



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 8OVJ / pdb_00008ovj
EMDB ID : EMD-17216
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
PARENTAL STRAIN
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2023-04-26
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

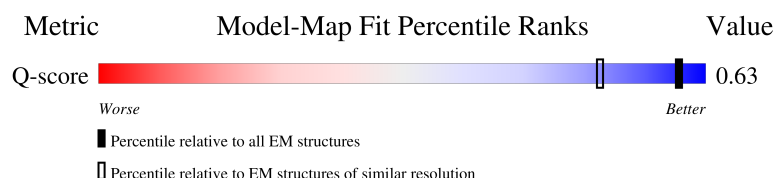
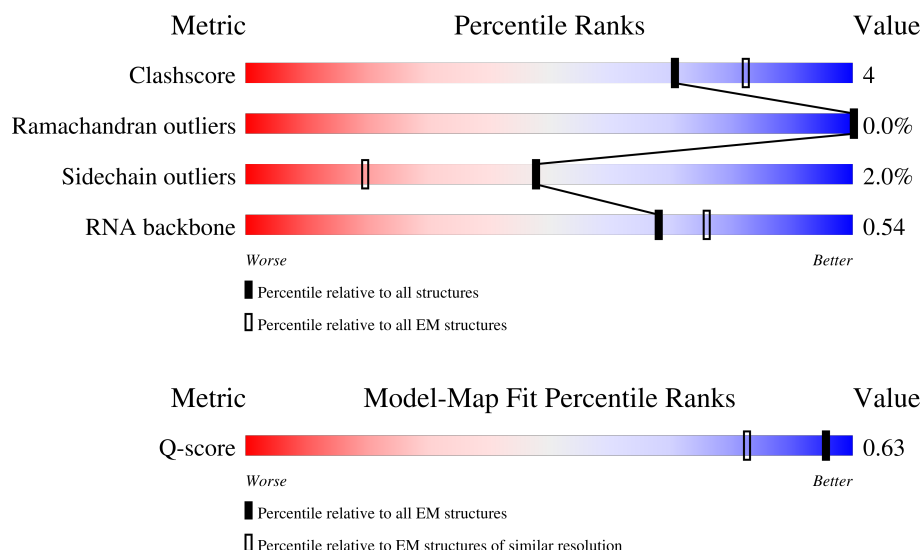
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

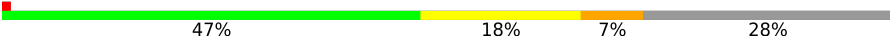
The reported resolution of this entry is 2.40 Å.

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.



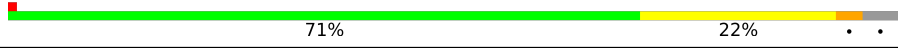
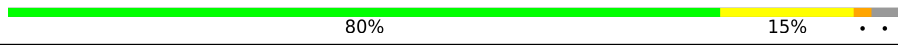
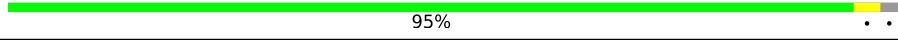
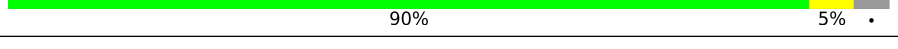
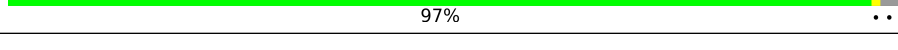
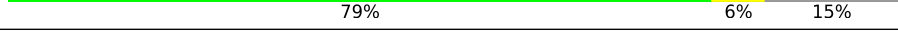
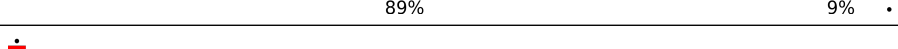
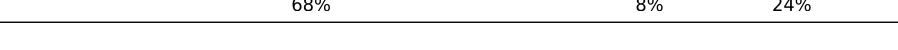
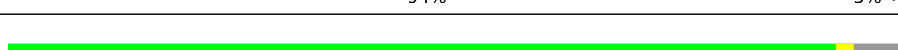
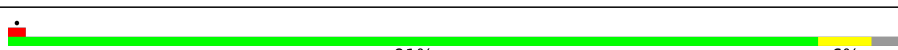
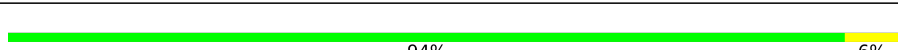
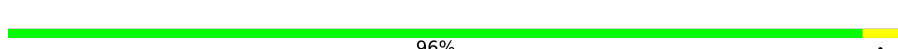
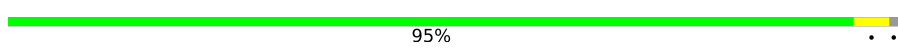
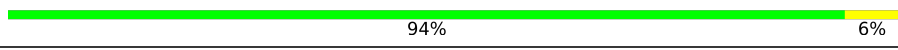
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	3	216	
3	4	183	

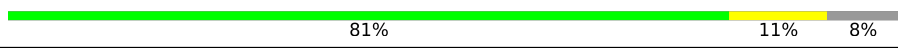
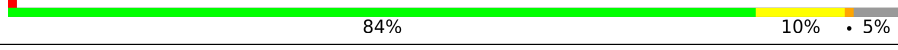
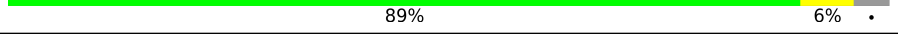
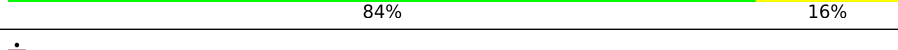
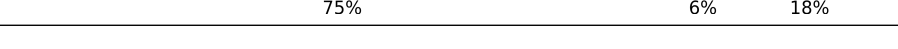
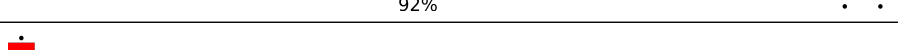
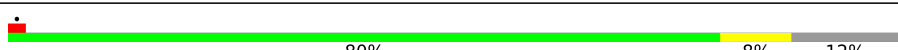
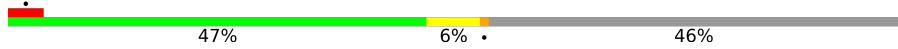
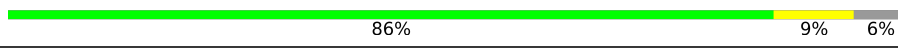
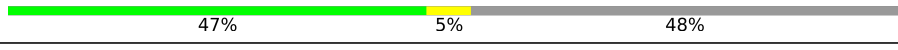
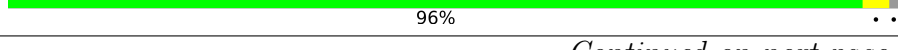
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	5	135	
5	6	73	
6	7	171	
7	8	123	
8	A	260	
9	B	419	
10	C	373	
11	D	188	
12	E	190	
13	F	195	
14	G	264	
15	H	222	
16	I	220	
17	J	139	
18	K	175	
19	L	145	
20	M	204	
21	N	213	
22	O	305	
23	P	198	
24	Q	254	
25	R	179	
26	S1	2204	
27	S4	20	
28	SA	264	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	SB	246	
30	SC	219	
31	SD	190	
32	SE	273	
33	SF	265	
34	SG	249	
35	SH	190	
36	SI	200	
37	SK	220	
38	SL	149	
39	SM	116	
40	SN	168	
41	SO	144	
42	SP	143	
43	SQ	141	
44	SR	153	
45	SS	57	
46	ST	151	
47	SU	173	
48	SV	143	
49	SW	152	
50	SX	161	
51	SY	164	
52	SZ	137	
53	S	159	

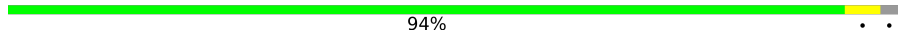
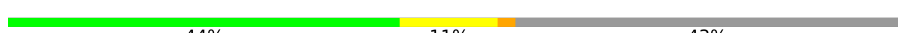
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Sa	120	
55	Sc	86	
56	Sb	112	
57	Sd	87	
58	Se	66	
59	Sg	312	
60	Sh	235	
61	SJ	130	
62	T	166	
63	U	129	
64	V	145	
65	W	143	
66	X	124	
67	Y	134	
68	Z	147	
69	a	127	
70	b	70	
71	c	252	
72	d	104	
73	e	188	
74	f	133	
75	g	144	
76	h	168	
77	i	105	
78	j	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	k	83	
80	l	51	
81	m	128	
82	n	34	
83	o	92	
84	p	106	
85	2	478	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 200822 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	1	0
			34587	15461	6344	11171	1611		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	164	G	U	conflict	GB 321438308
1	165	U	C	conflict	GB 321438308
1	198	A	C	conflict	GB 321438308
1	523	A	G	conflict	GB 321438308
1	588	U	A	conflict	GB 321438308
1	593	C	U	conflict	GB 321438308
1	1428	A	C	conflict	GB 321438308

- Molecule 2 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	156	Total	C	N	O	P	0	0
			3312	1481	577	1098	156		

- Molecule 3 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	183	Total	C	N	O	P	0	0
			3917	1747	710	1277	183		

- Molecule 4 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	115	Total	C	N	O	P	0	0
			2456	1095	445	801	115		

- Molecule 5 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 6 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	164	Total	C	N	O	P	0	0
			3485	1561	618	1143	163		

- Molecule 7 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 8 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	255	Total	C	N	O	S	1	0
			1893	1179	387	317	10		

- Molecule 9 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	401	Total	C	N	O	S	3	0
			3035	1923	595	504	13		

- Molecule 10 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	366	Total	C	N	O	S	0	0
			2664	1671	527	451	15		

- Molecule 11 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	160	Total	C	N	O	S	0	0
			1025	641	205	173	6		

- Molecule 12 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	186	Total	C	N	O	S	0	0
			1337	851	254	228	4		

- Molecule 13 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	148	Total	C	N	O	S	0	0
			1049	671	200	176	2		

- Molecule 14 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	226	Total	C	N	O	S	0	0
			1672	1061	328	276	7		

- Molecule 15 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	220	Total	C	N	O	S	0	0
			1652	1048	332	265	7		

- Molecule 16 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	208	Total	C	N	O	S	0	0
			1539	959	315	258	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 17 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	137	Total	C	N	O	S	0	0
			979	616	185	172	6		

- Molecule 18 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	170	Total	C	N	O	S	0	0
			1229	771	244	207	7		

- Molecule 19 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	144	Total	C	N	O	S	0	0
			1102	696	225	175	6		

- Molecule 20 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	203	Total	C	N	O	S	0	0
			1688	1065	359	256	8		

- Molecule 21 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	199	Total	C	N	O	S	0	0
			1615	1019	322	260	14		

- Molecule 22 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	276	Total	C	N	O	S	0	0
			1926	1226	370	327	3		

- Molecule 23 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	197	Total	C	N	O	S	0	0
			1500	943	300	251	6		

- Molecule 24 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	190	Total	C	N	O	S	0	0
			1427	884	313	224	6		

- Molecule 25 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	178	Total	C	N	O	S	0	0
			1405	898	271	231	5		

- Molecule 26 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S1	1755	Total	C	N	O	P	0	0
			37536	16792	6770	12219	1755		

- Molecule 27 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S4	20	Total	C	N	O	P	0	0
			427	191	81	136	19		

- Molecule 28 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SA	225	Total	C	N	O	S	2	0
			1828	1146	349	321	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SB	208	Total	C	N	O	S	0	0
			1590	1011	285	282	12		

- Molecule 30 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SC	212	Total	C	N	O	S	1	0
			1609	1018	295	283	13		

- Molecule 31 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SD	175	Total	C	N	O	S	0	0
			1422	897	283	234	8		

- Molecule 32 is a protein called 40S ribosomal protein S4.

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

- Molecule 33 is a protein called 40S ribosomal protein S2.

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

- Molecule 34 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SG	233	Total	C	N	O	S	0	0
			1826	1139	371	313	3		

- Molecule 35 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SH	182	Total	C	N	O	S	0	0
			1430	889	275	259	7		

- Molecule 36 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SI	199	Total	C	N	O	S	0	0
			1609	1024	311	267	7		

- Molecule 37 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SK	180	Total	C	N	O	S	0	0
			1430	898	303	227	2		

- Molecule 38 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SL	143	Total	C	N	O	S	0	0
			1118	721	203	191	3		

- Molecule 39 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SM	102	Total	C	N	O	S	0	0
			788	493	144	149	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SN	100	Total	C	N	O	S	0	0
			807	518	142	140	7		

- Molecule 41 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SO	136	Total	C	N	O	S	0	0
			995	615	195	178	7		

- Molecule 42 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SP	142	Total	C	N	O	S	2	0
			1117	704	223	187	3		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SQ	100	Total	C	N	O	S	0	0
			672	413	122	132	5		

- Molecule 44 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SR	135	Total	C	N	O	S	1	0
			1081	684	213	180	4		

- Molecule 45 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SS	54	Total	C	N	O	S	0	0
			434	268	89	71	6		

- Molecule 46 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	ST	143	Total	C	N	O	S	0	0
			1163	733	230	191	9		

- Molecule 47 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SU	158	Total	C	N	O	S	0	0
			1260	799	248	208	5		

- Molecule 48 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SV	77	Total	C	N	O	S	0	0
			636	403	121	110	2		

- Molecule 49 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SW	115	Total	C	N	O	S	0	0
			909	578	172	155	4		

- Molecule 50 is a protein called 40S ribosomal protein S19-like protein.

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

- Molecule 51 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SY	85	Total	C	N	O	S	0	0
			621	383	116	118	4		

- Molecule 52 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SZ	127	Total	C	N	O	S	0	0
			1021	656	196	166	3		

- Molecule 53 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S	157	Total	C	N	O	S	0	0
			1194	760	232	199	3		

- Molecule 54 is a protein called 40S ribosomal protein S25.

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

- Molecule 55 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Sc	76	Total	C	N	O	S	0	0
			586	366	110	106	4		

- Molecule 56 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Sb	103	Total	C	N	O	S	0	0
			820	508	176	129	7		

- Molecule 57 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Sd	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 58 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Se	54	Total	C	N	O	S	0	0
			430	270	91	68	1		

- Molecule 59 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sg	306	Total	C	N	O	S	0	0
			2313	1453	411	437	12		

- Molecule 60 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Sh	157	Total	C	N	O	S	0	0
			1094	698	200	194	2		

- Molecule 61 is a protein called Putative 40S ribosomal protein S15A.

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

- Molecule 62 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	T	152	Total	C	N	O	S	0	0
			1209	756	240	202	11		

- Molecule 63 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	U	107	Total	C	N	O	S	0	0
			688	440	126	120	2		

- Molecule 64 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	V	118	Total	C	N	O	S	0	0
			915	581	177	155	2		

- Molecule 65 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	W	118	Total	C	N	O	S	0	0
			925	579	194	148	4		

- Molecule 66 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	X	64	Total	C	N	O	S	0	0
			539	354	102	80	3		

- Molecule 67 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Y	132	Total	C	N	O	S	0	0
			997	641	197	157	2		

- Molecule 68 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Z	145	Total	C	N	O	S	0	0
			1068	653	225	185	5		

- Molecule 69 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	a	123	Total	C	N	O	S	0	0
			995	623	210	159	3		

- Molecule 70 is a protein called 60S ribosomal protein L29.

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

- Molecule 71 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	c	229	Total	C	N	O	S	0	0
			1866	1188	359	308	11		

- Molecule 72 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	d	93	Total	C	N	O	S	0	0
			713	444	130	134	5		

- Molecule 73 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	e	180	Total	C	N	O	S	0	0
			1414	889	287	234	4		

- Molecule 74 is a protein called 60S ribosomal protein L32.

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

- Molecule 75 is a protein called Putative ribosomal protein l35a.

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

- Molecule 76 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	h	127	Total	C	N	O	S	0	0
			1038	639	226	167	6		

- Molecule 77 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	i	86	Total	C	N	O	S	0	0
			660	421	133	104	2		

- Molecule 78 is a protein called Ribosomal protein L37.

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

- Molecule 79 is a protein called Putative ribosomal protein L38.

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

- Molecule 80 is a protein called Putative 60S ribosomal protein L39.

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

- Molecule 81 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	m	51	Total	C	N	O	S	0	0
			375	236	74	59	6		

- Molecule 82 is a protein called 60S ribosomal protein L41.

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

- Molecule 83 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	o	88	Total	C	N	O	S	0	0
			686	427	142	111	6		

- Molecule 84 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	p	97	Total	C	N	O	S	0	0
			780	494	158	123	5		

- Molecule 85 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	2	1105	Total	C	N	O	P	0	0
			23639	10583	4263	7688	1105		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	1	106	Total	Mg	0
			106	106	
86	3	1	Total	Mg	0
			1	1	
86	4	8	Total	Mg	0
			8	8	
86	5	1	Total	Mg	0
			1	1	
86	6	2	Total	Mg	0
			2	2	
86	7	2	Total	Mg	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	8	2	Total 2	Mg 2	0
86	I	1	Total 1	Mg 1	0
86	J	1	Total 1	Mg 1	0
86	M	1	Total 1	Mg 1	0
86	S1	107	Total 107	Mg 107	0
86	SH	1	Total 1	Mg 1	0
86	SS	1	Total 1	Mg 1	0
86	SX	1	Total 1	Mg 1	0
86	T	1	Total 1	Mg 1	0
86	2	66	Total 66	Mg 66	0

- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	1	3	Total 3	K 3	0
87	5	2	Total 2	K 2	0
87	7	2	Total 2	K 2	0
87	A	2	Total 2	K 2	0
87	B	1	Total 1	K 1	0
87	H	1	Total 1	K 1	0
87	M	1	Total 1	K 1	0
87	S1	25	Total 25	K 25	0
87	SG	1	Total 1	K 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	2	5	Total	K	0
			5	5	

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

Mol	Chain	Residues	Atoms		AltConf
88	1	5	Total	Na	0
			5	5	
88	4	1	Total	Na	0
			1	1	
88	A	1	Total	Na	0
			1	1	
88	M	1	Total	Na	0
			1	1	
88	S1	4	Total	Na	0
			4	4	
88	Sb	1	Total	Na	0
			1	1	
88	2	4	Total	Na	0
			4	4	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	SS	1	Total	Zn	0
			1	1	
89	Sb	1	Total	Zn	0
			1	1	
89	j	1	Total	Zn	0
			1	1	
89	o	1	Total	Zn	0
			1	1	
89	p	1	Total	Zn	0
			1	1	

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	1	9	Total	O	0
			9	9	
90	5	1	Total	O	0
			1	1	

Continued on next page...

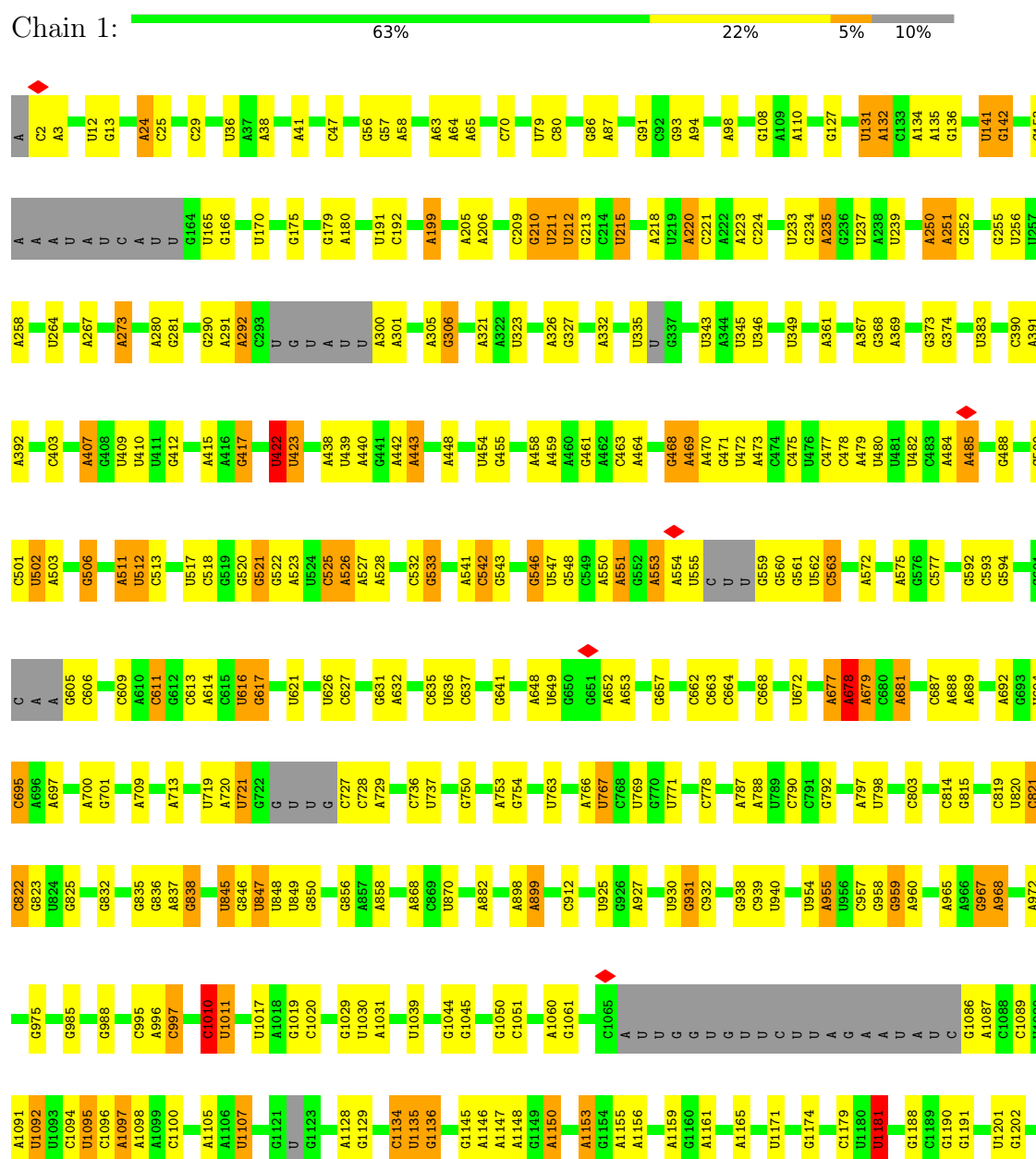
Continued from previous page...

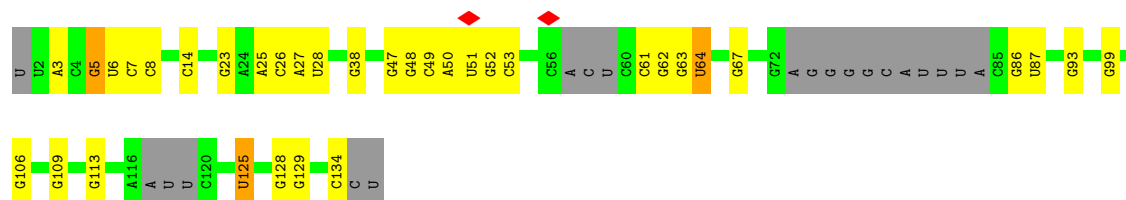
Mol	Chain	Residues	Atoms		AltConf
90	7	1	Total 1	O 1	0
90	A	1	Total 1	O 1	0
90	B	1	Total 1	O 1	0
90	H	1	Total 1	O 1	0
90	I	1	Total 1	O 1	0
90	M	4	Total 4	O 4	0
90	P	2	Total 2	O 2	0
90	S1	7	Total 7	O 7	0
90	SA	1	Total 1	O 1	0
90	S	1	Total 1	O 1	0
90	T	2	Total 2	O 2	0
90	2	17	Total 17	O 17	0

3 Residue-property plots

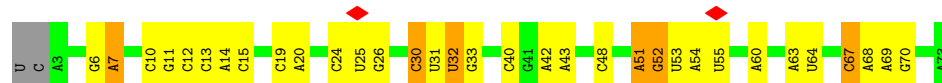
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

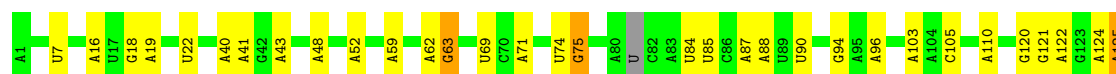




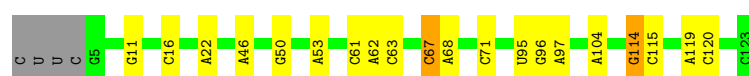
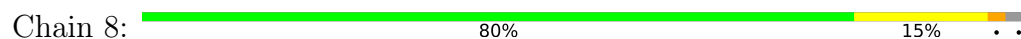
• Molecule 5: SR6_chain_6



• Molecule 6: 5.8S_rRNA_chain_7



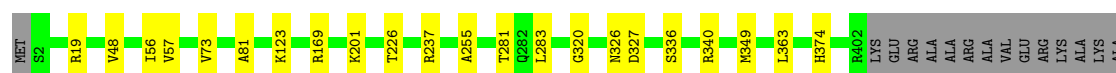
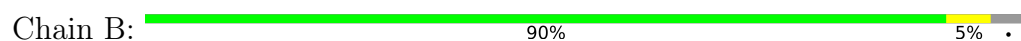
• Molecule 7: 5S_rRNA_chain_8



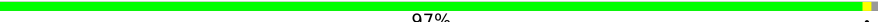
• Molecule 8: Putative 60S ribosomal protein L2



• Molecule 9: Putative ribosomal protein L3



• Molecule 10: Putative ribosomal protein L1a

Chain C:  97% ..



- Molecule 11: 60S ribosomal protein L11

Chain D:  79% 6% 15%



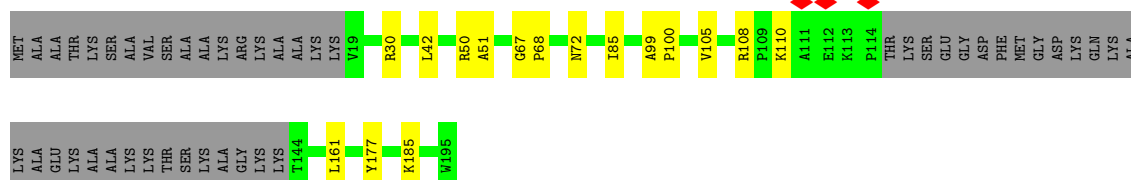
- Molecule 12: Putative 60S ribosomal protein L9

Chain E:  89% 9% .



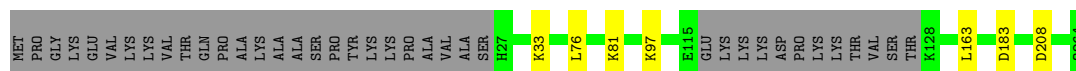
- Molecule 13: Putative 60S ribosomal protein L6

Chain F:  68% 8% 24%



- Molecule 14: 60S ribosomal protein L7a

Chain G:  83% 14%



- Molecule 15: Putative 60S ribosomal protein L13a

Chain H:  94% 5% .

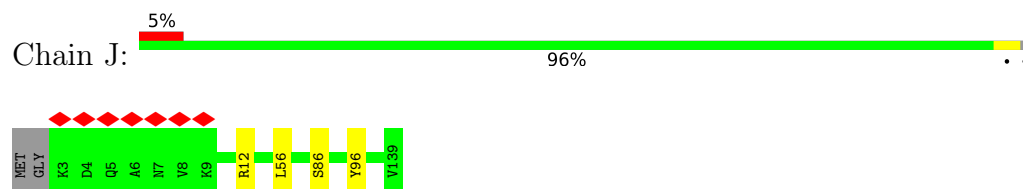


- Molecule 16: Putative 60S ribosomal protein L13

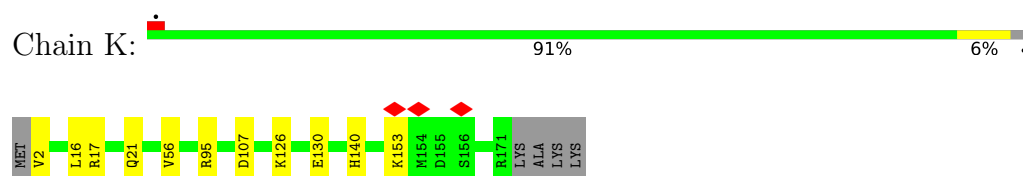
Chain I:  93% 5%



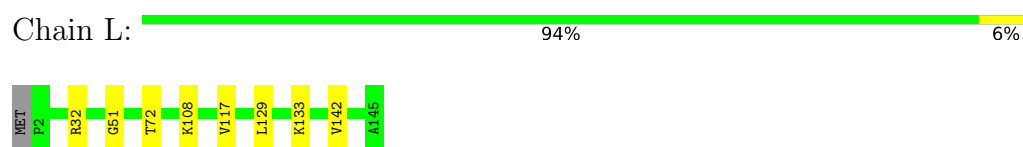
- Molecule 17: Putative 60S ribosomal protein L23



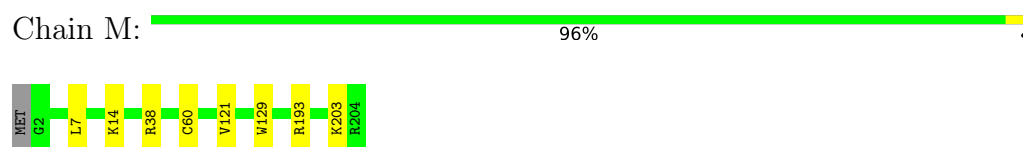
- Molecule 18: Putative 40S ribosomal protein L14



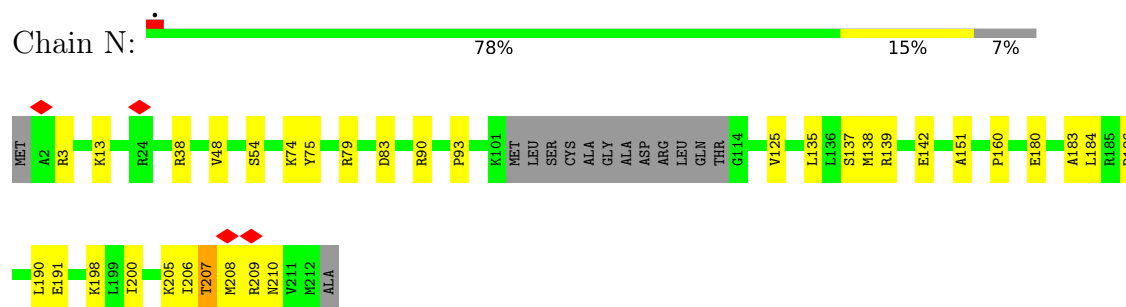
- Molecule 19: Putative 60S ribosomal protein L27A/L29



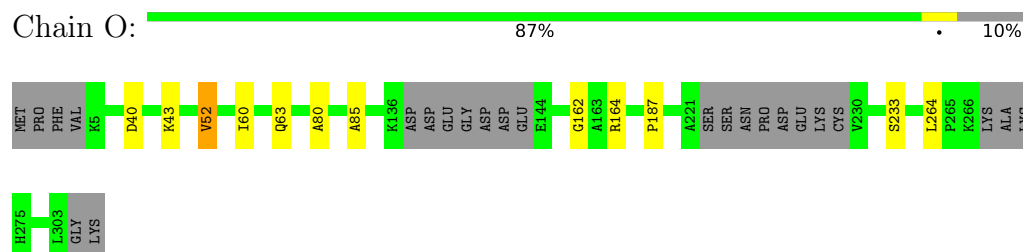
- Molecule 20: Ribosomal protein L15



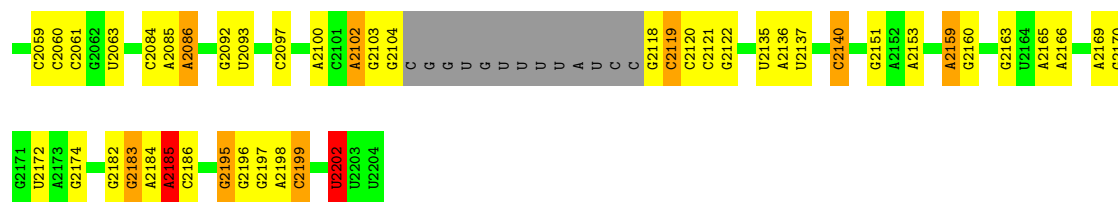
- Molecule 21: Putative 60S ribosomal protein L10



- Molecule 22: Putative 60S ribosomal protein L5



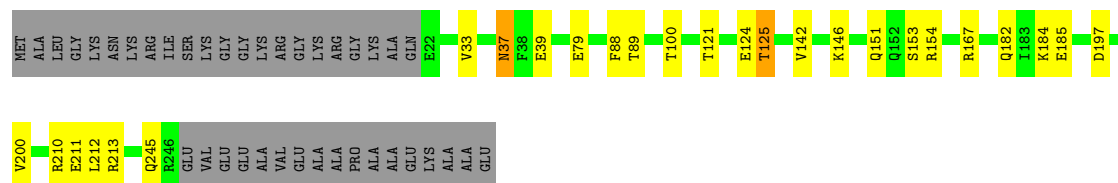
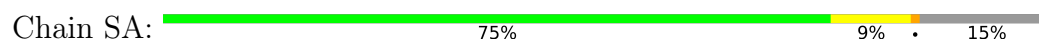




