:U:H3	28:S1:1401:G:H1	1.48	0.60
2:2:622:G:H2'	2:2:623:A:C8	2.37	0.60
2:2:1233:U:OP2	86:p:63:LYS:HG2	2.01	0.60
2:2:1519:U:H2'	2:2:1520:C:C6	2.37	0.60
27:S:84:THR:HG22	72:b:22:LYS:O	2.02	0.60
62:Sg:222:ASP:OD1	62:Sg:225:THR:N	2.35	0.60
73:c:30:GLN:HA	73:c:33:THR:HG22	1.82	0.60
2:2:721:G:H2'	2:2:722:C:C6	2.37	0.60
4:4:86:U:O4	75:e:141:LYS:NZ	2.23	0.60
28:S1:147:U:H5	28:S1:178:A:N1	2.00	0.60
28:S1:2012:A:H2'	28:S1:2013:G:C8	2.37	0.60
31:SB:28:ILE:HG22	31:SB:169:ARG:HH22	1.67	0.60
2:2:460:A:O2'	2:2:461:C:H6	1.84	0.60
4:4:28:A:N1	4:4:177:U:H5	2.00	0.60
22:N:55:ARG:HB2	22:N:162:ARG:HG2	1.84	0.60
25:Q:105:LEU:HD23	25:Q:138:LEU:HD23	1.84	0.60
28:S1:820:C:O3'	63:Sh:87:ARG:NH1	2.35	0.60
68:X:1:MET:HB2	68:X:15:PRO:HG3	1.82	0.60
1:1:60:A:OP2	91:1:1905:HOH:O	2.16	0.60
1:1:113:C:OP2	71:a:110:ARG:NH2	2.31	0.60
63:Sh:59:VAL:HB	63:Sh:91:ALA:HB3	1.83	0.60
1:1:93:G:H2'	1:1:94:A:C8	2.37	0.60
1:1:576:G:C8	11:C:323:ARG:NH2	2.70	0.60
28:S1:374:U:H2'	28:S1:375:G:C8	2.37	0.60
44:SO:60:ASP:O	44:SO:63:SER:OG	2.18	0.60
63:Sh:213:ARG:NH1	63:Sh:213:ARG:O	2.34	0.60
1:1:65:A:OP1	21:M:177:LYS:HE3	2.01	0.59
1:1:1243:G:OP2	26:R:2:VAL:N	2.35	0.59
28:S1:822:U:H2'	28:S1:823:G:H8	1.67	0.59
34:SE:150:HIS:O	34:SE:171:LYS:NZ	2.35	0.59
2:2:1122:C:O2'	2:2:1123:A:OP1	2.16	0.59
10:B:226:THR:HG22	10:B:336:SER:HB3	1.84	0.59
16:H:79:ARG:HA	16:H:88:PRO:HD2	1.85	0.59
17:I:98:ILE:HD11	17:I:130:LEU:HD13	1.83	0.59
22:N:193:ARG:HD3	22:N:198:LYS:HZ2	1.66	0.59
28:S1:1718:A:N7	56:Sa:85:ARG:NH2	2.49	0.59
35:SF:149:VAL:HG22	35:SF:150:PRO:HD2	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:e:116:VAL:HG11	75:e:168:THR:HG21	1.83	0.59
1:1:133:C:H5'	1:1:134:A:H5''	1.84	0.59
1:1:1057:A:N1	1:1:1095:U:H5	2.01	0.59
49:ST:87:ASP:OD2	49:ST:87:ASP:N	2.35	0.59
1:1:493:A:C2'	1:1:494:A:H5''	2.31	0.59
2:2:1078:OMG:N1	2:2:1236:C:N3	2.46	0.59
53:SX:46:CYS:O	53:SX:50:MET:HG2	2.03	0.59
1:1:1238:C:OP2	26:R:162:ARG:NH2	2.35	0.59
1:1:1276:U:H5	1:1:1353:A:N1	2.00	0.59
1:1:1739:A:H4'	78:h:12:MET:HE2	1.83	0.59
20:L:110:LEU:O	20:L:127:SER:OG	2.16	0.59
23:O:172:ALA:HB1	23:O:177:MET:HG3	1.84	0.59
28:S1:1573:A:H2'	28:S1:1574:G:C8	2.37	0.59
28:S1:2146:U:H2'	28:S1:2147:A:H8	1.66	0.59
6:6:6:G:H5''	6:6:7:A:OP2	2.03	0.59
28:S1:2117:C:O2'	28:S1:2118:G:N7	2.35	0.59
38:SI:132:MET:HE2	38:SI:175:VAL:HG12	1.85	0.59
28:S1:364:G:H2'	28:S1:365:U:C5	2.38	0.59
36:SG:149:ASN:HD22	36:SG:149:ASN:C	2.10	0.59
3:3:118:G:H2'	3:3:119:C:O2	2.02	0.59
28:S1:254:A:H61	28:S1:974:G:N2	1.98	0.59
28:S1:1281:C:HO2'	39:SJ:2:THR:N	2.00	0.59
47:SR:125:ARG:HD3	47:SR:130:LEU:HB2	1.85	0.59
62:Sg:2:ASN:OD1	62:Sg:307:SER:OG	2.21	0.59
2:2:748:C:O2'	2:2:749:G:OP1	2.20	0.59
2:2:954:A:C5	78:h:114:MET:HE1	2.38	0.59
7:7:18:G:H2'	7:7:19:A:C8	2.38	0.59
28:S1:1618:U:H2'	28:S1:1619:G:C8	2.37	0.59
28:S1:2170:G:OP1	28:S1:2173:A:H4'	2.03	0.59
30:SA:169:ARG:NH1	30:SA:202:ARG:O	2.36	0.59
38:SI:164:ARG:HH12	38:SI:165:ILE:HB	1.66	0.59
2:2:1132:A:H8	2:2:1132:A:OP1	1.85	0.59
2:2:1379:A:H5''	2:2:1381:G:H4'	1.85	0.59
28:S1:784:C:H41	28:S1:834:U:H3	1.50	0.59
30:SA:32:VAL:HG22	30:SA:98:LEU:HD12	1.85	0.59
46:SQ:104:VAL:HG22	46:SQ:115:THR:HG23	1.84	0.59
2:2:665:A:H2'	2:2:666:C:C6	2.38	0.58
11:C:257:GLN:HG2	11:C:260:LYS:CE	2.32	0.58
31:SB:1:MET:O	31:SB:66:ARG:NH1	2.35	0.58
56:Sa:95:SER:O	56:Sa:99:ARG:NH1	2.36	0.58
64:T:64:ASN:HB2	64:T:80:LYS:HE2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Y:72:LEU:O	69:Y:105:ARG:NH2	2.34	0.58
1:1:1019:G:H2'	1:1:1020:C:H6	1.68	0.58
8:8:31:A:H2'	8:8:32:C:H6	1.67	0.58
28:S1:133:G:H2'	28:S1:134:G:C8	2.38	0.58
28:S1:1143:U:OP1	30:SA:26:ARG:NH2	2.36	0.58
45:SP:60:LYS:HD2	45:SP:116:PRO:HA	1.84	0.58
68:X:45:MET:HE2	68:X:45:MET:HA	1.84	0.58
2:2:528:U:O2	2:2:556:U:H4'	2.04	0.58
9:A:119:LYS:O	9:A:122:ASP:HB2	2.03	0.58
28:S1:16:G:H2'	28:S1:17:C:C6	2.38	0.58
28:S1:1576:A:H61	28:S1:1611:C:N4	2.01	0.58
68:X:56:THR:HG22	68:X:58:THR:H	1.67	0.58
2:2:1124:A:H2'	2:2:1125:G:C8	2.38	0.58
28:S1:1586:A:OP1	48:SS:2:GLY:N	2.36	0.58
28:S1:2039:C:H2'	28:S1:2040:C:O2	2.04	0.58
31:SB:1:MET:HA	54:SY:83:MET:HA	1.85	0.58
53:SX:57:GLU:HG3	53:SX:58:ARG:HG3	1.84	0.58
2:2:846:G:H22	2:2:952:G:N2	2.02	0.58
6:6:40:C:H5'	19:K:91:ARG:CZ	2.33	0.58
15:G:95:ILE:HG23	15:G:133:VAL:HG11	1.84	0.58
28:S1:167:C:OP1	36:SG:84:GLY:N	2.25	0.58
28:S1:478:C:H5''	45:SP:48:LYS:HE3	1.83	0.58
33:SD:31:GLY:HA3	60:Se:40:TYR:CG	2.38	0.58
2:2:43:G:H2'	2:2:44:C:O2	2.04	0.58
7:7:21:U:OP1	67:W:9:ARG:NH2	2.33	0.58
10:B:112:VAL:O	10:B:116:ARG:HG3	2.03	0.58
28:S1:784:C:N4	28:S1:834:U:H3	2.01	0.58
28:S1:2132:C:H2'	28:S1:2133:G:O4'	2.03	0.58
28:S1:2135:U:H2'	28:S1:2136:A:C8	2.38	0.58
1:1:1426:A:N6	70:Z:86:GLY:O	2.36	0.58
2:2:1150:U:H2'	2:2:1151:U:O2	2.04	0.58
28:S1:1038:U:O2'	38:SI:84:GLU:OE2	2.22	0.58
28:S1:1689:G:H5'	28:S1:1690:C:OP2	2.03	0.58
29:S4:23:A:H62	29:S4:46:G:H21	1.51	0.58
42:SM:65:THR:OG1	42:SM:66:PRO:O	2.19	0.58
43:SN:94:MET:HG3	43:SN:98:GLN:HB2	1.85	0.58
1:1:1501:A:OP1	76:f:106:ARG:NH2	2.37	0.58
2:2:575:C:OP1	91:2:4303:HOH:O	2.17	0.58
28:S1:138:C:H2'	28:S1:139:C:C6	2.38	0.58
1:1:83:A:H61	1:1:98:A:H3'	1.69	0.58
1:1:1029:G:N2	1:1:1030:U:O4	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:603:A:H5'	64:T:137:THR:HG23	1.85	0.58
2:2:1136:U:H2'	2:2:1137:G:C8	2.38	0.58
2:2:1290:C:N3	22:N:158:LYS:NZ	2.51	0.58
11:C:204:ARG:HA	11:C:204:ARG:HE	1.69	0.58
20:L:75:LEU:HG	20:L:111:GLY:HA2	1.85	0.58
28:S1:1186:A:H2'	28:S1:1187:A:C8	2.39	0.58
62:Sg:247:ARG:HD2	62:Sg:249:TRP:CZ2	2.39	0.58
1:1:1567:C:H5''	75:e:123:LYS:HD2	1.85	0.58
1:1:1749:G:H2'	1:1:1751:A:N7	2.19	0.58
2:2:1369:C:OP1	18:J:42:LYS:NZ	2.37	0.58
33:SD:50:LYS:HG2	33:SD:53:ARG:HH22	1.69	0.58
1:1:592:G:H2'	1:1:593:C:C6	2.39	0.57
1:1:1238:C:H5''	1:1:1239:U:H5'	1.84	0.57
2:2:708:G:C2	2:2:709:G:H1'	2.38	0.57
28:S1:2137:U:H2'	28:S1:2138:U:C6	2.38	0.57
69:Y:92:GLU:O	69:Y:96:LYS:HG3	2.04	0.57
1:1:314:G:N7	91:1:1932:HOH:O	2.32	0.57
1:1:1574:C:O2'	1:1:1575:G:OP1	2.17	0.57
2:2:1038:U:H2'	2:2:1039:U:C6	2.40	0.57
23:O:76:MET:HE2	23:O:112:LYS:HD3	1.86	0.57
28:S1:787:G:H8	28:S1:833:G:H1	1.52	0.57
28:S1:1523:A:H2'	28:S1:1524:G:H8	1.69	0.57
63:Sh:164:ARG:HB3	63:Sh:176:TYR:HD2	1.69	0.57
79:i:61:GLN:HG2	79:i:97:LEU:HG	1.85	0.57
86:p:12:CYS:HA	86:p:23:PHE:HZ	1.69	0.57
1:1:1264:A:H2'	1:1:1265:A:C8	2.40	0.57
2:2:1398:C:H2'	2:2:1399:G:C8	2.40	0.57
5:5:53:G:N2	5:5:63:G:H22	2.02	0.57
13:E:18:VAL:HB	13:E:27:VAL:HG22	1.86	0.57
28:S1:639:C:H5''	60:Se:57:MET:HE2	1.86	0.57
1:1:576:G:O2'	1:1:577:C:OP1	2.20	0.57
4:4:136:G:H3'	4:4:148:C:H41	1.69	0.57
5:5:26:A:O2'	10:B:124:GLN:OE1	2.23	0.57
28:S1:568:U:O2'	28:S1:569:U:OP1	2.21	0.57
36:SG:125:GLU:N	36:SG:125:GLU:OE2	2.32	0.57
69:Y:57:MET:HB2	69:Y:61:THR:HG21	1.86	0.57
1:1:12:U:H2'	1:1:13:G:H8	1.69	0.57
1:1:998:A:OP1	76:f:56:LYS:N	2.37	0.57
1:1:1667:G:OP2	21:M:34:HIS:NE2	2.37	0.57
5:5:8:C:H2'	5:5:9:C:H6	1.69	0.57
22:N:171:TRP:HB2	22:N:178:ARG:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:1572:C:H5	28:S1:1615:G:H22	1.52	0.57
1:1:1597:G:O6	82:l:2:GLY:N	2.38	0.57
2:2:382:A2M:H8	2:2:382:A2M:O5'	2.04	0.57
28:S1:1781:U:O2'	28:S1:1782:G:N7	2.32	0.57
30:SA:97:ASN:OD1	30:SA:240:SER:HB2	2.04	0.57
62:Sg:109:ASP:OD2	62:Sg:127:ARG:NH1	2.38	0.57
62:Sg:132:ARG:HG2	62:Sg:143:GLU:HG2	1.87	0.57
2:2:780:G:H2'	2:2:781:G:H8	1.70	0.57
23:O:107:ARG:NH2	23:O:119:PHE:O	2.38	0.57
28:S1:123:A:N1	28:S1:336:U:H5	2.02	0.57
31:SB:56:MET:HG2	58:Sc:3:PHE:CE2	2.40	0.57
1:1:542:C:H2'	1:1:544:A:H5'	1.86	0.57
2:2:506:U:HO2'	2:2:507:G:H8	1.53	0.57
2:2:723:G:H8	2:2:725:A:C6	2.22	0.57
2:2:1024:U:H2'	2:2:1025:G:C8	2.40	0.57
13:E:95:TYR:O	83:m:78:MET:CE	2.49	0.57
76:f:12:LYS:NZ	91:f:202:HOH:O	2.36	0.57
1:1:24:A:H2'	1:1:25:C:H6	1.70	0.57
4:4:20:U:H2'	4:4:21:C:C6	2.39	0.57
28:S1:263:G:OP1	63:Sh:145:ARG:NH1	2.38	0.57
28:S1:286:G:H1'	36:SG:217:ALA:HB1	1.87	0.57
28:S1:836:C:H2'	28:S1:837:G:H8	1.70	0.57
31:SB:79:VAL:HG23	31:SB:126:VAL:HB	1.85	0.57
35:SF:63:LEU:HD12	35:SF:83:ILE:HD11	1.86	0.57
59:Sd:75:LEU:HD12	59:Sd:78:THR:HG22	1.85	0.57
10:B:47:MET:HB2	10:B:84:MET:HE3	1.86	0.57
28:S1:307:C:H2'	28:S1:308:C:C6	2.40	0.57
28:S1:822:U:H2'	28:S1:823:G:C8	2.40	0.57
43:SN:87:LEU:HD12	43:SN:89:LEU:HD11	1.86	0.57
7:7:169:A:H2'	7:7:170:A:C5	2.40	0.56
28:S1:234:C:HO2'	28:S1:235:C:H6	1.52	0.56
28:S1:1599:U:H2'	28:S1:1600:C:O2	2.05	0.56
39:SJ:18:GLU:HG3	39:SJ:69:LEU:HB3	1.87	0.56
1:1:795:U:HO2'	1:1:796:G:H8	1.53	0.56
22:N:193:ARG:HH11	22:N:198:LYS:HE3	1.69	0.56
28:S1:327:U:H2'	28:S1:328:C:C6	2.40	0.56
61:Sf:93:GLU:N	61:Sf:93:GLU:OE2	2.35	0.56
62:Sg:249:TRP:HB2	62:Sg:261:TYR:O	2.06	0.56
1:1:130:U:H2'	1:1:132:A:N6	2.20	0.56
1:1:586:U:C5'	11:C:335:ARG:HD2	2.32	0.56
2:2:1216:A:C2'	2:2:1217:C:H5'	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1510:A:N1	10:B:326:ASN:ND2	2.54	0.56
20:L:92:LYS:HG3	20:L:138:GLY:HA3	1.87	0.56
25:Q:185:ARG:NH1	28:S1:993:U:O4'	2.38	0.56
28:S1:315:A:H5''	28:S1:333:G:H22	1.70	0.56
28:S1:547:U:H3'	28:S1:548:G:H8	1.69	0.56
28:S1:1556:C:OP1	91:S1:2401:HOH:O	2.18	0.56
28:S1:1966:A:N1	28:S1:1983:U:H5	2.02	0.56
31:SB:203:ASP:HA	31:SB:206:PHE:CE2	2.40	0.56
37:SH:21:GLU:OE1	37:SH:132:ARG:NH2	2.38	0.56
38:SI:75:ARG:NH1	38:SI:131:ASP:OD1	2.30	0.56
40:SK:57:ALA:HB2	40:SK:196:GLY:HA2	1.85	0.56
1:1:687:C:H2'	1:1:688:A:H8	1.71	0.56
2:2:553:G:O2'	2:2:556:U:OP2	2.16	0.56
15:G:28:PHE:CD1	69:Y:55:ARG:HG2	2.40	0.56
28:S1:2045:A:H2'	28:S1:2046:PSU:C6	2.40	0.56
34:SE:158:VAL:HG22	34:SE:167:VAL:HB	1.87	0.56
1:1:790:C:H4'	73:c:38:LYS:HB3	1.87	0.56
13:E:36:LYS:HD3	13:E:38:LEU:HD21	1.88	0.56
26:R:14:ARG:HD2	26:R:24:PRO:HG2	1.88	0.56
31:SB:25:ARG:HH11	31:SB:28:ILE:HG13	1.70	0.56
56:Sa:50:LEU:HD12	56:Sa:54:VAL:HG21	1.88	0.56
2:2:723:G:H8	2:2:725:A:C5	2.23	0.56
2:2:1239:A:O2'	2:2:1240:A:H2'	2.06	0.56
28:S1:83:A:O3'	55:SZ:126:GLY:HA2	2.05	0.56
28:S1:260:A:H2'	28:S1:261:A:H8	1.69	0.56
28:S1:1830:G:H2'	28:S1:1831:U:C6	2.41	0.56
28:S1:1891:A:O2'	28:S1:1908:A:N6	2.38	0.56
2:2:12:G:H5'	2:2:13:A:OP1	2.04	0.56
11:C:146:VAL:HG22	70:Z:74:PRO:HG2	1.88	0.56
28:S1:2124:A:H2'	28:S1:2125:A:H5''	1.87	0.56
4:4:128:U:H5	4:4:162:A:N1	2.03	0.56
23:O:166:PHE:HA	23:O:169:LEU:HB3	1.88	0.56
77:g:74:ARG:HG2	77:g:141:PRO:HD3	1.88	0.56
1:1:510:U:H5	1:1:544:A:N1	2.02	0.56
2:2:496:G:O2'	2:2:497:G:OP1	2.19	0.56
28:S1:1115:G:H2'	28:S1:1116:U:C6	2.41	0.56
63:Sh:190:LYS:O	63:Sh:193:THR:OG1	2.22	0.56
85:o:11:MET:HG3	85:o:27:LYS:HB2	1.87	0.56
1:1:141:U:H1'	1:1:142:G:H5''	1.87	0.56
1:1:631:G:H1'	1:1:632:A:H2'	1.87	0.56
1:1:1374:C:H2'	1:1:1375:G:O4'	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:382:A2M:OP2	91:2:4304:HOH:O	2.18	0.56
2:2:1500:U:OP1	10:B:134:LYS:NZ	2.31	0.56
11:C:83:THR:HG22	11:C:85:THR:H	1.71	0.56
28:S1:1601:U:OP2	61:Sf:91:LYS:NZ	2.39	0.56
31:SB:96:HIS:CE1	31:SB:200:GLU:HG2	2.42	0.55
45:SP:109:GLY:O	45:SP:119:ARG:NE	2.31	0.55
62:Sg:109:ASP:HB2	62:Sg:127:ARG:HG3	1.87	0.55
1:1:1369:G:C4	16:H:78:LYS:HD2	2.41	0.55
2:2:111:G:C8	85:o:16:THR:HG22	2.42	0.55
11:C:133:PRO:O	11:C:137:MET:HG3	2.05	0.55
35:SF:257:GLU:H	35:SF:257:GLU:CD	2.13	0.55
39:SJ:32:LYS:O	39:SJ:36:LYS:HG2	2.05	0.55
1:1:1638:C:H2'	1:1:1639:U:C6	2.41	0.55
2:2:1290:C:HO2'	2:2:1291:G:H8	1.54	0.55
14:F:90:THR:O	14:F:174:LYS:NZ	2.37	0.55
17:I:175:ARG:NH2	17:I:181:GLU:OE1	2.39	0.55
23:O:38:LEU:O	23:O:48:LYS:NZ	2.37	0.55
28:S1:905:A:H2'	28:S1:906:U:O2	2.07	0.55
28:S1:966:G:H2'	28:S1:967:A:C8	2.41	0.55
33:SD:93:ASP:OD1	35:SF:158:ASN:ND2	2.39	0.55
38:SI:34:HIS:HB3	38:SI:37:LEU:HB2	1.88	0.55
69:Y:97:ILE:HG22	69:Y:111:LEU:HD23	1.88	0.55
73:c:126:PHE:CZ	73:c:157:MET:HE3	2.41	0.55
1:1:636:U:H2'	1:1:637:C:C6	2.41	0.55
3:3:64:U:H2'	3:3:65:U:C6	2.42	0.55
28:S1:1272:A:H2'	28:S1:1274:A:H5''	1.88	0.55
28:S1:1554:A:O2'	28:S1:1558:U:H5	1.89	0.55
44:SO:27:PHE:HB3	44:SO:34:PHE:HB2	1.87	0.55
49:ST:130:LYS:NZ	49:ST:139:TRP:O	2.37	0.55
69:Y:98:ASN:OD1	69:Y:104:LYS:HD2	2.07	0.55
1:1:486:C:H5	1:1:647:G:H1	1.55	0.55
5:5:6:G:H2'	5:5:7:U:C6	2.42	0.55
6:6:38:C:H2'	6:6:39:U:H5''	1.89	0.55
28:S1:1496:U:H2'	28:S1:1497:U:C6	2.42	0.55
32:SC:32:GLY:HA3	32:SC:52:THR:HB	1.89	0.55
69:Y:26:VAL:HG11	69:Y:97:ILE:HD11	1.89	0.55
69:Y:44:ALA:HB1	69:Y:112:VAL:HG21	1.87	0.55
1:1:208:C:H2'	1:1:209:C:O4'	2.06	0.55
1:1:1017:PSU:OP1	20:L:44:ASN:ND2	2.40	0.55
4:4:150:A:O2'	4:4:151:A:H5'	2.07	0.55
28:S1:1695:C:H5	28:S1:1780:C:H42	1.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:1701:A:H2'	28:S1:1702:A:C8	2.42	0.55
1:1:1099:A:H2'	22:N:22:PHE:CZ	2.42	0.55
5:5:48:G:H2'	5:5:49:G:N3	2.21	0.55
1:1:938:G:H2'	1:1:939:C:C6	2.42	0.55
2:2:1208:A:H2'	2:2:1209:A:C8	2.42	0.55
2:2:1369:C:N3	2:2:1373:C:H5	2.04	0.55
54:SY:39:ILE:O	54:SY:57:LEU:HD23	2.07	0.55
1:1:254:U:H5	1:1:258:A:N7	2.04	0.55
2:2:652:C:H2'	2:2:653:C:H6	1.72	0.55
28:S1:1656:G:H1'	28:S1:1674:A:C2	2.42	0.55
28:S1:2174:G:N2	84:n:3:THR:HG21	2.21	0.55
33:SD:27:MET:HE2	60:Se:40:TYR:HB2	1.88	0.55
70:Z:121:THR:HG23	76:f:115:GLU:HG2	1.88	0.55
1:1:1147:A:O2'	1:1:1150:A:N1	2.35	0.55
39:SJ:93:ILE:HD11	39:SJ:102:VAL:HG22	1.88	0.55
54:SY:23:HIS:CE1	54:SY:58:CYS:HG	2.24	0.55
1:1:472:U:H2'	1:1:473:A:C8	2.41	0.54
1:1:1533:PSU:H2'	1:1:1534:G:C8	2.41	0.54
6:6:34:C:H2'	6:6:35:U:C6	2.42	0.54
22:N:39:ARG:H	22:N:39:ARG:HD2	1.72	0.54
30:SA:125:THR:HG23	30:SA:167:ARG:HG3	1.88	0.54
1:1:1087:A:H2'	1:1:1088:C:C6	2.42	0.54
2:2:1082:U:O4	86:p:8:LYS:NZ	2.39	0.54
28:S1:114:U:H2'	28:S1:115:C:C6	2.43	0.54
28:S1:155:U:H5	28:S1:169:A:N1	2.05	0.54
28:S1:305:U:O2	40:SK:64:ASN:ND2	2.39	0.54
28:S1:748:C:H4'	38:SI:148:ASP:HB2	1.88	0.54
44:SO:94:GLY:HA2	44:SO:99:LYS:HD3	1.89	0.54
57:Sb:21:LYS:HG3	57:Sb:22:PRO:HD2	1.90	0.54
62:Sg:243:PHE:HE1	62:Sg:263:LEU:HD11	1.72	0.54
65:U:19:LEU:HD23	65:U:19:LEU:H	1.72	0.54
5:5:122:U:O2'	5:5:123:G:H5'	2.07	0.54
28:S1:815:U:O2'	28:S1:817:A:OP2	2.18	0.54
28:S1:1512:A:HO2'	28:S1:2040:C:H5	1.55	0.54
28:S1:1788:U:H5'	51:SV:48:ASN:CB	2.35	0.54
34:SE:117:GLN:CG	34:SE:162:LYS:HD2	2.31	0.54
56:Sa:81:LYS:HB2	56:Sa:81:LYS:NZ	2.22	0.54
1:1:586:U:O2'	1:1:587:G:OP2	2.22	0.54
1:1:1394:U:O2	73:c:246:ARG:NH1	2.41	0.54
2:2:382:A2M:H2	2:2:389:A:N7	2.23	0.54
6:6:48:C:C2	14:F:185:LYS:HD3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:26:A:H2'	8:8:27:A:C8	2.42	0.54
38:SI:19:LEU:HD22	38:SI:62:LEU:HD11	1.89	0.54
70:Z:22:ARG:HH21	76:f:77:ILE:HA	1.72	0.54
82:l:28:ARG:HD3	82:l:36:LYS:HA	1.89	0.54
82:l:38:ASN:O	82:l:40:LYS:N	2.41	0.54
1:1:335:U:H1'	1:1:337:G:C5	2.42	0.54
1:1:345:U:H2'	1:1:346:U:C6	2.43	0.54
1:1:1541:C:OP1	91:1:1908:HOH:O	2.18	0.54
28:S1:1471:U:H2'	28:S1:1472:U:C6	2.42	0.54
31:SB:94:SER:OG	31:SB:101:PHE:HB3	2.08	0.54
38:SI:9:ARG:HG2	38:SI:12:LYS:HG2	1.90	0.54
1:1:1422:A:HO2'	1:1:1423:A:H8	1.55	0.54
2:2:1447:A:OP2	10:B:93:ARG:NH2	2.40	0.54
19:K:100:LYS:O	19:K:104:VAL:HG22	2.08	0.54
28:S1:1908:A:H5''	28:S1:1909:C:C5	2.41	0.54
28:S1:2174:G:H21	84:n:3:THR:HG21	1.71	0.54
31:SB:107:ILE:O	31:SB:110:THR:OG1	2.21	0.54
62:Sg:203:SER:HB2	62:Sg:208:LEU:HB2	1.90	0.54
1:1:1127:U:O2'	72:b:43:ASN:OD1	2.20	0.54
1:1:1777:U:H2'	1:1:1778:G:C8	2.43	0.54
19:K:147:MET:HE1	77:g:13:LYS:HB3	1.89	0.54
28:S1:552:U:H2'	28:S1:553:U:C6	2.43	0.54
28:S1:2200:A:N6	57:Sb:88:VAL:HG22	2.23	0.54
73:c:146:TYR:CZ	73:c:239:ASN:HB2	2.43	0.54
1:1:196:C:O2'	1:1:198:A:OP2	2.25	0.54
1:1:553:A:H2'	1:1:554:A:C8	2.43	0.54
1:1:1171:PSU:H6	1:1:1171:PSU:C5'	2.20	0.54
2:2:488:A:H5''	9:A:244:GLY:HA3	1.89	0.54
2:2:729:G:H21	2:2:732:A:P	2.30	0.54
3:3:105:C:H2'	3:3:106:U:H6	1.72	0.54
4:4:115:A:OP1	91:4:301:HOH:O	2.18	0.54
4:4:126:G:H5'	10:B:283:LEU:CD1	2.37	0.54
11:C:167:MET:HA	11:C:167:MET:CE	2.34	0.54
21:M:40:ARG:HG2	21:M:41:ARG:HG3	1.90	0.54
22:N:193:ARG:HD3	22:N:198:LYS:NZ	2.22	0.54
28:S1:1907:A:O2'	28:S1:1908:A:O5'	2.26	0.54
82:l:38:ASN:HB3	82:l:41:ARG:HG2	1.90	0.54
28:S1:1112:A:H5''	49:ST:3:ARG:HB2	1.89	0.54
32:SC:98:MET:HE3	32:SC:172:ARG:NH2	2.21	0.54
1:1:1479:A:H5''	1:1:1481:G:O4'	2.08	0.54
1:1:1728:A:O2'	1:1:1729:A:C8	2.60	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:590:U:H2'	2:2:591:A2M:H8	1.89	0.54
3:3:58:U:C5	65:U:99:LYS:HD3	2.43	0.54
6:6:70:G:O2'	6:6:71:A:H5'	2.08	0.54
7:7:161:C:H2'	7:7:162:A2M:H8	1.89	0.54
28:S1:263:G:H1	28:S1:274:C:H5	1.55	0.54
28:S1:503:C:N4	55:SZ:106:ALA:O	2.28	0.54
36:SG:56:GLY:C	36:SG:64:MET:HG3	2.33	0.54
40:SK:68:ALA:HB2	40:SK:201:ILE:HD11	1.90	0.54
1:1:994:U:H5	1:1:1521:G:OP1	1.91	0.53
1:1:1629:G:O6	78:h:11:ARG:NH2	2.40	0.53
2:2:959:A:H2'	2:2:960:C:C6	2.43	0.53
2:2:1003:G:O2'	2:2:1004:G:O5'	2.25	0.53
4:4:55:A:H2'	4:4:56:G:O4'	2.08	0.53
28:S1:1133:U:O2'	44:SO:128:ILE:O	2.26	0.53
28:S1:2121:C:H2'	28:S1:2122:G:C8	2.43	0.53
1:1:409:U:O2'	82:l:34:ARG:NH1	2.38	0.53
1:1:700:A:H2'	1:1:701:G:C8	2.44	0.53
1:1:839:U:H2'	1:1:840:G:C8	2.44	0.53
1:1:1030:U:H4'	1:1:1031:A:O5'	2.07	0.53
1:1:1170:G:H2'	1:1:1171:PSU:H5'	1.91	0.53
9:A:108:THR:HG21	85:o:86:LEU:HD22	1.90	0.53
13:E:91:VAL:HG12	13:E:180:VAL:HG22	1.89	0.53
28:S1:122:A:N1	28:S1:337:U:H5	2.06	0.53
28:S1:1965:G:H2'	28:S1:1966:A:C8	2.43	0.53
45:SP:40:PRO:HA	45:SP:79:LYS:HD2	1.89	0.53
1:1:1006:U:H2'	1:1:1007:U:C6	2.43	0.53
2:2:1290:C:O2'	2:2:1291:G:H8	1.91	0.53
3:3:138:U:H2'	3:3:139:C:O2	2.08	0.53
28:S1:436:C:H2'	28:S1:437:C:C6	2.43	0.53
28:S1:2096:U:H2'	28:S1:2097:C:C6	2.43	0.53
32:SC:139:GLY:HA3	32:SC:181:ILE:HD13	1.90	0.53
1:1:1613:C:OP1	64:T:127:ARG:NH2	2.35	0.53
2:2:459:A:H2'	2:2:460:A:C8	2.43	0.53
2:2:691:A:H2'	2:2:692:U:C6	2.44	0.53
2:2:1138:C:O2'	2:2:1139:U:H6	1.91	0.53
2:2:1175:A:H2'	2:2:1176:A:C8	2.43	0.53
28:S1:1672:C:O2'	28:S1:1673:A:OP1	2.22	0.53
28:S1:1875:G:H2'	28:S1:1876:U:C6	2.42	0.53
30:SA:28:GLU:HG3	30:SA:50:LYS:HG2	1.91	0.53
2:2:610:G:H22	2:2:642:G:H1'	1.72	0.53
3:3:115:C:H42	74:d:86:HIS:CE1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:7:U:H2'	5:5:8:C:C6	2.44	0.53
19:K:151:ALA:O	19:K:155:ASP:HB2	2.09	0.53
28:S1:1600:C:OP1	61:Sf:89:ARG:NH1	2.42	0.53
30:SA:24:MET:HG3	30:SA:24:MET:O	2.08	0.53
1:1:519:G:H2'	1:1:520:G:O4'	2.08	0.53
1:1:553:A:N3	11:C:323:ARG:HD2	2.24	0.53
28:S1:2012:A:H2'	28:S1:2013:G:H8	1.74	0.53
28:S1:2016:C:OP2	48:SS:33:ARG:NH1	2.42	0.53
46:SQ:110:GLY:O	46:SQ:113:THR:OG1	2.20	0.53
53:SX:19:LEU:HD22	53:SX:78:TYR:CD1	2.44	0.53
62:Sg:300:ASP:OD1	62:Sg:304:ARG:NH2	2.42	0.53
80:j:38:ALA:HB2	80:j:45:ARG:HG3	1.89	0.53
1:1:687:C:H2'	1:1:688:A:C8	2.44	0.53
1:1:823:G:H2'	1:1:823:G:N3	2.24	0.53
2:2:653:C:H2'	2:2:654:U:C6	2.43	0.53
5:5:26:A:H5''	10:B:123:LYS:HG3	1.90	0.53
28:S1:1688:A:H5'	28:S1:1689:G:OP2	2.09	0.53
1:1:225:C:O2'	1:1:226:C:H5'	2.09	0.53
1:1:521:G:H2'	1:1:522:G:C8	2.44	0.53
2:2:693:C:H2'	2:2:694:U:O4'	2.09	0.53
2:2:1251:A:H2'	2:2:1252:G:O4'	2.09	0.53
28:S1:1437:A:H2'	28:S1:1438:A:C8	2.44	0.53
82:l:38:ASN:C	82:l:40:LYS:H	2.17	0.53
1:1:306:G:OP2	21:M:14:LYS:NZ	2.34	0.53
28:S1:447:G:H2'	28:S1:448:C:C6	2.44	0.53
54:SY:42:ALA:HA	54:SY:54:THR:HG23	1.90	0.53
56:Sa:43:ASP:H	56:Sa:46:THR:HG22	1.74	0.53
1:1:405:A:H1'	11:C:83:THR:HG23	1.91	0.53
1:1:483:C:H5	1:1:650:G:N1	2.05	0.53
1:1:1474:U:OP1	11:C:139:ARG:NH2	2.40	0.53
5:5:88:C:O2'	5:5:89:C:H6	1.93	0.53
13:E:184:THR:OG1	13:E:185:ASN:N	2.38	0.53
28:S1:447:G:H2'	28:S1:448:C:H6	1.73	0.53
1:1:494:A:OP1	14:F:82:ARG:NE	2.33	0.52
1:1:1060:A:N1	1:1:1092:U:H5	2.07	0.52
2:2:453:A:C6	2:2:454:A:H1'	2.44	0.52
2:2:603:A:H2'	2:2:604:A2M:H8	1.91	0.52
2:2:1508:A:H2'	2:2:1509:C:C6	2.44	0.52
27:S:53:PRO:HG3	27:S:91:VAL:HG11	1.92	0.52
28:S1:2059:C:H2'	28:S1:2060:C:O4'	2.09	0.52
28:S1:2190:C:H2'	28:S1:2191:A:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:o:6:VAL:HG12	85:o:7:LYS:HG3	1.91	0.52
1:1:423:U:HO2'	1:1:424:G:H8	1.57	0.52
1:1:736:C:H2'	1:1:737:U:O4'	2.09	0.52
1:1:1445:G:H3'	1:1:1446:C:H5'	1.90	0.52
1:1:1452:C:H2'	1:1:1453:G:H8	1.73	0.52
1:1:1670:A:H61	66:V:32:ARG:NH2	2.08	0.52
2:2:1042:G:H2'	2:2:1043:C:H6	1.74	0.52
28:S1:106:A:H2'	28:S1:107:G:C8	2.45	0.52
28:S1:276:G:H1'	28:S1:277:U:H5'	1.90	0.52
28:S1:2151:OMG:H8	28:S1:2151:OMG:H5''	1.73	0.52
62:Sg:300:ASP:OD1	62:Sg:304:ARG:NH1	2.40	0.52
85:o:5:THR:OG1	85:o:8:MET:O	2.14	0.52
1:1:1092:U:O2'	1:1:1093:U:H5'	2.09	0.52
1:1:1239:U:OP1	16:H:141:ARG:NH1	2.41	0.52
7:7:154:A:H2'	7:7:155:U:O4'	2.09	0.52
8:8:16:C:OP2	8:8:71:C:O2'	2.26	0.52
28:S1:1683:A:H4'	51:SV:46:LEU:HD13	1.92	0.52
52:SW:55:HIS:CD2	52:SW:58:ARG:HH21	2.26	0.52
56:Sa:44:LYS:O	56:Sa:48:ASP:OD2	2.27	0.52
1:1:1038:U:H2'	1:1:1039:PSU:C6	2.45	0.52
1:1:1728:A:O2'	1:1:1729:A:H8	1.92	0.52
28:S1:284:C:O2'	28:S1:285:A:OP1	2.25	0.52
2:2:1492:G:H2'	2:2:1493:C:C6	2.45	0.52
15:G:231:ARG:NH1	15:G:231:ARG:HB2	2.24	0.52
28:S1:1578:G:C5	46:SQ:116:LEU:HD11	2.44	0.52
31:SB:201:LYS:HE2	31:SB:203:ASP:HB2	1.90	0.52
33:SD:109:GLN:NE2	33:SD:125:ARG:HB2	2.24	0.52
34:SE:121:MET:HE3	34:SE:138:THR:HG21	1.92	0.52
1:1:79:U:H2'	1:1:80:C:C6	2.45	0.52
1:1:148:U:O2'	1:1:149:G:H8	1.93	0.52
1:1:148:U:O2'	1:1:149:G:O4'	2.28	0.52
1:1:547:U:O2'	1:1:548:G:H8	1.92	0.52
1:1:879:A:H2'	1:1:880:C:C6	2.44	0.52
1:1:1275:G:H2'	1:1:1276:U:O2	2.09	0.52
28:S1:259:C:H42	28:S1:969:A:H61	1.58	0.52
34:SE:208:LYS:HE3	34:SE:214:GLU:HG2	1.91	0.52
37:SH:45:ARG:HH11	37:SH:45:ARG:HG3	1.74	0.52
1:1:794:U:O2'	1:1:795:U:H6	1.93	0.52
1:1:924:C:H5''	1:1:925:U:OP2	2.09	0.52
1:1:1017:PSU:H2'	1:1:1018:A:C8	2.45	0.52
2:2:979:A:OP2	2:2:979:A:H4'	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:89:C:H2'	5:5:90:C:O2	2.10	0.52
21:M:107:GLY:HA3	21:M:160:GLU:OE2	2.10	0.52
28:S1:6:G:OP2	35:SF:217:ARG:HD2	2.09	0.52
28:S1:197:U:H3'	28:S1:198:C:H5''	1.90	0.52
56:Sa:60:ILE:HB	56:Sa:101:TYR:HB2	1.92	0.52
73:c:25:ARG:NE	73:c:29:LYS:HB3	2.16	0.52
2:2:640:G:N3	10:B:264:ARG:HA	2.25	0.52
3:3:101:G:N1	3:3:139:C:H5	1.93	0.52
13:E:89:PHE:CZ	13:E:183:LYS:HG2	2.44	0.52
28:S1:56:U:OP1	28:S1:446:A:N6	2.38	0.52
28:S1:1692:G:H2'	28:S1:1693:C:C6	2.45	0.52
62:Sg:247:ARG:HD2	62:Sg:249:TRP:CE2	2.45	0.52
1:1:575:A:C2	11:C:334:LYS:HG2	2.45	0.52
1:1:843:C:H2'	1:1:844:C:C6	2.44	0.52
2:2:780:G:H2'	2:2:781:G:C8	2.45	0.52
7:7:156:A:OP1	7:7:158:U:H5	1.92	0.52
9:A:83:PHE:HB3	85:o:64:VAL:HG22	1.91	0.52
25:Q:65:LYS:NZ	25:Q:65:LYS:HB3	2.24	0.52
26:R:40:LYS:NZ	73:c:241:ASP:OD2	2.42	0.52
28:S1:1013:U:H2'	28:S1:1014:C:C6	2.45	0.52
40:SK:76:VAL:HG12	40:SK:108:PRO:HG2	1.92	0.52
1:1:745:U:O2'	1:1:815:G:N3	2.42	0.52
5:5:87:U:H2'	5:5:88:C:C6	2.45	0.52
6:6:35:U:H2'	6:6:36:C:C6	2.45	0.52
28:S1:1527:U:H2'	28:S1:1528:G:C8	2.45	0.52
28:S1:2151:OMG:H5''	28:S1:2151:OMG:C8	2.45	0.52
31:SB:59:GLU:OE1	54:SY:84:ARG:HG3	2.10	0.52
1:1:6:C:O2'	1:1:7:C:OP2	2.25	0.51
1:1:216:G:O6	70:Z:140:LYS:HD2	2.10	0.51
2:2:715:G:H2'	2:2:716:C:C6	2.45	0.51
2:2:1131:A:H3'	2:2:1131:A:OP2	2.09	0.51
4:4:54:G:H21	4:4:57:A:H2	1.58	0.51
4:4:126:G:H5'	10:B:283:LEU:HD11	1.91	0.51
62:Sg:230:PHE:CD1	62:Sg:230:PHE:C	2.87	0.51
1:1:581:G:H1	1:1:625:C:H5	1.56	0.51
1:1:1728:A:HO2'	1:1:1729:A:H8	1.51	0.51
2:2:21:C:H5''	2:2:22:A:H5'	1.90	0.51
2:2:1225:A:H2'	2:2:1226:C:C6	2.45	0.51
7:7:20:C:H2'	7:7:21:U:H5''	1.91	0.51
8:8:52:G:H2'	8:8:53:A:C8	2.45	0.51
28:S1:2121:C:H2'	28:S1:2122:G:H8	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SE:171:LYS:HE2	34:SE:173:ARG:NH2	2.25	0.51
64:T:23:ARG:HG3	64:T:23:ARG:O	2.11	0.51
68:X:54:PRO:HA	68:X:59:TYR:CG	2.45	0.51
1:1:837:A:H4'	1:1:838:G:O5'	2.11	0.51
2:2:1329:U:H5	2:2:1350:G:O6	1.93	0.51
4:4:126:G:O2'	4:4:127:G:N2	2.44	0.51
6:6:39:U:C4'	19:K:91:ARG:HH22	2.21	0.51
18:J:111:MET:HE1	18:J:131:ILE:HA	1.90	0.51
28:S1:1588:A:H2'	28:S1:1589:G:H8	1.75	0.51
28:S1:1932:A:O2'	28:S1:1934:A:OP2	2.23	0.51
32:SC:7:LYS:HG3	42:SM:58:LEU:HD21	1.93	0.51
47:SR:101:SER:OG	47:SR:102:SER:N	2.35	0.51
69:Y:45:GLY:HA3	69:Y:71:PHE:CZ	2.45	0.51
1:1:306:G:H5''	21:M:14:LYS:HE3	1.92	0.51
1:1:793:U:C2'	1:1:794:U:H5'	2.40	0.51
1:1:1582:A:H2'	1:1:1583:C:C6	2.46	0.51
7:7:71:A:H4'	7:7:72:A:O5'	2.11	0.51
7:7:134:G:H2'	7:7:135:U:H6	1.75	0.51
15:G:28:PHE:CE1	69:Y:55:ARG:HG2	2.45	0.51
28:S1:60:U:H5'	28:S1:496:A:H4'	1.93	0.51
28:S1:914:G:H5'	49:ST:73:ARG:NH1	2.25	0.51
28:S1:1139:G:H22	28:S1:1167:A:H2	1.59	0.51
31:SB:144:ASN:ND2	54:SY:36:ALA:O	2.35	0.51
1:1:55:A:H5''	21:M:157:LYS:HE3	1.92	0.51
1:1:225:C:HO2'	1:1:226:C:H6	1.57	0.51
1:1:1061:G:OP1	22:N:39:ARG:NH1	2.43	0.51
2:2:452:G:H2'	2:2:452:G:N3	2.24	0.51
2:2:1216:A:H2'	2:2:1217:C:H5'	1.92	0.51
4:4:167:C:H2'	4:4:168:A:O4'	2.10	0.51
22:N:87:MET:HE2	22:N:136:LEU:HB3	1.92	0.51
28:S1:105:C:OP1	28:S1:426:G:O2'	2.19	0.51
28:S1:133:G:P	28:S1:133:G:H8	2.33	0.51
43:SN:46:CYS:SG	91:SN:202:HOH:O	2.49	0.51
44:SO:114:ARG:HG2	44:SO:114:ARG:HH11	1.76	0.51
1:1:925:U:OP2	2:2:91:C:O2'	2.29	0.51
1:1:1405:U:H2'	1:1:1406:C:C6	2.46	0.51
1:1:1473:G:OP1	11:C:204:ARG:HD2	2.10	0.51
2:2:382:A2M:H2'	2:2:388:A:N6	2.26	0.51
2:2:1412:U:H2'	2:2:1413:PSU:C6	2.46	0.51
28:S1:17:C:H2'	28:S1:18:OMC:C6	2.46	0.51
28:S1:162:A:H2'	28:S1:163:A:C8	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:326:U:HO2'	28:S1:327:U:H6	1.57	0.51
28:S1:2137:U:H2'	28:S1:2138:U:H6	1.75	0.51
41:SL:10:LYS:HA	41:SL:102:TYR:CZ	2.45	0.51
69:Y:89:MET:HG3	69:Y:93:LEU:HD23	1.91	0.51
1:1:292:A:O2'	1:1:293:C:H5''	2.10	0.51
1:1:586:U:O2'	1:1:587:G:H8	1.94	0.51
3:3:72:A:H2'	3:3:73:A:C8	2.46	0.51
6:6:35:U:H2'	6:6:36:C:H6	1.76	0.51
11:C:46:ASN:O	91:C:402:HOH:O	2.19	0.51
45:SP:101:LEU:HB3	45:SP:124:LYS:HB2	1.93	0.51
47:SR:87:ARG:HD2	47:SR:99:LEU:HD11	1.92	0.51
1:1:369:A:OP2	91:1:1909:HOH:O	2.19	0.51
1:1:599:G:H1	1:1:606:C:H5	1.58	0.51
1:1:1092:U:O2'	1:1:1093:U:H6	1.93	0.51
1:1:1389:A:H5'	19:K:19:PRO:HD3	1.91	0.51
3:3:28:A:H5''	9:A:71:ARG:HG3	1.93	0.51
3:3:123:G:OP1	25:Q:128:LYS:NZ	2.43	0.51
5:5:39:G:H4'	10:B:372:ILE:O	2.10	0.51
5:5:63:G:H3'	5:5:64:G:N2	2.23	0.51
28:S1:1193:U:H2'	28:S1:1194:C:C6	2.46	0.51
52:SW:91:VAL:HG22	52:SW:122:TYR:HE1	1.76	0.51
56:Sa:51:ARG:NH2	56:Sa:86:GLU:OE2	2.42	0.51
1:1:423:U:O2'	1:1:424:G:H8	1.93	0.51
2:2:714:A:N3	2:2:723:G:N2	2.54	0.51
4:4:44:G:N1	4:4:66:C:H5	2.02	0.51
11:C:147:PRO:HA	70:Z:75:ARG:HG2	1.93	0.51
20:L:110:LEU:O	20:L:130:ALA:HB2	2.11	0.51
28:S1:140:G:H2'	28:S1:141:C:C6	2.46	0.51
28:S1:148:G:H2'	28:S1:149:G:H8	1.73	0.51
28:S1:363:G:H4'	28:S1:367:A:C8	2.46	0.51
28:S1:450:A:H2'	28:S1:451:C:H6	1.74	0.51
28:S1:1512:A:H2'	28:S1:1513:C:C6	2.46	0.51
33:SD:87:GLU:H	33:SD:87:GLU:CD	2.18	0.51
35:SF:83:ILE:HG21	35:SF:88:LEU:HG	1.93	0.51
62:Sg:220:LEU:HD13	62:Sg:230:PHE:CE1	2.46	0.51
1:1:817:C:H2'	1:1:818:C:O4'	2.11	0.51
2:2:460:A:N6	2:2:477:G:O2'	2.44	0.51
2:2:653:C:H2'	2:2:654:U:H6	1.76	0.51
4:4:180:C:H1'	5:5:5:C:H1'	1.93	0.51
6:6:50:A:H2'	6:6:52:G:C2	2.46	0.51
10:B:305:TYR:CD2	10:B:364:LYS:HA	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:69:MET:HG3	14:F:73:GLY:HA2	1.93	0.51
26:R:46:MET:HE1	27:S:148:ARG:HD3	1.93	0.51
28:S1:177:C:OP2	91:S1:2405:HOH:O	2.19	0.51
28:S1:228:G:OP1	40:SK:164:ARG:NH2	2.44	0.51
31:SB:36:ALA:HB1	31:SB:157:LEU:HD22	1.93	0.51
38:SI:3:PRO:HB2	38:SI:28:PHE:CZ	2.46	0.51
38:SI:164:ARG:HH12	38:SI:165:ILE:HD12	1.76	0.51
40:SK:166:ARG:HA	40:SK:169:HIS:HB3	1.93	0.51
1:1:145:U:O2'	15:G:193:ARG:NH1	2.44	0.50
1:1:219:U:H5'	1:1:220:A:H5'	1.93	0.50
1:1:326:A:H2'	1:1:327:G:C8	2.46	0.50
1:1:559:G:H2'	1:1:560:G:H5'	1.93	0.50
1:1:691:G:N7	91:1:1936:HOH:O	2.34	0.50
1:1:738:C:H2'	1:1:739:U:C6	2.46	0.50
2:2:974:G:O2'	2:2:975:A:O5'	2.29	0.50
5:5:51:A:H1'	5:5:52:U:H5'	1.92	0.50
9:A:112:ILE:HG13	85:o:79:VAL:HG22	1.93	0.50
28:S1:71:G:O6	36:SG:173:ARG:NH1	2.45	0.50
28:S1:664:U:O2'	28:S1:670:A:N1	2.41	0.50
28:S1:1795:G:H22	28:S1:1803:A:H2	1.57	0.50
49:ST:115:LEU:O	49:ST:119:GLU:HG3	2.11	0.50
56:Sa:71:ILE:HB	56:Sa:75:ILE:HD11	1.93	0.50
63:Sh:85:LEU:HA	63:Sh:91:ALA:HA	1.92	0.50
84:n:3:THR:O	84:n:4:VAL:HG13	2.11	0.50
1:1:273:A:C6	80:j:79:LYS:HA	2.46	0.50
2:2:479:C:H3'	2:2:480:G:H8	1.76	0.50
4:4:98:A:H2'	4:4:99:A:H8	1.76	0.50
17:I:57:LYS:HB2	17:I:159:GLY:HA3	1.94	0.50
28:S1:83:A:H4'	55:SZ:126:GLY:O	2.11	0.50
28:S1:699:A:H62	28:S1:747:C:H42	1.60	0.50
62:Sg:148:GLY:HA2	62:Sg:179:TRP:HH2	1.77	0.50
1:1:24:A:H2'	1:1:25:C:C6	2.46	0.50
1:1:1238:C:C5'	1:1:1239:U:H5'	2.41	0.50
1:1:1272:U:O2'	1:1:1273:U:H5'	2.11	0.50
4:4:148:C:O2'	4:4:149:U:OP2	2.25	0.50
28:S1:1366:A:H61	28:S1:1404:U:H5	1.60	0.50
32:SC:163:HIS:CD2	32:SC:164:LYS:HG2	2.46	0.50
38:SI:31:GLU:O	38:SI:38:ARG:HG3	2.11	0.50
1:1:496:C:H2'	1:1:497:A:C8	2.46	0.50
1:1:904:G:N7	85:o:2:ALA:N	2.59	0.50
1:1:1450:U:H2'	1:1:1451:C:C6	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:121:U:H2'	2:2:122:PSU:C6	2.47	0.50
4:4:165:C:H5''	10:B:281:THR:HG21	1.94	0.50
7:7:93:C:C2'	7:7:94:G:H5''	2.41	0.50
18:J:129:PRO:O	18:J:133:THR:HG23	2.11	0.50
24:P:71:MET:HE1	24:P:85:PRO:O	2.12	0.50
25:Q:179:LYS:HD2	25:Q:180:LYS:N	2.26	0.50
28:S1:1036:G:OP2	28:S1:1036:G:N2	2.35	0.50
28:S1:2045:A:H2'	28:S1:2046:PSU:H6	1.76	0.50
47:SR:27:VAL:HG11	47:SR:51:ILE:HD11	1.94	0.50
61:Sf:94:LYS:HG3	61:Sf:95:MET:N	2.26	0.50
73:c:230:HIS:CE1	73:c:238:GLY:HA3	2.47	0.50
1:1:171:U:O2'	1:1:172:G:H5'	2.11	0.50
1:1:1153:A:H2'	1:1:1155:A:H62	1.76	0.50
1:1:1582:A:H2'	1:1:1583:C:H6	1.76	0.50
2:2:698:G:C4	2:2:740:A:N6	2.79	0.50
6:6:19:C:H2'	6:6:20:A:C8	2.46	0.50
8:8:65:C:H5''	23:O:283:LEU:HD21	1.93	0.50
28:S1:550:C:H2'	28:S1:551:A:C8	2.46	0.50
41:SL:89:GLN:HE22	41:SL:125:ALA:HA	1.77	0.50
49:ST:99:ARG:CZ	49:ST:143:SER:HB2	2.42	0.50
65:U:24:LYS:HD3	65:U:26:PHE:CZ	2.46	0.50
68:X:10:HIS:ND1	91:X:201:HOH:O	2.25	0.50
1:1:1177:U:H2'	1:1:1178:U:H6	1.76	0.50
1:1:1586:G:N1	78:h:3:CYS:SG	2.81	0.50
2:2:386:U:H1'	2:2:1416:U:H5''	1.94	0.50
2:2:1122:C:HO2'	2:2:1123:A:P	2.34	0.50
4:4:13:A:H2'	4:4:14:G:C8	2.47	0.50
4:4:64:C:C2'	4:4:65:C:H5'	2.42	0.50
15:G:224:LEU:O	15:G:227:SER:OG	2.29	0.50
22:N:129:VAL:HG11	22:N:135:LEU:HD21	1.94	0.50
28:S1:528:G:H1	28:S1:553:U:H3	1.60	0.50
28:S1:1836:G:O6	43:SN:71:TYR:OH	2.28	0.50
28:S1:2004:G:N2	28:S1:2031:A:OP2	2.36	0.50
30:SA:40:LYS:HB2	30:SA:75:GLN:OE1	2.11	0.50
74:d:92:LEU:HD21	74:d:94:VAL:HG23	1.93	0.50
1:1:199:A:H1'	70:Z:141:SER:OG	2.12	0.50
1:1:967:G:H5'	1:1:968:A:OP1	2.12	0.50
2:2:1003:G:O2'	2:2:1004:G:C8	2.64	0.50
3:3:129:A:C6	85:o:42:CYS:HA	2.46	0.50
4:4:75:C:O2'	4:4:76:C:H5'	2.12	0.50
5:5:116:A:N6	5:5:119:U:HO2'	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:777:A:H4'	28:S1:778:G:O5'	2.10	0.50
28:S1:1718:A:O2'	28:S1:1719:G:O5'	2.30	0.50
28:S1:1940:G:OP2	53:SX:80:ARG:NH2	2.38	0.50
31:SB:125:LEU:HD23	31:SB:147:VAL:HG22	1.93	0.50
34:SE:8:ARG:HD2	34:SE:22:GLY:O	2.12	0.50
59:Sd:30:LEU:HD12	59:Sd:41:GLN:HG2	1.94	0.50
1:1:116:U:C2'	1:1:117:G:H5'	2.42	0.50
1:1:1044:G:N3	2:2:1064:A:H2'	2.27	0.50
1:1:1574:C:H2'	1:1:1575:G:H8	1.75	0.50
2:2:846:G:H1	2:2:952:G:H22	1.58	0.50
2:2:1131:A:O2'	2:2:1132:A:O5'	2.28	0.50
2:2:1497:C:H2'	2:2:1498:G:O4'	2.11	0.50
11:C:27:PHE:CD1	11:C:131:SER:HB3	2.46	0.50
28:S1:180:G:H22	28:S1:316:A:H5'	1.76	0.50
28:S1:1813:A:H1'	28:S1:1814:U:C5	2.47	0.50
45:SP:84:PHE:CE2	45:SP:86:PRO:HA	2.47	0.50
1:1:636:U:H2'	1:1:637:C:H6	1.77	0.50
1:1:904:G:O2'	1:1:905:G:O5'	2.14	0.50
1:1:1055:U:H5	1:1:1097:A:N1	2.10	0.50
2:2:450:C:O2'	2:2:451:U:O2	2.26	0.50
2:2:460:A:O2'	2:2:461:C:O5'	2.29	0.50
2:2:1462:A:O2'	16:H:189:LYS:NZ	2.44	0.50
22:N:52:VAL:HG21	22:N:136:LEU:HD12	1.93	0.50
28:S1:915:A:H61	28:S1:1102:G:HO2'	1.60	0.50
31:SB:109:GLY:N	31:SB:139:GLU:OE2	2.37	0.50
49:ST:130:LYS:HE2	49:ST:139:TRP:HB3	1.94	0.50
1:1:472:U:H2'	1:1:473:A:H8	1.77	0.49
1:1:1662:G:H4'	1:1:1663:U:OP1	2.12	0.49
2:2:811:U:H5	2:2:1007:U:O2	1.94	0.49
5:5:37:C:O3'	10:B:380:LYS:NZ	2.44	0.49
28:S1:1588:A:H2'	28:S1:1589:G:C8	2.46	0.49
70:Z:8:GLN:HB3	70:Z:46:LEU:HD11	1.94	0.49
70:Z:22:ARG:HH22	76:f:82:ASP:CG	2.20	0.49
80:j:4:GLY:O	80:j:8:MET:HG2	2.12	0.49
1:1:591:U:O2'	1:1:592:G:H5'	2.11	0.49
1:1:958:G:H2'	1:1:977:A:H62	1.77	0.49
2:2:4:C:H1'	2:2:5:A:C8	2.47	0.49
2:2:1194:PSU:H2'	2:2:1195:U:C6	2.48	0.49
2:2:1253:OMG:H2'	2:2:1308:5MC:HM51	1.94	0.49
4:4:183:C:H2'	4:4:184:U:O4'	2.12	0.49
11:C:63:ALA:HB3	11:C:91:PHE:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:154:GLU:HA	24:P:154:GLU:OE1	2.11	0.49
28:S1:2185:MA6:H5'	28:S1:2186:C:OP2	2.11	0.49
30:SA:196:SER:O	30:SA:200:VAL:HG12	2.11	0.49
31:SB:70:ALA:HB2	54:SY:42:ALA:HB2	1.94	0.49
33:SD:70:LEU:HD23	34:SE:247:ILE:HD13	1.94	0.49
75:e:154:LYS:HG3	75:e:167:TYR:CZ	2.47	0.49
2:2:471:U:O2'	2:2:472:PSU:O4'	2.30	0.49
5:5:8:C:H2'	5:5:9:C:C6	2.47	0.49
6:6:44:G:H2'	6:6:45:G:C8	2.48	0.49
10:B:71:GLU:OE1	10:B:364:LYS:NZ	2.32	0.49
28:S1:1590:A:O2'	28:S1:1591:U:H6	1.95	0.49
28:S1:2146:U:H2'	28:S1:2147:A:C8	2.48	0.49
28:S1:2198:A:O2'	28:S1:2200:A:N7	2.43	0.49
32:SC:210:ILE:HD11	51:SV:40:ILE:HD11	1.94	0.49
74:d:15:LYS:O	74:d:19:VAL:HG13	2.12	0.49
1:1:6:C:O2'	1:1:7:C:C6	2.62	0.49
1:1:1352:C:H2'	1:1:1353:A:H8	1.77	0.49
1:1:1576:U:H2'	1:1:1577:U:C6	2.48	0.49
1:1:1588:G:O2'	1:1:1590:G:OP2	2.20	0.49
7:7:62:A:OP1	71:a:53:LYS:NZ	2.44	0.49
11:C:357:LEU:O	11:C:361:THR:HG23	2.12	0.49
28:S1:1809:U:H2'	28:S1:1810:G:O4'	2.12	0.49
1:1:256:U:H5	1:1:1479:A:O2'	1.94	0.49
1:1:573:U:H4'	1:1:574:G:H5'	1.94	0.49
1:1:1672:U:O4	66:V:39:HIS:NE2	2.41	0.49
2:2:5:A:O2'	2:2:6:A:OP2	2.23	0.49
2:2:749:G:O2'	2:2:750:U:H6	1.95	0.49
2:2:1318:PSU:H1'	10:B:255:ALA:HB3	1.94	0.49
2:2:1364:A:C2'	2:2:1365:C:H5'	2.43	0.49
4:4:13:A:H2'	4:4:14:G:H8	1.77	0.49
28:S1:242:A:H2'	28:S1:243:U:C6	2.46	0.49
28:S1:656:G:H5'	28:S1:662:G:N2	2.27	0.49
28:S1:951:U:O2	28:S1:984:G:N2	2.30	0.49
31:SB:97:VAL:HG13	31:SB:189:ARG:HH12	1.78	0.49
33:SD:122:HIS:CE1	60:Se:37:ARG:HD2	2.48	0.49
50:SU:42:ASN:HB2	50:SU:65:ASN:HA	1.95	0.49
79:i:56:LEU:HD13	79:i:79:ARG:HG3	1.95	0.49
83:m:87:LYS:HG2	83:m:91:TRP:CD2	2.47	0.49
1:1:1489:U:HO2'	1:1:1490:G:H8	1.58	0.49
2:2:712:G:H3'	2:2:713:A:C8	2.43	0.49
2:2:1012:U:OP1	15:G:49:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:145:U:H2'	3:3:146:G:O4'	2.13	0.49
7:7:128:U:O4	7:7:134:G:O6	2.30	0.49
18:J:8:VAL:HB	18:J:127:LEU:HD13	1.94	0.49
23:O:40:ASP:HB2	23:O:43:LYS:HG2	1.93	0.49
28:S1:550:C:O2'	28:S1:551:A:OP1	2.27	0.49
28:S1:991:G:O6	38:SI:76:LYS:NZ	2.46	0.49
34:SE:121:MET:HE1	34:SE:144:ILE:HD11	1.94	0.49
55:SZ:34:HIS:HB2	55:SZ:37:TRP:HB2	1.94	0.49
65:U:11:ARG:O	65:U:11:ARG:HG2	2.13	0.49
65:U:67:LYS:O	65:U:81:THR:HA	2.12	0.49
1:1:221:C:H2'	1:1:222:A:C8	2.47	0.49
1:1:479:A:H2'	1:1:480:U:C6	2.47	0.49
1:1:1178:U:H2'	1:1:1179:C:C6	2.47	0.49
2:2:615:G:H2'	2:2:616:G:C8	2.47	0.49
2:2:1499:G:H1	2:2:1522:U:H3	1.60	0.49
10:B:47:MET:HB2	10:B:84:MET:CE	2.43	0.49
26:R:29:PHE:HB2	27:S:146:LEU:HD23	1.95	0.49
27:S:137:ILE:HD13	73:c:79:ALA:HB2	1.95	0.49
28:S1:491:G:OP1	34:SE:26:PRO:HD3	2.12	0.49
28:S1:1449:U:C4	35:SF:213:ARG:HD3	2.48	0.49
28:S1:1870:A:OP2	91:S1:2406:HOH:O	2.19	0.49
31:SB:56:MET:HE3	58:Sc:3:PHE:CE1	2.48	0.49
62:Sg:81:LEU:CD1	62:Sg:91:MET:HG3	2.43	0.49
67:W:77:ILE:HG23	67:W:98:PRO:HG3	1.95	0.49
1:1:116:U:H2'	1:1:117:G:H5'	1.95	0.49
1:1:248:A:OP2	11:C:221:ASN:HB2	2.13	0.49
1:1:513:C:H2'	1:1:514:C:O2	2.13	0.49
1:1:739:U:H2'	1:1:740:C:C6	2.48	0.49
2:2:846:G:N2	2:2:952:G:H22	2.07	0.49
3:3:150:A:H4'	81:k:26:LYS:HE2	1.95	0.49
6:6:47:G:P	19:K:125:ARG:HH22	2.36	0.49
11:C:264:THR:HG22	11:C:265:PHE:H	1.76	0.49
22:N:76:MET:HE2	22:N:138:MET:SD	2.52	0.49
28:S1:52:U:H2'	28:S1:53:G:C8	2.48	0.49
28:S1:788:A:N1	28:S1:832:C:H5	2.11	0.49
28:S1:828:G:H2'	28:S1:829:G:C8	2.47	0.49
28:S1:1512:A:O2'	28:S1:2040:C:H5	1.94	0.49
28:S1:1514:A:H5'	59:Sd:36:ARG:HE	1.77	0.49
28:S1:2035:C:O2'	28:S1:2036:G:OP2	2.26	0.49
30:SA:123:MET:HE2	30:SA:145:THR:HG23	1.95	0.49
31:SB:161:ASP:OD1	54:SY:69:SER:OG	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53: SX:19: LEU: HD11	53: SX:75: ARG: HG3	1.95	0.49
73: c:142: PRO: HA	73: c:237: TYR: CG	2.47	0.49
1:1:476: U: H5	1:1:657: G: O6	1.96	0.49
1:1:1368: G: C6	16: H:80: LYS: HA	2.48	0.49
2:2:762: U: H2'	2:2:763: C: H6	1.77	0.49
4:4:77: U: C2	10: B:75: PRO: HB3	2.47	0.49
4:4:136: G: H3'	4:4:148: C: N4	2.28	0.49
10: B:261: HIS: HA	10: B:262: PRO: C	2.38	0.49
23: O:36: MET: HE1	23: O:153: ASP: OD1	2.13	0.49
25: Q:179: LYS: HD2	25: Q:179: LYS: C	2.38	0.49
28: S1:1138: G: H2'	28: S1:1139: G: H8	1.75	0.49
62: Sg:172: TRP: HA	62: Sg:196: TYR: HB2	1.94	0.49
74: d:40: ARG: HG2	74: d:40: ARG: HH11	1.77	0.49
77: g:57: ARG: HB2	77: g:116: MET: SD	2.53	0.49
79: i:7: ARG: HD3	79: i:17: GLY: HA3	1.94	0.49
1:1:624: U: O2'	1:1:625: C: H4'	2.12	0.49
1:1:626: U: O2'	1:1:627: C: H6	1.94	0.49
1:1:835: G: H2'	1:1:835: G: N3	2.28	0.49
2:2:806: C: H2'	2:2:807: A: O4'	2.13	0.49
2:2:947: U: H2'	2:2:948: G: C8	2.47	0.49
2:2:1262: G: H2'	2:2:1263: C: H6	1.78	0.49
22: N:66: GLU: OE1	22: N:69: ARG: NH2	2.43	0.49
31: SB:25: ARG: O	31: SB:167: ASN: ND2	2.40	0.49
46: SQ:50: VAL: O	46: SQ:53: THR: OG1	2.29	0.49
68: X:9: SER: HA	68: X:56: THR: HG23	1.94	0.49
1:1:637: C: H2'	1:1:638: C: C6	2.48	0.48
1:1:1451: C: H2'	1:1:1452: C: C6	2.47	0.48
2:2:1231: OMG: H5''	86: p:66: LYS: HG2	1.94	0.48
5:5:126: C: O2	75: e:76: ARG: HB3	2.13	0.48
22: N:36: ILE: HD13	22: N:69: ARG: HH11	1.78	0.48
28: S1:558: U: H5	28: S1:587: A: N7	2.10	0.48
28: S1:1572: C: H5	28: S1:1615: G: H1	1.59	0.48
28: S1:1612: C: O2'	28: S1:1613: C: H5'	2.13	0.48
37: SH:45: ARG: HG3	37: SH:45: ARG: NH1	2.27	0.48
38: SI:60: THR: OG1	38: SI:92: CYS: SG	2.60	0.48
44: SO:62: SER: O	44: SO:103: PRO: HG2	2.13	0.48
1:1:828: U: H2'	1:1:829: U: C6	2.49	0.48
1:1:1426: A: N1	70: Z:86: GLY: HA2	2.28	0.48
2:2:1170: U: H2'	2:2:1171: G: H8	1.78	0.48
2:2:1289: A: H2'	2:2:1290: C: H5'	1.94	0.48
28: S1:1682: G: H22	32: SC:205: ASP: HB2	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:1832:C:O2	28:S1:1838:U:H5	1.96	0.48
28:S1:1870:A:H2'	28:S1:1871:C:C6	2.49	0.48
32:SC:27:GLU:HG2	32:SC:68:LEU:HD21	1.95	0.48
33:SD:76:MET:HE1	33:SD:95:VAL:HG23	1.95	0.48
38:SI:143:TRP:CZ3	39:SJ:54:ASP:HB2	2.47	0.48
1:1:848:U:H2'	1:1:849:U:C6	2.48	0.48
1:1:1419:C:H5	1:1:1440:G:N1	1.93	0.48
1:1:1723:A:HO2'	1:1:1724:C:H6	1.61	0.48
2:2:27:C:OP1	91:2:4305:HOH:O	2.20	0.48
2:2:762:U:H2'	2:2:763:C:C6	2.48	0.48
2:2:956:C:O5'	2:2:956:C:H6	1.96	0.48
27:S:39:TYR:CE2	27:S:63:ILE:HD11	2.48	0.48
2:2:715:G:O6	2:2:723:G:N1	2.47	0.48
2:2:1379:A:N7	10:B:261:HIS:HE1	2.12	0.48
3:3:112:C:O2	3:3:112:C:H2'	2.13	0.48
6:6:40:C:H5'	19:K:91:ARG:NH2	2.27	0.48
28:S1:569:U:O2'	28:S1:571:A:N7	2.45	0.48
30:SA:241:VAL:HG12	44:SO:13:ASN:HD22	1.78	0.48
47:SR:25:ARG:HB2	47:SR:30:ALA:HB2	1.95	0.48
1:1:315:U:H2'	1:1:316:U:C6	2.49	0.48
1:1:576:G:O6	11:C:324:ARG:HG3	2.13	0.48
1:1:767:U:H2'	1:1:768:C:O4'	2.13	0.48
1:1:860:G:OP1	91:1:1907:HOH:O	2.18	0.48
1:1:1484:G:N7	91:1:1938:HOH:O	2.35	0.48
2:2:122:PSU:H1'	25:Q:78:VAL:HG12	1.96	0.48
3:3:212:G:H5'	69:Y:131:ARG:HH12	1.79	0.48
7:7:27:U:H2'	7:7:28:C:O2	2.13	0.48
10:B:56:ILE:O	10:B:73:VAL:HA	2.13	0.48
15:G:183:ASP:OD2	15:G:186:ARG:NH1	2.46	0.48
28:S1:1572:C:H41	28:S1:1615:G:H1	1.61	0.48
28:S1:1573:A:H2'	28:S1:1574:G:H8	1.78	0.48
28:S1:1999:G:H2'	28:S1:2000:U:C6	2.48	0.48
31:SB:63:LEU:HD12	54:SY:41:ILE:HD13	1.96	0.48
37:SH:83:LEU:HD22	37:SH:94:PRO:HB2	1.94	0.48
56:Sa:42:PHE:HD1	56:Sa:46:THR:HG23	1.78	0.48
63:Sh:139:PHE:HE1	63:Sh:172:PHE:HB2	1.78	0.48
64:T:13:LYS:HA	64:T:107:LEU:HD21	1.94	0.48
69:Y:66:SER:O	69:Y:117:GLN:NE2	2.43	0.48
1:1:592:G:H2'	1:1:593:C:H6	1.78	0.48
1:1:623:U:H2'	1:1:624:U:O2	2.13	0.48
2:2:496:G:HO2'	2:2:497:G:P	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1115:U:H5	23:O:17:GLN:O	1.97	0.48
2:2:1225:A:H2'	2:2:1226:C:H6	1.78	0.48
11:C:332:TYR:CZ	73:c:59:ARG:HG3	2.48	0.48
28:S1:546:U:H2'	28:S1:547:U:O4'	2.14	0.48
28:S1:992:C:H4'	28:S1:993:U:H5''	1.95	0.48
28:S1:1170:A:H2'	28:S1:1171:A:C8	2.49	0.48
28:S1:1367:U:H1'	30:SA:150:ASN:ND2	2.29	0.48
31:SB:96:HIS:HE1	31:SB:200:GLU:HG2	1.75	0.48
33:SD:89:LYS:HB2	33:SD:94:TYR:CD2	2.48	0.48
53:SX:6:ASN:O	53:SX:9:HIS:ND1	2.45	0.48
55:SZ:44:GLN:O	55:SZ:48:LYS:HG2	2.14	0.48
1:1:351:U:H2'	1:1:352:G:C8	2.49	0.48
1:1:508:A:OP2	11:C:356:LYS:NZ	2.47	0.48
1:1:606:C:H2'	1:1:607:C:O4'	2.13	0.48
1:1:1097:A:H2'	1:1:1100:C:C5	2.48	0.48
1:1:1185:U:H2'	1:1:1186:A:O4'	2.14	0.48
1:1:1520:U:OP1	91:1:1910:HOH:O	2.20	0.48
2:2:1519:U:H2'	2:2:1520:C:H6	1.77	0.48
6:6:46:C:H5'	19:K:121:ALA:CB	2.44	0.48
10:B:5:LYS:HG3	10:B:6:PHE:H	1.78	0.48
11:C:116:LEU:HA	11:C:119:LYS:HD3	1.95	0.48
12:D:35:ALA:HB2	12:D:125:TYR:CE1	2.49	0.48
28:S1:192:U:H5'	40:SK:158:LEU:HD13	1.96	0.48
28:S1:251:A:H1'	28:S1:784:C:H1'	1.94	0.48
28:S1:547:U:H3'	28:S1:548:G:C8	2.48	0.48
28:S1:836:C:H2'	28:S1:837:G:C8	2.49	0.48
28:S1:1471:U:H2'	28:S1:1472:U:H6	1.79	0.48
30:SA:39:GLU:OE1	30:SA:76:SER:OG	2.30	0.48
38:SI:52:VAL:HG12	38:SI:174:TYR:HE2	1.79	0.48
49:ST:4:MET:HE2	49:ST:5:HIS:CE1	2.47	0.48
65:U:56:LYS:O	65:U:85:TYR:OH	2.26	0.48
65:U:64:LEU:HD23	65:U:64:LEU:N	2.29	0.48
67:W:47:VAL:HG21	67:W:98:PRO:HB3	1.96	0.48
73:c:213:TRP:O	91:c:301:HOH:O	2.20	0.48
78:h:2:SER:O	78:h:2:SER:OG	2.29	0.48
1:1:416:A:H5''	67:W:92:VAL:HG21	1.95	0.48
1:1:498:G:O3'	11:C:316:PRO:HA	2.13	0.48
1:1:662:C:H2'	1:1:663:C:H6	1.78	0.48
1:1:694:U:H2'	1:1:695:OMC:C6	2.48	0.48
1:1:699:C:H2'	1:1:700:A:C8	2.48	0.48
1:1:744:C:O2'	1:1:745:U:H6	1.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:394:U:H2'	2:2:395:A:C5	2.49	0.48
2:2:775:C:OP1	2:2:776:C:O2'	2.27	0.48
3:3:206:A:H2'	3:3:207:C:O4'	2.13	0.48
28:S1:255:A:H2'	28:S1:256:A:C8	2.49	0.48
28:S1:913:G:N2	49:ST:133:LYS:HD3	2.28	0.48
28:S1:1510:C:H5	28:S1:1515:A:N6	2.11	0.48
28:S1:2026:U:H2'	28:S1:2027:G:C8	2.48	0.48
38:SI:141:ARG:HD2	38:SI:143:TRP:CZ2	2.48	0.48
44:SO:135:ARG:HG2	44:SO:136:LYS:N	2.29	0.48
55:SZ:28:PHE:CZ	55:SZ:50:LEU:HD21	2.49	0.48
1:1:118:C:H5	1:1:150:G:N1	1.90	0.48
1:1:744:C:O2'	1:1:745:U:OP2	2.29	0.48
1:1:1771:U:H6	1:1:1771:U:H5''	1.79	0.48
4:4:95:U:H5	4:4:102:G:O6	1.97	0.48
4:4:124:A:H2'	4:4:125:C:C6	2.48	0.48
10:B:4:CYS:N	91:B:506:HOH:O	2.47	0.48
28:S1:752:C:H2'	28:S1:753:A:C8	2.47	0.48
28:S1:983:C:H2'	28:S1:984:G:C8	2.48	0.48
28:S1:1101:A:H2'	28:S1:1102:G:C4	2.48	0.48
33:SD:105:GLU:OE1	33:SD:105:GLU:HA	2.14	0.48
34:SE:8:ARG:HD3	34:SE:18:SER:O	2.13	0.48
38:SI:61:VAL:HG11	38:SI:175:VAL:HG21	1.95	0.48
43:SN:12:ASN:OD1	43:SN:15:ARG:NE	2.46	0.48
49:ST:4:MET:HE2	49:ST:121:ARG:HD3	1.96	0.48
64:T:36:ILE:HD12	64:T:114:ILE:HD13	1.95	0.48
1:1:64:A:N6	1:1:74:G:H1'	2.29	0.48
2:2:696:A:H4'	2:2:697:G:OP1	2.11	0.48
2:2:1217:C:HO2'	2:2:1218:A:H8	1.62	0.48
15:G:48:SER:HA	15:G:51:MET:HE2	1.96	0.48
27:S:158:PRO:HG2	27:S:159:TYR:CE2	2.49	0.48
28:S1:2:A:N6	39:SJ:91:LYS:HE2	2.27	0.48
28:S1:30:G:H2'	28:S1:31:C:C6	2.47	0.48
28:S1:275:A:O2'	28:S1:276:G:N3	2.39	0.48
28:S1:288:A:H5'	36:SG:213:LEU:HD22	1.96	0.48
28:S1:979:U:H2'	28:S1:980:G:C8	2.49	0.48
63:Sh:185:LYS:HD2	63:Sh:185:LYS:C	2.38	0.48
77:g:55:LEU:HB3	77:g:116:MET:CE	2.44	0.48
1:1:412:G:H2'	1:1:414:A:H2	1.78	0.47
3:3:63:U:H3'	3:3:64:U:H5'	1.96	0.47
4:4:17:A:H2'	4:4:18:U:C6	2.48	0.47
28:S1:307:C:H3'	28:S1:308:C:H2'	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:461:G:O2'	36:SG:60:ASP:OD2	2.27	0.47
40:SK:24:ARG:HG2	91:SK:309:HOH:O	2.14	0.47
50:SU:14:ASP:OD1	50:SU:14:ASP:O	2.32	0.47
1:1:56:G:H2'	1:1:57:G:C8	2.49	0.47
1:1:172:G:H1'	1:1:173:G:OP1	2.14	0.47
1:1:620:U:H5''	1:1:621:U:OP1	2.14	0.47
1:1:662:C:H2'	1:1:663:C:C6	2.49	0.47
2:2:591:A2M:HM'3	2:2:591:A2M:H1'	1.78	0.47
2:2:701:U:O2	2:2:729:G:H5''	2.15	0.47
3:3:122:U:O4'	25:Q:96:MET:HG2	2.14	0.47
4:4:59:G:C2'	4:4:60:A:H5''	2.44	0.47
17:I:52:PHE:CD1	17:I:153:GLN:HB2	2.49	0.47
28:S1:1708:A:H4'	53:SX:138:ARG:NH1	2.29	0.47
28:S1:2122:G:H2'	28:S1:2123:A:O4'	2.14	0.47
29:S4:73:A:H2'	29:S4:74:C:O4'	2.14	0.47
41:SL:88:ARG:NH2	41:SL:119:ASP:OD2	2.47	0.47
1:1:69:A:OP1	20:L:67:PRO:HG3	2.14	0.47
1:1:1409:U:H2'	1:1:1410:U:C6	2.49	0.47
2:2:14:C:H2'	2:2:15:C:C6	2.49	0.47
5:5:116:A:N6	5:5:119:U:O2'	2.47	0.47
8:8:62:A:H2'	8:8:63:C:C6	2.49	0.47
42:SM:40:ALA:HB1	42:SM:47:ILE:HD11	1.96	0.47
82:l:38:ASN:O	82:l:38:ASN:ND2	2.47	0.47
1:1:200:A:P	70:Z:139:ARG:HH12	2.37	0.47
2:2:66:A:H2'	2:2:67:G:O4'	2.15	0.47
2:2:767:U:H5''	9:A:31:ILE:HG12	1.97	0.47
2:2:803:A:H2'	2:2:804:U:O4'	2.14	0.47
2:2:975:A:O2'	2:2:976:A:O4'	2.31	0.47
5:5:7:U:H2'	5:5:8:C:H6	1.78	0.47
8:8:96:G:H2'	8:8:97:A:C8	2.49	0.47
17:I:97:THR:HG21	71:a:118:PHE:HB3	1.95	0.47
18:J:74:LYS:HE2	18:J:76:LEU:HD21	1.96	0.47
24:P:46:LYS:O	24:P:50:GLN:HG2	2.14	0.47
28:S1:315:A:H5''	28:S1:333:G:N2	2.30	0.47
28:S1:1555:A:C2	28:S1:1975:A:C4	3.03	0.47
28:S1:2178:U:H2'	28:S1:2179:A:C8	2.50	0.47
30:SA:130:LYS:HA	30:SA:136:THR:HA	1.97	0.47
58:Sc:20:HIS:HB3	58:Sc:23:ARG:HG2	1.96	0.47
71:a:20:LYS:O	71:a:24:GLU:HG2	2.15	0.47
1:1:385:G:O2'	7:7:24:G:N3	2.47	0.47
1:1:491:A:O2'	6:6:65:C:H5	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:575:A:N1	11:C:334:LYS:HG2	2.29	0.47
1:1:1402:PSU:H2'	1:1:1403:A:H8	1.79	0.47
1:1:1422:A:H5''	73:c:29:LYS:HE3	1.96	0.47
2:2:133:G:H22	2:2:345:C:H5	1.62	0.47
2:2:747:A:H1'	2:2:748:C:O4'	2.15	0.47
2:2:1319:C:H2'	2:2:1320:U:C6	2.49	0.47
4:4:149:U:H4'	4:4:150:A:OP1	2.15	0.47
23:O:129:TYR:HB2	23:O:183:PRO:HB3	1.97	0.47
28:S1:109:C:H5	28:S1:347:A:C2	2.32	0.47
28:S1:905:A:C8	39:SJ:107:SER:HA	2.50	0.47
31:SB:72:GLU:HG3	31:SB:73:ASN:N	2.30	0.47
38:SI:41:LEU:N	38:SI:42:PRO:HD2	2.29	0.47
38:SI:143:TRP:HZ3	39:SJ:54:ASP:HB2	1.80	0.47
44:SO:77:ARG:O	44:SO:80:GLU:HG2	2.13	0.47
51:SV:14:ARG:HG2	51:SV:69:ILE:HD11	1.97	0.47
51:SV:35:ILE:HD13	51:SV:50:ILE:HG22	1.97	0.47
52:SW:113:GLU:HG2	52:SW:115:LYS:HD3	1.95	0.47
73:c:26:ALA:O	73:c:30:GLN:HG2	2.15	0.47
73:c:109:GLN:HG3	73:c:140:VAL:HG12	1.96	0.47
74:d:31:GLN:O	74:d:35:THR:HG23	2.15	0.47
1:1:1169:A:H2'	1:1:1170:G:C8	2.49	0.47
1:1:1727:A:C2'	1:1:1728:A:H5'	2.43	0.47
8:8:30:C:H2'	8:8:31:A:O4'	2.15	0.47
13:E:91:VAL:HG21	13:E:160:LEU:HD23	1.96	0.47
28:S1:555:C:H5'	28:S1:556:A:OP2	2.14	0.47
28:S1:1623:OMG:HM23	28:S1:1623:OMG:H1'	1.59	0.47
28:S1:2084:C:H2'	28:S1:2085:A:C8	2.49	0.47
35:SF:182:VAL:HB	35:SF:209:TYR:HB2	1.96	0.47
38:SI:62:LEU:HA	38:SI:62:LEU:HD12	1.77	0.47
67:W:74:LYS:HB2	67:W:76:VAL:HG22	1.97	0.47
1:1:151:C:OP1	71:a:109:SER:OG	2.32	0.47
1:1:165:U:O2'	1:1:166:G:H5'	2.15	0.47
1:1:613:C:H2'	1:1:614:A:C8	2.49	0.47
1:1:652:A:O2'	1:1:653:A:C8	2.68	0.47
1:1:727:C:O3'	1:1:728:C:H2'	2.14	0.47
1:1:1540:OMG:H2'	1:1:1541:C:C6	2.50	0.47
2:2:512:PSU:H2'	2:2:513:C:C6	2.49	0.47
2:2:700:G:N2	2:2:730:A:H2'	2.29	0.47
2:2:1510:A:O2'	10:B:170:LYS:HE3	2.15	0.47
3:3:42:U:H2'	3:3:43:C:C6	2.49	0.47
3:3:204:A:H2'	3:3:205:A:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:38:A:H2	4:4:164:U:O4	1.97	0.47
8:8:34:A:H2'	8:8:35:U:O4'	2.14	0.47
14:F:144:THR:OG1	14:F:145:LEU:N	2.47	0.47
20:L:72:THR:HG22	20:L:108:LYS:HB3	1.95	0.47
23:O:109:THR:HG21	23:O:177:MET:CE	2.45	0.47
28:S1:307:C:H2'	28:S1:308:C:C5	2.49	0.47
28:S1:1018:G:C2	28:S1:1035:G:C2	3.03	0.47
30:SA:31:ASP:O	30:SA:98:LEU:N	2.46	0.47
30:SA:115:LEU:HD11	30:SA:213:ARG:HE	1.80	0.47
36:SG:146:LYS:NZ	36:SG:146:LYS:HB3	2.29	0.47
37:SH:38:THR:O	37:SH:38:THR:OG1	2.32	0.47
52:SW:118:MET:HE2	52:SW:126:PHE:CD1	2.50	0.47
62:Sg:300:ASP:CG	62:Sg:304:ARG:HH12	2.22	0.47
64:T:16:LYS:O	64:T:101:ASN:ND2	2.41	0.47
1:1:225:C:O2'	1:1:226:C:H6	1.98	0.47
1:1:1422:A:O2'	1:1:1423:A:H8	1.97	0.47
2:2:1183:C:H2'	2:2:1184:C:O4'	2.14	0.47
2:2:1290:C:O2'	2:2:1291:G:O4'	2.32	0.47
11:C:282:LEU:HD13	24:P:25:TYR:HB3	1.97	0.47
16:H:86:LYS:HB3	16:H:86:LYS:HE2	1.55	0.47
16:H:194:ARG:O	16:H:198:LYS:HG3	2.15	0.47
27:S:57:TYR:OH	27:S:87:LYS:HD3	2.15	0.47
28:S1:245:A:O3'	50:SU:33:MET:HE2	2.15	0.47
28:S1:671:G:O2'	28:S1:1279:G:H5'	2.14	0.47
28:S1:1518:C:O2'	28:S1:2007:G:H4'	2.15	0.47
28:S1:1965:G:OP1	47:SR:122:ARG:NH1	2.48	0.47
34:SE:92:THR:HG22	55:SZ:21:LYS:HB2	1.97	0.47
38:SI:57:SER:OG	38:SI:58:LYS:N	2.48	0.47
53:SX:17:ALA:HB3	53:SX:149:PHE:HA	1.96	0.47
69:Y:77:HIS:HB3	74:d:37:ARG:HD3	1.96	0.47
1:1:581:G:H22	1:1:625:C:H5	1.62	0.47
1:1:1062:A:H2'	1:1:1063:G:C8	2.49	0.47
7:7:71:A:H3'	67:W:48:ARG:HG3	1.97	0.47
8:8:97:A:O2'	26:R:122:ASN:OD1	2.33	0.47
20:L:51:GLY:HA2	24:P:181:LYS:C	2.40	0.47
28:S1:294:G:HO2'	28:S1:295:A:P	2.38	0.47
28:S1:1179:U:OP2	30:SA:157:TYR:OH	2.30	0.47
28:S1:1718:A:H1'	28:S1:1719:G:H5'	1.97	0.47
28:S1:1834:G:H22	48:SS:46:GLU:CD	2.22	0.47
28:S1:1921:A:N3	28:S1:1982:G:O2'	2.44	0.47
28:S1:2199:C:O2	57:Sb:96:ARG:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:SD:158:ALA:O	33:SD:161:SER:OG	2.32	0.47
37:SH:153:LYS:NZ	37:SH:161:ASP:OD2	2.47	0.47
41:SL:75:VAL:HG12	41:SL:83:GLN:HG2	1.97	0.47
52:SW:67:LEU:HD21	52:SW:101:VAL:HG22	1.95	0.47
53:SX:147:LEU:HA	53:SX:147:LEU:HD23	1.69	0.47
62:Sg:122:ILE:HB	62:Sg:134:TRP:HB2	1.97	0.47
1:1:663:C:H2'	1:1:664:C:O2	2.15	0.47
1:1:1602:C:H2'	1:1:1603:G:C8	2.49	0.47
1:1:1603:G:H2'	1:1:1604:U:C6	2.49	0.47
4:4:60:A:H2'	4:4:61:A:C8	2.50	0.47
8:8:79:G:C8	26:R:52:LYS:HG2	2.50	0.47
21:M:46:GLU:O	21:M:50:MET:HG3	2.15	0.47
28:S1:595:U:H2'	28:S1:596:U:C6	2.50	0.47
28:S1:1580:G:H3'	28:S1:1581:G:H5'	1.96	0.47
28:S1:2022:A:H2'	28:S1:2023:C:C6	2.50	0.47
31:SB:15:GLU:HG3	31:SB:15:GLU:O	2.15	0.47
34:SE:97:ARG:HB2	34:SE:111:LEU:HD11	1.97	0.47
35:SF:65:GLU:OE1	35:SF:251:PRO:HD3	2.14	0.47
75:e:85:SER:HA	75:e:151:ILE:O	2.15	0.47
77:g:69:TRP:CZ2	77:g:144:ILE:HD11	2.49	0.47
1:1:5:A:O2'	1:1:6:C:H5'	2.15	0.46
1:1:1087:A:H2'	1:1:1088:C:H6	1.80	0.46
1:1:1098:A:N3	2:2:1060:PSU:O2'	2.48	0.46
1:1:1165:A:H2'	1:1:1166:C:C6	2.50	0.46
2:2:1116:A:H2'	2:2:1116:A:N3	2.30	0.46
2:2:1450:G:N2	2:2:1452:U:O4'	2.40	0.46
6:6:46:C:H5'	19:K:121:ALA:HB2	1.97	0.46
22:N:71:GLN:CD	22:N:154:ARG:HB3	2.40	0.46
28:S1:2159:A:H4'	28:S1:2159:A:OP1	2.16	0.46
29:S4:68:C:H2'	29:S4:69:G:O4'	2.15	0.46
31:SB:166:CYS:HB2	31:SB:177:MET:CE	2.41	0.46
52:SW:41:LYS:NZ	52:SW:53:ASN:OD1	2.46	0.46
1:1:618:G:H2'	1:1:619:U:O4'	2.15	0.46
1:1:898:A:H2'	1:1:899:A:C8	2.50	0.46
1:1:1237:A:H4'	1:1:1238:C:OP2	2.14	0.46
1:1:1513:C:H2'	1:1:1514:C:O2	2.15	0.46
1:1:1619:U:O4	2:2:24:C:O2'	2.29	0.46
5:5:122:U:C2'	5:5:123:G:H5'	2.45	0.46
11:C:288:THR:HG22	70:Z:6:ASP:OD2	2.15	0.46
26:R:91:ARG:HD2	26:R:126:LEU:HD22	1.98	0.46
28:S1:259:C:N4	28:S1:969:A:H61	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SA:241:VAL:HG12	44:SO:13:ASN:ND2	2.31	0.46
35:SF:185:PRO:HD2	35:SF:188:THR:HG21	1.96	0.46
40:SK:203:LEU:HD22	40:SK:207:GLU:HG2	1.97	0.46
75:e:131:LEU:HA	75:e:172:ASN:HB2	1.98	0.46
1:1:254:U:C5	1:1:258:A:N7	2.83	0.46
1:1:412:G:H4'	1:1:437:A:N1	2.30	0.46
1:1:508:A:P	11:C:352:ARG:HH22	2.37	0.46
1:1:1095:U:O2'	1:1:1096:C:H5'	2.15	0.46
1:1:1578:G:H5'	25:Q:24:LEU:O	2.15	0.46
1:1:1675:A:H3'	1:1:1676:G:C8	2.51	0.46
2:2:390:A:H1'	2:2:527:A2M:N6	2.29	0.46
2:2:534:OMG:H2'	2:2:535:U:C6	2.51	0.46
2:2:1000:U:H2'	2:2:1001:C:C6	2.50	0.46
2:2:1042:G:H2'	2:2:1043:C:C6	2.49	0.46
2:2:1137:G:O2'	2:2:1138:C:H5'	2.15	0.46
2:2:1441:C:H5	6:6:6:G:N1	1.97	0.46
5:5:30:G:N1	5:5:124:C:H5	1.96	0.46
8:8:13:C:OP1	27:S:28:SER:OG	2.32	0.46
8:8:115:C:H2'	8:8:116:C:C6	2.50	0.46
17:I:189:PHE:O	17:I:193:ASN:ND2	2.37	0.46
20:L:2:PRO:HG2	20:L:5:PHE:CD2	2.50	0.46
28:S1:15:U:H2'	28:S1:16:G:O4'	2.14	0.46
28:S1:811:C:H2'	28:S1:812:A:H8	1.80	0.46
31:SB:116:GLN:HA	31:SB:116:GLN:NE2	2.30	0.46
42:SM:96:LYS:HD3	42:SM:96:LYS:HA	1.58	0.46
1:1:480:U:H2'	1:1:481:U:C6	2.50	0.46
1:1:822:C:H4'	1:1:823:G:H5'	1.97	0.46
2:2:453:A:H1'	28:S1:1160:A:C8	2.50	0.46
2:2:560:OMU:H4'	2:2:561:G:OP2	2.16	0.46
2:2:824:G:C2	2:2:825:U:H2'	2.50	0.46
2:2:1493:C:H2'	2:2:1494:G:O4'	2.16	0.46
4:4:98:A:H2'	4:4:99:A:C8	2.51	0.46
4:4:131:U:H2'	4:4:132:U:O4'	2.15	0.46
7:7:122:A:H2'	7:7:123:G:O4'	2.16	0.46
7:7:134:G:H2'	7:7:135:U:C6	2.50	0.46
28:S1:594:A:H61	28:S1:643:A:H5''	1.80	0.46
35:SF:90:ASP:OD2	35:SF:90:ASP:C	2.58	0.46
45:SP:52:LEU:HD12	45:SP:71:ARG:HG2	1.97	0.46
49:ST:4:MET:HE2	49:ST:5:HIS:ND1	2.29	0.46
52:SW:59:ARG:HG3	52:SW:60:PRO:HD2	1.97	0.46
55:SZ:44:GLN:H	55:SZ:44:GLN:CD	2.12	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SZ:89:LEU:O	55:SZ:93:GLU:HB2	2.15	0.46
1:1:1452:C:H2'	1:1:1453:G:C8	2.50	0.46
1:1:1562:C:C4	1:1:1563:U:C4	3.03	0.46
1:1:1773:C:O2'	7:7:139:A:N3	2.47	0.46
15:G:183:ASP:OD2	15:G:185:ALA:HB3	2.15	0.46
28:S1:982:G:H2'	28:S1:983:C:O4'	2.15	0.46
28:S1:1209:C:H2'	28:S1:1210:C:C6	2.50	0.46
30:SA:88:PHE:HB3	30:SA:100:THR:HB	1.98	0.46
58:Sc:13:VAL:O	58:Sc:17:ARG:HB2	2.15	0.46
59:Sd:60:VAL:HG12	59:Sd:82:ALA:HB3	1.97	0.46
69:Y:50:PRO:HD3	69:Y:68:VAL:HG22	1.98	0.46
69:Y:53:VAL:HA	69:Y:57:MET:CE	2.46	0.46
1:1:426:A:H2'	1:1:427:A:C8	2.50	0.46
1:1:1765:A:H2'	1:1:1766:G:O4'	2.16	0.46
2:2:343:U:H2'	2:2:344:G:H8	1.81	0.46
4:4:148:C:H2'	83:m:111:ARG:NH1	2.30	0.46
11:C:345:ASN:HB3	11:C:348:ASN:HB2	1.97	0.46
28:S1:476:C:H2'	28:S1:477:G:O4'	2.15	0.46
28:S1:1685:C:H1'	32:SC:161:THR:HG21	1.97	0.46
28:S1:1911:U:H5	28:S1:1928:G:H1	1.63	0.46
38:SI:132:MET:CE	38:SI:175:VAL:HG12	2.45	0.46
80:j:39:TYR:CD1	80:j:40:PRO:HA	2.51	0.46
1:1:1403:A:H2'	1:1:1404:U:C6	2.51	0.46
2:2:728:U:C4	2:2:732:A:C6	3.03	0.46
3:3:200:G:C6	85:o:50:LYS:O	2.69	0.46
6:6:50:A:O2'	6:6:54:A:N6	2.49	0.46
7:7:7:OMU:HM23	7:7:7:OMU:H1'	1.71	0.46
11:C:63:ALA:HA	11:C:77:ARG:O	2.16	0.46
28:S1:1177:A:H2'	30:SA:116:LEU:HD22	1.98	0.46
28:S1:1248:A:H2'	28:S1:1249:G:C8	2.51	0.46
28:S1:1693:C:OP1	62:Sg:102:LYS:NZ	2.46	0.46
28:S1:1920:A:H2'	28:S1:1921:A:C8	2.50	0.46
55:SZ:112:LYS:HB2	55:SZ:112:LYS:HE2	1.58	0.46
67:W:54:ILE:HB	67:W:64:GLU:HG2	1.98	0.46
1:1:29:C:H4'	21:M:96:LYS:HG3	1.98	0.46
1:1:109:A:H4'	1:1:110:A:C5'	2.44	0.46
1:1:720:A:C8	1:1:721:U:H2'	2.50	0.46
1:1:1024:U:H6	1:1:1024:U:H5''	1.81	0.46
2:2:760:U:H5'	15:G:69:ARG:HG3	1.97	0.46
2:2:1320:U:H2'	2:2:1321:U:C6	2.50	0.46
13:E:66:ILE:O	13:E:69:LEU:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:1154:A:H2'	28:S1:1155:U:H6	1.81	0.46
28:S1:1683:A:H2	32:SC:204:PRO:HG2	1.81	0.46
31:SB:200:GLU:HA	31:SB:200:GLU:OE1	2.14	0.46
40:SK:79:LEU:HD12	40:SK:183:ARG:HG2	1.98	0.46
43:SN:64:GLU:HG3	43:SN:73:TRP:CD1	2.50	0.46
45:SP:85:VAL:HA	45:SP:86:PRO:HD3	1.76	0.46
1:1:52:C:HO2'	1:1:1653:U:HO2'	1.62	0.46
1:1:83:A:OP2	20:L:65:LYS:NZ	2.48	0.46
1:1:458:A:H2'	1:1:459:A:O4'	2.16	0.46
1:1:493:A:H5'	14:F:82:ARG:HG3	1.98	0.46
1:1:1169:A:OP2	91:1:1914:HOH:O	2.21	0.46
1:1:1214:G:H2'	1:1:1215:C:O4'	2.15	0.46
2:2:715:G:O2'	2:2:716:C:O4'	2.31	0.46
2:2:784:U:C2	15:G:85:ARG:HG3	2.51	0.46
6:6:60:A:C4	14:F:69:MET:HE1	2.50	0.46
8:8:7:G:H2'	8:8:8:U:C6	2.51	0.46
10:B:80:GLU:OE1	10:B:321:TYR:OH	2.28	0.46
28:S1:257:A:H8	28:S1:965:G:N2	2.02	0.46
28:S1:1718:A:O2'	28:S1:1719:G:H8	1.99	0.46
28:S1:2011:C:H2'	28:S1:2012:A:H8	1.80	0.46
35:SF:242:TRP:CE2	39:SJ:68:ARG:HG2	2.51	0.46
62:Sg:42:LYS:NZ	62:Sg:56:LEU:HB2	2.31	0.46
81:k:7:THR:HG22	81:k:9:LYS:H	1.81	0.46
86:p:68:ILE:HB	86:p:85:LEU:HB2	1.98	0.46
1:1:191:U:H5	1:1:258:A:N1	2.14	0.46
1:1:523:A:H2'	1:1:524:U:C6	2.50	0.46
2:2:348:A:H8	2:2:348:A:OP2	1.99	0.46
4:4:21:C:H2'	4:4:22:G:H8	1.80	0.46
15:G:163:LEU:HA	21:M:7:LEU:HD11	1.98	0.46
22:N:38:ARG:HG3	22:N:41:ALA:HB2	1.98	0.46
26:R:44:TRP:CH2	26:R:58:GLY:HA3	2.51	0.46
28:S1:109:C:H5	28:S1:347:A:H2	1.65	0.46
28:S1:954:A:H5'	28:S1:955:A:OP2	2.15	0.46
28:S1:1110:G:H1'	58:Sc:23:ARG:NH1	2.31	0.46
28:S1:1404:U:O2'	30:SA:150:ASN:OD1	2.20	0.46
36:SG:94:GLU:OE2	36:SG:96:ARG:NH1	2.48	0.46
39:SJ:18:GLU:OE2	39:SJ:65:LEU:HB3	2.16	0.46
40:SK:37:ARG:HB2	40:SK:59:ARG:NH1	2.31	0.46
47:SR:21:VAL:HG13	47:SR:30:ALA:HB1	1.97	0.46
50:SU:39:LYS:HG2	50:SU:40:HIS:CE1	2.51	0.46
62:Sg:240:GLN:HG3	62:Sg:241:ILE:N	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3:A:C6	7:7:169:A:H1'	2.51	0.45
1:1:126:G:H2'	1:1:127:G:H8	1.80	0.45
1:1:1128:A:C6	72:b:46:ARG:HD3	2.51	0.45
1:1:1571:C:H5	64:T:85:ARG:NH2	2.05	0.45
2:2:978:C:O2	3:3:25:G:N2	2.49	0.45
16:H:85:THR:O	16:H:86:LYS:HG2	2.16	0.45
19:K:146:LYS:HB2	19:K:146:LYS:HE3	1.77	0.45
28:S1:256:A:OP2	28:S1:965:G:H1'	2.16	0.45
28:S1:1879:OMG:HM23	28:S1:1879:OMG:H1'	1.59	0.45
28:S1:1907:A:H2'	28:S1:1908:A:C8	2.50	0.45
31:SB:81:SER:OG	31:SB:128:THR:OG1	2.08	0.45
1:1:51:G:H4'	1:1:863:G:H4'	1.97	0.45
2:2:35:G:H1'	80:j:9:GLY:HA3	1.98	0.45
2:2:519:G:N2	2:2:557:G:H2'	2.30	0.45
3:3:198:A:H5'	85:o:52:VAL:HB	1.97	0.45
3:3:203:A:H2'	3:3:204:A:C8	2.51	0.45
20:L:110:LEU:HD23	20:L:110:LEU:HA	1.63	0.45
28:S1:29:OMU:HM23	28:S1:29:OMU:H1'	1.69	0.45
28:S1:262:U:H3	28:S1:966:G:H1	1.64	0.45
28:S1:1202:A:OP1	49:ST:2:VAL:HG12	2.15	0.45
28:S1:1207:U:H1'	49:ST:52:MET:HG3	1.98	0.45
28:S1:1510:C:H2'	28:S1:1510:C:O2	2.16	0.45
55:SZ:55:LYS:HB2	55:SZ:55:LYS:HE2	1.72	0.45
62:Sg:102:LYS:HD2	62:Sg:104:LEU:HD21	1.98	0.45
64:T:67:ILE:HD11	64:T:80:LYS:HB3	1.97	0.45
66:V:71:THR:HG21	71:a:38:THR:HG22	1.98	0.45
1:1:148:U:O2'	1:1:149:G:C8	2.66	0.45
1:1:185:C:O2'	67:W:118:ARG:HD2	2.17	0.45
1:1:550:A:O3'	1:1:551:A:H8	1.99	0.45
1:1:1561:A:N6	64:T:46:GLN:OE1	2.50	0.45
2:2:501:A:N1	28:S1:2064:C:O2'	2.45	0.45
2:2:506:U:O2'	2:2:507:G:H8	1.98	0.45
2:2:619:A:N3	2:2:1262:G:O2'	2.38	0.45
2:2:1218:A:H2'	2:2:1219:A:H8	1.81	0.45
7:7:75:OMG:HM23	7:7:75:OMG:H1'	1.71	0.45
10:B:295:ALA:O	75:e:54:HIS:NE2	2.49	0.45
15:G:134:VAL:HB	15:G:200:ALA:HB3	1.99	0.45
28:S1:12:PSU:H2'	28:S1:13:U:C6	2.51	0.45
28:S1:492:U:OP1	34:SE:78:LYS:NZ	2.45	0.45
28:S1:772:A:O2'	28:S1:773:A:O5'	2.34	0.45
28:S1:962:A:H2'	28:S1:963:U:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:1875:G:H2'	28:S1:1876:U:H6	1.81	0.45
28:S1:2140:OMC:HM23	28:S1:2140:OMC:H1'	1.82	0.45
34:SE:33:HIS:NE2	34:SE:140:ASP:OD1	2.50	0.45
44:SO:71:ALA:HB3	44:SO:111:ALA:HB3	1.98	0.45
70:Z:49:LYS:O	70:Z:100:ARG:HD3	2.17	0.45
74:d:27:LEU:HD11	74:d:85:LYS:HE3	1.98	0.45
1:1:7:C:H5''	15:G:184:MET:HE3	1.99	0.45
1:1:191:U:OP1	1:1:192:C:H5''	2.17	0.45
1:1:1605:G:O2'	1:1:1606:C:H5'	2.16	0.45
2:2:342:U:HO2'	2:2:343:U:H6	1.61	0.45
2:2:625:U:H2'	2:2:626:PSU:C6	2.52	0.45
2:2:1335:C:C2	2:2:1337:C:H5'	2.52	0.45
11:C:111:HIS:HB3	21:M:203:LYS:HD3	1.98	0.45
19:K:138:SER:O	19:K:142:VAL:HG13	2.16	0.45
19:K:141:LYS:HD3	19:K:141:LYS:HA	1.74	0.45
28:S1:297:U:C4	50:SU:28:ALA:HB2	2.51	0.45
28:S1:1551:G:O6	42:SM:62:THR:HG22	2.16	0.45
28:S1:1782:G:H2'	28:S1:1783:C:C6	2.52	0.45
37:SH:132:ARG:NH1	59:Sd:74:SER:OG	2.49	0.45
38:SI:40:GLU:HG3	38:SI:77:VAL:HG11	1.97	0.45
63:Sh:67:VAL:HG13	63:Sh:70:ALA:H	1.80	0.45
83:m:78:MET:HE2	83:m:78:MET:HA	1.99	0.45
1:1:546:G:O2'	1:1:1393:A:H1'	2.16	0.45
1:1:699:C:H2'	1:1:700:A:H8	1.80	0.45
2:2:79:C:O2'	4:4:81:G:H4'	2.16	0.45
2:2:590:U:H2'	2:2:591:A2M:C8	2.46	0.45
2:2:1200:A:C2'	2:2:1201:G:H5'	2.46	0.45
2:2:1512:G:OP1	5:5:113:G:N2	2.44	0.45
5:5:32:A:H2'	5:5:33:U:C6	2.51	0.45
17:I:131:PHE:CE2	17:I:148:VAL:HG13	2.52	0.45
28:S1:639:C:H5''	60:Se:57:MET:CE	2.45	0.45
33:SD:46:MET:HE3	33:SD:46:MET:HB2	1.86	0.45
35:SF:79:VAL:HG12	35:SF:88:LEU:HD11	1.99	0.45
52:SW:79:LYS:CE	52:SW:113:GLU:OE1	2.53	0.45
57:Sb:81:CYS:O	57:Sb:85:SER:OG	2.34	0.45
64:T:23:ARG:NH2	64:T:125:MET:HE1	2.31	0.45
73:c:126:PHE:CZ	73:c:157:MET:CE	3.00	0.45
1:1:235:A2M:O5'	1:1:235:A2M:H8	2.16	0.45
1:1:1012:C:OP2	91:1:1915:HOH:O	2.21	0.45
3:3:10:U:O2'	69:Y:79:HIS:ND1	2.42	0.45
6:6:72:C:OP1	6:6:72:C:H3'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:210:ASN:O	22:N:210:ASN:OD1	2.35	0.45
28:S1:262:U:H2'	28:S1:263:G:H8	1.80	0.45
28:S1:643:A:OP1	33:SD:36:ARG:NH1	2.49	0.45
28:S1:1906:G:HO2'	28:S1:1907:A:H8	1.61	0.45
28:S1:2175:C:H4'	84:n:4:VAL:HG11	1.98	0.45
29:S4:1:G:C2'	29:S4:2:C:H5'	2.47	0.45
35:SF:55:VAL:HG21	35:SF:78:ILE:HG23	1.98	0.45
35:SF:137:ILE:O	35:SF:141:MET:HG3	2.17	0.45
38:SI:4:HIS:H	38:SI:4:HIS:CD2	2.35	0.45
62:Sg:216:GLY:HA2	62:Sg:236:SER:O	2.17	0.45
63:Sh:215:ARG:O	63:Sh:215:ARG:NH1	2.43	0.45
85:o:8:MET:HE3	85:o:12:GLY:HA2	1.98	0.45
2:2:4:C:H4'	2:2:5:A:OP1	2.16	0.45
2:2:511:C:H2'	2:2:512:PSU:O4'	2.15	0.45
2:2:1294:G:H5''	2:2:1294:G:H8	1.81	0.45
6:6:49:C:N4	77:g:29:LYS:O	2.50	0.45
9:A:116:VAL:HB	9:A:126:LEU:HB2	1.99	0.45
11:C:182:VAL:HG11	11:C:224:GLY:HA2	1.99	0.45
38:SI:6:ARG:HH22	38:SI:28:PHE:HE1	1.65	0.45
49:ST:2:VAL:HG23	49:ST:3:ARG:N	2.22	0.45
53:SX:40:LYS:HB2	53:SX:40:LYS:HE2	1.55	0.45
75:e:29:SER:HG	75:e:33:ARG:NH2	2.13	0.45
1:1:200:A:P	70:Z:139:ARG:NH1	2.88	0.45
1:1:252:G:OP1	11:C:199:ARG:HD2	2.17	0.45
1:1:496:C:H2'	1:1:497:A:H8	1.82	0.45
1:1:659:G:H2'	1:1:660:U:C6	2.52	0.45
2:2:451:U:OP1	2:2:452:G:N2	2.50	0.45
2:2:604:A2M:H2'	2:2:605:C:O4'	2.17	0.45
5:5:4:A:H2'	5:5:5:C:O2	2.17	0.45
11:C:139:ARG:HD3	11:C:245:GLY:C	2.42	0.45
13:E:93:CYS:HB3	13:E:100:ILE:HD12	1.98	0.45
23:O:262:LYS:HB2	23:O:262:LYS:HE3	1.77	0.45
28:S1:1646:G:O2'	28:S1:1673:A:N1	2.48	0.45
28:S1:2103:G:H2'	28:S1:2104:G:C8	2.51	0.45
31:SB:27:HIS:O	31:SB:51:ILE:HA	2.16	0.45
35:SF:198:LYS:HA	35:SF:198:LYS:HD3	1.67	0.45
59:Sd:61:ARG:HA	59:Sd:61:ARG:HD2	1.86	0.45
69:Y:4:PHE:HE2	74:d:36:LEU:O	1.99	0.45
70:Z:56:ALA:HB3	70:Z:60:ALA:HB3	1.99	0.45
1:1:1357:G:H2'	1:1:1358:C:C6	2.51	0.45
1:1:1489:U:O2'	1:1:1490:G:H8	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1539:A2M:H2'	1:1:1540:OMG:O4'	2.17	0.45
2:2:3:C:O2'	2:2:4:C:H5'	2.17	0.45
2:2:570:A2M:HM'2	2:2:570:A2M:H1'	1.69	0.45
6:6:52:G:H5''	19:K:122:HIS:NE2	2.32	0.45
7:7:22:U:OP1	67:W:13:ARG:NH2	2.43	0.45
8:8:67:C:H1'	23:O:292:ALA:HB1	1.99	0.45
21:M:85:LYS:HE3	21:M:85:LYS:HB3	1.78	0.45
22:N:150:GLU:OE2	22:N:153:ARG:NH1	2.50	0.45
24:P:126:GLU:OE2	24:P:128:LEU:HD21	2.16	0.45
28:S1:1108:A:H5''	49:ST:16:LEU:HD12	1.97	0.45
28:S1:1522:G:C2	28:S1:1523:A:C8	3.05	0.45
28:S1:1587:C:C2	28:S1:1588:A:C8	3.05	0.45
46:SQ:97:LEU:C	46:SQ:97:LEU:HD13	2.41	0.45
79:i:40:LEU:O	79:i:44:LYS:HG3	2.17	0.45
1:1:493:A:C3'	1:1:494:A:H5''	2.47	0.45
1:1:951:G:H1'	1:1:1739:A:N6	2.32	0.45
2:2:750:U:H1'	2:2:751:U:H5'	1.99	0.45
2:2:760:U:OP2	2:2:1012:U:H5	1.98	0.45
2:2:1151:U:OP1	27:S:87:LYS:HE2	2.17	0.45
27:S:133:ARG:HB3	73:c:90:LYS:HB2	1.98	0.45
28:S1:529:U:H2'	28:S1:530:U:C6	2.52	0.45
28:S1:949:U:H2'	28:S1:950:U:C6	2.52	0.45
28:S1:1145:A:N3	28:S1:1146:G:H1'	2.32	0.45
28:S1:1251:A:H62	28:S1:2183:G:H8	1.65	0.45
28:S1:1910:C:H2'	28:S1:1911:U:O4'	2.17	0.45
28:S1:2015:U:H5'	28:S1:2016:C:OP2	2.17	0.45
29:S4:14:A:C2	29:S4:15:G:H1'	2.52	0.45
33:SD:76:MET:HE3	33:SD:92:LEU:HD12	1.99	0.45
63:Sh:121:VAL:HG22	63:Sh:122:PRO:HD2	1.98	0.45
1:1:503:A:H2'	1:1:504:C:C6	2.52	0.44
1:1:947:A:H2'	91:1:2260:HOH:O	2.16	0.44
1:1:1571:C:H2'	1:1:1572:A:O4'	2.16	0.44
91:1:2173:HOH:O	21:M:105:ARG:HG3	2.16	0.44
2:2:1211:U:H2'	2:2:1212:A:H8	1.82	0.44
2:2:1386:C:OP1	10:B:249:ARG:NH2	2.49	0.44
2:2:1503:G:H5'	2:2:1504:U:OP2	2.16	0.44
3:3:65:U:H5''	25:Q:61:ALA:HB2	1.99	0.44
13:E:46:ARG:CZ	19:K:2:VAL:HG21	2.47	0.44
20:L:51:GLY:C	24:P:179:GLU:HA	2.41	0.44
26:R:97:ARG:HG2	26:R:141:ILE:HG23	1.99	0.44
28:S1:1459:G:O2'	28:S1:1460:G:H5'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:2005:U:H4'	41:SL:141:ARG:HD2	1.99	0.44
28:S1:2162:C:H2'	28:S1:2163:G:O4'	2.17	0.44
31:SB:14:LYS:C	31:SB:16:SER:H	2.25	0.44
31:SB:19:GLN:CD	31:SB:19:GLN:H	2.25	0.44
36:SG:164:ARG:NH2	36:SG:174:LEU:HD11	2.32	0.44
39:SJ:111:MET:SD	39:SJ:115:GLU:HG2	2.56	0.44
46:SQ:94:ARG:NH1	46:SQ:117:LYS:HB3	2.33	0.44
51:SV:35:ILE:HD12	51:SV:51:ALA:HA	1.99	0.44
74:d:88:ARG:NH2	85:o:44:LYS:HE2	2.31	0.44
75:e:42:LEU:HA	75:e:45:MET:HE2	1.98	0.44
79:i:8:THR:HG23	79:i:15:ASN:HB2	1.99	0.44
1:1:80:C:H2'	1:1:81:U:O4'	2.18	0.44
1:1:207:C:N3	70:Z:80:LYS:NZ	2.57	0.44
1:1:755:A:H2'	1:1:756:U:C6	2.53	0.44
2:2:659:A:H2'	2:2:660:G:H8	1.80	0.44
2:2:718:C:H2'	2:2:719:A:O4'	2.17	0.44
2:2:978:C:OP1	15:G:33:LYS:NZ	2.51	0.44
2:2:1038:U:H2'	2:2:1039:U:H6	1.80	0.44
2:2:1398:C:H2'	2:2:1399:G:H8	1.82	0.44
7:7:7:OMU:H2'	7:7:8:C:C6	2.52	0.44
8:8:92:U:H2'	8:8:93:G:O4'	2.16	0.44
16:H:63:GLY:O	16:H:155:THR:HG22	2.17	0.44
28:S1:1171:A:H2'	28:S1:1172:G:C8	2.52	0.44
28:S1:1624:U:H5	28:S1:1839:G:O6	2.00	0.44
51:SV:26:PHE:HZ	51:SV:62:ALA:HB2	1.82	0.44
55:SZ:89:LEU:HD21	55:SZ:101:MET:HE1	1.98	0.44
67:W:20:PRO:O	67:W:24:ARG:HG3	2.17	0.44
1:1:480:U:H2'	1:1:481:U:H6	1.83	0.44
1:1:590:C:O2'	1:1:591:U:O5'	2.31	0.44
1:1:717:G:OP1	17:I:40:ARG:HD2	2.16	0.44
1:1:743:A:H4'	1:1:744:C:H5'	1.99	0.44
1:1:812:A:H2'	1:1:813:C:C6	2.52	0.44
1:1:885:U:H2'	1:1:886:G:O4'	2.17	0.44
1:1:1468:U:H2'	1:1:1469:G:H8	1.82	0.44
2:2:729:G:H2'	2:2:731:A:OP2	2.17	0.44
2:2:743:C:H2'	2:2:744:G:C8	2.51	0.44
2:2:1046:OMG:H1'	2:2:1046:OMG:HM23	1.58	0.44
10:B:46:PHE:CZ	10:B:84:MET:HG3	2.53	0.44
28:S1:1647:OMG:HM22	28:S1:1648:A:H5'	1.99	0.44
31:SB:74:PRO:O	31:SB:99:THR:HA	2.18	0.44
50:SU:7:TYR:CE1	50:SU:36:PRO:HB3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SY:55:THR:HG23	54:SY:80:ARG:HH21	1.82	0.44
55:SZ:14:THR:HG23	55:SZ:28:PHE:HB2	1.99	0.44
57:Sb:44:ARG:HH11	57:Sb:44:ARG:HG3	1.81	0.44
58:Sc:34:MET:HE3	58:Sc:74:LEU:HD21	1.98	0.44
1:1:328:U:H2'	1:1:329:G:C8	2.52	0.44
1:1:620:U:H1'	1:1:621:U:C4	2.53	0.44
1:1:637:C:H2'	1:1:638:C:H6	1.83	0.44
2:2:1287:C:H1'	2:2:1288:G:H5'	1.99	0.44
28:S1:72:C:H2'	28:S1:73:A:O4'	2.16	0.44
28:S1:146:U:H4'	36:SG:183:ILE:HG13	2.00	0.44
28:S1:479:A2M:O5'	28:S1:479:A2M:H8	2.18	0.44
28:S1:1180:A:H3'	28:S1:1181:C:H5''	2.00	0.44
28:S1:2145:A:O5'	45:SP:37:LYS:NZ	2.47	0.44
52:SW:105:ASN:HB2	52:SW:129:SER:HA	2.00	0.44
70:Z:80:LYS:HB3	70:Z:83:HIS:CD2	2.52	0.44
77:g:69:TRP:HZ2	77:g:144:ILE:HD11	1.82	0.44
77:g:76:CYS:SG	77:g:102:ALA:HB1	2.58	0.44
1:1:262:C:H5'	67:W:31:PRO:HD3	2.00	0.44
1:1:351:U:H2'	1:1:352:G:H8	1.82	0.44
1:1:514:C:H5	1:1:537:G:N1	2.05	0.44
1:1:827:G:H2'	1:1:828:U:O4'	2.17	0.44
1:1:1676:G:H8	1:1:1676:G:OP2	2.00	0.44
2:2:343:U:H2'	2:2:344:G:C8	2.53	0.44
2:2:686:G:O2'	30:SA:53:GLY:HA2	2.17	0.44
2:2:1007:U:H2'	2:2:1008:C:C6	2.53	0.44
8:8:100:C:OP1	26:R:41:SER:OG	2.24	0.44
9:A:129:ALA:HB3	9:A:132:ASP:OD2	2.18	0.44
11:C:116:LEU:O	11:C:119:LYS:HG2	2.18	0.44
21:M:168:GLY:HA2	21:M:171:HIS:CD2	2.53	0.44
28:S1:30:G:H2'	28:S1:31:C:H6	1.83	0.44
28:S1:133:G:H2'	28:S1:134:G:H8	1.82	0.44
28:S1:1227:G:H4'	28:S1:2179:A:H4'	2.00	0.44
28:S1:1559:U:H4'	28:S1:1560:A:O4'	2.17	0.44
28:S1:2011:C:H2'	28:S1:2012:A:C8	2.53	0.44
50:SU:13:VAL:HG23	50:SU:18:GLN:HG3	1.99	0.44
69:Y:52:LYS:N	69:Y:65:ARG:HH21	2.15	0.44
85:o:11:MET:HE3	85:o:27:LYS:HA	2.00	0.44
1:1:199:A:N3	70:Z:141:SER:OG	2.51	0.44
1:1:595:C:C2	1:1:596:A:C8	3.06	0.44
1:1:737:U:H2'	1:1:738:C:C6	2.52	0.44
2:2:708:G:C6	2:2:740:A:C8	3.05	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:714:A:C2	2:2:734:A:C5	3.06	0.44
2:2:801:C:H2'	2:2:802:U:C6	2.53	0.44
4:4:64:C:O2'	4:4:65:C:H5'	2.18	0.44
23:O:80:ALA:O	23:O:92:LEU:HD22	2.18	0.44
27:S:130:LYS:HA	27:S:130:LYS:HD3	1.78	0.44
28:S1:58:C:OP1	28:S1:504:G:O2'	2.36	0.44
28:S1:340:G:O2'	28:S1:341:A:C8	2.70	0.44
28:S1:551:A:H2'	28:S1:552:U:O4'	2.17	0.44
28:S1:688:G:OP2	38:SI:122:THR:HG23	2.18	0.44
28:S1:991:G:N2	38:SI:43:ARG:HH21	2.00	0.44
28:S1:1560:A:H5'	28:S1:1561:C:OP2	2.18	0.44
28:S1:1645:U:H3	28:S1:1674:A:N6	2.08	0.44
31:SB:184:GLU:HA	31:SB:184:GLU:OE2	2.17	0.44
44:SO:75:VAL:O	44:SO:79:LYS:HG2	2.17	0.44
46:SQ:103:LEU:HB3	46:SQ:116:LEU:HB2	1.99	0.44
73:c:90:LYS:HD3	73:c:90:LYS:HA	1.76	0.44
75:e:48:GLU:O	75:e:51:LYS:HG2	2.17	0.44
79:i:87:LYS:HB2	79:i:87:LYS:HE3	1.57	0.44
1:1:1177:U:H2'	1:1:1178:U:C6	2.53	0.44
2:2:382:A2M:HM'3	2:2:382:A2M:H1'	1.82	0.44
2:2:447:G:H1'	9:A:222:PRO:HG2	2.00	0.44
4:4:175:G:H21	10:B:101:THR:HG21	1.83	0.44
5:5:51:A:H1'	5:5:52:U:C5'	2.48	0.44
8:8:94:A:C5	8:8:95:U:H1'	2.52	0.44
9:A:67:TYR:O	9:A:68:LYS:HD3	2.17	0.44
18:J:103:VAL:HG21	18:J:131:ILE:HG12	2.00	0.44
28:S1:123:A:N1	28:S1:336:U:C5	2.85	0.44
28:S1:1709:A:O2'	53:SX:145:ASP:OD1	2.30	0.44
42:SM:94:GLN:O	42:SM:98:ILE:HG13	2.16	0.44
52:SW:102:ALA:HB1	52:SW:109:PHE:HB3	2.00	0.44
59:Sd:25:LEU:HB2	59:Sd:47:MET:SD	2.58	0.44
63:Sh:83:VAL:HG13	63:Sh:93:VAL:HG22	1.99	0.44
65:U:29:ASP:HA	65:U:76:VAL:HG12	1.99	0.44
85:o:11:MET:CG	85:o:27:LYS:HB2	2.47	0.44
1:1:707:C:H5'	11:C:117:HIS:CE1	2.53	0.44
1:1:758:C:H2'	1:1:759:A:O4'	2.17	0.44
1:1:1061:G:N2	22:N:193:ARG:HE	2.16	0.44
2:2:110:C:N4	91:2:4324:HOH:O	2.39	0.44
2:2:641:OMG:H4'	10:B:263:ALA:HB1	1.98	0.44
2:2:1003:G:O2'	2:2:1004:G:H8	2.00	0.44
4:4:117:C:H2'	4:4:118:C:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:332:TYR:OH	73:c:59:ARG:HG3	2.17	0.44
15:G:92:LEU:HD13	15:G:190:ALA:HB2	2.00	0.44
28:S1:294:G:O2'	28:S1:295:A:OP1	2.30	0.44
28:S1:336:U:H2'	28:S1:337:U:O2	2.18	0.44
28:S1:435:G:OP1	40:SK:24:ARG:NH1	2.48	0.44
28:S1:1889:G:H3'	28:S1:1932:A:N6	2.33	0.44
28:S1:1975:A:C6	28:S1:1979:OMU:H1'	2.53	0.44
30:SA:226:ASP:HB3	30:SA:229:ALA:HB3	1.98	0.44
31:SB:2:SER:OG	54:SY:84:ARG:HD3	2.17	0.44
40:SK:167:ARG:HD2	40:SK:167:ARG:HA	1.85	0.44
46:SQ:47:LEU:HD13	46:SQ:73:TYR:CE1	2.53	0.44
46:SQ:64:LEU:HD11	46:SQ:74:LYS:HA	2.00	0.44
52:SW:67:LEU:HD22	52:SW:99:SER:HB2	2.00	0.44
62:Sg:13:TRP:HB3	62:Sg:283:ILE:HD11	2.00	0.44
69:Y:83:THR:HG23	69:Y:85:TYR:H	1.83	0.44
82:l:14:ALA:HA	82:l:17:MET:HE3	1.99	0.44
1:1:954:U:H2'	1:1:955:A2M:H8	2.00	0.44
2:2:771:G:N7	9:A:67:TYR:OH	2.33	0.44
2:2:1502:G:P	75:e:33:ARG:HH21	2.40	0.44
7:7:75:OMG:OP2	82:l:31:THR:OG1	2.32	0.44
10:B:5:LYS:HG3	10:B:6:PHE:N	2.33	0.44
13:E:56:VAL:HG22	13:E:69:LEU:HD23	2.00	0.44
13:E:123:GLN:HE22	13:E:159:VAL:HG23	1.83	0.44
13:E:175:LEU:HD22	83:m:86:ALA:HB1	1.99	0.44
22:N:75:TYR:HD2	22:N:151:ALA:HB2	1.83	0.44
22:N:139:ARG:HD3	22:N:173:PHE:CG	2.53	0.44
23:O:82:GLU:HA	23:O:264:LEU:HD21	2.00	0.44
23:O:230:VAL:O	23:O:233:SER:OG	2.35	0.44
24:P:141:LYS:HE3	24:P:141:LYS:HB3	1.61	0.44
28:S1:17:C:O2'	28:S1:1489:A:N1	2.47	0.44
28:S1:825:C:H1'	28:S1:826:A:H8	1.83	0.44
28:S1:1402:A:O2'	30:SA:206:ILE:O	2.33	0.44
28:S1:2164:U:O4'	28:S1:2185:MA6:H2	2.17	0.44
30:SA:67:GLU:OE2	30:SA:85:LYS:HD2	2.18	0.44
30:SA:118:LYS:O	30:SA:120:CYS:N	2.44	0.44
33:SD:31:GLY:HA3	60:Se:40:TYR:CD1	2.53	0.44
43:SN:94:MET:HB3	43:SN:99:LYS:HG3	1.99	0.44
47:SR:87:ARG:NH2	47:SR:111:ASP:OD2	2.50	0.44
61:Sf:94:LYS:HE2	61:Sf:94:LYS:HB2	1.72	0.44
82:l:34:ARG:HG2	82:l:34:ARG:HH11	1.83	0.44
1:1:1095:U:C2'	1:1:1096:C:H5'	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1260:G:C4'	1:1:1261:U:H5'	2.45	0.43
2:2:1364:A:O2'	2:2:1365:C:H5'	2.18	0.43
18:J:44:TYR:CE2	18:J:52:PRO:HG3	2.53	0.43
22:N:84:VAL:HG23	22:N:141:LYS:NZ	2.33	0.43
23:O:170:LYS:HB2	23:O:186:PHE:CE1	2.53	0.43
24:P:197:HIS:HB3	27:S:88:ARG:NH1	2.33	0.43
28:S1:168:A:H2'	28:S1:169:A:C8	2.53	0.43
28:S1:827:G:H2'	28:S1:828:G:H8	1.82	0.43
28:S1:1145:A:C5'	44:SO:53:MET:HE3	2.42	0.43
28:S1:1484:A:H2'	28:S1:1485:A:C8	2.53	0.43
28:S1:1906:G:O2'	28:S1:1907:A:H8	2.00	0.43
28:S1:2100:A:H3'	28:S1:2101:C:H6	1.82	0.43
35:SF:185:PRO:O	35:SF:188:THR:HG23	2.18	0.43
36:SG:126:GLY:N	36:SG:129:ASP:OD1	2.49	0.43
38:SI:108:ASP:OD1	38:SI:111:LYS:HG3	2.18	0.43
40:SK:107:ALA:HA	40:SK:110:LYS:HE2	2.00	0.43
46:SQ:67:ASP:OD2	46:SQ:67:ASP:N	2.47	0.43
56:Sa:91:LEU:HD11	56:Sa:94:CYS:HB2	2.00	0.43
62:Sg:81:LEU:HD21	62:Sg:122:ILE:HG23	1.99	0.43
65:U:100:LYS:HE3	65:U:100:LYS:HB3	1.64	0.43
72:b:22:LYS:HB3	72:b:22:LYS:HE3	1.78	0.43
1:1:415:A:N3	1:1:417:G:H5''	2.34	0.43
1:1:599:G:OP1	27:S:139:ARG:HD3	2.18	0.43
1:1:1403:A:OP1	24:P:2:GLY:N	2.51	0.43
2:2:464:G:H2'	2:2:465:A:H8	1.83	0.43
2:2:717:G:H1	2:2:720:A:H1'	1.83	0.43
2:2:1108:U:H5'	12:D:52:ALA:HA	2.00	0.43
9:A:62:GLU:OE1	9:A:71:ARG:NH1	2.50	0.43
12:D:98:PHE:HB2	12:D:158:LYS:HE3	1.99	0.43
28:S1:328:C:O2'	28:S1:329:C:OP1	2.32	0.43
28:S1:1405:A:H2'	28:S1:1406:U:C6	2.52	0.43
31:SB:40:TYR:CD2	31:SB:56:MET:HE2	2.54	0.43
32:SC:131:LYS:HA	32:SC:131:LYS:HD2	1.79	0.43
32:SC:131:LYS:HG3	32:SC:155:TYR:HE2	1.83	0.43
33:SD:117:LEU:HB3	33:SD:157:PHE:CE1	2.52	0.43
38:SI:6:ARG:NH2	38:SI:28:PHE:HE1	2.15	0.43
42:SM:26:ALA:HB2	42:SM:82:TYR:CZ	2.54	0.43
52:SW:128:MET:O	52:SW:131:ARG:NH1	2.50	0.43
52:SW:130:TYR:C	52:SW:130:TYR:CD2	2.96	0.43
54:SY:22:CYS:HB2	54:SY:29:ILE:HD11	1.98	0.43
62:Sg:73:LEU:HD22	62:Sg:94:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:Sh:84:GLN:HE22	63:Sh:90:TYR:HE2	1.66	0.43
64:T:137:THR:HG23	64:T:138:PRO:HD2	2.00	0.43
1:1:551:A:C6	73:c:151:LEU:HD23	2.52	0.43
1:1:575:A:C6	11:C:334:LYS:HG2	2.53	0.43
1:1:739:U:O2'	1:1:740:C:H5'	2.18	0.43
1:1:1087:A:H2'	1:1:1088:C:O4'	2.18	0.43
2:2:717:G:N1	2:2:720:A:H1'	2.33	0.43
7:7:70:C:H5''	67:W:115:ILE:HD11	1.99	0.43
7:7:89:U:H2'	7:7:90:U:O4'	2.19	0.43
8:8:27:A:H8	8:8:27:A:O5'	1.99	0.43
11:C:75:ILE:HG13	11:C:76:PRO:HD2	2.00	0.43
17:I:186:VAL:HG21	20:L:141:VAL:O	2.18	0.43
22:N:71:GLN:NE2	22:N:154:ARG:HB3	2.33	0.43
22:N:164:ILE:O	22:N:164:ILE:HG13	2.18	0.43
28:S1:2015:U:H5''	28:S1:2016:C:C5	2.54	0.43
30:SA:141:VAL:HG22	30:SA:214:ILE:HG12	2.00	0.43
31:SB:150:LEU:HD23	31:SB:164:ILE:HB	1.98	0.43
34:SE:148:ASP:O	34:SE:151:THR:OG1	2.31	0.43
34:SE:176:LYS:HD3	34:SE:227:LYS:HA	1.99	0.43
45:SP:101:LEU:HD23	45:SP:124:LYS:HG3	2.00	0.43
54:SY:8:ASN:HB2	54:SY:10:GLU:H	1.83	0.43
78:h:109:LYS:HD3	78:h:109:LYS:HA	1.84	0.43
86:p:2:VAL:N	86:p:90:HIS:O	2.52	0.43
1:1:121:A:H4'	1:1:122:A:O5'	2.19	0.43
1:1:531:C:OP1	26:R:74:ARG:HD3	2.18	0.43
1:1:1510:C:N4	11:C:188:ILE:O	2.43	0.43
3:3:13:OMU:H5'	3:3:13:OMU:H6	1.99	0.43
4:4:129:G:N1	4:4:161:C:H5	1.88	0.43
13:E:63:LYS:HE3	13:E:63:LYS:HB3	1.77	0.43
16:H:91:HIS:HB3	16:H:96:ASP:HB3	1.99	0.43
17:I:65:CYS:HB2	17:I:70:HIS:O	2.19	0.43
28:S1:438:U:H2'	28:S1:439:G:O4'	2.18	0.43
28:S1:1203:U:OP1	28:S1:1410:C:O2'	2.32	0.43
28:S1:2174:G:O2'	84:n:2:GLY:O	2.32	0.43
30:SA:139:LEU:HD13	30:SA:217:VAL:HG22	2.00	0.43
41:SL:56:GLU:HA	41:SL:59:THR:OG1	2.18	0.43
55:SZ:97:ARG:O	55:SZ:101:MET:HG3	2.19	0.43
78:h:12:MET:SD	78:h:19:ASN:ND2	2.92	0.43
82:l:13:TYR:CE2	82:l:51:TYR:HB2	2.53	0.43
83:m:110:CYS:SG	83:m:118:CYS:N	2.92	0.43
1:1:311:A:H2'	1:1:312:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:334:G:O2'	1:1:335:U:H5''	2.17	0.43
1:1:355:A:OP2	91:1:1902:HOH:O	2.21	0.43
1:1:374:G:N1	7:7:28:C:H5	1.94	0.43
1:1:574:G:N3	1:1:574:G:H2'	2.33	0.43
1:1:610:A:H3'	1:1:611:C:H5'	2.00	0.43
1:1:663:C:OP1	16:H:111:LYS:NZ	2.37	0.43
1:1:1121:G:O2'	1:1:1123:G:H5'	2.19	0.43
1:1:1153:A:H5'	27:S:131:SER:N	2.34	0.43
1:1:1255:G:H2'	1:1:1256:A:C8	2.53	0.43
2:2:396:G:O2'	2:2:435:U:OP1	2.18	0.43
2:2:729:G:H8	2:2:729:G:O5'	2.02	0.43
2:2:1359:OMU:O5'	2:2:1359:OMU:H6	2.19	0.43
2:2:1370:U:O2	2:2:1372:A2M:H8	2.17	0.43
2:2:1408:C:H4'	2:2:1409:A:C6	2.53	0.43
2:2:1519:U:C2	2:2:1520:C:C5	3.06	0.43
5:5:46:G:H2'	5:5:47:C:O4'	2.18	0.43
5:5:50:C:H1'	5:5:64:G:C6	2.53	0.43
15:G:166:TRP:CD1	15:G:166:TRP:H	2.36	0.43
18:J:47:ARG:HH11	18:J:47:ARG:HG3	1.82	0.43
28:S1:381:G:H3'	50:SU:148:LYS:HB2	2.00	0.43
28:S1:1178:C:OP2	28:S1:1179:U:O2'	2.33	0.43
30:SA:151:GLN:HE21	30:SA:153:SER:HB2	1.84	0.43
31:SB:137:ILE:CG2	31:SB:159:TYR:HB2	2.48	0.43
44:SO:54:LYS:HE2	44:SO:69:MET:HB3	2.00	0.43
76:f:33:TRP:CZ2	76:f:54:PRO:HD2	2.52	0.43
1:1:215:U:OP1	70:Z:129:LYS:NZ	2.25	0.43
1:1:291:A:H2'	1:1:292:A:H5'	2.00	0.43
2:2:404:A:O4'	2:2:406:G:C8	2.71	0.43
2:2:583:OMC:OP2	91:2:4306:HOH:O	2.21	0.43
2:2:723:G:H2'	2:2:725:A:C4	2.54	0.43
2:2:766:A:H4'	9:A:121:GLY:O	2.19	0.43
7:7:1:A:O2'	7:7:2:A:H8	1.80	0.43
10:B:5:LYS:HE2	10:B:5:LYS:HB2	1.74	0.43
13:E:149:ASP:CB	13:E:152:GLN:HG3	2.49	0.43
28:S1:292:U:H2'	28:S1:293:U:C6	2.53	0.43
28:S1:492:U:H2'	28:S1:493:C:C6	2.53	0.43
52:SW:88:ARG:HB3	52:SW:124:GLY:HA3	2.00	0.43
70:Z:143:ARG:HH21	70:Z:145:LYS:HZ1	1.67	0.43
86:p:70:LEU:HD21	86:p:91:PHE:CZ	2.54	0.43
1:1:1746:C:H5''	3:3:73:A:H4'	2.00	0.43
2:2:44:C:H5	2:2:52:G:N1	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:824:G:OP1	2:2:824:G:H4'	2.18	0.43
7:7:1:A:C4	7:7:2:A:C8	3.06	0.43
7:7:162:A2M:H2'	7:7:163:G:C8	2.53	0.43
11:C:261:ILE:HA	11:C:271:VAL:CG1	2.49	0.43
18:J:59:MET:HE3	18:J:128:TRP:CH2	2.54	0.43
23:O:128:SER:O	23:O:170:LYS:NZ	2.50	0.43
27:S:65:TRP:CE2	27:S:88:ARG:HD3	2.53	0.43
28:S1:293:U:O2'	28:S1:295:A:N7	2.41	0.43
28:S1:1203:U:H2'	28:S1:1204:A:H8	1.83	0.43
28:S1:1478:OMG:O5'	84:n:20:LYS:HE2	2.18	0.43
28:S1:2185:MA6:H8	28:S1:2185:MA6:H5''	2.01	0.43
35:SF:198:LYS:HD2	35:SF:202:PHE:CE1	2.53	0.43
38:SI:191:ASN:HB3	38:SI:196:GLN:HB2	1.99	0.43
44:SO:75:VAL:HG22	44:SO:117:MET:HG3	2.00	0.43
62:Sg:154:SER:OG	62:Sg:197:VAL:O	2.22	0.43
63:Sh:174:TYR:CD2	63:Sh:207:ARG:HD2	2.53	0.43
65:U:88:LYS:HE3	65:U:88:LYS:HB3	1.65	0.43
69:Y:126:MET:O	69:Y:130:GLN:HG2	2.18	0.43
1:1:3:A:H2'	1:1:4:G:O4'	2.19	0.43
1:1:478:C:H2'	1:1:479:A:H8	1.83	0.43
1:1:836:G:OP1	24:P:63:SER:OG	2.19	0.43
2:2:39:C:H2'	2:2:40:C:C6	2.54	0.43
2:2:569:G:O2'	2:2:571:G:OP2	2.24	0.43
2:2:683:G:N1	2:2:756:C:H5	2.08	0.43
2:2:1151:U:C5	2:2:1161:A:N1	2.81	0.43
4:4:154:C:H4'	13:E:155:ARG:HD2	2.00	0.43
5:5:5:C:H2'	5:5:6:G:O4'	2.19	0.43
7:7:128:U:O2	7:7:134:G:N2	2.31	0.43
8:8:39:C:H2'	8:8:40:C:O4'	2.18	0.43
8:8:46:A:OP1	8:8:47:U:H5	2.02	0.43
8:8:95:U:O5'	22:N:57:LEU:HD23	2.19	0.43
12:D:93:LEU:O	12:D:172:ILE:HA	2.19	0.43
25:Q:3:SER:OG	25:Q:5:LYS:HG3	2.19	0.43
28:S1:133:G:H8	28:S1:133:G:OP1	2.02	0.43
28:S1:291:G:N1	28:S1:298:C:H5	2.07	0.43
28:S1:1945:A:OP1	37:SH:77:ARG:NH2	2.51	0.43
28:S1:2063:U:P	84:n:18:ARG:HH12	2.42	0.43
36:SG:140:ARG:HB3	36:SG:143:LYS:HD2	2.00	0.43
47:SR:99:LEU:HD22	47:SR:103:MET:HG3	1.99	0.43
57:Sb:48:ASP:OD2	57:Sb:51:SER:OG	2.29	0.43
69:Y:89:MET:HG2	69:Y:94:ARG:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Y:101:ASP:O	69:Y:105:ARG:HB3	2.19	0.43
80:j:67:LEU:HD12	80:j:67:LEU:HA	1.85	0.43
1:1:99:A:H2'	1:1:100:G:N3	2.34	0.43
1:1:768:C:O2'	1:1:769:U:H5''	2.19	0.43
1:1:911:G:O2'	1:1:946:G:H4'	2.19	0.43
1:1:1120:C:C2'	1:1:1121:G:H5'	2.49	0.43
1:1:1254:C:N4	1:1:1377:U:O4	2.52	0.43
6:6:46:C:O3'	19:K:125:ARG:NH2	2.51	0.43
13:E:155:ARG:O	13:E:159:VAL:HG22	2.19	0.43
28:S1:46:U:O4	28:S1:476:C:H4'	2.19	0.43
28:S1:128:C:H1'	28:S1:129:U:OP2	2.18	0.43
30:SA:66:PHE:O	30:SA:87:ARG:HA	2.19	0.43
31:SB:198:TRP:HD1	31:SB:199:GLU:H	1.67	0.43
32:SC:207:ILE:HD12	51:SV:8:THR:HG22	2.00	0.43
33:SD:96:LEU:HB3	35:SF:186:ARG:O	2.18	0.43
1:1:147:G:H8	1:1:147:G:OP2	2.02	0.43
1:1:219:U:OP2	70:Z:131:ARG:NH2	2.52	0.43
1:1:998:A:H2'	1:1:999:U:C6	2.54	0.43
1:1:1583:C:H2'	1:1:1584:U:C6	2.53	0.43
2:2:455:U:H5'	2:2:455:U:O2	2.19	0.43
2:2:461:C:H2'	2:2:462:G:O4'	2.19	0.43
2:2:516:A:H2'	2:2:517:A:C8	2.53	0.43
2:2:527:A2M:H8	2:2:527:A2M:H2'	1.87	0.43
2:2:729:G:H2'	2:2:730:A:H3'	2.01	0.43
2:2:1382:PSU:H1'	10:B:256:CYS:SG	2.59	0.43
5:5:101:A:H2'	5:5:102:C:O4'	2.19	0.43
10:B:46:PHE:CE1	10:B:84:MET:HG3	2.54	0.43
10:B:165:HIS:HA	10:B:182:HIS:O	2.19	0.43
18:J:106:ASN:OD1	18:J:110:GLU:N	2.51	0.43
19:K:131:LYS:HE2	19:K:131:LYS:HB2	1.88	0.43
19:K:147:MET:HE2	77:g:14:LEU:CD2	2.49	0.43
28:S1:5:U:H2'	28:S1:6:G:H8	1.84	0.43
28:S1:769:A:H3'	28:S1:770:A:H8	1.82	0.43
28:S1:1494:A:H2'	28:S1:1495:A:C8	2.54	0.43
29:S4:39:U:H2'	29:S4:40:C:C6	2.54	0.43
35:SF:191:VAL:O	35:SF:210:THR:HB	2.19	0.43
37:SH:109:GLU:HG3	37:SH:186:ALA:HB3	2.01	0.43
43:SN:36:THR:HG22	43:SN:40:ASN:O	2.19	0.43
50:SU:20:GLU:O	50:SU:21:LYS:HB3	2.19	0.43
53:SX:125:LEU:HD23	53:SX:139:LYS:HG2	2.01	0.43
57:Sb:31:LEU:HD23	57:Sb:31:LEU:HA	1.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:503:A:N6	1:1:554:A:OP1	2.52	0.42
1:1:588:A:C6	1:1:589:G:C5	3.07	0.42
1:1:700:A:H4'	24:P:172:TYR:CE1	2.53	0.42
1:1:1122:U:H5'	1:1:1123:G:H5''	2.01	0.42
5:5:51:A:H2'	5:5:51:A:N3	2.34	0.42
5:5:124:C:O2'	5:5:125:U:H5'	2.19	0.42
7:7:169:A:H2'	7:7:170:A:C8	2.54	0.42
8:8:38:C:H2'	23:O:204:ARG:HH12	1.84	0.42
13:E:37:ASP:OD2	13:E:39:THR:OG1	2.31	0.42
13:E:160:LEU:HA	13:E:163:MET:HE2	2.01	0.42
22:N:152:LEU:O	22:N:156:LYS:HB2	2.19	0.42
28:S1:234:C:C2	28:S1:235:C:C5	3.06	0.42
28:S1:835:C:H2'	28:S1:836:C:H6	1.84	0.42
28:S1:876:G:H1	28:S1:885:C:H5	1.67	0.42
28:S1:989:A:N6	38:SI:119:LYS:HG2	2.34	0.42
28:S1:1979:OMU:HM23	28:S1:2018:U:O2	2.19	0.42
28:S1:2079:U:H2'	28:S1:2080:G:C8	2.54	0.42
30:SA:160:GLN:O	30:SA:164:LYS:HG3	2.19	0.42
37:SH:69:ASN:HD22	37:SH:69:ASN:HA	1.66	0.42
38:SI:59:LYS:HB2	38:SI:59:LYS:HE3	1.83	0.42
59:Sd:27:ILE:HD11	59:Sd:43:ARG:HG2	2.01	0.42
65:U:19:LEU:HD21	65:U:22:GLY:HA2	2.00	0.42
1:1:743:A:C4'	1:1:744:C:H5'	2.49	0.42
1:1:996:A:O2'	1:1:997:C:H5'	2.19	0.42
1:1:1410:U:H2'	1:1:1411:G:C8	2.54	0.42
1:1:1630:U:H5'	2:2:13:A:OP2	2.19	0.42
2:2:1086:G:H4'	2:2:1179:A:O2'	2.19	0.42
2:2:1289:A:C2'	2:2:1290:C:H5'	2.49	0.42
4:4:50:G:H1'	4:4:51:U:H5	1.84	0.42
16:H:149:ARG:HD3	16:H:149:ARG:HA	1.87	0.42
28:S1:294:G:H2'	28:S1:295:A:C8	2.54	0.42
28:S1:668:A2M:HM'3	28:S1:668:A2M:H1'	1.78	0.42
28:S1:1862:C:H2'	28:S1:1863:G:H8	1.84	0.42
28:S1:1976:U:H5''	28:S1:1979:OMU:OP2	2.20	0.42
30:SA:50:LYS:HE3	30:SA:50:LYS:HB3	1.85	0.42
30:SA:183:ILE:O	30:SA:187:VAL:HG23	2.19	0.42
34:SE:87:VAL:HB	34:SE:96:PHE:CE1	2.54	0.42
57:Sb:44:ARG:HG3	57:Sb:44:ARG:NH1	2.35	0.42
68:X:50:PRO:HB3	68:X:56:THR:HG21	2.00	0.42
1:1:126:G:H2'	1:1:127:G:C8	2.54	0.42
1:1:141:U:C1'	1:1:142:G:H5''	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:453:G:H2'	1:1:454:U:C6	2.54	0.42
1:1:589:G:O2'	1:1:590:C:H5'	2.19	0.42
1:1:663:C:O2	77:g:128:ALA:HB3	2.19	0.42
1:1:744:C:H1'	91:1:2045:HOH:O	2.20	0.42
1:1:1264:A:H2'	1:1:1265:A:H8	1.81	0.42
2:2:734:A:H5''	2:2:737:A:H61	1.85	0.42
22:N:62:SER:HA	22:N:65:LEU:HD12	2.00	0.42
28:S1:102:A:H4'	28:S1:103:A:OP2	2.19	0.42
28:S1:276:G:H1'	28:S1:277:U:C5'	2.49	0.42
28:S1:639:C:H2'	28:S1:640:A:C8	2.54	0.42
28:S1:1571:A:H3'	28:S1:1572:C:O2	2.19	0.42
30:SA:171:THR:HG22	30:SA:175:LYS:HD2	2.01	0.42
31:SB:177:MET:HE2	31:SB:177:MET:HB2	1.74	0.42
34:SE:121:MET:HB3	34:SE:138:THR:HB	2.01	0.42
38:SI:165:ILE:O	38:SI:169:LEU:HG	2.19	0.42
43:SN:15:ARG:HB3	43:SN:37:LEU:HD11	2.02	0.42
61:Sf:100:TYR:HB3	61:Sf:115:ARG:HD2	2.01	0.42
65:U:73:ASN:OD1	65:U:73:ASN:N	2.52	0.42
71:a:5:MET:HE3	71:a:25:TYR:OH	2.19	0.42
1:1:429:G:H4'	64:T:18:LYS:O	2.20	0.42
1:1:675:U:O2'	1:1:1210:A:N1	2.50	0.42
1:1:955:A2M:HM'3	1:1:955:A2M:H1'	1.76	0.42
2:2:512:PSU:H2'	2:2:513:C:H6	1.85	0.42
2:2:644:A:OP1	2:2:1311:U:H4'	2.20	0.42
2:2:748:C:HO2'	2:2:749:G:P	2.41	0.42
2:2:1039:U:H2'	2:2:1040:U:C6	2.55	0.42
2:2:1440:G:H4'	2:2:1441:C:O2	2.20	0.42
4:4:128:U:C5	4:4:162:A:N1	2.86	0.42
4:4:148:C:O2'	83:m:111:ARG:NH1	2.53	0.42
7:7:25:C:O2'	11:C:52:ALA:O	2.32	0.42
7:7:157:U:H5'	7:7:158:U:O4'	2.19	0.42
19:K:7:ILE:HD11	19:K:58:PRO:HG3	2.02	0.42
24:P:188:ARG:O	24:P:190:TYR:N	2.52	0.42
25:Q:66:MET:HG3	25:Q:70:LYS:HD2	2.01	0.42
28:S1:585:C:H2'	28:S1:586:G:O4'	2.19	0.42
28:S1:846:U:H2'	28:S1:847:A:C8	2.54	0.42
28:S1:1696:A:N1	28:S1:1779:U:H5	2.17	0.42
35:SF:80:ASP:N	35:SF:80:ASP:OD2	2.52	0.42
37:SH:8:LEU:HD21	37:SH:55:VAL:HG11	2.01	0.42
62:Sg:90:ARG:HD3	62:Sg:92:TRP:CZ2	2.54	0.42
63:Sh:57:VAL:HG12	63:Sh:93:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:V:69:PRO:HA	66:V:87:PHE:HA	2.01	0.42
79:i:61:GLN:NE2	79:i:93:MET:SD	2.91	0.42
82:l:16:LYS:HD3	82:l:16:LYS:HA	1.88	0.42
2:2:665:A:H2'	2:2:666:C:H6	1.82	0.42
2:2:769:A:O2'	15:G:50:PHE:O	2.28	0.42
2:2:1024:U:H2'	2:2:1025:G:H8	1.83	0.42
2:2:1339:G:O2'	4:4:52:A:N1	2.52	0.42
3:3:72:A:H2'	3:3:73:A:H8	1.84	0.42
16:H:159:ASN:HA	16:H:162:LYS:HG2	2.02	0.42
22:N:192:GLN:OE1	22:N:192:GLN:HA	2.20	0.42
27:S:52:MET:HG2	27:S:53:PRO:HD2	2.01	0.42
28:S1:986:C:H2'	28:S1:987:A:O4'	2.19	0.42
28:S1:1108:A:H8	28:S1:1108:A:OP2	2.02	0.42
28:S1:1701:A:H2'	28:S1:1702:A:H8	1.83	0.42
28:S1:2139:U:H2'	28:S1:2140:OMC:C6	2.55	0.42
31:SB:60:LYS:HE3	31:SB:60:LYS:HB3	1.83	0.42
84:n:29:MET:HA	84:n:29:MET:HE3	2.01	0.42
1:1:43:A:OP2	21:M:85:LYS:HE2	2.19	0.42
1:1:328:U:H2'	1:1:329:G:H8	1.85	0.42
1:1:941:C:O2	2:2:570:A2M:H2	2.19	0.42
2:2:728:U:H2'	2:2:729:G:O4'	2.19	0.42
3:3:10:U:H1'	69:Y:76:ASN:HB2	2.02	0.42
5:5:6:G:H2'	5:5:7:U:H6	1.84	0.42
6:6:51:A:H4'	6:6:52:G:O5'	2.18	0.42
9:A:22:LYS:HA	9:A:22:LYS:HD2	1.92	0.42
16:H:189:LYS:O	16:H:190:GLN:HB2	2.20	0.42
19:K:108:PHE:O	19:K:112:GLN:HG3	2.20	0.42
22:N:208:MET:SD	22:N:208:MET:N	2.90	0.42
28:S1:433:G:H2'	28:S1:434:A:O4'	2.20	0.42
28:S1:578:C:H2'	28:S1:579:C:C6	2.55	0.42
28:S1:1839:G:H4'	32:SC:177:ARG:O	2.20	0.42
30:SA:220:VAL:O	30:SA:221:ARG:HD2	2.20	0.42
41:SL:53:LYS:HE2	41:SL:85:TYR:CZ	2.55	0.42
45:SP:32:THR:HG22	45:SP:33:PHE:N	2.34	0.42
1:1:405:A:OP2	91:1:1911:HOH:O	2.20	0.42
1:1:522:G:OP2	1:1:522:G:H8	2.03	0.42
1:1:652:A:O2'	1:1:653:A:H8	2.02	0.42
1:1:1174:G:H2'	1:1:1175:C:C6	2.54	0.42
1:1:1554:G:H1'	1:1:1616:U:O2	2.19	0.42
2:2:524:5MC:H2'	2:2:525:A:H5''	2.02	0.42
2:2:658:G:H2'	2:2:659:A:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:719:A:H5''	2:2:720:A:OP2	2.18	0.42
2:2:1000:U:H2'	2:2:1001:C:H6	1.84	0.42
3:3:6:G:H2'	3:3:7:U:O4'	2.20	0.42
5:5:121:A:H2'	5:5:122:U:O4'	2.19	0.42
6:6:53:U:OP2	19:K:119:SER:OG	2.31	0.42
13:E:87:TYR:CE2	13:E:150:LEU:HB2	2.54	0.42
28:S1:65:A:H2'	28:S1:65:A:N3	2.34	0.42
28:S1:154:C:H2'	28:S1:155:U:O2	2.19	0.42
28:S1:565:U:C4	28:S1:566:A:H1'	2.54	0.42
28:S1:2179:A:H2'	28:S1:2180:G:C8	2.54	0.42
44:SO:118:LYS:HD3	44:SO:118:LYS:HA	1.81	0.42
67:W:41:ASN:O	67:W:121:ARG:HG3	2.19	0.42
69:Y:104:LYS:HA	69:Y:107:ARG:HD2	2.02	0.42
70:Z:7:LEU:O	70:Z:11:LEU:HG	2.19	0.42
1:1:409:U:O2'	1:1:410:U:OP1	2.36	0.42
1:1:719:U:O2'	1:1:720:A:H5''	2.20	0.42
1:1:793:U:H2'	1:1:794:U:H5'	2.00	0.42
2:2:445:G:H2'	2:2:446:U:C6	2.54	0.42
2:2:770:A:C2	15:G:47:LEU:HD21	2.55	0.42
8:8:34:A:OP1	12:D:136:ARG:NH1	2.53	0.42
10:B:349:MET:HE2	10:B:349:MET:HB2	1.95	0.42
11:C:161:GLU:HA	11:C:217:ARG:HD2	2.00	0.42
22:N:190:LEU:HD22	22:N:197:CYS:SG	2.60	0.42
28:S1:98:A2M:OP1	91:S1:2412:HOH:O	2.21	0.42
28:S1:1202:A:P	49:ST:2:VAL:HG12	2.59	0.42
28:S1:1632:C:H2'	28:S1:1633:G:C8	2.55	0.42
46:SQ:62:CYS:HA	46:SQ:122:ALA:HA	2.02	0.42
59:Sd:38:ASN:OD1	59:Sd:38:ASN:N	2.48	0.42
74:d:38:GLN:HG3	74:d:40:ARG:HD3	2.02	0.42
80:j:80:THR:HG22	80:j:81:PRO:HD2	2.02	0.42
1:1:12:U:H2'	1:1:13:G:C8	2.52	0.42
1:1:627:C:H2'	1:1:628:C:H6	1.84	0.42
1:1:727:C:H1'	1:1:728:C:C2	2.55	0.42
1:1:1647:A:H2'	1:1:1648:C:O4'	2.20	0.42
2:2:69:A:O4'	5:5:18:A:H5'	2.19	0.42
2:2:104:U:O2'	2:2:116:A:N7	2.43	0.42
2:2:1083:A:C5	2:2:1085:G:C8	3.06	0.42
2:2:1136:U:H2'	2:2:1137:G:H8	1.82	0.42
2:2:1384:A2M:H1'	2:2:1384:A2M:HM'3	1.80	0.42
17:I:43:LEU:HD12	17:I:43:LEU:HA	1.88	0.42
25:Q:60:ARG:O	25:Q:64:ARG:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:82:TYR:HE1	26:R:92:MET:HE3	1.85	0.42
27:S:39:TYR:CZ	27:S:63:ILE:HD11	2.54	0.42
28:S1:342:C:H1'	34:SE:30:PRO:HG3	2.01	0.42
28:S1:353:C:H2'	28:S1:354:C:O2	2.20	0.42
28:S1:641:A:O2'	28:S1:645:C:OP1	2.37	0.42
28:S1:846:U:H2'	28:S1:847:A:H8	1.83	0.42
28:S1:1614:U:H2'	28:S1:1615:G:C8	2.55	0.42
28:S1:2127:U:H2'	28:S1:2128:U:C6	2.54	0.42
28:S1:2139:U:H2'	28:S1:2140:OMC:H6	1.84	0.42
42:SM:64:LYS:HG2	42:SM:75:ASP:CG	2.45	0.42
44:SO:96:VAL:HG12	44:SO:132:SER:HB2	2.01	0.42
49:ST:56:ASP:HA	58:Sc:48:TYR:HB2	2.01	0.42
49:ST:110:ASP:O	49:ST:114:ARG:HG2	2.19	0.42
74:d:88:ARG:HH21	85:o:44:LYS:HE2	1.85	0.42
1:1:515:U:H2'	1:1:516:G:H8	1.84	0.42
1:1:791:C:OP2	73:c:38:LYS:HD2	2.20	0.42
1:1:881:A:O2'	2:2:49:A:OP1	2.34	0.42
1:1:1165:A:H2'	1:1:1166:C:H6	1.85	0.42
1:1:1550:A:H5'	75:e:127:ILE:O	2.20	0.42
2:2:95:A2M:HM'3	2:2:95:A2M:H1'	1.85	0.42
2:2:708:G:H2'	2:2:709:G:H4'	2.02	0.42
2:2:736:C:C4	2:2:737:A:C5	3.08	0.42
2:2:968:U:H2'	2:2:969:A:C8	2.55	0.42
6:6:34:C:H2'	6:6:35:U:H6	1.85	0.42
10:B:216:GLN:O	10:B:287:ILE:HB	2.19	0.42
11:C:70:ARG:H	11:C:70:ARG:HG2	1.52	0.42
13:E:95:TYR:CD2	13:E:100:ILE:HG13	2.55	0.42
21:M:80:THR:OG1	21:M:87:SER:HA	2.20	0.42
28:S1:1123:G:O2'	91:S1:2411:HOH:O	2.20	0.42
28:S1:1178:C:O2'	30:SA:120:CYS:O	2.33	0.42
50:SU:42:ASN:ND2	50:SU:46:HIS:HB2	2.29	0.42
62:Sg:298:HIS:HB2	62:Sg:300:ASP:OD2	2.20	0.42
69:Y:23:ALA:HA	69:Y:45:GLY:HA2	2.02	0.42
78:h:58:LYS:HE2	78:h:72:GLU:OE1	2.19	0.42
1:1:29:C:H4'	21:M:96:LYS:HE3	2.02	0.41
1:1:561:G:H2'	1:1:562:U:O2	2.20	0.41
1:1:731:U:C2	1:1:732:A:C8	3.08	0.41
1:1:1670:A:H61	66:V:32:ARG:CZ	2.33	0.41
2:2:723:G:HO2'	2:2:724:C:H6	1.66	0.41
3:3:71:U:H3	3:3:150:A:H2	1.61	0.41
3:3:139:C:OP1	78:h:58:LYS:NZ	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:82:U:H2'	4:4:83:U:H5'	2.02	0.41
7:7:169:A:H2'	7:7:170:A:N7	2.35	0.41
8:8:62:A:H2'	8:8:63:C:H6	1.85	0.41
15:G:46:ASP:OD2	66:V:29:SER:OG	2.23	0.41
16:H:27:ILE:HB	16:H:53:VAL:HG12	2.02	0.41
18:J:4:ASP:HA	18:J:128:TRP:CE3	2.55	0.41
28:S1:491:G:O6	28:S1:506:U:H5	2.03	0.41
28:S1:1637:A:H62	28:S1:1822:A:N6	2.18	0.41
28:S1:1804:C:H2'	28:S1:1805:A:C8	2.56	0.41
29:S4:14:A:C5	29:S4:15:G:C8	3.08	0.41
31:SB:114:GLN:HG2	31:SB:115:ILE:N	2.34	0.41
62:Sg:16:SER:HB3	62:Sg:32:THR:OG1	2.20	0.41
79:i:37:HIS:O	79:i:41:ARG:HB2	2.20	0.41
1:1:657:G:N2	1:1:1490:G:OP1	2.47	0.41
1:1:715:G:H2'	1:1:716:A:O4'	2.20	0.41
1:1:1388:U:O4	1:1:1396:G:H1'	2.20	0.41
2:2:725:A:H3'	2:2:725:A:N3	2.34	0.41
2:2:954:A:H5'	2:2:955:C:O4'	2.20	0.41
2:2:1132:A:OP1	2:2:1132:A:C8	2.70	0.41
2:2:1146:A:H5''	2:2:1147:C:OP2	2.20	0.41
2:2:1385:G:OP2	2:2:1385:G:H4'	2.20	0.41
3:3:195:U:H2'	3:3:196:U:C5	2.55	0.41
4:4:56:G:H2'	4:4:57:A:N3	2.35	0.41
4:4:163:A:H2'	4:4:164:U:H6	1.85	0.41
7:7:43:A2M:H5''	7:7:43:A2M:H8	2.02	0.41
8:8:50:G:OP1	23:O:164:ARG:HG3	2.20	0.41
12:D:50:SER:O	12:D:66:LYS:HA	2.20	0.41
15:G:209:GLU:O	15:G:213:LYS:HG3	2.20	0.41
22:N:66:GLU:O	22:N:70:ILE:HG13	2.20	0.41
22:N:189:LYS:O	22:N:199:LEU:HD12	2.21	0.41
28:S1:379:U:H2'	28:S1:380:G:O4'	2.20	0.41
28:S1:634:A:H2'	28:S1:635:G:C8	2.55	0.41
28:S1:1166:C:H2'	28:S1:1167:A:C8	2.56	0.41
28:S1:1511:C:N4	28:S1:1637:A:O5'	2.51	0.41
29:S4:4:C:H2'	29:S4:5:G:C8	2.54	0.41
31:SB:183:ARG:HG3	31:SB:198:TRP:CE3	2.55	0.41
40:SK:74:HIS:NE2	40:SK:108:PRO:HB3	2.34	0.41
70:Z:27:MET:HE3	70:Z:27:MET:HB3	1.89	0.41
75:e:133:THR:O	75:e:137:HIS:HB3	2.20	0.41
1:1:589:G:H3'	1:1:590:C:C6	2.55	0.41
1:1:611:C:C5	11:C:359:ARG:HD3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:622:C:O2'	1:1:623:U:H6	2.02	0.41
2:2:708:G:C6	2:2:709:G:H1'	2.56	0.41
2:2:1184:C:O2'	27:S:8:LYS:HD2	2.20	0.41
2:2:1262:G:H2'	2:2:1263:C:C6	2.55	0.41
2:2:1451:A:OP1	2:2:1454:A:H8	2.04	0.41
4:4:65:C:H5''	10:B:355:ARG:NH2	2.35	0.41
15:G:95:ILE:HD11	15:G:153:VAL:HG21	2.02	0.41
26:R:12:VAL:O	26:R:61:LEU:N	2.53	0.41
28:S1:844:U:O2'	38:SI:108:ASP:OD2	2.38	0.41
28:S1:967:A:H2'	28:S1:968:G:O4'	2.19	0.41
28:S1:1444:G:O2'	28:S1:1445:A:H3'	2.20	0.41
28:S1:1550:OMG:HM21	42:SM:67:CYS:HA	2.02	0.41
28:S1:1911:U:H2'	28:S1:1912:A:C8	2.55	0.41
28:S1:2061:5MC:H2'	28:S1:2062:G:C8	2.55	0.41
29:S4:27:G:C2	29:S4:28:G:C8	3.08	0.41
31:SB:12:ARG:HE	31:SB:12:ARG:HB2	1.62	0.41
42:SM:17:VAL:HG22	42:SM:113:ILE:HD13	2.01	0.41
52:SW:32:LEU:HA	52:SW:32:LEU:HD23	1.83	0.41
73:c:237:TYR:C	73:c:237:TYR:CD1	2.99	0.41
76:f:3:LYS:HA	76:f:3:LYS:HD2	1.80	0.41
76:f:16:LYS:HE3	76:f:16:LYS:HB3	1.65	0.41
82:l:4:PHE:CZ	82:l:6:PRO:HD3	2.55	0.41
1:1:5:A:H2'	1:1:6:C:C6	2.55	0.41
2:2:383:U:C6	2:2:387:U:C4	3.08	0.41
2:2:613:A:H2'	2:2:614:A:C8	2.55	0.41
2:2:708:G:N1	2:2:709:G:H1'	2.34	0.41
2:2:1248:OMC:H1'	2:2:1248:OMC:HM23	1.81	0.41
4:4:60:A:H2'	4:4:61:A:H8	1.85	0.41
4:4:144:G:H3'	4:4:145:C:H6	1.85	0.41
4:4:174:A:C6	16:H:4:PRO:HD3	2.55	0.41
11:C:178:ASP:HB3	11:C:206:PRO:HD3	2.03	0.41
17:I:175:ARG:HH22	17:I:181:GLU:CD	2.28	0.41
22:N:175:ASN:OD1	22:N:175:ASN:N	2.53	0.41
28:S1:131:G:H2'	28:S1:132:C:C6	2.55	0.41
28:S1:183:C:H2'	28:S1:184:C:O4'	2.20	0.41
28:S1:274:C:H2'	28:S1:966:G:OP2	2.20	0.41
28:S1:447:G:H4'	36:SG:91:TYR:HE2	1.84	0.41
28:S1:628:A:H2'	32:SC:144:GLN:OE1	2.20	0.41
28:S1:1553:G:N2	28:S1:2019:C:H2'	2.36	0.41
28:S1:2090:A:H2'	28:S1:2091:G:O4'	2.19	0.41
35:SF:166:ILE:HD12	35:SF:168:MET:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SY:39:ILE:HB	54:SY:57:LEU:HD21	2.03	0.41
56:Sa:66:SER:OG	56:Sa:71:ILE:O	2.30	0.41
63:Sh:67:VAL:HG22	63:Sh:68:ALA:H	1.85	0.41
68:X:59:TYR:C	68:X:59:TYR:CD2	2.98	0.41
1:1:980:A:H2'	1:1:981:C:O4'	2.21	0.41
2:2:4:C:H1'	2:2:5:A:N7	2.36	0.41
2:2:791:A:H2'	2:2:792:G:H8	1.86	0.41
2:2:1170:U:H2'	2:2:1171:G:C8	2.54	0.41
2:2:1214:G:N1	2:2:1222:C:H5	2.10	0.41
4:4:50:G:N2	4:4:59:G:H2'	2.35	0.41
9:A:198:LYS:NZ	91:A:403:HOH:O	2.43	0.41
21:M:181:ALA:HB1	21:M:184:LEU:HD11	2.01	0.41
28:S1:284:C:O2'	28:S1:285:A:P	2.79	0.41
28:S1:848:C:H4'	39:SJ:80:ASP:OD1	2.20	0.41
28:S1:853:A:H5''	34:SE:216:ALA:O	2.20	0.41
28:S1:1592:U:H1'	28:S1:1596:U:O4	2.21	0.41
28:S1:2084:C:H2'	28:S1:2085:A:H8	1.85	0.41
31:SB:143:VAL:HG23	31:SB:145:ILE:HD12	2.03	0.41
34:SE:48:ARG:HA	34:SE:48:ARG:HD2	1.96	0.41
49:ST:26:LEU:HD21	49:ST:60:ILE:HD13	2.03	0.41
51:SV:67:ARG:HG2	51:SV:67:ARG:HH11	1.84	0.41
54:SY:41:ILE:HG12	54:SY:82:ILE:HG21	2.01	0.41
54:SY:78:ILE:HD12	54:SY:85:ILE:HA	2.01	0.41
62:Sg:128:ASP:HB3	62:Sg:130:VAL:HG12	2.02	0.41
75:e:116:VAL:CG1	75:e:168:THR:HG21	2.51	0.41
1:1:52:C:O2'	1:1:1653:U:H1'	2.21	0.41
1:1:175:G:O2'	1:1:176:C:H5'	2.20	0.41
1:1:464:A:N1	2:2:608:C:O2'	2.50	0.41
1:1:478:C:H2'	1:1:479:A:C8	2.55	0.41
1:1:559:G:C2'	1:1:560:G:H5'	2.50	0.41
1:1:734:U:H2'	1:1:735:U:C6	2.55	0.41
1:1:1001:G:H5'	1:1:1022:G:OP1	2.20	0.41
2:2:1321:U:H2'	2:2:1322:C:C6	2.55	0.41
2:2:1385:G:N3	10:B:255:ALA:HB1	2.36	0.41
8:8:83:U:H2'	8:8:84:G:C8	2.56	0.41
10:B:67:VAL:HG11	18:J:90:LYS:HG2	2.02	0.41
11:C:356:LYS:HE2	11:C:356:LYS:HB3	1.57	0.41
27:S:78:LYS:HD3	27:S:87:LYS:HD2	2.01	0.41
27:S:126:PRO:HA	27:S:127:PRO:HD3	1.98	0.41
28:S1:170:G:P	36:SG:8:PRO:HB3	2.60	0.41
28:S1:1864:C:H2'	28:S1:1865:OMG:H8	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:2071:U:H2'	28:S1:2072:C:C6	2.56	0.41
33:SD:57:LEU:HD11	33:SD:67:ARG:HH21	1.86	0.41
44:SO:91:ARG:HA	44:SO:126:THR:HG22	2.03	0.41
61:Sf:95:MET:CE	61:Sf:98:LEU:HD12	2.50	0.41
63:Sh:70:ALA:O	63:Sh:73:VAL:HG12	2.19	0.41
70:Z:33:ASN:OD1	70:Z:36:GLY:N	2.48	0.41
82:l:20:ASN:ND2	82:l:42:ARG:O	2.43	0.41
1:1:65:A:O2'	1:1:353:C:O2	2.38	0.41
1:1:794:U:C2	1:1:795:U:C5	3.08	0.41
1:1:1007:U:H2'	1:1:1008:C:C6	2.56	0.41
1:1:1176:C:H2'	1:1:1177:U:C6	2.56	0.41
1:1:1396:G:H2'	1:1:1397:C:O4'	2.21	0.41
6:6:39:U:H4'	19:K:91:ARG:NH2	2.31	0.41
8:8:94:A:H8	8:8:94:A:OP2	2.03	0.41
28:S1:832:C:C5	28:S1:833:G:C8	3.08	0.41
28:S1:1192:PSU:H2'	28:S1:1193:U:C6	2.55	0.41
28:S1:1206:C:O5'	58:Sc:29:PRO:HB3	2.20	0.41
28:S1:2202:PSU:H2'	30:SA:118:LYS:HB2	2.02	0.41
30:SA:66:PHE:CE2	44:SO:41:SER:HB3	2.55	0.41
30:SA:131:THR:OG1	30:SA:135:TYR:HB2	2.21	0.41
46:SQ:35:GLN:NE2	46:SQ:100:TRP:O	2.54	0.41
51:SV:2:GLY:O	51:SV:3:LYS:HD2	2.21	0.41
75:e:48:GLU:HA	75:e:51:LYS:HE2	2.02	0.41
79:i:69:GLU:H	79:i:69:GLU:HG2	1.74	0.41
85:o:49:ARG:HB2	85:o:55:TRP:CH2	2.56	0.41
1:1:613:C:H2'	1:1:614:A:H8	1.86	0.41
2:2:506:U:H1'	2:2:507:G:H5'	2.02	0.41
2:2:691:A:H61	2:2:748:C:H42	1.68	0.41
2:2:1285:A:C4	2:2:1286:G:C8	3.09	0.41
2:2:1385:G:C2	10:B:255:ALA:HB1	2.56	0.41
2:2:1425:A:H2'	2:2:1426:C:C6	2.56	0.41
2:2:1496:G:H2'	2:2:1497:C:O4'	2.21	0.41
3:3:180:U:O2'	3:3:181:G:O5'	2.27	0.41
7:7:66:G:H2'	7:7:67:U:C6	2.56	0.41
11:C:189:ARG:O	11:C:194:LYS:HE3	2.20	0.41
23:O:109:THR:HG21	23:O:177:MET:HE2	2.02	0.41
25:Q:109:TYR:CE2	25:Q:114:LYS:HD2	2.56	0.41
28:S1:746:C:H2'	28:S1:747:C:C6	2.56	0.41
28:S1:1516:G:O2'	28:S1:1517:A:H5'	2.21	0.41
28:S1:1660:G:H2'	28:S1:1661:G:C8	2.56	0.41
28:S1:1975:A:N1	28:S1:1979:OMU:H1'	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SA:145:THR:HG21	30:SA:158:ALA:HB2	2.03	0.41
31:SB:198:TRP:CD1	31:SB:199:GLU:N	2.89	0.41
34:SE:181:THR:C	34:SE:186:ARG:HG3	2.45	0.41
36:SG:171:LYS:HE2	36:SG:171:LYS:HB2	1.95	0.41
43:SN:87:LEU:HB2	43:SN:89:LEU:HG	2.01	0.41
59:Sd:44:VAL:HG11	59:Sd:73:LEU:HD12	2.02	0.41
1:1:70:C:O2	17:I:66:PRO:O	2.39	0.41
1:1:89:C:OP1	1:1:320:G:H1'	2.21	0.41
1:1:517:U:H2'	1:1:518:C:O2	2.20	0.41
1:1:573:U:O4	1:1:630:U:O2'	2.31	0.41
1:1:576:G:C6	11:C:324:ARG:HG3	2.56	0.41
1:1:820:U:H5	1:1:823:G:H22	1.68	0.41
1:1:828:U:O5'	2:2:1148:G:H4'	2.21	0.41
1:1:1061:G:N2	22:N:193:ARG:HH21	2.18	0.41
1:1:1119:C:H2'	1:1:1120:C:H6	1.85	0.41
1:1:1561:A:C6	1:1:1562:C:N4	2.89	0.41
1:1:1763:A:H5'	81:k:67:ILE:HD11	2.01	0.41
2:2:127:C:H5'	5:5:69:G:H4'	2.02	0.41
2:2:464:G:H2'	2:2:465:A:C8	2.56	0.41
2:2:825:U:N3	2:2:953:U:O2	2.54	0.41
2:2:979:A:H2'	2:2:980:A:C8	2.56	0.41
2:2:1127:G:O2'	2:2:1132:A:N1	2.43	0.41
2:2:1188:G:C4	2:2:1233:U:C5	3.08	0.41
2:2:1399:G:H2'	2:2:1400:U:C6	2.55	0.41
2:2:1501:G:C2	2:2:1502:G:C8	3.09	0.41
2:2:1512:G:C2	75:e:67:GLY:HA2	2.56	0.41
3:3:8:G:N7	69:Y:17:ARG:NE	2.67	0.41
10:B:73:VAL:HG22	18:J:88:ARG:NH2	2.36	0.41
11:C:299:VAL:HG21	24:P:138:PRO:HB2	2.02	0.41
12:D:12:ARG:HA	12:D:135:ARG:HD3	2.02	0.41
13:E:41:LEU:HD23	13:E:41:LEU:HA	1.79	0.41
14:F:20:SER:O	14:F:23:SER:HB3	2.21	0.41
21:M:65:ARG:HD3	21:M:127:PHE:CE1	2.55	0.41
22:N:78:LYS:O	22:N:78:LYS:HG2	2.21	0.41
28:S1:105:C:H2'	28:S1:106:A:H8	1.85	0.41
28:S1:364:G:H2'	28:S1:365:U:C6	2.55	0.41
28:S1:434:A:OP2	40:SK:23:LYS:NZ	2.53	0.41
28:S1:793:G:O6	28:S1:830:G:O6	2.39	0.41
28:S1:1178:C:O3'	30:SA:118:LYS:O	2.39	0.41
28:S1:1368:C:H42	28:S1:1402:A:H61	1.69	0.41
28:S1:1906:G:O2'	28:S1:1907:A:C8	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:2094:G:H1'	40:SK:32:LEU:HD12	2.02	0.41
30:SA:58:ALA:O	30:SA:62:ARG:HG3	2.21	0.41
31:SB:11:LEU:HD11	54:SY:44:VAL:HG21	2.03	0.41
31:SB:13:MET:HG3	31:SB:58:TRP:CD2	2.56	0.41
33:SD:28:LYS:NZ	33:SD:28:LYS:HB2	2.35	0.41
37:SH:171:SER:O	37:SH:177:LYS:HG3	2.21	0.41
38:SI:132:MET:HE2	38:SI:175:VAL:CG1	2.50	0.41
44:SO:68:MET:O	44:SO:72:GLN:HG3	2.20	0.41
44:SO:114:ARG:HG2	44:SO:114:ARG:NH1	2.35	0.41
47:SR:121:HIS:HA	47:SR:124:VAL:HG12	2.03	0.41
52:SW:40:PHE:CE1	52:SW:94:PRO:HD3	2.56	0.41
58:Sc:35:ASP:OD2	58:Sc:83:LYS:HE2	2.21	0.41
62:Sg:112:ALA:HB1	62:Sg:156:ILE:HG12	2.02	0.41
62:Sg:230:PHE:HE1	62:Sg:232:ILE:CD1	2.33	0.41
64:T:61:LYS:O	64:T:62:ARG:HB3	2.20	0.41
65:U:96:LYS:HE3	65:U:96:LYS:HB3	1.95	0.41
68:X:6:CYS:HB2	68:X:36:SER:HB2	2.03	0.41
69:Y:22:LYS:NZ	69:Y:130:GLN:O	2.39	0.41
69:Y:89:MET:HE3	69:Y:89:MET:HB2	1.78	0.41
73:c:142:PRO:HA	73:c:237:TYR:CD1	2.56	0.41
76:f:23:TYR:CE2	76:f:31:SER:HB3	2.56	0.41
78:h:99:GLU:O	78:h:103:ILE:HG22	2.21	0.41
82:l:26:TRP:HA	82:l:29:LEU:HD12	2.02	0.41
1:1:622:C:C2	1:1:623:U:C5	3.09	0.41
1:1:714:G:H2'	1:1:715:G:O4'	2.21	0.41
1:1:1534:G:H2'	1:1:1535:G:O4'	2.21	0.41
2:2:427:C:H2'	2:2:428:A:C8	2.55	0.41
2:2:742:U:H2'	2:2:743:C:C6	2.56	0.41
2:2:1333:G:O2'	83:m:100:TYR:O	2.34	0.41
2:2:1510:A:H62	10:B:327:ASP:CG	2.29	0.41
4:4:77:U:H4'	10:B:371:LYS:HE3	2.03	0.41
24:P:17:HIS:CE1	24:P:18:HIS:ND1	2.89	0.41
28:S1:28:A:H2'	28:S1:29:OMU:H6	2.02	0.41
28:S1:120:G:H2'	28:S1:121:C:C6	2.56	0.41
28:S1:133:G:C8	28:S1:133:G:OP2	2.74	0.41
28:S1:1493:A:H2'	28:S1:1494:A:C8	2.56	0.41
28:S1:1953:C:C2	56:Sa:73:VAL:HB	2.56	0.41
28:S1:1977:U:OP1	28:S1:1978:A:O2'	2.32	0.41
28:S1:2035:C:P	37:SH:46:ARG:HH11	2.43	0.41
31:SB:176:MET:HE3	31:SB:176:MET:O	2.20	0.41
37:SH:25:ARG:HD3	37:SH:25:ARG:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:SL:47:PRO:HD2	41:SL:50:LEU:HD12	2.03	0.41
45:SP:79:LYS:HE3	45:SP:79:LYS:HB2	1.82	0.41
54:SY:50:ILE:HD13	54:SY:50:ILE:HA	1.83	0.41
75:e:45:MET:HG2	75:e:49:LYS:HB2	2.02	0.41
75:e:148:ARG:HD3	75:e:181:LEU:HD13	2.03	0.41
79:i:59:ARG:HE	79:i:59:ARG:HB3	1.73	0.41
1:1:326:A:H2'	1:1:327:G:H8	1.86	0.40
1:1:610:A:C3'	1:1:611:C:H5'	2.51	0.40
1:1:1675:A:C6	1:1:1676:G:C6	3.09	0.40
1:1:1746:C:H2'	1:1:1757:U:O2	2.21	0.40
2:2:377:A:N6	85:o:17:ARG:O	2.46	0.40
3:3:38:U:H2'	3:3:39:C:C6	2.56	0.40
15:G:177:PRO:HA	15:G:224:LEU:HD22	2.03	0.40
28:S1:1215:U:OP1	28:S1:1280:A:O2'	2.36	0.40
28:S1:1581:G:H8	28:S1:1581:G:OP2	2.04	0.40
31:SB:130:PRO:HG3	31:SB:149:ALA:HB1	2.03	0.40
32:SC:199:PRO:HB2	32:SC:201:GLU:OE2	2.20	0.40
43:SN:37:LEU:HD23	43:SN:37:LEU:HA	1.95	0.40
44:SO:13:ASN:ND2	44:SO:13:ASN:O	2.54	0.40
59:Sd:45:ARG:HD3	59:Sd:56:ASN:HA	2.03	0.40
62:Sg:144:PHE:HZ	62:Sg:181:VAL:HA	1.85	0.40
64:T:22:LEU:O	64:T:23:ARG:HB3	2.20	0.40
75:e:6:MET:HE3	75:e:16:LYS:NZ	2.36	0.40
85:o:89:LEU:HA	85:o:89:LEU:HD12	1.85	0.40
1:1:484:A:H2'	1:1:648:A:H2	1.85	0.40
1:1:563:C:O2	1:1:563:C:H2'	2.21	0.40
1:1:1478:G:O2'	1:1:1508:A:N1	2.49	0.40
1:1:1622:A:H2'	1:1:1623:C:C6	2.55	0.40
2:2:1007:U:H2'	2:2:1008:C:H6	1.85	0.40
3:3:117:C:H2'	3:3:118:G:C8	2.56	0.40
9:A:83:PHE:CZ	9:A:86:GLN:HB2	2.57	0.40
28:S1:752:C:H2'	28:S1:753:A:H8	1.86	0.40
28:S1:785:G:O4'	28:S1:787:G:N2	2.54	0.40
28:S1:949:U:H2'	28:S1:950:U:H6	1.87	0.40
28:S1:1201:G:H2'	28:S1:1202:A:C8	2.56	0.40
28:S1:1516:G:H2'	28:S1:1517:A:C8	2.55	0.40
28:S1:1527:U:H2'	28:S1:1528:G:H8	1.85	0.40
28:S1:1792:U:H2'	28:S1:1793:U:C6	2.57	0.40
31:SB:37:MET:HE3	31:SB:157:LEU:CD1	2.50	0.40
31:SB:79:VAL:HG13	31:SB:90:ILE:HG23	2.03	0.40
32:SC:7:LYS:HG3	42:SM:58:LEU:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:SG:7:TYR:HD1	36:SG:7:TYR:HA	1.77	0.40
38:SI:54:VAL:HA	38:SI:55:PRO:HD3	1.95	0.40
51:SV:43:SER:HB3	51:SV:46:LEU:HB2	2.03	0.40
71:a:92:THR:HB	71:a:95:ARG:HD2	2.04	0.40
75:e:106:PRO:O	75:e:110:LYS:HG3	2.21	0.40
81:k:22:CYS:HA	81:k:64:VAL:HG22	2.03	0.40
86:p:65:THR:OG1	86:p:87:ARG:HB3	2.22	0.40
1:1:37:A:H5''	20:L:35:ALA:HB2	2.03	0.40
1:1:415:A:H4'	1:1:416:A:OP1	2.19	0.40
1:1:1549:U:H2'	1:1:1550:A:C8	2.55	0.40
1:1:1602:C:H2'	1:1:1603:G:H8	1.87	0.40
1:1:1726:G:H5''	66:V:39:HIS:CE1	2.55	0.40
2:2:16:G:N3	82:l:3:ARG:NH1	2.69	0.40
2:2:735:C:O2	2:2:735:C:H2'	2.22	0.40
2:2:748:C:C4	2:2:749:G:N7	2.89	0.40
8:8:52:G:OP2	23:O:94:ASN:HB3	2.22	0.40
24:P:43:GLY:O	24:P:47:VAL:HG22	2.21	0.40
28:S1:693:C:H2'	28:S1:694:U:C6	2.56	0.40
28:S1:1016:G:H5'	38:SI:90:PRO:HA	2.02	0.40
28:S1:1669:C:H2'	28:S1:1670:G:O4'	2.21	0.40
28:S1:1790:C:H2'	28:S1:1791:C:H6	1.87	0.40
28:S1:2059:C:H5	28:S1:2166:A:N6	2.09	0.40
31:SB:166:CYS:SG	31:SB:167:ASN:N	2.94	0.40
40:SK:214:ARG:HH12	50:SU:21:LYS:HA	1.75	0.40
43:SN:94:MET:SD	43:SN:95:PRO:HD2	2.62	0.40
52:SW:75:LYS:HB2	52:SW:75:LYS:HE2	1.74	0.40
55:SZ:93:GLU:HB3	55:SZ:98:LYS:HG3	2.03	0.40
1:1:376:A:O2'	1:1:377:G:H5'	2.21	0.40
1:1:434:U:H2'	1:1:435:G:O4'	2.21	0.40
1:1:541:A:H4'	1:1:542:C:H5'	2.03	0.40
1:1:1657:G:H2'	1:1:1658:U:C6	2.56	0.40
2:2:645:A:H2'	2:2:646:G:O4'	2.20	0.40
2:2:749:G:O2'	2:2:750:U:O5'	2.40	0.40
2:2:784:U:C4	15:G:182:LYS:HD2	2.56	0.40
2:2:1391:U:H2'	2:2:1392:U:H2'	2.04	0.40
3:3:188:C:H2'	3:3:189:U:O4'	2.21	0.40
11:C:83:THR:HG22	11:C:85:THR:HG22	2.04	0.40
15:G:184:MET:HG3	15:G:195:THR:CG2	2.52	0.40
16:H:22:PRO:HG2	16:H:24:ILE:HD11	2.02	0.40
21:M:47:LYS:HA	21:M:47:LYS:HD2	1.90	0.40
22:N:12:CYS:HB2	22:N:13:LYS:H	1.77	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S1:105:C:H2'	28:S1:106:A:C8	2.56	0.40
28:S1:340:G:O2'	28:S1:341:A:H8	2.04	0.40
28:S1:531:G:H2'	28:S1:532:U:H6	1.87	0.40
28:S1:1403:A:H2'	28:S1:1404:U:O4'	2.22	0.40
28:S1:1487:U:H2'	28:S1:1488:U:C6	2.56	0.40
28:S1:1606:C:H3'	28:S1:1607:G:C8	2.56	0.40
29:S4:31:A:O2'	37:SH:122:ARG:NH2	2.53	0.40
29:S4:69:G:H5'	29:S4:70:C:OP2	2.21	0.40
33:SD:48:LEU:HD12	33:SD:48:LEU:HA	1.95	0.40
36:SG:138:PRO:HG2	36:SG:144:ILE:HG12	2.04	0.40
45:SP:11:ARG:HD2	45:SP:15:ARG:NH1	2.36	0.40
45:SP:119:ARG:HG3	45:SP:120:PHE:CE2	2.57	0.40
58:Sc:24:ARG:NH2	58:Sc:30:ASN:OD1	2.54	0.40
67:W:63:ARG:HG2	67:W:82:VAL:HG12	2.03	0.40
83:m:115:CYS:SG	83:m:118:CYS:HB3	2.62	0.40
1:1:6:C:O2'	1:1:7:C:H5'	2.22	0.40
1:1:484:A:H2'	1:1:648:A:C2	2.57	0.40
1:1:515:U:H2'	1:1:516:G:C8	2.56	0.40
1:1:574:G:O2'	1:1:577:C:N4	2.54	0.40
1:1:740:C:O2'	1:1:741:G:H5''	2.22	0.40
1:1:1521:G:H5''	91:1:2299:HOH:O	2.21	0.40
2:2:506:U:H6	2:2:506:U:OP2	2.04	0.40
2:2:667:OMU:HM23	2:2:667:OMU:H1'	1.93	0.40
2:2:723:G:C8	2:2:725:A:C5	3.07	0.40
2:2:1274:C:H4'	22:N:157:MET:HG3	2.03	0.40
11:C:320:MET:HE3	11:C:320:MET:HB3	1.93	0.40
16:H:199:SER:OG	19:K:131:LYS:NZ	2.55	0.40
23:O:106:ALA:HA	23:O:177:MET:HE2	2.04	0.40
24:P:165:PRO:HB3	24:P:193:LYS:HB2	2.02	0.40
28:S1:413:A:N3	39:SJ:91:LYS:NZ	2.66	0.40
28:S1:2025:G:OP2	41:SL:133:LYS:NZ	2.44	0.40
28:S1:2083:G:O2'	28:S1:2084:C:H5'	2.22	0.40
31:SB:40:TYR:HD2	31:SB:56:MET:HE2	1.86	0.40
35:SF:114:ASN:HB2	35:SF:140:SER:OG	2.21	0.40
42:SM:56:ARG:HA	42:SM:56:ARG:HD3	1.90	0.40
48:SS:34:LYS:HE2	48:SS:35:TYR:CZ	2.56	0.40
53:SX:96:LYS:HD3	53:SX:98:TYR:CZ	2.56	0.40
56:Sa:36:LEU:H	56:Sa:36:LEU:HD23	1.87	0.40
64:T:91:MET:HE3	64:T:91:MET:HB3	1.91	0.40
64:T:129:THR:HG22	64:T:137:THR:O	2.22	0.40
69:Y:61:THR:O	69:Y:65:ARG:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Y:70:VAL:HG11	69:Y:112:VAL:HG13	2.04	0.40
71:a:84:PRO:HD2	71:a:87:LEU:HD12	2.03	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	
9	A	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
10	B	397/419 (95%)	389 (98%)	8 (2%)	0	100	100
11	C	364/373 (98%)	351 (96%)	13 (4%)	0	100	100
12	D	152/188 (81%)	143 (94%)	9 (6%)	0	100	100
13	E	184/190 (97%)	172 (94%)	12 (6%)	0	100	100
14	F	144/195 (74%)	136 (94%)	8 (6%)	0	100	100
15	G	222/264 (84%)	216 (97%)	6 (3%)	0	100	100
16	H	218/222 (98%)	217 (100%)	1 (0%)	0	100	100
17	I	206/220 (94%)	199 (97%)	5 (2%)	2 (1%)	12	13
18	J	135/139 (97%)	131 (97%)	4 (3%)	0	100	100
19	K	168/175 (96%)	162 (96%)	6 (4%)	0	100	100
20	L	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
21	M	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
22	N	195/213 (92%)	190 (97%)	5 (3%)	0	100	100
23	O	268/305 (88%)	261 (97%)	7 (3%)	0	100	100
24	P	195/198 (98%)	187 (96%)	8 (4%)	0	100	100
25	Q	185/254 (73%)	185 (100%)	0	0	100	100
26	R	176/179 (98%)	172 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	S	155/159 (98%)	151 (97%)	4 (3%)	0	100	100
30	SA	224/264 (85%)	216 (96%)	8 (4%)	0	100	100
31	SB	206/246 (84%)	194 (94%)	12 (6%)	0	100	100
32	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
33	SD	165/190 (87%)	165 (100%)	0	0	100	100
34	SE	258/273 (94%)	253 (98%)	5 (2%)	0	100	100
35	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100
36	SG	229/249 (92%)	224 (98%)	4 (2%)	1 (0%)	30	36
37	SH	178/190 (94%)	174 (98%)	4 (2%)	0	100	100
38	SI	197/200 (98%)	194 (98%)	3 (2%)	0	100	100
39	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
40	SK	178/220 (81%)	174 (98%)	4 (2%)	0	100	100
41	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
42	SM	100/116 (86%)	99 (99%)	1 (1%)	0	100	100
43	SN	97/168 (58%)	92 (95%)	5 (5%)	0	100	100
44	SO	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
45	SP	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
46	SQ	96/141 (68%)	94 (98%)	2 (2%)	0	100	100
47	SR	128/153 (84%)	127 (99%)	1 (1%)	0	100	100
48	SS	54/57 (95%)	54 (100%)	0	0	100	100
49	ST	140/151 (93%)	135 (96%)	5 (4%)	0	100	100
50	SU	154/173 (89%)	149 (97%)	5 (3%)	0	100	100
51	SV	69/143 (48%)	66 (96%)	3 (4%)	0	100	100
52	SW	111/152 (73%)	109 (98%)	2 (2%)	0	100	100
53	SX	150/161 (93%)	144 (96%)	6 (4%)	0	100	100
54	SY	82/164 (50%)	78 (95%)	4 (5%)	0	100	100
55	SZ	125/137 (91%)	123 (98%)	2 (2%)	0	100	100
56	Sa	69/120 (58%)	69 (100%)	0	0	100	100
57	Sb	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
58	Sc	67/86 (78%)	64 (96%)	3 (4%)	0	100	100
59	Sd	64/87 (74%)	63 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	Se	47/66 (71%)	47 (100%)	0	0	100	100
61	Sf	29/152 (19%)	26 (90%)	3 (10%)	0	100	100
62	Sg	290/312 (93%)	284 (98%)	6 (2%)	0	100	100
63	Sh	120/235 (51%)	113 (94%)	7 (6%)	0	100	100
64	T	149/166 (90%)	143 (96%)	6 (4%)	0	100	100
65	U	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
66	V	116/145 (80%)	116 (100%)	0	0	100	100
67	W	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
68	X	62/124 (50%)	61 (98%)	1 (2%)	0	100	100
69	Y	130/134 (97%)	127 (98%)	3 (2%)	0	100	100
70	Z	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
71	a	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
72	b	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
73	c	227/252 (90%)	219 (96%)	8 (4%)	0	100	100
74	d	90/104 (86%)	88 (98%)	2 (2%)	0	100	100
75	e	176/188 (94%)	173 (98%)	3 (2%)	0	100	100
76	f	123/133 (92%)	119 (97%)	4 (3%)	0	100	100
77	g	140/144 (97%)	140 (100%)	0	0	100	100
78	h	125/168 (74%)	122 (98%)	2 (2%)	1 (1%)	16	18
79	i	84/105 (80%)	83 (99%)	1 (1%)	0	100	100
80	j	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
81	k	70/83 (84%)	68 (97%)	2 (3%)	0	100	100
82	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
83	m	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
84	n	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
85	o	86/92 (94%)	79 (92%)	7 (8%)	0	100	100
86	p	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
All	All	11096/12926 (86%)	10802 (97%)	290 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	SG	172	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	h	62	HIS
17	I	16	HIS
17	I	152	THR