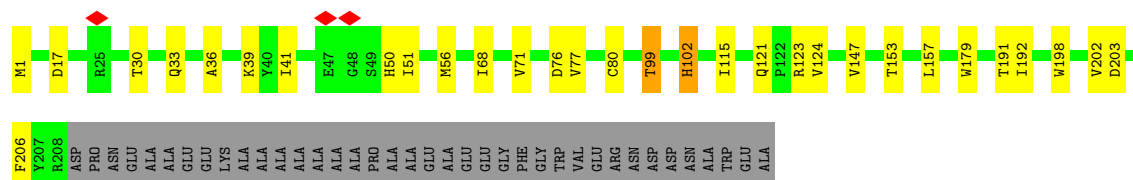
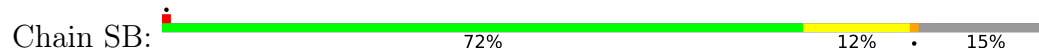
• Molecule 27: E-site_tRNA_chain_S4



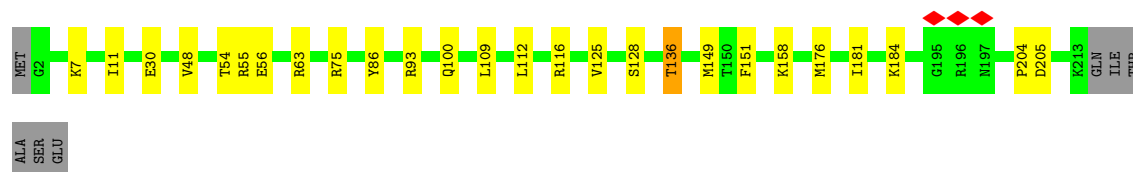
• Molecule 28: 40S ribosomal protein S3a



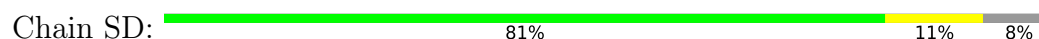
• Molecule 29: 40S ribosomal protein SA



• Molecule 30: Putative 40S ribosomal protein S3

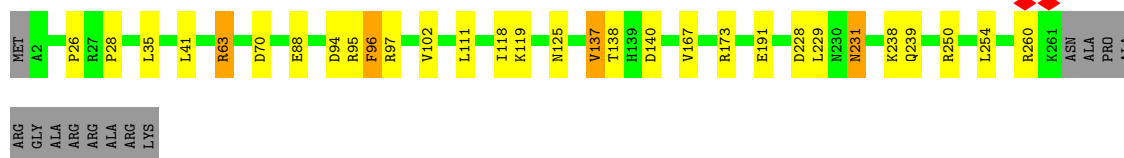
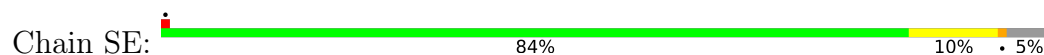


• Molecule 31: Putative 40S ribosomal protein S9

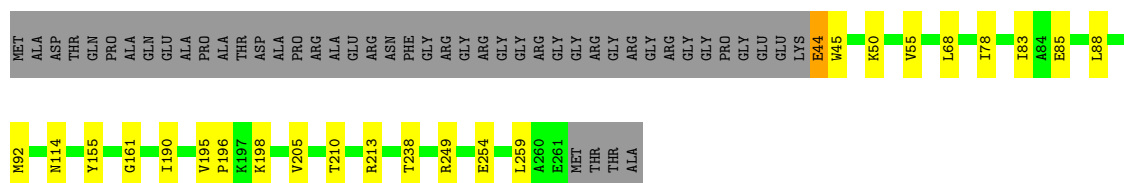




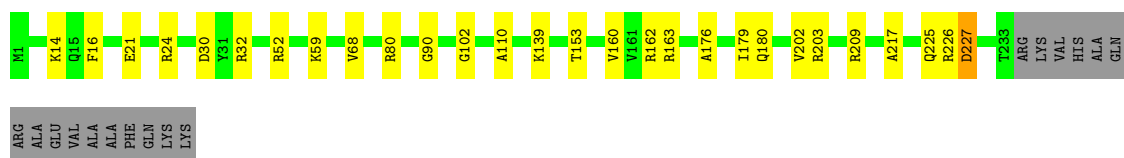
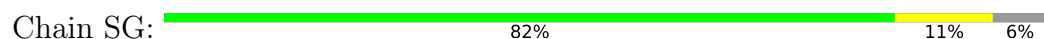
- Molecule 32: 40S ribosomal protein S4



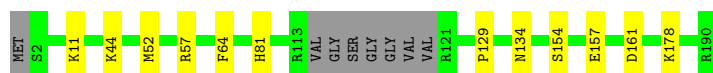
- Molecule 33: 40S ribosomal protein S2



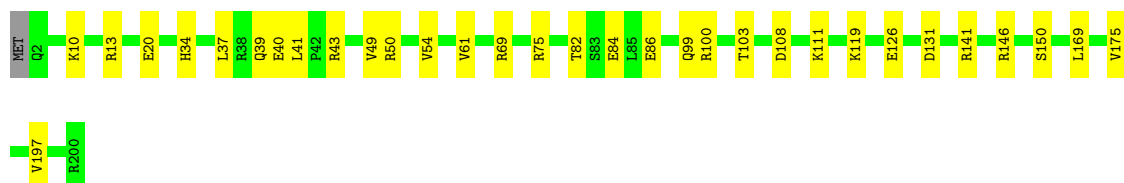
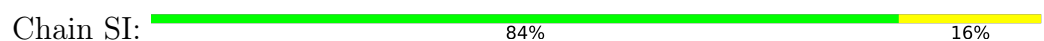
- Molecule 34: 40S ribosomal protein S6



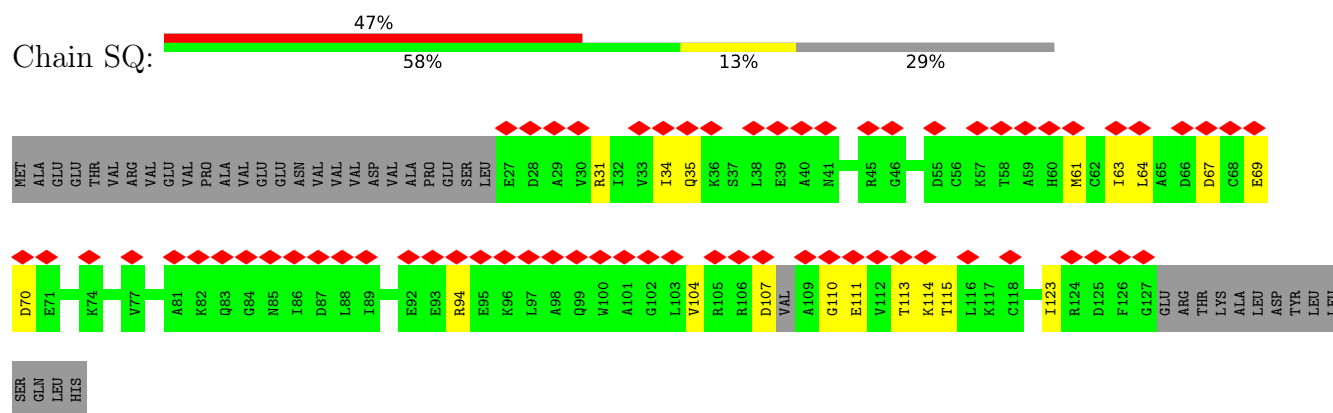
- Molecule 35: 40S ribosomal protein S5



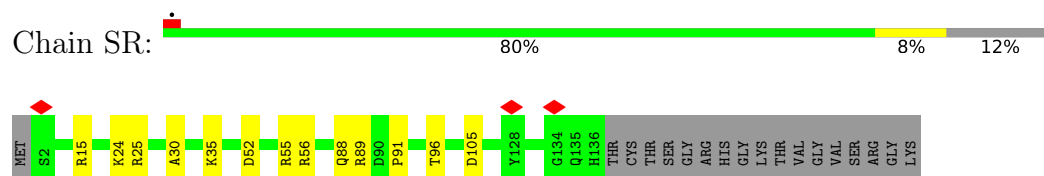
- Molecule 36: 40S ribosomal protein S7



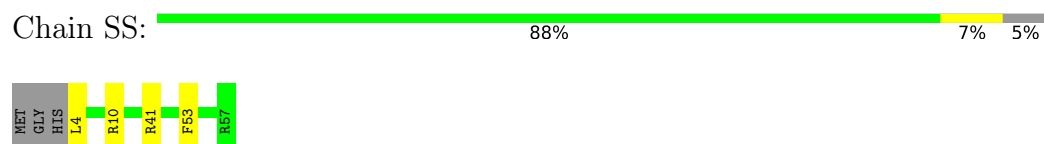
- Molecule 43: 40S ribosomal protein S12



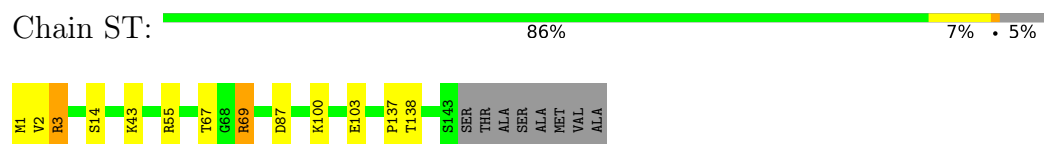
- Molecule 44: Putative 40S ribosomal protein S18



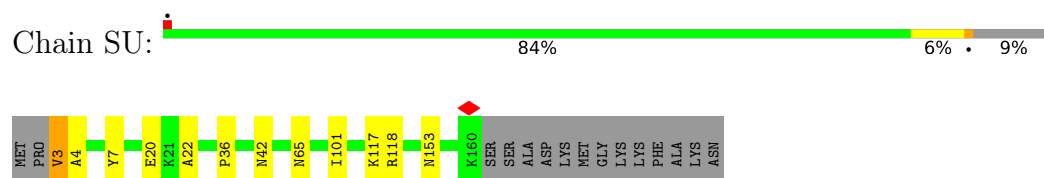
- Molecule 45: Putative ribosomal protein S29



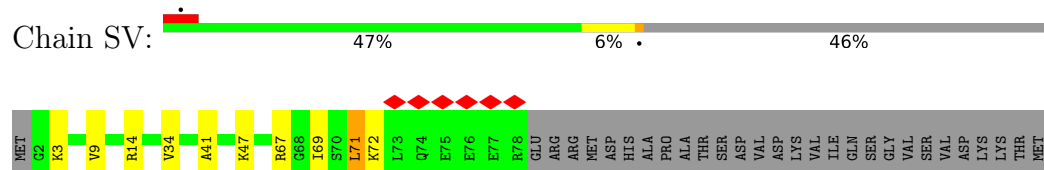
- Molecule 46: Putative 40S ribosomal protein S13



- Molecule 47: Putative 40S ribosomal protein S11



- Molecule 48: Putative 40S ribosomal protein S17



ALA
GLU
ALA
ALA
ALA
ALA
PRO
ALA
ALA
GLU

- Molecule 55: Putative 40S ribosomal protein S27-1

Chain Sc:  79% 9% 12%

MET C2 F3 F4 V36 S37 CYS PRO ARG CYS ARG Q43 V44 T45 C57 LYS GLY CYS S61 L64 T68 G69 G70 D85 HIS

- Molecule 56: 40S ribosomal protein S26

Chain Sb:  85% 7% 8%

MET T2 R6 T32 V42 L47 N65 M68 R96 K103 V104 PRO PHE ARG PRO ALA GLY LYS LYS

- Molecule 57: Putative 40S ribosomal protein S33

Chain Sd:  69% 6% 25%

MET ALA ASP LYS HIS LYS ASP ASN LYS THR GLU VAL VAL THR GLN THR ASP GLN A21 L25 V44 M47 M72 L75 L85 ARG

- Molecule 58: 40S ribosomal protein S30

Chain Se:  77% 18%

MET GLY LYS ILE HIS GLY S7 T41 L45 S46 K47 T48 VAL LYS PRO GLY E53 K64 ALA GLY

- Molecule 59: Guanine nucleotide-binding protein subunit beta-like protein

Chain Sg:  87% 12%

H1 E4 M13 Q22 A23 Q24 R34 H48 S49 V50 D51 S52 T77 R87 F103 F115 I122 D128 N129 V134 N135 G138 E139 L145 R146 L162 E163 S171 W172 D173 M180 V181 N182 T199 P205 L220 L223 Q228

L239 F230 V234 I241 N246 R247 R256 K266 A267 V268 L272 T273 P274 ASP GLY ALA K278 N301 S307 I308 S309 ASP ALA GLU

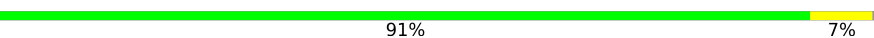
- Molecule 60: Putative RNA binding protein

Chain Sh:  21% 57% 9% 33%

MET PRO ALA LYS ALA ALA LYS VAL PRO PRO ALA ALA LYS PRO PRO LYS PRO ALA ASN LYS ALA PRO PRO ALA LYS VAL ALA ALA ALA ALA PRO PRO LYS LYS ALA ALA PRO PRO ARG ALA ALA SER GLY SER SER ASN GLY V57 K60 N61

ARG
ALA
GLU
VAL
ALA
GLU
ARG
LYS
ALA
LYS
LYS
LYS

- Molecule 67: 60S ribosomal protein L27

Chain Y:  91% 7% .

MET THR K3 A23 G45 I46 K47 Q67 N76 H77 V99 Q117 M126 Q130 F134

- Molecule 68: Putative 60S ribosomal protein L28

Chain Z:  93% 5% ..

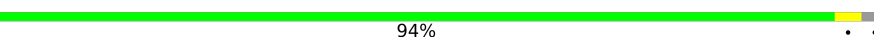
MET S2 K21 R22 R26 T81 V99 R109 R120 R143 A144 K145 R146 ASN

- Molecule 69: Putative 60S ribosomal protein L35

Chain a:  91% 5% . .

MET SER HIS H4 K26 K53 R77 R80 T92 R93 R94 R95 M112 K126 ILE

- Molecule 70: 60S ribosomal protein L29

Chain b:  94% . .

MET A2 K5 T8 K69 ASN

- Molecule 71: Putative 60S ribosomal protein L7

Chain c:  87% . 9%

MET ALA THR HIS SER VAL TYR GLY ASN ALA SER ASP MET PRO VAL VAL PRO ALA PRO GLU SER ALA ILE K24 R25 K29 Q30 Q31 Q32 T33 E34 R43 L87 Q109 V140 I152

- Molecule 72: 60S ribosomal protein L30

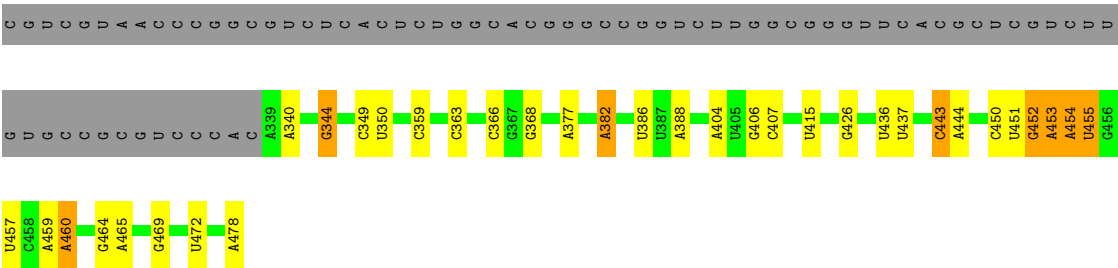
Chain d:  75% 13% . 11%

MET ALA LYS LYS THR LYS SER LYS VAL D10 T11 K24 Q38 G39 R40 N49 C50 P51 P52 L77 T89 C90 V94 T95 N96 V97 S100 D101 I102 ALA ALA

- Molecule 73: Putative 60S ribosomal subunit protein L31

Chain e:  84% 12% .

- [illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212912	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 ($e^-/\text{\AA}^2$)	0.83	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	0.162	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, C4J, OMU, 1MA, OMC, MG, 7MG, MA6, ZN, NA, A2M, 5MC, K

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	0.21	3/37759 (0.0%)	0.31	0/58867
2	3	0.19	0/3671	0.32	0/5704
3	4	0.18	0/4354	0.29	0/6788
4	5	0.18	0/2742	0.30	0/4266
5	6	0.17	0/1683	0.34	0/2618
6	7	0.23	2/3748 (0.1%)	0.27	0/5834
7	8	0.16	0/2829	0.27	0/4405
8	A	0.16	0/1935	0.32	0/2606
9	B	0.15	0/3109	0.29	0/4214
10	C	0.15	0/2714	0.28	0/3679
11	D	0.10	0/1045	0.30	0/1423
12	E	0.13	0/1357	0.30	0/1850
13	F	0.14	0/1071	0.27	0/1466
14	G	0.15	0/1696	0.29	0/2303
15	H	0.15	0/1687	0.30	0/2291
16	I	0.15	0/1572	0.28	0/2129
17	J	0.15	0/996	0.30	0/1355
18	K	0.12	0/1248	0.23	0/1695
19	L	0.16	0/1129	0.34	0/1511
20	M	0.17	0/1728	0.33	0/2312
21	N	0.13	0/1647	0.27	0/2202
22	O	0.12	0/1963	0.26	0/2665
23	P	0.16	0/1524	0.29	0/2045
24	Q	0.17	0/1446	0.27	0/1940
25	R	0.14	0/1439	0.28	0/1949
26	S1	0.28	4/40844 (0.0%)	0.32	0/63606
27	S4	0.15	0/476	0.28	0/739
28	SA	0.22	0/1859	0.30	0/2501
29	SB	0.18	0/1623	0.29	0/2204
30	SC	0.13	0/1636	0.22	0/2192
31	SD	0.20	0/1447	0.28	0/1942
32	SE	0.21	0/2088	0.28	0/2814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SF	0.23	0/1698	0.28	0/2301
34	SG	0.18	0/1849	0.23	0/2477
35	SH	0.16	0/1452	0.26	0/1948
36	SI	0.20	0/1639	0.27	0/2209
37	SK	0.22	0/1451	0.28	0/1944
38	SL	0.15	0/1139	0.25	0/1533
39	SM	0.14	0/798	0.22	0/1084
40	SN	0.12	0/830	0.22	0/1126
41	SO	0.23	0/1010	0.31	0/1362
42	SP	0.23	0/1143	0.29	0/1531
43	SQ	0.09	0/674	0.27	0/916
44	SR	0.14	0/1103	0.24	0/1481
45	SS	0.15	0/439	0.26	0/583
46	ST	0.25	0/1186	0.28	0/1590
47	SU	0.24	0/1290	0.29	0/1740
48	SV	0.17	0/643	0.25	0/854
49	SW	0.12	0/929	0.23	0/1255
50	SX	0.15	0/1233	0.24	0/1656
51	SY	0.15	0/630	0.24	0/858
52	SZ	0.18	0/1041	0.28	0/1388
53	S	0.14	0/1222	0.24	0/1656
54	Sa	0.14	0/563	0.25	0/757
55	Sc	0.21	0/596	0.28	0/801
56	Sb	0.28	0/837	0.27	0/1120
57	Sd	0.16	0/468	0.26	0/630
58	Se	0.19	0/436	0.24	0/577
59	Sg	0.11	0/2371	0.27	0/3233
60	Sh	0.09	0/1113	0.25	0/1514
61	SJ	0.25	0/1038	0.30	0/1391
62	T	0.16	0/1233	0.29	0/1656
63	U	0.09	0/695	0.23	0/939
64	V	0.14	0/930	0.24	0/1256
65	W	0.13	0/938	0.26	0/1254
66	X	0.14	0/560	0.25	0/757
67	Y	0.12	0/1018	0.22	0/1376
68	Z	0.13	0/1083	0.22	0/1461
69	a	0.13	0/1005	0.21	0/1339
70	b	0.14	0/557	0.25	0/743
71	c	0.15	0/1900	0.27	0/2544
72	d	0.15	0/723	0.24	0/979
73	e	0.13	0/1432	0.26	0/1904
74	f	0.15	0/1031	0.27	0/1380
75	g	0.15	0/1165	0.27	0/1563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	h	0.13	0/1054	0.25	0/1399
77	i	0.12	0/668	0.27	0/889
78	j	0.16	0/682	0.31	0/910
79	k	0.09	0/542	0.21	0/733
80	l	0.16	0/463	0.29	0/617
81	m	0.12	0/381	0.29	0/515
82	n	0.23	0/296	0.32	0/386
83	o	0.18	0/698	0.35	0/930
84	p	0.14	0/793	0.26	0/1048
85	2	0.23	8/25035 (0.0%)	0.32	0/39014
All	All	0.21	17/211768 (0.0%)	0.30	0/311222

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	668	A2M	O3'-P	5.77	1.62	1.56
85	2	1372	A2M	O3'-P	5.62	1.61	1.56
85	2	527	A2M	O3'-P	5.35	1.61	1.56
85	2	570	A2M	O3'-P	5.30	1.61	1.56
85	2	1384	A2M	O3'-P	5.28	1.61	1.56
26	S1	479	A2M	O3'-P	5.23	1.61	1.56
85	2	572	A2M	O3'-P	5.22	1.61	1.56
85	2	604	A2M	O3'-P	5.17	1.61	1.56
1	1	697	A2M	O3'-P	5.17	1.61	1.56
85	2	1185	A2M	O3'-P	5.14	1.61	1.56
26	S1	2021	A2M	O3'-P	5.13	1.61	1.56
85	2	591	A2M	O3'-P	5.06	1.61	1.56
6	7	43	A2M	O3'-P	5.06	1.61	1.56
6	7	162	A2M	O3'-P	5.04	1.61	1.56
26	S1	98	A2M	O3'-P	5.03	1.61	1.56
1	1	955	A2M	O3'-P	5.02	1.61	1.56
1	1	858	A2M	O3'-P	5.01	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	34587	0	17450	214	0
2	3	3312	0	1681	28	0
3	4	3917	0	1979	19	0
4	5	2456	0	1247	14	0
5	6	1506	0	768	12	0
6	7	3485	0	1770	13	0
7	8	2531	0	1283	11	0
8	A	1893	0	1905	6	0
9	B	3035	0	3004	16	0
10	C	2664	0	2626	4	0
11	D	1025	0	787	6	0
12	E	1337	0	1269	8	0
13	F	1049	0	1025	11	0
14	G	1672	0	1696	4	0
15	H	1652	0	1644	7	0
16	I	1539	0	1491	2	0
17	J	979	0	968	2	0
18	K	1229	0	1194	7	0
19	L	1102	0	1124	4	0
20	M	1688	0	1748	5	0
21	N	1615	0	1685	23	0
22	O	1926	0	1761	8	0
23	P	1500	0	1568	4	0
24	Q	1427	0	1383	4	0
25	R	1405	0	1411	7	0
26	S1	37536	0	18968	359	0
27	S4	427	0	222	6	0
28	SA	1828	0	1917	12	0
29	SB	1590	0	1570	17	0
30	SC	1609	0	1655	16	0
31	SD	1422	0	1467	15	0
32	SE	2050	0	2144	20	0
33	SF	1662	0	1708	13	0
34	SG	1826	0	1914	23	0
35	SH	1430	0	1456	9	0
36	SI	1609	0	1668	21	0
37	SK	1430	0	1512	7	0
38	SL	1118	0	1168	1	0
39	SM	788	0	823	9	0
40	SN	807	0	782	6	0
41	SO	995	0	997	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	SP	1117	0	1166	8	0
43	SQ	672	0	602	11	0
44	SR	1081	0	1126	8	0
45	SS	434	0	438	5	0
46	ST	1163	0	1232	10	0
47	SU	1260	0	1277	6	0
48	SV	636	0	687	8	0
49	SW	909	0	909	10	0
50	SX	1202	0	1227	16	0
51	SY	621	0	601	6	0
52	SZ	1021	0	1083	12	0
53	S	1194	0	1184	3	0
54	Sa	558	0	606	7	0
55	Sc	586	0	570	4	0
56	Sb	820	0	854	5	0
57	Sd	466	0	476	2	0
58	Se	430	0	473	2	0
59	Sg	2313	0	2189	16	0
60	Sh	1094	0	1005	11	0
61	SJ	1021	0	1050	0	0
62	T	1209	0	1236	8	0
63	U	688	0	536	3	0
64	V	915	0	956	6	0
65	W	925	0	991	8	0
66	X	539	0	535	2	0
67	Y	997	0	988	5	0
68	Z	1068	0	1057	6	0
69	a	995	0	1076	5	0
70	b	546	0	575	1	0
71	c	1866	0	1970	7	0
72	d	713	0	730	5	0
73	e	1414	0	1532	14	0
74	f	1011	0	1054	4	0
75	g	1142	0	1196	11	0
76	h	1038	0	1109	6	0
77	i	660	0	714	1	0
78	j	668	0	680	4	0
79	k	534	0	534	4	0
80	l	450	0	483	1	0
81	m	375	0	370	4	0
82	n	292	0	331	5	0
83	o	686	0	702	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	p	780	0	838	4	0
85	2	23639	0	11982	156	0
86	1	106	0	0	0	0
86	2	66	0	0	0	0
86	3	1	0	0	0	0
86	4	8	0	0	0	0
86	5	1	0	0	0	0
86	6	2	0	0	0	0
86	7	2	0	0	0	0
86	8	2	0	0	0	0
86	I	1	0	0	0	0
86	J	1	0	0	0	0
86	M	1	0	0	0	0
86	S1	107	0	0	0	0
86	SH	1	0	0	0	0
86	SS	1	0	0	0	0
86	SX	1	0	0	0	0
86	T	1	0	0	0	0
87	1	3	0	0	0	0
87	2	5	0	0	0	0
87	5	2	0	0	0	0
87	7	2	0	0	0	0
87	A	2	0	0	0	0
87	B	1	0	0	0	0
87	H	1	0	0	0	0
87	M	1	0	0	0	0
87	S1	25	0	0	0	0
87	SG	1	0	0	0	0
88	1	5	0	0	0	0
88	2	4	0	0	0	0
88	4	1	0	0	0	0
88	A	1	0	0	0	0
88	M	1	0	0	0	0
88	S1	4	0	0	0	0
88	Sb	1	0	0	0	0
89	SS	1	0	0	0	0
89	Sb	1	0	0	0	0
89	j	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	1	9	0	0	0	0
90	2	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	5	1	0	0	0	0
90	7	1	0	0	0	0
90	A	1	0	0	0	0
90	B	1	0	0	0	0
90	H	1	0	0	0	0
90	I	1	0	0	0	0
90	M	4	0	0	0	0
90	P	2	0	0	0	0
90	S	1	0	0	0	0
90	S1	7	0	0	0	0
90	SA	1	0	0	0	0
90	T	2	0	0	0	0
All	All	200822	0	145368	1194	0