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	
9	A	190/204 (93%)	189 (100%)	1 (0%)	81	87
10	B	303/351 (86%)	298 (98%)	5 (2%)	53	66
11	C	277/301 (92%)	269 (97%)	8 (3%)	37	49
12	D	61/162 (38%)	60 (98%)	1 (2%)	55	68
13	E	139/172 (81%)	134 (96%)	5 (4%)	31	42
14	F	99/153 (65%)	97 (98%)	2 (2%)	48	62
15	G	170/221 (77%)	167 (98%)	3 (2%)	51	64
16	H	175/188 (93%)	170 (97%)	5 (3%)	37	49
17	I	161/183 (88%)	158 (98%)	3 (2%)	50	63
18	J	100/111 (90%)	99 (99%)	1 (1%)	68	77
19	K	118/145 (81%)	117 (99%)	1 (1%)	73	81
20	L	113/114 (99%)	111 (98%)	2 (2%)	51	64
21	M	174/180 (97%)	173 (99%)	1 (1%)	78	85
22	N	166/179 (93%)	159 (96%)	7 (4%)	26	37
23	O	162/242 (67%)	158 (98%)	4 (2%)	42	54
24	P	159/164 (97%)	158 (99%)	1 (1%)	78	85
25	Q	125/198 (63%)	123 (98%)	2 (2%)	55	68
26	R	146/159 (92%)	143 (98%)	3 (2%)	47	60
27	S	126/134 (94%)	120 (95%)	6 (5%)	23	32
30	SA	197/222 (89%)	194 (98%)	3 (2%)	57	69
31	SB	173/202 (86%)	168 (97%)	5 (3%)	37	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	SC	170/184 (92%)	166 (98%)	4 (2%)	43	56
33	SD	144/164 (88%)	142 (99%)	2 (1%)	59	70
34	SE	215/225 (96%)	210 (98%)	5 (2%)	44	57
35	SF	174/208 (84%)	174 (100%)	0	100	100
36	SG	189/208 (91%)	185 (98%)	4 (2%)	47	60
37	SH	151/159 (95%)	150 (99%)	1 (1%)	76	83
38	SI	175/186 (94%)	171 (98%)	4 (2%)	44	57
39	SJ	110/111 (99%)	108 (98%)	2 (2%)	51	64
40	SK	141/176 (80%)	137 (97%)	4 (3%)	38	51
41	SL	113/120 (94%)	111 (98%)	2 (2%)	51	64
42	SM	92/104 (88%)	92 (100%)	0	100	100
43	SN	86/128 (67%)	82 (95%)	4 (5%)	23	33
44	SO	103/113 (91%)	100 (97%)	3 (3%)	37	49
45	SP	114/117 (97%)	110 (96%)	4 (4%)	32	44
46	SQ	58/120 (48%)	57 (98%)	1 (2%)	53	66
47	SR	107/130 (82%)	104 (97%)	3 (3%)	38	51
48	SS	47/49 (96%)	46 (98%)	1 (2%)	47	60
49	ST	124/132 (94%)	124 (100%)	0	100	100
50	SU	132/152 (87%)	130 (98%)	2 (2%)	57	69
51	SV	62/126 (49%)	61 (98%)	1 (2%)	55	68
52	SW	95/130 (73%)	93 (98%)	2 (2%)	47	60
53	SX	121/131 (92%)	120 (99%)	1 (1%)	73	81
54	SY	64/116 (55%)	61 (95%)	3 (5%)	23	33
55	SZ	109/118 (92%)	105 (96%)	4 (4%)	30	41
56	Sa	63/95 (66%)	62 (98%)	1 (2%)	55	68
57	Sb	84/93 (90%)	81 (96%)	3 (4%)	31	42
58	Sc	60/76 (79%)	59 (98%)	1 (2%)	53	66
59	Sd	49/75 (65%)	47 (96%)	2 (4%)	27	38
60	Se	41/54 (76%)	40 (98%)	1 (2%)	43	56
61	Sf	32/126 (25%)	30 (94%)	2 (6%)	16	21
62	Sg	243/265 (92%)	236 (97%)	7 (3%)	37	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	Sh	80/177 (45%)	71 (89%)	9 (11%)	5	5
64	T	127/143 (89%)	125 (98%)	2 (2%)	55	68
65	U	57/114 (50%)	57 (100%)	0	100	100
66	V	96/124 (77%)	92 (96%)	4 (4%)	26	37
67	W	99/122 (81%)	97 (98%)	2 (2%)	48	62
68	X	58/104 (56%)	58 (100%)	0	100	100
69	Y	100/116 (86%)	96 (96%)	4 (4%)	28	39
70	Z	108/118 (92%)	104 (96%)	4 (4%)	30	41
71	a	106/118 (90%)	105 (99%)	1 (1%)	70	80
72	b	56/58 (97%)	56 (100%)	0	100	100
73	c	191/209 (91%)	187 (98%)	4 (2%)	47	60
74	d	80/89 (90%)	75 (94%)	5 (6%)	16	21
75	e	148/158 (94%)	145 (98%)	3 (2%)	48	62
76	f	106/115 (92%)	105 (99%)	1 (1%)	70	80
77	g	119/121 (98%)	118 (99%)	1 (1%)	73	81
78	h	104/146 (71%)	101 (97%)	3 (3%)	37	49
79	i	68/88 (77%)	67 (98%)	1 (2%)	57	69
80	j	67/70 (96%)	67 (100%)	0	100	100
81	k	52/74 (70%)	52 (100%)	0	100	100
82	l	46/47 (98%)	45 (98%)	1 (2%)	45	59
83	m	37/113 (33%)	36 (97%)	1 (3%)	39	52
84	n	30/32 (94%)	30 (100%)	0	100	100
85	o	69/74 (93%)	67 (97%)	2 (3%)	37	49
86	p	80/92 (87%)	80 (100%)	0	100	100
All	All	8886/10798 (82%)	8695 (98%)	191 (2%)	45	60