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

All (1194) 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)
26:S1:955:A:N6	26:S1:980:G:H1	1.53	1.06
26:S1:1366:A:N1	26:S1:1416:G:N2	2.05	1.04
26:S1:781:A:H2	26:S1:839:G:H1	1.03	0.97
85:2:984:G:H1	85:2:1000:U:H3	0.92	0.92
1:1:520:G:HO2'	1:1:521:G:H8	0.95	0.92
1:1:1676:G:H1	1:1:1723:A:H61	1.15	0.88
26:S1:781:A:C2	26:S1:839:G:N1	2.42	0.88
1:1:1676:G:H1	1:1:1723:A:N6	1.70	0.87
26:S1:999:A:N6	26:S1:1095:G:H1	1.72	0.86
85:2:1472:U:H3	85:2:1492:G:H1	1.24	0.86
26:S1:1019:U:H3	26:S1:1033:G:H1	0.92	0.85
26:S1:1912:A:H2	26:S1:1929:G:H1	1.25	0.83
26:S1:783:A:H2	26:S1:837:G:H22	1.23	0.82
26:S1:2085:A:HO2'	26:S1:2086:A:H8	1.28	0.82
26:S1:559:G:H1	26:S1:592:C:H5	1.27	0.82
31:SD:158:ALA:O	31:SD:164:GLY:N	2.13	0.82
26:S1:781:A:H2	26:S1:839:G:N1	1.78	0.81
26:S1:275:A:H3'	26:S1:276:G:H21	1.46	0.81
26:S1:782:C:H42	26:S1:838:U:H3	1.29	0.81
4:5:53:C:H42	4:5:61:C:H42	1.31	0.79
26:S1:354:C:H5	26:S1:400:G:H1	1.31	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:503:A:N6	1:1:553:A:N7	2.32	0.78
26:S1:999:A:N6	26:S1:1095:G:N1	2.31	0.77
26:S1:996:C:N3	26:S1:1098:U:O4	2.18	0.76
5:6:10:C:H5	5:6:70:G:H1	1.34	0.76
57:Sd:25:LEU:HB2	57:Sd:47:MET:HE3	1.68	0.76
1:1:1443:U:H5'	1:1:1464:G:H21	1.51	0.75
3:4:154:C:H4'	12:E:155:ARG:HE	1.52	0.75
26:S1:497:A:OP2	32:SE:63:ARG:NH1	2.20	0.74
26:S1:528:G:H1	26:S1:553:U:H3	1.30	0.74
26:S1:983:C:H2'	26:S1:984:G:H8	1.53	0.74
26:S1:955:A:N1	26:S1:980:G:N2	2.30	0.74
1:1:1239:U:OP1	15:H:141:ARG:NH1	2.21	0.74
33:SF:249:ARG:HH21	33:SF:254:GLU:HA	1.51	0.74
1:1:511:A:H4'	1:1:512:U:H5''	1.69	0.74
26:S1:958:G:H22	26:S1:977:G:H1	1.33	0.74
26:S1:756:C:N3	26:S1:773:A:N6	2.36	0.74
26:S1:955:A:H61	26:S1:980:G:H1	0.78	0.73
1:1:1051:C:H5	1:1:1097:A:H62	1.34	0.73
26:S1:691:G:H22	26:S1:754:G:H22	1.36	0.73
26:S1:790:U:H3	34:SG:226:ARG:HE	1.35	0.73
85:2:781:G:H1	85:2:808:C:H5	1.34	0.73
85:2:684:C:N4	85:2:755:U:O4	2.19	0.73
24:Q:174:ARG:NH2	26:S1:1102:G:OP2	2.21	0.73
26:S1:1645:U:H3	26:S1:1674:A:H62	1.37	0.73
26:S1:790:U:H3	34:SG:226:ARG:NE	1.87	0.73
83:o:42:CYS:HB3	83:o:60:CYS:SG	2.28	0.72
26:S1:1142:G:H21	41:SO:45:THR:HG21	1.54	0.72
1:1:251:A:N1	65:W:5:LYS:N	2.36	0.72
26:S1:1035:G:H2'	26:S1:1036:G:C8	2.24	0.72
26:S1:771:G:N2	26:S1:772:A:N1	2.36	0.72
85:2:569:G:O2'	85:2:571:G:OP2	2.08	0.72
26:S1:810:G:OP1	60:Sh:125:THR:OG1	2.08	0.72
26:S1:1016:G:H22	26:S1:1036:G:N2	1.87	0.72
69:a:92:THR:HG22	69:a:95:ARG:H	1.54	0.72
26:S1:951:U:O2	26:S1:984:G:N2	2.21	0.71
26:S1:1016:G:H22	26:S1:1036:G:H22	1.38	0.71
81:m:110:CYS:SG	81:m:118:CYS:N	2.63	0.71
26:S1:2059:C:H5	26:S1:2166:A:H61	1.37	0.71
26:S1:780:A:H61	26:S1:840:A:H62	1.37	0.71
26:S1:1706:A:H62	26:S1:1766:G:H1	1.37	0.71
30:SC:63:ARG:HH21	40:SN:98:GLN:HE22	1.36	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:951:U:H3	26:S1:984:G:H1	1.39	0.70
26:S1:836:C:H2'	26:S1:837:G:C8	2.26	0.70
26:S1:691:G:H22	26:S1:754:G:N2	1.90	0.70
2:3:41:A:H8	2:3:188:C:H42	1.39	0.70
1:1:1588:G:O2'	1:1:1590:G:OP2	2.10	0.70
26:S1:585:C:OP2	31:SD:181:ARG:NH1	2.25	0.70
25:R:173:THR:HG22	25:R:175:ARG:H	1.55	0.69
26:S1:253:U:H3	26:S1:974:G:H1	1.39	0.69
49:SW:35:LEU:HG	49:SW:39:GLU:HG3	1.74	0.69
26:S1:875:A:H62	26:S1:887:U:H5	1.39	0.69
60:Sh:62:TRP:NE1	60:Sh:65:GLY:O	2.25	0.69
72:d:49:ASN:ND2	83:o:42:CYS:O	2.25	0.69
26:S1:2102:A:OP2	34:SG:52:ARG:NH2	2.26	0.69
85:2:978:C:H5'	85:2:979:A:H5''	1.75	0.69
26:S1:1016:G:H1	26:S1:1036:G:H22	1.39	0.68
26:S1:1878:A:O2'	50:SX:60:PRO:O	2.11	0.68
26:S1:789:G:OP2	32:SE:173:ARG:NH1	2.25	0.68
60:Sh:163:GLN:NE2	60:Sh:178:ASP:OD1	2.26	0.68
85:2:134:C:H5	85:2:344:G:H1	1.42	0.68
1:1:593:C:H42	1:1:614:A:H61	1.42	0.67
28:SA:211:GLU:OE2	28:SA:213:ARG:NH1	2.27	0.67
33:SF:92:MET:SD	33:SF:114:ASN:ND2	2.66	0.67
26:S1:822:U:O2'	34:SG:226:ARG:NH1	2.23	0.67
36:SI:126:GLU:OE2	36:SI:141:ARG:NH1	2.26	0.67
85:2:818:U:H3	85:2:958:A:H61	1.43	0.67
3:4:4:G:H1	3:4:20:U:H3	1.43	0.67
26:S1:983:C:H2'	26:S1:984:G:C8	2.29	0.67
26:S1:1160:A:C8	85:2:452:G:H4'	2.29	0.67
36:SI:75:ARG:NH2	36:SI:131:ASP:OD1	2.25	0.67
26:S1:999:A:N1	26:S1:1095:G:N2	2.43	0.66
26:S1:558:U:H2'	26:S1:559:G:C8	2.30	0.66
26:S1:692:G:H22	26:S1:753:A:H2	1.42	0.66
26:S1:1138:G:H2'	26:S1:1139:G:C8	2.31	0.66
26:S1:1670:G:OP1	48:SV:67:ARG:NH1	2.18	0.66
2:3:7:U:OP1	67:Y:47:LYS:NZ	2.29	0.66
26:S1:65:A:OP1	34:SG:139:LYS:NZ	2.26	0.66
26:S1:1033:G:H2'	26:S1:1034:G:C8	2.31	0.66
32:SE:102:VAL:HG12	32:SE:239:GLN:HE21	1.60	0.66
44:SR:35:LYS:NZ	44:SR:105:ASP:OD1	2.28	0.65
9:B:374:HIS:O	66:X:37:ARG:NH2	2.30	0.65
26:S1:1881:G:OP1	50:SX:91:ARG:NH1	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:57:VAL:HG22	9:B:73:VAL:HG22	1.79	0.65
43:SQ:107:ASP:OD2	43:SQ:113:THR:OG1	2.14	0.65
1:1:700:A:N1	1:1:845:OMU:H5	2.12	0.65
1:1:1672:U:O2'	1:1:1673:G:N2	2.27	0.65
26:S1:148:G:H2'	26:S1:149:G:C8	2.32	0.64
21:N:74:LYS:HE2	85:2:1276:A:H4'	1.80	0.64
39:SM:23:SER:HB3	39:SM:29:VAL:HG22	1.80	0.64
1:1:521:G:H2'	1:1:522:G:C8	2.33	0.64
42:SP:11:ARG:NH2	47:SU:117:LYS:O	2.31	0.64
37:SK:160:ARG:HB3	37:SK:164:ARG:HH21	1.63	0.64
67:Y:126:MET:O	67:Y:130:GLN:NE2	2.30	0.64
26:S1:1578:G:N7	43:SQ:114:LYS:NZ	2.46	0.63
37:SK:34:ALA:HB2	37:SK:56:ARG:HD2	1.79	0.63
26:S1:661:OMU:OP2	42:SP:3:LYS:NZ	2.32	0.63
59:Sg:122:ILE:HG12	59:Sg:134:TRP:HB2	1.80	0.63
49:SW:69:GLU:OE2	49:SW:73:HIS:NE2	2.31	0.63
1:1:502:U:O4	1:1:553:A:N6	2.31	0.63
26:S1:1015:G:H1	26:S1:1037:U:H3	1.47	0.63
26:S1:1659:U:H3	26:S1:1670:G:H22	1.46	0.63
85:2:1024:U:H2'	85:2:1025:G:C8	2.33	0.63
26:S1:1017:U:H2'	26:S1:1018:G:C8	2.34	0.62
36:SI:146:ARG:NH1	36:SI:150:SER:OG	2.32	0.62
85:2:957:C:H3'	85:2:958:A:C8	2.34	0.62
59:Sg:171:SER:OG	59:Sg:173:ASP:OD1	2.16	0.62
1:1:321:A:OP2	84:p:41:ARG:NH1	2.31	0.62
1:1:1095:U:OP1	21:N:90:ARG:NE	2.17	0.62
2:3:200:G:N1	83:o:50:LYS:O	2.32	0.62
26:S1:285:A:H2'	26:S1:817:A:H2	1.65	0.62
1:1:199:A:N6	1:1:215:U:O2'	2.32	0.62
21:N:93:PRO:HB2	21:N:125:VAL:HG12	1.82	0.62
26:S1:2102:A:H61	26:S1:2121:C:H42	1.47	0.62
39:SM:77:PHE:HB3	45:SS:53:PHE:HB3	1.82	0.62
4:5:26:C:N3	4:5:125:U:O2'	2.28	0.62
39:SM:48:HIS:HB2	39:SM:87:ASP:HB2	1.82	0.62
85:2:984:G:O6	85:2:1000:U:O4	2.18	0.62
1:1:482:U:OP1	74:f:3:LYS:NZ	2.33	0.61
26:S1:259:C:H2'	26:S1:260:A:C8	2.35	0.61
85:2:451:U:H3	85:2:483:C:H42	1.47	0.61
26:S1:814:G:HO2'	26:S1:817:A:H62	1.49	0.61
85:2:459:A:H2'	85:2:460:A:C8	2.36	0.61
1:1:1730:A:O5'	64:V:32:ARG:NH2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:2085:A:O2'	26:S1:2086:A:H8	1.82	0.61
73:e:101:PHE:HB3	73:e:141:LYS:HG2	1.82	0.61
85:2:382:A2M:O5'	85:2:382:A2M:H8	2.01	0.61
32:SE:97:ARG:NH2	32:SE:118:ILE:O	2.33	0.61
63:U:29:ASP:HA	63:U:76:VAL:HG12	1.82	0.61
1:1:1672:U:H6	1:1:1727:A:H62	1.49	0.61
4:5:64:U:H3	4:5:93:G:H1	1.49	0.61
26:S1:1035:G:H2'	26:S1:1036:G:H8	1.62	0.61
26:S1:1920:A:N7	50:SX:45:ASN:N	2.47	0.61
54:Sa:95:SER:O	54:Sa:99:ARG:NH1	2.33	0.61
64:V:102:MET:HE3	64:V:127:ILE:HD13	1.80	0.61
1:1:141:U:H1'	1:1:142:G:H5''	1.82	0.60
1:1:1264:A:H2'	1:1:1265:A:C8	2.36	0.60
26:S1:45:U:O2'	26:S1:46:U:H2'	2.01	0.60
30:SC:112:LEU:HD11	30:SC:116:ARG:HD2	1.82	0.60
26:S1:1114:G:H1	26:S1:1207:U:H3	1.47	0.60
26:S1:781:A:N1	26:S1:839:G:O6	2.34	0.60
26:S1:1881:G:H2'	26:S1:1882:A:C8	2.36	0.60
1:1:2:C:H5	6:7:169:A:H1'	1.64	0.60
26:S1:1670:G:O5'	48:SV:67:ARG:NH2	2.35	0.60
1:1:165:U:H3	1:1:290:G:H1	1.50	0.60
1:1:520:G:O2'	1:1:521:G:O5'	2.20	0.60
32:SE:228:ASP:OD1	32:SE:229:LEU:N	2.34	0.60
84:p:6:LYS:NZ	84:p:95:ASP:OD2	2.33	0.60
85:2:453:A:H1'	85:2:454:A:O4'	2.02	0.60
26:S1:1186:A:H2'	26:S1:1187:A:C8	2.36	0.60
26:S1:1511:C:N4	26:S1:1637:A:H5'	2.16	0.60
28:SA:37:ASN:OD1	28:SA:184:LYS:NZ	2.32	0.60
3:4:54:G:H21	3:4:57:A:H2	1.48	0.60
26:S1:1171:A:H2'	26:S1:1172:G:C8	2.36	0.60
44:SR:88:GLN:HA	44:SR:96:THR:HG23	1.82	0.60
1:1:846:G:H2'	1:1:847:OMU:H6	1.83	0.60
26:S1:1976:U:OP2	26:S1:1978:A:O2'	2.17	0.60
52:SZ:19:VAL:HG12	52:SZ:26:LYS:HG2	1.84	0.60
1:1:485:A:N3	13:F:110:LYS:NZ	2.47	0.59
26:S1:1016:G:N2	26:S1:1036:G:H22	1.99	0.59
33:SF:85:GLU:OE1	33:SF:85:GLU:N	2.31	0.59
4:5:25:A:H5''	9:B:123:LYS:HG3	1.84	0.59
26:S1:640:A:H2'	26:S1:641:A:C8	2.38	0.59
26:S1:822:U:H4'	34:SG:226:ARG:NH2	2.18	0.59
62:T:41:LEU:HD13	62:T:150:MET:HE1	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:1295:G:H1	26:S1:1420:U:H3	1.51	0.59
69:a:77:ARG:HA	69:a:80:ARG:HG2	1.83	0.59
1:1:522:G:H2'	1:1:523:A:C8	2.38	0.59
26:S1:691:G:N2	26:S1:754:G:H22	2.01	0.59
26:S1:978:C:H2'	26:S1:979:U:H6	1.67	0.59
12:E:17:THR:OG1	12:E:28:THR:OG1	2.21	0.59
26:S1:2202:PSU:OP2	56:Sb:103:LYS:NZ	2.35	0.59
42:SP:32:THR:HG22	42:SP:34:SER:H	1.67	0.59
26:S1:1132:G:H2'	26:S1:1133:U:C6	2.38	0.59
85:2:1398:C:H2'	85:2:1399:G:C8	2.38	0.59
59:Sg:234:VAL:O	59:Sg:256:ARG:NH2	2.36	0.58
26:S1:975:G:H3'	26:S1:976:A:H8	1.68	0.58
26:S1:1113:G:OP1	46:ST:1:MET:N	2.35	0.58
52:SZ:34:HIS:HB2	52:SZ:37:TRP:HB2	1.86	0.58
26:S1:87:G:N2	26:S1:495:A:OP1	2.37	0.58
26:S1:1988:C:H5''	26:S1:1989:A:H5''	1.83	0.58
36:SI:10:LYS:HA	36:SI:13:ARG:HG3	1.85	0.58
26:S1:3:U:O2	31:SD:16:ARG:NH1	2.36	0.58
26:S1:1580:G:N1	43:SQ:69:GLU:OE2	2.36	0.58
9:B:327:ASP:H	85:2:1510:A:H61	1.51	0.58
26:S1:1121:C:H2'	26:S1:1122:G:C8	2.38	0.58
1:1:12:U:H2'	1:1:13:G:H8	1.69	0.58
1:1:1264:A:O2'	85:2:1294:G:OP1	2.21	0.58
52:SZ:44:GLN:O	52:SZ:48:LYS:NZ	2.36	0.58
1:1:1029:G:N2	1:1:1030:U:O4	2.34	0.58
5:6:32:U:O2'	12:E:46:ARG:NH1	2.28	0.58
26:S1:759:U:O2	36:SI:99:GLN:NE2	2.34	0.58
26:S1:1292:U:H3	26:S1:1423:G:H1	1.51	0.58
1:1:417:G:O2'	1:1:442:A:N6	2.37	0.58
1:1:1779:G:H1	85:2:3:C:H5	1.51	0.58
3:4:149:U:H1'	3:4:150:A:H5''	1.84	0.58
6:7:153:C:OP1	20:M:38:ARG:NH1	2.36	0.58
1:1:291:A:H2'	1:1:292:A:H5''	1.85	0.57
1:1:1536:C:OP1	62:T:66:LYS:NZ	2.37	0.57
26:S1:785:G:O4'	26:S1:787:G:N2	2.37	0.57
56:Sb:47:LEU:HD12	56:Sb:68:MET:HE1	1.86	0.57
59:Sg:199:THR:HG21	59:Sg:241:ILE:H	1.68	0.57
1:1:264:U:O2'	65:W:5:LYS:NZ	2.37	0.57
1:1:210:G:H4'	1:1:211:U:O5'	2.05	0.57
5:6:43:A:OP2	18:K:95:ARG:NH1	2.37	0.57
52:SZ:62:VAL:HG12	52:SZ:82:ILE:HG12	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:2:1398:C:H2'	85:2:1399:G:H8	1.70	0.57
1:1:472:U:H2'	1:1:473:A:H8	1.69	0.57
26:S1:750:U:H2'	26:S1:751:G:C8	2.39	0.57
26:S1:1594:A:OP1	49:SW:66:ARG:NH1	2.37	0.57
85:2:553:G:O2'	85:2:556:U:OP2	2.21	0.57
73:e:44:ASN:ND2	85:2:1506:G:OP1	2.36	0.57
1:1:472:U:H2'	1:1:473:A:C8	2.40	0.57
29:SB:77:VAL:O	29:SB:99:THR:OG1	2.22	0.57
59:Sg:13:TRP:HB2	59:Sg:34:ARG:HD2	1.86	0.57
26:S1:1288:G:H1	26:S1:1427:U:H3	1.52	0.57
26:S1:1670:G:P	48:SV:67:ARG:HH22	2.28	0.57
85:2:453:A:H2	85:2:455:U:H5	1.52	0.57
1:1:1147:A:O2'	1:1:1150:A:N1	2.38	0.56
2:3:100:U:HO2'	2:3:101:G:H8	1.51	0.56
26:S1:185:A:OP1	34:SG:203:ARG:NH2	2.37	0.56
85:2:968:U:O4	85:2:969:A:N6	2.38	0.56
36:SI:39:GLN:OE1	36:SI:39:GLN:N	2.38	0.56
1:1:1060:A:H2'	1:1:1061:G:C8	2.41	0.56
2:3:16:G:N7	76:h:71:HIS:NE2	2.52	0.56
2:3:39:C:H5''	24:Q:96:MET:HE1	1.86	0.56
3:4:92:U:H2'	3:4:93:U:C6	2.40	0.56
33:SF:83:ILE:HG21	33:SF:88:LEU:HD13	1.86	0.56
85:2:755:U:HO2'	85:2:756:C:H6	1.52	0.56
21:N:207:THR:HB	21:N:209:ARG:HD2	1.88	0.56
10:C:113:LYS:HG2	20:M:203:LYS:HB3	1.86	0.56
17:J:12:ARG:NH1	17:J:56:LEU:O	2.38	0.56
30:SC:56:GLU:OE1	30:SC:56:GLU:N	2.38	0.56
85:2:619:A:N3	85:2:1262:G:O2'	2.36	0.56
30:SC:54:THR:OG1	30:SC:55:ARG:NH1	2.39	0.56
85:2:558:A:OP1	85:2:560:OMU:H5	2.06	0.56
37:SK:57:ALA:HB2	37:SK:196:GLY:HA2	1.86	0.56
1:1:727:C:O2'	1:1:728:C:H2'	2.06	0.56
8:A:36:GLU:HG3	8:A:91:GLY:HA2	1.88	0.56
26:S1:978:C:H2'	26:S1:979:U:C6	2.40	0.56
85:2:454:A:O3'	85:2:455:U:H3'	2.06	0.56
85:2:1024:U:H2'	85:2:1025:G:H8	1.71	0.56
1:1:70:C:O2'	16:I:71:ASN:OD1	2.24	0.55
1:1:611:C:OP2	10:C:359:ARG:NH1	2.38	0.55
26:S1:1972:G:O6	49:SW:50:ARG:NH1	2.38	0.55
26:S1:259:C:H2'	26:S1:260:A:H8	1.69	0.55
26:S1:285:A:H62	26:S1:816:C:H2'	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:1612:C:HO2'	26:S1:1613:C:H6	1.53	0.55
26:S1:1718:A:H4'	54:Sa:87:LYS:HE2	1.89	0.55
79:k:23:VAL:HG12	79:k:36:VAL:HG22	1.88	0.55
85:2:782:G:OP2	85:2:782:G:N2	2.32	0.55
85:2:1424:U:H2'	85:2:1425:A:H8	1.71	0.55
1:1:687:C:H2'	1:1:688:A:H8	1.71	0.55
2:3:204:A:H2'	2:3:205:A:C8	2.42	0.55
26:S1:450:A:H2'	26:S1:451:C:C6	2.42	0.55
26:S1:1033:G:H2'	26:S1:1034:G:H8	1.68	0.55
13:F:68:PRO:HG3	13:F:161:LEU:HD23	1.89	0.55
30:SC:48:VAL:HG12	30:SC:86:TYR:HB2	1.88	0.55
71:c:31:GLN:OE1	71:c:31:GLN:N	2.35	0.55
1:1:475:C:OP1	75:g:83:LYS:NZ	2.35	0.55
1:1:790:C:H5	10:C:305:LEU:H	1.55	0.55
26:S1:1278:U:H5	26:S1:1445:A:N7	2.04	0.55
51:SY:80:ARG:HB2	51:SY:82:ILE:HG12	1.89	0.55
26:S1:1918:U:H4'	26:S1:1919:C:H5'	1.89	0.55
85:2:622:G:H2'	85:2:623:A:C8	2.42	0.55
26:S1:1794:U:H2'	26:S1:1795:G:C8	2.42	0.54
26:S1:1982:G:OP1	50:SX:96:LYS:NZ	2.38	0.54
26:S1:691:G:H1	26:S1:754:G:H1	1.54	0.54
68:Z:120:ARG:NH1	74:f:114:MET:O	2.40	0.54
1:1:652:A:H2'	1:1:653:A:C8	2.43	0.54
34:SG:160:VAL:HG21	34:SG:179:ILE:HD11	1.90	0.54
1:1:594:G:H1	1:1:613:C:H5	1.56	0.54
1:1:1255:G:H2'	1:1:1256:A:C8	2.43	0.54
1:1:1571:C:H5	62:T:85:ARG:HH21	1.55	0.54
24:Q:105:LEU:HD23	24:Q:138:LEU:HD23	1.90	0.54
21:N:3:ARG:NH2	85:2:1292:U:OP2	2.39	0.54
85:2:1282:C:H5	85:2:1336:G:H1	1.56	0.54
18:K:140:HIS:CE1	75:g:20:LYS:HZ3	2.26	0.54
26:S1:1117:A:H2'	26:S1:1118:G:C8	2.43	0.54
26:S1:992:C:H4'	26:S1:993:U:H5'	1.89	0.54
26:S1:1701:A:H2'	26:S1:1702:A:C8	2.43	0.54
40:SN:95:PRO:HD2	40:SN:98:GLN:HG3	1.90	0.54
26:S1:1207:U:H5'	46:ST:55:ARG:HD3	1.89	0.54
26:S1:1539:PSU:HN3	26:S1:1550:OMG:HN1	1.55	0.54
1:1:412:G:N1	1:1:415:A:OP2	2.36	0.54
22:O:40:ASP:OD1	53:S:70:ARG:NH1	2.40	0.54
26:S1:814:G:O2'	26:S1:817:A:N6	2.28	0.54
36:SI:20:GLU:HG3	36:SI:49:VAL:HG12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Sh:67:VAL:HG22	60:Sh:69:ASP:H	1.73	0.54
1:1:1251:U:O2	15:H:74:GLN:NE2	2.41	0.54
5:6:32:U:HO2'	12:E:46:ARG:HH11	1.55	0.54
26:S1:450:A:H2'	26:S1:451:C:H6	1.73	0.54
26:S1:750:U:H2'	26:S1:751:G:H8	1.73	0.54
1:1:898:A:H2'	1:1:899:A:C8	2.43	0.53
26:S1:979:U:H2'	26:S1:980:G:C8	2.42	0.53
1:1:179:G:H2'	1:1:180:A:H8	1.73	0.53
1:1:403:C:OP2	78:j:56:ARG:NH2	2.37	0.53
1:1:442:A:O3'	1:1:443:A:H4'	2.07	0.53
32:SE:88:GLU:HG2	32:SE:95:ARG:HG2	1.90	0.53
85:2:999:U:O2'	85:2:1000:U:O5'	2.22	0.53
1:1:1355:C:O2'	1:1:1356:G:H5''	2.09	0.53
1:1:1365:A:O2'	1:1:1366:A:O4'	2.13	0.53
26:S1:1038:U:O2'	36:SI:84:GLU:OE1	2.26	0.53
26:S1:1708:A:O3'	50:SX:138:ARG:NH1	2.41	0.53
26:S1:1971:U:OP2	49:SW:50:ARG:NH2	2.41	0.53
84:p:34:ARG:NH2	85:2:1224:U:OP2	2.40	0.53
85:2:97:A:O2'	85:2:366:C:O2	2.22	0.53
26:S1:2160:G:H5'	85:2:502:A:C6	2.43	0.53
85:2:956:C:H2'	85:2:957:C:H4'	1.90	0.53
26:S1:964:U:H5'	26:S1:965:G:H5''	1.91	0.53
26:S1:1019:U:O2	26:S1:1033:G:N2	2.29	0.53
36:SI:39:GLN:O	36:SI:43:ARG:NH2	2.42	0.53
7:8:16:C:OP2	7:8:71:C:O2'	2.26	0.53
26:S1:971:U:H2'	26:S1:972:A:C8	2.43	0.53
51:SY:76:ILE:O	51:SY:80:ARG:HG2	2.09	0.53
33:SF:50:LYS:HD2	33:SF:259:LEU:HD13	1.90	0.53
68:Z:21:LYS:HG3	68:Z:26:ARG:HG2	1.91	0.53
76:h:120:ARG:NH2	85:2:817:U:OP2	2.41	0.53
1:1:1181:PSU:HN1	1:1:1191:G:H1	1.56	0.53
26:S1:1890:A:C6	26:S1:1891:A:H1'	2.43	0.53
29:SB:33:GLN:HE21	29:SB:50:HIS:CE1	2.27	0.53
55:Sc:37:SER:HB3	55:Sc:44:VAL:HG22	1.91	0.53
1:1:209:C:OP2	1:1:210:G:O2'	2.26	0.53
1:1:1675:A:H3'	1:1:1676:G:C8	2.44	0.53
26:S1:1100:U:H5''	26:S1:1101:A:OP1	2.08	0.53
26:S1:1133:U:O2'	41:SO:128:ILE:O	2.27	0.53
85:2:1124:A:H2'	85:2:1125:G:C8	2.44	0.53
1:1:1263:A:O2'	1:1:1264:A:OP2	2.21	0.53
39:SM:67:CYS:SG	39:SM:68:GLY:N	2.82	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:1273:A:H61	82:n:3:THR:HG22	1.75	0.52
26:S1:1701:A:H2'	26:S1:1702:A:H8	1.73	0.52
25:R:153:LEU:HB3	25:R:156:ARG:HD2	1.92	0.52
26:S1:792:G:O6	26:S1:833:G:O6	2.27	0.52
26:S1:1795:G:H22	26:S1:1803:A:H2	1.57	0.52
35:SH:52:MET:HE3	35:SH:57:ARG:HD3	1.91	0.52
54:Sa:60:ILE:HB	54:Sa:101:TYR:HB2	1.92	0.52
1:1:700:A:C2	1:1:845:OMU:H5	2.43	0.52
21:N:191:GLU:HB2	21:N:200:ILE:HD11	1.90	0.52
21:N:207:THR:HG22	21:N:208:MET:H	1.74	0.52
32:SE:191:GLU:HG2	32:SE:229:LEU:HD13	1.92	0.52
26:S1:760:G:OP1	36:SI:50:ARG:NH1	2.38	0.52
26:S1:820:C:H3'	26:S1:821:A:H5'	1.91	0.52
26:S1:1523:A:H2'	26:S1:1524:G:C8	2.45	0.52
62:T:112:MET:HE3	62:T:150:MET:HG3	1.90	0.52
1:1:235:A2M:O5'	1:1:235:A2M:H8	2.08	0.52
1:1:1153:A:H2'	1:1:1155:A:H62	1.74	0.52
26:S1:953:U:H3	26:S1:982:G:H1	1.56	0.52
26:S1:1911:U:H5	26:S1:1930:G:H1	1.57	0.52
31:SD:101:PRO:O	31:SD:105:GLU:HG2	2.10	0.52
1:1:1673:G:H2'	1:1:1674:A:O4'	2.09	0.52
30:SC:136:THR:HG23	30:SC:184:LYS:HB2	1.92	0.52
58:Se:41:THR:HG22	58:Se:45:LEU:HD12	1.91	0.52
1:1:2:C:N4	6:7:169:A:O3'	2.43	0.52
1:1:1260:G:H4'	1:1:1261:U:H5'	1.91	0.52
6:7:71:A:OP1	65:W:25:ARG:NH1	2.42	0.52
1:1:250:A:C8	65:W:5:LYS:HG2	2.45	0.52
2:3:111:A:O2'	2:3:112:C:H5''	2.10	0.52
6:7:125:A:H3'	6:7:126:G:H8	1.73	0.52
26:S1:2026:U:H2'	26:S1:2027:G:C8	2.44	0.52
14:G:33:LYS:NZ	85:2:978:C:OP1	2.43	0.52
26:S1:1293:G:H1	26:S1:1422:U:H3	1.57	0.52
59:Sg:180:ASN:ND2	59:Sg:182:ASN:OD1	2.43	0.52
85:2:958:A:H2'	85:2:959:A:C8	2.44	0.52
85:2:1136:U:H2'	85:2:1137:G:C8	2.45	0.52
4:5:3:A:H62	4:5:134:C:H5	1.58	0.51
26:S1:1101:A:H2'	26:S1:1102:G:C5	2.45	0.51
29:SB:41:ILE:HD11	29:SB:153:THR:HG22	1.92	0.51
39:SM:104:GLU:N	39:SM:104:GLU:OE1	2.42	0.51
1:1:179:G:H2'	1:1:180:A:C8	2.44	0.51
26:S1:694:U:H3	26:S1:751:G:H22	1.56	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1092:U:O3'	21:N:198:LYS:NZ	2.44	0.51
11:D:158:LYS:HG2	11:D:162:MET:HE2	1.93	0.51
1:1:736:C:H2'	1:1:737:U:O4'	2.11	0.51
5:6:67:C:OP1	75:g:96:ARG:NH2	2.44	0.51
26:S1:966:G:H2'	26:S1:967:A:C8	2.45	0.51
42:SP:84:PHE:CE2	42:SP:86:PRO:HA	2.45	0.51
1:1:594:G:H22	1:1:613:C:H5	1.57	0.51
1:1:938:G:H2'	1:1:939:C:C6	2.46	0.51
30:SC:125:VAL:O	30:SC:128:SER:OG	2.28	0.51
1:1:520:G:O2'	1:1:521:G:H8	1.76	0.51
6:7:128:U:H2'	6:7:129:C:C6	2.46	0.51
17:J:86:SER:HA	17:J:96:TYR:HB3	1.91	0.51
19:L:129:LEU:HG	19:L:133:LYS:HD2	1.93	0.51
26:S1:752:C:H2'	26:S1:753:A:C8	2.46	0.51
26:S1:1014:C:H2'	26:S1:1015:G:C8	2.45	0.51
56:Sb:65:ASN:OD1	56:Sb:65:ASN:N	2.43	0.51
60:Sh:161:LYS:H	60:Sh:161:LYS:HD3	1.76	0.51
26:S1:315:A:H5''	26:S1:333:G:H22	1.75	0.51
52:SZ:17:PHE:HZ	52:SZ:26:LYS:HD2	1.76	0.51
64:V:91:SER:HA	64:V:123:LYS:HD2	1.92	0.51
26:S1:1206:C:H5''	46:ST:14:SER:HB2	1.93	0.51
26:S1:1019:U:O4	26:S1:1033:G:O6	2.28	0.51
26:S1:1618:U:H2'	26:S1:1619:G:C8	2.46	0.51
33:SF:155:TYR:OH	33:SF:161:GLY:O	2.25	0.51
26:S1:1000:U:H3	26:S1:1094:G:H1	1.59	0.51
83:o:21:ASN:ND2	85:2:436:U:OP1	2.38	0.51
1:1:300:A:O2'	1:1:301:A:O4'	2.23	0.50
21:N:184:LEU:HD23	21:N:190:LEU:HD21	1.93	0.50
26:S1:780:A:H2'	26:S1:781:A:C8	2.46	0.50
85:2:653:C:H2'	85:2:654:U:H6	1.76	0.50
2:3:105:C:H2'	2:3:106:U:C6	2.46	0.50
26:S1:580:A:OP2	31:SD:181:ARG:NH2	2.34	0.50
26:S1:779:A:H2'	26:S1:780:A:H8	1.77	0.50
32:SE:28:PRO:HG2	32:SE:35:LEU:HG	1.93	0.50
2:3:192:G:O6	76:h:44:HIS:NE2	2.39	0.50
6:7:18:G:H2'	6:7:19:A:C8	2.46	0.50
9:B:326:ASN:HB3	85:2:1510:A:H61	1.75	0.50
60:Sh:195:PHE:HB3	60:Sh:200:LEU:HD11	1.93	0.50
85:2:603:A:H2'	85:2:604:A2M:H8	1.94	0.50
1:1:1778:G:H2'	1:1:1779:G:C8	2.47	0.50
26:S1:995:U:C4	26:S1:996:C:C4	3.00	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:SI:37:LEU:HB3	36:SI:41:LEU:HD23	1.94	0.50
85:2:406:G:H2'	85:2:407:C:C6	2.47	0.50
26:S1:106:A:H2'	26:S1:107:G:C8	2.45	0.50
26:S1:781:A:N1	26:S1:839:G:C6	2.80	0.50
26:S1:1940:G:N2	50:SX:91:ARG:HH21	2.09	0.50
1:1:93:G:H2'	1:1:94:A:C8	2.47	0.50
1:1:1726:G:OP2	1:1:1726:G:N2	2.20	0.50
9:B:320:GLY:O	9:B:340:ARG:NH1	2.44	0.50
25:R:70:LYS:O	25:R:74:ARG:NH2	2.44	0.50
26:S1:580:A:O2'	26:S1:583:A:OP2	2.22	0.50
60:Sh:112:GLU:HA	60:Sh:117:THR:HA	1.94	0.50
1:1:532:C:H2'	1:1:533:G:H5''	1.94	0.50
13:F:42:LEU:HD11	13:F:85:ILE:HG13	1.94	0.50
26:S1:1645:U:H3	26:S1:1674:A:N6	2.07	0.50
30:SC:109:LEU:HD23	30:SC:176:MET:HE1	1.93	0.50
85:2:83:G:O2'	85:2:580:U:O4	2.23	0.50
1:1:1060:A:H2'	1:1:1061:G:H8	1.76	0.50
1:1:1242:U:OP1	18:K:17:ARG:NH2	2.45	0.50
3:4:158:A:OP1	85:2:1330:A:O2'	2.26	0.50
26:S1:2092:G:H2'	26:S1:2093:U:C6	2.47	0.50
31:SD:163:PHE:C	31:SD:164:GLY:HA2	2.37	0.50
37:SK:76:VAL:HG12	37:SK:108:PRO:HG2	1.93	0.50
43:SQ:104:VAL:HG23	43:SQ:115:THR:HA	1.93	0.50
1:1:626:U:H2'	1:1:627:C:H6	1.76	0.50
9:B:327:ASP:H	85:2:1510:A:N6	2.09	0.50
33:SF:55:VAL:HG21	33:SF:78:ILE:HG23	1.94	0.50
85:2:68:A:O2'	85:2:69:A:OP1	2.28	0.50
26:S1:276:G:H2'	26:S1:277:U:O4'	2.12	0.49
26:S1:1421:C:H2'	26:S1:1422:U:C6	2.46	0.49
26:S1:2118:G:O2'	26:S1:2119:C:O4'	2.29	0.49
67:Y:67:GLN:HA	67:Y:117:GLN:NE2	2.27	0.49
1:1:273:A:H4'	78:j:82:LYS:HD3	1.94	0.49
1:1:719:U:O2'	1:1:720:A:H5''	2.13	0.49
14:G:163:LEU:HD23	20:M:7:LEU:HD21	1.94	0.49
22:O:85:ALA:HB2	22:O:264:LEU:HD23	1.93	0.49
26:S1:1016:G:H1	26:S1:1036:G:N2	2.09	0.49
32:SE:138:THR:OG1	32:SE:140:ASP:OD1	2.20	0.49
43:SQ:110:GLY:O	43:SQ:113:THR:OG1	2.22	0.49
73:e:53:PHE:HD2	73:e:56:VAL:HG11	1.77	0.49
6:7:121:G:H2'	6:7:122:A:C8	2.48	0.49
7:8:96:G:H2'	7:8:97:A:C8	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:2084:C:O2'	26:S1:2085:A:H5'	2.12	0.49
55:Sc:36:VAL:HG21	55:Sc:64:LEU:HD22	1.93	0.49
67:Y:76:ASN:OD1	67:Y:77:HIS:N	2.45	0.49
26:S1:996:C:H2'	26:S1:997:C:C6	2.47	0.49
26:S1:1170:A:H2'	26:S1:1171:A:C8	2.47	0.49
26:S1:1915:U:H3	26:S1:1926:G:H1	1.60	0.49
85:2:1470:C:H5	85:2:1600:C:H2'	1.77	0.49
26:S1:772:A:H1'	26:S1:773:A:H5'	1.95	0.49
53:S:9:SER:O	53:S:55:LYS:NZ	2.46	0.49
85:2:525:A:N7	85:2:532:U:H5	2.11	0.49
85:2:957:C:H3'	85:2:958:A:H8	1.74	0.49
1:1:422:PSU:H2'	1:1:423:U:C6	2.48	0.49
26:S1:746:C:H2'	26:S1:747:C:C6	2.47	0.49
26:S1:1968:G:OP1	44:SR:89:ARG:NH2	2.45	0.49
27:S4:68:C:H2'	27:S4:69:G:H8	1.76	0.49
85:2:1472:U:O4	85:2:1492:G:O6	2.30	0.49
1:1:512:U:N3	25:R:30:GLU:OE2	2.41	0.49
36:SI:108:ASP:HB3	36:SI:111:LYS:HG3	1.94	0.49
48:SV:41:ALA:HB3	48:SV:47:LYS:HE3	1.93	0.49
26:S1:99:U:O2	37:SK:21:HIS:HB2	2.13	0.49
26:S1:819:G:H5'	26:S1:820:C:H2'	1.95	0.49
26:S1:1415:C:H2'	26:S1:1416:G:C8	2.47	0.49
26:S1:1551:G:OP2	45:SS:41:ARG:NH1	2.42	0.49
46:ST:67:THR:O	46:ST:69:ARG:NH1	2.46	0.49
73:e:82:ASP:OD2	73:e:164:LYS:NZ	2.42	0.49
83:o:16:THR:HG22	85:2:111:G:C8	2.48	0.49
1:1:737:U:OP1	16:I:73:LYS:NZ	2.33	0.49
26:S1:822:U:H4'	34:SG:226:ARG:HH22	1.77	0.49
26:S1:2021:A2M:H5''	26:S1:2021:A2M:H8	1.95	0.49
12:E:135:ASP:OD2	12:E:137:SER:OG	2.31	0.49
26:S1:1296:G:H1	26:S1:1419:U:H3	1.61	0.49
34:SG:21:GLU:HA	34:SG:24:ARG:HH11	1.77	0.49
43:SQ:34:ILE:HG22	43:SQ:123:ILE:HD11	1.94	0.49
35:SH:57:ARG:NH2	35:SH:134:ASN:OD1	2.31	0.48
44:SR:91:PRO:HA	49:SW:25:ARG:HH11	1.78	0.48
51:SY:47:ASN:HD21	51:SY:49:VAL:HG22	1.77	0.48
26:S1:327:U:H2'	26:S1:328:C:C6	2.48	0.48
26:S1:1018:G:N2	26:S1:1034:G:H22	2.12	0.48
39:SM:65:THR:O	45:SS:41:ARG:NH2	2.46	0.48
85:2:984:G:H2'	85:2:985:A:C8	2.49	0.48
26:S1:790:U:H3	34:SG:226:ARG:CD	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:e:66:ARG:NH1	85:2:1512:G:OP2	2.47	0.48
12:E:184:THR:OG1	12:E:185:ASN:N	2.46	0.48
26:S1:991:G:H21	36:SI:43:ARG:NH2	2.11	0.48
64:V:60:ILE:HG13	69:a:26:LYS:HG3	1.94	0.48
1:1:345:U:H2'	1:1:346:U:C6	2.48	0.48
1:1:1392:G:H2'	1:1:1392:G:N3	2.29	0.48
2:3:98:C:H2'	2:3:99:U:H6	1.77	0.48
14:G:97:LYS:NZ	14:G:208:ASP:OD2	2.40	0.48
26:S1:2185:MA6:H8	26:S1:2185:MA6:H5''	1.95	0.48
28:SA:146:LYS:HB3	28:SA:210:ARG:HB2	1.95	0.48
30:SC:93:ARG:O	30:SC:100:GLN:NE2	2.45	0.48
1:1:636:U:H2'	1:1:637:C:C6	2.47	0.48
13:F:50:ARG:O	13:F:72:ASN:ND2	2.47	0.48
26:S1:16:G:H2'	26:S1:17:C:C6	2.48	0.48
26:S1:1037:U:H2'	26:S1:1038:U:C6	2.48	0.48
26:S1:1037:U:H2'	26:S1:1038:U:H6	1.78	0.48
26:S1:1366:A:N6	26:S1:1416:G:H22	2.11	0.48
32:SE:125:ASN:HB3	32:SE:137:VAL:HG13	1.95	0.48
85:2:1492:G:H2'	85:2:1493:C:C6	2.48	0.48
1:1:479:A:H2'	1:1:480:U:C6	2.49	0.48
1:1:636:U:H2'	1:1:637:C:H6	1.79	0.48
22:O:162:GLY:HA2	22:O:187:PRO:HG3	1.96	0.48
26:S1:958:G:N2	26:S1:977:G:H22	2.12	0.48
26:S1:1672:C:O2'	26:S1:1673:A:OP1	2.29	0.48
26:S1:1891:A:H2	26:S1:1932:A:C5	2.31	0.48
85:2:94:A:H2'	85:2:95:A2M:H8	1.95	0.48
85:2:646:G:O2'	85:2:647:A:OP1	2.30	0.48
85:2:653:C:H2'	85:2:654:U:C6	2.49	0.48
4:5:64:U:O2	4:5:93:G:N2	2.39	0.48
26:S1:148:G:H2'	26:S1:149:G:H8	1.77	0.48
29:SB:179:TRP:CG	29:SB:202:VAL:HG12	2.49	0.48
32:SE:97:ARG:HB2	32:SE:111:LEU:HD11	1.96	0.48
1:1:252:G:OP1	65:W:9:ARG:NH1	2.45	0.48
26:S1:779:A:N6	26:S1:842:U:O4	2.46	0.48
26:S1:1969:A:OP2	49:SW:49:ARG:NH1	2.46	0.48
11:D:51:ARG:HA	11:D:66:LYS:HA	1.96	0.48
24:Q:7:GLN:NE2	24:Q:35:ALA:O	2.35	0.48
26:S1:1572:C:H2'	26:S1:1573:A:H8	1.79	0.48
59:Sg:103:PHE:HE2	59:Sg:138:GLY:HA2	1.78	0.48
66:X:59:TYR:CZ	66:X:63:HIS:HD2	2.32	0.48
1:1:1135:U:H4'	1:1:1136:G:O5'	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:177:TYR:OH	18:K:107:ASP:OD2	2.24	0.47
26:S1:557:A:OP2	31:SD:175:ARG:N	2.47	0.47
26:S1:558:U:H2'	26:S1:559:G:H8	1.78	0.47
26:S1:1916:G:H22	50:SX:85:TYR:HE2	1.62	0.47
72:d:24:LYS:HB2	72:d:96:ASN:HB3	1.95	0.47
85:2:591:A2M:HM'3	85:2:591:A2M:H1'	1.72	0.47
1:1:213:G:O6	68:Z:143:ARG:NH2	2.47	0.47
1:1:454:U:H2'	1:1:455:G:C8	2.48	0.47
1:1:1677:G:N2	1:1:1722:A:N7	2.63	0.47
4:5:6:U:H2'	4:5:7:C:C6	2.49	0.47
26:S1:2135:U:H2'	26:S1:2136:A:H8	1.79	0.47
72:d:97:VAL:HG23	72:d:100:SER:HB2	1.96	0.47
1:1:1524:OMG:H5''	1:1:1527:OMC:H5	1.79	0.47
26:S1:491:G:OP1	32:SE:26:PRO:HD3	2.15	0.47
40:SN:10:ARG:NH1	40:SN:86:TYR:OH	2.46	0.47
71:c:25:ARG:HH21	71:c:29:LYS:HD2	1.78	0.47
85:2:615:G:H2'	85:2:616:G:C8	2.49	0.47
1:1:36:U:H4'	19:L:32:ARG:HD3	1.97	0.47
26:S1:1459:G:O2'	26:S1:1460:G:H5'	2.14	0.47
1:1:438:A:H4'	1:1:439:U:H3'	1.96	0.47
11:D:81:LEU:O	11:D:82:LEU:HB3	2.15	0.47
26:S1:1016:G:H1	26:S1:1036:G:H1	1.62	0.47
34:SG:68:VAL:HG23	34:SG:102:GLY:HA2	1.96	0.47
34:SG:225:GLN:O	34:SG:226:ARG:NH1	2.47	0.47
26:S1:817:A:C8	26:S1:819:G:H2'	2.50	0.47
26:S1:1656:G:H1'	26:S1:1674:A:C2	2.50	0.47
49:SW:102:ALA:HB1	49:SW:109:PHE:HB3	1.97	0.47
1:1:300:A:H2'	1:1:301:A:C8	2.50	0.47
1:1:687:C:H2'	1:1:688:A:C8	2.48	0.47
1:1:688:A:H2'	1:1:689:A:C8	2.50	0.47
1:1:814:C:H2'	1:1:815:G:H8	1.79	0.47
5:6:14:A:N6	85:2:1450:G:O2'	2.39	0.47
26:S1:254:A:H2'	26:S1:255:A:C8	2.50	0.47
26:S1:558:U:H5	26:S1:587:A:N7	2.13	0.47
26:S1:1368:C:H42	26:S1:1414:A:H61	1.63	0.47
46:ST:87:ASP:OD1	46:ST:87:ASP:N	2.48	0.47
85:2:1189:A:H2'	85:2:1190:U:O2	2.15	0.47
1:1:471:G:H5'	75:g:124:ALA:HB1	1.97	0.47
12:E:20:VAL:HG11	12:E:45:LEU:HB2	1.96	0.47
85:2:1334:C:O2'	85:2:1335:C:OP1	2.31	0.47
26:S1:67:C:H5	26:S1:81:G:H21	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:1512:A:O2'	26:S1:2040:C:H5	1.98	0.47
28:SA:200:VAL:HG22	28:SA:212:LEU:HB3	1.97	0.47
85:2:665:A:H2'	85:2:666:C:C6	2.50	0.47
85:2:1183:C:H2'	85:2:1184:C:O4'	2.14	0.47
1:1:2:C:H2'	1:1:3:A:O4'	2.15	0.47
34:SG:162:ARG:HG2	34:SG:176:ALA:HB2	1.96	0.47
49:SW:57:ASP:OD1	49:SW:57:ASP:N	2.40	0.47
1:1:1778:G:H2'	1:1:1779:G:H8	1.80	0.46
26:S1:173:A:OP2	34:SG:139:LYS:HD2	2.16	0.46
26:S1:1765:C:H2'	26:S1:1766:G:C8	2.50	0.46
26:S1:2135:U:H2'	26:S1:2136:A:C8	2.50	0.46
46:ST:137:PRO:O	46:ST:138:THR:OG1	2.25	0.46
1:1:250:A:H8	65:W:5:LYS:HG2	1.81	0.46
1:1:819:C:H2'	1:1:820:U:O4'	2.15	0.46
1:1:1264:A:H2'	1:1:1265:A:H8	1.80	0.46
21:N:205:LYS:O	21:N:210:ASN:ND2	2.49	0.46
26:S1:864:G:OP1	32:SE:250:ARG:NH2	2.44	0.46
26:S1:1692:G:H2'	26:S1:1693:C:C6	2.50	0.46
34:SG:80:ARG:NH1	34:SG:90:GLY:O	2.48	0.46
48:SV:14:ARG:HG2	48:SV:69:ILE:HD11	1.97	0.46
59:Sg:22:GLN:N	59:Sg:22:GLN:OE1	2.48	0.46
62:T:42:ARG:NH1	62:T:99:GLU:OE2	2.49	0.46
7:8:62:A:H2'	7:8:63:C:C6	2.51	0.46
19:L:72:THR:HG22	19:L:108:LYS:HB3	1.97	0.46
85:2:1496:G:H2'	85:2:1497:C:C6	2.50	0.46
6:7:40:A:H2'	6:7:41:A:C8	2.50	0.46
26:S1:753:A:H2'	26:S1:754:G:C8	2.50	0.46
26:S1:1366:A:H2'	26:S1:1366:A:N3	2.30	0.46
28:SA:79:GLU:OE1	28:SA:79:GLU:N	2.45	0.46
59:Sg:230:PHE:CD1	59:Sg:266:LYS:HE3	2.50	0.46
85:2:1195:U:H2'	85:2:1196:G:H8	1.80	0.46
1:1:837:A:H4'	1:1:838:G:O5'	2.16	0.46
7:8:53:A:H5''	22:O:233:SER:HB3	1.98	0.46
26:S1:998:C:H2'	26:S1:999:A:O4'	2.16	0.46
85:2:1452:U:OP1	85:2:1454:A:N6	2.37	0.46
1:1:967:G:H5'	1:1:968:A:OP1	2.15	0.46
2:3:180:U:O2'	2:3:181:G:O5'	2.32	0.46
26:S1:306:U:H4'	37:SK:64:ASN:HD21	1.80	0.46
26:S1:1853:U:OP1	45:SS:10:ARG:NH2	2.46	0.46
26:S1:1966:A:N1	26:S1:1983:U:H5	2.14	0.46
29:SB:203:ASP:HA	29:SB:206:PHE:CD2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SU:3:VAL:HB	47:SU:4:ALA:H	1.58	0.46
81:m:100:TYR:O	85:2:1333:G:O2'	2.32	0.46
85:2:1424:U:C2	85:2:1425:A:C8	3.04	0.46
1:1:468:G:H2'	1:1:469:A:C8	2.51	0.46
1:1:626:U:H2'	1:1:627:C:C6	2.51	0.46
1:1:664:C:O2	75:g:49:GLN:NE2	2.45	0.46
1:1:882:A:O2'	85:2:47:A:N3	2.46	0.46