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	A	161	THR
10	B	45	SER
10	B	73	VAL
10	B	101	THR
10	B	217	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	B	308	THR
11	C	13	SER
11	C	70	ARG
11	C	146	VAL
11	C	225	LEU
11	C	271	VAL
11	C	285	THR
11	C	356	LYS
11	C	362	LYS
12	D	45	GLN
13	E	2	VAL
13	E	18	VAL
13	E	28	THR
13	E	84	THR
13	E	127	ASN
14	F	91	VAL
14	F	144	THR
15	G	147	LYS
15	G	219	VAL
15	G	262	ILE
16	H	79	ARG
16	H	86	LYS
16	H	150	SER
16	H	155	THR
16	H	184	SER
17	I	46	LEU
17	I	68	VAL
17	I	116	VAL
18	J	7	ASN
19	K	135	THR
20	L	104	SER
20	L	136	LYS
21	M	117	ASN
22	N	12	CYS
22	N	36	ILE
22	N	43	VAL
22	N	74	LYS
22	N	125	VAL
22	N	140	THR
22	N	145	VAL
23	O	53	VAL
23	O	66	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	O	93	THR
23	O	130	SER
24	P	3	VAL
25	Q	115	ILE
25	Q	177	GLU
26	R	2	VAL
26	R	156	ARG
26	R	173	THR
27	S	28	SER
27	S	70	ARG
27	S	80	VAL
27	S	84	THR
27	S	137	ILE
27	S	150	VAL
30	SA	110	ASP
30	SA	116	LEU
30	SA	194	VAL
31	SB	96	HIS
31	SB	100	SER
31	SB	102	HIS
31	SB	143	VAL
31	SB	160	VAL
32	SC	109	LEU
32	SC	144	GLN
32	SC	194	THR
32	SC	208	THR
33	SD	60	THR
33	SD	151	SER
34	SE	35	LEU
34	SE	68	HIS
34	SE	158	VAL
34	SE	161	VAL
34	SE	247	ILE
36	SG	26	VAL
36	SG	57	SER
36	SG	71	SER
36	SG	104	VAL
37	SH	64	PHE
38	SI	54	VAL
38	SI	113	GLN
38	SI	115	VAL
38	SI	139	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	SJ	30	SER
39	SJ	118	SER
40	SK	58	LEU
40	SK	76	VAL
40	SK	81	VAL
40	SK	184	VAL
41	SL	27	VAL
41	SL	142	THR
43	SN	3	THR
43	SN	22	VAL
43	SN	44	VAL
43	SN	60	ASN
44	SO	45	THR
44	SO	74	VAL
44	SO	126	THR
45	SP	55	ILE
45	SP	72	VAL
45	SP	100	VAL
45	SP	118	VAL
46	SQ	62	CYS
47	SR	51	ILE
47	SR	100	SER
47	SR	106	THR
48	SS	54	THR
50	SU	89	VAL
50	SU	116	GLN
51	SV	66	VAL
52	SW	44	VAL
52	SW	76	VAL
53	SX	26	ARG
54	SY	23	HIS
54	SY	50	ILE
54	SY	82	ILE
55	SZ	6	LYS
55	SZ	30	VAL
55	SZ	41	VAL
55	SZ	125	ARG
56	Sa	46	THR
57	Sb	65	ASN
57	Sb	87	THR
57	Sb	88	VAL
58	Sc	15	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	Sd	20	GLN
59	Sd	81	GLU
60	Se	7	SER
61	Sf	81	THR
61	Sf	98	LEU
62	Sg	113	VAL
62	Sg	130	VAL
62	Sg	150	GLU
62	Sg	154	SER
62	Sg	273	THR
62	Sg	280	SER
62	Sg	308	ILE
63	Sh	73	VAL
63	Sh	81	VAL
63	Sh	83	VAL
63	Sh	118	VAL
63	Sh	121	VAL
63	Sh	162	VAL
63	Sh	187	VAL
63	Sh	193	THR
63	Sh	199	THR
64	T	66	LYS
64	T	137	THR
66	V	34	GLN
66	V	77	LYS
66	V	91	SER
66	V	108	VAL
67	W	82	VAL
67	W	92	VAL
69	Y	11	VAL
69	Y	48	LYS
69	Y	83	THR
69	Y	97	ILE
70	Z	17	ARG
70	Z	62	CYS
70	Z	87	VAL
70	Z	138	SER
71	a	92	THR
73	c	34	GLU
73	c	56	LEU
73	c	60	LYS
73	c	131	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
74	d	19	VAL
74	d	38	GLN
74	d	73	SER
74	d	90	CYS
74	d	97	VAL
75	e	10	VAL
75	e	123	LYS
75	e	185	THR
76	f	87	VAL
77	g	14	LEU
78	h	2	SER
78	h	69	SER
78	h	116	LEU
79	i	21	THR
82	l	29	LEU
83	m	117	HIS
85	o	41	PHE
85	o	42	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
10	B	248	HIS
11	C	42	ASN
11	C	145	ASN
11	C	158	GLN
11	C	183	ASN
11	C	345	ASN
13	E	107	GLN
14	F	59	HIS
14	F	194	ASN
15	G	169	ASN
16	H	44	GLN
16	H	163	HIS
16	H	186	HIS
16	H	187	HIS
17	I	10	HIS
17	I	139	GLN
19	K	21	GLN
20	L	62	HIS
20	L	66	ASN
21	M	156	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	N	71	GLN
22	N	100	ASN
26	R	5	HIS
30	SA	75	GLN
31	SB	33	GLN
31	SB	95	GLN
31	SB	135	GLN
34	SE	64	GLN
34	SE	231	ASN
36	SG	35	ASN
36	SG	86	ASN
36	SG	92	GLN
37	SH	123	GLN
37	SH	189	ASN
38	SI	45	HIS
39	SJ	9	ASN
40	SK	35	ASN
40	SK	52	ASN
40	SK	116	HIS
41	SL	13	GLN
41	SL	34	ASN
41	SL	43	GLN
44	SO	13	ASN
44	SO	72	GLN
45	SP	73	GLN
45	SP	87	ASN
47	SR	12	HIS
48	SS	50	HIS
50	SU	104	ASN
50	SU	107	HIS
50	SU	116	GLN
51	SV	15	GLN
52	SW	110	ASN
56	Sa	82	GLN
57	Sb	65	ASN
59	Sd	22	GLN
60	Se	16	ASN
62	Sg	2	ASN
62	Sg	59	HIS
63	Sh	191	ASN
64	T	28	ASN
64	T	133	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	V	107	GLN
66	V	114	ASN
66	V	140	ASN
67	W	16	HIS
68	X	14	HIS
69	Y	77	HIS
72	b	19	ASN
72	b	28	HIS
73	c	82	HIS
73	c	177	GLN
75	e	152	GLN
75	e	172	ASN
76	f	21	HIS
76	f	28	GLN
77	g	27	ASN
79	i	26	GLN
80	j	76	ASN
85	o	76	ASN
86	p	73	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1600/1782 (89%)	410 (25%)	33 (2%)
2	2	1147/1526 (75%)	308 (26%)	25 (2%)
28	S1	1762/2204 (79%)	413 (23%)	25 (1%)
29	S4	45/76 (59%)	24 (53%)	1 (2%)
3	3	151/216 (69%)	31 (20%)	5 (3%)
4	4	183/184 (99%)	37 (20%)	1 (0%)
5	5	112/135 (82%)	26 (23%)	2 (1%)
6	6	70/73 (95%)	31 (44%)	3 (4%)
7	7	160/171 (93%)	34 (21%)	3 (1%)
8	8	118/123 (95%)	17 (14%)	0
All	All	5348/6490 (82%)	1331 (24%)	98 (1%)