1:1:1134:C:O2'	1:1:1135:U:O4'	2.30	0.46
2:3:72:A:H2'	2:3:73:A:C8	2.50	0.46
15:H:131:VAL:HG12	15:H:132:ARG:HG3	1.96	0.46
26:S1:286:G:H1'	34:SG:217:ALA:HB1	1.97	0.46
26:S1:1879:OMG:HM23	26:S1:1879:OMG:H1'	1.73	0.46
1:1:1549:U:H2'	1:1:1550:A:C8	2.50	0.46
2:3:105:C:H2'	2:3:106:U:H6	1.80	0.46
26:S1:954:A:H5'	26:S1:955:A:OP2	2.15	0.46
32:SE:94:ASP:HB3	32:SE:96:PHE:CZ	2.51	0.46
1:1:1565:A:N6	73:e:79:ARG:HG3	2.31	0.46
3:4:24:A:H5''	15:H:7:LYS:HB2	1.98	0.46
5:6:51:A:H4'	5:6:52:G:O5'	2.16	0.46
13:F:30:ARG:NH2	75:g:144:ILE:OXT	2.46	0.46
23:P:23:ASN:HB3	23:P:26:ILE:HB	1.97	0.46
26:S1:779:A:H2'	26:S1:780:A:C8	2.51	0.46
85:2:998:G:O2'	85:2:999:U:O5'	2.34	0.46
21:N:75:TYR:CZ	21:N:79:ARG:HG3	2.52	0.46
26:S1:363:G:H4'	26:S1:367:A:C8	2.50	0.46
26:S1:988:A:OP2	36:SI:69:ARG:NH2	2.48	0.46
85:2:998:G:H1'	85:2:999:U:H5'	1.97	0.46
1:1:955:A2M:HM'3	1:1:955:A2M:H1'	1.79	0.45
1:1:959[A]:OMG:N1	85:2:660:G:OP1	2.36	0.45
1:1:1266:A:H61	1:1:1361:C:H42	1.62	0.45
4:5:128:G:OP1	73:e:16:LYS:NZ	2.48	0.45
18:K:153:LYS:HE2	18:K:153:LYS:HB2	1.80	0.45
26:S1:93:G:HO2'	26:S1:508:A:HO2'	1.58	0.45
26:S1:953:U:H3	26:S1:982:G:H22	1.63	0.45
26:S1:999:A:N6	26:S1:1095:G:C6	2.81	0.45
26:S1:1927:U:H2'	26:S1:1928:G:C8	2.51	0.45
36:SI:100:ARG:NH2	36:SI:131:ASP:OD2	2.49	0.45
60:Sh:60:LYS:NZ	60:Sh:61:ASN:H	2.14	0.45
1:1:954:U:H2'	1:1:955:A2M:H8	1.98	0.45
1:1:1365:A:H1'	85:2:1323:C:O2'	2.16	0.45
26:S1:997:C:H42	26:S1:1097:C:H42	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:2:816:G:H2'	85:2:817:U:H6	1.81	0.45
85:2:1320:U:H2'	85:2:1321:U:C6	2.51	0.45
1:1:1638:C:H2'	1:1:1639:U:C6	2.52	0.45
8:A:34:TYR:OH	85:2:965:C:OP1	2.24	0.45
15:H:185:ARG:NH1	85:2:1462:A:OP1	2.42	0.45
26:S1:1437:A:H2'	26:S1:1438:A:C8	2.51	0.45
26:S1:2005:U:H4'	38:SL:141:ARG:HD2	1.98	0.45
26:S1:2174:G:H21	82:n:3:THR:HG21	1.82	0.45
31:SD:92:LEU:O	31:SD:95:VAL:HG12	2.16	0.45
34:SG:59:LYS:HD3	34:SG:110:ALA:HB2	1.97	0.45
34:SG:227:ASP:OD1	34:SG:227:ASP:N	2.49	0.45
40:SN:34:THR:HB	40:SN:43:THR:HG22	1.98	0.45
85:2:478:A:H2'	85:2:479:C:O2	2.15	0.45
1:1:478:C:H2'	1:1:479:A:H8	1.81	0.45
1:1:845:OMU:H1'	1:1:845:OMU:HM23	1.77	0.45
1:1:1374:C:H2'	1:1:1375:G:O4'	2.16	0.45
1:1:1777:U:H2'	1:1:1778:G:H8	1.81	0.45
5:6:30:C:O2'	5:6:31:U:H2'	2.16	0.45
28:SA:151:GLN:HE21	28:SA:153:SER:HB2	1.80	0.45
85:2:1365:C:H2'	85:2:1366:C:C6	2.52	0.45
1:1:525:C:HO2'	1:1:526:A:H8	1.63	0.45
1:1:1050:G:H2'	1:1:1051:C:C2	2.52	0.45
1:1:1771:U:H2'	1:1:1772:G:H8	1.81	0.45
1:1:1779:G:H22	85:2:3:C:H5	1.63	0.45
26:S1:258:C:H42	26:S1:969:A:H61	1.64	0.45
26:S1:1702:A:H2'	26:S1:1703:U:C6	2.51	0.45
85:2:1170:U:H2'	85:2:1171:G:H8	1.82	0.45
1:1:1135:U:O2	1:1:1135:U:H2'	2.16	0.45
2:3:76:C:H42	2:3:145:U:H3	1.64	0.45
2:3:204:A:H2'	2:3:205:A:H8	1.79	0.45
13:F:185:LYS:HB2	13:F:185:LYS:HE3	1.72	0.45
14:G:76:LEU:HD23	14:G:76:LEU:HA	1.82	0.45
26:S1:1912:A:H2	26:S1:1929:G:N1	2.03	0.45
1:1:563:C:H2'	1:1:563:C:O2	2.16	0.45
1:1:1409:U:H2'	1:1:1410:U:C6	2.51	0.45
21:N:90:ARG:NH1	21:N:137:SER:OG	2.49	0.45
52:SZ:8:ALA:HB1	52:SZ:37:TRP:CE3	2.52	0.45
1:1:326:A:H2'	1:1:327:G:C8	2.52	0.45
2:3:25:G:N2	85:2:978:C:O2	2.50	0.45
7:8:62:A:H2'	7:8:63:C:H6	1.81	0.45
21:N:38:ARG:HG3	21:N:83:ASP:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:958:G:N2	26:S1:977:G:H1	2.08	0.45
26:S1:1160:A:N7	85:2:452:G:H4'	2.31	0.45
26:S1:2136:A:H2'	26:S1:2137:U:C6	2.51	0.45
30:SC:176:MET:HG2	30:SC:181:ILE:HG13	1.99	0.45
43:SQ:67:ASP:OD1	43:SQ:67:ASP:N	2.49	0.45
2:3:192:G:H4'	2:3:193:C:OP1	2.16	0.45
29:SB:68:ILE:O	29:SB:71:VAL:HG12	2.17	0.45
85:2:95:A2M:HM'3	85:2:95:A2M:H1'	1.84	0.45
85:2:570:A2M:H8	85:2:570:A2M:H2'	1.81	0.45
85:2:958:A:H2'	85:2:959:A:H8	1.82	0.45
29:SB:1:MET:N	51:SY:82:ILE:HG22	2.32	0.45
60:Sh:161:LYS:HE3	60:Sh:178:ASP:HB2	1.99	0.45
71:c:25:ARG:NH1	71:c:33:THR:OG1	2.35	0.45
75:g:7:HIS:HA	75:g:10:ARG:NH1	2.32	0.45
85:2:451:U:H3	85:2:483:C:N4	2.13	0.45
1:1:652:A:H2'	1:1:653:A:H8	1.81	0.44
1:1:1238:C:H41	25:R:179:ALA:HB1	1.82	0.44
2:3:203:A:H2'	2:3:204:A:C8	2.52	0.44
4:5:47:G:O2'	4:5:48:G:H5'	2.17	0.44
23:P:153:ARG:O	23:P:157:ARG:HG2	2.17	0.44
26:S1:263:G:H2'	26:S1:264:C:C6	2.53	0.44
26:S1:1974:A:OP2	49:SW:54:ARG:NH2	2.49	0.44
36:SI:39:GLN:HG2	36:SI:40:GLU:OE1	2.16	0.44
36:SI:82:THR:O	36:SI:86:GLU:HG2	2.17	0.44
59:Sg:4:GLU:OE2	59:Sg:307:SER:OG	2.21	0.44
59:Sg:246:ASN:OD1	59:Sg:247:ARG:N	2.47	0.44
79:k:49:ASP:OD2	79:k:52:LYS:N	2.45	0.44
85:2:1492:G:H2'	85:2:1493:C:H6	1.82	0.44
3:4:167:C:H2'	3:4:168:A:O4'	2.17	0.44
26:S1:161:A:H2'	26:S1:162:A:O4'	2.18	0.44
26:S1:751:G:H2'	26:S1:752:C:H6	1.81	0.44
26:S1:1366:A:H61	26:S1:1416:G:H22	1.64	0.44
26:S1:2010:G:H1	26:S1:2026:U:H3	1.65	0.44
26:S1:2199:C:H5	56:Sb:6:ARG:H	1.65	0.44
52:SZ:45:LEU:O	52:SZ:49:LYS:HG2	2.18	0.44
75:g:21:THR:OG1	75:g:22:SER:N	2.50	0.44
85:2:1470:C:C5	85:2:1600:C:H2'	2.52	0.44
85:2:1525:C:H2'	85:2:1600:C:O4'	2.17	0.44
1:1:550:A:O2'	1:1:551:A:N3	2.48	0.44
1:1:1657:G:H2'	1:1:1658:U:H6	1.83	0.44
1:1:1749:G:H2'	1:1:1751:A:N7	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:50:G:H4'	3:4:51:U:O5'	2.18	0.44
3:4:149:U:OP2	81:m:111:ARG:NH1	2.50	0.44
26:S1:173:A:O4'	26:S1:173:A:P	2.76	0.44
26:S1:351:G:OP1	47:SU:118:ARG:NH1	2.46	0.44
30:SC:7:LYS:HG2	39:SM:58:LEU:HD21	1.99	0.44
54:Sa:50:LEU:HD12	54:Sa:54:VAL:HG21	2.00	0.44
74:f:16:LYS:HE2	74:f:16:LYS:HB3	1.81	0.44
85:2:957:C:H2'	85:2:957:C:O2	2.17	0.44
85:2:1412:U:H2'	85:2:1413:PSU:C6	2.51	0.44
1:1:517:U:H2'	1:1:518:C:C6	2.52	0.44
1:1:657:G:O2'	1:1:1491:G:OP2	2.35	0.44
1:1:821:C:H5''	1:1:822:C:H5	1.83	0.44
1:1:1746:C:H2'	1:1:1747:U:C6	2.52	0.44
4:5:53:C:H42	4:5:61:C:N4	2.09	0.44
6:7:161:C:H2'	6:7:162:A2M:H8	2.00	0.44
21:N:142:GLU:H	21:N:142:GLU:CD	2.25	0.44
26:S1:582:U:OP2	52:SZ:5:LYS:HE2	2.17	0.44
62:T:137:THR:CG2	85:2:603:A:H5'	2.47	0.44
73:e:37:ARG:NH2	85:2:1513:G:N7	2.65	0.44
85:2:1082:U:H4'	85:2:1083:A:O4'	2.17	0.44
1:1:469:A:H2'	1:1:470:A:C8	2.52	0.44
2:3:64:U:H2'	2:3:65:U:C6	2.53	0.44
11:D:81:LEU:C	11:D:83:GLU:H	2.26	0.44
18:K:126:LYS:O	18:K:130:GLU:HG2	2.17	0.44
26:S1:2103:G:H2'	26:S1:2104:G:C8	2.53	0.44
32:SE:231:ASN:OD1	32:SE:231:ASN:N	2.50	0.44
75:g:20:LYS:HE3	75:g:20:LYS:HB3	1.85	0.44
85:2:1239:A:O2'	85:2:1240:A:H2'	2.18	0.44
1:1:541:A:H4'	1:1:542:C:H5''	2.00	0.44
4:5:5:G:H2'	4:5:6:U:C6	2.52	0.44
26:S1:1:G:N2	33:SF:190:ILE:O	2.50	0.44
26:S1:746:C:H4'	26:S1:747:C:OP1	2.17	0.44
35:SH:81:HIS:HD1	54:Sa:93:SER:HG	1.64	0.44
1:1:1086:G:H2'	1:1:1087:A:C8	2.52	0.44
26:S1:1830:G:H2'	26:S1:1831:U:C6	2.53	0.44
27:S4:76:A:O2'	85:2:1191:C:H5	2.00	0.44
30:SC:30:GLU:OE1	30:SC:30:GLU:N	2.44	0.44
85:2:1491:G:H2'	85:2:1492:G:C8	2.53	0.44
21:N:183:ALA:HA	21:N:186:ASP:OD2	2.18	0.44
26:S1:519:A:O2'	31:SD:8:ASN:O	2.29	0.44
26:S1:692:G:N2	26:S1:753:A:H2	2.14	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:1093:C:H2'	26:S1:1094:G:C8	2.53	0.44
44:SR:25:ARG:HG3	44:SR:30:ALA:HB2	1.99	0.44
55:Sc:68:THR:HG22	55:Sc:70:GLY:H	1.83	0.44
84:p:98:LYS:HD2	84:p:98:LYS:HA	1.78	0.44
85:2:751:U:H2'	85:2:752:G:H8	1.83	0.44
85:2:1278:C:H2'	85:2:1279:G:O4'	2.18	0.44
1:1:662:C:H2'	1:1:663:C:C6	2.53	0.44
1:1:957:C:O2'	1:1:960:A:N3	2.49	0.44
26:S1:479:A2M:OP2	26:S1:479:A2M:H8	2.18	0.44
30:SC:205:ASP:N	30:SC:205:ASP:OD1	2.50	0.44
48:SV:72:LYS:HB3	48:SV:72:LYS:HE3	1.60	0.44
62:T:137:THR:HG23	85:2:603:A:H5'	2.00	0.44
73:e:25:LYS:HA	73:e:25:LYS:HD3	1.83	0.44
1:1:700:A:H2'	1:1:701:G:C8	2.53	0.43
1:1:1263:A:O2'	1:1:1363:A:N6	2.48	0.43
1:1:1771:U:H2'	1:1:1772:G:C8	2.53	0.43
8:A:206:PRO:HG3	8:A:213:GLY:HA3	2.00	0.43
26:S1:992:C:H4'	26:S1:993:U:C5'	2.47	0.43
26:S1:2159:A:O2'	26:S1:2160:G:H8	2.01	0.43
41:SO:106:GLN:HE21	41:SO:106:GLN:HB2	1.59	0.43
42:SP:139:GLU:OE1	42:SP:139:GLU:N	2.51	0.43
26:S1:751:G:H2'	26:S1:752:C:C6	2.53	0.43
26:S1:989:A:N6	36:SI:119:LYS:HG2	2.33	0.43
26:S1:1708:A:H4'	50:SX:138:ARG:HH22	1.83	0.43
26:S1:1940:G:N2	50:SX:91:ARG:HE	2.16	0.43
26:S1:2037:U:H2'	26:S1:2038:C:C6	2.53	0.43
85:2:1492:G:O5'	85:2:1492:G:H8	2.01	0.43
1:1:677:1MA:H8	1:1:677:1MA:H2'	1.36	0.43
22:O:52:VAL:HG13	22:O:63:GLN:HB2	2.00	0.43
26:S1:1573:A:H2'	26:S1:1574:G:C8	2.54	0.43
26:S1:1712:G:N2	50:SX:8:ILE:O	2.41	0.43
43:SQ:67:ASP:OD1	43:SQ:94:ARG:HB2	2.19	0.43
50:SX:44:PRO:HG2	50:SX:47:THR:HG23	2.01	0.43
71:c:30:GLN:O	71:c:34:GLU:HG2	2.19	0.43
85:2:1399:G:H2'	85:2:1400:U:C6	2.53	0.43
1:1:79:U:H2'	1:1:80:C:C6	2.53	0.43
1:1:631:G:N7	71:c:43:ARG:NH2	2.65	0.43
26:S1:1015:G:H2'	26:S1:1016:G:C8	2.53	0.43
26:S1:1512:A:HO2'	26:S1:2040:C:H5	1.65	0.43
26:S1:1601:U:H2'	26:S1:1602:U:C6	2.53	0.43
26:S1:1870:A:H2'	26:S1:1871:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:1915:U:OP1	50:SX:134:GLN:NE2	2.38	0.43
31:SD:28:LYS:HE2	31:SD:28:LYS:HB2	1.72	0.43
39:SM:25:ASN:O	39:SM:29:VAL:HG23	2.18	0.43
50:SX:29:LYS:HE3	50:SX:29:LYS:HB2	1.88	0.43
73:e:45:MET:HG2	73:e:49:LYS:HB2	2.00	0.43
79:k:39:SER:OG	85:2:8:U:OP1	2.36	0.43
85:2:604:A2M:HM'3	85:2:604:A2M:H1'	1.82	0.43
85:2:1042:G:H2'	85:2:1043:C:H6	1.83	0.43
85:2:1253:OMG:HM21	85:2:1255:A:H2'	2.00	0.43
7:8:119:A:H2'	7:8:120:C:H6	1.83	0.43
7:8:119:A:H2'	7:8:120:C:C6	2.54	0.43
26:S1:285:A:H3'	26:S1:285:A:N3	2.33	0.43
26:S1:886:U:H3'	32:SE:238:LYS:NZ	2.34	0.43
28:SA:39:GLU:OE1	28:SA:39:GLU:N	2.50	0.43
29:SB:192:ILE:HG12	29:SB:198:TRP:CD1	2.53	0.43
35:SH:178:LYS:HE2	35:SH:178:LYS:HB2	1.82	0.43
37:SK:210:PHE:O	37:SK:214:ARG:HG2	2.19	0.43
50:SX:155:LYS:HD2	50:SX:155:LYS:HA	1.90	0.43
85:2:451:U:H2'	85:2:452:G:C2	2.53	0.43
85:2:652:C:H2'	85:2:653:C:C6	2.54	0.43
85:2:1151:U:H2'	85:2:1152:U:H6	1.83	0.43
1:1:448:A:C2	6:7:16:A:H1'	2.54	0.43
1:1:1722:A:N3	1:1:1722:A:H2'	2.34	0.43
2:3:63:U:N3	63:U:16:GLN:OE1	2.38	0.43
4:5:128:G:H2'	4:5:129:G:H8	1.83	0.43
7:8:67:C:C6	21:N:206:ILE:HG12	2.53	0.43
26:S1:232:C:H2'	26:S1:233:G:H8	1.83	0.43
26:S1:792:G:H5'	26:S1:792:G:N3	2.34	0.43
26:S1:1018:G:N2	26:S1:1034:G:H1	2.16	0.43
26:S1:1096:C:H2'	26:S1:1097:C:C6	2.53	0.43
26:S1:2199:C:O2	56:Sb:96:ARG:HB3	2.19	0.43
36:SI:61:VAL:HG11	36:SI:175:VAL:HG21	1.99	0.43
85:2:625:U:H2'	85:2:626:PSU:C6	2.54	0.43
1:1:500:C:H2'	1:1:501:C:H6	1.83	0.43
1:1:1010:OMC:HM22	1:1:1010:OMC:H1'	1.61	0.43
3:4:127:G:C6	9:B:283:LEU:HD11	2.53	0.43
9:B:226:THR:HG22	9:B:336:SER:HB3	2.01	0.43
25:R:61:LEU:HD23	71:c:87:LEU:HD13	2.00	0.43
26:S1:1513:C:H2'	26:S1:1514:A:H8	1.84	0.43
48:SV:71:LEU:O	48:SV:72:LYS:HB3	2.19	0.43
1:1:500:C:H2'	1:1:501:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:161:CYS:HA	15:H:164:VAL:HG22	2.00	0.43
21:N:38:ARG:HH11	21:N:83:ASP:HB3	1.83	0.43
26:S1:285:A:C8	26:S1:816:C:C2	3.07	0.43
26:S1:656:G:H5'	26:S1:662:G:N2	2.34	0.43
26:S1:976:A:C4	26:S1:977:G:C8	3.07	0.43
26:S1:1702:A:H2'	26:S1:1703:U:H6	1.83	0.43
26:S1:2012:A:H2'	26:S1:2013:G:H8	1.84	0.43
27:S4:63:G:H2'	27:S4:64:A:O4'	2.19	0.43
35:SH:11:LYS:HE3	35:SH:11:LYS:HB3	1.85	0.43
62:T:137:THR:HG23	62:T:138:PRO:HD2	2.00	0.43
69:a:53:LYS:HA	69:a:53:LYS:HD3	1.81	0.43
85:2:755:U:O2'	85:2:756:C:H6	2.00	0.43
1:1:1764:A:H3'	1:1:1766:G:OP2	2.18	0.43
2:3:100:U:O2'	2:3:101:G:H8	2.01	0.43
8:A:130:SER:OG	8:A:174:ARG:NH1	2.52	0.43
21:N:48:VAL:O	21:N:139:ARG:HA	2.18	0.43
26:S1:114:U:H2'	26:S1:115:C:C6	2.54	0.43
41:SO:47:VAL:HG11	41:SO:77:ARG:HG2	2.01	0.43
42:SP:96:GLU:OE1	42:SP:96:GLU:N	2.49	0.43
72:d:38:GLN:OE1	72:d:40:ARG:NE	2.51	0.43
72:d:51:PRO:HA	72:d:52:PRO:HD3	1.95	0.43
85:2:1116:A:N3	85:2:1116:A:H2'	2.34	0.43
1:1:559:G:H2'	1:1:560:G:O4'	2.19	0.43
9:B:255:ALA:HB1	85:2:1385:G:C2	2.54	0.43
26:S1:282:C:H2'	26:S1:283:C:C6	2.54	0.43
26:S1:815:U:H5'	26:S1:816:C:OP1	2.19	0.43
26:S1:820:C:C3'	26:S1:821:A:H5'	2.49	0.43
26:S1:1115:G:H2'	26:S1:1116:U:C6	2.53	0.43
26:S1:1202:A:OP1	46:ST:2:VAL:HG12	2.19	0.43
26:S1:1496:U:H2'	26:S1:1497:U:C6	2.54	0.43
29:SB:80:CYS:HA	29:SB:102:HIS:O	2.19	0.43
47:SU:7:TYR:CZ	47:SU:36:PRO:HG3	2.53	0.43
85:2:80:A:H61	85:2:585:C:H42	1.66	0.43
85:2:590:U:H2'	85:2:591:A2M:H8	2.01	0.43
85:2:1453:U:H4'	85:2:1454:A:H5''	2.00	0.43
1:1:131:U:H3'	1:1:132:A:C8	2.54	0.42
1:1:766:A:H2'	1:1:767:U:C6	2.54	0.42
1:1:1019:G:H2'	1:1:1020:C:H6	1.84	0.42
26:S1:1510:C:H2'	26:S1:1510:C:O2	2.19	0.42
26:S1:1615:G:H2'	26:S1:1616:A:O4'	2.18	0.42
26:S1:2102:A:N6	26:S1:2121:C:H42	2.15	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50: SX:19: LEU: HD12	50: SX:19: LEU: HA	1.90	0.42
73: e:122: THR: HG22	73: e:124: ASP: H	1.83	0.42
1:1:24: A: H2'	1:1:25: C: H6	1.84	0.42
1:1:1443: U: O2'	1:1:1444: A: H3'	2.19	0.42
1:1:1451: C: H2'	1:1:1452: C: C6	2.53	0.42
8: A:68: LYS: HD3	8: A:70: ARG: NH2	2.34	0.42
26: S1:66: U: H6	34: SG:163: ARG: NH1	2.17	0.42
26: S1:629: A: O2'	26: S1:631: U: OP1	2.36	0.42
26: S1:789: G: H4'	26: S1:790: U: OP2	2.19	0.42
28: SA:197: ASP: OD1	28: SA:197: ASP: N	2.52	0.42
31: SD:159: ASP: OD1	31: SD:159: ASP: N	2.50	0.42
35: SH:154: SER: OG	35: SH:157: GLU: OE1	2.22	0.42
46: ST:43: LYS: HE2	46: ST:43: LYS: HB2	1.89	0.42
75: g:12: LYS: HB2	75: g:12: LYS: HE3	1.81	0.42
79: k:7: THR: HG22	79: k:9: LYS: H	1.84	0.42
85:2:1454: A: O2'	85:2:1455: U: H2'	2.18	0.42
1:1:546: G: N3	1:1:546: G: H2'	2.34	0.42
1:1:1603: G: H2'	1:1:1604: U: C6	2.53	0.42
3:4:51: U: H2'	3:4:52: A: H8	1.84	0.42
4:5:7: C: H2'	4:5:8: C: H6	1.83	0.42
27: S4:68: C: C2	27: S4:69: G: C8	3.07	0.42
29: SB:36: ALA: HB1	29: SB:157: LEU: HD12	2.00	0.42
36: SI:34: HIS: HB3	36: SI:37: LEU: HB2	2.01	0.42
42: SP:109: GLY: O	42: SP:119: ARG: NE	2.42	0.42
85:2:1364: A: H2'	85:2:1365: C: C6	2.55	0.42
1:1:468: G: HO2'	1:1:469: A: P	2.42	0.42
1:1:678: A2M: O2'	1:1:679: A: C8	2.72	0.42
1:1:996: A: H2'	1:1:997: C: C6	2.53	0.42
5:6:48: C: C2	13: F:185: LYS: HD3	2.54	0.42
6:7:63: G: H22	6:7:96: A: H2	1.63	0.42
26: S1:285: A: N6	26: S1:816: C: H2'	2.33	0.42
26: S1:811: C: H2'	26: S1:812: A: H8	1.84	0.42
26: S1:977: G: N3	26: S1:977: G: H2'	2.35	0.42
26: S1:2182: G: H2'	26: S1:2183: G: H5'	2.01	0.42
27: S4:64: A: H2'	27: S4:65: G: C8	2.54	0.42
76: h:125: LYS: HA	76: h:125: LYS: HD3	1.80	0.42
85:2:455: U: C2	85:2:482: G: N2	2.87	0.42
85:2:1175: A: H2'	85:2:1176: A: C8	2.55	0.42
85:2:1456: C: H5	85:2:1468: G: H1	1.68	0.42
1:1:220: A: H2'	1:1:221: C: C6	2.55	0.42
9: B:48: VAL: HG12	9: B:81: ALA: HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:51:ALA:HA	13:F:67:GLY:HA2	2.01	0.42
26:S1:552:U:O2'	26:S1:553:U:H5''	2.20	0.42
26:S1:1018:G:H22	26:S1:1034:G:N2	2.18	0.42
26:S1:1367:U:H2'	26:S1:1368:C:C6	2.54	0.42
59:Sg:1:MET:HB3	59:Sg:272:LEU:HD11	2.00	0.42
59:Sg:220:LEU:HD22	59:Sg:230:PHE:CZ	2.54	0.42
70:b:5:LYS:HE2	70:b:8:THR:HB	2.02	0.42
85:2:659:A:H2'	85:2:660:G:H8	1.83	0.42
85:2:748:C:H3'	85:2:749:G:H5''	2.02	0.42
1:1:57:G:OP2	69:a:94:ARG:NH2	2.52	0.42
1:1:458:A:H2'	1:1:459:A:O4'	2.20	0.42
1:1:1761:A:H2'	64:V:128:ARG:NH2	2.34	0.42
22:O:60:ILE:HG12	22:O:80:ALA:HB2	2.00	0.42
26:S1:838:U:H2'	26:S1:839:G:H8	1.84	0.42
26:S1:1368:C:H2'	26:S1:1369:U:C6	2.54	0.42
26:S1:1512:A:H2'	26:S1:1513:C:C6	2.54	0.42
26:S1:1670:G:P	48:SV:67:ARG:HH12	2.35	0.42
26:S1:1792:U:H2'	26:S1:1793:U:C6	2.55	0.42
35:SH:129:PRO:HG3	57:Sd:72:MET:O	2.20	0.42
44:SR:15:ARG:HA	44:SR:15:ARG:HD2	1.88	0.42
47:SU:20:GLU:C	47:SU:22:ALA:H	2.26	0.42
52:SZ:47:ARG:HB3	52:SZ:48:LYS:HZ2	1.85	0.42
71:c:109:GLN:HG3	71:c:140:VAL:HG12	2.02	0.42
1:1:787:A:H2'	1:1:788:A:C8	2.54	0.42
1:1:1777:U:H2'	1:1:1778:G:C8	2.55	0.42
2:3:106:U:H2'	2:3:107:U:C6	2.55	0.42
18:K:16:LEU:O	18:K:21:GLN:HG3	2.19	0.42
26:S1:66:U:H6	34:SG:163:ARG:HH11	1.67	0.42
26:S1:668:A2M:H8	26:S1:668:A2M:H2'	1.91	0.42
26:S1:877:U:O2	32:SE:260:ARG:NH2	2.49	0.42
26:S1:1014:C:H2'	26:S1:1015:G:H8	1.85	0.42
26:S1:1036:G:C2	26:S1:1037:U:C5	3.07	0.42
85:2:459:A:H2'	85:2:460:A:H8	1.81	0.42
7:8:50:G:OP1	22:O:164:ARG:HG3	2.19	0.42
26:S1:1015:G:H22	26:S1:1037:U:H3	1.68	0.42
26:S1:1875:G:H2'	26:S1:1876:U:C6	2.53	0.42
27:S4:68:C:H2'	27:S4:69:G:C8	2.53	0.42
85:2:1323:C:O2'	85:2:1324:U:H5'	2.19	0.42
15:H:209:PRO:O	15:H:213:VAL:HG23	2.20	0.42
26:S1:997:C:O2'	26:S1:998:C:H5'	2.20	0.42
29:SB:39:LYS:HB2	55:Sc:2:GLY:HA3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SB:76:ASP:OD1	29:SB:123:ARG:N	2.53	0.42
31:SD:86:ASP:OD1	31:SD:86:ASP:N	2.46	0.42
31:SD:180:LYS:NZ	31:SD:181:ARG:HE	2.17	0.42
35:SH:81:HIS:ND1	54:Sa:93:SER:OG	2.48	0.42
85:2:527:A2M:H8	85:2:527:A2M:H2'	1.89	0.42
5:6:6:G:H5'	5:6:7:A:OP2	2.19	0.42
21:N:180:GLU:OE1	21:N:180:GLU:N	2.53	0.42
26:S1:230:G:H2'	26:S1:231:A:C8	2.55	0.42
26:S1:1836:G:O6	40:SN:71:TYR:OH	2.25	0.42
28:SA:88:PHE:HB3	28:SA:100:THR:HB	2.01	0.42
35:SH:44:LYS:HD2	35:SH:44:LYS:HA	1.94	0.42
60:Sh:190:LYS:HA	60:Sh:190:LYS:HD2	1.86	0.42
76:h:2:SER:OG	76:h:3:CYS:N	2.42	0.42
85:2:464:G:H2'	85:2:465:A:H8	1.84	0.42
1:1:592:G:H2'	1:1:593:C:C6	2.55	0.41
1:1:720:A:C8	1:1:721:U:H2'	2.55	0.41
1:1:1019:G:H2'	1:1:1020:C:C6	2.55	0.41
1:1:1677:G:H8	1:1:1677:G:OP2	2.03	0.41
3:4:140:G:N1	3:4:149:U:OP1	2.40	0.41
7:8:114:G:H2'	7:8:115:C:C6	2.55	0.41
11:D:168:VAL:HG12	11:D:169:HIS:CE1	2.55	0.41
26:S1:315:A:H5''	26:S1:333:G:N2	2.34	0.41
26:S1:2059:C:H2'	26:S1:2060:C:O4'	2.19	0.41
26:S1:2102:A:H61	26:S1:2121:C:N4	2.16	0.41
29:SB:77:VAL:HG22	29:SB:124:VAL:HB	2.02	0.41
44:SR:52:ASP:O	44:SR:55:ARG:HG2	2.20	0.41
46:ST:100:LYS:O	46:ST:103:GLU:HG2	2.20	0.41
47:SU:42:ASN:HB2	47:SU:65:ASN:HB3	2.02	0.41
53:S:24:VAL:HB	53:S:25:PRO:HD2	2.01	0.41
63:U:87:LYS:HG2	63:U:117:TYR:CE2	2.55	0.41
85:2:1262:G:H2'	85:2:1263:C:H6	1.85	0.41
1:1:306:G:H5''	20:M:14:LYS:HE2	2.02	0.41
2:3:66:C:H2'	2:3:67:A:H8	1.85	0.41
3:4:157:A:H2'	3:4:158:A:H5''	2.02	0.41
5:6:19:C:H2'	5:6:20:A:C8	2.56	0.41
21:N:142:GLU:OE1	21:N:142:GLU:N	2.42	0.41
21:N:160:PRO:HG3	85:2:1292:U:H5''	2.02	0.41
26:S1:691:G:H1	26:S1:754:G:H22	1.68	0.41
26:S1:1890:A:H2'	26:S1:1891:A:O3'	2.20	0.41
28:SA:124:GLU:HG2	28:SA:142:VAL:HG23	2.02	0.41
29:SB:179:TRP:CD1	29:SB:202:VAL:HG12	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Sa:91:LEU:HD21	54:Sa:94:CYS:HB2	2.02	0.41
83:o:67:GLY:HA3	83:o:70:THR:O	2.20	0.41
85:2:349:C:H2'	85:2:350:U:C6	2.56	0.41
1:1:141:U:C1'	1:1:142:G:H5''	2.50	0.41
1:1:1436:G:OP2	68:Z:109:ARG:NH1	2.53	0.41
1:1:1676:G:N1	1:1:1723:A:N6	2.35	0.41
23:P:62:ILE:HG12	23:P:63:SER:H	1.84	0.41
26:S1:1099:C:H2'	26:S1:1100:U:O4'	2.19	0.41
26:S1:1683:A:H2	30:SC:204:PRO:HG2	1.84	0.41
26:S1:1911:U:H5	26:S1:1930:G:H22	1.66	0.41
43:SQ:104:VAL:HG21	43:SQ:111:GLU:HG2	2.02	0.41
77:i:64:LEU:HD13	77:i:94:GLU:HG3	2.01	0.41
1:1:694:U:H2'	1:1:695:OMC:C6	2.55	0.41
1:1:1201:U:H1'	1:1:1202:G:C8	2.55	0.41
2:3:41:A:N6	2:3:187:U:O2	2.50	0.41
3:4:165:C:H5''	9:B:281:THR:HG21	2.03	0.41
26:S1:52:U:H2'	26:S1:53:G:C8	2.55	0.41
26:S1:436:C:H2'	26:S1:437:C:C6	2.55	0.41
26:S1:1276:G:O2'	26:S1:1278:U:O2	2.38	0.41
26:S1:1809:U:H2'	26:S1:1810:G:O4'	2.20	0.41
40:SN:29:ARG:HD2	40:SN:29:ARG:HA	1.85	0.41
58:Se:41:THR:O	58:Se:46:SER:HB3	2.21	0.41
85:2:349:C:H2'	85:2:350:U:H6	1.86	0.41
85:2:749:G:H2'	85:2:750:U:C6	2.54	0.41
85:2:1038:U:H2'	85:2:1039:U:C6	2.55	0.41
1:1:1410:U:H2'	1:1:1411:G:C8	2.55	0.41
5:6:63:A:C6	13:F:108:ARG:HD3	2.55	0.41
11:D:126:GLY:HA3	85:2:1101:A:N1	2.36	0.41
21:N:75:TYR:HD2	21:N:151:ALA:HB2	1.86	0.41
26:S1:328:C:HO2'	26:S1:329:C:H6	1.67	0.41
26:S1:1413:C:H2'	26:S1:1414:A:C8	2.56	0.41
73:e:15:LYS:HE3	73:e:15:LYS:HB2	1.81	0.41
85:2:1452:U:H4'	85:2:1453:U:O5'	2.19	0.41
3:4:19:C:H2'	3:4:20:U:C6	2.56	0.41
7:8:61:C:H2'	7:8:62:A:H8	1.85	0.41
19:L:51:GLY:O	23:P:179:GLU:HA	2.20	0.41
26:S1:2195:G:O2'	82:n:3:THR:HG23	2.19	0.41
32:SE:70:ASP:OD2	32:SE:119:LYS:NZ	2.38	0.41
52:SZ:55:LYS:HE2	52:SZ:55:LYS:HB2	1.89	0.41
65:W:80:ASP:OD1	65:W:81:LYS:N	2.53	0.41
76:h:3:CYS:HA	76:h:4:PRO:HD3	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:2:803:A:H2'	85:2:804:U:O4'	2.20	0.41
85:2:1424:U:H2'	85:2:1425:A:C8	2.52	0.41
26:S1:966:G:H2'	26:S1:967:A:H8	1.84	0.41
26:S1:2174:G:O2'	82:n:2:GLY:O	2.32	0.41
34:SG:14:LYS:HE2	34:SG:16:PHE:CZ	2.55	0.41
44:SR:24:LYS:O	44:SR:56:ARG:HD2	2.21	0.41
52:SZ:58:ASP:O	52:SZ:61:GLN:HG2	2.21	0.41
59:Sg:145:LEU:HD23	59:Sg:145:LEU:HA	1.90	0.41
68:Z:81:THR:O	68:Z:81:THR:OG1	2.37	0.41
83:o:46:ALA:HB1	83:o:58:ASP:HB2	2.03	0.41
1:1:2:C:H5''	6:7:169:A:H2	1.86	0.41
1:1:821:C:O2'	1:1:823:G:N2	2.53	0.41
1:1:1657:G:H2'	1:1:1658:U:C6	2.55	0.41
2:3:117:C:H2'	2:3:118:G:C8	2.56	0.41
8:A:174:ARG:NH2	85:2:426:G:OP1	2.54	0.41
12:E:41:LEU:HD23	12:E:41:LEU:HA	1.85	0.41
29:SB:121:GLN:O	33:SF:50:LYS:NZ	2.54	0.41
30:SC:149:MET:HE2	30:SC:151:PHE:HZ	1.85	0.41
33:SF:198:LYS:HE2	33:SF:198:LYS:HB2	1.92	0.41
39:SM:26:ALA:HB2	39:SM:82:TYR:CZ	2.55	0.41
85:2:1347:U:H2'	85:2:1348:A:O4'	2.20	0.41
1:1:56:G:H2'	1:1:57:G:C8	2.56	0.41
1:1:1145:G:H2'	1:1:1146:A:C8	2.56	0.41
1:1:1676:G:C6	1:1:1723:A:N6	2.85	0.41
3:4:148:C:H5''	81:m:111:ARG:HH12	1.86	0.41
26:S1:1882:A:H2'	26:S1:1883:G:O4'	2.21	0.41
29:SB:30:THR:HG22	29:SB:153:THR:OG1	2.21	0.41
31:SD:89:LYS:HG3	31:SD:94:TYR:CG	2.56	0.41
32:SE:41:LEU:HD23	32:SE:41:LEU:HA	1.86	0.41
33:SF:44:GLU:OE1	33:SF:45:TRP:N	2.53	0.41
36:SI:103:THR:HG23	36:SI:119:LYS:HB3	2.03	0.41
43:SQ:61:MET:HE2	43:SQ:61:MET:HB3	1.93	0.41
59:Sg:49:SER:O	59:Sg:52:SER:N	2.36	0.41
59:Sg:135:ASN:OD1	59:Sg:139:GLU:HG3	2.21	0.41
64:V:72:THR:O	64:V:76:MET:HG2	2.20	0.41
80:l:38:ASN:HB3	80:l:41:ARG:HG2	2.03	0.41
83:o:42:CYS:SG	83:o:43:GLY:N	2.93	0.41
85:2:1510:A:H4'	85:2:1511:U:C5	2.55	0.41
1:1:506:G:OP2	10:C:349:ARG:NH1	2.53	0.41
1:1:517:U:H2'	1:1:518:C:H6	1.86	0.41
1:1:1554:G:N1	1:1:1557:A:OP1	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:72:A:H2'	2:3:73:A:H8	1.86	0.41
26:S1:694:U:H3	26:S1:751:G:H1	1.67	0.41
31:SD:87:GLU:OE1	31:SD:87:GLU:N	2.54	0.41
33:SF:195:VAL:HB	33:SF:196:PRO:HD3	2.02	0.41
60:Sh:186:PHE:O	60:Sh:190:LYS:HB2	2.21	0.41
78:j:4:GLY:O	78:j:8:MET:HG2	2.21	0.41
78:j:39:TYR:CD1	78:j:40:PRO:HA	2.56	0.41
85:2:1089:A:H2'	85:2:1090:G:C8	2.55	0.41
85:2:1195:U:H2'	85:2:1196:G:C8	2.55	0.41
1:1:848:U:H2'	1:1:849:U:C6	2.56	0.40
9:B:56:ILE:HD13	9:B:363:LEU:HD22	2.03	0.40
26:S1:185:A:H4'	26:S1:186:A:H5'	2.02	0.40
26:S1:814:G:N2	26:S1:819:G:O2'	2.49	0.40
26:S1:995:U:O2'	26:S1:996:C:OP1	2.36	0.40
28:SA:125:THR:HB	28:SA:167:ARG:HG3	2.02	0.40
67:Y:23:ALA:HA	67:Y:45:GLY:HA2	2.03	0.40
85:2:965:C:O2	85:2:965:C:H2'	2.21	0.40
1:1:415:A:N3	1:1:417:G:H5''	2.36	0.40
1:1:1044:G:N3	85:2:1064:A:H2'	2.36	0.40
1:1:1489:U:H2'	1:1:1490:G:C8	2.56	0.40
1:1:1722:A:H1'	1:1:1723:A:C8	2.56	0.40
3:4:20:U:H2'	3:4:21:C:C6	2.57	0.40
9:B:19:ARG:HB2	9:B:237:ARG:NH2	2.36	0.40
13:F:99:ALA:N	13:F:100:PRO:HD2	2.34	0.40
26:S1:639:C:H2'	26:S1:640:A:C8	2.56	0.40
26:S1:1692:G:H2'	26:S1:1693:C:H6	1.87	0.40
26:S1:1704:U:H2'	26:S1:1705:C:C6	2.57	0.40
26:S1:2153:A:H4'	82:n:22:LEU:HD21	2.03	0.40
33:SF:88:LEU:HD12	33:SF:88:LEU:HA	1.90	0.40
42:SP:71[A]:ARG:HG2	42:SP:82:ILE:HG12	2.02	0.40
43:SQ:31:ARG:O	43:SQ:35:GLN:HG2	2.21	0.40
68:Z:22:ARG:HB3	74:f:76:PRO:HG2	2.02	0.40
1:1:1565:A:H2'	1:1:1565:A:N3	2.37	0.40
26:S1:1852:C:OP1	45:SS:10:ARG:HB3	2.21	0.40
52:SZ:47:ARG:HG3	52:SZ:62:VAL:HG23	2.03	0.40
65:W:81:LYS:HD3	65:W:81:LYS:HA	1.84	0.40
85:2:689:A:H2'	85:2:690:C:C6	2.56	0.40
2:3:99:U:O2'	2:3:100:U:H5'	2.21	0.40
3:4:124:A:H2'	3:4:125:C:C6	2.57	0.40
4:5:48:G:OP2	4:5:48:G:N2	2.42	0.40
9:B:201:LYS:HE3	9:B:201:LYS:HB3	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:54:SER:HB3	21:N:135:LEU:HD11	2.02	0.40
22:O:40:ASP:HB2	22:O:43:LYS:HD2	2.03	0.40
26:S1:174:A:H5'	34:SG:180:GLN:HG2	2.03	0.40
30:SC:75:ARG:HD3	30:SC:75:ARG:C	2.47	0.40
32:SE:254:LEU:HD23	32:SE:254:LEU:HA	1.87	0.40
46:ST:2:VAL:HG23	46:ST:3:ARG:H	1.86	0.40
73:e:6:MET:HE3	73:e:6:MET:HB3	1.97	0.40
1:1:211:U:O2'	1:1:212:U:OP1	2.40	0.40
1:1:616:U:H4'	1:1:617:G:C5'	2.51	0.40
1:1:931:G:O2'	1:1:932:C:H3'	2.22	0.40
1:1:1393:A:H2'	1:1:1394:U:H5	1.86	0.40
9:B:349:MET:HB3	9:B:349:MET:HE2	1.86	0.40
20:M:121:VAL:HG12	20:M:129:TRP:O	2.21	0.40
25:R:19:GLU:OE1	25:R:19:GLU:N	2.53	0.40
26:S1:29:OMU:H1'	26:S1:29:OMU:HM23	1.79	0.40
26:S1:1108:A:H8	26:S1:1108:A:OP2	2.04	0.40
26:S1:1704:U:H2'	26:S1:1705:C:H6	1.87	0.40
26:S1:1916:G:N2	50:SX:85:TYR:HE2	2.20	0.40
26:S1:2012:A:H2'	26:S1:2013:G:C8	2.56	0.40
28:SA:182:GLN:HB2	28:SA:185:GLU:OE1	2.20	0.40
29:SB:192:ILE:HD12	29:SB:192:ILE:HA	1.96	0.40
51:SY:63:LEU:HD12	51:SY:63:LEU:HA	1.97	0.40
51:SY:83:MET:HE3	51:SY:83:MET:HB2	1.94	0.40
73:e:36:LYS:O	73:e:40:ARG:HG3	2.22	0.40
75:g:61:VAL:HG13	75:g:66:ASP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	A	254/260 (98%)	248 (98%)	6 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	B	402/419 (96%)	397 (99%)	5 (1%)	0	100	100
10	C	364/373 (98%)	353 (97%)	11 (3%)	0	100	100
11	D	156/188 (83%)	145 (93%)	11 (7%)	0	100	100
12	E	184/190 (97%)	176 (96%)	8 (4%)	0	100	100
13	F	144/195 (74%)	135 (94%)	9 (6%)	0	100	100
14	G	222/264 (84%)	218 (98%)	3 (1%)	1 (0%)	24	37
15	H	218/222 (98%)	218 (100%)	0	0	100	100
16	I	206/220 (94%)	202 (98%)	4 (2%)	0	100	100
17	J	135/139 (97%)	135 (100%)	0	0	100	100
18	K	168/175 (96%)	165 (98%)	3 (2%)	0	100	100
19	L	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
20	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
21	N	195/213 (92%)	193 (99%)	2 (1%)	0	100	100
22	O	268/305 (88%)	260 (97%)	8 (3%)	0	100	100
23	P	195/198 (98%)	188 (96%)	7 (4%)	0	100	100
24	Q	188/254 (74%)	185 (98%)	3 (2%)	0	100	100
25	R	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
28	SA	225/264 (85%)	215 (96%)	10 (4%)	0	100	100
29	SB	206/246 (84%)	199 (97%)	7 (3%)	0	100	100
30	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
31	SD	169/190 (89%)	167 (99%)	2 (1%)	0	100	100
32	SE	258/273 (94%)	254 (98%)	4 (2%)	0	100	100
33	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100
34	SG	231/249 (93%)	228 (99%)	3 (1%)	0	100	100
35	SH	178/190 (94%)	175 (98%)	3 (2%)	0	100	100
36	SI	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
37	SK	176/220 (80%)	174 (99%)	2 (1%)	0	100	100
38	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
39	SM	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
40	SN	98/168 (58%)	98 (100%)	0	0	100	100
41	SO	134/144 (93%)	131 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	SP	142/143 (99%)	139 (98%)	3 (2%)	0	100	100
43	SQ	96/141 (68%)	85 (88%)	11 (12%)	0	100	100
44	SR	134/153 (88%)	131 (98%)	3 (2%)	0	100	100
45	SS	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
46	ST	141/151 (93%)	139 (99%)	2 (1%)	0	100	100
47	SU	156/173 (90%)	151 (97%)	5 (3%)	0	100	100
48	SV	75/143 (52%)	73 (97%)	2 (3%)	0	100	100
49	SW	113/152 (74%)	109 (96%)	4 (4%)	0	100	100
50	SX	150/161 (93%)	143 (95%)	7 (5%)	0	100	100
51	SY	83/164 (51%)	81 (98%)	2 (2%)	0	100	100
52	SZ	125/137 (91%)	124 (99%)	1 (1%)	0	100	100
53	S	155/159 (98%)	154 (99%)	1 (1%)	0	100	100
54	Sa	69/120 (58%)	68 (99%)	1 (1%)	0	100	100
55	Sc	70/86 (81%)	70 (100%)	0	0	100	100
56	Sb	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
57	Sd	63/87 (72%)	62 (98%)	1 (2%)	0	100	100
58	Se	50/66 (76%)	48 (96%)	2 (4%)	0	100	100
59	Sg	302/312 (97%)	290 (96%)	12 (4%)	0	100	100
60	Sh	153/235 (65%)	146 (95%)	7 (5%)	0	100	100
61	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
62	T	150/166 (90%)	148 (99%)	2 (1%)	0	100	100
63	U	99/129 (77%)	98 (99%)	1 (1%)	0	100	100
64	V	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
65	W	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
66	X	62/124 (50%)	61 (98%)	1 (2%)	0	100	100
67	Y	130/134 (97%)	129 (99%)	1 (1%)	0	100	100
68	Z	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
69	a	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
70	b	66/70 (94%)	66 (100%)	0	0	100	100
71	c	227/252 (90%)	220 (97%)	7 (3%)	0	100	100
72	d	91/104 (88%)	90 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	e	176/188 (94%)	172 (98%)	4 (2%)	0	100	100
74	f	123/133 (92%)	117 (95%)	6 (5%)	0	100	100
75	g	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
76	h	125/168 (74%)	122 (98%)	3 (2%)	0	100	100
77	i	82/105 (78%)	81 (99%)	1 (1%)	0	100	100
78	j	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
79	k	70/83 (84%)	70 (100%)	0	0	100	100
80	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
81	m	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
82	n	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
83	o	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
84	p	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
All	All	11140/12774 (87%)	10878 (98%)	261 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	G	183	ASP