All (1331) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	C
1	1	8	U
1	1	16	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	24	A
1	1	29	C
1	1	38	A
1	1	41	A
1	1	47	C
1	1	55	A
1	1	58	A
1	1	63	A
1	1	64	A
1	1	67	C
1	1	70	C
1	1	72	G
1	1	84	G
1	1	86	G
1	1	87	A
1	1	91	G
1	1	98	A
1	1	110	A
1	1	117	G
1	1	118	C
1	1	127	G
1	1	129	C
1	1	131	U
1	1	134	A
1	1	135	A
1	1	136	G
1	1	141	U
1	1	142	G
1	1	144	G
1	1	145	U
1	1	146	U
1	1	147	G
1	1	149	G
1	1	153	C
1	1	165	U
1	1	170	U
1	1	171	U
1	1	172	G
1	1	173	G
1	1	176	C
1	1	178	G
1	1	179	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	182	U
1	1	188	A
1	1	191	U
1	1	192	C
1	1	197	G
1	1	199	A
1	1	201	A
1	1	205	A
1	1	209	C
1	1	216	G
1	1	218	A
1	1	219	U
1	1	223	A
1	1	224	C
1	1	226	C
1	1	233	U
1	1	234	G
1	1	237	U
1	1	242	A
1	1	243	G
1	1	257	U
1	1	265	U
1	1	266	G
1	1	273	A
1	1	280	A
1	1	292	A
1	1	293	C
1	1	305	A2M
1	1	306	G
1	1	307	U
1	1	322	A
1	1	323	U
1	1	324	G
1	1	332	A
1	1	335	U
1	1	336	U
1	1	342	G
1	1	343	U
1	1	344	A
1	1	357	A
1	1	367	A
1	1	368	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	369	A
1	1	371	U
1	1	373	G
1	1	374	G
1	1	383	U
1	1	391	A
1	1	392	A
1	1	409	U
1	1	410	U
1	1	416	A
1	1	417	G
1	1	419	A
1	1	424	G
1	1	439	U
1	1	440	A
1	1	443	A
1	1	444	C
1	1	461	G
1	1	463	C
1	1	464	A
1	1	471	G
1	1	477	C
1	1	485	A
1	1	486	C
1	1	488	G
1	1	489	C
1	1	494	A
1	1	501	C
1	1	502	U
1	1	504	C
1	1	510	U
1	1	515	U
1	1	518	C
1	1	521	G
1	1	522	G
1	1	524	U
1	1	527	A
1	1	535	C
1	1	536	G
1	1	538	G
1	1	542	C
1	1	543	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	546	G
1	1	547	U
1	1	551	A
1	1	552	G
1	1	553	A
1	1	560	G
1	1	561	G
1	1	565	U
1	1	569	G
1	1	570	A
1	1	571	A
1	1	572	A
1	1	573	U
1	1	574	G
1	1	577	C
1	1	578	G
1	1	580	A
1	1	585	U
1	1	586	U
1	1	590	C
1	1	591	U
1	1	592	G
1	1	594	G
1	1	597	C
1	1	598	G
1	1	599	G
1	1	601	G
1	1	606	C
1	1	607	C
1	1	609	C
1	1	611	C
1	1	612	G
1	1	616	U
1	1	617	G
1	1	621	U
1	1	623	U
1	1	625	C
1	1	627	C
1	1	630	U
1	1	631	G
1	1	632	A
1	1	633	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	634	G
1	1	635	C
1	1	639	A
1	1	641	G
1	1	648	A
1	1	651	G
1	1	652	A
1	1	653	A
1	1	666	C
1	1	668	C
1	1	669	C
1	1	678	A2M
1	1	680	C
1	1	681	A2M
1	1	692	A
1	1	694	U
1	1	709	A
1	1	710	G
1	1	718	A
1	1	719	U
1	1	721	U
1	1	722	G
1	1	728	C
1	1	735	U
1	1	736	C
1	1	740	C
1	1	741	G
1	1	743	A
1	1	744	C
1	1	745	U
1	1	748	A
1	1	753	A
1	1	761	A
1	1	763	U
1	1	771	U
1	1	775	G
1	1	778	C
1	1	779	A
1	1	782	C
1	1	783	G
1	1	790	C
1	1	792	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	794	U
1	1	795	U
1	1	803	C
1	1	810	C
1	1	818	C
1	1	823	G
1	1	828	U
1	1	832	G
1	1	835	G
1	1	836	G
1	1	838	G
1	1	850	G
1	1	852	A
1	1	868	A
1	1	895	G
1	1	900	C
1	1	903	A
1	1	905	G
1	1	912	C
1	1	922	U
1	1	925	U
1	1	930	U
1	1	947	A
1	1	948	U
1	1	957	C
1	1	965	A
1	1	967	G
1	1	968	A
1	1	972	A
1	1	975	G
1	1	976	A
1	1	985	G
1	1	988	G
1	1	995	C
1	1	998	A
1	1	1011	PSU
1	1	1013	A
1	1	1025	G
1	1	1030	U
1	1	1031	A
1	1	1036	U
1	1	1045	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1053	A
1	1	1061	G
1	1	1063	G
1	1	1064	G
1	1	1089	C
1	1	1092	U
1	1	1093	U
1	1	1094	C
1	1	1097	A
1	1	1098	A
1	1	1100	C
1	1	1108	G
1	1	1114	A
1	1	1116	A
1	1	1121	G
1	1	1122	U
1	1	1123	G
1	1	1124	C
1	1	1129	G
1	1	1133	A
1	1	1135	U
1	1	1136	G
1	1	1137	C
1	1	1141	G
1	1	1144	G
1	1	1148	A
1	1	1150	A
1	1	1153	A
1	1	1156	A
1	1	1159	A
1	1	1161	A
1	1	1162	G
1	1	1165	A
1	1	1171	PSU
1	1	1172	G
1	1	1174	G
1	1	1188	G
1	1	1196	G
1	1	1201	U
1	1	1207	A
1	1	1210	A
1	1	1216	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1217	U
1	1	1220	G
1	1	1231	G
1	1	1239	U
1	1	1240	U
1	1	1242	U
1	1	1243	G
1	1	1249	A
1	1	1250	U
1	1	1251	U
1	1	1252	C
1	1	1253	U
1	1	1254	C
1	1	1258	A
1	1	1261	U
1	1	1262	G
1	1	1263	A
1	1	1267	G
1	1	1274	G
1	1	1280	U
1	1	1351	C
1	1	1352	C
1	1	1364	A
1	1	1367	U
1	1	1369	G
1	1	1371	OMU
1	1	1378	U
1	1	1379	A
1	1	1388	U
1	1	1389	A
1	1	1390	G
1	1	1391	U
1	1	1395	U
1	1	1401	U
1	1	1413	U
1	1	1420	G
1	1	1421	G
1	1	1422	A
1	1	1423	A
1	1	1424	A
1	1	1426	A
1	1	1427	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1438	A
1	1	1439	A
1	1	1441	U
1	1	1445	G
1	1	1446	C
1	1	1455	U
1	1	1464	G
1	1	1465	G
1	1	1470	G
1	1	1476	A
1	1	1480	C
1	1	1489	U
1	1	1490	G
1	1	1504	A
1	1	1505	U
1	1	1508	A
1	1	1509	C
1	1	1519	G
1	1	1524	OMG
1	1	1527	OMC
1	1	1536	C
1	1	1540	OMG
1	1	1545	G
1	1	1547	U
1	1	1557	A
1	1	1560	U
1	1	1566	A
1	1	1569	U
1	1	1574	C
1	1	1575	G
1	1	1586	G
1	1	1590	G
1	1	1613	C
1	1	1636	A
1	1	1639	U
1	1	1653	U
1	1	1654	A
1	1	1655	U
1	1	1661	U
1	1	1662	G
1	1	1663	U
1	1	1666	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1667	G
1	1	1672	U
1	1	1674	A
1	1	1676	G
1	1	1723	A
1	1	1724	C
1	1	1726	G
1	1	1727	A
1	1	1728	A
1	1	1729	A
1	1	1730	A
1	1	1731	G
1	1	1734	G
1	1	1737	A
1	1	1739	A
1	1	1743	A
1	1	1744	A
1	1	1746	C
1	1	1747	U
1	1	1751	A
1	1	1757	U
1	1	1758	U
1	1	1762	A
1	1	1763	A
1	1	1766	G
1	1	1771	U
1	1	1772	G
1	1	1776	G
1	1	1780	G
2	2	4	C
2	2	5	A
2	2	6	A
2	2	7	C
2	2	22	A
2	2	25	A
2	2	29	C
2	2	49	A
2	2	61	C
2	2	62	A
2	2	63	U
2	2	68	A
2	2	69	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	75	C
2	2	77	C
2	2	90	G
2	2	97	A
2	2	98	G
2	2	122	PSU
2	2	123	G
2	2	125	C
2	2	127	C
2	2	134	C
2	2	340	A
2	2	342	U
2	2	343	U
2	2	347	A
2	2	348	A
2	2	349	C
2	2	350	U
2	2	351	C
2	2	358	G
2	2	368	G
2	2	377	A
2	2	386	U
2	2	388	A
2	2	404	A
2	2	415	U
2	2	416	G
2	2	434	A
2	2	436	U
2	2	443	OMC
2	2	444	A
2	2	451	U
2	2	452	G
2	2	453	A
2	2	454	A
2	2	455	U
2	2	456	G
2	2	458	C
2	2	459	A
2	2	460	A
2	2	461	C
2	2	471	U
2	2	472	PSU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	478	A
2	2	490	A
2	2	492	G
2	2	495	G
2	2	496	G
2	2	497	G
2	2	498	A
2	2	499	G
2	2	500	U
2	2	501	A
2	2	502	A
2	2	503	C
2	2	504	U
2	2	506	U
2	2	507	G
2	2	511	C
2	2	518	G
2	2	519	G
2	2	527	A2M
2	2	529	G
2	2	530	C
2	2	534	OMG
2	2	544	U
2	2	552	C
2	2	554	C
2	2	556	U
2	2	559	A
2	2	561	G
2	2	571	G
2	2	580	U
2	2	582	U
2	2	602	A
2	2	616	G
2	2	619	A
2	2	620	C
2	2	621	G
2	2	623	A
2	2	637	G
2	2	639	G
2	2	640	G
2	2	643	A
2	2	648	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	649	G
2	2	650	A
2	2	657	U
2	2	658	G
2	2	688	G
2	2	695	G
2	2	696	A
2	2	697	G
2	2	698	G
2	2	703	G
2	2	709	G
2	2	711	G
2	2	712	G
2	2	714	A
2	2	715	G
2	2	716	C
2	2	718	C
2	2	720	A
2	2	724	C
2	2	725	A
2	2	726	A
2	2	728	U
2	2	731	A
2	2	732	A
2	2	733	U
2	2	734	A
2	2	735	C
2	2	738	C
2	2	739	C
2	2	741	C
2	2	745	G
2	2	746	A
2	2	747	A
2	2	748	C
2	2	749	G
2	2	750	U
2	2	751	U
2	2	752	G
2	2	758	C
2	2	760	U
2	2	761	A
2	2	777	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	778	A
2	2	779	U
2	2	783	U
2	2	784	U
2	2	789	G
2	2	799	G
2	2	805	G
2	2	808	C
2	2	810	G
2	2	811	U
2	2	819	U
2	2	820	G
2	2	822	G
2	2	823	A
2	2	824	G
2	2	825	U
2	2	845	C
2	2	846	G
2	2	848	C
2	2	851	C
2	2	947	U
2	2	951	G
2	2	952	G
2	2	953	U
2	2	954	A
2	2	955	C
2	2	974	G
2	2	975	A
2	2	976	A
2	2	979	A
2	2	980	A
2	2	1004	G
2	2	1010	U
2	2	1011	G
2	2	1012	U
2	2	1019	A
2	2	1020	C
2	2	1021	A
2	2	1025	G
2	2	1033	G
2	2	1034	G
2	2	1041	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1046	OMG
2	2	1053	A
2	2	1058	PSU
2	2	1064	A
2	2	1075	G
2	2	1078	OMG
2	2	1079	U
2	2	1083	A
2	2	1084	A
2	2	1096	U
2	2	1101	A
2	2	1111	C
2	2	1112	A
2	2	1115	U
2	2	1116	A
2	2	1118	A
2	2	1121	A
2	2	1122	C
2	2	1123	A
2	2	1129	A
2	2	1132	A
2	2	1137	G
2	2	1139	U
2	2	1141	G
2	2	1147	C
2	2	1148	G
2	2	1156	G
2	2	1157	U
2	2	1161	A
2	2	1162	A
2	2	1165	G
2	2	1171	G
2	2	1178	C
2	2	1179	A
2	2	1180	A
2	2	1181	G
2	2	1185	A2M
2	2	1189	A
2	2	1199	A
2	2	1201	G
2	2	1203	A
2	2	1204	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1206	G
2	2	1207	G
2	2	1209	A
2	2	1215	A
2	2	1216	A
2	2	1217	C
2	2	1218	A
2	2	1223	A
2	2	1229	OMG
2	2	1233	U
2	2	1234	G
2	2	1237	A
2	2	1238	G
2	2	1239	A
2	2	1240	A
2	2	1241	U
2	2	1246	A
2	2	1248	OMC
2	2	1252	G
2	2	1255	A
2	2	1271	G
2	2	1274	C
2	2	1278	C
2	2	1281	U
2	2	1283	A
2	2	1284	U
2	2	1288	G
2	2	1289	A
2	2	1290	C
2	2	1291	G
2	2	1294	G
2	2	1297	U
2	2	1300	U
2	2	1305	C
2	2	1309	G
2	2	1313	U
2	2	1314	C
2	2	1325	A
2	2	1336	G
2	2	1337	C
2	2	1342	G
2	2	1349	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1354	PSU
2	2	1361	PSU
2	2	1363	C
2	2	1365	C
2	2	1366	C
2	2	1373	C
2	2	1374	A
2	2	1379	A
2	2	1380	C
2	2	1385	G
2	2	1389	G
2	2	1392	U
2	2	1409	A
2	2	1416	U
2	2	1421	C
2	2	1428	U
2	2	1433	G
2	2	1437	A
2	2	1441	C
2	2	1443	A
2	2	1444	G
2	2	1445	A
2	2	1448	A
2	2	1450	G
2	2	1454	A
2	2	1455	U
2	2	1458	G
2	2	1463	A
2	2	1465	G
2	2	1492	G
2	2	1494	G
2	2	1500	U
2	2	1501	G
2	2	1503	G
2	2	1504	U
2	2	1510	A
2	2	1511	U
2	2	1512	G
2	2	1513	G
2	2	1514	U
2	2	1522	U
2	2	1524	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1525	C
3	3	35	A
3	3	41	A
3	3	42	U
3	3	59	U
3	3	60	U
3	3	63	U
3	3	64	U
3	3	99	U
3	3	109	U
3	3	110	U
3	3	111	A
3	3	112	C
3	3	113	U
3	3	116	U
3	3	124	U
3	3	125	U
3	3	142	G
3	3	149	A
3	3	150	A
3	3	151	A
3	3	180	U
3	3	181	G
3	3	184	A
3	3	187	U
3	3	188	C
3	3	192	G
3	3	199	A
3	3	201	C
3	3	202	A
3	3	210	G
3	3	214	U
4	4	4	G
4	4	9	G
4	4	16	G
4	4	24	A
4	4	40	G
4	4	50	G
4	4	51	U
4	4	52	A
4	4	60	A
4	4	61	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	64	C
4	4	65	C
4	4	66	C
4	4	69	G
4	4	83	U
4	4	85	C
4	4	86	U
4	4	102	G
4	4	106	G
4	4	114	A
4	4	120	U
4	4	121	C
4	4	127	G
4	4	128	U
4	4	133	C
4	4	144	G
4	4	148	C
4	4	149	U
4	4	150	A
4	4	151	A
4	4	153	C
4	4	157	A
4	4	158	A
4	4	159	G
4	4	168	A
4	4	170	G
4	4	173	C
5	5	6	G
5	5	15	C
5	5	24	G
5	5	29	U
5	5	39	G
5	5	50	C
5	5	51	A
5	5	52	U
5	5	53	G
5	5	65	U
5	5	68	G
5	5	87	U
5	5	88	C
5	5	89	C
5	5	92	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	5	99	G
5	5	105	U
5	5	106	G
5	5	109	G
5	5	113	G
5	5	117	U
5	5	118	U
5	5	119	U
5	5	120	C
5	5	123	G
5	5	124	C
6	6	5	C
6	6	7	A
6	6	12	C
6	6	15	C
6	6	22	G
6	6	24	C
6	6	25	U
6	6	26	G
6	6	33	G
6	6	39	U
6	6	40	C
6	6	41	G
6	6	42	A
6	6	43	A
6	6	44	G
6	6	45	G
6	6	51	A
6	6	52	G
6	6	54	A
6	6	55	U
6	6	56	A
6	6	57	U
6	6	64	U
6	6	65	C
6	6	67	C
6	6	68	A
6	6	69	A
6	6	70	G
6	6	71	A
6	6	72	C
6	6	73	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	7	2	A
7	7	5	U
7	7	6	G
7	7	16	A
7	7	19	A
7	7	22	U
7	7	31	A
7	7	33	U
7	7	43	A2M
7	7	59	A
7	7	62	A
7	7	63	G
7	7	71	A
7	7	72	A
7	7	84	U
7	7	85	U
7	7	87	A
7	7	88	A
7	7	89	U
7	7	90	U
7	7	94	G
7	7	96	A
7	7	103	A
7	7	104	A
7	7	105	C
7	7	110	A
7	7	119	G
7	7	120	G
7	7	127	C
7	7	128	U
7	7	136	G
7	7	157	U
7	7	158	U
7	7	169	A
8	8	11	G
8	8	22	A
8	8	26	A
8	8	34	A
8	8	37	U
8	8	45	G
8	8	46	A
8	8	52	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	8	57	U
8	8	63	C
8	8	67	C
8	8	68	A
8	8	70	G
8	8	94	A
8	8	95	U
8	8	104	A
8	8	114	G
28	S1	3	U
28	S1	17	C
28	S1	25	C
28	S1	26	A
28	S1	34	G
28	S1	42	G
28	S1	45	U
28	S1	47	A
28	S1	55	A
28	S1	61	C
28	S1	65	A
28	S1	66	U
28	S1	68	A
28	S1	98	A2M
28	S1	102	A
28	S1	103	A
28	S1	109	C
28	S1	112	A
28	S1	114	U
28	S1	117	G
28	S1	122	A
28	S1	129	U
28	S1	133	G
28	S1	144	A
28	S1	145	A
28	S1	146	U
28	S1	147	U
28	S1	149	G
28	S1	150	A
28	S1	158	G
28	S1	164	C
28	S1	165	G
28	S1	167	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	168	A
28	S1	170	G
28	S1	171	C
28	S1	174	A
28	S1	175	U
28	S1	181	A
28	S1	182	A
28	S1	194	U
28	S1	195	U
28	S1	197	U
28	S1	198	C
28	S1	199	C
28	S1	232	C
28	S1	234	C
28	S1	235	C
28	S1	237	A
28	S1	247	U
28	S1	249	A
28	S1	252	G
28	S1	253	U
28	S1	254	A
28	S1	255	A
28	S1	264	C
28	S1	275	A
28	S1	276	G
28	S1	277	U
28	S1	278	A
28	S1	284	C
28	S1	285	A
28	S1	287	C
28	S1	288	A
28	S1	295	A
28	S1	308	C
28	S1	309	G
28	S1	310	U
28	S1	311	G
28	S1	316	A
28	S1	321	G
28	S1	327	U
28	S1	329	C
28	S1	340	G
28	S1	341	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	349	C
28	S1	356	A
28	S1	358	C
28	S1	360	G
28	S1	364	G
28	S1	381	G
28	S1	382	A
28	S1	387	C
28	S1	396	G
28	S1	404	C
28	S1	433	G
28	S1	443	A
28	S1	444	A
28	S1	445	U
28	S1	446	A
28	S1	447	G
28	S1	451	C
28	S1	454	C
28	S1	462	G
28	S1	464	G
28	S1	467	C
28	S1	469	G
28	S1	474	C
28	S1	477	G
28	S1	481	A
28	S1	482	U
28	S1	487	C
28	S1	497	A
28	S1	500	A
28	S1	501	A
28	S1	502	A
28	S1	516	A
28	S1	523	A
28	S1	525	A
28	S1	528	G
28	S1	548	G
28	S1	551	A
28	S1	552	U
28	S1	553	U
28	S1	554	U
28	S1	555	C
28	S1	556	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	559	G
28	S1	565	U
28	S1	566	A
28	S1	569	U
28	S1	574	C
28	S1	576	A
28	S1	580	A
28	S1	581	A
28	S1	585	C
28	S1	588	G
28	S1	590	A
28	S1	591	A
28	S1	592	C
28	S1	594	A
28	S1	606	G
28	S1	614	C
28	S1	617	G
28	S1	628	A
28	S1	631	U
28	S1	632	C
28	S1	643	A
28	S1	660	U
28	S1	668	A2M
28	S1	669	A
28	S1	671	G
28	S1	672	G
28	S1	673	G
28	S1	685	A
28	S1	688	G
28	S1	689	U
28	S1	690	G
28	S1	693	C
28	S1	698	C
28	S1	749	U
28	S1	754	G
28	S1	755	C
28	S1	757	C
28	S1	760	G
28	S1	772	A
28	S1	773	A
28	S1	775	C
28	S1	776	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	777	A
28	S1	778	G
28	S1	782	C
28	S1	785	G
28	S1	786	G
28	S1	788	A
28	S1	790	U
28	S1	791	G
28	S1	792	G
28	S1	793	G
28	S1	794	U
28	S1	810	G
28	S1	815	U
28	S1	816	C
28	S1	818	U
28	S1	819	G
28	S1	820	C
28	S1	825	C
28	S1	826	A
28	S1	827	G
28	S1	833	G
28	S1	834	U
28	S1	839	G
28	S1	840	A
28	S1	844	U
28	S1	845	U
28	S1	856	A
28	S1	857	A
28	S1	866	G
28	S1	867	A
28	S1	868	C
28	S1	879	A
28	S1	882	U
28	S1	883	G
28	S1	886	U
28	S1	887	U
28	S1	890	A
28	S1	892	U
28	S1	895	A
28	S1	914	G
28	S1	916	G
28	S1	917	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	918	A
28	S1	950	U
28	S1	951	U
28	S1	953	U
28	S1	954	A
28	S1	955	A
28	S1	956	A
28	S1	964	U
28	S1	965	G
28	S1	968	G
28	S1	969	A
28	S1	970	U
28	S1	972	A
28	S1	976	A
28	S1	977	G
28	S1	978	C
28	S1	984	G
28	S1	986	C
28	S1	987	A
28	S1	989	A
28	S1	990	U
28	S1	991	G
28	S1	992	C
28	S1	993	U
28	S1	994	U
28	S1	996	C
28	S1	1015	G
28	S1	1016	G
28	S1	1039	U
28	S1	1102	G
28	S1	1105	A
28	S1	1108	A
28	S1	1109	A
28	S1	1115	G
28	S1	1119	U
28	S1	1123	G
28	S1	1130	A
28	S1	1133	U
28	S1	1139	G
28	S1	1160	A
28	S1	1170	A
28	S1	1180	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	1181	C
28	S1	1182	A
28	S1	1197	C
28	S1	1198	A
28	S1	1199	A
28	S1	1207	U
28	S1	1210	C
28	S1	1213	A
28	S1	1235	A
28	S1	1245	A
28	S1	1251	A
28	S1	1252	A
28	S1	1271	C
28	S1	1272	A
28	S1	1273	A
28	S1	1275	C
28	S1	1404	U
28	S1	1443	U
28	S1	1444	G
28	S1	1446	G
28	S1	1448	U
28	S1	1449	U
28	S1	1452	A
28	S1	1466	G
28	S1	1467	U
28	S1	1490	A
28	S1	1502	G
28	S1	1510	C
28	S1	1531	G
28	S1	1537	U
28	S1	1543	B8N
28	S1	1546	A
28	S1	1548	A
28	S1	1551	G
28	S1	1552	G
28	S1	1554	A
28	S1	1566	PSU
28	S1	1569	G
28	S1	1570	G
28	S1	1581	G
28	S1	1591	U
28	S1	1595	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	1596	U
28	S1	1597	G
28	S1	1606	C
28	S1	1611	C
28	S1	1613	C
28	S1	1614	U
28	S1	1616	A
28	S1	1621	OMU
28	S1	1637	A
28	S1	1638	U
28	S1	1640	G
28	S1	1651	G
28	S1	1653	U
28	S1	1658	U
28	S1	1666	U
28	S1	1667	U
28	S1	1673	A
28	S1	1675	C
28	S1	1676	G
28	S1	1677	G
28	S1	1679	C
28	S1	1688	A
28	S1	1689	G
28	S1	1690	C
28	S1	1693	C
28	S1	1694	C
28	S1	1696	A
28	S1	1699	A
28	S1	1703	U
28	S1	1706	A
28	S1	1712	G
28	S1	1713	C
28	S1	1718	A
28	S1	1719	G
28	S1	1720	G
28	S1	1725	C
28	S1	1764	U
28	S1	1767	G
28	S1	1773	U
28	S1	1782	G
28	S1	1788	U
28	S1	1789	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	1806	A
28	S1	1814	U
28	S1	1816	U
28	S1	1825	A
28	S1	1826	G
28	S1	1828	A
28	S1	1829	OMG
28	S1	1832	C
28	S1	1833	OMU
28	S1	1836	G
28	S1	1860	C
28	S1	1861	A
28	S1	1867	A
28	S1	1872	A
28	S1	1879	OMG
28	S1	1880	U
28	S1	1884	A
28	S1	1887	A
28	S1	1889	G
28	S1	1890	A
28	S1	1891	A
28	S1	1906	G
28	S1	1907	A
28	S1	1908	A
28	S1	1916	G
28	S1	1918	U
28	S1	1923	A
28	S1	1926	G
28	S1	1928	G
28	S1	1933	A
28	S1	1948	U
28	S1	1949	A
28	S1	1950	G
28	S1	1954	C
28	S1	1955	A
28	S1	1956	C
28	S1	1961	G
28	S1	1977	U
28	S1	1979	OMU
28	S1	1988	C
28	S1	1989	A
28	S1	2004	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	2010	G
28	S1	2016	C
28	S1	2020	A
28	S1	2021	A2M
28	S1	2030	G
28	S1	2031	A
28	S1	2036	G
28	S1	2054	C
28	S1	2055	A
28	S1	2069	U
28	S1	2078	A
28	S1	2080	G
28	S1	2095	A
28	S1	2097	C
28	S1	2099	G
28	S1	2101	C
28	S1	2118	G
28	S1	2119	C
28	S1	2120	C
28	S1	2121	C
28	S1	2125	A
28	S1	2134	A
28	S1	2136	A
28	S1	2137	U
28	S1	2144	A
28	S1	2145	A
28	S1	2151	OMG
28	S1	2152	A
28	S1	2158	A
28	S1	2159	A
28	S1	2160	G
28	S1	2163	G
28	S1	2169	A
28	S1	2170	G
28	S1	2172	U
28	S1	2183	G
28	S1	2185	MA6
28	S1	2186	C
28	S1	2195	G
28	S1	2196	G
28	S1	2197	G
28	S1	2199	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	2202	PSU
28	S1	2203	U
29	S4	2	C
29	S4	4	C
29	S4	5	G
29	S4	14	A
29	S4	15	G
29	S4	16	U
29	S4	22	G
29	S4	25	C
29	S4	27	G
29	S4	31	A
29	S4	44	G
29	S4	46	G
29	S4	51	U
29	S4	63	G
29	S4	64	A
29	S4	65	G
29	S4	66	U
29	S4	68	C
29	S4	69	G
29	S4	70	C
29	S4	71	G
29	S4	73	A
29	S4	74	C
29	S4	76	A

All (98) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	141	U
1	1	148	U
1	1	170	U
1	1	172	G
1	1	208	C
1	1	215	U
1	1	334	G
1	1	415	A
1	1	423	U
1	1	488	G
1	1	509	U
1	1	560	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	584	U
1	1	589	G
1	1	606	C
1	1	611	C
1	1	620	U
1	1	679	A
1	1	774	U
1	1	835	G
1	1	947	A
1	1	967	G
1	1	1011	PSU
1	1	1030	U
1	1	1044	G
1	1	1171	PSU
1	1	1390	G
1	1	1479	A
1	1	1565	A
1	1	1574	C
1	1	1662	G
1	1	1730	A
1	1	1742	G
2	2	4	C
2	2	122	PSU
2	2	350	U
2	2	443	OMC
2	2	496	G
2	2	497	G
2	2	510	PSU
2	2	618	A
2	2	696	A
2	2	748	C
2	2	1083	A
2	2	1122	C
2	2	1131	A
2	2	1136	U
2	2	1146	A
2	2	1156	G
2	2	1170	U
2	2	1188	G
2	2	1222	C
2	2	1239	A
2	2	1313	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1388	G
2	2	1416	U
2	2	1437	A
2	2	1512	G
3	3	112	C
3	3	149	A
3	3	150	A
3	3	179	U
3	3	180	U
4	4	149	U
5	5	51	A
5	5	106	G
6	6	23	A
6	6	51	A
6	6	71	A
7	7	71	A
7	7	93	C
7	7	95	A
28	S1	65	A
28	S1	128	C
28	S1	236	C
28	S1	276	G
28	S1	284	C
28	S1	294	G
28	S1	308	C
28	S1	310	U
28	S1	328	C
28	S1	550	C
28	S1	568	U
28	S1	777	A
28	S1	790	U
28	S1	889	A
28	S1	1209	C
28	S1	1403	A
28	S1	1639	G
28	S1	1672	C
28	S1	1879	OMG
28	S1	1889	G
28	S1	1907	A
28	S1	1915	U
28	S1	2035	C
28	S1	2119	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	S1	2151	OMG
29	S4	13	C

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

153 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$
7	OMU	7	7	1,7	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)
2	A2M	2	591	2	22,25,26	3.42	10 (45%)	31,36,39	2.30	9 (29%)
1	OMC	1	695	1	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
2	OMG	2	1231	2	23,26,27	2.44	8 (34%)	33,38,41	2.04	10 (30%)
2	OMG	2	1229	2	23,26,27	2.44	8 (34%)	33,38,41	1.99	10 (30%)
2	OMC	2	1397	2	19,22,23	2.91	8 (42%)	26,31,34	0.74	0
1	A2M	1	858	1	22,25,26	3.41	10 (45%)	31,36,39	2.46	12 (38%)
2	OMG	2	534	2	23,26,27	2.46	8 (34%)	33,38,41	2.02	9 (27%)
28	A2M	S1	98	87,28	22,25,26	3.41	10 (45%)	31,36,39	2.35	10 (32%)
28	PSU	S1	1539	28	18,21,22	4.52	8 (44%)	22,30,33	1.71	4 (18%)
2	OMG	2	71	2	23,26,27	2.46	8 (34%)	33,38,41	2.10	11 (33%)
28	PSU	S1	1566	28	18,21,22	4.54	8 (44%)	22,30,33	1.69	4 (18%)
2	OMG	2	1253	2	23,26,27	2.46	8 (34%)	33,38,41	2.03	10 (30%)
28	PSU	S1	2202	28	18,21,22	4.50	8 (44%)	22,30,33	1.67	5 (22%)
7	PSU	7	74	7	18,21,22	4.51	7 (38%)	22,30,33	1.76	5 (22%)
2	OMU	2	560	2,87	19,22,23	2.98	8 (42%)	26,31,34	2.13	7 (26%)
2	OMG	2	1078	2	23,26,27	2.77	7 (30%)	33,38,41	2.28	10 (30%)
2	OMC	2	1317	2	19,22,23	2.95	8 (42%)	26,31,34	0.77	0
2	PSU	2	597	2	18,21,22	4.49	7 (38%)	22,30,33	1.84	5 (22%)
2	A2M	2	604	2,1	22,25,26	3.42	9 (40%)	31,36,39	2.42	11 (35%)
28	7MG	S1	1995	28	22,26,27	4.32	10 (45%)	29,39,42	1.99	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	1017	1	18,21,22	4.50	7 (38%)	22,30,33	1.83	5 (22%)
28	OMU	S1	8	87,28	19,22,23	2.99	8 (42%)	26,31,34	1.80	5 (19%)
28	OMC	S1	38	28	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
1	OMC	1	1010	1	19,22,23	2.98	8 (42%)	26,31,34	0.73	0
2	PSU	2	1265	2	18,21,22	4.51	7 (38%)	22,30,33	1.83	5 (22%)
28	MA6	S1	2185	28	23,26,27	1.43	4 (17%)	34,38,41	2.87	11 (32%)
2	OMU	2	1359	2	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
28	OMU	S1	29	28	19,22,23	3.06	8 (42%)	26,31,34	1.68	5 (19%)
2	OMG	2	655	2	23,26,27	2.46	8 (34%)	33,38,41	2.06	10 (30%)
1	OMG	1	1626	1	23,26,27	2.42	8 (34%)	33,38,41	2.02	10 (30%)
2	PSU	2	472	2	18,21,22	4.43	7 (38%)	22,30,33	1.85	5 (22%)
28	OMG	S1	1647	28	23,26,27	2.44	8 (34%)	33,38,41	2.10	10 (30%)
2	PSU	2	593	2	18,21,22	4.50	8 (44%)	22,30,33	1.72	5 (22%)
2	OMC	2	1248	2	19,22,23	2.99	8 (42%)	26,31,34	0.84	0
2	OMC	2	583	2	19,22,23	2.97	8 (42%)	26,31,34	0.68	0
2	PSU	2	1413	2	18,21,22	4.49	7 (38%)	22,30,33	1.75	5 (22%)
1	OMU	1	1107	1	19,22,23	3.02	8 (42%)	26,31,34	1.78	6 (23%)
28	PSU	S1	1246	28	18,21,22	4.47	7 (38%)	22,30,33	1.89	5 (22%)
1	PSU	1	940	1	18,21,22	4.49	7 (38%)	22,30,33	1.91	5 (22%)
2	A2M	2	1384	2,87	22,25,26	0.17	0	31,36,39	0.65	0
1	A2M	1	678	2,1	22,25,26	0.18	0	31,36,39	0.32	0
2	PSU	2	1060	2	18,21,22	4.50	7 (38%)	22,30,33	1.93	5 (22%)
1	A2M	1	1539	2,1,87	22,25,26	3.39	10 (45%)	31,36,39	2.40	12 (38%)
2	OMG	2	1046	2	23,26,27	2.43	8 (34%)	33,38,41	2.03	10 (30%)
2	OMU	2	1419	2	19,22,23	0.24	0	26,31,34	0.42	0
28	OMG	S1	1879	28	23,26,27	2.45	8 (34%)	33,38,41	2.02	10 (30%)
28	OMG	S1	1623	87,28	23,26,27	2.45	8 (34%)	33,38,41	1.99	9 (27%)
2	A2M	2	628	2	22,25,26	3.39	9 (40%)	31,36,39	2.45	11 (35%)
2	OMU	2	667	2	19,22,23	3.03	8 (42%)	26,31,34	1.78	5 (19%)
2	PSU	2	510	2	18,21,22	4.54	7 (38%)	22,30,33	1.82	5 (22%)
28	PSU	S1	1657	28	18,21,22	4.48	7 (38%)	22,30,33	1.75	5 (22%)
1	OMG	1	959	1	23,26,27	2.44	8 (34%)	33,38,41	2.05	10 (30%)
28	PSU	S1	609	28	18,21,22	4.53	7 (38%)	22,30,33	1.81	5 (22%)
1	A2M	1	697	1	22,25,26	3.38	9 (40%)	31,36,39	2.37	11 (35%)
2	PSU	2	1361	2	18,21,22	4.52	7 (38%)	22,30,33	1.87	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	2	1185	2	22,25,26	3.39	10 (45%)	31,36,39	2.48	12 (38%)
2	A2M	2	1372	2	22,25,26	3.49	9 (40%)	31,36,39	2.30	9 (29%)
1	PSU	1	1171	1	18,21,22	4.44	8 (44%)	22,30,33	1.77	4 (18%)
1	OMU	1	1371	1	19,22,23	3.12	8 (42%)	26,31,34	1.88	6 (23%)
28	OMG	S1	2151	89,28	23,26,27	2.42	9 (39%)	33,38,41	2.05	10 (30%)
2	PSU	2	437	2	18,21,22	4.48	7 (38%)	22,30,33	1.76	4 (18%)
28	A2M	S1	512	28	22,25,26	3.40	9 (40%)	31,36,39	2.37	11 (35%)
7	OMG	7	75	7	23,26,27	2.40	8 (34%)	33,38,41	2.06	10 (30%)
2	A2M	2	570	2,1	22,25,26	0.22	0	31,36,39	0.49	0
2	OMG	2	1360	2	23,26,27	2.46	8 (34%)	33,38,41	2.04	10 (30%)
28	PSU	S1	1192	28	18,21,22	4.51	7 (38%)	22,30,33	1.75	5 (22%)
28	PSU	S1	2046	28	18,21,22	4.44	7 (38%)	22,30,33	1.80	5 (22%)
2	PSU	2	1058	2	18,21,22	4.45	7 (38%)	22,30,33	1.70	4 (18%)
3	OMU	3	13	3	19,22,23	3.04	8 (42%)	26,31,34	1.68	5 (19%)
2	PSU	2	1403	2	18,21,22	4.52	7 (38%)	22,30,33	1.88	6 (27%)
2	PSU	2	78	2	18,21,22	4.52	7 (38%)	22,30,33	1.80	5 (22%)
28	OMC	S1	1866	28	19,22,23	3.02	8 (42%)	26,31,34	0.80	0
1	PSU	1	1664	1	18,21,22	4.56	7 (38%)	22,30,33	1.71	4 (18%)
28	OMU	S1	661	28	19,22,23	3.02	8 (42%)	26,31,34	1.70	5 (19%)
1	PSU	1	1011	2,1	18,21,22	4.46	9 (50%)	22,30,33	1.71	6 (27%)
28	A2M	S1	479	28	22,25,26	3.36	9 (40%)	31,36,39	2.38	10 (32%)
28	OMG	S1	1865	28	23,26,27	2.43	8 (34%)	33,38,41	2.04	9 (27%)
1	PSU	1	1039	1	18,21,22	4.52	7 (38%)	22,30,33	1.70	4 (18%)
1	PSU	1	1528	1	18,21,22	4.57	7 (38%)	22,30,33	1.77	5 (22%)
28	OMG	S1	1550	28	23,26,27	2.44	8 (34%)	33,38,41	2.07	10 (30%)
2	OMC	2	443	2	19,22,23	3.00	8 (42%)	26,31,34	0.75	0
28	PSU	S1	1841	28	18,21,22	4.52	8 (44%)	22,30,33	1.66	4 (18%)
2	PSU	2	1264	2	18,21,22	4.50	8 (44%)	22,30,33	1.75	4 (18%)
28	5MC	S1	1544	28	18,22,23	3.61	7 (38%)	26,32,35	0.99	1 (3%)
2	PSU	2	1318	2	18,21,22	4.50	7 (38%)	22,30,33	1.80	5 (22%)
2	PSU	2	662	2,87	18,21,22	4.51	7 (38%)	22,30,33	1.90	6 (27%)
1	PSU	1	672	1,87	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
28	PSU	S1	455	28	18,21,22	4.50	8 (44%)	22,30,33	1.68	4 (18%)
28	A2M	S1	2021	28	22,25,26	3.40	10 (45%)	31,36,39	2.41	10 (32%)
28	MA6	S1	2184	28	23,26,27	1.41	4 (17%)	34,38,41	2.92	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1	845	1	19,22,23	2.99	8 (42%)	26,31,34	2.31	8 (30%)
1	A2M	1	927	1	22,25,26	3.41	10 (45%)	31,36,39	2.35	10 (32%)
2	A2M	2	95	2	22,25,26	3.44	9 (40%)	31,36,39	2.47	9 (29%)
2	PSU	2	1144	2	18,21,22	4.49	7 (38%)	22,30,33	1.92	5 (22%)
2	PSU	2	1303	2	18,21,22	4.50	7 (38%)	22,30,33	1.89	6 (27%)
7	PSU	7	69	7	18,21,22	4.52	7 (38%)	22,30,33	1.91	6 (27%)
1	OMC	1	1527	1	19,22,23	2.97	8 (42%)	26,31,34	0.72	0
2	A2M	2	527	2,87	22,25,26	3.34	10 (45%)	31,36,39	2.68	12 (38%)
2	PSU	2	1194	2	18,21,22	4.48	7 (38%)	22,30,33	1.84	5 (22%)
1	A2M	1	305	1	22,25,26	3.40	10 (45%)	31,36,39	2.41	11 (35%)
28	5MC	S1	2061	28	18,22,23	3.56	7 (38%)	26,32,35	0.99	3 (11%)
28	PSU	S1	33	28	18,21,22	4.54	7 (38%)	22,30,33	1.87	5 (22%)
1	OMG	1	1524	1	23,26,27	2.45	8 (34%)	33,38,41	2.14	10 (30%)
28	OMU	S1	1979	28	19,22,23	3.08	8 (42%)	26,31,34	1.66	5 (19%)
2	OMC	2	359	2	19,22,23	3.00	8 (42%)	26,31,34	0.67	0
2	A2M	2	382	2	22,25,26	3.40	8 (36%)	31,36,39	2.32	9 (29%)
1	PSU	1	1402	1	18,21,22	4.45	9 (50%)	22,30,33	1.68	4 (18%)
28	PSU	S1	12	28	18,21,22	4.49	7 (38%)	22,30,33	1.81	5 (22%)
28	OMC	S1	2140	28	19,22,23	3.01	8 (42%)	26,31,34	0.79	0
2	OMU	2	56	2,1	19,22,23	3.00	8 (42%)	26,31,34	1.73	5 (19%)
2	PSU	2	1382	2	18,21,22	0.87	1 (5%)	22,30,33	0.69	0
1	PSU	1	1181	1	18,21,22	4.58	8 (44%)	22,30,33	1.63	3 (13%)
28	OMG	S1	600	28	23,26,27	2.46	8 (34%)	33,38,41	2.00	9 (27%)
28	OMU	S1	1833	28	19,22,23	3.02	8 (42%)	26,31,34	1.85	5 (19%)
28	OMC	S1	18	28	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
28	PSU	S1	104	28	18,21,22	4.52	7 (38%)	22,30,33	1.87	5 (22%)
4	OMG	4	74	4	23,26,27	2.43	8 (34%)	33,38,41	1.94	10 (30%)
1	A2M	1	681	1	22,25,26	0.20	0	31,36,39	0.34	0
28	PSU	S1	1533	28	18,21,22	4.53	7 (38%)	22,30,33	1.81	5 (22%)
1	PSU	1	1533	2,1	18,21,22	4.52	7 (38%)	22,30,33	1.85	6 (27%)
1	OMG	1	856	1	23,26,27	2.44	8 (34%)	33,38,41	2.05	10 (30%)
2	OMU	2	1077	2	19,22,23	3.06	8 (42%)	26,31,34	1.76	5 (19%)
7	A2M	7	43	7	22,25,26	3.40	10 (45%)	31,36,39	2.52	11 (35%)
1	A2M	1	235	1	22,25,26	3.42	9 (40%)	31,36,39	2.38	10 (32%)
1	1MA	1	677	1,87	21,25,26	0.45	0	31,37,40	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1	1190	1	23,26,27	2.43	8 (34%)	33,38,41	2.12	10 (30%)
28	OMG	S1	1829	87,28	23,26,27	2.45	8 (34%)	33,38,41	2.00	10 (30%)
2	5MC	2	1308	2	18,22,23	4.65	13 (72%)	26,32,35	1.35	2 (7%)
28	A2M	S1	668	87,28	22,25,26	3.38	10 (45%)	31,36,39	2.47	11 (35%)
1	PSU	1	422	1	18,21,22	4.52	7 (38%)	22,30,33	1.78	5 (22%)
1	OMU	1	1659	1	19,22,23	3.02	8 (42%)	26,31,34	1.71	5 (19%)
2	OMG	2	641	2,87	23,26,27	2.43	8 (34%)	33,38,41	2.03	10 (30%)
1	PSU	1	239	1	18,21,22	4.52	7 (38%)	22,30,33	1.87	5 (22%)
1	A2M	1	407	1	22,25,26	3.42	9 (40%)	31,36,39	2.40	10 (32%)
2	A2M	2	572	2	22,25,26	3.39	9 (40%)	31,36,39	2.55	12 (38%)
1	A2M	1	955	1	22,25,26	3.38	10 (45%)	31,36,39	2.40	10 (32%)
1	OMU	1	847	1	19,22,23	3.00	8 (42%)	26,31,34	1.66	5 (19%)
28	OMU	S1	1621	28	19,22,23	3.02	8 (42%)	26,31,34	1.71	5 (19%)
28	PSU	S1	2048	28	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
2	PSU	2	512	2	18,21,22	4.53	7 (38%)	22,30,33	1.72	5 (22%)
7	A2M	7	162	1,7	22,25,26	3.42	10 (45%)	31,36,39	2.40	11 (35%)
2	PSU	2	1354	2	18,21,22	4.49	8 (44%)	22,30,33	1.68	5 (22%)
2	PSU	2	626	2	18,21,22	4.45	7 (38%)	22,30,33	1.73	5 (22%)
28	OMG	S1	1478	28	23,26,27	2.43	8 (34%)	33,38,41	1.99	10 (30%)
2	PSU	2	122	2	18,21,22	4.54	8 (44%)	22,30,33	1.95	6 (27%)
2	5MC	2	524	2,87	18,22,23	3.51	7 (38%)	26,32,35	1.01	2 (7%)
28	PSU	S1	607	28	18,21,22	4.55	8 (44%)	22,30,33	1.69	4 (18%)
2	OMC	2	1159	2	19,22,23	3.00	8 (42%)	26,31,34	0.84	0
28	PSU	S1	1156	28	18,21,22	4.54	7 (38%)	22,30,33	1.77	5 (22%)
1	OMG	1	1540	2,1	23,26,27	2.40	8 (34%)	33,38,41	2.01	10 (30%)
28	B8N	S1	1543	28	24,29,30	3.06	5 (20%)	29,42,45	1.72	6 (20%)
2	OMU	2	73	2	19,22,23	2.97	8 (42%)	26,31,34	1.50	4 (15%)

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
7	OMU	7	7	1,7	-	1/9/27/28	0/2/2/2
2	A2M	2	591	2	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
2	OMG	2	1231	2	-	0/9/27/28	0/3/3/3
2	OMG	2	1229	2	-	2/9/27/28	0/3/3/3
2	OMC	2	1397	2	-	0/9/27/28	0/2/2/2
1	A2M	1	858	1	-	1/9/27/28	0/3/3/3
2	OMG	2	534	2	-	2/9/27/28	0/3/3/3
28	A2M	S1	98	87,28	-	2/9/27/28	0/3/3/3
28	PSU	S1	1539	28	-	0/7/25/26	0/2/2/2
2	OMG	2	71	2	-	0/9/27/28	0/3/3/3
28	PSU	S1	1566	28	-	2/7/25/26	0/2/2/2
2	OMG	2	1253	2	-	0/9/27/28	0/3/3/3
28	PSU	S1	2202	28	-	1/7/25/26	0/2/2/2
7	PSU	7	74	7	-	0/7/25/26	0/2/2/2
2	OMU	2	560	2,87	-	2/9/27/28	0/2/2/2
2	OMG	2	1078	2	-	2/9/27/28	0/3/3/3
2	OMC	2	1317	2	-	0/9/27/28	0/2/2/2
2	PSU	2	597	2	-	0/7/25/26	0/2/2/2
2	A2M	2	604	2,1	-	0/9/27/28	0/3/3/3
28	7MG	S1	1995	28	-	2/7/37/38	0/3/3/3
1	PSU	1	1017	1	-	0/7/25/26	0/2/2/2
28	OMU	S1	8	87,28	-	7/9/27/28	0/2/2/2
28	OMC	S1	38	28	-	0/9/27/28	0/2/2/2
1	OMC	1	1010	1	-	2/9/27/28	0/2/2/2
2	PSU	2	1265	2	-	0/7/25/26	0/2/2/2
28	MA6	S1	2185	28	-	1/11/29/30	0/3/3/3
2	OMU	2	1359	2	-	0/9/27/28	0/2/2/2
28	OMU	S1	29	28	-	1/9/27/28	0/2/2/2
2	OMG	2	655	2	-	1/9/27/28	0/3/3/3
1	OMG	1	1626	1	-	0/9/27/28	0/3/3/3
2	PSU	2	472	2	-	0/7/25/26	0/2/2/2
28	OMG	S1	1647	28	-	0/9/27/28	0/3/3/3
2	PSU	2	593	2	-	0/7/25/26	0/2/2/2
2	OMC	2	1248	2	-	2/9/27/28	0/2/2/2
2	OMC	2	583	2	-	0/9/27/28	0/2/2/2
2	PSU	2	1413	2	-	0/7/25/26	0/2/2/2
1	OMU	1	1107	1	-	0/9/27/28	0/2/2/2
28	PSU	S1	1246	28	-	0/7/25/26	0/2/2/2
1	PSU	1	940	1	-	0/7/25/26	0/2/2/2
2	A2M	2	1384	2,87	-	1/9/27/28	0/3/3/3
1	A2M	1	678	2,1	-	2/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	1060	2	-	0/7/25/26	0/2/2/2
1	A2M	1	1539	2,1,87	-	1/9/27/28	0/3/3/3
2	OMG	2	1046	2	-	3/9/27/28	0/3/3/3
2	OMU	2	1419	2	-	0/9/27/28	0/2/2/2
28	OMG	S1	1879	28	-	3/9/27/28	0/3/3/3
28	OMG	S1	1623	87,28	-	1/9/27/28	0/3/3/3
2	A2M	2	628	2	-	0/9/27/28	0/3/3/3
2	OMU	2	667	2	-	0/9/27/28	0/2/2/2
2	PSU	2	510	2	-	0/7/25/26	0/2/2/2
28	PSU	S1	1657	28	-	1/7/25/26	0/2/2/2
1	OMG	1	959	1	-	0/9/27/28	0/3/3/3
28	PSU	S1	609	28	-	0/7/25/26	0/2/2/2
1	A2M	1	697	1	-	0/9/27/28	0/3/3/3
2	PSU	2	1361	2	-	1/7/25/26	0/2/2/2
2	A2M	2	1185	2	-	2/9/27/28	0/3/3/3
2	A2M	2	1372	2	-	0/9/27/28	0/3/3/3
1	PSU	1	1171	1	-	4/7/25/26	0/2/2/2
1	OMU	1	1371	1	-	3/9/27/28	0/2/2/2
28	OMG	S1	2151	89,28	-	2/9/27/28	0/3/3/3
2	PSU	2	437	2	-	0/7/25/26	0/2/2/2
28	A2M	S1	512	28	-	1/9/27/28	0/3/3/3
7	OMG	7	75	7	-	1/9/27/28	0/3/3/3
2	A2M	2	570	2,1	-	4/9/27/28	0/3/3/3
2	OMG	2	1360	2	-	1/9/27/28	0/3/3/3
28	PSU	S1	1192	28	-	2/7/25/26	0/2/2/2
28	PSU	S1	2046	28	-	0/7/25/26	0/2/2/2
2	PSU	2	1058	2	-	2/7/25/26	0/2/2/2
3	OMU	3	13	3	-	0/9/27/28	0/2/2/2
2	PSU	2	1403	2	-	0/7/25/26	0/2/2/2
2	PSU	2	78	2	-	0/7/25/26	0/2/2/2
28	OMC	S1	1866	28	-	0/9/27/28	0/2/2/2
1	PSU	1	1664	1	-	0/7/25/26	0/2/2/2
28	OMU	S1	661	28	-	0/9/27/28	0/2/2/2
1	PSU	1	1011	2,1	-	1/7/25/26	0/2/2/2
28	A2M	S1	479	28	-	0/9/27/28	0/3/3/3
28	OMG	S1	1865	28	-	0/9/27/28	0/3/3/3
1	PSU	1	1039	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1528	1	-	0/7/25/26	0/2/2/2
28	OMG	S1	1550	28	-	0/9/27/28	0/3/3/3
2	OMC	2	443	2	-	4/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PSU	S1	1841	28	-	2/7/25/26	0/2/2/2
2	PSU	2	1264	2	-	2/7/25/26	0/2/2/2
28	5MC	S1	1544	28	-	2/7/25/26	0/2/2/2
2	PSU	2	1318	2	-	0/7/25/26	0/2/2/2
2	PSU	2	662	2,87	-	0/7/25/26	0/2/2/2
1	PSU	1	672	1,87	-	0/7/25/26	0/2/2/2
28	PSU	S1	455	28	-	3/7/25/26	0/2/2/2
28	A2M	S1	2021	28	-	3/9/27/28	0/3/3/3
28	MA6	S1	2184	28	-	0/11/29/30	0/3/3/3
1	OMU	1	845	1	-	3/9/27/28	0/2/2/2
1	A2M	1	927	1	-	0/9/27/28	0/3/3/3
2	A2M	2	95	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1144	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1303	2	-	0/7/25/26	0/2/2/2
7	PSU	7	69	7	-	0/7/25/26	0/2/2/2
1	OMC	1	1527	1	-	1/9/27/28	0/2/2/2
2	A2M	2	527	2,87	-	2/9/27/28	0/3/3/3
2	PSU	2	1194	2	-	0/7/25/26	0/2/2/2
1	A2M	1	305	1	-	2/9/27/28	0/3/3/3
28	5MC	S1	2061	28	-	0/7/25/26	0/2/2/2
28	PSU	S1	33	28	-	0/7/25/26	0/2/2/2
1	OMG	1	1524	1	-	0/9/27/28	0/3/3/3
28	OMU	S1	1979	28	-	3/9/27/28	0/2/2/2
2	OMC	2	359	2	-	0/9/27/28	0/2/2/2
2	A2M	2	382	2	-	1/9/27/28	0/3/3/3
1	PSU	1	1402	1	-	0/7/25/26	0/2/2/2
28	PSU	S1	12	28	-	0/7/25/26	0/2/2/2
28	OMC	S1	2140	28	-	0/9/27/28	0/2/2/2
2	OMU	2	56	2,1	-	0/9/27/28	0/2/2/2
2	PSU	2	1382	2	-	0/7/25/26	0/2/2/2
1	PSU	1	1181	1	-	2/7/25/26	0/2/2/2
28	OMG	S1	600	28	-	0/9/27/28	0/3/3/3
28	OMU	S1	1833	28	-	2/9/27/28	0/2/2/2
28	OMC	S1	18	28	-	0/9/27/28	0/2/2/2
28	PSU	S1	104	28	-	0/7/25/26	0/2/2/2
4	OMG	4	74	4	-	0/9/27/28	0/3/3/3
1	A2M	1	681	1	-	3/9/27/28	0/3/3/3
28	PSU	S1	1533	28	-	0/7/25/26	0/2/2/2
1	PSU	1	1533	2,1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1	856	1	-	0/9/27/28	0/3/3/3
2	OMU	2	1077	2	-	0/9/27/28	0/2/2/2
7	A2M	7	43	7	-	0/9/27/28	0/3/3/3
1	A2M	1	235	1	-	0/9/27/28	0/3/3/3
1	1MA	1	677	1,87	-	2/7/25/26	0/3/3/3
1	OMG	1	1190	1	-	0/9/27/28	0/3/3/3
28	OMG	S1	1829	87,28	-	1/9/27/28	0/3/3/3
2	5MC	2	1308	2	-	4/7/25/26	0/2/2/2
28	A2M	S1	668	87,28	-	5/9/27/28	0/3/3/3
1	PSU	1	422	1	-	0/7/25/26	0/2/2/2
1	OMU	1	1659	1	-	0/9/27/28	0/2/2/2
2	OMG	2	641	2,87	-	0/9/27/28	0/3/3/3
1	PSU	1	239	1	-	0/7/25/26	0/2/2/2
1	A2M	1	407	1	-	0/9/27/28	0/3/3/3
2	A2M	2	572	2	-	0/9/27/28	0/3/3/3
1	A2M	1	955	1	-	1/9/27/28	0/3/3/3
1	OMU	1	847	1	-	0/9/27/28	0/2/2/2
28	OMU	S1	1621	28	-	1/9/27/28	0/2/2/2
28	PSU	S1	2048	28	-	0/7/25/26	0/2/2/2
2	PSU	2	512	2	-	0/7/25/26	0/2/2/2
7	A2M	7	162	1,7	-	1/9/27/28	0/3/3/3
2	PSU	2	1354	2	-	1/7/25/26	0/2/2/2
2	PSU	2	626	2	-	0/7/25/26	0/2/2/2
28	OMG	S1	1478	28	-	1/9/27/28	0/3/3/3
2	PSU	2	122	2	-	2/7/25/26	0/2/2/2
2	5MC	2	524	2,87	-	0/7/25/26	0/2/2/2
28	PSU	S1	607	28	-	3/7/25/26	0/2/2/2
2	OMC	2	1159	2	-	0/9/27/28	0/2/2/2
28	PSU	S1	1156	28	-	0/7/25/26	0/2/2/2
1	OMG	1	1540	2,1	-	2/9/27/28	0/3/3/3
28	B8N	S1	1543	28	-	9/16/34/35	0/2/2/2
2	OMU	2	73	2	-	0/9/27/28	0/2/2/2