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	
8	A	186/204 (91%)	186 (100%)	0	100	100
9	B	294/351 (84%)	293 (100%)	1 (0%)	86	93
10	C	250/301 (83%)	249 (100%)	1 (0%)	84	92
11	D	62/162 (38%)	60 (97%)	2 (3%)	34	56
12	E	122/172 (71%)	116 (95%)	6 (5%)	22	39
13	F	94/153 (61%)	93 (99%)	1 (1%)	65	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	G	156/221 (71%)	155 (99%)	1 (1%)	78	89
15	H	155/188 (82%)	154 (99%)	1 (1%)	78	89
16	I	145/183 (79%)	143 (99%)	2 (1%)	59	79
17	J	95/111 (86%)	95 (100%)	0	100	100
18	K	109/145 (75%)	107 (98%)	2 (2%)	51	73
19	L	107/114 (94%)	105 (98%)	2 (2%)	50	71
20	M	172/180 (96%)	170 (99%)	2 (1%)	63	81
21	N	168/179 (94%)	165 (98%)	3 (2%)	51	73
22	O	148/242 (61%)	147 (99%)	1 (1%)	76	88
23	P	152/164 (93%)	151 (99%)	1 (1%)	76	88
24	Q	120/198 (61%)	117 (98%)	3 (2%)	42	64
25	R	144/159 (91%)	144 (100%)	0	100	100
28	SA	198/222 (89%)	191 (96%)	7 (4%)	32	53
29	SB	165/202 (82%)	157 (95%)	8 (5%)	23	40
30	SC	167/184 (91%)	164 (98%)	3 (2%)	51	73
31	SD	148/164 (90%)	145 (98%)	3 (2%)	48	70
32	SE	215/225 (96%)	210 (98%)	5 (2%)	44	66
33	SF	174/208 (84%)	168 (97%)	6 (3%)	32	54
34	SG	186/208 (89%)	180 (97%)	6 (3%)	34	56
35	SH	150/159 (94%)	148 (99%)	2 (1%)	61	80
36	SI	172/186 (92%)	169 (98%)	3 (2%)	53	74
37	SK	139/176 (79%)	135 (97%)	4 (3%)	37	60
38	SL	112/120 (93%)	107 (96%)	5 (4%)	24	42
39	SM	90/104 (86%)	87 (97%)	3 (3%)	33	55
40	SN	84/128 (66%)	79 (94%)	5 (6%)	17	31
41	SO	97/113 (86%)	94 (97%)	3 (3%)	35	57
42	SP	115/117 (98%)	112 (97%)	3 (3%)	40	63
43	SQ	57/120 (48%)	54 (95%)	3 (5%)	20	36
44	SR	112/130 (86%)	112 (100%)	0	100	100
45	SS	45/49 (92%)	44 (98%)	1 (2%)	45	67
46	ST	125/132 (95%)	123 (98%)	2 (2%)	55	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	SU	132/152 (87%)	129 (98%)	3 (2%)	44	66
48	SV	69/126 (55%)	65 (94%)	4 (6%)	18	32
49	SW	93/130 (72%)	92 (99%)	1 (1%)	65	82
50	SX	121/131 (92%)	120 (99%)	1 (1%)	73	86
51	SY	64/116 (55%)	63 (98%)	1 (2%)	55	76
52	SZ	107/118 (91%)	102 (95%)	5 (5%)	23	41
53	S	116/134 (87%)	116 (100%)	0	100	100
54	Sa	63/95 (66%)	62 (98%)	1 (2%)	55	76
55	Sc	62/76 (82%)	61 (98%)	1 (2%)	55	76
56	Sb	85/93 (91%)	83 (98%)	2 (2%)	43	65
57	Sd	46/75 (61%)	44 (96%)	2 (4%)	26	44
58	Se	45/54 (83%)	44 (98%)	1 (2%)	45	67
59	Sg	246/265 (93%)	239 (97%)	7 (3%)	38	60
60	Sh	91/177 (51%)	85 (93%)	6 (7%)	15	26
61	SJ	110/111 (99%)	108 (98%)	2 (2%)	51	73
62	T	125/143 (87%)	123 (98%)	2 (2%)	55	76
63	U	41/114 (36%)	41 (100%)	0	100	100
64	V	93/124 (75%)	91 (98%)	2 (2%)	45	67
65	W	96/122 (79%)	96 (100%)	0	100	100
66	X	56/104 (54%)	54 (96%)	2 (4%)	31	52
67	Y	93/116 (80%)	92 (99%)	1 (1%)	65	82
68	Z	102/118 (86%)	100 (98%)	2 (2%)	48	70
69	a	103/118 (87%)	100 (97%)	3 (3%)	37	60
70	b	56/58 (97%)	56 (100%)	0	100	100
71	c	192/209 (92%)	192 (100%)	0	100	100
72	d	81/89 (91%)	74 (91%)	7 (9%)	10	16
73	e	146/158 (92%)	144 (99%)	2 (1%)	59	79
74	f	106/115 (92%)	105 (99%)	1 (1%)	70	85
75	g	119/121 (98%)	118 (99%)	1 (1%)	73	86
76	h	110/146 (75%)	106 (96%)	4 (4%)	31	52
77	i	64/88 (73%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	j	67/70 (96%)	67 (100%)	0	100	100
79	k	52/74 (70%)	50 (96%)	2 (4%)	29	49
80	l	46/47 (98%)	46 (100%)	0	100	100
81	m	36/113 (32%)	36 (100%)	0	100	100
82	n	30/32 (94%)	29 (97%)	1 (3%)	33	55
83	o	68/74 (92%)	66 (97%)	2 (3%)	37	60
84	p	82/92 (89%)	81 (99%)	1 (1%)	63	81
All	All	8644/10672 (81%)	8473 (98%)	171 (2%)	48	70