All (1148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1181	PSU	C6-C5	12.07	1.49	1.35
1	1	1664	PSU	C6-C5	11.96	1.49	1.35
1	1	1528	PSU	C6-C5	11.94	1.49	1.35
28	S1	1566	PSU	C6-C5	11.92	1.49	1.35
1	1	1171	PSU	C6-C5	11.91	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1058	PSU	C6-C5	11.90	1.49	1.35
7	7	69	PSU	C6-C5	11.87	1.49	1.35
28	S1	607	PSU	C6-C5	11.87	1.49	1.35
2	2	510	PSU	C6-C5	11.84	1.49	1.35
2	2	1264	PSU	C6-C5	11.84	1.49	1.35
28	S1	1539	PSU	C6-C5	11.83	1.49	1.35
1	1	422	PSU	C6-C5	11.80	1.49	1.35
2	2	512	PSU	C6-C5	11.80	1.49	1.35
28	S1	609	PSU	C6-C5	11.79	1.49	1.35
28	S1	1156	PSU	C6-C5	11.78	1.49	1.35
28	S1	33	PSU	C6-C5	11.78	1.49	1.35
7	7	74	PSU	C6-C5	11.77	1.49	1.35
1	1	1017	PSU	C6-C5	11.75	1.49	1.35
28	S1	455	PSU	C6-C5	11.75	1.49	1.35
2	2	593	PSU	C6-C5	11.75	1.49	1.35
28	S1	1533	PSU	C6-C5	11.74	1.49	1.35
28	S1	1841	PSU	C6-C5	11.74	1.49	1.35
28	S1	104	PSU	C6-C5	11.73	1.49	1.35
2	2	1413	PSU	C6-C5	11.72	1.49	1.35
2	2	437	PSU	C6-C5	11.72	1.49	1.35
28	S1	1192	PSU	C6-C5	11.72	1.49	1.35
2	2	1318	PSU	C6-C5	11.71	1.49	1.35
2	2	122	PSU	C6-C5	11.70	1.48	1.35
2	2	1403	PSU	C6-C5	11.70	1.48	1.35
1	1	1039	PSU	C6-C5	11.70	1.48	1.35
1	1	1533	PSU	C6-C5	11.70	1.48	1.35
2	2	662	PSU	C6-C5	11.69	1.48	1.35
1	1	940	PSU	C6-C5	11.69	1.48	1.35
28	S1	2202	PSU	C6-C5	11.69	1.48	1.35
2	2	78	PSU	C6-C5	11.68	1.48	1.35
2	2	1354	PSU	C6-C5	11.67	1.48	1.35
28	S1	12	PSU	C6-C5	11.67	1.48	1.35
2	2	1144	PSU	C6-C5	11.66	1.48	1.35
2	2	1265	PSU	C6-C5	11.66	1.48	1.35
2	2	597	PSU	C6-C5	11.65	1.48	1.35
2	2	1060	PSU	C6-C5	11.65	1.48	1.35
2	2	1303	PSU	C6-C5	11.64	1.48	1.35
2	2	1361	PSU	C6-C5	11.63	1.48	1.35
1	1	239	PSU	C6-C5	11.63	1.48	1.35
1	1	1402	PSU	C6-C5	11.63	1.48	1.35
2	2	626	PSU	C6-C5	11.60	1.48	1.35
2	2	1194	PSU	C6-C5	11.60	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	1246	PSU	C6-C5	11.54	1.48	1.35
1	1	1011	PSU	C6-C5	11.50	1.48	1.35
28	S1	1657	PSU	C6-C5	11.49	1.48	1.35
28	S1	2046	PSU	C6-C5	11.47	1.48	1.35
28	S1	1995	7MG	C8-N9	11.45	1.52	1.46
2	2	472	PSU	C6-C5	11.27	1.48	1.35
1	1	1181	PSU	C2-N1	9.97	1.50	1.36
1	1	1528	PSU	C2-N1	9.85	1.50	1.36
2	2	510	PSU	C2-N1	9.82	1.50	1.36
2	2	1361	PSU	C2-N1	9.82	1.50	1.36
2	2	78	PSU	C2-N1	9.80	1.50	1.36
1	1	239	PSU	C2-N1	9.79	1.50	1.36
1	1	1533	PSU	C2-N1	9.79	1.50	1.36
28	S1	33	PSU	C2-N1	9.79	1.50	1.36
28	S1	607	PSU	C2-N1	9.79	1.50	1.36
28	S1	1156	PSU	C2-N1	9.78	1.50	1.36
28	S1	104	PSU	C2-N1	9.76	1.49	1.36
28	S1	1533	PSU	C2-N1	9.75	1.49	1.36
2	2	1264	PSU	C2-N1	9.75	1.49	1.36
2	2	1403	PSU	C2-N1	9.75	1.49	1.36
2	2	512	PSU	C2-N1	9.74	1.49	1.36
1	1	1664	PSU	C2-N1	9.73	1.49	1.36
2	2	122	PSU	C2-N1	9.73	1.49	1.36
1	1	1039	PSU	C2-N1	9.72	1.49	1.36
2	2	1303	PSU	C2-N1	9.71	1.49	1.36
2	2	1318	PSU	C2-N1	9.70	1.49	1.36
1	1	940	PSU	C2-N1	9.70	1.49	1.36
28	S1	1192	PSU	C2-N1	9.70	1.49	1.36
2	2	1060	PSU	C2-N1	9.70	1.49	1.36
2	2	1194	PSU	C2-N1	9.69	1.49	1.36
28	S1	1657	PSU	C2-N1	9.69	1.49	1.36
7	7	74	PSU	C2-N1	9.69	1.49	1.36
28	S1	1995	7MG	C5-N7	9.69	1.46	1.35
28	S1	609	PSU	C2-N1	9.68	1.49	1.36
2	2	593	PSU	C2-N1	9.68	1.49	1.36
2	2	597	PSU	C2-N1	9.68	1.49	1.36
28	S1	1566	PSU	C2-N1	9.68	1.49	1.36
2	2	1265	PSU	C2-N1	9.67	1.49	1.36
28	S1	1841	PSU	C2-N1	9.65	1.49	1.36
2	2	1413	PSU	C2-N1	9.65	1.49	1.36
28	S1	455	PSU	C2-N1	9.65	1.49	1.36
28	S1	12	PSU	C2-N1	9.64	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	662	PSU	C2-N1	9.64	1.49	1.36
28	S1	2202	PSU	C2-N1	9.62	1.49	1.36
1	1	1017	PSU	C2-N1	9.60	1.49	1.36
1	1	422	PSU	C2-N1	9.60	1.49	1.36
28	S1	1246	PSU	C2-N1	9.60	1.49	1.36
2	2	1144	PSU	C2-N1	9.60	1.49	1.36
28	S1	1539	PSU	C2-N1	9.58	1.49	1.36
2	2	437	PSU	C2-N1	9.58	1.49	1.36
2	2	1354	PSU	C2-N1	9.53	1.49	1.36
2	2	472	PSU	C2-N1	9.51	1.49	1.36
1	1	1011	PSU	C2-N1	9.51	1.49	1.36
7	7	69	PSU	C2-N1	9.50	1.49	1.36
2	2	626	PSU	C2-N1	9.45	1.49	1.36
28	S1	2046	PSU	C2-N1	9.44	1.49	1.36
1	1	1402	PSU	C2-N1	9.40	1.49	1.36
28	S1	2061	5MC	C6-C5	9.28	1.49	1.34
28	S1	1544	5MC	C6-C5	9.27	1.49	1.34
2	2	1308	5MC	C6-C5	9.24	1.49	1.34
1	1	1171	PSU	C2-N1	9.12	1.49	1.36
2	2	524	5MC	C6-C5	9.04	1.49	1.34
2	2	1058	PSU	C2-N1	9.02	1.48	1.36
2	2	1372	A2M	C2'-C1'	-8.81	1.30	1.53
2	2	95	A2M	O4'-C1'	8.73	1.62	1.42
1	1	305	A2M	C2'-C1'	-8.72	1.30	1.53
2	2	604	A2M	C2'-C1'	-8.72	1.30	1.53
1	1	407	A2M	O4'-C1'	8.71	1.62	1.42
2	2	527	A2M	C2'-C1'	-8.65	1.30	1.53
2	2	591	A2M	C2'-C1'	-8.62	1.30	1.53
1	1	927	A2M	C2'-C1'	-8.62	1.30	1.53
2	2	1308	5MC	C3'-C4'	-8.59	1.31	1.53
7	7	162	A2M	C2'-C1'	-8.59	1.31	1.53
1	1	1539	A2M	O4'-C1'	8.59	1.62	1.42
7	7	43	A2M	O4'-C1'	8.59	1.62	1.42
2	2	1372	A2M	O4'-C1'	8.58	1.62	1.42
28	S1	98	A2M	C2'-C1'	-8.58	1.31	1.53
1	1	1539	A2M	C2'-C1'	-8.57	1.31	1.53
28	S1	98	A2M	O4'-C1'	8.57	1.62	1.42
1	1	407	A2M	C2'-C1'	-8.56	1.31	1.53
28	S1	512	A2M	C2'-C1'	-8.56	1.31	1.53
7	7	43	A2M	C2'-C1'	-8.56	1.31	1.53
2	2	382	A2M	C2'-C1'	-8.55	1.31	1.53
2	2	604	A2M	O4'-C1'	8.54	1.62	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	512	A2M	O4'-C1'	8.54	1.62	1.42
2	2	382	A2M	O4'-C1'	8.54	1.62	1.42
2	2	572	A2M	C2'-C1'	-8.53	1.31	1.53
2	2	95	A2M	C2'-C1'	-8.53	1.31	1.53
2	2	1185	A2M	O4'-C1'	8.53	1.62	1.42
1	1	235	A2M	O4'-C1'	8.48	1.62	1.42
1	1	697	A2M	O4'-C1'	8.48	1.62	1.42
1	1	235	A2M	C2'-C1'	-8.46	1.31	1.53
2	2	572	A2M	O4'-C1'	8.45	1.62	1.42
28	S1	2021	A2M	O4'-C1'	8.45	1.62	1.42
1	1	955	A2M	O4'-C1'	8.44	1.62	1.42
1	1	927	A2M	O4'-C1'	8.43	1.62	1.42
2	2	628	A2M	O4'-C1'	8.43	1.62	1.42
28	S1	479	A2M	O4'-C1'	8.42	1.62	1.42
7	7	162	A2M	O4'-C1'	8.42	1.62	1.42
1	1	858	A2M	C2'-C1'	-8.42	1.31	1.53
1	1	955	A2M	C2'-C1'	-8.42	1.31	1.53
2	2	628	A2M	C2'-C1'	-8.42	1.31	1.53
1	1	697	A2M	C2'-C1'	-8.42	1.31	1.53
2	2	1185	A2M	C2'-C1'	-8.38	1.31	1.53
28	S1	2021	A2M	C2'-C1'	-8.38	1.31	1.53
2	2	591	A2M	O4'-C1'	8.37	1.61	1.42
1	1	858	A2M	O4'-C1'	8.37	1.61	1.42
28	S1	479	A2M	C2'-C1'	-8.37	1.31	1.53
28	S1	1543	B8N	C6-N1	8.29	1.57	1.36
28	S1	668	A2M	C2'-C1'	-8.27	1.31	1.53
28	S1	668	A2M	O4'-C1'	8.20	1.61	1.42
1	1	305	A2M	O4'-C1'	8.14	1.61	1.42
2	2	527	A2M	O4'-C1'	7.95	1.60	1.42
2	2	472	PSU	C2-N3	7.74	1.50	1.37
2	2	122	PSU	C2-N3	7.67	1.50	1.37
2	2	1078	OMG	C4-N3	7.67	1.52	1.34
2	2	1265	PSU	C2-N3	7.66	1.50	1.37
28	S1	1533	PSU	C2-N3	7.63	1.50	1.37
2	2	662	PSU	C2-N3	7.63	1.50	1.37
1	1	1371	OMU	C2-N1	7.63	1.50	1.38
2	2	1058	PSU	C2-N3	7.62	1.50	1.37
28	S1	33	PSU	C2-N3	7.61	1.50	1.37
28	S1	1841	PSU	C2-N3	7.61	1.50	1.37
28	S1	2046	PSU	C2-N3	7.61	1.50	1.37
28	S1	1539	PSU	C2-N3	7.60	1.50	1.37
28	S1	607	PSU	C2-N3	7.58	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1533	PSU	C2-N3	7.58	1.50	1.37
1	1	239	PSU	C2-N3	7.57	1.50	1.37
1	1	422	PSU	C2-N3	7.56	1.50	1.37
28	S1	609	PSU	C2-N3	7.56	1.50	1.37
28	S1	1156	PSU	C2-N3	7.56	1.50	1.37
28	S1	1566	PSU	C2-N3	7.56	1.50	1.37
1	1	1039	PSU	C2-N3	7.54	1.50	1.37
2	2	510	PSU	C2-N3	7.53	1.50	1.37
2	2	1403	PSU	C2-N3	7.53	1.50	1.37
28	S1	12	PSU	C2-N3	7.53	1.50	1.37
1	1	1171	PSU	C2-N3	7.53	1.50	1.37
28	S1	2202	PSU	C2-N3	7.53	1.50	1.37
28	S1	104	PSU	C2-N3	7.53	1.50	1.37
1	1	1011	PSU	C2-N3	7.52	1.50	1.37
1	1	1664	PSU	C2-N3	7.51	1.50	1.37
1	1	1017	PSU	C2-N3	7.51	1.50	1.37
2	2	512	PSU	C2-N3	7.51	1.50	1.37
28	S1	1192	PSU	C2-N3	7.51	1.50	1.37
2	2	1354	PSU	C2-N3	7.50	1.50	1.37
2	2	1144	PSU	C2-N3	7.50	1.50	1.37
28	S1	1246	PSU	C2-N3	7.50	1.50	1.37
7	7	69	PSU	C2-N3	7.49	1.50	1.37
1	1	845	OMU	C2-N1	7.49	1.50	1.38
2	2	1303	PSU	C2-N3	7.48	1.50	1.37
2	2	1194	PSU	C2-N3	7.48	1.50	1.37
2	2	1361	PSU	C2-N3	7.48	1.50	1.37
2	2	1060	PSU	C2-N3	7.48	1.50	1.37
1	1	1528	PSU	C2-N3	7.47	1.50	1.37
28	S1	455	PSU	C2-N3	7.46	1.50	1.37
28	S1	1657	PSU	C2-N3	7.46	1.50	1.37
7	7	74	PSU	C2-N3	7.45	1.50	1.37
2	2	597	PSU	C2-N3	7.45	1.50	1.37
1	1	1402	PSU	C2-N3	7.45	1.50	1.37
2	2	626	PSU	C2-N3	7.43	1.50	1.37
2	2	78	PSU	C2-N3	7.41	1.50	1.37
28	S1	1543	B8N	C4-N3	-7.40	1.26	1.40
2	2	437	PSU	C2-N3	7.39	1.50	1.37
2	2	1318	PSU	C2-N3	7.38	1.50	1.37
1	1	940	PSU	C2-N3	7.37	1.50	1.37
1	1	1181	PSU	C2-N3	7.36	1.50	1.37
2	2	593	PSU	C2-N3	7.35	1.50	1.37
2	2	1413	PSU	C2-N3	7.29	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	1995	7MG	C4-N9	7.25	1.46	1.37
28	S1	1979	OMU	C2-N1	7.17	1.49	1.38
2	2	1264	PSU	C2-N3	7.16	1.49	1.37
2	2	1308	5MC	O4'-C4'	7.10	1.60	1.45
2	2	560	OMU	C2-N1	7.09	1.49	1.38
28	S1	29	OMU	C2-N1	7.08	1.49	1.38
2	2	1077	OMU	C2-N1	7.07	1.49	1.38
2	2	1359	OMU	C2-N1	7.04	1.49	1.38
28	S1	1979	OMU	C2-N3	7.00	1.50	1.38
2	2	56	OMU	C2-N1	6.98	1.49	1.38
1	1	847	OMU	C2-N1	6.98	1.49	1.38
28	S1	1833	OMU	C2-N1	6.98	1.49	1.38
3	3	13	OMU	C2-N1	6.97	1.49	1.38
1	1	1107	OMU	C2-N1	6.94	1.49	1.38
2	2	1077	OMU	C2-N3	6.91	1.50	1.38
28	S1	1833	OMU	C2-N3	6.89	1.50	1.38
1	1	1371	OMU	C2-N3	6.89	1.50	1.38
28	S1	29	OMU	C2-N3	6.86	1.50	1.38
28	S1	661	OMU	C2-N1	6.86	1.49	1.38
1	1	1659	OMU	C2-N1	6.85	1.49	1.38
1	1	1107	OMU	C2-N3	6.84	1.50	1.38
28	S1	1621	OMU	C2-N1	6.82	1.49	1.38
7	7	7	OMU	C2-N1	6.80	1.49	1.38
2	2	73	OMU	C2-N1	6.80	1.49	1.38
28	S1	668	A2M	O4'-C4'	-6.79	1.29	1.45
2	2	667	OMU	C2-N1	6.78	1.49	1.38
28	S1	8	OMU	C2-N1	6.78	1.49	1.38
3	3	13	OMU	C2-N3	6.78	1.50	1.38
1	1	1659	OMU	C2-N3	6.77	1.50	1.38
1	1	847	OMU	C2-N3	6.77	1.50	1.38
28	S1	1621	OMU	C2-N3	6.76	1.50	1.38
2	2	1359	OMU	C2-N3	6.75	1.50	1.38
2	2	667	OMU	C2-N3	6.73	1.50	1.38
2	2	1078	OMG	C2-N3	6.72	1.49	1.33
28	S1	661	OMU	C2-N3	6.70	1.49	1.38
1	1	858	A2M	O4'-C4'	-6.70	1.30	1.45
7	7	7	OMU	C2-N3	6.70	1.49	1.38
2	2	56	OMU	C2-N3	6.63	1.49	1.38
2	2	534	OMG	C4-N3	6.60	1.50	1.34
28	S1	600	OMG	C4-N3	6.59	1.49	1.34
2	2	655	OMG	C4-N3	6.58	1.49	1.34
28	S1	8	OMU	C2-N3	6.58	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	560	OMU	C2-N3	6.58	1.49	1.38
2	2	1372	A2M	O4'-C4'	-6.57	1.30	1.45
2	2	1253	OMG	C4-N3	6.57	1.49	1.34
2	2	628	A2M	O4'-C4'	-6.55	1.30	1.45
28	S1	1829	OMG	C4-N3	6.50	1.49	1.34
1	1	235	A2M	O4'-C4'	-6.50	1.30	1.45
28	S1	1623	OMG	C4-N3	6.49	1.49	1.34
2	2	71	OMG	C4-N3	6.49	1.49	1.34
28	S1	1550	OMG	C4-N3	6.48	1.49	1.34
28	S1	1544	5MC	C4-N3	6.48	1.45	1.34
2	2	1231	OMG	C4-N3	6.48	1.49	1.34
2	2	73	OMU	C2-N3	6.48	1.49	1.38
1	1	959	OMG	C4-N3	6.48	1.49	1.34
28	S1	2140	OMC	C2-N3	6.48	1.49	1.36
1	1	1626	OMG	C4-N3	6.47	1.49	1.34
4	4	74	OMG	C4-N3	6.47	1.49	1.34
28	S1	2021	A2M	O4'-C4'	-6.46	1.30	1.45
1	1	856	OMG	C4-N3	6.46	1.49	1.34
2	2	1360	OMG	C4-N3	6.46	1.49	1.34
1	1	305	A2M	O4'-C4'	-6.45	1.30	1.45
2	2	1229	OMG	C4-N3	6.45	1.49	1.34
1	1	1524	OMG	C4-N3	6.44	1.49	1.34
28	S1	1647	OMG	C4-N3	6.44	1.49	1.34
28	S1	1879	OMG	C4-N3	6.42	1.49	1.34
2	2	591	A2M	O4'-C4'	-6.42	1.30	1.45
1	1	845	OMU	C2-N3	6.41	1.49	1.38
2	2	1046	OMG	C4-N3	6.41	1.49	1.34
2	2	1185	A2M	O4'-C4'	-6.41	1.30	1.45
2	2	641	OMG	C4-N3	6.40	1.49	1.34
7	7	75	OMG	C4-N3	6.39	1.49	1.34
1	1	695	OMC	C2-N3	6.38	1.49	1.36
1	1	1190	OMG	C4-N3	6.37	1.49	1.34
28	S1	1865	OMG	C4-N3	6.37	1.49	1.34
2	2	524	5MC	C4-N3	6.36	1.44	1.34
1	1	927	A2M	O4'-C4'	-6.36	1.30	1.45
7	7	162	A2M	O4'-C4'	-6.35	1.30	1.45
1	1	955	A2M	O4'-C4'	-6.34	1.30	1.45
28	S1	1478	OMG	C4-N3	6.33	1.49	1.34
1	1	1010	OMC	C2-N3	6.33	1.49	1.36
28	S1	2061	5MC	C4-N3	6.32	1.44	1.34
28	S1	1866	OMC	C2-N3	6.32	1.49	1.36
1	1	697	A2M	O4'-C4'	-6.31	1.30	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	2151	OMG	C4-N3	6.31	1.49	1.34
28	S1	479	A2M	O4'-C4'	-6.30	1.30	1.45
2	2	95	A2M	O4'-C4'	-6.30	1.30	1.45
1	1	1539	A2M	O4'-C4'	-6.28	1.31	1.45
28	S1	18	OMC	C2-N3	6.26	1.49	1.36
2	2	359	OMC	C2-N3	6.26	1.49	1.36
2	2	572	A2M	O4'-C4'	-6.26	1.31	1.45
2	2	382	A2M	O4'-C4'	-6.25	1.31	1.45
28	S1	1995	7MG	C2-N3	6.25	1.48	1.33
2	2	604	A2M	O4'-C4'	-6.24	1.31	1.45
28	S1	98	A2M	O4'-C4'	-6.23	1.31	1.45
2	2	443	OMC	C2-N3	6.22	1.49	1.36
28	S1	38	OMC	C2-N3	6.21	1.49	1.36
2	2	1159	OMC	C2-N3	6.20	1.48	1.36
1	1	1540	OMG	C4-N3	6.18	1.49	1.34
28	S1	512	A2M	O4'-C4'	-6.18	1.31	1.45
2	2	527	A2M	O4'-C4'	-6.18	1.31	1.45
1	1	407	A2M	O4'-C4'	-6.17	1.31	1.45
2	2	583	OMC	C2-N3	6.17	1.48	1.36
2	2	1248	OMC	C2-N3	6.15	1.48	1.36
1	1	1527	OMC	C2-N3	6.13	1.48	1.36
28	S1	1544	5MC	C2-N3	6.11	1.48	1.36
2	2	1308	5MC	C4-N3	6.07	1.44	1.34
2	2	443	OMC	C6-C5	6.07	1.49	1.35
2	2	1317	OMC	C6-C5	6.05	1.49	1.35
2	2	1317	OMC	C2-N3	6.05	1.48	1.36
7	7	43	A2M	O4'-C4'	-6.04	1.31	1.45
2	2	1248	OMC	C6-C5	6.03	1.49	1.35
28	S1	38	OMC	C6-C5	6.02	1.49	1.35
2	2	524	5MC	C2-N3	6.02	1.48	1.36
2	2	583	OMC	C6-C5	6.00	1.49	1.35
2	2	1397	OMC	C6-C5	5.99	1.49	1.35
2	2	1159	OMC	C6-C5	5.95	1.48	1.35
28	S1	1866	OMC	C6-C5	5.94	1.48	1.35
2	2	1078	OMG	C2-N2	5.94	1.48	1.34
28	S1	18	OMC	C6-C5	5.93	1.48	1.35
2	2	359	OMC	C6-C5	5.92	1.48	1.35
1	1	1527	OMC	C6-C5	5.91	1.48	1.35
28	S1	2061	5MC	C2-N3	5.90	1.48	1.36
1	1	695	OMC	C6-C5	5.89	1.48	1.35
2	2	1397	OMC	C2-N3	5.84	1.48	1.36
28	S1	2140	OMC	C6-C5	5.84	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1308	5MC	C2-N3	5.83	1.48	1.36
28	S1	1543	B8N	C2-N1	5.82	1.56	1.39
1	1	1010	OMC	C6-C5	5.80	1.48	1.35
2	2	1359	OMU	C6-C5	5.79	1.48	1.35
2	2	667	OMU	C6-C5	5.77	1.48	1.35
28	S1	8	OMU	C6-C5	5.77	1.48	1.35
2	2	73	OMU	C6-C5	5.75	1.48	1.35
28	S1	661	OMU	C6-C5	5.74	1.48	1.35
28	S1	1621	OMU	C6-C5	5.74	1.48	1.35
2	2	1077	OMU	C6-C5	5.73	1.48	1.35
3	3	13	OMU	C6-C5	5.72	1.48	1.35
28	S1	600	OMG	C2-N3	5.71	1.46	1.33
2	2	655	OMG	C2-N3	5.69	1.46	1.33
1	1	1659	OMU	C6-C5	5.69	1.48	1.35
28	S1	29	OMU	C6-C5	5.69	1.48	1.35
7	7	7	OMU	C6-C5	5.68	1.48	1.35
2	2	534	OMG	C2-N3	5.67	1.46	1.33
1	1	847	OMU	C6-C5	5.64	1.48	1.35
1	1	1181	PSU	C6-N1	5.63	1.45	1.36
2	2	1360	OMG	C2-N3	5.62	1.46	1.33
2	2	71	OMG	C2-N3	5.61	1.46	1.33
28	S1	1623	OMG	C2-N3	5.61	1.46	1.33
28	S1	1979	OMU	C6-C5	5.61	1.48	1.35
2	2	56	OMU	C6-C5	5.60	1.48	1.35
2	2	1253	OMG	C2-N3	5.60	1.46	1.33
1	1	1371	OMU	C6-C5	5.59	1.48	1.35
4	4	74	OMG	C2-N3	5.59	1.46	1.33
28	S1	1829	OMG	C2-N3	5.58	1.46	1.33
2	2	1231	OMG	C2-N3	5.58	1.46	1.33
28	S1	1550	OMG	C2-N3	5.58	1.46	1.33
1	1	856	OMG	C2-N3	5.57	1.46	1.33
28	S1	1879	OMG	C2-N3	5.56	1.46	1.33
2	2	1229	OMG	C2-N3	5.56	1.46	1.33
28	S1	1478	OMG	C2-N3	5.51	1.46	1.33
2	2	560	OMU	C6-C5	5.51	1.47	1.35
1	1	959	OMG	C2-N3	5.51	1.46	1.33
1	1	1626	OMG	C2-N3	5.51	1.46	1.33
1	1	1107	OMU	C6-C5	5.50	1.47	1.35
2	2	1361	PSU	C6-N1	5.50	1.45	1.36
28	S1	1647	OMG	C2-N3	5.50	1.46	1.33
2	2	641	OMG	C2-N3	5.50	1.46	1.33
2	2	1046	OMG	C2-N3	5.49	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1039	PSU	C6-N1	5.48	1.45	1.36
28	S1	1865	OMG	C2-N3	5.48	1.46	1.33
1	1	1528	PSU	C6-N1	5.47	1.45	1.36
1	1	1524	OMG	C2-N3	5.47	1.46	1.33
1	1	1664	PSU	C6-N1	5.46	1.45	1.36
1	1	1190	OMG	C2-N3	5.44	1.46	1.33
28	S1	607	PSU	C6-N1	5.42	1.45	1.36
28	S1	1156	PSU	C6-N1	5.42	1.45	1.36
2	2	78	PSU	C6-N1	5.41	1.45	1.36
2	2	1264	PSU	C6-N1	5.41	1.45	1.36
28	S1	1841	PSU	C6-N1	5.41	1.45	1.36
2	2	512	PSU	C6-N1	5.41	1.45	1.36
28	S1	1833	OMU	C6-C5	5.40	1.47	1.35
28	S1	1995	7MG	C4-N3	5.39	1.47	1.34
28	S1	1533	PSU	C6-N1	5.39	1.45	1.36
28	S1	1192	PSU	C6-N1	5.39	1.45	1.36
7	7	75	OMG	C2-N3	5.38	1.46	1.33
28	S1	1543	B8N	C6-C5	5.37	1.42	1.34
2	2	593	PSU	C6-N1	5.37	1.45	1.36
28	S1	1566	PSU	C6-N1	5.37	1.45	1.36
28	S1	1657	PSU	C6-N1	5.36	1.45	1.36
2	2	1413	PSU	C6-N1	5.36	1.45	1.36
2	2	510	PSU	C6-N1	5.35	1.45	1.36
28	S1	33	PSU	C6-N1	5.34	1.45	1.36
28	S1	2151	OMG	C2-N3	5.34	1.46	1.33
28	S1	455	PSU	C6-N1	5.34	1.45	1.36
1	1	1540	OMG	C2-N3	5.33	1.46	1.33
28	S1	609	PSU	C6-N1	5.33	1.45	1.36
2	2	1403	PSU	C6-N1	5.33	1.45	1.36
2	2	1318	PSU	C6-N1	5.32	1.45	1.36
7	7	69	PSU	C6-N1	5.32	1.45	1.36
2	2	597	PSU	C6-N1	5.31	1.45	1.36
28	S1	104	PSU	C6-N1	5.31	1.45	1.36
28	S1	12	PSU	C6-N1	5.30	1.45	1.36
28	S1	2140	OMC	C4-N3	5.30	1.45	1.34
1	1	422	PSU	C6-N1	5.28	1.45	1.36
7	7	74	PSU	C6-N1	5.28	1.45	1.36
1	1	239	PSU	C6-N1	5.27	1.45	1.36
2	2	1060	PSU	C6-N1	5.26	1.45	1.36
2	2	437	PSU	C6-N1	5.26	1.45	1.36
28	S1	1539	PSU	C6-N1	5.25	1.44	1.36
2	2	1354	PSU	C6-N1	5.25	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1010	OMC	C4-N3	5.24	1.45	1.34
2	2	1303	PSU	C6-N1	5.24	1.44	1.36
2	2	1265	PSU	C6-N1	5.22	1.44	1.36
2	2	359	OMC	C4-N3	5.22	1.45	1.34
28	S1	2202	PSU	C6-N1	5.22	1.44	1.36
1	1	1533	PSU	C6-N1	5.21	1.44	1.36
1	1	845	OMU	C6-C5	5.20	1.47	1.35
2	2	662	PSU	C6-N1	5.17	1.44	1.36
2	2	443	OMC	C4-N3	5.17	1.44	1.34
1	1	940	PSU	C6-N1	5.16	1.44	1.36
2	2	1159	OMC	C4-N3	5.16	1.44	1.34
28	S1	38	OMC	C4-N3	5.16	1.44	1.34
28	S1	1866	OMC	C4-N3	5.16	1.44	1.34
2	2	1194	PSU	C6-N1	5.15	1.44	1.36
1	1	1017	PSU	C6-N1	5.15	1.44	1.36
1	1	1011	PSU	C6-N1	5.13	1.44	1.36
2	2	1144	PSU	C6-N1	5.12	1.44	1.36
28	S1	1246	PSU	C6-N1	5.12	1.44	1.36
28	S1	18	OMC	C4-N3	5.10	1.44	1.34
2	2	626	PSU	C6-N1	5.09	1.44	1.36
2	2	472	PSU	C6-N1	5.08	1.44	1.36
1	1	1402	PSU	C6-N1	5.07	1.44	1.36
1	1	1527	OMC	C4-N3	5.07	1.44	1.34
2	2	122	PSU	C6-N1	5.05	1.44	1.36
28	S1	2046	PSU	C6-N1	5.04	1.44	1.36
2	2	1308	5MC	O4'-C1'	-5.04	1.30	1.42
1	1	695	OMC	C4-N3	5.00	1.44	1.34
2	2	1058	PSU	C6-N1	4.99	1.44	1.36
2	2	1248	OMC	C4-N3	4.99	1.44	1.34
2	2	583	OMC	C4-N3	4.95	1.44	1.34
2	2	1397	OMC	C4-N3	4.91	1.44	1.34
1	1	1171	PSU	C6-N1	4.88	1.44	1.36
2	2	359	OMC	C4-N4	4.85	1.45	1.33
28	S1	1866	OMC	C4-N4	4.85	1.45	1.33
2	2	443	OMC	C4-N4	4.83	1.45	1.33
28	S1	38	OMC	C4-N4	4.80	1.45	1.33
28	S1	2140	OMC	C4-N4	4.79	1.45	1.33
28	S1	18	OMC	C4-N4	4.79	1.45	1.33
1	1	1524	OMG	C2-N2	4.78	1.45	1.34
2	2	1317	OMC	C4-N4	4.78	1.45	1.33
2	2	1317	OMC	C4-N3	4.77	1.44	1.34
2	2	1360	OMG	C2-N2	4.77	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	1550	OMG	C2-N2	4.77	1.45	1.34
2	2	1159	OMC	C4-N4	4.76	1.45	1.33
1	1	1527	OMC	C4-N4	4.76	1.45	1.33
2	2	1248	OMC	C4-N4	4.75	1.45	1.33
2	2	583	OMC	C4-N4	4.74	1.45	1.33
28	S1	1623	OMG	C2-N2	4.73	1.45	1.34
2	2	1231	OMG	C2-N2	4.73	1.45	1.34
28	S1	1544	5MC	C6-N1	4.73	1.46	1.38
28	S1	1829	OMG	C2-N2	4.73	1.45	1.34
28	S1	1879	OMG	C2-N2	4.72	1.45	1.34
2	2	71	OMG	C2-N2	4.72	1.45	1.34
1	1	1010	OMC	C4-N4	4.72	1.45	1.33
28	S1	1647	OMG	C2-N2	4.72	1.45	1.34
1	1	959	OMG	C2-N2	4.71	1.45	1.34
28	S1	1865	OMG	C2-N2	4.70	1.45	1.34
28	S1	2061	5MC	C6-N1	4.69	1.46	1.38
1	1	1190	OMG	C2-N2	4.69	1.45	1.34
2	2	1046	OMG	C2-N2	4.68	1.45	1.34
2	2	655	OMG	C2-N2	4.68	1.45	1.34
1	1	856	OMG	C2-N2	4.68	1.45	1.34
1	1	695	OMC	C4-N4	4.67	1.44	1.33
28	S1	600	OMG	C2-N2	4.67	1.45	1.34
2	2	1229	OMG	C2-N2	4.64	1.45	1.34
2	2	534	OMG	C2-N2	4.62	1.45	1.34
2	2	1397	OMC	C4-N4	4.62	1.44	1.33
7	7	75	OMG	C2-N2	4.61	1.45	1.34
2	2	1253	OMG	C2-N2	4.61	1.45	1.34
28	S1	2140	OMC	C2-N1	4.60	1.50	1.40
4	4	74	OMG	C2-N2	4.60	1.45	1.34
2	2	641	OMG	C2-N2	4.59	1.45	1.34
1	1	1626	OMG	C2-N2	4.58	1.45	1.34
28	S1	2151	OMG	C2-N2	4.58	1.45	1.34
2	2	1248	OMC	C2-N1	4.58	1.49	1.40
1	1	1540	OMG	C2-N2	4.57	1.45	1.34
28	S1	1478	OMG	C2-N2	4.57	1.45	1.34
2	2	1308	5MC	C6-N1	4.57	1.45	1.38
2	2	1159	OMC	C2-N1	4.56	1.49	1.40
28	S1	2021	A2M	C6-N6	4.54	1.45	1.34
1	1	235	A2M	C6-N6	4.53	1.45	1.34
1	1	940	PSU	C1'-C5	-4.52	1.39	1.50
2	2	95	A2M	C6-N6	4.52	1.45	1.34
2	2	1060	PSU	C1'-C5	-4.51	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	1866	OMC	C2-N1	4.50	1.49	1.40
7	7	162	A2M	C6-N6	4.49	1.45	1.34
2	2	1372	A2M	C6-N6	4.48	1.45	1.34
1	1	305	A2M	C6-N6	4.48	1.45	1.34
1	1	927	A2M	C6-N6	4.48	1.45	1.34
28	S1	98	A2M	C6-N6	4.48	1.45	1.34
7	7	43	A2M	C6-N6	4.47	1.45	1.34
28	S1	1246	PSU	C1'-C5	-4.47	1.40	1.50
28	S1	479	A2M	C6-N6	4.47	1.45	1.34
2	2	572	A2M	C6-N6	4.47	1.45	1.34
2	2	591	A2M	C6-N6	4.47	1.45	1.34
1	1	1539	A2M	C6-N6	4.47	1.45	1.34
28	S1	668	A2M	C6-N6	4.46	1.45	1.34
1	1	407	A2M	C6-N6	4.46	1.45	1.34
28	S1	512	A2M	C6-N6	4.45	1.45	1.34
28	S1	1543	B8N	C1'-C5	-4.45	1.40	1.50
2	2	604	A2M	C6-N6	4.45	1.45	1.34
2	2	1185	A2M	C6-N6	4.45	1.45	1.34
2	2	1144	PSU	C1'-C5	-4.45	1.40	1.50
1	1	1010	OMC	C2-N1	4.44	1.49	1.40
1	1	1527	OMC	C2-N1	4.44	1.49	1.40
28	S1	104	PSU	C1'-C5	-4.44	1.40	1.50
1	1	858	A2M	C6-N6	4.43	1.45	1.34
2	2	524	5MC	C6-N1	4.40	1.45	1.38
2	2	382	A2M	C6-N6	4.40	1.45	1.34
1	1	695	OMC	C2-N1	4.39	1.49	1.40
1	1	697	A2M	C6-N6	4.39	1.45	1.34
2	2	628	A2M	C6-N6	4.39	1.45	1.34
1	1	239	PSU	C1'-C5	-4.39	1.40	1.50
28	S1	33	PSU	C1'-C5	-4.38	1.40	1.50
2	2	122	PSU	C1'-C5	-4.38	1.40	1.50
7	7	69	PSU	C1'-C5	-4.37	1.40	1.50
2	2	1303	PSU	C1'-C5	-4.37	1.40	1.50
2	2	1317	OMC	C2-N1	4.36	1.49	1.40
2	2	662	PSU	C1'-C5	-4.36	1.40	1.50
28	S1	18	OMC	C2-N1	4.36	1.49	1.40
1	1	955	A2M	C6-N6	4.36	1.45	1.34
28	S1	1544	5MC	C4-N4	4.35	1.45	1.34
28	S1	609	PSU	C1'-C5	-4.35	1.40	1.50
2	2	583	OMC	C2-N1	4.35	1.49	1.40
2	2	472	PSU	C1'-C5	-4.34	1.40	1.50
28	S1	2061	5MC	C4-N4	4.34	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	359	OMC	C2-N1	4.34	1.49	1.40
28	S1	1533	PSU	C1'-C5	-4.33	1.40	1.50
28	S1	1833	OMU	C4-N3	4.32	1.46	1.38
2	2	1403	PSU	C1'-C5	-4.31	1.40	1.50
28	S1	1657	PSU	C1'-C5	-4.31	1.40	1.50
2	2	1194	PSU	C1'-C5	-4.31	1.40	1.50
1	1	422	PSU	C1'-C5	-4.29	1.40	1.50
2	2	510	PSU	C1'-C5	-4.29	1.40	1.50
7	7	74	PSU	C1'-C5	-4.28	1.40	1.50
2	2	1361	PSU	C1'-C5	-4.28	1.40	1.50
1	1	1107	OMU	C4-N3	4.27	1.46	1.38
28	S1	2046	PSU	C1'-C5	-4.27	1.40	1.50
28	S1	1979	OMU	C4-N3	4.26	1.46	1.38
28	S1	1544	5MC	C2-N1	4.26	1.49	1.40
28	S1	1156	PSU	C1'-C5	-4.25	1.40	1.50
2	2	597	PSU	C1'-C5	-4.25	1.40	1.50
2	2	443	OMC	C2-N1	4.25	1.49	1.40
2	2	1308	5MC	C4-N4	4.24	1.45	1.34
1	1	1017	PSU	C1'-C5	-4.24	1.40	1.50
28	S1	1621	OMU	C4-N3	4.24	1.46	1.38
1	1	1533	PSU	C1'-C5	-4.24	1.40	1.50
2	2	524	5MC	C4-N4	4.23	1.45	1.34
2	2	437	PSU	C1'-C5	-4.22	1.40	1.50
2	2	78	PSU	C1'-C5	-4.22	1.40	1.50
1	1	1039	PSU	C1'-C5	-4.22	1.40	1.50
2	2	1265	PSU	C1'-C5	-4.21	1.40	1.50
28	S1	38	OMC	C2-N1	4.21	1.49	1.40
2	2	1397	OMC	C2-N1	4.21	1.49	1.40
2	2	1413	PSU	C1'-C5	-4.18	1.40	1.50
2	2	1318	PSU	C1'-C5	-4.17	1.40	1.50
28	S1	2202	PSU	C1'-C5	-4.17	1.40	1.50
2	2	1354	PSU	C1'-C5	-4.17	1.40	1.50
28	S1	29	OMU	C4-N3	4.17	1.46	1.38
2	2	593	PSU	C1'-C5	-4.17	1.40	1.50
1	1	1659	OMU	C4-N3	4.16	1.46	1.38
2	2	1058	PSU	C4-N3	4.16	1.46	1.38
28	S1	12	PSU	C1'-C5	-4.16	1.40	1.50
1	1	1528	PSU	C1'-C5	-4.15	1.40	1.50
2	2	1077	OMU	C4-N3	4.14	1.46	1.38
2	2	527	A2M	C6-N6	4.13	1.44	1.34
28	S1	1841	PSU	C1'-C5	-4.12	1.40	1.50
2	2	626	PSU	C1'-C5	-4.12	1.40	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	607	PSU	C1'-C5	-4.11	1.40	1.50
28	S1	1192	PSU	C1'-C5	-4.11	1.40	1.50
3	3	13	OMU	C4-N3	4.11	1.45	1.38
2	2	1359	OMU	C4-N3	4.11	1.45	1.38
2	2	667	OMU	C4-N3	4.11	1.45	1.38
1	1	1664	PSU	C1'-C5	-4.09	1.40	1.50
28	S1	1539	PSU	C1'-C5	-4.07	1.40	1.50
2	2	524	5MC	C2-N1	4.07	1.48	1.40
2	2	512	PSU	C1'-C5	-4.06	1.40	1.50
28	S1	1539	PSU	C4-N3	4.04	1.46	1.38
2	2	626	PSU	C4-N3	4.03	1.46	1.38
2	2	512	PSU	C4-N3	4.02	1.46	1.38
1	1	1371	OMU	C4-N3	4.02	1.45	1.38
28	S1	1566	PSU	C4-N3	4.02	1.46	1.38
28	S1	455	PSU	C1'-C5	-4.02	1.41	1.50
28	S1	661	OMU	C4-N3	4.02	1.45	1.38
1	1	1402	PSU	C1'-C5	-4.02	1.41	1.50
1	1	1171	PSU	C4-N3	4.00	1.46	1.38
2	2	56	OMU	C4-N3	3.99	1.45	1.38
28	S1	609	PSU	C4-N3	3.99	1.46	1.38
28	S1	2061	5MC	C2-N1	3.98	1.48	1.40
28	S1	607	PSU	C4-N3	3.98	1.46	1.38
28	S1	1841	PSU	C4-N3	3.98	1.46	1.38
28	S1	1566	PSU	C1'-C5	-3.97	1.41	1.50
2	2	1308	5MC	C2-N1	3.97	1.48	1.40
1	1	1011	PSU	C4-N3	3.96	1.46	1.38
1	1	1011	PSU	C1'-C5	-3.95	1.41	1.50
28	S1	2046	PSU	C4-N3	3.95	1.46	1.38
28	S1	1657	PSU	C4-N3	3.94	1.46	1.38
2	2	122	PSU	C4-N3	3.93	1.46	1.38
2	2	662	PSU	C4-N3	3.93	1.46	1.38
2	2	1265	PSU	C4-N3	3.93	1.46	1.38
2	2	472	PSU	C4-N3	3.93	1.46	1.38
28	S1	8	OMU	C4-N3	3.93	1.45	1.38
7	7	7	OMU	C4-N3	3.92	1.45	1.38
1	1	1039	PSU	C4-N3	3.92	1.46	1.38
28	S1	1533	PSU	C4-N3	3.91	1.46	1.38
28	S1	455	PSU	C4-N3	3.91	1.46	1.38
1	1	1402	PSU	C4-N3	3.90	1.46	1.38
28	S1	104	PSU	C4-N3	3.90	1.46	1.38
28	S1	1156	PSU	C4-N3	3.89	1.46	1.38
28	S1	1192	PSU	C4-N3	3.89	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1181	PSU	C1'-C5	-3.89	1.41	1.50
1	1	1017	PSU	C4-N3	3.89	1.46	1.38
2	2	1264	PSU	C1'-C5	-3.88	1.41	1.50
1	1	239	PSU	C4-N3	3.87	1.46	1.38
2	2	560	OMU	C4-N3	3.87	1.45	1.38
1	1	422	PSU	C4-N3	3.87	1.46	1.38
2	2	1318	PSU	C4-N3	3.87	1.46	1.38
2	2	1354	PSU	C4-N3	3.87	1.46	1.38
2	2	1303	PSU	C4-N3	3.87	1.46	1.38
1	1	1533	PSU	C4-N3	3.86	1.46	1.38
28	S1	33	PSU	C4-N3	3.86	1.46	1.38
7	7	74	PSU	C4-N3	3.86	1.46	1.38
2	2	1194	PSU	C4-N3	3.86	1.46	1.38
28	S1	1246	PSU	C4-N3	3.86	1.46	1.38
2	2	510	PSU	C4-N3	3.84	1.46	1.38
2	2	1144	PSU	C4-N3	3.83	1.45	1.38
2	2	437	PSU	C4-N3	3.83	1.45	1.38
2	2	1413	PSU	C4-N3	3.81	1.45	1.38
7	7	69	PSU	C4-N3	3.80	1.45	1.38
1	1	1664	PSU	C4-N3	3.80	1.45	1.38
1	1	1528	PSU	C4-N3	3.80	1.45	1.38
28	S1	12	PSU	C4-N3	3.80	1.45	1.38
2	2	78	PSU	C4-N3	3.80	1.45	1.38
2	2	1361	PSU	C4-N3	3.78	1.45	1.38
28	S1	2202	PSU	C4-N3	3.78	1.45	1.38
2	2	593	PSU	C4-N3	3.77	1.45	1.38
2	2	597	PSU	C4-N3	3.77	1.45	1.38
2	2	1403	PSU	C4-N3	3.76	1.45	1.38
2	2	73	OMU	C4-N3	3.76	1.45	1.38
2	2	1060	PSU	C4-N3	3.76	1.45	1.38
1	1	847	OMU	C4-N3	3.75	1.45	1.38
28	S1	1995	7MG	C6-N1	3.73	1.45	1.38
2	2	1264	PSU	C4-N3	3.73	1.45	1.38
1	1	1181	PSU	C4-N3	3.71	1.45	1.38
1	1	940	PSU	C4-N3	3.65	1.45	1.38
28	S1	2184	MA6	C6-N6	3.63	1.47	1.36
1	1	845	OMU	O2-C2	-3.61	1.16	1.23
28	S1	2185	MA6	C6-N6	3.60	1.47	1.36
28	S1	1995	7MG	C2-N1	3.60	1.46	1.37
28	S1	1995	7MG	C5-C6	3.53	1.52	1.43
2	2	1058	PSU	C1'-C5	-3.51	1.42	1.50
2	2	1317	OMC	C6-N1	3.38	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	534	OMG	C5-N7	-3.38	1.32	1.39
1	1	672	PSU	C6-C5	3.38	1.39	1.35
28	S1	1866	OMC	C6-N1	3.38	1.46	1.38
2	2	1382	PSU	C6-C5	3.37	1.39	1.35
2	2	1159	OMC	C6-N1	3.35	1.46	1.38
1	1	1527	OMC	C6-N1	3.35	1.46	1.38
2	2	1397	OMC	C6-N1	3.35	1.46	1.38
28	S1	1995	7MG	C2-N2	3.35	1.42	1.34
2	2	583	OMC	C6-N1	3.34	1.46	1.38
28	S1	1829	OMG	C5-N7	-3.33	1.32	1.39
28	S1	2048	PSU	C6-C5	3.33	1.39	1.35
1	1	1171	PSU	C1'-C5	-3.33	1.42	1.50
2	2	641	OMG	C5-N7	-3.33	1.32	1.39
1	1	695	OMC	C6-N1	3.31	1.46	1.38
2	2	655	OMG	C5-N7	-3.31	1.32	1.39
2	2	1229	OMG	C5-N7	-3.30	1.32	1.39
2	2	359	OMC	C6-N1	3.29	1.45	1.38
28	S1	1478	OMG	C5-N7	-3.29	1.32	1.39
28	S1	38	OMC	C6-N1	3.29	1.45	1.38
2	2	1248	OMC	C6-N1	3.27	1.45	1.38
28	S1	600	OMG	C5-N7	-3.26	1.32	1.39
2	2	1253	OMG	C5-N7	-3.26	1.32	1.39
1	1	1540	OMG	C5-N7	-3.26	1.32	1.39
28	S1	18	OMC	C6-N1	3.25	1.45	1.38
4	4	74	OMG	C5-N7	-3.25	1.32	1.39
2	2	443	OMC	C6-N1	3.24	1.45	1.38
2	2	1360	OMG	C5-N7	-3.23	1.32	1.39
28	S1	1833	OMU	O4-C4	-3.23	1.18	1.24
28	S1	2151	OMG	C5-N7	-3.22	1.32	1.39
7	7	162	A2M	O2'-C2'	3.21	1.50	1.42
2	2	71	OMG	C5-N7	-3.20	1.32	1.39
2	2	1078	OMG	C5-N7	-3.20	1.32	1.39
2	2	560	OMU	O4-C4	-3.18	1.18	1.24
1	1	235	A2M	O3'-C3'	-3.16	1.35	1.43
1	1	856	OMG	C5-N7	-3.16	1.33	1.39
2	2	667	OMU	O4-C4	-3.16	1.18	1.24
28	S1	1879	OMG	C5-N7	-3.15	1.33	1.39
1	1	845	OMU	C4-N3	3.15	1.44	1.38
28	S1	2140	OMC	C6-N1	3.15	1.45	1.38
7	7	162	A2M	O3'-C3'	-3.14	1.35	1.43
1	1	1190	OMG	C5-N7	-3.14	1.33	1.39
2	2	56	OMU	O4-C4	-3.13	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	845	OMU	O4-C4	-3.13	1.18	1.24
28	S1	1623	OMG	C5-N7	-3.12	1.33	1.39
28	S1	8	OMU	O4-C4	-3.11	1.18	1.24
2	2	591	A2M	O3'-C3'	-3.11	1.35	1.43
2	2	1046	OMG	C5-N7	-3.11	1.33	1.39
1	1	1010	OMC	C6-N1	3.10	1.45	1.38
1	1	1626	OMG	C5-N7	-3.10	1.33	1.39
28	S1	1995	7MG	O6-C6	-3.10	1.17	1.23
28	S1	661	OMU	O4-C4	-3.09	1.18	1.24
28	S1	1647	OMG	C5-N7	-3.09	1.33	1.39
7	7	43	A2M	O3'-C3'	-3.08	1.35	1.43
28	S1	2021	A2M	O2'-C2'	3.08	1.50	1.42
2	2	95	A2M	O3'-C3'	-3.07	1.35	1.43
2	2	73	OMU	O4-C4	-3.06	1.18	1.24
1	1	1107	OMU	O4-C4	-3.06	1.18	1.24
1	1	1371	OMU	O4-C4	-3.06	1.18	1.24
3	3	13	OMU	O4-C4	-3.05	1.18	1.24
1	1	1524	OMG	C5-N7	-3.05	1.33	1.39
2	2	1359	OMU	C6-N1	3.04	1.45	1.38
2	2	1308	5MC	O2'-C2'	-3.04	1.35	1.43
1	1	959	OMG	C5-N7	-3.03	1.33	1.39
28	S1	1550	OMG	C5-N7	-3.03	1.33	1.39
1	1	847	OMU	O4-C4	-3.02	1.18	1.24
2	2	73	OMU	C6-N1	3.02	1.45	1.38
28	S1	1865	OMG	C5-N7	-3.02	1.33	1.39
1	1	407	A2M	O3'-C3'	-3.01	1.35	1.43
7	7	7	OMU	C6-N1	3.01	1.45	1.38
2	2	667	OMU	C6-N1	3.01	1.45	1.38
28	S1	98	A2M	O3'-C3'	-3.00	1.35	1.43
2	2	527	A2M	C5-C4	-3.00	1.33	1.39
28	S1	29	OMU	C6-N1	3.00	1.45	1.38
2	2	382	A2M	O2'-C2'	3.00	1.50	1.42
2	2	1359	OMU	O4-C4	-3.00	1.18	1.24
1	1	1659	OMU	C6-N1	2.99	1.45	1.38
2	2	1185	A2M	O3'-C3'	-2.99	1.35	1.43
3	3	13	OMU	C6-N1	2.99	1.45	1.38
2	2	1231	OMG	C5-N7	-2.99	1.33	1.39
28	S1	1621	OMU	O4-C4	-2.99	1.18	1.24
2	2	572	A2M	C5-C4	-2.99	1.33	1.39
2	2	443	OMC	O2-C2	-2.98	1.18	1.23
28	S1	1979	OMU	C6-N1	2.98	1.45	1.38
28	S1	661	OMU	C6-N1	2.98	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	75	OMG	C5-N7	-2.98	1.33	1.39
2	2	95	A2M	O2'-C2'	2.97	1.50	1.42
1	1	955	A2M	O3'-C3'	-2.97	1.36	1.43
2	2	1077	OMU	C6-N1	2.97	1.45	1.38
28	S1	1621	OMU	C6-N1	2.96	1.45	1.38
7	7	7	OMU	O4-C4	-2.96	1.18	1.24
2	2	382	A2M	O3'-C3'	-2.96	1.36	1.43
28	S1	29	OMU	O4-C4	-2.96	1.18	1.24
1	1	1659	OMU	O4-C4	-2.95	1.18	1.24
1	1	1371	OMU	C6-N1	2.95	1.45	1.38
28	S1	668	A2M	O2'-C2'	2.94	1.50	1.42
1	1	847	OMU	C6-N1	2.94	1.45	1.38
2	2	572	A2M	O3'-C3'	-2.93	1.36	1.43
28	S1	2185	MA6	C5-C4	-2.93	1.33	1.39
1	1	235	A2M	O2'-C2'	2.92	1.50	1.42
1	1	858	A2M	O3'-C3'	-2.92	1.36	1.43
28	S1	1979	OMU	O4-C4	-2.91	1.18	1.24
2	2	628	A2M	C5-C4	-2.90	1.33	1.39
2	2	1077	OMU	O4-C4	-2.90	1.18	1.24
2	2	1264	PSU	O4-C4	-2.89	1.18	1.23
1	1	927	A2M	O3'-C3'	-2.89	1.36	1.43
1	1	858	A2M	C5-C4	-2.89	1.33	1.39
28	S1	8	OMU	C6-N1	2.88	1.44	1.38
1	1	235	A2M	C5-C4	-2.88	1.33	1.39
2	2	1372	A2M	C5-C4	-2.87	1.33	1.39
2	2	78	PSU	O4-C4	-2.87	1.18	1.23
1	1	697	A2M	C5-C4	-2.87	1.33	1.39
2	2	56	OMU	C6-N1	2.86	1.44	1.38
2	2	1372	A2M	O3'-C3'	-2.86	1.36	1.43
1	1	407	A2M	C5-C4	-2.86	1.33	1.39
2	2	604	A2M	O3'-C3'	-2.86	1.36	1.43
28	S1	479	A2M	O2'-C2'	2.86	1.49	1.42
1	1	305	A2M	C5-C4	-2.86	1.33	1.39
2	2	1397	OMC	O2-C2	-2.86	1.18	1.23
28	S1	2021	A2M	O3'-C3'	-2.85	1.36	1.43
28	S1	512	A2M	O3'-C3'	-2.85	1.36	1.43
28	S1	512	A2M	C5-C4	-2.85	1.33	1.39
2	2	1317	OMC	O2-C2	-2.85	1.18	1.23
2	2	560	OMU	C6-N1	2.84	1.44	1.38
1	1	927	A2M	C5-C4	-2.84	1.33	1.39
1	1	697	A2M	O3'-C3'	-2.84	1.36	1.43
2	2	628	A2M	O3'-C3'	-2.84	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	858	A2M	O2'-C2'	2.83	1.49	1.42
2	2	591	A2M	O2'-C2'	2.83	1.49	1.42
2	2	604	A2M	O2'-C2'	2.83	1.49	1.42
1	1	697	A2M	O2'-C2'	2.83	1.49	1.42
1	1	1527	OMC	O2-C2	-2.83	1.18	1.23
7	7	43	A2M	C5-C4	-2.81	1.33	1.39
28	S1	479	A2M	O3'-C3'	-2.81	1.36	1.43
1	1	305	A2M	O3'-C3'	-2.81	1.36	1.43
2	2	591	A2M	C5-C4	-2.81	1.33	1.39
2	2	604	A2M	C5-C4	-2.80	1.33	1.39
1	1	955	A2M	O2'-C2'	2.80	1.49	1.42
28	S1	38	OMC	O2-C2	-2.80	1.18	1.23
2	2	359	OMC	O2-C2	-2.80	1.18	1.23
28	S1	98	A2M	O2'-C2'	2.79	1.49	1.42
2	2	583	OMC	O2-C2	-2.79	1.18	1.23
28	S1	668	A2M	O3'-C3'	-2.79	1.36	1.43
1	1	955	A2M	C5-C4	-2.78	1.33	1.39
7	7	162	A2M	C5-C4	-2.78	1.33	1.39
2	2	1248	OMC	O2-C2	-2.78	1.18	1.23
2	2	1308	5MC	O2-C2	-2.78	1.18	1.23
7	7	43	A2M	O2'-C2'	2.78	1.49	1.42
2	2	626	PSU	O4-C4	-2.78	1.18	1.23
2	2	527	A2M	O2'-C2'	2.78	1.49	1.42
2	2	1372	A2M	O2'-C2'	2.78	1.49	1.42
28	S1	668	A2M	C5-C4	-2.77	1.33	1.39
1	1	1539	A2M	O3'-C3'	-2.77	1.36	1.43
28	S1	2021	A2M	C5-C4	-2.77	1.33	1.39
28	S1	1833	OMU	C6-N1	2.77	1.44	1.38
28	S1	98	A2M	C5-C4	-2.77	1.33	1.39
1	1	1107	OMU	C6-N1	2.77	1.44	1.38
2	2	1159	OMC	O2-C2	-2.76	1.18	1.23
28	S1	512	A2M	O2'-C2'	2.76	1.49	1.42
1	1	1664	PSU	O4-C4	-2.76	1.18	1.23
1	1	239	PSU	O4-C4	-2.75	1.18	1.23
2	2	572	A2M	O2'-C2'	2.75	1.49	1.42
28	S1	18	OMC	O2-C2	-2.75	1.18	1.23
2	2	437	PSU	O4-C4	-2.75	1.18	1.23
1	1	1181	PSU	O4-C4	-2.74	1.18	1.23
2	2	1078	OMG	O6-C6	-2.74	1.18	1.23
28	S1	1866	OMC	O2-C2	-2.74	1.18	1.23
2	2	382	A2M	C5-C4	-2.74	1.33	1.39
2	2	1185	A2M	O2'-C2'	2.73	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1528	PSU	O4-C4	-2.73	1.18	1.23
1	1	695	OMC	O2-C2	-2.73	1.18	1.23
1	1	927	A2M	O2'-C2'	2.72	1.49	1.42
2	2	1185	A2M	C5-C4	-2.72	1.33	1.39
28	S1	2061	5MC	O2-C2	-2.72	1.18	1.23
28	S1	1865	OMG	C2-N1	2.72	1.44	1.37
2	2	628	A2M	O2'-C2'	2.72	1.49	1.42
2	2	1413	PSU	O4-C4	-2.72	1.18	1.23
2	2	95	A2M	C5-N7	-2.72	1.33	1.39
2	2	1253	OMG	O6-C6	-2.72	1.18	1.23
28	S1	1879	OMG	C2-N1	2.71	1.44	1.37
2	2	1372	A2M	C5-N7	-2.71	1.33	1.39
2	2	1403	PSU	O4-C4	-2.71	1.18	1.23
7	7	43	A2M	C5-N7	-2.71	1.33	1.39
2	2	524	5MC	O2-C2	-2.71	1.18	1.23
2	2	591	A2M	C5-N7	-2.71	1.33	1.39
2	2	71	OMG	O6-C6	-2.71	1.18	1.23
1	1	1539	A2M	C5-C4	-2.70	1.34	1.39
28	S1	1623	OMG	C2-N1	2.70	1.44	1.37
2	2	1046	OMG	C2-N1	2.70	1.44	1.37
2	2	1360	OMG	C2-N1	2.70	1.44	1.37
1	1	959	OMG	C2-N1	2.69	1.44	1.37
2	2	382	A2M	C5-N7	-2.69	1.33	1.39
1	1	1539	A2M	O2'-C2'	2.69	1.49	1.42
28	S1	1829	OMG	C2-N1	2.69	1.44	1.37
1	1	697	A2M	C5-N7	-2.69	1.33	1.39
2	2	662	PSU	O4-C4	-2.68	1.18	1.23
28	S1	1478	OMG	C2-N1	2.68	1.44	1.37
28	S1	1647	OMG	C2-N1	2.68	1.44	1.37
28	S1	479	A2M	C5-C4	-2.68	1.34	1.39
1	1	407	A2M	C5-N7	-2.68	1.34	1.39
1	1	1010	OMC	O2-C2	-2.68	1.18	1.23
1	1	407	A2M	O2'-C2'	2.68	1.49	1.42
1	1	1524	OMG	C2-N1	2.68	1.44	1.37
1	1	305	A2M	C5-N7	-2.67	1.34	1.39
2	2	1308	5MC	O3'-C3'	2.67	1.49	1.43
1	1	856	OMG	O6-C6	-2.67	1.18	1.23
2	2	534	OMG	O6-C6	-2.67	1.18	1.23
28	S1	2046	PSU	O4-C4	-2.67	1.18	1.23
28	S1	1544	5MC	O2-C2	-2.67	1.18	1.23
2	2	593	PSU	O4-C4	-2.67	1.18	1.23
1	1	1533	PSU	O4-C4	-2.66	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1361	PSU	O4-C4	-2.66	1.18	1.23
2	2	1318	PSU	O4-C4	-2.65	1.18	1.23
1	1	1540	OMG	C2-N1	2.65	1.44	1.37
2	2	1229	OMG	C2-N1	2.65	1.44	1.37
2	2	95	A2M	C5-C4	-2.65	1.34	1.39
2	2	527	A2M	C5-N7	-2.65	1.34	1.39
2	2	1231	OMG	O6-C6	-2.65	1.18	1.23
1	1	1171	PSU	O4-C4	-2.65	1.18	1.23
1	1	927	A2M	C5-N7	-2.64	1.34	1.39
2	2	534	OMG	C2-N1	2.64	1.44	1.37
1	1	1017	PSU	O4-C4	-2.63	1.18	1.23
28	S1	2184	MA6	C5-C4	-2.63	1.34	1.39
1	1	1539	A2M	C5-N7	-2.63	1.34	1.39
28	S1	600	OMG	C2-N1	2.63	1.44	1.37
28	S1	1657	PSU	O4-C4	-2.63	1.18	1.23
2	2	583	OMC	C5-C4	2.63	1.48	1.42
2	2	655	OMG	O6-C6	-2.63	1.18	1.23
7	7	75	OMG	C2-N1	2.63	1.44	1.37
2	2	1144	PSU	O4-C4	-2.63	1.18	1.23
28	S1	479	A2M	C5-N7	-2.63	1.34	1.39
7	7	69	PSU	O4-C4	-2.63	1.18	1.23
2	2	1229	OMG	O6-C6	-2.63	1.18	1.23
1	1	305	A2M	O2'-C2'	2.63	1.49	1.42
28	S1	1550	OMG	C2-N1	2.63	1.44	1.37
2	2	71	OMG	C2-N1	2.63	1.44	1.37
2	2	1253	OMG	C2-N1	2.63	1.44	1.37
1	1	1039	PSU	O4-C4	-2.63	1.18	1.23
2	2	1194	PSU	O4-C4	-2.62	1.18	1.23
1	1	422	PSU	O4-C4	-2.62	1.18	1.23
1	1	1402	PSU	O4-C4	-2.62	1.18	1.23
2	2	1354	PSU	O4-C4	-2.61	1.18	1.23
7	7	74	PSU	O4-C4	-2.61	1.18	1.23
2	2	1303	PSU	O4-C4	-2.61	1.18	1.23
28	S1	2184	MA6	C5-N7	-2.61	1.34	1.39
1	1	856	OMG	C2-N1	2.60	1.44	1.37
28	S1	1550	OMG	O6-C6	-2.60	1.18	1.23
2	2	641	OMG	C2-N1	2.60	1.44	1.37
2	2	597	PSU	O4-C4	-2.60	1.18	1.23
2	2	604	A2M	C5-N7	-2.60	1.34	1.39
2	2	443	OMC	C5-C4	2.59	1.48	1.42
2	2	641	OMG	O6-C6	-2.59	1.18	1.23
28	S1	2151	OMG	C2-N1	2.59	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	74	OMG	O6-C6	-2.59	1.18	1.23
28	S1	512	A2M	C5-N7	-2.59	1.34	1.39
1	1	955	A2M	C5-N7	-2.59	1.34	1.39
2	2	1248	OMC	C5-C4	2.59	1.48	1.42
28	S1	2140	OMC	O2-C2	-2.59	1.18	1.23
2	2	1231	OMG	C2-N1	2.58	1.44	1.37
2	2	527	A2M	O3'-C3'	-2.58	1.36	1.43
2	2	1185	A2M	C5-N7	-2.58	1.34	1.39
4	4	74	OMG	C2-N1	2.58	1.44	1.37
2	2	122	PSU	O4-C4	-2.58	1.18	1.23
1	1	940	PSU	O4-C4	-2.58	1.18	1.23
28	S1	33	PSU	O4-C4	-2.58	1.18	1.23
2	2	655	OMG	C2-N1	2.57	1.44	1.37
2	2	1060	PSU	O4-C4	-2.57	1.18	1.23
2	2	122	PSU	O4'-C1'	-2.57	1.40	1.43
28	S1	98	A2M	C5-N7	-2.57	1.34	1.39
28	S1	455	PSU	O4-C4	-2.57	1.18	1.23
2	2	1360	OMG	O6-C6	-2.57	1.18	1.23
28	S1	668	A2M	C5-N7	-2.57	1.34	1.39
1	1	959	OMG	C5-C6	2.57	1.53	1.44
1	1	235	A2M	C5-N7	-2.56	1.34	1.39
28	S1	12	PSU	O4-C4	-2.56	1.18	1.23
28	S1	2202	PSU	O4-C4	-2.56	1.18	1.23
28	S1	1647	OMG	O6-C6	-2.56	1.18	1.23
1	1	1540	OMG	C5-C6	2.55	1.53	1.44
28	S1	1866	OMC	C5-C4	2.55	1.48	1.42
1	1	1626	OMG	C2-N1	2.55	1.44	1.37
1	1	1626	OMG	O6-C6	-2.55	1.18	1.23
2	2	1397	OMC	C5-C4	2.55	1.48	1.42
2	2	1046	OMG	O6-C6	-2.55	1.18	1.23
1	1	1190	OMG	C2-N1	2.55	1.44	1.37
28	S1	600	OMG	O6-C6	-2.55	1.18	1.23
1	1	858	A2M	C5-N7	-2.54	1.34	1.39
2	2	1058	PSU	O4-C4	-2.54	1.18	1.23
28	S1	1623	OMG	O6-C6	-2.54	1.18	1.23
2	2	359	OMC	C5-C4	2.54	1.48	1.42
28	S1	1841	PSU	O4-C4	-2.53	1.18	1.23
1	1	959	OMG	O6-C6	-2.53	1.18	1.23
1	1	1626	OMG	C5-C6	2.53	1.53	1.44
28	S1	607	PSU	O4-C4	-2.53	1.18	1.23
2	2	512	PSU	O4-C4	-2.53	1.18	1.23
28	S1	38	OMC	C5-C4	2.53	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	472	PSU	O4-C4	-2.52	1.18	1.23
28	S1	1550	OMG	C5-C6	2.52	1.53	1.44
2	2	641	OMG	C5-C6	2.52	1.53	1.44
2	2	1159	OMC	C5-C4	2.52	1.48	1.42
28	S1	1192	PSU	O4-C4	-2.52	1.18	1.23
28	S1	1246	PSU	O4-C4	-2.52	1.18	1.23
2	2	1265	PSU	O4-C4	-2.52	1.18	1.23
28	S1	1478	OMG	O6-C6	-2.52	1.18	1.23
28	S1	2185	MA6	C5-N7	-2.52	1.34	1.39
1	1	1371	OMU	O2-C2	-2.51	1.18	1.23
28	S1	1879	OMG	C5-C6	2.51	1.53	1.44
28	S1	609	PSU	O4-C4	-2.51	1.18	1.23
2	2	655	OMG	C5-C6	2.51	1.53	1.44
1	1	1540	OMG	O6-C6	-2.51	1.18	1.23
2	2	1046	OMG	C5-C6	2.51	1.53	1.44
28	S1	1865	OMG	O6-C6	-2.51	1.18	1.23
1	1	1010	OMC	C5-C4	2.51	1.48	1.42
28	S1	2151	OMG	C5-C6	2.50	1.53	1.44
1	1	1190	OMG	O6-C6	-2.50	1.18	1.23
1	1	1524	OMG	C5-C6	2.50	1.53	1.44
2	2	1253	OMG	C5-C6	2.50	1.53	1.44
2	2	510	PSU	O4-C4	-2.50	1.18	1.23
2	2	572	A2M	C5-N7	-2.50	1.34	1.39
7	7	75	OMG	O6-C6	-2.50	1.18	1.23
2	2	1317	OMC	C5-C4	2.49	1.48	1.42
28	S1	1647	OMG	C6-N1	2.49	1.43	1.38
2	2	667	OMU	C5-C4	2.49	1.49	1.43
28	S1	1865	OMG	C5-C6	2.49	1.53	1.44
28	S1	8	OMU	C5-C4	2.49	1.49	1.43
28	S1	1566	PSU	O4-C4	-2.49	1.18	1.23
28	S1	1621	OMU	C5-C4	2.49	1.49	1.43
28	S1	1533	PSU	O4-C4	-2.48	1.18	1.23
28	S1	1539	PSU	O4-C4	-2.48	1.18	1.23
1	1	1190	OMG	C5-C6	2.48	1.53	1.44
1	1	305	A2M	O5'-C5'	-2.48	1.38	1.44
1	1	856	OMG	C5-C6	2.48	1.53	1.44
28	S1	2151	OMG	O6-C6	-2.48	1.18	1.23
28	S1	1156	PSU	O4-C4	-2.48	1.18	1.23
28	S1	661	OMU	C5-C4	2.47	1.49	1.43
2	2	1359	OMU	C5-C4	2.47	1.49	1.43
1	1	1011	PSU	O4-C4	-2.47	1.18	1.23
2	2	628	A2M	C5-N7	-2.47	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	2021	A2M	C5-N7	-2.47	1.34	1.39
28	S1	1647	OMG	C5-C6	2.46	1.53	1.44
1	1	1527	OMC	C5-C4	2.46	1.48	1.42
1	1	1524	OMG	O6-C6	-2.46	1.18	1.23
28	S1	1879	OMG	O6-C6	-2.46	1.18	1.23
2	2	1231	OMG	C5-C6	2.46	1.53	1.44
28	S1	1623	OMG	C6-N1	2.46	1.43	1.38
1	1	1659	OMU	O2-C2	-2.46	1.18	1.23
2	2	1077	OMU	C5-C4	2.45	1.49	1.43
2	2	1229	OMG	C5-C6	2.45	1.53	1.44
1	1	1107	OMU	C5-C4	2.45	1.49	1.43
7	7	75	OMG	C5-C6	2.45	1.53	1.44
1	1	695	OMC	C5-C4	2.44	1.48	1.42
28	S1	2151	OMG	C6-N1	2.44	1.43	1.38
1	1	1524	OMG	C6-N1	2.44	1.43	1.38
28	S1	104	PSU	O4-C4	-2.44	1.19	1.23
4	4	74	OMG	C5-C6	2.44	1.53	1.44
2	2	1078	OMG	C2-N1	2.44	1.43	1.37
2	2	1360	OMG	C5-C6	2.43	1.53	1.44
28	S1	1865	OMG	C6-N1	2.43	1.43	1.38
28	S1	600	OMG	C5-C6	2.43	1.53	1.44
28	S1	1478	OMG	C5-C6	2.43	1.53	1.44
7	7	162	A2M	C5-N7	-2.43	1.34	1.39
28	S1	1829	OMG	O6-C6	-2.42	1.19	1.23
28	S1	18	OMC	C5-C4	2.42	1.48	1.42
28	S1	1623	OMG	C5-C6	2.42	1.53	1.44
2	2	1046	OMG	C6-N1	2.41	1.43	1.38
28	S1	1829	OMG	C5-C6	2.41	1.53	1.44
1	1	1171	PSU	O4'-C1'	-2.40	1.40	1.43
3	3	13	OMU	C5-C4	2.40	1.48	1.43
28	S1	29	OMU	C5-C4	2.40	1.48	1.43
1	1	959	OMG	C6-N1	2.40	1.43	1.38
1	1	1190	OMG	C6-N1	2.40	1.43	1.38
2	2	73	OMU	C5-C4	2.40	1.48	1.43
2	2	73	OMU	O2-C2	-2.40	1.18	1.23
2	2	56	OMU	C5-C4	2.40	1.48	1.43
3	3	13	OMU	O2-C2	-2.40	1.18	1.23
28	S1	661	OMU	O2-C2	-2.40	1.18	1.23
1	1	1540	OMG	C6-N1	2.40	1.43	1.38
1	1	1659	OMU	C5-C4	2.39	1.48	1.43
2	2	71	OMG	C5-C6	2.39	1.53	1.44
28	S1	1879	OMG	C6-N1	2.38	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	7	OMU	C5-C4	2.38	1.48	1.43
7	7	7	OMU	O2-C2	-2.37	1.18	1.23
1	1	845	OMU	C6-N1	2.37	1.43	1.38
2	2	534	OMG	C5-C6	2.36	1.53	1.44
28	S1	1550	OMG	C6-N1	2.36	1.43	1.38
7	7	75	OMG	C6-N1	2.36	1.43	1.38
2	2	667	OMU	O2-C2	-2.35	1.18	1.23
2	2	527	A2M	O5'-C5'	-2.35	1.39	1.44
1	1	847	OMU	O2-C2	-2.35	1.18	1.23
2	2	1372	A2M	C8-N9	-2.35	1.33	1.37
2	2	1077	OMU	O2-C2	-2.35	1.18	1.23
28	S1	600	OMG	C6-N1	2.34	1.43	1.38
28	S1	2140	OMC	C5-C4	2.34	1.48	1.42
2	2	56	OMU	O2-C2	-2.33	1.18	1.23
2	2	1078	OMG	C5-C6	2.33	1.53	1.44
28	S1	1478	OMG	C6-N1	2.33	1.43	1.38
2	2	534	OMG	C6-N1	2.32	1.43	1.38
28	S1	1829	OMG	C6-N1	2.32	1.43	1.38
28	S1	1979	OMU	C5-C4	2.32	1.48	1.43
2	2	1360	OMG	C6-N1	2.32	1.43	1.38
28	S1	8	OMU	O2-C2	-2.32	1.18	1.23
28	S1	2185	MA6	C4-N9	-2.31	1.32	1.37
2	2	560	OMU	O2-C2	-2.31	1.18	1.23
1	1	1011	PSU	O4'-C1'	-2.31	1.40	1.43
1	1	1371	OMU	C5-C4	2.28	1.48	1.43
1	1	1626	OMG	C6-N1	2.28	1.43	1.38
2	2	1229	OMG	C6-N1	2.28	1.43	1.38
1	1	847	OMU	C5-C4	2.28	1.48	1.43
2	2	1359	OMU	O2-C2	-2.27	1.18	1.23
1	1	1107	OMU	O2-C2	-2.27	1.18	1.23
2	2	1253	OMG	C6-N1	2.26	1.43	1.38
1	1	856	OMG	C6-N1	2.26	1.43	1.38
1	1	1011	PSU	C4-C5	2.26	1.50	1.44
28	S1	1833	OMU	C5-C4	2.25	1.48	1.43
2	2	655	OMG	C6-N1	2.25	1.43	1.38
4	4	74	OMG	C6-N1	2.25	1.43	1.38
28	S1	29	OMU	O2-C2	-2.24	1.18	1.23
28	S1	1979	OMU	O2-C2	-2.24	1.18	1.23
2	2	628	A2M	O5'-C5'	-2.24	1.39	1.44
28	S1	668	A2M	C8-N9	-2.24	1.33	1.37
2	2	71	OMG	C6-N1	2.23	1.43	1.38
2	2	1231	OMG	C6-N1	2.22	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	1833	OMU	O2-C2	-2.22	1.19	1.23
2	2	560	OMU	C5-C4	2.20	1.48	1.43
2	2	641	OMG	C6-N1	2.20	1.42	1.38
28	S1	1621	OMU	O2-C2	-2.20	1.19	1.23
28	S1	1566	PSU	C4-C5	2.19	1.50	1.44
1	1	845	OMU	C5-C4	2.19	1.48	1.43
1	1	858	A2M	C8-N9	-2.18	1.33	1.37
1	1	927	A2M	C8-N9	-2.17	1.33	1.37
2	2	95	A2M	C8-N9	-2.17	1.33	1.37
1	1	1402	PSU	C4-C5	2.16	1.50	1.44
1	1	955	A2M	O5'-C5'	-2.15	1.39	1.44
7	7	43	A2M	O5'-C5'	-2.14	1.39	1.44
28	S1	668	A2M	O5'-C5'	-2.14	1.39	1.44
28	S1	607	PSU	C4-C5	2.13	1.50	1.44
28	S1	455	PSU	C4-C5	2.12	1.50	1.44
2	2	1354	PSU	C4-C5	2.12	1.50	1.44
2	2	1185	A2M	C8-N9	-2.11	1.33	1.37
1	1	305	A2M	C8-N9	-2.11	1.33	1.37
1	1	955	A2M	C8-N9	-2.10	1.33	1.37
7	7	43	A2M	C8-N9	-2.10	1.33	1.37
1	1	927	A2M	O5'-C5'	-2.09	1.39	1.44
28	S1	2202	PSU	C4-C5	2.09	1.50	1.44
2	2	604	A2M	C8-N9	-2.09	1.33	1.37
2	2	1308	5MC	O5'-C5'	-2.08	1.39	1.44
28	S1	2021	A2M	C8-N9	-2.08	1.33	1.37
1	1	1539	A2M	O5'-C5'	-2.08	1.39	1.44
2	2	591	A2M	O5'-C5'	-2.08	1.39	1.44
7	7	162	A2M	O5'-C5'	-2.08	1.39	1.44
28	S1	479	A2M	C8-N9	-2.07	1.33	1.37
2	2	527	A2M	C8-N9	-2.07	1.33	1.37
2	2	1185	A2M	O5'-C5'	-2.07	1.39	1.44
28	S1	98	A2M	C8-N9	-2.07	1.33	1.37
1	1	858	A2M	O5'-C5'	-2.06	1.39	1.44
28	S1	1539	PSU	C4-C5	2.05	1.50	1.44
2	2	572	A2M	O5'-C5'	-2.05	1.39	1.44
2	2	591	A2M	C8-N9	-2.04	1.33	1.37
28	S1	512	A2M	C8-N9	-2.03	1.33	1.37
1	1	1539	A2M	C8-N9	-2.03	1.33	1.37
1	1	697	A2M	C8-N9	-2.03	1.33	1.37
28	S1	2021	A2M	O5'-C5'	-2.03	1.39	1.44
1	1	407	A2M	C8-N9	-2.02	1.33	1.37
2	2	593	PSU	C4-C5	2.02	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S1	98	A2M	O5'-C5'	-2.02	1.39	1.44
1	1	235	A2M	C8-N9	-2.02	1.33	1.37
28	S1	1841	PSU	C4-C5	2.01	1.49	1.44
28	S1	2184	MA6	C4-N9	-2.01	1.33	1.37
2	2	1264	PSU	C4-C5	2.01	1.49	1.44
28	S1	2151	OMG	C4-N9	-2.01	1.32	1.38
1	1	1402	PSU	O4'-C1'	-2.01	1.41	1.43
7	7	162	A2M	C8-N9	-2.01	1.33	1.37
1	1	1181	PSU	C4-C5	2.00	1.49	1.44