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	B	169	ARG
10	C	183	ASN
11	D	16	VAL
11	D	131	VAL
12	E	8	CYS
12	E	25	VAL
12	E	55	THR
12	E	83	VAL
12	E	122	ARG
12	E	175	LEU
13	F	105	VAL
14	G	81	LYS
15	H	155	THR
16	I	116	VAL
16	I	186	VAL
18	K	2	VAL
18	K	56	VAL
19	L	117	VAL
19	L	142	VAL
20	M	60	CYS
20	M	193	ARG
21	N	13	LYS
21	N	138	MET
21	N	207	THR
22	O	52	VAL
23	P	3	VAL
24	Q	55	VAL
24	Q	142	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Q	181	ARG
28	SA	33	VAL
28	SA	37	ASN
28	SA	89	THR
28	SA	121	THR
28	SA	125	THR
28	SA	154	ARG
28	SA	245	GLN
29	SB	17	ASP
29	SB	51	ILE
29	SB	56	MET
29	SB	99	THR
29	SB	102	HIS
29	SB	115	ILE
29	SB	147	VAL
29	SB	191	THR
30	SC	11	ILE
30	SC	136	THR
30	SC	158	LYS
31	SD	98	LEU
31	SD	121	VAL
31	SD	147	VAL
32	SE	63	ARG
32	SE	96	PHE
32	SE	137	VAL
32	SE	167	VAL
32	SE	231	ASN
33	SF	44	GLU
33	SF	68	LEU
33	SF	205	VAL
33	SF	210	THR
33	SF	213	ARG
33	SF	238	THR
34	SG	30	ASP
34	SG	32	ARG
34	SG	153	THR
34	SG	202	VAL
34	SG	209	ARG
34	SG	227	ASP
35	SH	64	PHE
35	SH	161	ASP
36	SI	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	SI	169	LEU
36	SI	197	VAL
37	SK	38	LEU
37	SK	69	SER
37	SK	79	LEU
37	SK	160	ARG
38	SL	29	LYS
38	SL	37	VAL
38	SL	44	GLN
38	SL	75	VAL
38	SL	123	LEU
39	SM	45	VAL
39	SM	59	LYS
39	SM	67	CYS
40	SN	4	TYR
40	SN	32	THR
40	SN	34	THR
40	SN	36	THR
40	SN	60	ASN
41	SO	47	VAL
41	SO	77	ARG
41	SO	106	GLN
42	SP	2	THR
42	SP	55	ILE
42	SP	105	PHE
43	SQ	63	ILE
43	SQ	64	LEU
43	SQ	70	ASP
45	SS	4	LEU
46	ST	3	ARG
46	ST	69	ARG
47	SU	3	VAL
47	SU	101	ILE
47	SU	153	ASN
48	SV	3	LYS
48	SV	9	VAL
48	SV	34	VAL
48	SV	71	LEU
49	SW	76	VAL
50	SX	105	THR
51	SY	55	THR
52	SZ	10	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	SZ	30	VAL
52	SZ	32	VAL
52	SZ	56	VAL
52	SZ	60	SER
54	Sa	104	ILE
55	Sc	45	THR
56	Sb	32	THR
56	Sb	42	VAL
57	Sd	44	VAL
57	Sd	75	LEU
58	Se	46	SER
59	Sg	87	ARG
59	Sg	115	PHE
59	Sg	128	ASP
59	Sg	129	ASN
59	Sg	228	GLN
59	Sg	268	VAL
59	Sg	301	ASN
60	Sh	84	GLN
60	Sh	93	VAL
60	Sh	143	ILE
60	Sh	177	LEU
60	Sh	184	LYS
60	Sh	204	LEU
61	SJ	63	VAL
61	SJ	114	GLU
62	T	13	LYS
62	T	128	ARG
64	V	34	GLN
64	V	60	ILE
66	X	27	LEU
66	X	29	THR
67	Y	99	VAL
68	Z	81	THR
68	Z	99	VAL
69	a	77	ARG
69	a	92	THR
69	a	112	MET
72	d	11	THR
72	d	77	LEU
72	d	89	THR
72	d	90	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	d	94	VAL
72	d	97	VAL
72	d	101	ASP
73	e	52	LYS
73	e	140	VAL
74	f	56	LYS
75	g	33	LEU
76	h	5	ARG
76	h	12	MET
76	h	75	VAL
76	h	116	LEU
79	k	5	ILE
79	k	63	SER
82	n	4	VAL
83	o	41	PHE
83	o	47	PHE
84	p	2	VAL

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

Mol	Chain	Res	Type
8	A	216	HIS
8	A	218	HIS
8	A	221	HIS
9	B	11	HIS
10	C	42	ASN
10	C	64	HIS
11	D	97	ASN
11	D	155	HIS
12	E	162	GLN
15	H	143	GLN
18	K	5	HIS
18	K	21	GLN
18	K	112	GLN
19	L	40	HIS
19	L	62	HIS
19	L	116	GLN
20	M	23	GLN
20	M	112	ASN
20	M	156	HIS
21	N	73	ASN
22	O	31	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Q	134	ASN
24	Q	137	ASN
25	R	122	ASN
28	SA	155	ASN
29	SB	33	GLN
30	SC	77	ASN
31	SD	165	ASN
32	SE	239	GLN
34	SG	15	GLN
36	SI	178	GLN
36	SI	181	HIS
37	SK	52	ASN
37	SK	99	ASN
38	SL	11	GLN
38	SL	80	GLN
39	SM	48	HIS
40	SN	65	GLN
40	SN	88	HIS
42	SP	73	GLN
42	SP	87	ASN
43	SQ	99	GLN
45	SS	38	ASN
46	ST	62	GLN
46	ST	134	GLN
47	SU	24	GLN
47	SU	32	ASN
47	SU	40	HIS
47	SU	104	ASN
47	SU	113	GLN
47	SU	119	HIS
47	SU	125	HIS
49	SW	121	HIS
50	SX	141	HIS
54	Sa	37	GLN
57	Sd	56	ASN
57	Sd	70	ASN
59	Sg	180	ASN
60	Sh	84	GLN
60	Sh	170	GLN
61	SJ	70	ASN
62	T	78	GLN
62	T	97	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	X	63	HIS
67	Y	67	GLN
67	Y	86	ASN
67	Y	130	GLN
68	Z	15	ASN
69	a	31	GLN
71	c	30	GLN
73	e	32	ASN
74	f	21	HIS
74	f	50	GLN
75	g	47	HIS
75	g	60	ASN
75	g	113	ASN
76	h	7	GLN
76	h	19	ASN
76	h	85	HIS
76	h	101	GLN
77	i	26	GLN
78	j	30	GLN
80	l	50	ASN
81	m	90	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1598/1782 (89%)	281 (17%)	16 (1%)
2	3	151/216 (69%)	32 (21%)	4 (2%)
26	S1	1729/2204 (78%)	314 (18%)	12 (0%)
27	S4	18/20 (90%)	6 (33%)	0
3	4	182/183 (99%)	31 (17%)	3 (1%)
4	5	111/135 (82%)	21 (18%)	0
5	6	70/73 (95%)	22 (31%)	2 (2%)
6	7	161/171 (94%)	24 (14%)	0
7	8	118/123 (95%)	8 (6%)	0
85	2	1097/478 (229%)	208 (18%)	13 (1%)
All	All	5235/5385 (97%)	947 (18%)	50 (0%)

All (947) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	24	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	29	C
1	1	38	A
1	1	41	A
1	1	47	C
1	1	58	A
1	1	63	A
1	1	64	A
1	1	65	A
1	1	86	G
1	1	87	A
1	1	91	G
1	1	98	A
1	1	108	G
1	1	110	A
1	1	127	G
1	1	131	U
1	1	132	A
1	1	134	A
1	1	135	A
1	1	136	G
1	1	141	U
1	1	142	G
1	1	153	C
1	1	166	G
1	1	170	U
1	1	175	G
1	1	191	U
1	1	192	C
1	1	199	A
1	1	205	A
1	1	206	A
1	1	211	U
1	1	212	U
1	1	215	U
1	1	218	A
1	1	220	A
1	1	223	A
1	1	224	C
1	1	233	U
1	1	234	G
1	1	237	U
1	1	250	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	251	A
1	1	255	G
1	1	256	U
1	1	258	A
1	1	267	A
1	1	273	A
1	1	280	A
1	1	281	G
1	1	292	A
1	1	306	G
1	1	323	U
1	1	332	A
1	1	335	U
1	1	343	U
1	1	349	U
1	1	361	A
1	1	367	A
1	1	368	G
1	1	369	A
1	1	373	G
1	1	374	G
1	1	383	U
1	1	390	C
1	1	391	A
1	1	392	A
1	1	407	A2M
1	1	409	U
1	1	410	U
1	1	417	G
1	1	423	U
1	1	440	A
1	1	443	A
1	1	461	G
1	1	463	C
1	1	464	A
1	1	469	A
1	1	477	C
1	1	484	A
1	1	485	A
1	1	488	G
1	1	502	U
1	1	506	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	511	A
1	1	512	U
1	1	513	C
1	1	521	G
1	1	525	C
1	1	526	A
1	1	527	A
1	1	528	A
1	1	533	G
1	1	542	C
1	1	543	G
1	1	546	G
1	1	547	U
1	1	548	G
1	1	551	A
1	1	553	A
1	1	554	A
1	1	555	U
1	1	561	G
1	1	562	U
1	1	563	C
1	1	572	A
1	1	575	A
1	1	577	C
1	1	606	C
1	1	609	C
1	1	611	C
1	1	616	U
1	1	617	G
1	1	621	U
1	1	632	A
1	1	635	C
1	1	641	G
1	1	648	A
1	1	649	U
1	1	668	C
1	1	678	A2M
1	1	679	A
1	1	681	A2M
1	1	692	A
1	1	709	A
1	1	713	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	721	U
1	1	729	A
1	1	750	G
1	1	753	A
1	1	754	G
1	1	763	U
1	1	767	U
1	1	769	U
1	1	771	U
1	1	778	C
1	1	792	G
1	1	797	A
1	1	798	U
1	1	803	C
1	1	821	C
1	1	822	C
1	1	825	G
1	1	832	G
1	1	835	G
1	1	836	G
1	1	838	G
1	1	850	G
1	1	868	A
1	1	899	A
1	1	912	C
1	1	925	U
1	1	930	U
1	1	931	G
1	1	958	G
1	1	965	A
1	1	967	G
1	1	968	A
1	1	972	A
1	1	975	G
1	1	985	G
1	1	988	G
1	1	995	C
1	1	997	C
1	1	1010	OMC
1	1	1011	PSU
1	1	1031	A
1	1	1045	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1089	C
1	1	1091	A
1	1	1092	U
1	1	1094	C
1	1	1095	U
1	1	1097	A
1	1	1098	A
1	1	1100	C
1	1	1105	A
1	1	1107	OMU
1	1	1128	A
1	1	1129	G
1	1	1135	U
1	1	1136	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	1165	A
1	1	1174	G
1	1	1179	C
1	1	1181	PSU
1	1	1188	G
1	1	1210	A
1	1	1216	U
1	1	1235	A
1	1	1238	C
1	1	1239	U
1	1	1240	U
1	1	1242	U
1	1	1243	G
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	1277	G
1	1	1279	A
1	1	1353	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1355	C
1	1	1356	G
1	1	1357	G
1	1	1369	G
1	1	1371	OMU
1	1	1375	G
1	1	1378	U
1	1	1379	A
1	1	1389	A
1	1	1390	G
1	1	1392	G
1	1	1393	A
1	1	1394	U
1	1	1395	U
1	1	1401	U
1	1	1413	U
1	1	1420	G
1	1	1422	A
1	1	1426	A
1	1	1427	A
1	1	1434	G
1	1	1438	A
1	1	1443	U
1	1	1445	G
1	1	1464	G
1	1	1476	A
1	1	1481	G
1	1	1490	G
1	1	1504	A
1	1	1509	C
1	1	1524	OMG
1	1	1527	OMC
1	1	1536	C
1	1	1540	OMG
1	1	1545	G
1	1	1557	A
1	1	1560	U
1	1	1561	A
1	1	1565	A
1	1	1566	A
1	1	1569	U
1	1	1586	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1589	C
1	1	1590	G
1	1	1612	G
1	1	1613	C
1	1	1625	A
1	1	1654	A
1	1	1655	U
1	1	1661	U
1	1	1662	G
1	1	1663	U
1	1	1666	G
1	1	1667	G
1	1	1670	A
1	1	1672	U
1	1	1673	G
1	1	1675	A
1	1	1676	G
1	1	1677	G
1	1	1727	A
1	1	1729	A
1	1	1730	A
1	1	1738	C
1	1	1739	A
1	1	1744	A
1	1	1751	A
1	1	1753	U
1	1	1762	A
1	1	1766	G
2	3	34	C
2	3	35	A
2	3	36	A
2	3	41	A
2	3	52	G
2	3	72	A
2	3	76	C
2	3	99	U
2	3	100	U
2	3	101	G
2	3	108	U
2	3	109	U
2	3	110	U
2	3	111	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	3	112	C
2	3	116	U
2	3	124	U
2	3	125	U
2	3	126	C
2	3	146	G
2	3	149	A
2	3	150	A
2	3	151	A
2	3	180	U
2	3	181	G
2	3	183	G
2	3	187	U
2	3	188	C
2	3	192	G
2	3	193	C
2	3	201	C
2	3	202	A
3	4	5	G
3	4	9	G
3	4	11	G
3	4	12	A
3	4	15	G
3	4	24	A
3	4	25	G
3	4	40	G
3	4	50	G
3	4	51	U
3	4	58	G
3	4	85	C
3	4	86	U
3	4	87	G
3	4	102	G
3	4	114	A
3	4	120	U
3	4	121	C
3	4	127	G
3	4	141	A
3	4	143	C
3	4	144	G
3	4	148	C
3	4	149	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	4	150	A
3	4	157	A
3	4	158	A
3	4	159	G
3	4	168	A
3	4	171	A
3	4	173	C
4	5	5	G
4	5	14	C
4	5	23	G
4	5	27	A
4	5	28	U
4	5	38	G
4	5	49	C
4	5	50	A
4	5	51	U
4	5	52	G
4	5	62	G
4	5	63	G
4	5	64	U
4	5	67	G
4	5	86	G
4	5	87	U
4	5	99	G
4	5	106	G
4	5	109	G
4	5	113	G
4	5	125	U
5	6	7	A
5	6	11	G
5	6	12	C
5	6	13	C
5	6	15	C
5	6	24	C
5	6	25	U
5	6	26	G
5	6	30	C
5	6	32	U
5	6	33	G
5	6	40	C
5	6	42	A
5	6	52	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	6	53	U
5	6	54	A
5	6	55	U
5	6	60	A
5	6	64	U
5	6	67	C
5	6	68	A
5	6	69	A
6	7	22	U
6	7	48	A
6	7	52	A
6	7	59	A
6	7	62	A
6	7	63	G
6	7	75	OMG
6	7	84	U
6	7	85	U
6	7	87	A
6	7	88	A
6	7	90	U
6	7	94	G
6	7	103	A
6	7	105	C
6	7	110	A
6	7	120	G
6	7	124	A
6	7	125	A
6	7	126	G
6	7	135	U
6	7	136	G
6	7	157	U
6	7	158	U
7	8	11	G
7	8	22	A
7	8	46	A
7	8	67	C
7	8	68	A
7	8	95	U
7	8	104	A
7	8	114	G
26	S1	3	U
26	S1	4	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	17	C
26	S1	26	A
26	S1	33	PSU
26	S1	34	G
26	S1	42	G
26	S1	45	U
26	S1	47	A
26	S1	65	A
26	S1	73	A
26	S1	98	A2M
26	S1	102	A
26	S1	103	A
26	S1	104	PSU
26	S1	112	A
26	S1	114	U
26	S1	117	G
26	S1	128	C
26	S1	145	A
26	S1	146	U
26	S1	150	A
26	S1	151	U
26	S1	152	A
26	S1	158	G
26	S1	164	C
26	S1	165	G
26	S1	171	C
26	S1	173	A
26	S1	174	A
26	S1	176	A
26	S1	181	A
26	S1	184	C
26	S1	193	G
26	S1	197	U
26	S1	198	C
26	S1	235	C
26	S1	249	A
26	S1	252	G
26	S1	253	U
26	S1	257	A
26	S1	275	A
26	S1	278	A
26	S1	281	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	282	C
26	S1	284	C
26	S1	286	G
26	S1	288	A
26	S1	313	G
26	S1	316	A
26	S1	320	G
26	S1	329	C
26	S1	356	A
26	S1	358	C
26	S1	360	G
26	S1	364	G
26	S1	381	G
26	S1	382	A
26	S1	404	C
26	S1	413	A
26	S1	443	A
26	S1	444	A
26	S1	445	U
26	S1	447	G
26	S1	462	G
26	S1	467	C
26	S1	469	G
26	S1	473	G
26	S1	477	G
26	S1	479	A2M
26	S1	480	A
26	S1	481	A
26	S1	482	U
26	S1	483	U
26	S1	487	C
26	S1	488	A
26	S1	495	A
26	S1	499	A
26	S1	501	A
26	S1	503	C
26	S1	516	A
26	S1	523	A
26	S1	553	U
26	S1	554	U
26	S1	556	A
26	S1	580	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	581	A
26	S1	585	C
26	S1	588	G
26	S1	591	A
26	S1	600	OMG
26	S1	606	G
26	S1	614	C
26	S1	628	A
26	S1	631	U
26	S1	636	C
26	S1	643	A
26	S1	660	U
26	S1	668	A2M
26	S1	669	A
26	S1	671	G
26	S1	672	G
26	S1	673	G
26	S1	688	G
26	S1	689	U
26	S1	693	C
26	S1	694	U
26	S1	747	C
26	S1	754	G
26	S1	757	C
26	S1	758	G
26	S1	771	G
26	S1	773	A
26	S1	774	A
26	S1	782	C
26	S1	787	G
26	S1	788	A
26	S1	789	G
26	S1	790	U
26	S1	791	G
26	S1	792	G
26	S1	793	G
26	S1	810	G
26	S1	811	C
26	S1	814	G
26	S1	815	U
26	S1	816	C
26	S1	819	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	820	C
26	S1	821	A
26	S1	823	G
26	S1	835	C
26	S1	843	U
26	S1	856	A
26	S1	866	G
26	S1	867	A
26	S1	875	A
26	S1	876	G
26	S1	879	A
26	S1	883	G
26	S1	884	A
26	S1	886	U
26	S1	887	U
26	S1	895	A
26	S1	916	G
26	S1	917	C
26	S1	954	A
26	S1	955	A
26	S1	956	A
26	S1	957	G
26	S1	974	G
26	S1	977	G
26	S1	978	C
26	S1	982	G
26	S1	990	U
26	S1	992	C
26	S1	993	U
26	S1	994	U
26	S1	996	C
26	S1	997	C
26	S1	998	C
26	S1	999	A
26	S1	1015	G
26	S1	1098	U
26	S1	1101	A
26	S1	1102	G
26	S1	1105	A
26	S1	1109	A
26	S1	1119	U
26	S1	1123	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	1130	A
26	S1	1133	U
26	S1	1139	G
26	S1	1142	G
26	S1	1155	U
26	S1	1168	C
26	S1	1180	A
26	S1	1181	C
26	S1	1182	A
26	S1	1199	A
26	S1	1207	U
26	S1	1213	A
26	S1	1235	A
26	S1	1239	A
26	S1	1245	A
26	S1	1252	A
26	S1	1273	A
26	S1	1275	C
26	S1	1290	A
26	S1	1414	A
26	S1	1443	U
26	S1	1444	G
26	S1	1449	U
26	S1	1452	A
26	S1	1466	G
26	S1	1490	A
26	S1	1502	G
26	S1	1503	A
26	S1	1510	C
26	S1	1537	U
26	S1	1542	C
26	S1	1543	C4J
26	S1	1544	5MC
26	S1	1546	A
26	S1	1548	A
26	S1	1551	G
26	S1	1552	G
26	S1	1554	A
26	S1	1566	PSU
26	S1	1569	G
26	S1	1570	G
26	S1	1573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	1580	G
26	S1	1582	A
26	S1	1583	U
26	S1	1595	G
26	S1	1597	G
26	S1	1598	U
26	S1	1602	U
26	S1	1603	U
26	S1	1608	A
26	S1	1613	C
26	S1	1616	A
26	S1	1625	G
26	S1	1637	A
26	S1	1638	U
26	S1	1643	G
26	S1	1651	G
26	S1	1653	U
26	S1	1658	U
26	S1	1659	U
26	S1	1666	U
26	S1	1667	U
26	S1	1673	A
26	S1	1674	A
26	S1	1677	G
26	S1	1699	A
26	S1	1706	A
26	S1	1712	G
26	S1	1713	C
26	S1	1719	G
26	S1	1725	C
26	S1	1762	A
26	S1	1773	U
26	S1	1774	U
26	S1	1782	G
26	S1	1788	U
26	S1	1789	U
26	S1	1796	U
26	S1	1797	A
26	S1	1807	G
26	S1	1816	U
26	S1	1822	A
26	S1	1825	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	1826	G
26	S1	1828	A
26	S1	1829	OMG
26	S1	1833	OMU
26	S1	1836	G
26	S1	1846	A
26	S1	1847	A
26	S1	1848	U
26	S1	1849	G
26	S1	1861	A
26	S1	1872	A
26	S1	1890	A
26	S1	1891	A
26	S1	1919	C
26	S1	1921	A
26	S1	1924	G
26	S1	1932	A
26	S1	1933	A
26	S1	1939	G
26	S1	1944	C
26	S1	1948	U
26	S1	1949	A
26	S1	1950	G
26	S1	1955	A
26	S1	1956	C
26	S1	1976	U
26	S1	1977	U
26	S1	1978	A
26	S1	1988	C
26	S1	1989	A
26	S1	2004	G
26	S1	2010	G
26	S1	2021	A2M
26	S1	2039	C
26	S1	2054	C
26	S1	2055	A
26	S1	2063	U
26	S1	2086	A
26	S1	2097	C
26	S1	2100	A
26	S1	2102	A
26	S1	2119	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	S1	2120	C
26	S1	2122	G
26	S1	2140	OMC
26	S1	2159	A
26	S1	2163	G
26	S1	2165	A
26	S1	2169	A
26	S1	2170	G
26	S1	2172	U
26	S1	2183	G
26	S1	2185	MA6
26	S1	2186	C
26	S1	2195	G
26	S1	2196	G
26	S1	2197	G
26	S1	2198	A
26	S1	2199	C
26	S1	2202	PSU
27	S4	4	C
27	S4	5	G
27	S4	64	A
27	S4	70	C
27	S4	73	A
27	S4	76	A
85	2	5	A
85	2	6	A
85	2	7	C
85	2	22	A
85	2	25	A
85	2	29	C
85	2	33	A
85	2	62	A
85	2	63	U
85	2	68	A
85	2	69	A
85	2	75	C
85	2	90	G
85	2	91	C
85	2	136	A
85	2	340	A
85	2	344	G
85	2	363	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	2	368	G
85	2	377	A
85	2	386	U
85	2	388	A
85	2	404	A
85	2	415	U
85	2	443	OMC
85	2	444	A
85	2	450	C
85	2	452	G
85	2	453	A
85	2	454	A
85	2	455	U
85	2	457	U
85	2	460	A
85	2	469	G
85	2	490	A
85	2	495	G
85	2	498	A
85	2	502	A
85	2	503	C
85	2	505	A
85	2	508	A
85	2	518	G
85	2	519	G
85	2	527	A2M
85	2	528	U
85	2	529	G
85	2	530	C
85	2	534	OMG
85	2	544	U
85	2	552	C
85	2	553	G
85	2	554	C
85	2	556	U
85	2	559	A
85	2	561	G
85	2	570	A2M
85	2	571	G
85	2	580	U
85	2	582	U
85	2	602	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	2	618	A
85	2	619	A
85	2	620	C
85	2	621	G
85	2	639	G
85	2	643	A
85	2	647	A
85	2	648	A
85	2	649	G
85	2	650	A
85	2	657	U
85	2	658	G
85	2	675	G
85	2	681	G
85	2	685	G
85	2	749	G
85	2	750	U
85	2	751	U
85	2	752	G
85	2	753	C
85	2	754	U
85	2	755	U
85	2	756	C
85	2	760	U
85	2	761	A
85	2	768	G
85	2	769	A
85	2	777	A
85	2	778	A
85	2	779	U
85	2	780	G
85	2	783	U
85	2	784	U
85	2	797	C
85	2	799	G
85	2	805	G
85	2	810	G
85	2	811	U
85	2	812	C
85	2	950	G
85	2	955	C
85	2	957	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	2	958	A
85	2	959	A
85	2	960	C
85	2	964	G
85	2	965	C
85	2	966	U
85	2	970	A
85	2	979	A
85	2	980	A
85	2	999	U
85	2	1000	U
85	2	1001	C
85	2	1010	U
85	2	1011	G
85	2	1012	U
85	2	1017	A
85	2	1019	A
85	2	1023	C
85	2	1033	G
85	2	1034	G
85	2	1041	G
85	2	1045	G
85	2	1046	OMG
85	2	1053	A
85	2	1055	A
85	2	1064	A
85	2	1075	G
85	2	1079	U
85	2	1083	A
85	2	1093	C
85	2	1099	G
85	2	1116	A
85	2	1118	A
85	2	1120	C
85	2	1123	A
85	2	1131	A
85	2	1132	A
85	2	1141	G
85	2	1146	A
85	2	1147	C
85	2	1156	G
85	2	1181	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	2	1189	A
85	2	1198	G
85	2	1199	A
85	2	1200	A
85	2	1201	G
85	2	1202	A
85	2	1203	A
85	2	1204	U
85	2	1207	G
85	2	1215	A
85	2	1237	A
85	2	1238	G
85	2	1239	A
85	2	1241	U
85	2	1248	OMC
85	2	1252	G
85	2	1255	A
85	2	1271	G
85	2	1276	A
85	2	1280	U
85	2	1281	U
85	2	1283	A
85	2	1294	G
85	2	1309	G
85	2	1314	C
85	2	1325	A
85	2	1332	C
85	2	1335	C
85	2	1336	G
85	2	1337	C
85	2	1344	C
85	2	1368	A
85	2	1373	C
85	2	1374	A
85	2	1379	A
85	2	1380	C
85	2	1381	G
85	2	1385	G
85	2	1409	A
85	2	1416	U
85	2	1421	C
85	2	1428	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	2	1433	G
85	2	1436	A
85	2	1438	U
85	2	1441	C
85	2	1443	A
85	2	1448	A
85	2	1452	U
85	2	1453	U
85	2	1454	A
85	2	1456	C
85	2	1463	A
85	2	1470	C
85	2	1502	G
85	2	1503	G
85	2	1504	U
85	2	1505	A
85	2	1510	A
85	2	1511	U
85	2	1512	G
85	2	1513	G
85	2	1514	U
85	2	1516	C

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	141	U
1	1	191	U
1	1	210	G
1	1	422	PSU
1	1	468	G
1	1	546	G
1	1	547	U
1	1	605	G
1	1	616	U
1	1	967	G
1	1	1011	PSU
1	1	1094	C
1	1	1096	C
1	1	1134	C
1	1	1135	U
1	1	1394	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	3	98	C
2	3	150	A
2	3	180	U
2	3	192	G
3	4	11	G
3	4	50	G
3	4	157	A
5	6	24	C
5	6	51	A
26	S1	72	C
26	S1	234	C
26	S1	252	G
26	S1	277	U
26	S1	494	A
26	S1	746	C
26	S1	770	A
26	S1	790	U
26	S1	916	G
26	S1	992	C
26	S1	995	U
26	S1	1672	C
85	2	68	A
85	2	443	OMC
85	2	454	A
85	2	646	G
85	2	749	G
85	2	750	U
85	2	783	U
85	2	1022	U
85	2	1092	U
85	2	1293	C
85	2	1334	C
85	2	1343	A
85	2	1452	U