All (920) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	2184	MA6	N1-C6-N6	-10.55	105.55	117.08
28	S1	2185	MA6	N1-C6-N6	-10.38	105.73	117.08
2	2	1078	OMG	C5-C4-N3	-6.44	118.01	128.46
1	1	845	OMU	C4-N3-C2	-6.29	118.29	126.58
2	2	95	A2M	C5-C4-N3	-6.06	118.85	126.75
2	2	655	OMG	C5-C4-N3	-6.00	118.72	128.46
2	2	534	OMG	C5-C4-N3	-5.93	118.83	128.46
2	2	572	A2M	N3-C2-N1	-5.90	119.37	128.60
7	7	43	A2M	N3-C2-N1	-5.84	119.47	128.60
28	S1	600	OMG	C5-C4-N3	-5.79	119.07	128.46
7	7	162	A2M	N3-C2-N1	-5.77	119.57	128.60
1	1	845	OMU	N3-C2-N1	5.77	122.55	114.89
2	2	591	A2M	N3-C2-N1	-5.75	119.61	128.60
2	2	628	A2M	N3-C2-N1	-5.74	119.63	128.60
1	1	697	A2M	N3-C2-N1	-5.73	119.64	128.60
2	2	560	OMU	C4-N3-C2	-5.69	119.08	126.58
28	S1	1833	OMU	C4-N3-C2	-5.68	119.08	126.58
2	2	1372	A2M	N3-C2-N1	-5.67	119.73	128.60
1	1	235	A2M	N3-C2-N1	-5.67	119.73	128.60
1	1	927	A2M	N3-C2-N1	-5.63	119.79	128.60
28	S1	2021	A2M	N3-C2-N1	-5.60	119.84	128.60
28	S1	512	A2M	N3-C2-N1	-5.58	119.87	128.60
2	2	1253	OMG	C5-C4-N3	-5.57	119.42	128.46
1	1	858	A2M	N3-C2-N1	-5.56	119.90	128.60
2	2	604	A2M	N3-C2-N1	-5.56	119.90	128.60
2	2	1229	OMG	C5-C4-N3	-5.55	119.46	128.46
2	2	527	A2M	N3-C2-N1	-5.55	119.92	128.60
28	S1	668	A2M	N3-C2-N1	-5.54	119.93	128.60
28	S1	1829	OMG	C5-C4-N3	-5.54	119.47	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1078	OMG	N9-C4-N3	5.53	137.05	125.94
1	1	407	A2M	N3-C2-N1	-5.53	119.95	128.60
28	S1	2184	MA6	N1-C2-N3	-5.53	119.95	128.60
1	1	955	A2M	N3-C2-N1	-5.53	119.96	128.60
1	1	1107	OMU	C4-N3-C2	-5.52	119.29	126.58
2	2	382	A2M	C5-C4-N3	-5.52	119.55	126.75
2	2	667	OMU	C4-N3-C2	-5.51	119.31	126.58
28	S1	2184	MA6	C5-C6-N6	5.51	134.89	125.30
28	S1	479	A2M	N3-C2-N1	-5.49	120.01	128.60
28	S1	1550	OMG	C5-C4-N3	-5.49	119.56	128.46
28	S1	98	A2M	N3-C2-N1	-5.48	120.03	128.60
7	7	7	OMU	C4-N3-C2	-5.47	119.36	126.58
2	2	56	OMU	C4-N3-C2	-5.47	119.36	126.58
2	2	1077	OMU	C4-N3-C2	-5.47	119.37	126.58
2	2	1185	A2M	N3-C2-N1	-5.47	120.05	128.60
28	S1	8	OMU	C4-N3-C2	-5.46	119.37	126.58
1	1	1539	A2M	C5-C4-N3	-5.46	119.62	126.75
2	2	1046	OMG	C5-C4-N3	-5.46	119.60	128.46
2	2	71	OMG	C5-C4-N3	-5.45	119.62	128.46
1	1	305	A2M	N3-C2-N1	-5.44	120.09	128.60
4	4	74	OMG	C5-C4-N3	-5.43	119.65	128.46
7	7	43	A2M	C5-C4-N3	-5.42	119.68	126.75
28	S1	1879	OMG	C5-C4-N3	-5.41	119.68	128.46
1	1	959	OMG	C5-C4-N3	-5.41	119.69	128.46
2	2	1360	OMG	C5-C4-N3	-5.40	119.69	128.46
2	2	382	A2M	N3-C2-N1	-5.40	120.16	128.60
28	S1	661	OMU	C4-N3-C2	-5.38	119.48	126.58
1	1	1659	OMU	C4-N3-C2	-5.36	119.50	126.58
28	S1	1647	OMG	C5-C4-N3	-5.36	119.77	128.46
28	S1	1621	OMU	C4-N3-C2	-5.35	119.52	126.58
1	1	1539	A2M	N3-C2-N1	-5.35	120.23	128.60
1	1	1540	OMG	C5-C4-N3	-5.35	119.79	128.46
28	S1	2185	MA6	N1-C2-N3	-5.34	120.25	128.60
28	S1	1623	OMG	C5-C4-N3	-5.33	119.82	128.46
28	S1	98	A2M	C5-C4-N3	-5.32	119.81	126.75
2	2	641	OMG	C5-C4-N3	-5.32	119.83	128.46
2	2	604	A2M	C5-C4-N3	-5.31	119.82	126.75
28	S1	479	A2M	C5-C4-N3	-5.29	119.85	126.75
2	2	1231	OMG	C5-C4-N3	-5.27	119.90	128.46
1	1	1626	OMG	C5-C4-N3	-5.26	119.92	128.46
28	S1	668	A2M	C5-C4-N3	-5.26	119.89	126.75
28	S1	1478	OMG	C5-C4-N3	-5.26	119.93	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1185	A2M	C5-C4-N3	-5.26	119.89	126.75
28	S1	2185	MA6	C5-C6-N6	5.25	134.45	125.30
1	1	407	A2M	C5-C4-N3	-5.25	119.91	126.75
1	1	305	A2M	C5-C4-N3	-5.24	119.92	126.75
28	S1	2021	A2M	C5-C4-N3	-5.22	119.94	126.75
1	1	955	A2M	C5-C4-N3	-5.17	120.01	126.75
1	1	856	OMG	C5-C4-N3	-5.17	120.08	128.46
2	2	1359	OMU	C4-N3-C2	-5.17	119.76	126.58
1	1	235	A2M	C5-C4-N3	-5.16	120.01	126.75
2	2	95	A2M	N3-C2-N1	-5.16	120.52	128.60
28	S1	512	A2M	C5-C4-N3	-5.16	120.02	126.75
1	1	1524	OMG	C5-C4-N3	-5.13	120.14	128.46
1	1	1190	OMG	C5-C4-N3	-5.10	120.18	128.46
2	2	1078	OMG	C2-N3-C4	5.10	121.39	112.30
28	S1	29	OMU	C4-N3-C2	-5.10	119.86	126.58
28	S1	668	A2M	N6-C6-N1	-5.09	107.19	118.35
7	7	162	A2M	N6-C6-N1	-5.09	107.21	118.35
28	S1	2151	OMG	C5-C4-N3	-5.08	120.21	128.46
2	2	527	A2M	O4'-C1'-N9	5.08	118.07	108.06
28	S1	1865	OMG	C5-C4-N3	-5.07	120.23	128.46
3	3	13	OMU	C4-N3-C2	-5.07	119.89	126.58
1	1	1539	A2M	N6-C6-N1	-5.07	107.25	118.35
2	2	628	A2M	N6-C6-N1	-5.07	107.25	118.35
1	1	858	A2M	C5-C4-N3	-5.05	120.16	126.75
1	1	1371	OMU	C4-N3-C2	-5.01	119.97	126.58
7	7	75	OMG	C5-C4-N3	-5.01	120.34	128.46
7	7	43	A2M	N6-C6-N1	-5.00	107.40	118.35
1	1	955	A2M	N6-C6-N1	-4.99	107.42	118.35
2	2	527	A2M	C5-C4-N3	-4.99	120.24	126.75
28	S1	1543	B8N	C5-C4-N3	4.98	125.40	116.17
28	S1	1979	OMU	C4-N3-C2	-4.98	120.01	126.58
1	1	847	OMU	C4-N3-C2	-4.98	120.01	126.58
1	1	927	A2M	C5-C4-N3	-4.94	120.30	126.75
2	2	572	A2M	N6-C6-N1	-4.94	107.54	118.35
28	S1	479	A2M	N6-C6-N1	-4.93	107.54	118.35
1	1	697	A2M	C5-C4-N3	-4.93	120.31	126.75
2	2	1185	A2M	N6-C6-N1	-4.93	107.55	118.35
28	S1	1995	7MG	C5-C6-N1	4.93	119.67	110.99
2	2	604	A2M	N6-C6-N1	-4.90	107.62	118.35
28	S1	2021	A2M	N6-C6-N1	-4.89	107.64	118.35
1	1	235	A2M	N6-C6-N1	-4.88	107.65	118.35
2	2	95	A2M	N6-C6-N1	-4.88	107.67	118.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	591	A2M	C5-C4-N3	-4.86	120.41	126.75
2	2	572	A2M	C5-C4-N3	-4.85	120.42	126.75
2	2	628	A2M	C5-C4-N3	-4.84	120.44	126.75
1	1	305	A2M	N6-C6-N1	-4.84	107.75	118.35
1	1	927	A2M	N6-C6-N1	-4.83	107.77	118.35
1	1	858	A2M	N6-C6-N1	-4.83	107.78	118.35
28	S1	2184	MA6	C5-C4-N3	-4.83	120.45	126.75
2	2	382	A2M	N6-C6-N1	-4.78	107.88	118.35
2	2	527	A2M	N6-C6-N1	-4.77	107.91	118.35
7	7	162	A2M	C5-C4-N3	-4.76	120.54	126.75
2	2	78	PSU	C4-N3-C2	-4.72	119.53	126.34
1	1	407	A2M	N6-C6-N1	-4.72	108.02	118.35
2	2	591	A2M	N6-C6-N1	-4.71	108.03	118.35
28	S1	98	A2M	N6-C6-N1	-4.71	108.03	118.35
2	2	1361	PSU	C4-N3-C2	-4.71	119.55	126.34
2	2	655	OMG	C2-N3-C4	4.69	120.66	112.30
1	1	239	PSU	C4-N3-C2	-4.69	119.58	126.34
2	2	1318	PSU	C4-N3-C2	-4.67	119.61	126.34
2	2	437	PSU	C4-N3-C2	-4.67	119.61	126.34
28	S1	33	PSU	C4-N3-C2	-4.66	119.62	126.34
2	2	1403	PSU	C4-N3-C2	-4.65	119.63	126.34
2	2	1144	PSU	C4-N3-C2	-4.65	119.64	126.34
1	1	1524	OMG	C1'-N9-C4	-4.64	112.71	126.50
2	2	534	OMG	C2-N3-C4	4.64	120.56	112.30
7	7	69	PSU	C4-N3-C2	-4.64	119.66	126.34
28	S1	512	A2M	N6-C6-N1	-4.64	108.20	118.35
1	1	1017	PSU	C4-N3-C2	-4.64	119.66	126.34
2	2	1060	PSU	C4-N3-C2	-4.63	119.67	126.34
28	S1	1657	PSU	C4-N3-C2	-4.63	119.67	126.34
28	S1	1550	OMG	C2-N3-C4	4.61	120.52	112.30
2	2	1372	A2M	C5-C4-N3	-4.61	120.74	126.75
28	S1	2185	MA6	C5-C4-N3	-4.61	120.74	126.75
2	2	662	PSU	C4-N3-C2	-4.60	119.70	126.34
28	S1	2185	MA6	N9-C8-N7	-4.60	107.62	113.91
1	1	1533	PSU	C4-N3-C2	-4.58	119.73	126.34
2	2	1372	A2M	N6-C6-N1	-4.58	108.33	118.35
2	2	1264	PSU	C4-N3-C2	-4.56	119.77	126.34
1	1	858	A2M	N9-C8-N7	-4.55	107.68	113.91
1	1	697	A2M	N6-C6-N1	-4.55	108.38	118.35
28	S1	104	PSU	C4-N3-C2	-4.55	119.79	126.34
2	2	73	OMU	C4-N3-C2	-4.54	120.59	126.58
1	1	940	PSU	C4-N3-C2	-4.54	119.80	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	1647	OMG	C2-N3-C4	4.51	120.34	112.30
1	1	959	OMG	C2-N3-C4	4.51	120.33	112.30
2	2	597	PSU	C4-N3-C2	-4.51	119.84	126.34
2	2	572	A2M	C2'-C1'-N9	-4.51	105.94	113.53
28	S1	2184	MA6	N9-C8-N7	-4.51	107.75	113.91
7	7	74	PSU	C4-N3-C2	-4.50	119.85	126.34
28	S1	12	PSU	C4-N3-C2	-4.50	119.85	126.34
2	2	1060	PSU	N1-C2-N3	4.50	120.23	115.13
2	2	1144	PSU	N1-C2-N3	4.50	120.22	115.13
1	1	1540	OMG	C2-N3-C4	4.48	120.29	112.30
2	2	1253	OMG	C2-N3-C4	4.48	120.29	112.30
7	7	162	A2M	C5-C6-N6	4.48	133.18	123.43
28	S1	600	OMG	C2-N3-C4	4.48	120.27	112.30
28	S1	1246	PSU	C4-N3-C2	-4.48	119.89	126.34
2	2	1194	PSU	C4-N3-C2	-4.48	119.89	126.34
2	2	527	A2M	C2'-C1'-N9	-4.47	106.00	113.53
1	1	1664	PSU	C4-N3-C2	-4.47	119.90	126.34
1	1	1190	OMG	C2-N3-C4	4.46	120.25	112.30
2	2	1303	PSU	C4-N3-C2	-4.46	119.91	126.34
2	2	604	A2M	N9-C8-N7	-4.46	107.82	113.91
1	1	422	PSU	C4-N3-C2	-4.46	119.92	126.34
28	S1	1533	PSU	C4-N3-C2	-4.45	119.92	126.34
2	2	628	A2M	N9-C8-N7	-4.45	107.83	113.91
2	2	1046	OMG	C2-N3-C4	4.45	120.22	112.30
2	2	1413	PSU	C4-N3-C2	-4.44	119.94	126.34
2	2	527	A2M	N9-C8-N7	-4.44	107.84	113.91
7	7	75	OMG	C1'-N9-C4	-4.44	113.31	126.50
7	7	69	PSU	N1-C2-N3	4.44	120.16	115.13
2	2	510	PSU	C4-N3-C2	-4.43	119.95	126.34
1	1	940	PSU	N1-C2-N3	4.43	120.15	115.13
2	2	1231	OMG	C2-N3-C4	4.42	120.18	112.30
28	S1	1879	OMG	C2-N3-C4	4.42	120.18	112.30
1	1	1528	PSU	C4-N3-C2	-4.42	119.97	126.34
1	1	1190	OMG	C1'-N9-C4	-4.42	113.37	126.50
2	2	71	OMG	C2-N3-C4	4.42	120.17	112.30
1	1	1524	OMG	C1'-N9-C8	4.41	139.26	126.70
2	2	1229	OMG	C2-N3-C4	4.41	120.15	112.30
2	2	572	A2M	N9-C8-N7	-4.40	107.89	113.91
28	S1	668	A2M	C5-C6-N6	4.40	133.01	123.43
2	2	626	PSU	C4-N3-C2	-4.40	120.01	126.34
28	S1	1829	OMG	C2-N3-C4	4.39	120.11	112.30
28	S1	1156	PSU	C4-N3-C2	-4.38	120.02	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	668	A2M	N9-C8-N7	-4.38	107.92	113.91
2	2	1265	PSU	N1-C2-N3	4.38	120.09	115.13
28	S1	2151	OMG	C2-N3-C4	4.37	120.09	112.30
28	S1	1865	OMG	C2-N3-C4	4.37	120.09	112.30
28	S1	1623	OMG	C2-N3-C4	4.37	120.08	112.30
1	1	1524	OMG	C2-N3-C4	4.37	120.08	112.30
1	1	1626	OMG	C2-N3-C4	4.36	120.08	112.30
2	2	1361	PSU	N1-C2-N3	4.36	120.07	115.13
2	2	593	PSU	C4-N3-C2	-4.36	120.06	126.34
28	S1	609	PSU	C4-N3-C2	-4.36	120.06	126.34
1	1	305	A2M	N9-C8-N7	-4.36	107.95	113.91
2	2	472	PSU	C4-N3-C2	-4.36	120.06	126.34
2	2	1194	PSU	N1-C2-N3	4.35	120.06	115.13
28	S1	1192	PSU	C4-N3-C2	-4.34	120.08	126.34
28	S1	1478	OMG	C2-N3-C4	4.34	120.03	112.30
28	S1	104	PSU	N1-C2-N3	4.34	120.05	115.13
1	1	697	A2M	N9-C8-N7	-4.33	107.99	113.91
2	2	628	A2M	C5-C6-N6	4.33	132.86	123.43
2	2	512	PSU	C4-N3-C2	-4.33	120.10	126.34
28	S1	1246	PSU	N1-C2-N3	4.33	120.03	115.13
28	S1	2046	PSU	C4-N3-C2	-4.33	120.11	126.34
28	S1	1995	7MG	C2-N3-C4	4.33	120.01	112.30
7	7	43	A2M	C5-C6-N6	4.32	132.84	123.43
2	2	1360	OMG	C2-N3-C4	4.32	120.00	112.30
28	S1	512	A2M	N9-C8-N7	-4.32	108.01	113.91
1	1	1539	A2M	C5-C6-N6	4.32	132.82	123.43
2	2	122	PSU	C4-N3-C2	-4.31	120.13	126.34
1	1	1017	PSU	N1-C2-N3	4.31	120.01	115.13
28	S1	33	PSU	N1-C2-N3	4.31	120.01	115.13
2	2	597	PSU	N1-C2-N3	4.31	120.01	115.13
28	S1	1566	PSU	C4-N3-C2	-4.30	120.14	126.34
2	2	1308	5MC	C5-C6-N1	-4.29	118.92	123.34
2	2	1303	PSU	N1-C2-N3	4.29	119.99	115.13
4	4	74	OMG	C2-N3-C4	4.29	119.94	112.30
1	1	1039	PSU	C4-N3-C2	-4.29	120.16	126.34
1	1	235	A2M	N9-C8-N7	-4.28	108.06	113.91
2	2	122	PSU	N1-C2-N3	4.28	119.98	115.13
2	2	662	PSU	N1-C2-N3	4.28	119.98	115.13
28	S1	2021	A2M	N9-C8-N7	-4.28	108.06	113.91
2	2	1185	A2M	N9-C8-N7	-4.28	108.06	113.91
2	2	472	PSU	N1-C2-N3	4.26	119.96	115.13
1	1	955	A2M	C5-C6-N6	4.26	132.69	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	162	A2M	N9-C8-N7	-4.26	108.09	113.91
1	1	927	A2M	C5-C6-N6	4.25	132.68	123.43
2	2	641	OMG	C2-N3-C4	4.25	119.87	112.30
2	2	1265	PSU	C4-N3-C2	-4.25	120.22	126.34
1	1	239	PSU	N1-C2-N3	4.24	119.94	115.13
28	S1	2151	OMG	C1'-N9-C4	-4.24	113.90	126.50
2	2	1403	PSU	N1-C2-N3	4.23	119.92	115.13
2	2	572	A2M	C5-C6-N6	4.23	132.63	123.43
1	1	856	OMG	C2-N3-C4	4.23	119.83	112.30
7	7	75	OMG	C2-N3-C4	4.23	119.83	112.30
2	2	1372	A2M	N9-C8-N7	-4.22	108.14	113.91
1	1	1533	PSU	N1-C2-N3	4.22	119.91	115.13
1	1	955	A2M	N9-C8-N7	-4.22	108.14	113.91
28	S1	2046	PSU	N1-C2-N3	4.21	119.90	115.13
28	S1	609	PSU	N1-C2-N3	4.21	119.90	115.13
28	S1	2202	PSU	C4-N3-C2	-4.21	120.28	126.34
7	7	43	A2M	N9-C8-N7	-4.20	108.16	113.91
2	2	1354	PSU	C4-N3-C2	-4.19	120.30	126.34
28	S1	607	PSU	C4-N3-C2	-4.19	120.30	126.34
2	2	1318	PSU	N1-C2-N3	4.19	119.87	115.13
1	1	927	A2M	N9-C8-N7	-4.18	108.20	113.91
2	2	1185	A2M	C5-C6-N6	4.18	132.52	123.43
28	S1	2151	OMG	C1'-N9-C8	4.17	138.58	126.70
28	S1	12	PSU	N1-C2-N3	4.17	119.86	115.13
28	S1	479	A2M	C5-C6-N6	4.17	132.50	123.43
7	7	75	OMG	C1'-N9-C8	4.17	138.55	126.70
1	1	305	A2M	C5-C6-N6	4.17	132.49	123.43
2	2	591	A2M	C5-C6-N6	4.16	132.49	123.43
28	S1	1865	OMG	C1'-N9-C4	-4.16	114.14	126.50
28	S1	1539	PSU	C4-N3-C2	-4.16	120.35	126.34
28	S1	1543	B8N	C4-N3-C2	-4.16	120.20	125.46
28	S1	1192	PSU	N1-C2-N3	4.15	119.84	115.13
28	S1	98	A2M	N9-C8-N7	-4.15	108.24	113.91
1	1	1181	PSU	C4-N3-C2	-4.15	120.36	126.34
28	S1	455	PSU	C4-N3-C2	-4.15	120.36	126.34
1	1	407	A2M	N9-C8-N7	-4.14	108.25	113.91
1	1	856	OMG	C1'-N9-C4	-4.14	114.20	126.50
1	1	1402	PSU	C4-N3-C2	-4.14	120.38	126.34
28	S1	1156	PSU	N1-C2-N3	4.13	119.81	115.13
28	S1	2021	A2M	C5-C6-N6	4.13	132.42	123.43
2	2	534	OMG	N9-C4-N3	4.13	134.22	125.94
28	S1	1841	PSU	C4-N3-C2	-4.12	120.40	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	74	PSU	N1-C2-N3	4.11	119.79	115.13
1	1	1528	PSU	N1-C2-N3	4.11	119.79	115.13
2	2	604	A2M	C5-C6-N6	4.11	132.37	123.43
1	1	845	OMU	C1'-N1-C2	4.11	125.01	117.57
28	S1	1533	PSU	N1-C2-N3	4.11	119.78	115.13
1	1	422	PSU	N1-C2-N3	4.11	119.78	115.13
2	2	1413	PSU	N1-C2-N3	4.10	119.78	115.13
2	2	78	PSU	N1-C2-N3	4.10	119.78	115.13
2	2	1264	PSU	N1-C2-N3	4.09	119.76	115.13
2	2	591	A2M	N9-C8-N7	-4.09	108.32	113.91
1	1	1190	OMG	C1'-N9-C8	4.09	138.34	126.70
1	1	235	A2M	C5-C6-N6	4.09	132.33	123.43
1	1	1171	PSU	C6-N1-C2	-4.08	118.51	122.68
1	1	858	A2M	C5-C6-N6	4.08	132.31	123.43
28	S1	479	A2M	N9-C8-N7	-4.07	108.34	113.91
2	2	95	A2M	C5-C6-N6	4.06	132.26	123.43
2	2	510	PSU	N1-C2-N3	4.06	119.72	115.13
28	S1	1657	PSU	N1-C2-N3	4.05	119.72	115.13
28	S1	2202	PSU	N1-C2-N3	4.05	119.72	115.13
28	S1	1539	PSU	N1-C2-N3	4.05	119.71	115.13
28	S1	1833	OMU	C5-C4-N3	4.04	120.89	114.84
28	S1	1647	OMG	C1'-N9-C4	-4.04	114.51	126.50
2	2	1077	OMU	N3-C2-N1	4.03	120.25	114.89
1	1	1011	PSU	C4-N3-C2	-4.02	120.54	126.34
2	2	593	PSU	N1-C2-N3	4.02	119.69	115.13
28	S1	98	A2M	C5-C6-N6	4.01	132.16	123.43
28	S1	1566	PSU	N1-C2-N3	4.01	119.67	115.13
2	2	626	PSU	N1-C2-N3	4.00	119.67	115.13
28	S1	607	PSU	N1-C2-N3	3.98	119.64	115.13
1	1	407	A2M	C5-C6-N6	3.98	132.08	123.43
2	2	1372	A2M	C5-C6-N6	3.97	132.07	123.43
28	S1	455	PSU	N1-C2-N3	3.97	119.62	115.13
2	2	1354	PSU	N1-C2-N3	3.96	119.61	115.13
1	1	1371	OMU	C1'-N1-C2	3.95	124.73	117.57
2	2	1231	OMG	C1'-N9-C4	-3.95	114.76	126.50
1	1	1402	PSU	N1-C2-N3	3.95	119.61	115.13
2	2	512	PSU	N1-C2-N3	3.95	119.61	115.13
1	1	1539	A2M	N9-C8-N7	-3.95	108.52	113.91
2	2	382	A2M	C5-C6-N6	3.94	132.01	123.43
28	S1	512	A2M	C5-C6-N6	3.94	132.01	123.43
1	1	1664	PSU	N1-C2-N3	3.94	119.59	115.13
2	2	1078	OMG	N2-C2-N3	3.93	127.39	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1011	PSU	N1-C2-N3	3.93	119.59	115.13
2	2	437	PSU	N1-C2-N3	3.92	119.57	115.13
28	S1	1865	OMG	C1'-N9-C8	3.92	137.85	126.70
1	1	1039	PSU	N1-C2-N3	3.91	119.56	115.13
2	2	560	OMU	C2'-C1'-N1	-3.90	106.64	114.22
1	1	1626	OMG	C1'-N9-C4	-3.90	114.90	126.50
1	1	1659	OMU	N3-C2-N1	3.89	120.06	114.89
2	2	655	OMG	N9-C4-N3	3.89	133.76	125.94
28	S1	1841	PSU	N1-C2-N3	3.89	119.54	115.13
2	2	1359	OMU	N3-C2-N1	3.89	120.05	114.89
2	2	95	A2M	N3-C4-N9	3.88	133.47	127.08
1	1	697	A2M	C5-C6-N6	3.88	131.87	123.43
28	S1	1550	OMG	C1'-N9-C4	-3.86	115.04	126.50
2	2	1058	PSU	C4-N3-C2	-3.85	120.79	126.34
2	2	527	A2M	C5-C6-N6	3.85	131.80	123.43
28	S1	1995	7MG	C5-C4-N3	-3.84	120.82	128.13
28	S1	661	OMU	N3-C2-N1	3.84	119.98	114.89
2	2	667	OMU	N3-C2-N1	3.84	119.98	114.89
7	7	7	OMU	N3-C2-N1	3.82	119.97	114.89
28	S1	600	OMG	N9-C4-N3	3.82	133.62	125.94
2	2	95	A2M	N9-C8-N7	-3.82	108.68	113.91
28	S1	1833	OMU	O4-C4-C5	-3.82	118.44	125.16
1	1	1181	PSU	N1-C2-N3	3.80	119.43	115.13
1	1	959	OMG	C1'-N9-C4	-3.80	115.23	126.50
2	2	71	OMG	C1'-N9-C4	-3.78	115.27	126.50
1	1	847	OMU	N3-C2-N1	3.77	119.89	114.89
2	2	641	OMG	C1'-N9-C4	-3.76	115.33	126.50
2	2	560	OMU	N3-C2-N1	3.76	119.88	114.89
28	S1	1647	OMG	C1'-N9-C8	3.75	137.38	126.70
1	1	1171	PSU	C4-N3-C2	-3.74	120.95	126.34
2	2	382	A2M	N9-C8-N7	-3.74	108.80	113.91
1	1	856	OMG	C1'-N9-C8	3.73	137.32	126.70
7	7	43	A2M	C2-N3-C4	3.72	120.53	111.75
28	S1	8	OMU	N3-C2-N1	3.72	119.82	114.89
2	2	1046	OMG	C1'-N9-C4	-3.71	115.47	126.50
28	S1	1550	OMG	C1'-N9-C8	3.70	137.23	126.70
2	2	1231	OMG	C1'-N9-C8	3.67	137.14	126.70
28	S1	29	OMU	N3-C2-N1	3.67	119.76	114.89
2	2	1360	OMG	C1'-N9-C4	-3.67	115.61	126.50
28	S1	2184	MA6	C2-N1-C6	3.67	120.41	111.75
1	1	959	OMG	C1'-N9-C8	3.65	137.07	126.70
2	2	1253	OMG	C1'-N9-C4	-3.64	115.68	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	74	OMG	N9-C4-N3	3.63	133.24	125.94
2	2	95	A2M	C2-N3-C4	3.63	120.32	111.75
28	S1	1623	OMG	C1'-N9-C4	-3.62	115.74	126.50
2	2	1058	PSU	C6-N1-C2	-3.62	118.98	122.68
2	2	56	OMU	N3-C2-N1	3.62	119.70	114.89
1	1	1371	OMU	N3-C2-N1	3.62	119.69	114.89
28	S1	1621	OMU	N3-C2-N1	3.62	119.69	114.89
2	2	604	A2M	C2-N3-C4	3.62	120.30	111.75
1	1	235	A2M	C2-N3-C4	3.61	120.29	111.75
2	2	1058	PSU	N1-C2-N3	3.61	119.22	115.13
2	2	1060	PSU	C6-C5-C4	3.61	120.72	118.20
28	S1	8	OMU	C5-C4-N3	3.60	120.22	114.84
1	1	1626	OMG	C1'-N9-C8	3.60	136.94	126.70
28	S1	2184	MA6	C4-C5-C6	3.60	119.91	115.88
2	2	382	A2M	C2-N3-C4	3.60	120.25	111.75
2	2	56	OMU	C5-C4-N3	3.59	120.22	114.84
28	S1	1879	OMG	C1'-N9-C4	-3.59	115.83	126.50
1	1	1107	OMU	C5-C4-N3	3.59	120.21	114.84
28	S1	1478	OMG	C1'-N9-C4	-3.59	115.84	126.50
1	1	1171	PSU	N1-C2-N3	3.59	119.19	115.13
28	S1	1829	OMG	N9-C4-N3	3.58	133.14	125.94
28	S1	2021	A2M	C2-N3-C4	3.58	120.22	111.75
1	1	1539	A2M	C2-N3-C4	3.58	120.21	111.75
7	7	7	OMU	C5-C4-N3	3.58	120.20	114.84
2	2	572	A2M	C2-N3-C4	3.58	120.21	111.75
1	1	955	A2M	C2-N3-C4	3.58	120.21	111.75
2	2	628	A2M	C2-N3-C4	3.57	120.19	111.75
2	2	71	OMG	N9-C4-N3	3.57	133.12	125.94
28	S1	479	A2M	C2-N3-C4	3.56	120.17	111.75
2	2	560	OMU	C5-C4-N3	3.56	120.16	114.84
28	S1	1621	OMU	C5-C4-N3	3.55	120.14	114.84
2	2	1046	OMG	C1'-N9-C8	3.55	136.79	126.70
28	S1	668	A2M	C2-N3-C4	3.54	120.11	111.75
28	S1	1246	PSU	C6-C5-C4	3.53	120.66	118.20
2	2	1253	OMG	N9-C4-N3	3.52	133.02	125.94
2	2	667	OMU	C5-C4-N3	3.52	120.11	114.84
1	1	1540	OMG	C1'-N9-C4	-3.52	116.05	126.50
3	3	13	OMU	N3-C2-N1	3.52	119.56	114.89
1	1	407	A2M	C2-N3-C4	3.52	120.06	111.75
1	1	305	A2M	C2-N3-C4	3.51	120.05	111.75
28	S1	98	A2M	C2-N3-C4	3.51	120.05	111.75
2	2	1229	OMG	N9-C4-N3	3.50	132.98	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	524	5MC	C5-C6-N1	-3.50	119.73	123.34
28	S1	2046	PSU	C6-N1-C2	-3.50	119.10	122.68
28	S1	661	OMU	C5-C4-N3	3.50	120.08	114.84
28	S1	2185	MA6	C2-N1-C6	3.50	120.02	111.75
2	2	472	PSU	C6-N1-C2	-3.50	119.10	122.68
2	2	1185	A2M	C2-N3-C4	3.50	120.02	111.75
1	1	697	A2M	C2-N3-C4	3.49	120.01	111.75
1	1	858	A2M	C2-N3-C4	3.49	120.00	111.75
28	S1	512	A2M	C2-N3-C4	3.49	120.00	111.75
7	7	162	A2M	C2-N3-C4	3.48	119.97	111.75
1	1	927	A2M	C2-N3-C4	3.48	119.97	111.75
28	S1	1979	OMU	N3-C2-N1	3.48	119.50	114.89
2	2	604	A2M	C5-N7-C8	3.47	108.44	103.51
2	2	1360	OMG	N9-C4-N3	3.47	132.90	125.94
1	1	1107	OMU	N3-C2-N1	3.47	119.49	114.89
2	2	122	PSU	C6-N1-C2	-3.46	119.14	122.68
2	2	1265	PSU	C6-N1-C2	-3.46	119.14	122.68
28	S1	1544	5MC	C5-C6-N1	-3.46	119.78	123.34
2	2	1303	PSU	C6-C5-C4	3.46	120.61	118.20
2	2	1253	OMG	C1'-N9-C8	3.44	136.50	126.70
2	2	527	A2M	C2-N3-C4	3.44	119.87	111.75
2	2	73	OMU	N3-C2-N1	3.44	119.45	114.89
3	3	13	OMU	C5-C4-N3	3.43	119.98	114.84
1	1	940	PSU	C6-C5-C4	3.42	120.59	118.20
28	S1	668	A2M	C5-N7-C8	3.42	108.37	103.51
2	2	641	OMG	N9-C4-N3	3.42	132.80	125.94
2	2	71	OMG	C1'-N9-C8	3.42	136.42	126.70
28	S1	1879	OMG	C1'-N9-C8	3.41	136.42	126.70
28	S1	2061	5MC	C5-C6-N1	-3.40	119.84	123.34
28	S1	2185	MA6	C4-C5-C6	3.39	119.67	115.88
28	S1	1623	OMG	N9-C4-N3	3.38	132.73	125.94
2	2	591	A2M	C2-N3-C4	3.38	119.73	111.75
1	1	1659	OMU	C5-C4-N3	3.37	119.89	114.84
28	S1	2184	MA6	C2-N3-C4	3.37	119.72	111.75
2	2	641	OMG	C1'-N9-C8	3.37	136.28	126.70
2	2	1360	OMG	C1'-N9-C8	3.36	136.27	126.70
1	1	1540	OMG	C1'-N9-C8	3.36	136.27	126.70
2	2	1144	PSU	C6-C5-C4	3.36	120.54	118.20
2	2	628	A2M	C5-N7-C8	3.35	108.26	103.51
28	S1	1979	OMU	C5-C4-N3	3.34	119.84	114.84
2	2	1359	OMU	C5-C4-N3	3.33	119.83	114.84
2	2	662	PSU	C6-C5-C4	3.33	120.53	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	1478	OMG	C1'-N9-C8	3.33	136.18	126.70
28	S1	29	OMU	C5-C4-N3	3.33	119.82	114.84
1	1	845	OMU	C6-C5-C4	3.32	124.05	119.52
2	2	1077	OMU	C5-C4-N3	3.32	119.80	114.84
1	1	305	A2M	C5-N7-C8	3.31	108.21	103.51
28	S1	1623	OMG	C1'-N9-C8	3.31	136.12	126.70
28	S1	512	A2M	N3-C4-N9	3.30	132.53	127.08
2	2	1185	A2M	N3-C4-N9	3.30	132.53	127.08
1	1	1371	OMU	C5-C4-N3	3.30	119.77	114.84
28	S1	1879	OMG	N9-C4-N3	3.29	132.54	125.94
2	2	1372	A2M	C2-N3-C4	3.29	119.51	111.75
28	S1	2185	MA6	C2-N3-C4	3.28	119.51	111.75
7	7	43	A2M	N3-C4-N9	3.28	132.49	127.08
2	2	534	OMG	C2-N1-C6	-3.28	119.12	125.10
7	7	43	A2M	C5-N7-C8	3.28	108.17	103.51
28	S1	1829	OMG	C1'-N9-C4	-3.28	116.76	126.50
2	2	1046	OMG	N9-C4-N3	3.28	132.52	125.94
2	2	1229	OMG	C1'-N9-C4	-3.26	116.81	126.50
28	S1	1647	OMG	N9-C4-N3	3.26	132.49	125.94
2	2	382	A2M	N3-C4-N9	3.26	132.45	127.08
1	1	856	OMG	N9-C4-N3	3.26	132.48	125.94
2	2	1231	OMG	N9-C4-N3	3.25	132.47	125.94
1	1	858	A2M	C5-N7-C8	3.25	108.12	103.51
2	2	1403	PSU	C6-C5-C4	3.25	120.47	118.20
1	1	1626	OMG	N9-C4-N3	3.24	132.45	125.94
2	2	1185	A2M	C5-N7-C8	3.24	108.12	103.51
2	2	1308	5MC	C4'-O4'-C1'	-3.24	102.32	109.47
28	S1	1550	OMG	N9-C4-N3	3.24	132.44	125.94
7	7	69	PSU	C6-C5-C4	3.23	120.46	118.20
28	S1	1478	OMG	N9-C4-N3	3.22	132.41	125.94
2	2	655	OMG	C2-N1-C6	-3.22	119.23	125.10
1	1	697	A2M	C5-N7-C8	3.21	108.07	103.51
28	S1	98	A2M	N3-C4-N9	3.21	132.36	127.08
4	4	74	OMG	C1'-N9-C4	-3.20	116.99	126.50
2	2	560	OMU	O3'-C3'-C4'	3.20	120.31	111.05
1	1	235	A2M	C5-N7-C8	3.20	108.05	103.51
28	S1	104	PSU	C6-C5-C4	3.19	120.43	118.20
2	2	527	A2M	N3-C4-N9	3.19	132.34	127.08
1	1	407	A2M	N3-C4-N9	3.19	132.34	127.08
1	1	959	OMG	N9-C4-N3	3.19	132.34	125.94
7	7	43	A2M	C2'-C1'-N9	-3.19	108.16	113.53
1	1	1107	OMU	O4-C4-C5	-3.18	119.57	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1046	OMG	C2-N1-C6	-3.18	119.30	125.10
1	1	955	A2M	C5-N7-C8	3.18	108.03	103.51
28	S1	2184	MA6	C5-N7-C8	3.18	108.02	103.51
2	2	572	A2M	C5-N7-C8	3.16	108.00	103.51
1	1	1539	A2M	C5-N7-C8	3.16	108.00	103.51
28	S1	98	A2M	C5-N7-C8	3.16	108.00	103.51
1	1	858	A2M	N3-C4-N9	3.16	132.29	127.08
7	7	162	A2M	C5-N7-C8	3.16	107.99	103.51
28	S1	1539	PSU	C6-N1-C2	-3.15	119.46	122.68
28	S1	1995	7MG	C4-C5-N7	3.15	109.91	105.53
28	S1	1995	7MG	C5-C4-N9	3.15	110.44	106.35
1	1	927	A2M	C5-N7-C8	3.14	107.97	103.51
28	S1	2021	A2M	C5-N7-C8	3.14	107.97	103.51
2	2	591	A2M	N3-C4-N9	3.13	132.25	127.08
28	S1	1833	OMU	N3-C2-N1	3.13	119.05	114.89
2	2	73	OMU	C5-C4-N3	3.13	119.53	114.84
28	S1	2184	MA6	N3-C4-N9	3.13	132.24	127.08
28	S1	479	A2M	C5-N7-C8	3.13	107.95	103.51
2	2	1185	A2M	C2'-C1'-N9	-3.13	108.27	113.53
1	1	847	OMU	C5-C4-N3	3.12	119.51	114.84
2	2	1194	PSU	C6-N1-C2	-3.12	119.49	122.68
1	1	239	PSU	C6-C5-C4	3.12	120.38	118.20
2	2	95	A2M	C5-N7-C8	3.12	107.94	103.51
2	2	71	OMG	C2-N1-C6	-3.11	119.43	125.10
1	1	305	A2M	N3-C4-N9	3.11	132.21	127.08
28	S1	600	OMG	C2-N1-C6	-3.11	119.43	125.10
1	1	845	OMU	O2-C2-N3	-3.11	115.72	121.50
28	S1	1192	PSU	C6-N1-C2	-3.11	119.51	122.68
28	S1	479	A2M	N3-C4-N9	3.10	132.19	127.08
2	2	604	A2M	N3-C4-N9	3.09	132.18	127.08
2	2	1253	OMG	C2-N1-C6	-3.09	119.47	125.10
2	2	1229	OMG	C1'-N9-C8	3.09	135.49	126.70
28	S1	1879	OMG	C2-N1-C6	-3.08	119.48	125.10
1	1	1539	A2M	N3-C4-N9	3.08	132.16	127.08
2	2	655	OMG	C1'-N9-C4	-3.08	117.37	126.50
1	1	1540	OMG	C2-N1-C6	-3.07	119.50	125.10
28	S1	609	PSU	C6-N1-C2	-3.07	119.55	122.68
28	S1	2185	MA6	C5-N7-C8	3.07	107.87	103.51
1	1	407	A2M	C5-N7-C8	3.07	107.87	103.51
28	S1	1829	OMG	C2-N1-C6	-3.07	119.51	125.10
28	S1	1841	PSU	C6-N1-C2	-3.06	119.55	122.68
2	2	1229	OMG	C2-N1-C6	-3.06	119.52	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	1550	OMG	C2-N1-C6	-3.06	119.52	125.10
2	2	1265	PSU	C6-C5-C4	3.06	120.34	118.20
28	S1	1533	PSU	C6-C5-C4	3.06	120.34	118.20
28	S1	512	A2M	C5-N7-C8	3.05	107.84	103.51
28	S1	2021	A2M	N3-C4-N9	3.05	132.11	127.08
1	1	1190	OMG	N9-C4-N3	3.05	132.06	125.94
2	2	1360	OMG	C2-N1-C6	-3.05	119.55	125.10
28	S1	1623	OMG	C2-N1-C6	-3.05	119.55	125.10
1	1	1540	OMG	N9-C4-N3	3.04	132.05	125.94
2	2	1231	OMG	C2-N1-C6	-3.04	119.56	125.10
28	S1	668	A2M	N3-C4-N9	3.04	132.09	127.08
1	1	1039	PSU	C6-N1-C2	-3.02	119.59	122.68
28	S1	1979	OMU	O4-C4-C5	-3.02	119.85	125.16
28	S1	607	PSU	C6-N1-C2	-3.02	119.60	122.68
1	1	959	OMG	C2-N1-C6	-3.02	119.60	125.10
28	S1	600	OMG	C1'-N9-C4	-3.02	117.54	126.50
2	2	1078	OMG	C5-C6-N1	3.02	120.85	113.19
2	2	527	A2M	C5-N7-C8	3.01	107.79	103.51
28	S1	1478	OMG	C2-N1-C6	-3.01	119.61	125.10
28	S1	1647	OMG	C2-N1-C6	-3.01	119.61	125.10
2	2	641	OMG	N9-C8-N7	-3.00	107.74	113.39
1	1	235	A2M	N3-C4-N9	2.99	132.01	127.08
1	1	856	OMG	N9-C8-N7	-2.99	107.76	113.39
1	1	1524	OMG	C2-N1-C6	-2.99	119.65	125.10
28	S1	1829	OMG	C1'-N9-C8	2.99	135.20	126.70
1	1	1626	OMG	C2-N1-C6	-2.99	119.66	125.10
1	1	940	PSU	C6-N1-C2	-2.98	119.63	122.68
28	S1	33	PSU	C6-C5-C4	2.98	120.28	118.20
2	2	641	OMG	C2-N1-C6	-2.98	119.67	125.10
1	1	1402	PSU	C6-N1-C2	-2.97	119.64	122.68
28	S1	1865	OMG	C2-N1-C6	-2.97	119.69	125.10
2	2	655	OMG	C1'-N9-C8	2.97	135.14	126.70
1	1	1011	PSU	C6-N1-C2	-2.97	119.65	122.68
28	S1	1865	OMG	N9-C4-N3	2.96	131.89	125.94
1	1	856	OMG	C2-N1-C6	-2.96	119.70	125.10
1	1	1190	OMG	N9-C8-N7	-2.96	107.82	113.39
28	S1	1543	B8N	N3-C2-N1	2.95	120.93	116.76
28	S1	1621	OMU	O4-C4-C5	-2.95	119.98	125.16
28	S1	455	PSU	C6-N1-C2	-2.94	119.68	122.68
2	2	382	A2M	C5-N7-C8	2.93	107.67	103.51
2	2	1372	A2M	C5-N7-C8	2.93	107.67	103.51
1	1	1371	OMU	O4-C4-C5	-2.93	120.00	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	955	A2M	N3-C4-N9	2.93	131.91	127.08
1	1	697	A2M	N3-C4-N9	2.92	131.90	127.08
7	7	75	OMG	C2-N1-C6	-2.92	119.78	125.10
4	4	74	OMG	C2-N1-C6	-2.91	119.78	125.10
7	7	75	OMG	N9-C8-N7	-2.91	107.91	113.39
28	S1	2202	PSU	C6-N1-C2	-2.91	119.71	122.68
2	2	1361	PSU	C6-N1-C2	-2.90	119.72	122.68
2	2	472	PSU	O2-C2-N1	-2.90	119.60	122.79
2	2	591	A2M	C5-N7-C8	2.89	107.62	103.51
28	S1	29	OMU	O4-C4-C5	-2.89	120.08	125.16
28	S1	1156	PSU	C6-N1-C2	-2.89	119.73	122.68
1	1	1533	PSU	C6-C5-C4	2.89	120.22	118.20
2	2	597	PSU	C6-C5-C4	2.89	120.22	118.20
2	2	1303	PSU	C6-N1-C2	-2.89	119.73	122.68
3	3	13	OMU	O4-C4-C5	-2.88	120.09	125.16
1	1	1524	OMG	N9-C4-N3	2.88	131.72	125.94
1	1	1528	PSU	C6-N1-C2	-2.88	119.74	122.68
2	2	1144	PSU	C6-N1-C2	-2.87	119.74	122.68
4	4	74	OMG	C1'-N9-C8	2.87	134.88	126.70
28	S1	1246	PSU	C6-N1-C2	-2.87	119.75	122.68
2	2	597	PSU	C6-N1-C2	-2.87	119.75	122.68
7	7	75	OMG	N9-C4-N3	2.87	131.70	125.94
28	S1	104	PSU	C6-N1-C2	-2.87	119.75	122.68
28	S1	1647	OMG	N9-C8-N7	-2.87	107.99	113.39
2	2	1060	PSU	C6-N1-C2	-2.86	119.76	122.68
1	1	1190	OMG	C2-N1-C6	-2.85	119.89	125.10
1	1	1524	OMG	N9-C8-N7	-2.85	108.02	113.39
28	S1	33	PSU	C6-N1-C2	-2.85	119.77	122.68
2	2	1078	OMG	N1-C2-N3	-2.84	118.02	123.32
2	2	560	OMU	O4-C4-C5	-2.84	120.16	125.16
28	S1	2151	OMG	C2-N1-C6	-2.84	119.92	125.10
1	1	1533	PSU	C6-N1-C2	-2.83	119.79	122.68
2	2	1354	PSU	C6-N1-C2	-2.83	119.79	122.68
1	1	1181	PSU	C6-N1-C2	-2.82	119.80	122.68
1	1	1626	OMG	N9-C8-N7	-2.82	108.08	113.39
28	S1	609	PSU	C6-C5-C4	2.82	120.17	118.20
2	2	667	OMU	O4-C4-C5	-2.82	120.21	125.16
28	S1	600	OMG	C1'-N9-C8	2.81	134.71	126.70
2	2	510	PSU	C6-N1-C2	-2.80	119.82	122.68
2	2	534	OMG	C5-C6-N1	2.80	120.30	113.19
1	1	1659	OMU	O4-C4-C5	-2.80	120.24	125.16
1	1	927	A2M	N3-C4-N9	2.80	131.70	127.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	2151	OMG	N9-C4-N3	2.80	131.56	125.94
2	2	1231	OMG	C5-C6-N1	2.80	120.30	113.19
2	2	1077	OMU	O4-C4-C5	-2.80	120.24	125.16
2	2	1058	PSU	O2-C2-N1	-2.79	119.72	122.79
1	1	422	PSU	C6-N1-C2	-2.79	119.83	122.68
2	2	122	PSU	C6-C5-C4	2.79	120.15	118.20
2	2	1372	A2M	N3-C4-N9	2.79	131.68	127.08
28	S1	1995	7MG	C2-N1-C6	-2.78	120.02	125.10
2	2	71	OMG	N9-C8-N7	-2.78	108.15	113.39
2	2	1361	PSU	C6-C5-C4	2.78	120.14	118.20
1	1	1017	PSU	C6-N1-C2	-2.78	119.84	122.68
28	S1	12	PSU	C6-N1-C2	-2.78	119.84	122.68
28	S1	1995	7MG	O6-C6-C5	-2.78	120.72	127.54
2	2	1231	OMG	N9-C8-N7	-2.78	108.16	113.39
28	S1	1533	PSU	C6-N1-C2	-2.78	119.84	122.68
2	2	572	A2M	N3-C4-N9	2.77	131.65	127.08
28	S1	1657	PSU	C6-C5-C4	2.77	120.13	118.20
28	S1	12	PSU	C6-C5-C4	2.77	120.13	118.20
2	2	56	OMU	O4-C4-C5	-2.77	120.30	125.16
28	S1	1829	OMG	N9-C8-N7	-2.77	108.18	113.39
2	2	512	PSU	C6-N1-C2	-2.76	119.86	122.68
2	2	1413	PSU	C6-N1-C2	-2.76	119.87	122.68
28	S1	1865	OMG	N9-C8-N7	-2.76	108.20	113.39
2	2	71	OMG	C5-C6-N1	2.75	120.19	113.19
2	2	655	OMG	C5-C6-N1	2.75	120.18	113.19
28	S1	1478	OMG	N9-C8-N7	-2.75	108.21	113.39
2	2	626	PSU	C6-N1-C2	-2.75	119.87	122.68
28	S1	1550	OMG	C5-C6-N1	2.75	120.17	113.19
2	2	662	PSU	C6-N1-C2	-2.75	119.88	122.68
2	2	1194	PSU	C6-C5-C4	2.75	120.12	118.20
2	2	1360	OMG	N9-C8-N7	-2.74	108.23	113.39
28	S1	1566	PSU	C6-N1-C2	-2.73	119.89	122.68
28	S1	8	OMU	O4-C4-C5	-2.73	120.36	125.16
7	7	69	PSU	C6-N1-C2	-2.73	119.90	122.68
1	1	239	PSU	C6-N1-C2	-2.72	119.90	122.68
1	1	407	A2M	C2'-C1'-N9	-2.72	108.94	113.53
28	S1	2185	MA6	N3-C4-N9	2.72	131.57	127.08
28	S1	1550	OMG	N9-C8-N7	-2.72	108.27	113.39
2	2	1265	PSU	O2-C2-N1	-2.72	119.80	122.79
2	2	1253	OMG	C5-C6-N1	2.72	120.09	113.19
2	2	534	OMG	O6-C6-C5	-2.71	119.40	126.60
28	S1	1623	OMG	N9-C8-N7	-2.71	108.29	113.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	7	OMU	O4-C4-C5	-2.71	120.40	125.16
2	2	122	PSU	O2-C2-N1	-2.70	119.82	122.79
7	7	74	PSU	C6-N1-C2	-2.70	119.92	122.68
2	2	662	PSU	O2-C2-N1	-2.70	119.82	122.79
2	2	71	OMG	O6-C6-C5	-2.69	119.46	126.60
28	S1	1623	OMG	C5-C6-N1	2.69	120.02	113.19
1	1	847	OMU	O4-C4-C5	-2.68	120.44	125.16
28	S1	1543	B8N	O4-C4-N3	-2.68	115.43	119.98
2	2	1078	OMG	O6-C6-C5	-2.68	119.50	126.60
1	1	1626	OMG	C5-C6-N1	2.67	119.98	113.19
28	S1	2046	PSU	O2-C2-N1	-2.67	119.85	122.79
28	S1	1865	OMG	C5-C6-N1	2.66	119.95	113.19
2	2	510	PSU	C6-C5-C4	2.66	120.06	118.20
2	2	1046	OMG	C5-C6-N1	2.66	119.94	113.19
28	S1	1539	PSU	O2-C2-N1	-2.65	119.87	122.79
28	S1	2184	MA6	C4-N9-C8	2.65	108.60	105.73
28	S1	1829	OMG	O6-C6-C5	-2.65	119.57	126.60
28	S1	1879	OMG	C5-C6-N1	2.65	119.92	113.19
28	S1	1156	PSU	C6-C5-C4	2.65	120.05	118.20
1	1	1664	PSU	C6-N1-C2	-2.65	119.97	122.68
1	1	959	OMG	C5-C6-N1	2.65	119.92	113.19
1	1	1524	OMG	C5-C6-N1	2.65	119.91	113.19
1	1	1540	OMG	N9-C8-N7	-2.65	108.41	113.39
1	1	1190	OMG	C5-C6-N1	2.65	119.91	113.19
1	1	856	OMG	C5-C6-N1	2.64	119.91	113.19
28	S1	600	OMG	C5-C6-N1	2.64	119.91	113.19
2	2	626	PSU	O2-C2-N1	-2.64	119.88	122.79
28	S1	1647	OMG	C5-C6-N1	2.64	119.90	113.19
4	4	74	OMG	N9-C8-N7	-2.64	108.41	113.39
2	2	1046	OMG	N9-C8-N7	-2.64	108.43	113.39
2	2	1078	OMG	N9-C8-N7	-2.64	108.43	113.39
2	2	1359	OMU	O4-C4-C5	-2.63	120.53	125.16
1	1	1017	PSU	C6-C5-C4	2.63	120.04	118.20
2	2	95	A2M	C6-C5-C4	2.63	120.72	117.18
2	2	1253	OMG	N9-C8-N7	-2.63	108.44	113.39
2	2	1360	OMG	C5-C6-N1	2.63	119.86	113.19
2	2	534	OMG	C1'-N9-C4	-2.63	118.70	126.50
2	2	593	PSU	C6-N1-C2	-2.62	120.00	122.68
28	S1	1478	OMG	C5-C6-N1	2.62	119.85	113.19
28	S1	1829	OMG	C5-C6-N1	2.62	119.85	113.19
28	S1	661	OMU	O4-C4-C5	-2.62	120.55	125.16
2	2	1229	OMG	C5-C6-N1	2.62	119.84	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	422	PSU	C6-C5-C4	2.61	120.02	118.20
28	S1	1879	OMG	N9-C8-N7	-2.61	108.47	113.39
7	7	75	OMG	C5-C6-N1	2.61	119.81	113.19
2	2	1229	OMG	N9-C8-N7	-2.60	108.49	113.39
1	1	959	OMG	N9-C8-N7	-2.60	108.50	113.39
1	1	858	A2M	C4-N9-C8	2.60	108.54	105.73
28	S1	2151	OMG	N9-C8-N7	-2.60	108.50	113.39
28	S1	2185	MA6	C4-N9-C8	2.59	108.54	105.73
28	S1	1865	OMG	O6-C6-C5	-2.59	119.72	126.60
28	S1	600	OMG	O6-C6-C5	-2.59	119.72	126.60
1	1	1528	PSU	C6-C5-C4	2.59	120.01	118.20
1	1	1533	PSU	O2-C2-N1	-2.59	119.94	122.79
28	S1	1623	OMG	O6-C6-C5	-2.59	119.74	126.60
2	2	1403	PSU	C6-N1-C2	-2.58	120.04	122.68
2	2	437	PSU	C6-C5-C4	2.58	120.00	118.20
28	S1	1657	PSU	C6-N1-C2	-2.58	120.05	122.68
2	2	1264	PSU	C6-N1-C2	-2.58	120.05	122.68
2	2	1360	OMG	O6-C6-C5	-2.58	119.77	126.60
2	2	1318	PSU	C6-C5-C4	2.57	120.00	118.20
1	1	1011	PSU	O2-C2-N1	-2.57	119.96	122.79
2	2	667	OMU	O2-C2-N1	-2.57	119.37	122.79
2	2	1144	PSU	O2-C2-N1	-2.57	119.96	122.79
2	2	1194	PSU	O2-C2-N1	-2.57	119.97	122.79
1	1	1540	OMG	C5-C6-N1	2.56	119.70	113.19
2	2	1229	OMG	O6-C6-C5	-2.56	119.82	126.60
28	S1	1647	OMG	O6-C6-C5	-2.55	119.84	126.60
4	4	74	OMG	C5-C6-N1	2.55	119.67	113.19
28	S1	512	A2M	C2'-C1'-N9	-2.55	109.24	113.53
1	1	1171	PSU	O2-C2-N1	-2.54	119.99	122.79
1	1	1524	OMG	O6-C6-C5	-2.54	119.86	126.60
28	S1	2151	OMG	C5-C6-N1	2.54	119.64	113.19
2	2	641	OMG	C5-C6-N1	2.54	119.64	113.19
28	S1	1478	OMG	O6-C6-C5	-2.54	119.87	126.60
1	1	1659	OMU	O2-C2-N1	-2.53	119.43	122.79
2	2	527	A2M	C4-N9-C8	2.53	108.47	105.73
2	2	1318	PSU	C6-N1-C2	-2.52	120.10	122.68
2	2	472	PSU	C6-C5-C4	2.52	119.96	118.20
2	2	655	OMG	N9-C8-N7	-2.51	108.66	113.39
2	2	628	A2M	N3-C4-N9	2.51	131.22	127.08
7	7	7	OMU	O2-C2-N1	-2.51	119.45	122.79
28	S1	600	OMG	N9-C8-N7	-2.51	108.67	113.39
2	2	1046	OMG	O6-C6-C5	-2.51	119.95	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	74	OMG	O6-C6-C5	-2.50	119.95	126.60
7	7	162	A2M	N3-C4-N9	2.50	131.21	127.08
28	S1	1246	PSU	O2-C2-N1	-2.50	120.04	122.79
2	2	527	A2M	C4'-O4'-C1'	-2.50	103.96	109.47
28	S1	609	PSU	O2-C2-N1	-2.49	120.04	122.79
2	2	1231	OMG	O6-C6-C5	-2.49	119.98	126.60
7	7	74	PSU	C6-C5-C4	2.48	119.93	118.20
1	1	1190	OMG	O6-C6-C5	-2.48	120.02	126.60
2	2	78	PSU	C6-N1-C2	-2.48	120.15	122.68
7	7	75	OMG	O6-C6-C5	-2.48	120.02	126.60
1	1	858	A2M	C4'-O4'-C1'	-2.47	104.01	109.47
28	S1	1879	OMG	O6-C6-C5	-2.47	120.04	126.60
2	2	1253	OMG	O6-C6-C5	-2.47	120.05	126.60
2	2	628	A2M	C4-C5-N7	-2.47	107.61	110.62
28	S1	1621	OMU	O2-C2-N1	-2.47	119.51	122.79
28	S1	668	A2M	C4-C5-N7	-2.46	107.62	110.62
1	1	697	A2M	C2'-C1'-N9	-2.46	109.39	113.53
2	2	655	OMG	O6-C6-C5	-2.46	120.08	126.60
28	S1	2202	PSU	C6-C5-C4	2.46	119.92	118.20
2	2	534	OMG	N9-C8-N7	-2.45	108.77	113.39
2	2	78	PSU	C6-C5-C4	2.45	119.91	118.20
28	S1	1550	OMG	O6-C6-C5	-2.44	120.13	126.60
28	S1	8	OMU	O2-C2-N1	-2.43	119.56	122.79
2	2	641	OMG	C8-N7-C5	2.43	108.63	104.24
2	2	122	PSU	C3'-C2'-C1'	2.42	104.46	101.64
2	2	560	OMU	CM2-O2'-C2'	-2.42	108.17	114.52
1	1	940	PSU	O2-C2-N1	-2.42	120.13	122.79
1	1	239	PSU	O2-C2-N1	-2.42	120.13	122.79
2	2	604	A2M	C4-C5-N7	-2.42	107.68	110.62
1	1	959	OMG	O6-C6-C5	-2.41	120.19	126.60
2	2	1372	A2M	C4-N9-C8	2.41	108.34	105.73
2	2	534	OMG	C1'-N9-C8	2.40	133.54	126.70
28	S1	2151	OMG	O6-C6-C5	-2.40	120.23	126.60
2	2	1077	OMU	O2-C2-N1	-2.40	119.59	122.79
2	2	73	OMU	O4-C4-C5	-2.39	120.95	125.16
2	2	1354	PSU	O2-C2-N1	-2.39	120.16	122.79
2	2	593	PSU	C6-C5-C4	2.38	119.86	118.20
1	1	1107	OMU	O2-C2-N1	-2.38	119.63	122.79
1	1	1626	OMG	O6-C6-C5	-2.38	120.30	126.60
28	S1	33	PSU	O2-C2-N1	-2.37	120.18	122.79
28	S1	1841	PSU	O2-C2-N1	-2.37	120.18	122.79
1	1	1540	OMG	O6-C6-C5	-2.37	120.31	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	1543	B8N	C32-C31-N3	-2.37	107.56	112.00
28	S1	1657	PSU	O2-C2-N1	-2.36	120.19	122.79
28	S1	104	PSU	O2-C2-N1	-2.35	120.20	122.79
7	7	162	A2M	C4-C5-N7	-2.35	107.75	110.62
28	S1	512	A2M	C4-N9-C8	2.35	108.27	105.73
1	1	1402	PSU	O2-C2-N1	-2.35	120.21	122.79
2	2	1403	PSU	O2-C2-N1	-2.34	120.21	122.79
1	1	422	PSU	O2-C2-N1	-2.34	120.22	122.79
1	1	1017	PSU	O2-C2-N1	-2.33	120.23	122.79
28	S1	1192	PSU	C6-C5-C4	2.32	119.82	118.20
28	S1	661	OMU	O2-C2-N1	-2.32	119.70	122.79
28	S1	1533	PSU	O2-C2-N1	-2.32	120.24	122.79
1	1	856	OMG	O6-C6-C5	-2.32	120.45	126.60
1	1	1539	A2M	C4-C5-N7	-2.31	107.80	110.62
1	1	1011	PSU	O4'-C1'-C2'	2.31	108.40	105.14
2	2	1078	OMG	C2-N1-C6	-2.30	120.90	125.10
1	1	845	OMU	C5-C4-N3	2.30	118.28	114.84
2	2	1413	PSU	C6-C5-C4	2.30	119.80	118.20
28	S1	12	PSU	O2-C2-N1	-2.29	120.27	122.79
28	S1	607	PSU	O2-C2-N1	-2.29	120.27	122.79
2	2	1303	PSU	O2-C2-N1	-2.29	120.27	122.79
2	2	512	PSU	O2-C2-N1	-2.29	120.27	122.79
1	1	858	A2M	C2'-C1'-N9	-2.28	109.69	113.53
2	2	1318	PSU	O2-C2-N1	-2.28	120.28	122.79
1	1	955	A2M	C4-C5-N7	-2.27	107.85	110.62
2	2	510	PSU	O2-C2-N1	-2.27	120.29	122.79
28	S1	1192	PSU	O2-C2-N1	-2.27	120.29	122.79
2	2	641	OMG	O6-C6-C5	-2.26	120.61	126.60
2	2	597	PSU	O2-C2-N1	-2.26	120.31	122.79
2	2	1264	PSU	O4'-C1'-C2'	2.25	108.32	105.14
28	S1	1995	7MG	N9-C8-N7	2.25	106.60	103.38
7	7	69	PSU	O2-C2-N1	-2.25	120.32	122.79
1	1	856	OMG	C8-N7-C5	2.25	108.31	104.24
28	S1	2202	PSU	O2-C2-N1	-2.24	120.32	122.79
1	1	1371	OMU	C1'-N1-C6	-2.23	115.97	120.84
1	1	927	A2M	C4-C5-N7	-2.23	107.90	110.62
2	2	512	PSU	C6-C5-C4	2.23	119.76	118.20
1	1	847	OMU	O2-C2-N1	-2.23	119.83	122.79
2	2	572	A2M	C4-N9-C8	2.23	108.14	105.73
2	2	1185	A2M	C4-N9-C8	2.22	108.14	105.73
7	7	69	PSU	O4'-C1'-C2'	2.22	108.28	105.14
1	1	305	A2M	C4-C5-N7	-2.22	107.92	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1303	PSU	O4'-C1'-C2'	2.21	108.26	105.14
2	2	591	A2M	C4-N9-C8	2.20	108.11	105.73
2	2	628	A2M	C5-C4-N9	2.20	108.34	105.78
28	S1	1995	7MG	N9-C4-N3	2.19	128.74	125.47
3	3	13	OMU	O2-C2-N1	-2.19	119.87	122.79
2	2	1359	OMU	O2-C2-N1	-2.19	119.87	122.79
28	S1	1647	OMG	C8-N7-C5	2.19	108.20	104.24
1	1	1190	OMG	C8-N7-C5	2.19	108.20	104.24
28	S1	1156	PSU	O2-C2-N1	-2.19	120.38	122.79
1	1	235	A2M	C4-C5-N7	-2.18	107.96	110.62
28	S1	2021	A2M	C4-C5-N7	-2.18	107.97	110.62
2	2	437	PSU	C6-N1-C2	-2.18	120.46	122.68
1	1	1626	OMG	C8-N7-C5	2.17	108.17	104.24
2	2	1060	PSU	O2-C2-N1	-2.16	120.41	122.79
28	S1	1566	PSU	O2-C2-N1	-2.16	120.42	122.79
2	2	604	A2M	C4-N9-C8	2.16	108.06	105.73
28	S1	668	A2M	C4-N9-C8	2.16	108.06	105.73
28	S1	479	A2M	C4-C5-N7	-2.16	107.99	110.62
7	7	75	OMG	C8-N7-C5	2.16	108.14	104.24
28	S1	98	A2M	C6-C5-C4	2.15	120.08	117.18
1	1	1540	OMG	C8-N7-C5	2.15	108.14	104.24
1	1	697	A2M	C4-N9-C8	2.15	108.06	105.73
28	S1	1829	OMG	C8-N7-C5	2.15	108.12	104.24
28	S1	2021	A2M	C4-N9-C8	2.14	108.05	105.73
7	7	43	A2M	C4-C5-N7	-2.14	108.01	110.62
2	2	1403	PSU	O4'-C1'-C2'	2.14	108.16	105.14
2	2	655	OMG	C8-N7-C5	2.13	108.10	104.24
1	1	1039	PSU	O2-C2-N1	-2.13	120.44	122.79
1	1	305	A2M	C4-N9-C8	2.13	108.04	105.73
1	1	1524	OMG	C8-N7-C5	2.12	108.08	104.24
28	S1	2046	PSU	C6-C5-C4	2.12	119.68	118.20
2	2	572	A2M	C4-C5-N7	-2.12	108.04	110.62
7	7	162	A2M	C5-C4-N9	2.12	108.25	105.78
2	2	572	A2M	O4'-C1'-N9	2.12	112.23	108.06
1	1	305	A2M	C6-C5-C4	2.12	120.03	117.18
28	S1	98	A2M	C4-C5-N7	-2.11	108.05	110.62
2	2	524	5MC	CM5-C5-C6	-2.10	120.04	122.85
2	2	662	PSU	O4'-C1'-C2'	2.10	108.11	105.14
28	S1	1550	OMG	C8-N7-C5	2.10	108.05	104.24
28	S1	29	OMU	O2-C2-N1	-2.10	119.99	122.79
2	2	593	PSU	O2-C2-N1	-2.10	120.48	122.79
1	1	1539	A2M	C5-C4-N9	2.09	108.22	105.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S1	2061	5MC	CM5-C5-C6	-2.09	120.05	122.85
1	1	407	A2M	C6-C5-C4	2.09	119.99	117.18
2	2	626	PSU	C6-C5-C4	2.08	119.65	118.20
7	7	74	PSU	O2-C2-N1	-2.08	120.50	122.79
1	1	1664	PSU	C6-C5-C4	2.08	119.65	118.20
2	2	382	A2M	C6-C5-C4	2.08	119.97	117.18
2	2	1361	PSU	O2-C2-N1	-2.08	120.51	122.79
1	1	1528	PSU	O2-C2-N1	-2.07	120.51	122.79
1	1	858	A2M	C4-C5-N7	-2.07	108.10	110.62
2	2	1185	A2M	C4-C5-N7	-2.07	108.10	110.62
2	2	1360	OMG	C8-N7-C5	2.07	107.98	104.24
1	1	697	A2M	C4-C5-N7	-2.07	108.10	110.62
1	1	1539	A2M	C6-C5-C4	2.07	119.96	117.18
28	S1	512	A2M	C6-C5-C4	2.06	119.96	117.18
28	S1	1979	OMU	C1'-N1-C2	2.06	121.30	117.57
2	2	1253	OMG	C8-N7-C5	2.06	107.96	104.24
2	2	1413	PSU	O2-C2-N1	-2.06	120.53	122.79
2	2	1229	OMG	C8-N7-C5	2.06	107.96	104.24
28	S1	668	A2M	C3'-C2'-C1'	2.05	106.75	102.89
2	2	604	A2M	C6-C5-C4	2.05	119.94	117.18
2	2	1046	OMG	C8-N7-C5	2.05	107.96	104.24
28	S1	1478	OMG	C8-N7-C5	2.05	107.95	104.24
1	1	235	A2M	C4-N9-C8	2.05	107.95	105.73
2	2	1185	A2M	C6-C5-C4	2.05	119.94	117.18
2	2	628	A2M	C4-N9-C8	2.05	107.95	105.73
28	S1	455	PSU	O2-C2-N1	-2.04	120.54	122.79
28	S1	479	A2M	C6-C5-C4	2.04	119.93	117.18
2	2	78	PSU	O2-C2-N1	-2.04	120.55	122.79
1	1	1107	OMU	C2'-C1'-N1	-2.04	110.27	114.22
1	1	1533	PSU	O4'-C1'-C2'	2.04	108.02	105.14
2	2	1354	PSU	C6-C5-C4	2.03	119.62	118.20
2	2	71	OMG	C8-N7-C5	2.03	107.92	104.24
1	1	1011	PSU	C6-C5-C4	2.03	119.62	118.20
2	2	1078	OMG	C1'-N9-C4	-2.03	120.47	126.50
1	1	959	OMG	C8-N7-C5	2.03	107.92	104.24
28	S1	1879	OMG	C8-N7-C5	2.03	107.91	104.24
28	S1	2151	OMG	C8-N7-C5	2.03	107.91	104.24
7	7	43	A2M	C6-C5-C4	2.03	119.91	117.18
2	2	56	OMU	O2-C2-N1	-2.03	120.09	122.79
1	1	1539	A2M	C5'-C4'-C3'	-2.03	107.59	115.18
1	1	927	A2M	C4-N9-C8	2.02	107.92	105.73
4	4	74	OMG	C8-N7-C5	2.02	107.90	104.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	845	OMU	C5-C6-N1	-2.02	118.42	121.81
1	1	845	OMU	C6-N1-C2	-2.02	118.41	120.99
28	S1	2061	5MC	C5-C4-N3	-2.02	119.50	121.67
2	2	1231	OMG	C8-N7-C5	2.02	107.89	104.24
7	7	162	A2M	C4-N9-C8	2.01	107.91	105.73
2	2	71	OMG	C2'-C1'-N9	-2.01	110.32	114.22
28	S1	1543	B8N	O36-C34-C33	2.01	120.22	113.38
28	S1	1833	OMU	O2-C2-N1	-2.01	120.12	122.79
1	1	955	A2M	C4-N9-C8	2.00	107.90	105.73