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

105 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$
85	OMC	2	359	85	19,22,23	3.00	8 (42%)	25,31,34	0.70	0
1	PSU	1	1011	1	18,21,22	4.61	9 (50%)	21,30,33	1.91	6 (28%)
6	PSU	7	74	6	18,21,22	4.62	7 (38%)	21,30,33	1.95	5 (23%)
26	PSU	S1	1533	26	18,21,22	4.59	7 (38%)	21,30,33	1.89	5 (23%)
1	A2M	1	305	1	22,25,26	3.51	9 (40%)	30,36,39	2.45	11 (36%)
26	PSU	S1	1192	26	18,21,22	4.50	8 (44%)	21,30,33	1.86	5 (23%)
1	OMC	1	1010	86,1,88	19,22,23	2.96	8 (42%)	25,31,34	0.85	0
1	A2M	1	1539	86,85,1	22,25,26	3.55	9 (40%)	30,36,39	2.26	11 (36%)
26	PSU	S1	104	26	18,21,22	4.53	7 (38%)	21,30,33	1.89	5 (23%)
1	PSU	1	239	1	18,21,22	4.63	7 (38%)	21,30,33	1.95	5 (23%)
26	MA6	S1	2184	26	23,26,27	1.54	5 (21%)	33,38,41	2.89	12 (36%)
26	PSU	S1	33	26	18,21,22	4.59	8 (44%)	21,30,33	1.90	4 (19%)
1	OMU	1	845	1	19,22,23	3.01	8 (42%)	25,31,34	2.16	6 (24%)
6	A2M	7	162	1,6	22,25,26	3.55	9 (40%)	30,36,39	2.38	11 (36%)
26	OMG	S1	1829	86,26	23,26,27	2.40	9 (39%)	32,38,41	2.60	10 (31%)
1	PSU	1	940	1	18,21,22	4.61	7 (38%)	21,30,33	1.97	5 (23%)
1	PSU	1	422	1	18,21,22	4.64	7 (38%)	21,30,33	1.99	5 (23%)
26	PSU	S1	1156	26	18,21,22	4.51	7 (38%)	21,30,33	2.00	5 (23%)
26	OMG	S1	1623	26	23,26,27	2.41	9 (39%)	32,38,41	2.66	10 (31%)
85	OMU	2	56	85,1	19,22,23	3.03	8 (42%)	25,31,34	1.87	4 (16%)
26	OMU	S1	8	26	19,22,23	2.91	8 (42%)	25,31,34	1.94	5 (20%)
1	OMG	1	959[B]	1	23,26,27	2.44	8 (34%)	32,38,41	2.41	9 (28%)
85	OMG	2	71	86,85	23,26,27	2.42	9 (39%)	32,38,41	2.53	11 (34%)
26	PSU	S1	1539	26	18,21,22	4.57	7 (38%)	21,30,33	1.93	5 (23%)
26	C4J	S1	1543	26	25,29,30	2.87	9 (36%)	28,42,45	1.46	4 (14%)
1	PSU	1	1039	1	18,21,22	4.61	7 (38%)	21,30,33	2.01	5 (23%)
26	5MC	S1	1544	26	19,22,23	3.70	8 (42%)	26,32,35	1.05	1 (3%)
85	A2M	2	95	85	22,25,26	3.53	9 (40%)	30,36,39	2.31	11 (36%)
26	OMU	S1	1621	86,26	19,22,23	3.04	8 (42%)	25,31,34	1.83	5 (20%)
26	MA6	S1	2185	26	23,26,27	1.56	5 (21%)	33,38,41	2.91	13 (39%)
1	PSU	1	1528	1	18,21,22	4.61	7 (38%)	21,30,33	1.97	6 (28%)
1	A2M	1	955	1	22,25,26	3.56	9 (40%)	30,36,39	2.31	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	A2M	2	382	85	22,25,26	3.52	9 (40%)	30,36,39	2.33	11 (36%)
26	OMC	S1	18	26	19,22,23	2.82	8 (42%)	25,31,34	0.78	0
6	PSU	7	69	6	18,21,22	4.61	9 (50%)	21,30,33	1.89	5 (23%)
1	A2M	1	858	1	22,25,26	3.46	9 (40%)	30,36,39	2.45	12 (40%)
1	A2M	1	407	1	22,25,26	3.57	9 (40%)	30,36,39	2.41	13 (43%)
2	OMU	3	13	2	19,22,23	3.04	8 (42%)	25,31,34	1.84	5 (20%)
26	OMG	S1	1478	26	23,26,27	2.36	9 (39%)	32,38,41	2.48	11 (34%)
26	OMC	S1	2140	26	19,22,23	2.95	8 (42%)	25,31,34	0.87	1 (4%)
85	OMU	2	73	85	19,22,23	3.01	8 (42%)	25,31,34	1.80	5 (20%)
85	PSU	2	78	85	18,21,22	4.58	7 (38%)	21,30,33	1.99	5 (23%)
85	PSU	2	472	85	18,21,22	4.62	7 (38%)	21,30,33	2.01	5 (23%)
1	A2M	1	235	1	22,25,26	3.54	9 (40%)	30,36,39	2.32	10 (33%)
26	OMG	S1	2151	26	23,26,27	2.40	9 (39%)	32,38,41	2.57	10 (31%)
1	A2M	1	681	1	22,25,26	3.50	9 (40%)	30,36,39	2.39	11 (36%)
6	OMG	7	75	6	23,26,27	2.42	9 (39%)	32,38,41	2.56	10 (31%)
26	A2M	S1	2021	26	22,25,26	3.44	9 (40%)	30,36,39	2.42	11 (36%)
1	OMG	1	959[A]	1	23,26,27	2.45	9 (39%)	32,38,41	2.63	12 (37%)
26	PSU	S1	609	26	18,21,22	4.59	7 (38%)	21,30,33	2.04	5 (23%)
26	PSU	S1	2202	26	18,21,22	4.44	8 (44%)	21,30,33	1.79	4 (19%)
26	OMU	S1	1979	26	19,22,23	3.03	8 (42%)	25,31,34	1.84	5 (20%)
1	PSU	1	1017	86,1	18,21,22	4.53	7 (38%)	21,30,33	1.98	5 (23%)
26	PSU	S1	12	26	18,21,22	4.41	7 (38%)	21,30,33	1.97	5 (23%)
3	OMG	4	74	3	23,26,27	2.39	9 (39%)	32,38,41	2.53	11 (34%)
26	OMU	S1	29	86,26	19,22,23	2.98	8 (42%)	25,31,34	1.90	5 (20%)
1	A2M	1	697	1	22,25,26	3.50	9 (40%)	30,36,39	2.33	12 (40%)
26	OMU	S1	661	26	19,22,23	2.93	8 (42%)	25,31,34	1.89	5 (20%)
26	OMC	S1	38	26	19,22,23	2.89	8 (42%)	25,31,34	0.80	0
1	OMG	1	1524	1	23,26,27	2.42	9 (39%)	32,38,41	2.58	10 (31%)
26	PSU	S1	1246	86,26	18,21,22	4.49	7 (38%)	21,30,33	2.07	5 (23%)
1	OMC	1	695	1	19,22,23	2.95	8 (42%)	25,31,34	0.71	0
26	A2M	S1	479	26	22,25,26	3.51	9 (40%)	30,36,39	2.33	13 (43%)
1	OMU	1	1371	1	19,22,23	3.09	8 (42%)	25,31,34	1.98	6 (24%)
26	OMG	S1	600	26	23,26,27	2.40	9 (39%)	32,38,41	2.63	10 (31%)
26	PSU	S1	455	26	18,21,22	4.55	7 (38%)	21,30,33	2.05	5 (23%)
6	A2M	7	43	6	22,25,26	3.53	9 (40%)	30,36,39	2.33	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OMC	2	443	85,87	19,22,23	2.95	8 (42%)	25,31,34	0.83	0
26	PSU	S1	2048	26	18,21,22	4.40	7 (38%)	21,30,33	2.00	5 (23%)
1	PSU	1	1664	1	18,21,22	4.61	7 (38%)	21,30,33	1.99	6 (28%)
26	7MG	S1	1995	26	23,26,27	3.81	10 (43%)	27,39,42	2.19	9 (33%)
1	PSU	1	1402	1	18,21,22	4.57	7 (38%)	21,30,33	1.82	4 (19%)
1	OMU	1	1107	1	19,22,23	3.03	8 (42%)	25,31,34	1.87	5 (20%)
1	PSU	1	672	86,1	18,21,22	4.56	7 (38%)	21,30,33	2.00	6 (28%)
1	OMG	1	1626	1	23,26,27	2.42	9 (39%)	32,38,41	2.54	11 (34%)
1	1MA	1	677	86,1	21,25,26	2.96	5 (23%)	30,37,40	3.01	7 (23%)
26	PSU	S1	2046	26	18,21,22	4.46	7 (38%)	21,30,33	2.06	5 (23%)
1	PSU	1	1171	86,1	18,21,22	4.60	7 (38%)	21,30,33	1.98	6 (28%)
26	A2M	S1	98	86,26	22,25,26	3.56	9 (40%)	30,36,39	2.29	11 (36%)
85	PSU	2	437	85	18,21,22	4.55	7 (38%)	21,30,33	1.98	5 (23%)
26	OMG	S1	1550	26	23,26,27	2.42	9 (39%)	32,38,41	2.64	10 (31%)
26	PSU	S1	1657	26	18,21,22	4.49	7 (38%)	21,30,33	1.95	5 (23%)
1	PSU	1	870	1	18,21,22	4.58	7 (38%)	21,30,33	2.00	5 (23%)
1	OMG	1	1190	86,1	23,26,27	2.39	9 (39%)	32,38,41	2.48	13 (40%)
26	OMU	S1	1833	86,26	19,22,23	3.04	8 (42%)	25,31,34	1.88	5 (20%)
1	A2M	1	927	1	22,25,26	3.51	9 (40%)	30,36,39	2.36	11 (36%)
26	PSU	S1	1841	87,26	18,21,22	4.53	7 (38%)	21,30,33	2.09	5 (23%)
26	A2M	S1	668	86,26	22,25,26	3.48	9 (40%)	30,36,39	2.45	12 (40%)
1	OMU	1	1659	86,1	19,22,23	3.02	8 (42%)	25,31,34	1.84	5 (20%)
26	A2M	S1	512	86,26	22,25,26	3.55	9 (40%)	30,36,39	2.33	12 (40%)
26	OMG	S1	1647	26	23,26,27	2.37	8 (34%)	32,38,41	2.57	11 (34%)
1	PSU	1	1181	1	18,21,22	4.60	8 (44%)	21,30,33	1.87	5 (23%)
1	OMG	1	1540	85,1	23,26,27	2.37	9 (39%)	32,38,41	2.51	11 (34%)
6	OMU	7	7	1,6	19,22,23	3.02	8 (42%)	25,31,34	1.82	5 (20%)
26	PSU	S1	607	26	18,21,22	4.71	7 (38%)	21,30,33	1.88	6 (28%)
26	5MC	S1	2061	26	19,22,23	3.57	8 (42%)	26,32,35	0.98	2 (7%)
1	OMU	1	847	1	19,22,23	2.99	8 (42%)	25,31,34	1.87	5 (20%)
26	PSU	S1	1566	86,26	18,21,22	4.60	8 (44%)	21,30,33	1.85	4 (19%)
1	PSU	1	1533	85,1	18,21,22	4.60	7 (38%)	21,30,33	2.07	6 (28%)
26	OMC	S1	1866	26	19,22,23	2.91	8 (42%)	25,31,34	0.75	0
1	A2M	1	678	85,1	22,25,26	3.43	9 (40%)	30,36,39	3.11	16 (53%)
1	OMC	1	1527	1	19,22,23	2.95	8 (42%)	25,31,34	1.02	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1	856	1	23,26,27	2.39	9 (39%)	32,38,41	2.54	10 (31%)
26	OMG	S1	1865	26	23,26,27	2.39	9 (39%)	32,38,41	2.53	10 (31%)
26	OMG	S1	1879	26	23,26,27	2.41	9 (39%)	32,38,41	2.62	10 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OMC	2	359	85	-	0/9/27/28	0/2/2/2
1	PSU	1	1011	1	-	0/7/25/26	0/2/2/2
6	PSU	7	74	6	-	2/7/25/26	0/2/2/2
26	PSU	S1	1533	26	-	2/7/25/26	0/2/2/2
1	A2M	1	305	1	-	2/9/27/28	0/3/3/3
26	PSU	S1	1192	26	-	0/7/25/26	0/2/2/2
1	OMC	1	1010	86,1,88	-	1/9/27/28	0/2/2/2
1	A2M	1	1539	86,85,1	-	0/9/27/28	0/3/3/3
26	PSU	S1	104	26	-	2/7/25/26	0/2/2/2
1	PSU	1	239	1	-	0/7/25/26	0/2/2/2
26	MA6	S1	2184	26	-	0/11/29/30	0/3/3/3
26	PSU	S1	33	26	-	2/7/25/26	0/2/2/2
1	OMU	1	845	1	-	3/9/27/28	0/2/2/2
6	A2M	7	162	1,6	-	1/9/27/28	0/3/3/3
26	OMG	S1	1829	86,26	-	0/9/27/28	0/3/3/3
1	PSU	1	940	1	-	0/7/25/26	0/2/2/2
1	PSU	1	422	1	-	0/7/25/26	0/2/2/2
26	PSU	S1	1156	26	-	0/7/25/26	0/2/2/2
26	OMG	S1	1623	26	-	2/9/27/28	0/3/3/3
85	OMU	2	56	85,1	-	0/9/27/28	0/2/2/2
26	OMU	S1	8	26	-	5/9/27/28	0/2/2/2
1	OMG	1	959[B]	1	-	0/9/27/28	0/3/3/3
85	OMG	2	71	86,85	-	0/9/27/28	0/3/3/3
26	PSU	S1	1539	26	-	2/7/25/26	0/2/2/2
26	C4J	S1	1543	26	-	5/16/34/35	0/2/2/2
1	PSU	1	1039	1	-	0/7/25/26	0/2/2/2
26	5MC	S1	1544	26	-	0/7/25/26	0/2/2/2
85	A2M	2	95	85	-	0/9/27/28	0/3/3/3
26	OMU	S1	1621	86,26	-	0/9/27/28	0/2/2/2
26	MA6	S1	2185	26	-	1/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1528	1	-	0/7/25/26	0/2/2/2
1	A2M	1	955	1	-	0/9/27/28	0/3/3/3
85	A2M	2	382	85	-	1/9/27/28	0/3/3/3
26	OMC	S1	18	26	-	0/9/27/28	0/2/2/2
6	PSU	7	69	6	-	3/7/25/26	0/2/2/2
1	A2M	1	858	1	-	1/9/27/28	0/3/3/3
1	A2M	1	407	1	-	3/9/27/28	0/3/3/3
2	OMU	3	13	2	-	0/9/27/28	0/2/2/2
26	OMG	S1	1478	26	-	0/9/27/28	0/3/3/3
26	OMC	S1	2140	26	-	2/9/27/28	0/2/2/2
85	OMU	2	73	85	-	0/9/27/28	0/2/2/2
85	PSU	2	78	85	-	0/7/25/26	0/2/2/2
85	PSU	2	472	85	-	0/7/25/26	0/2/2/2
1	A2M	1	235	1	-	0/9/27/28	0/3/3/3
26	OMG	S1	2151	26	-	0/9/27/28	0/3/3/3
1	A2M	1	681	1	-	3/9/27/28	0/3/3/3
6	OMG	7	75	6	-	2/9/27/28	0/3/3/3
26	A2M	S1	2021	26	-	2/9/27/28	0/3/3/3
1	OMG	1	959[A]	1	-	2/9/27/28	0/3/3/3
26	PSU	S1	609	26	-	0/7/25/26	0/2/2/2
26	PSU	S1	2202	26	-	1/7/25/26	0/2/2/2
26	OMU	S1	1979	26	-	0/9/27/28	0/2/2/2
1	PSU	1	1017	86,1	-	0/7/25/26	0/2/2/2
26	PSU	S1	12	26	-	0/7/25/26	0/2/2/2
3	OMG	4	74	3	-	0/9/27/28	0/3/3/3
26	OMU	S1	29	86,26	-	0/9/27/28	0/2/2/2
1	A2M	1	697	1	-	0/9/27/28	0/3/3/3
26	OMU	S1	661	26	-	0/9/27/28	0/2/2/2
26	OMC	S1	38	26	-	0/9/27/28	0/2/2/2
1	OMG	1	1524	1	-	1/9/27/28	0/3/3/3
26	PSU	S1	1246	86,26	-	0/7/25/26	0/2/2/2
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
26	A2M	S1	479	26	-	2/9/27/28	0/3/3/3
1	OMU	1	1371	1	-	4/9/27/28	0/2/2/2
26	OMG	S1	600	26	-	2/9/27/28	0/3/3/3
26	PSU	S1	455	26	-	0/7/25/26	0/2/2/2
6	A2M	7	43	6	-	0/9/27/28	0/3/3/3
85	OMC	2	443	85,87	-	4/9/27/28	0/2/2/2
26	PSU	S1	2048	26	-	0/7/25/26	0/2/2/2
1	PSU	1	1664	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
26	7MG	S1	1995	26	-	2/7/37/38	0/3/3/3
1	PSU	1	1402	1	-	2/7/25/26	0/2/2/2
1	OMU	1	1107	1	-	3/9/27/28	0/2/2/2
1	PSU	1	672	86,1	-	0/7/25/26	0/2/2/2
1	OMG	1	1626	1	-	0/9/27/28	0/3/3/3
1	1MA	1	677	86,1	-	0/7/25/26	0/3/3/3
26	PSU	S1	2046	26	-	0/7/25/26	0/2/2/2
1	PSU	1	1171	86,1	-	0/7/25/26	0/2/2/2
26	A2M	S1	98	86,26	-	2/9/27/28	0/3/3/3
85	PSU	2	437	85	-	0/7/25/26	0/2/2/2
26	OMG	S1	1550	26	-	3/9/27/28	0/3/3/3
26	PSU	S1	1657	26	-	2/7/25/26	0/2/2/2
1	PSU	1	870	1	-	0/7/25/26	0/2/2/2
1	OMG	1	1190	86,1	-	0/9/27/28	0/3/3/3
26	OMU	S1	1833	86,26	-	1/9/27/28	0/2/2/2
1	A2M	1	927	1	-	1/9/27/28	0/3/3/3
26	PSU	S1	1841	87,26	-	1/7/25/26	0/2/2/2
26	A2M	S1	668	86,26	-	4/9/27/28	0/3/3/3
1	OMU	1	1659	86,1	-	0/9/27/28	0/2/2/2
26	A2M	S1	512	86,26	-	2/9/27/28	0/3/3/3
26	OMG	S1	1647	26	-	0/9/27/28	0/3/3/3
1	PSU	1	1181	1	-	4/7/25/26	0/2/2/2
1	OMG	1	1540	85,1	-	2/9/27/28	0/3/3/3
6	OMU	7	7	1,6	-	1/9/27/28	0/2/2/2
26	PSU	S1	607	26	-	2/7/25/26	0/2/2/2
26	5MC	S1	2061	26	-	0/7/25/26	0/2/2/2
1	OMU	1	847	1	-	0/9/27/28	0/2/2/2
26	PSU	S1	1566	86,26	-	2/7/25/26	0/2/2/2
1	PSU	1	1533	85,1	-	0/7/25/26	0/2/2/2
26	OMC	S1	1866	26	-	0/9/27/28	0/2/2/2
1	A2M	1	678	85,1	-	3/9/27/28	0/3/3/3
1	OMC	1	1527	1	-	1/9/27/28	0/2/2/2
1	OMG	1	856	1	-	0/9/27/28	0/3/3/3
26	OMG	S1	1865	26	-	0/9/27/28	0/3/3/3
26	OMG	S1	1879	26	-	1/9/27/28	0/3/3/3