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	7	7	OMU	C1'-C2'-O2'-CM2
7	7	75	OMG	C1'-C2'-O2'-CM2
7	7	162	A2M	C1'-C2'-O2'-CM'
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	C3'-C4'-C5'-O5'
1	1	845	OMU	O4'-C1'-N1-C2
1	1	845	OMU	O4'-C1'-N1-C6
1	1	845	OMU	C1'-C2'-O2'-CM2
1	1	955	A2M	C1'-C2'-O2'-CM'
1	1	1011	PSU	C2'-C1'-C5-C4
1	1	1171	PSU	C3'-C4'-C5'-O5'
1	1	1171	PSU	O4'-C4'-C5'-O5'
1	1	1371	OMU	O4'-C1'-N1-C2
1	1	1371	OMU	O4'-C1'-N1-C6
1	1	1540	OMG	O4'-C4'-C5'-O5'
2	2	122	PSU	O4'-C4'-C5'-O5'
2	2	382	A2M	C1'-C2'-O2'-CM'
2	2	443	OMC	C2'-C1'-N1-C6
2	2	534	OMG	O4'-C4'-C5'-O5'
2	2	534	OMG	C3'-C4'-C5'-O5'
2	2	570	A2M	C1'-C2'-O2'-CM'
2	2	591	A2M	C1'-C2'-O2'-CM'
2	2	1046	OMG	C1'-C2'-O2'-CM2
2	2	1058	PSU	C3'-C4'-C5'-O5'
2	2	1229	OMG	O4'-C4'-C5'-O5'
2	2	1229	OMG	C3'-C4'-C5'-O5'
2	2	1248	OMC	C1'-C2'-O2'-CM2
2	2	1264	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	2	1264	PSU	O4'-C1'-C5-C6
2	2	1384	A2M	C1'-C2'-O2'-CM'
28	S1	29	OMU	C1'-C2'-O2'-CM2
28	S1	455	PSU	C2'-C1'-C5-C4
28	S1	455	PSU	O4'-C1'-C5-C4
28	S1	455	PSU	O4'-C1'-C5-C6
28	S1	607	PSU	O4'-C1'-C5-C4
28	S1	607	PSU	O4'-C1'-C5-C6
28	S1	668	A2M	C1'-C2'-O2'-CM'
28	S1	1543	B8N	O4'-C4'-C5'-O5'
28	S1	1543	B8N	C3'-C4'-C5'-O5'
28	S1	1543	B8N	N3-C31-C32-C33
28	S1	1543	B8N	C31-C32-C33-C34
28	S1	1543	B8N	C31-C32-C33-N34
28	S1	1566	PSU	C3'-C4'-C5'-O5'
28	S1	1566	PSU	O4'-C4'-C5'-O5'
28	S1	1623	OMG	C1'-C2'-O2'-CM2
28	S1	1841	PSU	C3'-C4'-C5'-O5'
28	S1	1879	OMG	O4'-C4'-C5'-O5'
28	S1	1879	OMG	C3'-C4'-C5'-O5'
28	S1	1879	OMG	C1'-C2'-O2'-CM2
28	S1	2021	A2M	C3'-C4'-C5'-O5'
28	S1	2021	A2M	C1'-C2'-O2'-CM'
28	S1	2151	OMG	C3'-C4'-C5'-O5'
2	2	443	OMC	C2'-C1'-N1-C2
1	1	305	A2M	O4'-C4'-C5'-O5'
1	1	678	A2M	O4'-C4'-C5'-O5'
1	1	1181	PSU	C3'-C4'-C5'-O5'
1	1	1540	OMG	C3'-C4'-C5'-O5'
2	2	122	PSU	C3'-C4'-C5'-O5'
2	2	527	A2M	O4'-C4'-C5'-O5'
2	2	1046	OMG	O4'-C4'-C5'-O5'
28	S1	668	A2M	O4'-C4'-C5'-O5'
28	S1	668	A2M	C3'-C4'-C5'-O5'
28	S1	1621	OMU	O4'-C4'-C5'-O5'
28	S1	1841	PSU	O4'-C4'-C5'-O5'
1	1	678	A2M	C3'-C4'-C5'-O5'
1	1	1181	PSU	O4'-C4'-C5'-O5'
2	2	527	A2M	C3'-C4'-C5'-O5'
2	2	1046	OMG	C3'-C4'-C5'-O5'
2	2	1058	PSU	O4'-C4'-C5'-O5'
28	S1	98	A2M	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	S1	2021	A2M	O4'-C4'-C5'-O5'
2	2	1308	5MC	C2'-C1'-N1-C6
28	S1	8	OMU	C2'-C1'-N1-C6
2	2	1078	OMG	C3'-C4'-C5'-O5'
2	2	1078	OMG	O4'-C4'-C5'-O5'
28	S1	1544	5MC	O4'-C4'-C5'-O5'
28	S1	2151	OMG	O4'-C4'-C5'-O5'
1	1	305	A2M	C3'-C4'-C5'-O5'
2	2	1185	A2M	C3'-C4'-C5'-O5'
28	S1	1979	OMU	C3'-C4'-C5'-O5'
28	S1	1543	B8N	N34-C33-C34-O35
1	1	1010	OMC	O4'-C4'-C5'-O5'
2	2	1248	OMC	C4'-C5'-O5'-P
2	2	1361	PSU	C4'-C5'-O5'-P
28	S1	1829	OMG	C4'-C5'-O5'-P
2	2	570	A2M	C2'-C1'-N9-C8
28	S1	668	A2M	C2'-C1'-N9-C8
28	S1	8	OMU	O4'-C1'-N1-C6
28	S1	8	OMU	O4'-C4'-C5'-O5'
28	S1	98	A2M	C3'-C4'-C5'-O5'
28	S1	1192	PSU	C3'-C4'-C5'-O5'
28	S1	1995	7MG	O4'-C4'-C5'-O5'
2	2	1308	5MC	C2'-C1'-N1-C2
2	2	443	OMC	O4'-C1'-N1-C6
2	2	1308	5MC	O4'-C1'-N1-C6
1	1	677	1MA	C2'-C1'-N9-C8
1	1	681	A2M	C4'-C5'-O5'-P
2	2	560	OMU	C4'-C5'-O5'-P
2	2	1185	A2M	C4'-C5'-O5'-P
28	S1	1192	PSU	O4'-C4'-C5'-O5'
28	S1	1979	OMU	O4'-C4'-C5'-O5'
2	2	443	OMC	O4'-C1'-N1-C2
28	S1	1833	OMU	C4'-C5'-O5'-P
28	S1	2185	MA6	C4'-C5'-O5'-P
2	2	1354	PSU	C4'-C5'-O5'-P
1	1	677	1MA	C2'-C1'-N9-C4
28	S1	1995	7MG	C3'-C4'-C5'-O5'
2	2	1308	5MC	O4'-C1'-N1-C2
28	S1	8	OMU	O4'-C1'-N1-C2
28	S1	1543	B8N	C32-C33-C34-O35
1	1	1171	PSU	O4'-C1'-C5-C4
28	S1	1657	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	2	655	OMG	C3'-C2'-O2'-CM2
28	S1	8	OMU	C3'-C2'-O2'-CM2
28	S1	8	OMU	C2'-C1'-N1-C2
2	2	570	A2M	O4'-C1'-N9-C8
28	S1	1543	B8N	N34-C33-C34-O36
28	S1	1544	5MC	C3'-C4'-C5'-O5'
2	2	560	OMU	C3'-C4'-C5'-O5'
28	S1	1979	OMU	C2'-C1'-N1-C2
1	1	1527	OMC	O4'-C4'-C5'-O5'
28	S1	1543	B8N	C32-C33-C34-O36
1	1	1171	PSU	O4'-C1'-C5-C6
28	S1	2202	PSU	O4'-C1'-C5-C6
1	1	858	A2M	O4'-C1'-N9-C8
28	S1	668	A2M	O4'-C1'-N9-C8
1	1	1010	OMC	C3'-C4'-C5'-O5'
28	S1	512	A2M	O4'-C4'-C5'-O5'
28	S1	1478	OMG	C3'-C4'-C5'-O5'
28	S1	1833	OMU	O4'-C4'-C5'-O5'
1	1	1539	A2M	C3'-C2'-O2'-CM'
2	2	1360	OMG	C3'-C2'-O2'-CM2
1	1	1371	OMU	C4'-C5'-O5'-P
28	S1	607	PSU	C4'-C5'-O5'-P
28	S1	8	OMU	C3'-C4'-C5'-O5'
2	2	570	A2M	C2'-C1'-N9-C4

There are no ring outliers.

77 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	7	7	OMU	2	0
2	2	591	A2M	3	0
1	1	695	OMC	1	0
2	2	1231	OMG	1	0
2	2	534	OMG	1	0
28	S1	98	A2M	1	0
2	2	1253	OMG	1	0
28	S1	2202	PSU	1	0
2	2	560	OMU	2	0
2	2	1078	OMG	1	0
2	2	604	A2M	2	0
1	1	1017	PSU	2	0
28	S1	2185	MA6	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1359	OMU	1	0
28	S1	29	OMU	2	0
2	2	655	OMG	1	0
2	2	472	PSU	1	0
28	S1	1647	OMG	1	0
2	2	1248	OMC	1	0
2	2	583	OMC	1	0
2	2	1413	PSU	1	0
2	2	1384	A2M	1	0
2	2	1060	PSU	1	0
1	1	1539	A2M	1	0
2	2	1046	OMG	1	0
28	S1	1879	OMG	1	0
28	S1	1623	OMG	1	0
2	2	667	OMU	1	0
2	2	1372	A2M	1	0
1	1	1171	PSU	3	0
28	S1	2151	OMG	2	0
28	S1	512	A2M	1	0
7	7	75	OMG	2	0
2	2	570	A2M	2	0
28	S1	1192	PSU	1	0
28	S1	2046	PSU	2	0
2	2	1058	PSU	1	0
3	3	13	OMU	1	0
28	S1	479	A2M	1	0
28	S1	1865	OMG	1	0
1	1	1039	PSU	1	0
1	1	1528	PSU	1	0
28	S1	1550	OMG	1	0
2	2	1318	PSU	1	0
1	1	845	OMU	3	0
1	1	927	A2M	1	0
2	2	95	A2M	1	0
1	1	1527	OMC	1	0
2	2	527	A2M	2	0
2	2	1194	PSU	1	0
1	1	305	A2M	1	0
28	S1	2061	5MC	1	0
28	S1	1979	OMU	5	0
2	2	382	A2M	5	0
1	1	1402	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	S1	12	PSU	1	0
28	S1	2140	OMC	3	0
2	2	1382	PSU	1	0
28	S1	18	OMC	1	0
1	1	1533	PSU	1	0
7	7	43	A2M	1	0
1	1	235	A2M	1	0
2	2	1308	5MC	1	0
28	S1	668	A2M	1	0
2	2	641	OMG	1	0
1	1	407	A2M	1	0
1	1	955	A2M	2	0
1	1	847	OMU	1	0
28	S1	1621	OMU	1	0
2	2	512	PSU	3	0
7	7	162	A2M	2	0
2	2	626	PSU	1	0
28	S1	1478	OMG	1	0
2	2	122	PSU	2	0
2	2	524	5MC	1	0
1	1	1540	OMG	2	0
28	S1	1543	B8N	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 270 ligands modelled in this entry, 270 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	7	1
28	S1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	169:A	O3'	170:A	P	4.55
1	S1	1543:B8N	O3'	1544:5MC	P	4.07

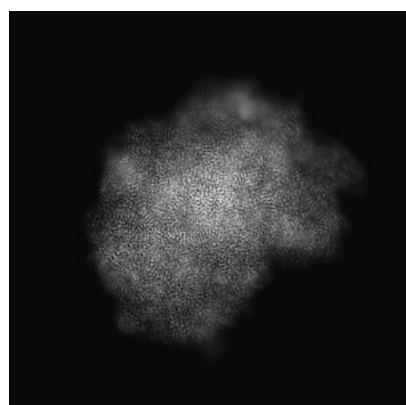
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18437. These allow visual inspection of the internal detail of the map and identification of artifacts.

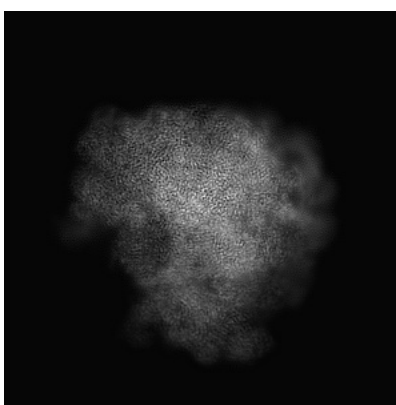
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

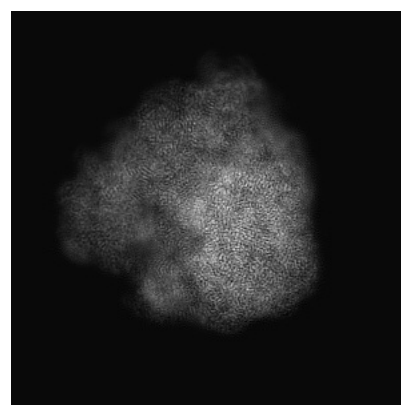
6.1.1 Primary map



X



Y

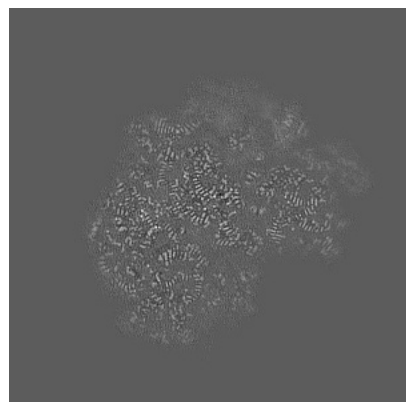


Z

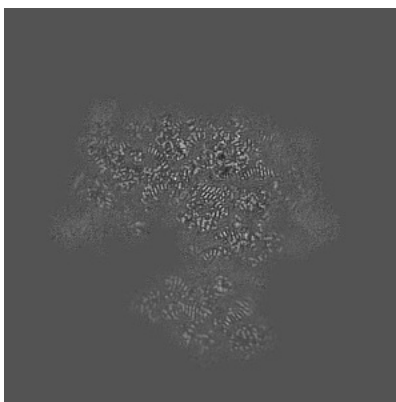
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

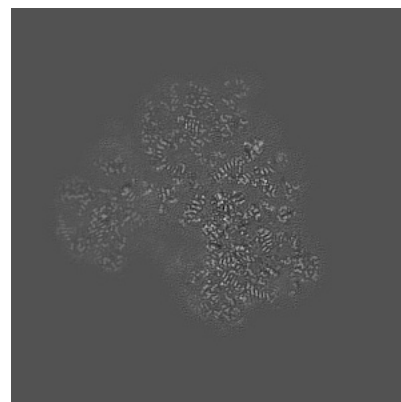
6.2.1 Primary map



X Index: 240



Y Index: 240

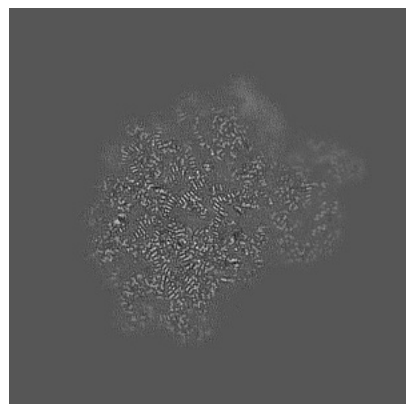


Z Index: 240

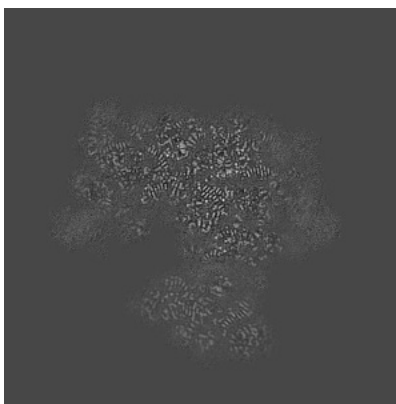
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

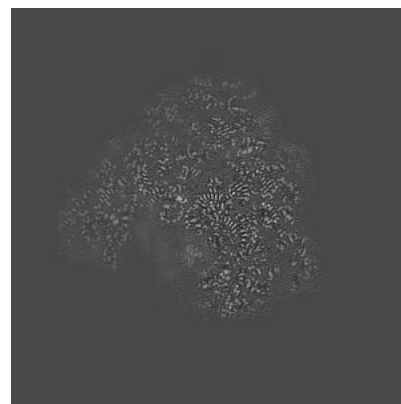
6.3.1 Primary map



X Index: 276



Y Index: 241

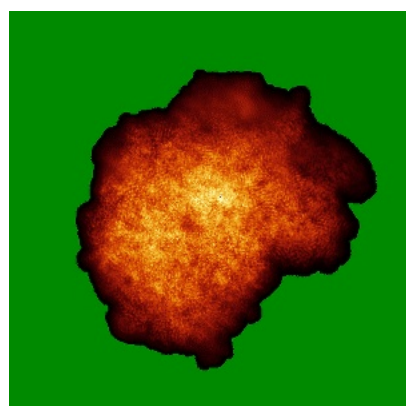


Z Index: 253

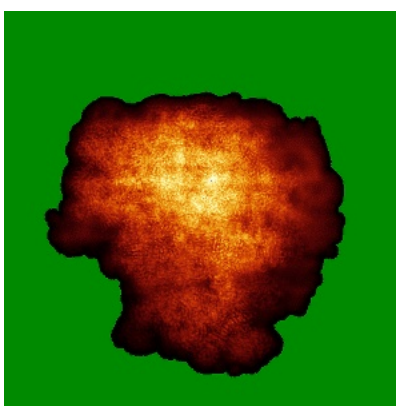
The images above show the largest variance slices of the map in three orthogonal directions.

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

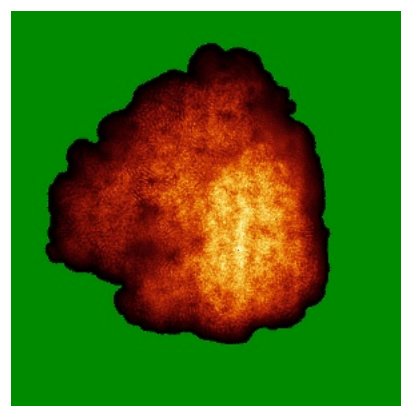
6.4.1 Primary map



X



Y

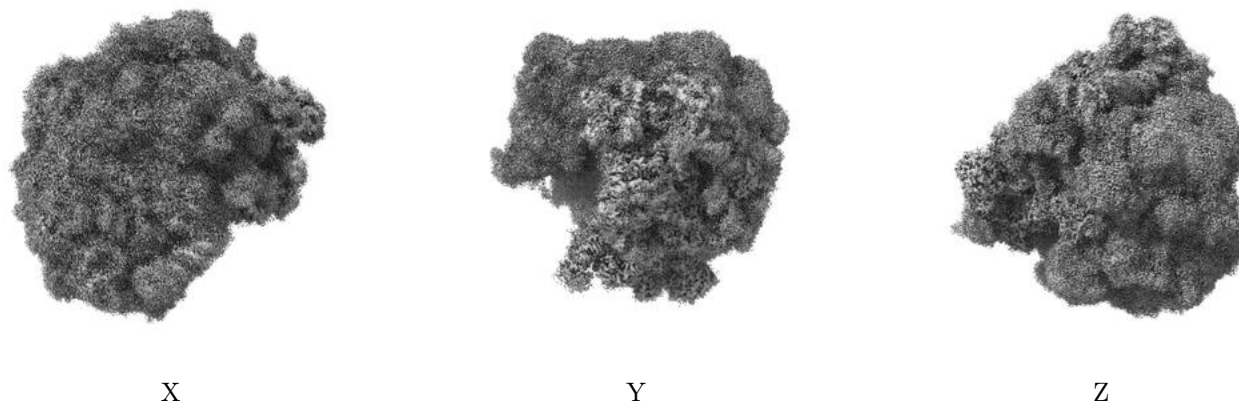


Z

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

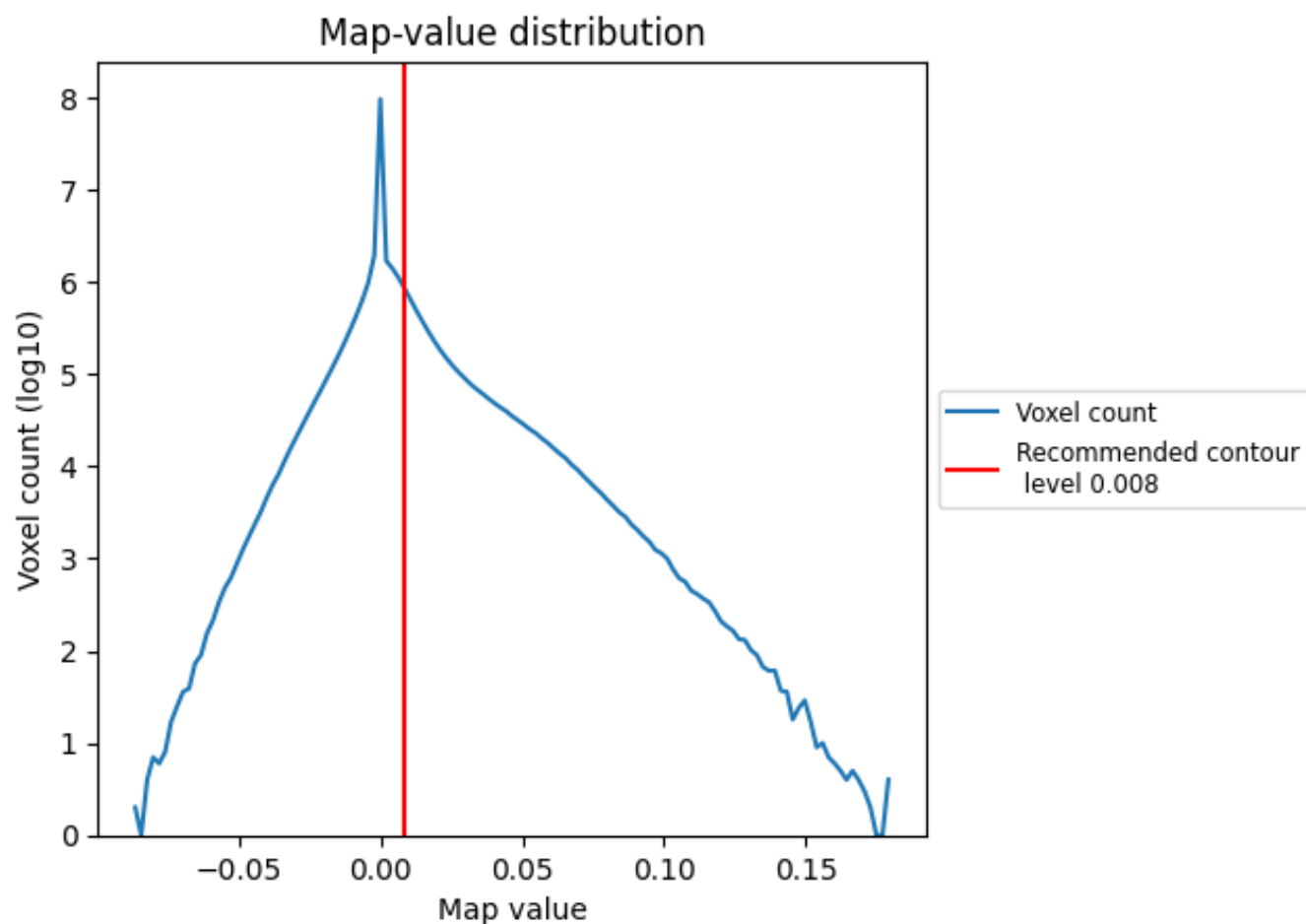
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

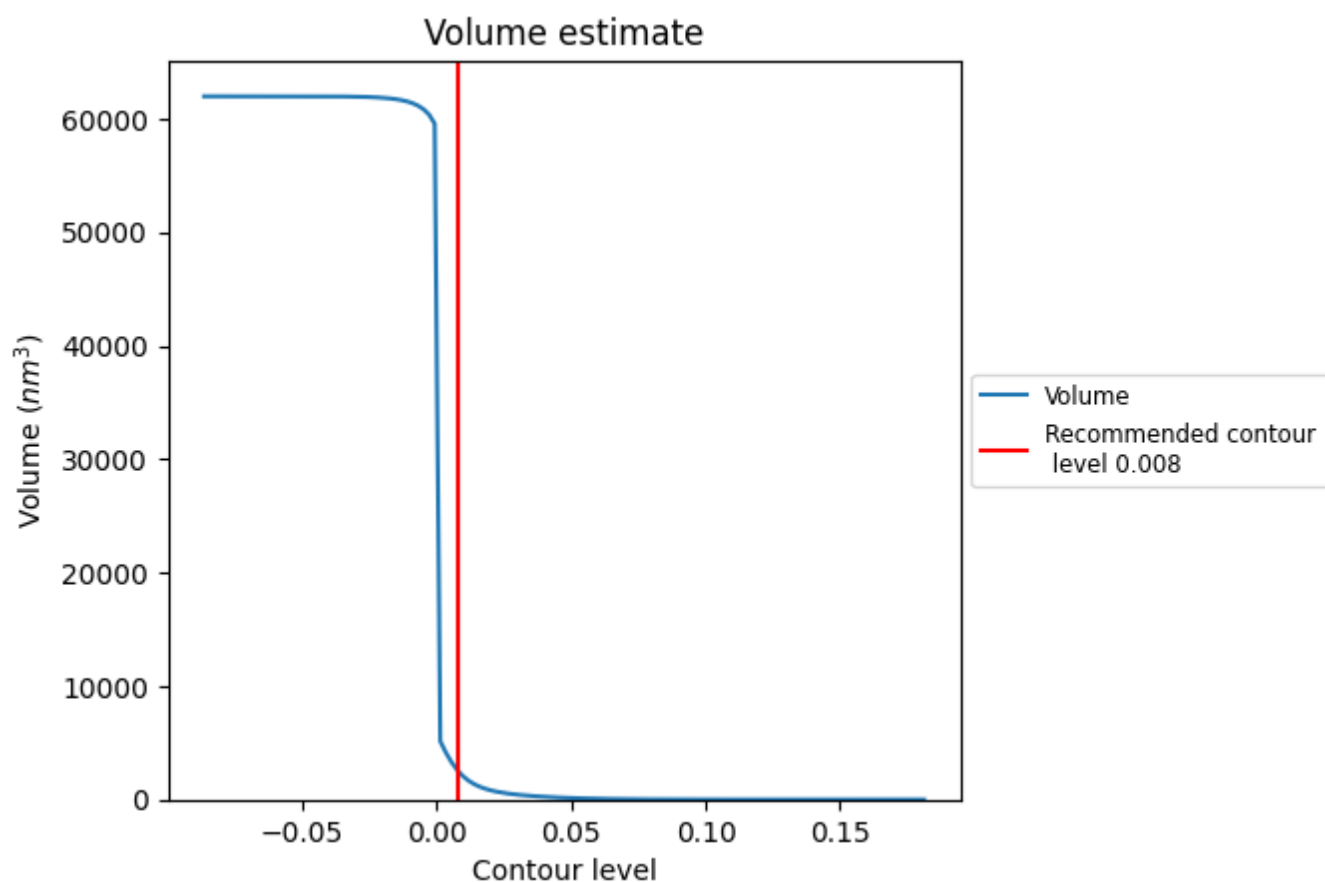
This section contains the results of statistical analysis of the map.

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.

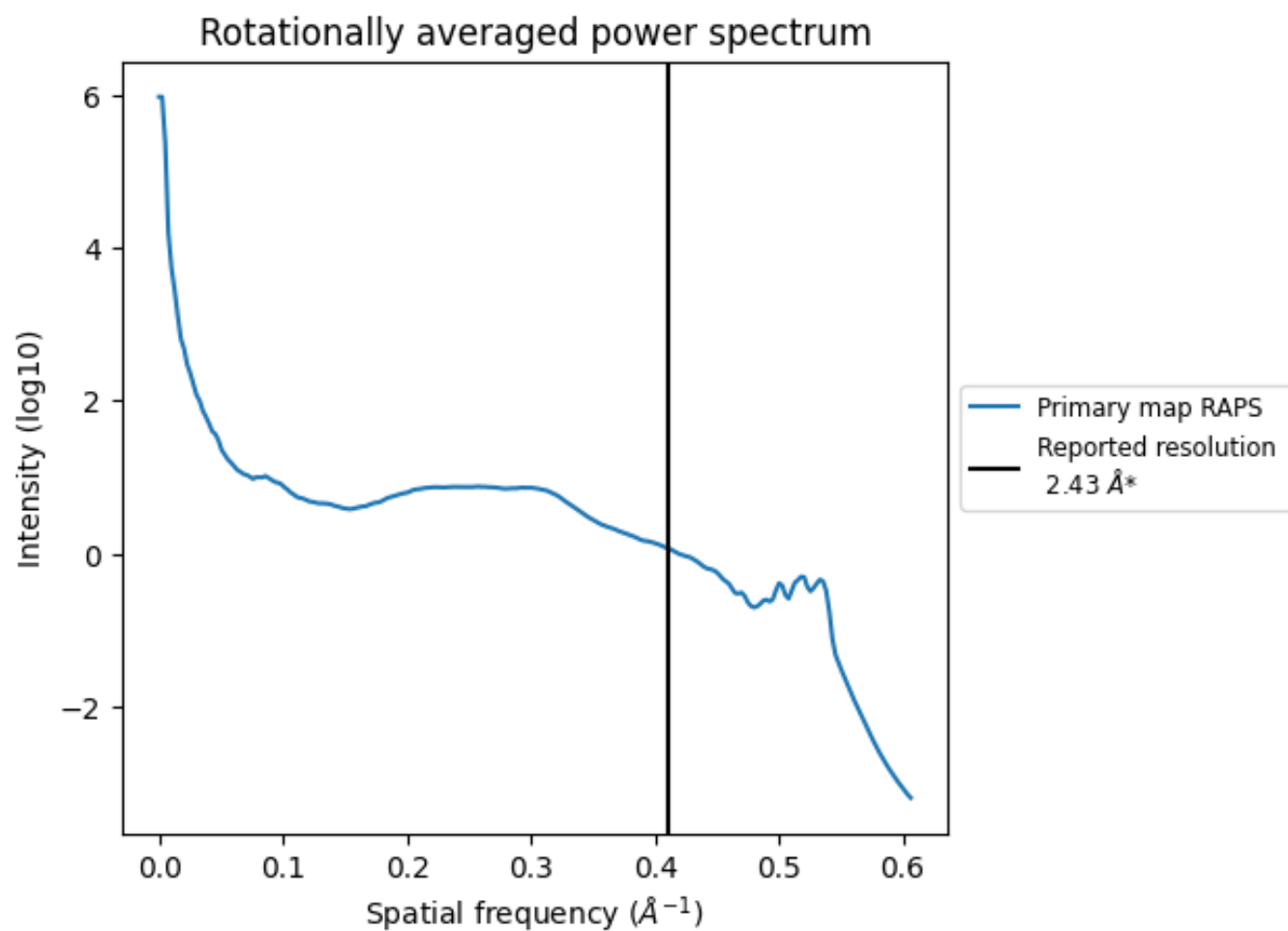
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2508 nm^3 ; this corresponds to an approximate mass of 2266 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 ⓘ

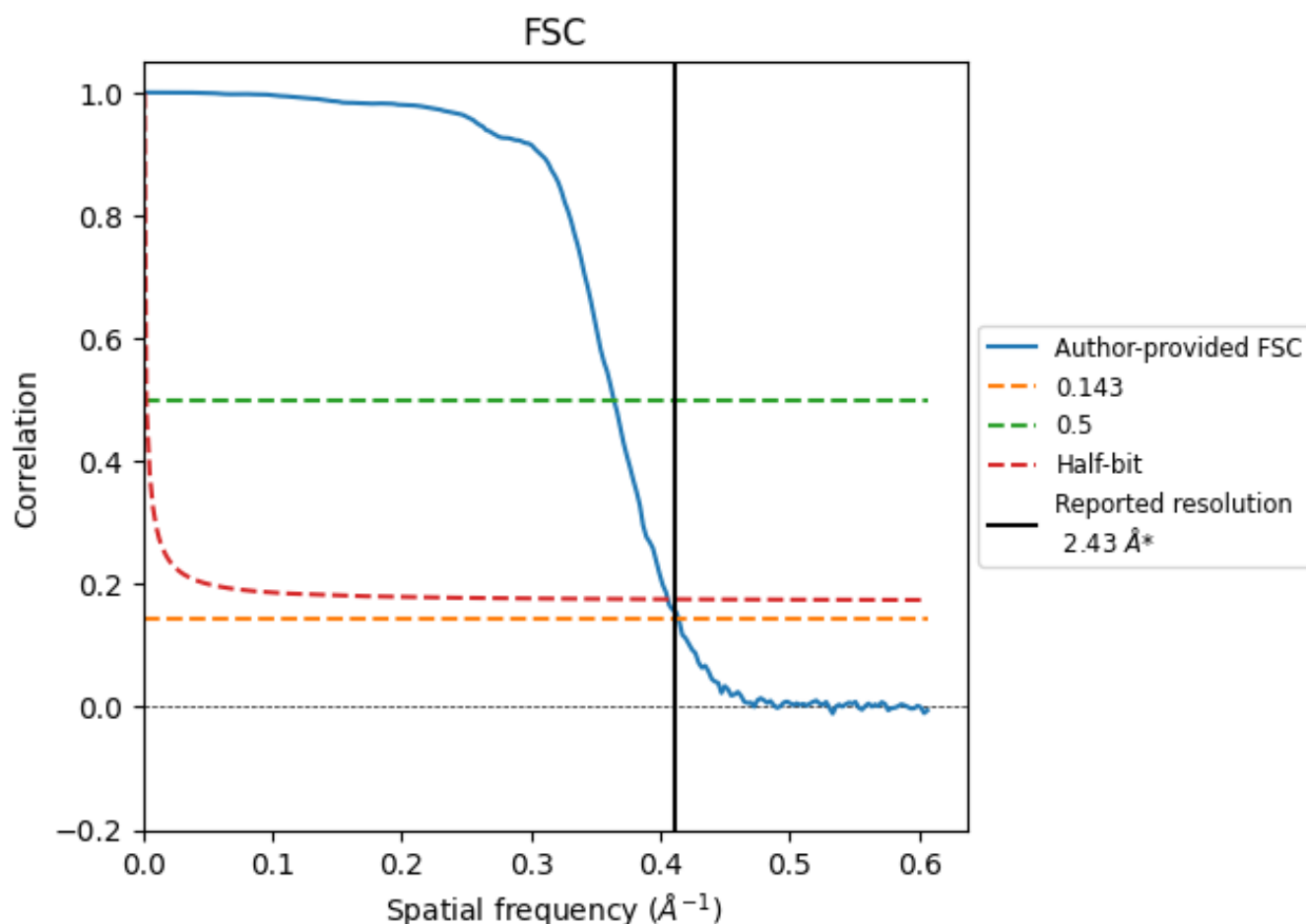


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

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 0.412 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

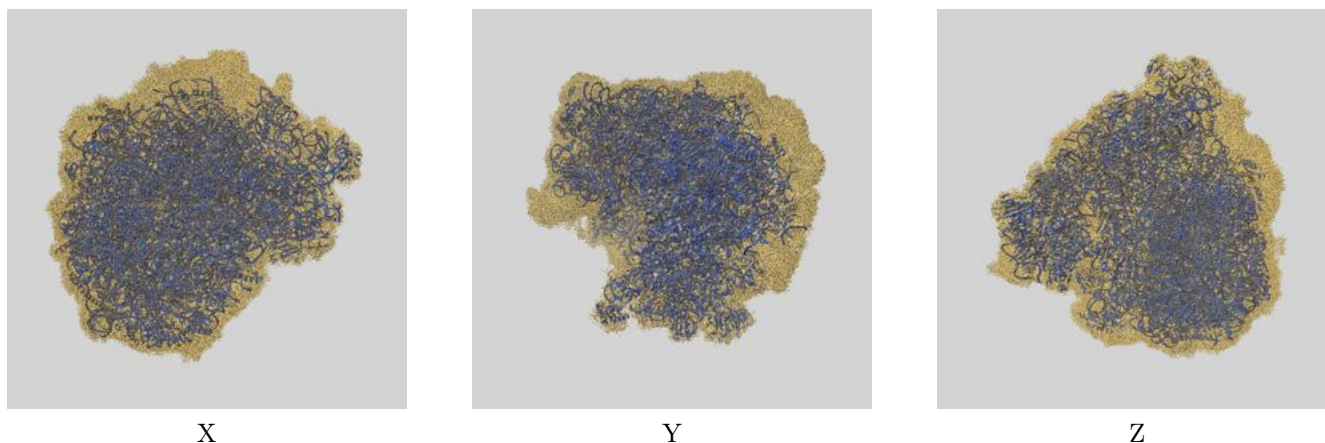
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.41	2.75	2.46
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

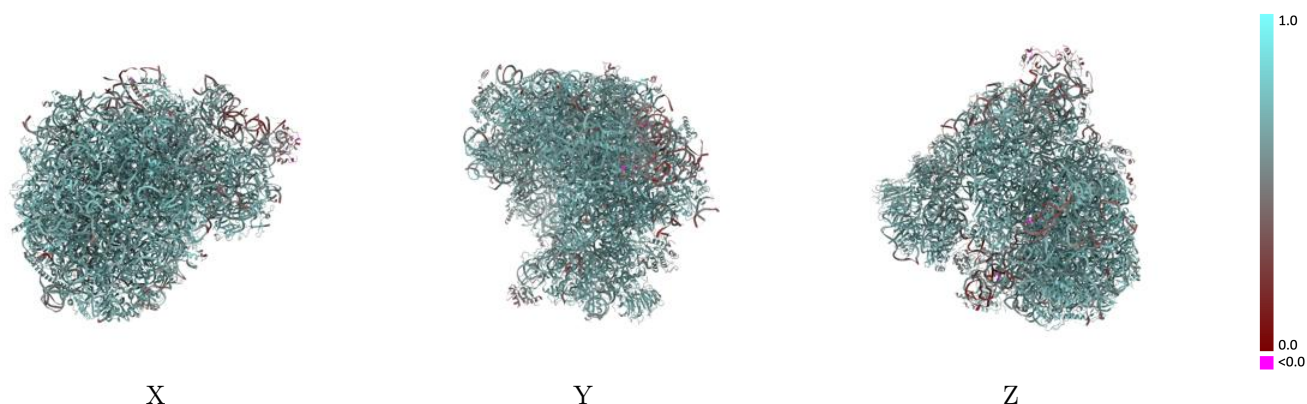
This section contains information regarding the fit between EMDB map EMD-18437 and PDB model 8QIE. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



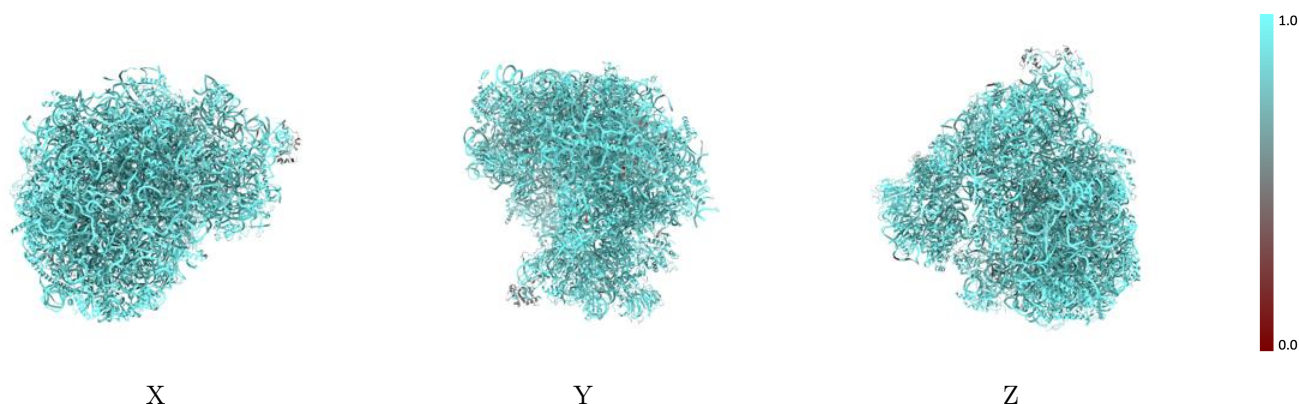
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



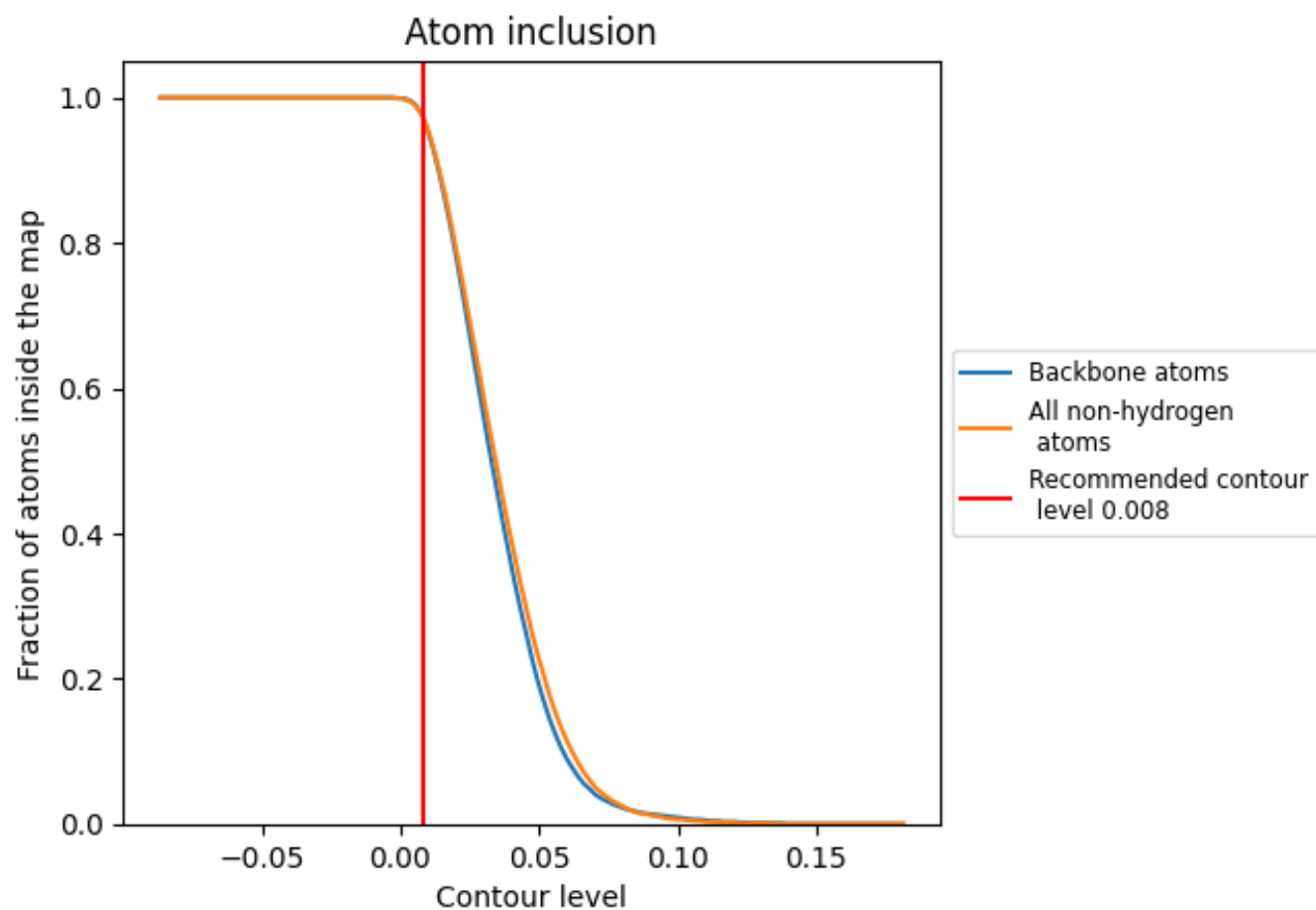
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6550
1	 0.9840	 0.6640
2	 0.9790	 0.6420
3	 0.9870	 0.6550
4	 0.9860	 0.6700
5	 0.9770	 0.6550
6	 0.9680	 0.6310
7	 0.9890	 0.6700
8	 0.9970	 0.6660
A	 0.9980	 0.7320
B	 0.9960	 0.7300
C	 0.9930	 0.6930
D	 0.9650	 0.5600
E	 0.9830	 0.6460
F	 0.9780	 0.6620
G	 0.9930	 0.6890
H	 0.9960	 0.7200
I	 0.9880	 0.6780
J	 0.9930	 0.7180
K	 0.9750	 0.6560
L	 0.9950	 0.7090
M	 0.9990	 0.7250
N	 0.9740	 0.6390
O	 0.9830	 0.6470
P	 0.9980	 0.7030
Q	 0.9960	 0.6880
R	 0.9960	 0.7110
S	 0.9840	 0.6840
S1	 0.9720	 0.6350
S4	 0.7840	 0.2720
SA	 0.9780	 0.6600
SB	 0.9400	 0.5660
SC	 0.9420	 0.6230
SD	 0.9840	 0.6660
SE	 0.9760	 0.6720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SF	 0.9640	 0.6660
SG	 0.9690	 0.6430
SH	 0.9830	 0.6710
SI	 0.9740	 0.6510
SJ	 0.9910	 0.7100
SK	 0.9800	 0.6710
SL	 0.9850	 0.6770
SM	 0.9270	 0.6290
SN	 0.9390	 0.6280
SO	 0.9930	 0.6870
SP	 0.9900	 0.6980
SQ	 0.5530	 0.4310
SR	 0.9460	 0.6300
SS	 0.9890	 0.6740
ST	 0.9960	 0.6970
SU	 0.9850	 0.6900
SV	 0.9840	 0.6580
SW	 0.9170	 0.6200
SX	 0.9640	 0.6570
SY	 0.9440	 0.6040
SZ	 0.9770	 0.6560
Sa	 0.9500	 0.6400
Sb	 0.9910	 0.7050
Sc	 0.9510	 0.6630
Sd	 0.9640	 0.6320
Se	 0.9950	 0.6520
Sf	 0.5610	 0.4380
Sg	 0.9430	 0.6280
Sh	 0.7140	 0.4000
T	 0.9960	 0.7300
U	 0.9350	 0.5420
V	 0.9980	 0.7070
W	 0.9950	 0.6870
X	 0.9980	 0.7150
Y	 0.9930	 0.6540
Z	 0.9820	 0.6660
a	 0.9870	 0.6650
b	 0.9850	 0.6810
c	 0.9930	 0.7020
d	 0.9930	 0.6750
e	 0.9790	 0.6840
f	 0.9970	 0.7070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.9920	 0.7010
h	 0.9650	 0.6540
i	 0.9870	 0.6600
j	 0.9950	 0.7250
k	 0.9540	 0.6040
l	 0.9930	 0.7130
m	 0.9400	 0.5970
n	 0.9960	 0.6810
o	 0.9920	 0.7150
p	 0.9710	 0.6610