All (843) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	422	PSU	C6-C5	12.54	1.49	1.35
26	S1	607	PSU	C6-C5	12.36	1.49	1.35
26	S1	33	PSU	C6-C5	12.16	1.48	1.35
6	7	69	PSU	C6-C5	12.15	1.48	1.35
26	S1	1566	PSU	C6-C5	12.15	1.48	1.35
1	1	1402	PSU	C6-C5	12.15	1.48	1.35
1	1	1171	PSU	C6-C5	12.13	1.48	1.35
1	1	239	PSU	C6-C5	12.13	1.48	1.35
1	1	1664	PSU	C6-C5	12.12	1.48	1.35
85	2	472	PSU	C6-C5	12.10	1.48	1.35
1	1	1181	PSU	C6-C5	12.09	1.48	1.35
6	7	74	PSU	C6-C5	12.09	1.48	1.35
1	1	1528	PSU	C6-C5	12.09	1.48	1.35
1	1	1039	PSU	C6-C5	12.08	1.48	1.35
26	S1	609	PSU	C6-C5	12.07	1.48	1.35
1	1	1011	PSU	C6-C5	12.07	1.48	1.35
1	1	940	PSU	C6-C5	12.07	1.48	1.35
26	S1	1539	PSU	C6-C5	12.03	1.48	1.35
26	S1	1533	PSU	C6-C5	11.99	1.48	1.35
1	1	870	PSU	C6-C5	11.99	1.48	1.35
1	1	1533	PSU	C6-C5	11.96	1.48	1.35
85	2	78	PSU	C6-C5	11.96	1.48	1.35
1	1	672	PSU	C6-C5	11.95	1.48	1.35
1	1	1017	PSU	C6-C5	11.90	1.48	1.35
26	S1	1192	PSU	C6-C5	11.88	1.48	1.35
26	S1	455	PSU	C6-C5	11.87	1.48	1.35
26	S1	104	PSU	C6-C5	11.86	1.48	1.35
85	2	437	PSU	C6-C5	11.84	1.48	1.35
26	S1	1841	PSU	C6-C5	11.82	1.48	1.35
26	S1	1156	PSU	C6-C5	11.78	1.48	1.35
26	S1	1657	PSU	C6-C5	11.66	1.48	1.35
26	S1	1246	PSU	C6-C5	11.63	1.48	1.35
26	S1	2202	PSU	C6-C5	11.63	1.48	1.35
26	S1	2046	PSU	C6-C5	11.55	1.48	1.35
26	S1	12	PSU	C6-C5	11.48	1.48	1.35
26	S1	2048	PSU	C6-C5	11.46	1.48	1.35
26	S1	607	PSU	C2-N1	10.24	1.50	1.36
1	1	239	PSU	C2-N1	10.01	1.49	1.36
1	1	940	PSU	C2-N1	9.98	1.49	1.36
6	7	69	PSU	C2-N1	9.98	1.49	1.36
1	1	1181	PSU	C2-N1	9.96	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	2	472	PSU	C2-N1	9.95	1.49	1.36
6	7	74	PSU	C2-N1	9.94	1.49	1.36
1	1	1039	PSU	C2-N1	9.94	1.49	1.36
1	1	870	PSU	C2-N1	9.92	1.49	1.36
1	1	1011	PSU	C2-N1	9.92	1.49	1.36
1	1	1533	PSU	C2-N1	9.91	1.49	1.36
26	S1	1566	PSU	C2-N1	9.91	1.49	1.36
1	1	1528	PSU	C2-N1	9.91	1.49	1.36
26	S1	1533	PSU	C2-N1	9.90	1.49	1.36
26	S1	455	PSU	C2-N1	9.89	1.49	1.36
1	1	1664	PSU	C2-N1	9.89	1.49	1.36
85	2	78	PSU	C2-N1	9.88	1.49	1.36
26	S1	104	PSU	C2-N1	9.87	1.49	1.36
1	1	1171	PSU	C2-N1	9.87	1.49	1.36
85	2	437	PSU	C2-N1	9.85	1.49	1.36
26	S1	1539	PSU	C2-N1	9.84	1.49	1.36
1	1	422	PSU	C2-N1	9.80	1.49	1.36
26	S1	609	PSU	C2-N1	9.79	1.49	1.36
26	S1	1841	PSU	C2-N1	9.77	1.49	1.36
1	1	672	PSU	C2-N1	9.77	1.49	1.36
26	S1	1156	PSU	C2-N1	9.74	1.49	1.36
26	S1	33	PSU	C2-N1	9.71	1.49	1.36
1	1	1017	PSU	C2-N1	9.69	1.49	1.36
1	1	1402	PSU	C2-N1	9.69	1.49	1.36
26	S1	1657	PSU	C2-N1	9.66	1.49	1.36
26	S1	1246	PSU	C2-N1	9.65	1.49	1.36
26	S1	1543	C4J	C6-C5	9.65	1.48	1.35
26	S1	2046	PSU	C2-N1	9.59	1.49	1.36
26	S1	1192	PSU	C2-N1	9.51	1.49	1.36
26	S1	12	PSU	C2-N1	9.51	1.49	1.36
26	S1	2202	PSU	C2-N1	9.49	1.49	1.36
26	S1	2048	PSU	C2-N1	9.38	1.48	1.36
26	S1	1995	7MG	C8-N9	9.37	1.51	1.45
6	7	162	A2M	C2'-C1'	-9.34	1.30	1.53
1	1	1539	A2M	C2'-C1'	-9.29	1.30	1.53
1	1	955	A2M	C2'-C1'	-9.18	1.30	1.53
26	S1	98	A2M	C2'-C1'	-9.16	1.30	1.53
26	S1	512	A2M	C2'-C1'	-9.14	1.30	1.53
1	1	305	A2M	C2'-C1'	-9.13	1.30	1.53
1	1	407	A2M	O4'-C1'	9.12	1.63	1.42
85	2	95	A2M	C2'-C1'	-9.12	1.30	1.53
85	2	382	A2M	C2'-C1'	-9.11	1.30	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	43	A2M	C2'-C1'	-9.11	1.30	1.53
1	1	927	A2M	C2'-C1'	-9.08	1.30	1.53
1	1	681	A2M	C2'-C1'	-9.04	1.30	1.53
1	1	235	A2M	O4'-C1'	9.04	1.62	1.42
1	1	697	A2M	C2'-C1'	-9.03	1.30	1.53
26	S1	1544	5MC	C6-C5	9.02	1.49	1.34
26	S1	668	A2M	C2'-C1'	-9.01	1.30	1.53
1	1	407	A2M	C2'-C1'	-9.00	1.30	1.53
1	1	235	A2M	C2'-C1'	-8.97	1.31	1.53
85	2	382	A2M	O4'-C1'	8.96	1.62	1.42
1	1	678	A2M	O4'-C1'	8.92	1.62	1.42
26	S1	479	A2M	C2'-C1'	-8.89	1.31	1.53
6	7	43	A2M	O4'-C1'	8.84	1.62	1.42
26	S1	98	A2M	O4'-C1'	8.82	1.62	1.42
26	S1	2021	A2M	C2'-C1'	-8.82	1.31	1.53
1	1	955	A2M	O4'-C1'	8.81	1.62	1.42
1	1	697	A2M	O4'-C1'	8.80	1.62	1.42
6	7	162	A2M	O4'-C1'	8.76	1.62	1.42
1	1	1539	A2M	O4'-C1'	8.76	1.62	1.42
1	1	858	A2M	C2'-C1'	-8.76	1.31	1.53
85	2	95	A2M	O4'-C1'	8.71	1.62	1.42
1	1	927	A2M	O4'-C1'	8.70	1.62	1.42
1	1	681	A2M	O4'-C1'	8.68	1.62	1.42
26	S1	512	A2M	O4'-C1'	8.67	1.62	1.42
1	1	305	A2M	O4'-C1'	8.65	1.62	1.42
26	S1	479	A2M	O4'-C1'	8.64	1.62	1.42
26	S1	2061	5MC	C6-C5	8.59	1.48	1.34
1	1	858	A2M	O4'-C1'	8.48	1.61	1.42
1	1	677	1MA	C2-N3	8.42	1.45	1.30
1	1	678	A2M	C2'-C1'	-8.41	1.32	1.53
26	S1	2021	A2M	O4'-C1'	8.36	1.61	1.42
26	S1	1995	7MG	C5-N7	8.33	1.46	1.35
26	S1	668	A2M	O4'-C1'	8.06	1.60	1.42
1	1	677	1MA	C4-N3	8.01	1.51	1.35
26	S1	607	PSU	C2-N3	7.82	1.50	1.37
85	2	472	PSU	C2-N3	7.80	1.50	1.37
1	1	1533	PSU	C2-N3	7.77	1.50	1.37
6	7	74	PSU	C2-N3	7.75	1.50	1.37
1	1	239	PSU	C2-N3	7.74	1.50	1.37
1	1	422	PSU	C2-N3	7.73	1.50	1.37
26	S1	33	PSU	C2-N3	7.72	1.50	1.37
1	1	1011	PSU	C2-N3	7.72	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	609	PSU	C2-N3	7.71	1.50	1.37
1	1	1664	PSU	C2-N3	7.71	1.50	1.37
1	1	1039	PSU	C2-N3	7.70	1.50	1.37
1	1	1528	PSU	C2-N3	7.68	1.50	1.37
1	1	940	PSU	C2-N3	7.68	1.50	1.37
1	1	1402	PSU	C2-N3	7.67	1.50	1.37
26	S1	1533	PSU	C2-N3	7.67	1.50	1.37
1	1	1181	PSU	C2-N3	7.65	1.50	1.37
1	1	672	PSU	C2-N3	7.61	1.50	1.37
26	S1	1841	PSU	C2-N3	7.61	1.50	1.37
85	2	78	PSU	C2-N3	7.60	1.50	1.37
26	S1	1539	PSU	C2-N3	7.60	1.50	1.37
1	1	1017	PSU	C2-N3	7.60	1.50	1.37
1	1	1371	OMU	C2-N1	7.58	1.50	1.38
26	S1	1566	PSU	C2-N3	7.58	1.50	1.37
6	7	69	PSU	C2-N3	7.56	1.49	1.37
85	2	437	PSU	C2-N3	7.55	1.49	1.37
1	1	870	PSU	C2-N3	7.54	1.49	1.37
1	1	1171	PSU	C2-N3	7.54	1.49	1.37
26	S1	455	PSU	C2-N3	7.52	1.49	1.37
26	S1	1192	PSU	C2-N3	7.45	1.49	1.37
26	S1	1246	PSU	C2-N3	7.45	1.49	1.37
26	S1	2046	PSU	C2-N3	7.44	1.49	1.37
26	S1	1657	PSU	C2-N3	7.43	1.49	1.37
26	S1	104	PSU	C2-N3	7.42	1.49	1.37
1	1	845	OMU	C2-N1	7.40	1.50	1.38
26	S1	2202	PSU	C2-N3	7.39	1.49	1.37
26	S1	1156	PSU	C2-N3	7.38	1.49	1.37
26	S1	2048	PSU	C2-N3	7.26	1.49	1.37
26	S1	12	PSU	C2-N3	7.20	1.49	1.37
85	2	56	OMU	C2-N1	7.13	1.49	1.38
26	S1	1833	OMU	C2-N1	7.10	1.49	1.38
26	S1	1621	OMU	C2-N1	7.04	1.49	1.38
2	3	13	OMU	C2-N1	7.01	1.49	1.38
26	S1	1979	OMU	C2-N1	7.00	1.49	1.38
1	1	1659	OMU	C2-N1	7.00	1.49	1.38
6	7	7	OMU	C2-N1	6.98	1.49	1.38
1	1	1107	OMU	C2-N1	6.94	1.49	1.38
85	2	73	OMU	C2-N1	6.93	1.49	1.38
26	S1	1621	OMU	C2-N3	6.88	1.50	1.38
2	3	13	OMU	C2-N3	6.88	1.50	1.38
1	1	1107	OMU	C2-N3	6.88	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	29	OMU	C2-N1	6.88	1.49	1.38
1	1	847	OMU	C2-N1	6.85	1.49	1.38
26	S1	668	A2M	O4'-C4'	-6.83	1.29	1.45
26	S1	1979	OMU	C2-N3	6.82	1.49	1.38
85	2	73	OMU	C2-N3	6.81	1.49	1.38
6	7	7	OMU	C2-N3	6.81	1.49	1.38
26	S1	1833	OMU	C2-N3	6.80	1.49	1.38
1	1	1371	OMU	C2-N3	6.80	1.49	1.38
1	1	1659	OMU	C2-N3	6.79	1.49	1.38
85	2	56	OMU	C2-N3	6.75	1.49	1.38
1	1	847	OMU	C2-N3	6.73	1.49	1.38
26	S1	29	OMU	C2-N3	6.70	1.49	1.38
1	1	858	A2M	O4'-C4'	-6.69	1.30	1.45
26	S1	661	OMU	C2-N1	6.65	1.48	1.38
26	S1	479	A2M	O4'-C4'	-6.65	1.30	1.45
1	1	845	OMU	C2-N3	6.62	1.49	1.38
26	S1	1544	5MC	C4-N3	6.59	1.44	1.34
1	1	407	A2M	O4'-C4'	-6.58	1.30	1.45
1	1	959[B]	OMG	C4-N3	6.58	1.49	1.34
26	S1	1995	7MG	C4-N9	6.58	1.45	1.37
26	S1	8	OMU	C2-N1	6.54	1.48	1.38
1	1	959[A]	OMG	C4-N3	6.54	1.49	1.34
26	S1	512	A2M	O4'-C4'	-6.51	1.30	1.45
26	S1	661	OMU	C2-N3	6.49	1.49	1.38
26	S1	8	OMU	C2-N3	6.49	1.49	1.38
85	2	71	OMG	C4-N3	6.45	1.49	1.34
6	7	75	OMG	C4-N3	6.45	1.49	1.34
1	1	955	A2M	O4'-C4'	-6.44	1.30	1.45
1	1	1524	OMG	C4-N3	6.42	1.49	1.34
1	1	1539	A2M	O4'-C4'	-6.42	1.30	1.45
1	1	235	A2M	O4'-C4'	-6.42	1.30	1.45
26	S1	1623	OMG	C4-N3	6.42	1.48	1.34
26	S1	1550	OMG	C4-N3	6.41	1.48	1.34
6	7	162	A2M	O4'-C4'	-6.41	1.30	1.45
85	2	359	OMC	C2-N3	6.41	1.49	1.36
1	1	1626	OMG	C4-N3	6.40	1.48	1.34
26	S1	1829	OMG	C4-N3	6.39	1.48	1.34
26	S1	600	OMG	C4-N3	6.39	1.48	1.34
26	S1	1865	OMG	C4-N3	6.39	1.48	1.34
26	S1	1879	OMG	C4-N3	6.38	1.48	1.34
26	S1	2061	5MC	C4-N3	6.38	1.44	1.34
1	1	1010	OMC	C2-N3	6.36	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	98	A2M	O4'-C4'	-6.35	1.30	1.45
1	1	856	OMG	C4-N3	6.35	1.48	1.34
26	S1	2021	A2M	O4'-C4'	-6.35	1.30	1.45
1	1	927	A2M	O4'-C4'	-6.33	1.30	1.45
26	S1	2151	OMG	C4-N3	6.32	1.48	1.34
85	2	95	A2M	O4'-C4'	-6.32	1.30	1.45
1	1	695	OMC	C2-N3	6.32	1.48	1.36
26	S1	2140	OMC	C2-N3	6.31	1.48	1.36
1	1	1527	OMC	C2-N3	6.31	1.48	1.36
1	1	697	A2M	O4'-C4'	-6.31	1.31	1.45
3	4	74	OMG	C4-N3	6.30	1.48	1.34
1	1	1190	OMG	C4-N3	6.29	1.48	1.34
85	2	443	OMC	C2-N3	6.29	1.48	1.36
1	1	681	A2M	O4'-C4'	-6.27	1.31	1.45
6	7	43	A2M	O4'-C4'	-6.27	1.31	1.45
1	1	1540	OMG	C4-N3	6.26	1.48	1.34
85	2	382	A2M	O4'-C4'	-6.22	1.31	1.45
26	S1	1866	OMC	C2-N3	6.18	1.48	1.36
26	S1	1995	7MG	C2-N3	6.17	1.48	1.33
26	S1	1478	OMG	C4-N3	6.15	1.48	1.34
26	S1	38	OMC	C2-N3	6.14	1.48	1.36
1	1	305	A2M	O4'-C4'	-6.12	1.31	1.45
26	S1	1647	OMG	C4-N3	6.11	1.48	1.34
26	S1	1544	5MC	C2-N3	6.09	1.48	1.36
26	S1	18	OMC	C2-N3	6.07	1.48	1.36
85	2	359	OMC	C6-C5	5.97	1.48	1.35
26	S1	1544	5MC	C5-C4	5.91	1.48	1.44
26	S1	1866	OMC	C6-C5	5.91	1.48	1.35
85	2	443	OMC	C6-C5	5.90	1.48	1.35
26	S1	2061	5MC	C2-N3	5.89	1.48	1.36
1	1	695	OMC	C6-C5	5.84	1.48	1.35
26	S1	38	OMC	C6-C5	5.84	1.48	1.35
1	1	1010	OMC	C6-C5	5.82	1.48	1.35
26	S1	1543	C4J	C2-N3	5.82	1.48	1.38
1	1	1527	OMC	C6-C5	5.82	1.48	1.35
26	S1	2140	OMC	C6-C5	5.81	1.48	1.35
1	1	678	A2M	O4'-C4'	-5.80	1.32	1.45
26	S1	2061	5MC	C5-C4	5.69	1.48	1.44
26	S1	1833	OMU	C6-C5	5.68	1.48	1.35
26	S1	18	OMC	C6-C5	5.65	1.48	1.35
1	1	1107	OMU	C6-C5	5.64	1.48	1.35
26	S1	1621	OMU	C6-C5	5.62	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	847	OMU	C6-C5	5.61	1.48	1.35
1	1	1659	OMU	C6-C5	5.61	1.48	1.35
2	3	13	OMU	C6-C5	5.61	1.48	1.35
85	2	73	OMU	C6-C5	5.59	1.48	1.35
85	2	56	OMU	C6-C5	5.59	1.48	1.35
26	S1	1979	OMU	C6-C5	5.59	1.48	1.35
6	7	7	OMU	C6-C5	5.58	1.48	1.35
1	1	1371	OMU	C6-C5	5.57	1.48	1.35
26	S1	29	OMU	C6-C5	5.54	1.47	1.35
26	S1	8	OMU	C6-C5	5.51	1.47	1.35
26	S1	661	OMU	C6-C5	5.49	1.47	1.35
26	S1	1995	7MG	C4-N3	5.48	1.46	1.34
26	S1	607	PSU	C6-N1	5.48	1.45	1.36
1	1	959[A]	OMG	C2-N3	5.40	1.46	1.33
1	1	959[B]	OMG	C2-N3	5.35	1.46	1.33
1	1	239	PSU	C6-N1	5.34	1.45	1.36
6	7	69	PSU	C6-N1	5.32	1.45	1.36
26	S1	1566	PSU	C6-N1	5.31	1.45	1.36
1	1	845	OMU	C6-C5	5.30	1.47	1.35
6	7	74	PSU	C6-N1	5.30	1.45	1.36
26	S1	1550	OMG	C2-N3	5.29	1.46	1.33
1	1	1171	PSU	C6-N1	5.28	1.44	1.36
1	1	1664	PSU	C6-N1	5.28	1.44	1.36
26	S1	1533	PSU	C6-N1	5.27	1.44	1.36
85	2	78	PSU	C6-N1	5.27	1.44	1.36
85	2	472	PSU	C6-N1	5.27	1.44	1.36
1	1	1528	PSU	C6-N1	5.25	1.44	1.36
1	1	1039	PSU	C6-N1	5.25	1.44	1.36
85	2	359	OMC	C4-N3	5.24	1.44	1.34
85	2	71	OMG	C2-N3	5.24	1.45	1.33
1	1	940	PSU	C6-N1	5.24	1.44	1.36
1	1	1524	OMG	C2-N3	5.23	1.45	1.33
6	7	75	OMG	C2-N3	5.23	1.45	1.33
26	S1	1623	OMG	C2-N3	5.23	1.45	1.33
1	1	870	PSU	C6-N1	5.22	1.44	1.36
1	1	422	PSU	C6-N1	5.21	1.44	1.36
1	1	1533	PSU	C6-N1	5.20	1.44	1.36
1	1	1011	PSU	C6-N1	5.20	1.44	1.36
1	1	1402	PSU	C6-N1	5.19	1.44	1.36
26	S1	1879	OMG	C2-N3	5.19	1.45	1.33
1	1	672	PSU	C6-N1	5.18	1.44	1.36
1	1	1181	PSU	C6-N1	5.17	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	600	OMG	C2-N3	5.17	1.45	1.33
26	S1	1156	PSU	C6-N1	5.17	1.44	1.36
26	S1	1539	PSU	C6-N1	5.16	1.44	1.36
1	1	1626	OMG	C2-N3	5.16	1.45	1.33
26	S1	455	PSU	C6-N1	5.16	1.44	1.36
1	1	1010	OMC	C4-N3	5.16	1.44	1.34
26	S1	1829	OMG	C2-N3	5.14	1.45	1.33
26	S1	609	PSU	C6-N1	5.13	1.44	1.36
26	S1	104	PSU	C6-N1	5.12	1.44	1.36
26	S1	2151	OMG	C2-N3	5.12	1.45	1.33
85	2	437	PSU	C6-N1	5.12	1.44	1.36
26	S1	1865	OMG	C2-N3	5.11	1.45	1.33
1	1	695	OMC	C4-N3	5.11	1.44	1.34
26	S1	1192	PSU	C6-N1	5.10	1.44	1.36
26	S1	1841	PSU	C6-N1	5.10	1.44	1.36
26	S1	1657	PSU	C6-N1	5.10	1.44	1.36
26	S1	2140	OMC	C4-N3	5.08	1.44	1.34
1	1	856	OMG	C2-N3	5.08	1.45	1.33
85	2	443	OMC	C4-N3	5.07	1.44	1.34
26	S1	33	PSU	C6-N1	5.06	1.44	1.36
26	S1	1246	PSU	C6-N1	5.05	1.44	1.36
3	4	74	OMG	C2-N3	5.04	1.45	1.33
26	S1	2046	PSU	C6-N1	5.04	1.44	1.36
26	S1	1866	OMC	C4-N3	5.02	1.44	1.34
1	1	1017	PSU	C6-N1	5.02	1.44	1.36
1	1	1527	OMC	C4-N3	4.99	1.44	1.34
1	1	1190	OMG	C2-N3	4.96	1.45	1.33
1	1	1540	OMG	C2-N3	4.93	1.45	1.33
26	S1	12	PSU	C6-N1	4.92	1.44	1.36
26	S1	1647	OMG	C2-N3	4.90	1.45	1.33
26	S1	38	OMC	C4-N3	4.90	1.44	1.34
26	S1	2202	PSU	C6-N1	4.89	1.44	1.36
26	S1	2048	PSU	C6-N1	4.86	1.44	1.36
26	S1	1478	OMG	C2-N3	4.77	1.44	1.33
1	1	959[A]	OMG	C2-N2	4.77	1.45	1.34
26	S1	2048	PSU	C1'-C5	-4.74	1.39	1.50
26	S1	18	OMC	C4-N3	4.73	1.43	1.34
26	S1	1246	PSU	C1'-C5	-4.72	1.39	1.50
1	1	959[B]	OMG	C2-N2	4.71	1.45	1.34
6	7	75	OMG	C2-N2	4.71	1.45	1.34
26	S1	1550	OMG	C2-N2	4.69	1.45	1.34
85	2	359	OMC	C4-N4	4.68	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1626	OMG	C2-N2	4.67	1.45	1.34
85	2	71	OMG	C2-N2	4.67	1.45	1.34
26	S1	1879	OMG	C2-N2	4.66	1.45	1.34
1	1	1527	OMC	C2-N1	4.65	1.49	1.40
26	S1	1623	OMG	C2-N2	4.65	1.45	1.34
1	1	1524	OMG	C2-N2	4.65	1.45	1.34
3	4	74	OMG	C2-N2	4.64	1.45	1.34
26	S1	455	PSU	C1'-C5	-4.62	1.39	1.50
26	S1	1829	OMG	C2-N2	4.61	1.45	1.34
26	S1	1865	OMG	C2-N2	4.61	1.45	1.34
1	1	856	OMG	C2-N2	4.60	1.44	1.34
26	S1	2140	OMC	C2-N1	4.60	1.49	1.40
26	S1	600	OMG	C2-N2	4.59	1.44	1.34
1	1	1010	OMC	C4-N4	4.59	1.45	1.33
1	1	1190	OMG	C2-N2	4.59	1.44	1.34
26	S1	1841	PSU	C1'-C5	-4.59	1.39	1.50
26	S1	2046	PSU	C1'-C5	-4.59	1.39	1.50
85	2	443	OMC	C4-N4	4.59	1.45	1.33
26	S1	1657	PSU	C1'-C5	-4.59	1.39	1.50
26	S1	12	PSU	C1'-C5	-4.59	1.39	1.50
26	S1	2140	OMC	C4-N4	4.58	1.45	1.33
26	S1	2151	OMG	C2-N2	4.58	1.44	1.34
85	2	78	PSU	C1'-C5	-4.58	1.39	1.50
1	1	1533	PSU	C1'-C5	-4.57	1.39	1.50
1	1	695	OMC	C4-N4	4.55	1.44	1.33
26	S1	1866	OMC	C4-N4	4.55	1.44	1.33
1	1	1540	OMG	C2-N2	4.55	1.44	1.34
26	S1	609	PSU	C1'-C5	-4.54	1.40	1.50
1	1	1527	OMC	C4-N4	4.54	1.44	1.33
26	S1	1647	OMG	C2-N2	4.54	1.44	1.34
26	S1	38	OMC	C4-N4	4.54	1.44	1.33
1	1	1039	PSU	C1'-C5	-4.53	1.40	1.50
26	S1	1156	PSU	C1'-C5	-4.53	1.40	1.50
1	1	940	PSU	C1'-C5	-4.51	1.40	1.50
85	2	472	PSU	C1'-C5	-4.51	1.40	1.50
26	S1	1478	OMG	C2-N2	4.48	1.44	1.34
6	7	74	PSU	C1'-C5	-4.48	1.40	1.50
1	1	870	PSU	C1'-C5	-4.47	1.40	1.50
1	1	1017	PSU	C1'-C5	-4.46	1.40	1.50
1	1	239	PSU	C1'-C5	-4.45	1.40	1.50
26	S1	104	PSU	C1'-C5	-4.44	1.40	1.50
1	1	672	PSU	C1'-C5	-4.44	1.40	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	18	OMC	C4-N4	4.43	1.44	1.33
26	S1	1192	PSU	C1'-C5	-4.42	1.40	1.50
85	2	437	PSU	C1'-C5	-4.42	1.40	1.50
1	1	1528	PSU	C1'-C5	-4.41	1.40	1.50
1	1	1664	PSU	C1'-C5	-4.41	1.40	1.50
85	2	359	OMC	C2-N1	4.40	1.49	1.40
1	1	695	OMC	C2-N1	4.39	1.49	1.40
1	1	1171	PSU	C1'-C5	-4.39	1.40	1.50
26	S1	1539	PSU	C1'-C5	-4.38	1.40	1.50
85	2	443	OMC	C2-N1	4.38	1.49	1.40
26	S1	1533	PSU	C1'-C5	-4.38	1.40	1.50
26	S1	1544	5MC	C6-N1	4.38	1.45	1.38
26	S1	2202	PSU	C1'-C5	-4.35	1.40	1.50
1	1	235	A2M	C6-N6	4.31	1.45	1.34
85	2	95	A2M	C6-N6	4.31	1.45	1.34
26	S1	1544	5MC	C4-N4	4.31	1.45	1.34
1	1	858	A2M	C6-N6	4.30	1.45	1.34
1	1	1010	OMC	C2-N1	4.27	1.49	1.40
26	S1	607	PSU	C1'-C5	-4.27	1.40	1.50
26	S1	33	PSU	C1'-C5	-4.27	1.40	1.50
26	S1	2021	A2M	C6-N6	4.25	1.45	1.34
6	7	162	A2M	C6-N6	4.25	1.45	1.34
1	1	1181	PSU	C1'-C5	-4.25	1.40	1.50
6	7	43	A2M	C6-N6	4.24	1.45	1.34
1	1	955	A2M	C6-N6	4.24	1.45	1.34
1	1	305	A2M	C6-N6	4.24	1.45	1.34
1	1	1539	A2M	C6-N6	4.24	1.45	1.34
1	1	697	A2M	C6-N6	4.23	1.45	1.34
1	1	1011	PSU	C1'-C5	-4.22	1.40	1.50
85	2	382	A2M	C6-N6	4.22	1.45	1.34
1	1	927	A2M	C6-N6	4.22	1.45	1.34
1	1	681	A2M	C6-N6	4.22	1.45	1.34
26	S1	479	A2M	C6-N6	4.21	1.45	1.34
1	1	407	A2M	C6-N6	4.21	1.45	1.34
26	S1	1566	PSU	C1'-C5	-4.20	1.40	1.50
2	3	13	OMU	C4-N3	4.20	1.45	1.38
1	1	678	A2M	C6-N6	4.20	1.44	1.34
26	S1	1866	OMC	C2-N1	4.20	1.48	1.40
26	S1	512	A2M	C6-N6	4.19	1.44	1.34
26	S1	1979	OMU	C4-N3	4.19	1.45	1.38
26	S1	1621	OMU	C4-N3	4.19	1.45	1.38
26	S1	98	A2M	C6-N6	4.19	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	422	PSU	C1'-C5	-4.19	1.40	1.50
26	S1	2061	5MC	C4-N4	4.18	1.44	1.34
26	S1	668	A2M	C6-N6	4.18	1.44	1.34
6	7	7	OMU	C4-N3	4.16	1.45	1.38
1	1	1107	OMU	C4-N3	4.13	1.45	1.38
26	S1	2061	5MC	C6-N1	4.12	1.45	1.38
26	S1	38	OMC	C2-N1	4.11	1.48	1.40
1	1	1402	PSU	C1'-C5	-4.11	1.41	1.50
1	1	1659	OMU	C4-N3	4.10	1.45	1.38
26	S1	1833	OMU	C4-N3	4.09	1.45	1.38
26	S1	1543	C4J	C6-N1	4.08	1.46	1.36
85	2	73	OMU	C4-N3	4.06	1.45	1.38
85	2	56	OMU	C4-N3	4.05	1.45	1.38
26	S1	1544	5MC	C2-N1	4.03	1.48	1.40
6	7	69	PSU	C1'-C5	-4.03	1.41	1.50
26	S1	18	OMC	C2-N1	4.02	1.48	1.40
26	S1	29	OMU	C4-N3	4.01	1.45	1.38
1	1	847	OMU	C4-N3	3.98	1.45	1.38
1	1	1371	OMU	C4-N3	3.93	1.45	1.38
26	S1	607	PSU	C4-N3	3.87	1.46	1.38
26	S1	661	OMU	C4-N3	3.83	1.45	1.38
1	1	1011	PSU	C4-N3	3.82	1.46	1.38
1	1	422	PSU	C4-N3	3.79	1.45	1.38
6	7	74	PSU	C4-N3	3.78	1.45	1.38
1	1	239	PSU	C4-N3	3.77	1.45	1.38
26	S1	2061	5MC	C2-N1	3.77	1.48	1.40
26	S1	1566	PSU	C4-N3	3.76	1.45	1.38
85	2	472	PSU	C4-N3	3.75	1.45	1.38
26	S1	33	PSU	C4-N3	3.74	1.45	1.38
26	S1	8	OMU	C4-N3	3.74	1.45	1.38
1	1	1402	PSU	C4-N3	3.73	1.45	1.38
1	1	1533	PSU	C4-N3	3.73	1.45	1.38
1	1	1664	PSU	C4-N3	3.72	1.45	1.38
26	S1	1533	PSU	C4-N3	3.72	1.45	1.38
1	1	1181	PSU	C4-N3	3.72	1.45	1.38
26	S1	609	PSU	C4-N3	3.70	1.45	1.38
26	S1	1539	PSU	C4-N3	3.70	1.45	1.38
6	7	69	PSU	C4-N3	3.70	1.45	1.38
1	1	1039	PSU	C4-N3	3.69	1.45	1.38
1	1	1528	PSU	C4-N3	3.68	1.45	1.38
26	S1	2184	MA6	C6-N6	3.66	1.46	1.36
1	1	940	PSU	C4-N3	3.65	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	677	1MA	C2-N1	3.64	1.43	1.35
26	S1	2185	MA6	C6-N6	3.62	1.46	1.36
1	1	870	PSU	C4-N3	3.62	1.45	1.38
1	1	672	PSU	C4-N3	3.62	1.45	1.38
85	2	437	PSU	C4-N3	3.61	1.45	1.38
85	2	78	PSU	C4-N3	3.61	1.45	1.38
1	1	1017	PSU	C4-N3	3.60	1.45	1.38
1	1	1171	PSU	C4-N3	3.58	1.45	1.38
26	S1	104	PSU	C4-N3	3.58	1.45	1.38
1	1	845	OMU	C4-N3	3.56	1.44	1.38
26	S1	1192	PSU	C4-N3	3.55	1.45	1.38
26	S1	1156	PSU	C4-N3	3.54	1.45	1.38
26	S1	1841	PSU	C4-N3	3.54	1.45	1.38
26	S1	2046	PSU	C4-N3	3.53	1.45	1.38
1	1	677	1MA	C5-C6	3.50	1.53	1.43
26	S1	1995	7MG	C2-N1	3.50	1.46	1.37
26	S1	1657	PSU	C4-N3	3.48	1.45	1.38
26	S1	1246	PSU	C4-N3	3.48	1.45	1.38
26	S1	455	PSU	C4-N3	3.47	1.45	1.38
26	S1	668	A2M	C5-C4	-3.47	1.32	1.39
26	S1	1995	7MG	C6-N1	3.44	1.45	1.38
26	S1	2185	MA6	C5-C4	-3.41	1.33	1.39
26	S1	1995	7MG	C5-C6	3.40	1.52	1.43
1	1	678	A2M	C5-C4	-3.39	1.33	1.39
26	S1	2048	PSU	C4-N3	3.37	1.45	1.38
26	S1	12	PSU	C4-N3	3.34	1.45	1.38
1	1	677	1MA	C5-N7	-3.34	1.32	1.39
26	S1	2202	PSU	C4-N3	3.34	1.45	1.38
26	S1	661	OMU	O4-C4	-3.33	1.18	1.24
26	S1	1995	7MG	C2-N2	3.31	1.41	1.34
26	S1	98	A2M	C5-N7	-3.31	1.33	1.39
26	S1	512	A2M	C5-C4	-3.31	1.33	1.39
26	S1	479	A2M	C5-N7	-3.28	1.33	1.39
26	S1	8	OMU	O4-C4	-3.27	1.18	1.24
85	2	359	OMC	C6-N1	3.24	1.45	1.38
26	S1	2184	MA6	C5-C4	-3.24	1.33	1.39
26	S1	1995	7MG	O6-C6	-3.23	1.17	1.23
26	S1	479	A2M	C5-C4	-3.21	1.33	1.39
26	S1	98	A2M	C5-C4	-3.21	1.33	1.39
1	1	407	A2M	C5-C4	-3.21	1.33	1.39
26	S1	668	A2M	C5-N7	-3.20	1.33	1.39
1	1	695	OMC	C6-N1	3.19	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1539	A2M	C5-N7	-3.19	1.33	1.39
26	S1	18	OMC	O2-C2	-3.18	1.17	1.23
85	2	382	A2M	C5-N7	-3.18	1.33	1.39
26	S1	512	A2M	C5-N7	-3.18	1.33	1.39
1	1	845	OMU	O2-C2	-3.18	1.17	1.23
26	S1	512	A2M	O3'-C3'	-3.17	1.35	1.43
26	S1	29	OMU	O4-C4	-3.17	1.18	1.24
26	S1	1543	C4J	C2-N1	3.16	1.48	1.39
1	1	845	OMU	O4-C4	-3.16	1.18	1.24
1	1	955	A2M	C5-C4	-3.16	1.33	1.39
1	1	847	OMU	O4-C4	-3.15	1.18	1.24
1	1	697	A2M	C5-N7	-3.15	1.33	1.39
85	2	56	OMU	O4-C4	-3.15	1.18	1.24
1	1	235	A2M	C5-C4	-3.15	1.33	1.39
1	1	305	A2M	C5-C4	-3.14	1.33	1.39
85	2	73	OMU	O4-C4	-3.14	1.18	1.24
1	1	407	A2M	C5-N7	-3.14	1.33	1.39
1	1	235	A2M	C5-N7	-3.13	1.33	1.39
26	S1	1543	C4J	O4-C4	-3.13	1.16	1.23
26	S1	1543	C4J	C4-N3	3.13	1.45	1.40
1	1	927	A2M	C5-N7	-3.12	1.33	1.39
26	S1	2021	A2M	C5-C4	-3.12	1.33	1.39
26	S1	2202	PSU	O4-C4	-3.12	1.17	1.23
1	1	1539	A2M	C5-C4	-3.12	1.33	1.39
1	1	1010	OMC	C6-N1	3.11	1.45	1.38
26	S1	38	OMC	O2-C2	-3.11	1.17	1.23
1	1	955	A2M	C5-N7	-3.11	1.33	1.39
1	1	1371	OMU	O4-C4	-3.11	1.18	1.24
85	2	95	A2M	C5-N7	-3.11	1.33	1.39
1	1	678	A2M	C5-N7	-3.10	1.33	1.39
26	S1	2140	OMC	C6-N1	3.10	1.45	1.38
85	2	443	OMC	C6-N1	3.10	1.45	1.38
26	S1	1543	C4J	O4'-C1'	-3.09	1.39	1.43
1	1	681	A2M	C5-N7	-3.09	1.33	1.39
1	1	927	A2M	C5-C4	-3.08	1.33	1.39
1	1	1527	OMC	C6-N1	3.08	1.45	1.38
6	7	162	A2M	C5-C4	-3.08	1.33	1.39
6	7	7	OMU	O4-C4	-3.07	1.18	1.24
1	1	1659	OMU	O4-C4	-3.06	1.18	1.24
6	7	43	A2M	C5-C4	-3.06	1.33	1.39
2	3	13	OMU	O4-C4	-3.06	1.18	1.24
1	1	1107	OMU	O4-C4	-3.06	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	2	95	A2M	C5-C4	-3.06	1.33	1.39
26	S1	2021	A2M	C5-N7	-3.06	1.33	1.39
1	1	697	A2M	C5-C4	-3.05	1.33	1.39
26	S1	2061	5MC	O2-C2	-3.04	1.18	1.23
26	S1	1866	OMC	C6-N1	3.03	1.45	1.38
1	1	858	A2M	C5-C4	-3.03	1.33	1.39
6	7	43	A2M	C5-N7	-3.03	1.33	1.39
26	S1	1833	OMU	O4-C4	-3.02	1.18	1.24
26	S1	1647	OMG	C5-N7	-3.02	1.33	1.39
26	S1	1979	OMU	O4-C4	-3.02	1.18	1.24
26	S1	1621	OMU	O4-C4	-3.01	1.18	1.24
85	2	382	A2M	C5-C4	-3.01	1.33	1.39
1	1	1527	OMC	O2-C2	-3.01	1.18	1.23
26	S1	2185	MA6	C5-N7	-3.00	1.33	1.39
26	S1	1478	OMG	O6-C6	-3.00	1.17	1.23
26	S1	1478	OMG	C5-N7	-3.00	1.33	1.39
1	1	681	A2M	C5-C4	-3.00	1.33	1.39
1	1	305	A2M	C5-N7	-3.00	1.33	1.39
26	S1	2048	PSU	O4-C4	-2.99	1.17	1.23
26	S1	2021	A2M	O2'-C2'	2.98	1.50	1.42
1	1	959[B]	OMG	C5-N7	-2.98	1.33	1.39
26	S1	600	OMG	C5-N7	-2.98	1.33	1.39
26	S1	1866	OMC	O2-C2	-2.98	1.18	1.23
1	1	858	A2M	C5-N7	-2.96	1.33	1.39
26	S1	38	OMC	C6-N1	2.96	1.45	1.38
26	S1	12	PSU	O4-C4	-2.96	1.18	1.23
6	7	43	A2M	O3'-C3'	-2.95	1.35	1.43
1	1	1539	A2M	O3'-C3'	-2.95	1.35	1.43
6	7	162	A2M	C5-N7	-2.93	1.33	1.39
85	2	95	A2M	O3'-C3'	-2.93	1.35	1.43
1	1	407	A2M	O3'-C3'	-2.93	1.35	1.43
1	1	681	A2M	O3'-C3'	-2.92	1.35	1.43
26	S1	1623	OMG	C5-N7	-2.92	1.33	1.39
26	S1	1829	OMG	C5-N7	-2.92	1.33	1.39
1	1	305	A2M	O3'-C3'	-2.92	1.35	1.43
26	S1	1879	OMG	C5-N7	-2.89	1.33	1.39
26	S1	2184	MA6	C5-N7	-2.89	1.33	1.39
26	S1	1657	PSU	O4-C4	-2.89	1.18	1.23
26	S1	2151	OMG	C5-N7	-2.89	1.33	1.39
1	1	1010	OMC	O2-C2	-2.89	1.18	1.23
26	S1	1550	OMG	C5-N7	-2.89	1.33	1.39
1	1	695	OMC	O2-C2	-2.88	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	305	A2M	O2'-C2'	2.88	1.49	1.42
26	S1	1865	OMG	C5-N7	-2.88	1.33	1.39
1	1	955	A2M	O3'-C3'	-2.87	1.35	1.43
26	S1	1647	OMG	O6-C6	-2.87	1.18	1.23
1	1	1171	PSU	O4-C4	-2.87	1.18	1.23
1	1	235	A2M	O3'-C3'	-2.86	1.35	1.43
85	2	443	OMC	O2-C2	-2.86	1.18	1.23
1	1	1626	OMG	C5-N7	-2.86	1.33	1.39
85	2	437	PSU	O4-C4	-2.86	1.18	1.23
26	S1	1246	PSU	O4-C4	-2.85	1.18	1.23
1	1	927	A2M	O3'-C3'	-2.85	1.35	1.43
26	S1	600	OMG	O6-C6	-2.85	1.18	1.23
85	2	71	OMG	C5-N7	-2.84	1.33	1.39
85	2	382	A2M	O3'-C3'	-2.84	1.35	1.43
1	1	856	OMG	C5-N7	-2.84	1.33	1.39
26	S1	98	A2M	O3'-C3'	-2.84	1.35	1.43
1	1	955	A2M	C8-N9	-2.84	1.32	1.37
1	1	1371	OMU	C6-N1	2.84	1.44	1.38
26	S1	1544	5MC	O2-C2	-2.83	1.18	1.23
3	4	74	OMG	C5-N7	-2.83	1.33	1.39
26	S1	2046	PSU	O4-C4	-2.83	1.18	1.23
26	S1	1156	PSU	O4-C4	-2.83	1.18	1.23
1	1	672	PSU	O4-C4	-2.83	1.18	1.23
26	S1	18	OMC	C6-N1	2.82	1.44	1.38
1	1	1524	OMG	C5-N7	-2.82	1.33	1.39
1	1	1017	PSU	O4-C4	-2.81	1.18	1.23
1	1	1540	OMG	O6-C6	-2.81	1.18	1.23
1	1	870	PSU	O4-C4	-2.81	1.18	1.23
26	S1	8	OMU	O2-C2	-2.81	1.18	1.23
6	7	162	A2M	C8-N9	-2.81	1.32	1.37
1	1	678	A2M	O3'-C3'	-2.80	1.36	1.43
85	2	78	PSU	O4-C4	-2.80	1.18	1.23
6	7	75	OMG	C5-N7	-2.79	1.33	1.39
1	1	959[A]	OMG	C2-N1	2.79	1.44	1.37
26	S1	455	PSU	O4-C4	-2.79	1.18	1.23
2	3	13	OMU	C6-N1	2.78	1.44	1.38
1	1	1190	OMG	O6-C6	-2.78	1.18	1.23
6	7	162	A2M	O3'-C3'	-2.78	1.36	1.43
26	S1	2140	OMC	O2-C2	-2.77	1.18	1.23
26	S1	98	A2M	C8-N9	-2.77	1.32	1.37
1	1	1659	OMU	C6-N1	2.77	1.44	1.38
1	1	1540	OMG	C5-N7	-2.77	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	940	PSU	O4-C4	-2.77	1.18	1.23
85	2	359	OMC	O2-C2	-2.77	1.18	1.23
6	7	7	OMU	C6-N1	2.76	1.44	1.38
26	S1	661	OMU	O2-C2	-2.76	1.18	1.23
85	2	73	OMU	C6-N1	2.76	1.44	1.38
1	1	1528	PSU	O4-C4	-2.76	1.18	1.23
26	S1	1979	OMU	C6-N1	2.76	1.44	1.38
1	1	1626	OMG	C2-N1	2.76	1.44	1.37
1	1	959[B]	OMG	C2-N1	2.76	1.44	1.37
26	S1	1833	OMU	C6-N1	2.76	1.44	1.38
6	7	75	OMG	C2-N1	2.76	1.44	1.37
1	1	1107	OMU	C6-N1	2.75	1.44	1.38
26	S1	1621	OMU	C6-N1	2.75	1.44	1.38
26	S1	2151	OMG	O6-C6	-2.75	1.18	1.23
26	S1	1478	OMG	C4-N9	-2.75	1.31	1.38
1	1	927	A2M	C8-N9	-2.75	1.32	1.37
1	1	697	A2M	O3'-C3'	-2.75	1.36	1.43
26	S1	104	PSU	O4-C4	-2.75	1.18	1.23
26	S1	1829	OMG	O6-C6	-2.74	1.18	1.23
1	1	1181	PSU	O4-C4	-2.74	1.18	1.23
1	1	856	OMG	O6-C6	-2.74	1.18	1.23
1	1	858	A2M	O3'-C3'	-2.74	1.36	1.43
1	1	1626	OMG	O6-C6	-2.74	1.18	1.23
26	S1	1879	OMG	O6-C6	-2.74	1.18	1.23
1	1	1190	OMG	C5-N7	-2.73	1.33	1.39
26	S1	609	PSU	O4-C4	-2.73	1.18	1.23
6	7	69	PSU	O4-C4	-2.73	1.18	1.23
85	2	56	OMU	C6-N1	2.73	1.44	1.38
26	S1	1192	PSU	O4-C4	-2.73	1.18	1.23
1	1	847	OMU	C6-N1	2.73	1.44	1.38
85	2	71	OMG	O6-C6	-2.72	1.18	1.23
1	1	1402	PSU	O4-C4	-2.72	1.18	1.23
1	1	1664	PSU	O4-C4	-2.72	1.18	1.23
85	2	95	A2M	C8-N9	-2.72	1.32	1.37
3	4	74	OMG	C2-N1	2.72	1.44	1.37
1	1	681	A2M	O2'-C2'	2.72	1.49	1.42
1	1	1039	PSU	O4-C4	-2.71	1.18	1.23
26	S1	1539	PSU	O4-C4	-2.71	1.18	1.23
26	S1	2021	A2M	O3'-C3'	-2.71	1.36	1.43
1	1	959[A]	OMG	C5-N7	-2.71	1.33	1.39
1	1	1533	PSU	O4-C4	-2.70	1.18	1.23
26	S1	1841	PSU	O4-C4	-2.70	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	305	A2M	C8-N9	-2.70	1.33	1.37
1	1	1524	OMG	C2-N1	2.70	1.44	1.37
26	S1	1623	OMG	O6-C6	-2.70	1.18	1.23
26	S1	1533	PSU	O4-C4	-2.70	1.18	1.23
1	1	239	PSU	O4-C4	-2.69	1.18	1.23
26	S1	1865	OMG	O6-C6	-2.69	1.18	1.23
3	4	74	OMG	O6-C6	-2.69	1.18	1.23
26	S1	1550	OMG	C2-N1	2.69	1.44	1.37
6	7	162	A2M	O2'-C2'	2.69	1.49	1.42
1	1	1190	OMG	C2-N1	2.68	1.44	1.37
26	S1	1829	OMG	C2-N1	2.68	1.44	1.37
1	1	678	A2M	O2'-C2'	2.68	1.49	1.42
1	1	681	A2M	C8-N9	-2.67	1.33	1.37
1	1	235	A2M	O2'-C2'	2.67	1.49	1.42
1	1	422	PSU	O4-C4	-2.67	1.18	1.23
26	S1	1879	OMG	C2-N1	2.67	1.44	1.37
26	S1	1623	OMG	C2-N1	2.67	1.44	1.37
26	S1	1865	OMG	C2-N1	2.67	1.44	1.37
26	S1	29	OMU	O2-C2	-2.67	1.18	1.23
85	2	71	OMG	C2-N1	2.66	1.44	1.37
1	1	1540	OMG	C2-N1	2.66	1.44	1.37
85	2	95	A2M	O2'-C2'	2.66	1.49	1.42
1	1	1539	A2M	O2'-C2'	2.65	1.49	1.42
1	1	856	OMG	C2-N1	2.65	1.44	1.37
26	S1	33	PSU	O4-C4	-2.65	1.18	1.23
26	S1	1647	OMG	C4-N9	-2.64	1.31	1.38
6	7	74	PSU	O4-C4	-2.64	1.18	1.23
26	S1	512	A2M	O2'-C2'	2.64	1.49	1.42
1	1	1011	PSU	O4-C4	-2.64	1.18	1.23
26	S1	1566	PSU	O4-C4	-2.64	1.18	1.23
6	7	43	A2M	O2'-C2'	2.63	1.49	1.42
1	1	858	A2M	O2'-C2'	2.63	1.49	1.42
6	7	75	OMG	O6-C6	-2.62	1.18	1.23
1	1	959[B]	OMG	O6-C6	-2.62	1.18	1.23
26	S1	1478	OMG	C2-N1	2.62	1.44	1.37
26	S1	607	PSU	O4-C4	-2.62	1.18	1.23
26	S1	479	A2M	O2'-C2'	2.62	1.49	1.42
1	1	1540	OMG	C4-N9	-2.62	1.31	1.38
85	2	472	PSU	O4-C4	-2.62	1.18	1.23
26	S1	668	A2M	C8-N9	-2.61	1.33	1.37
1	1	407	A2M	O2'-C2'	2.61	1.49	1.42
26	S1	479	A2M	C8-N9	-2.61	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1371	OMU	O2-C2	-2.61	1.18	1.23
1	1	1659	OMU	O2-C2	-2.61	1.18	1.23
85	2	56	OMU	O2-C2	-2.60	1.18	1.23
85	2	382	A2M	O2'-C2'	2.60	1.49	1.42
6	7	43	A2M	C8-N9	-2.59	1.33	1.37
1	1	955	A2M	O2'-C2'	2.59	1.49	1.42
26	S1	661	OMU	C6-N1	2.59	1.44	1.38
1	1	847	OMU	O2-C2	-2.59	1.18	1.23
26	S1	29	OMU	C6-N1	2.59	1.44	1.38
1	1	1524	OMG	O6-C6	-2.58	1.18	1.23
85	2	73	OMU	O2-C2	-2.58	1.18	1.23
26	S1	2151	OMG	C2-N1	2.58	1.43	1.37
26	S1	1550	OMG	O6-C6	-2.58	1.18	1.23
1	1	927	A2M	O2'-C2'	2.58	1.49	1.42
1	1	1190	OMG	C4-N9	-2.58	1.31	1.38
1	1	697	A2M	C8-N9	-2.57	1.33	1.37
26	S1	1543	C4J	O2-C2	-2.57	1.17	1.22
26	S1	668	A2M	O2'-C2'	2.56	1.49	1.42
6	7	7	OMU	O2-C2	-2.56	1.18	1.23
26	S1	1979	OMU	O2-C2	-2.55	1.18	1.23
26	S1	8	OMU	C6-N1	2.55	1.44	1.38
26	S1	98	A2M	O2'-C2'	2.54	1.48	1.42
1	1	678	A2M	C8-N9	-2.54	1.33	1.37
3	4	74	OMG	C4-N9	-2.54	1.31	1.38
1	1	697	A2M	O2'-C2'	2.54	1.48	1.42
1	1	1539	A2M	C8-N9	-2.54	1.33	1.37
26	S1	600	OMG	C2-N1	2.54	1.43	1.37
26	S1	2185	MA6	C4-N9	-2.53	1.32	1.37
1	1	959[A]	OMG	O6-C6	-2.52	1.18	1.23
26	S1	1647	OMG	C2-N1	2.52	1.43	1.37
26	S1	1621	OMU	O2-C2	-2.51	1.18	1.23
1	1	845	OMU	C6-N1	2.51	1.44	1.38
26	S1	512	A2M	C8-N9	-2.51	1.33	1.37
26	S1	1833	OMU	O2-C2	-2.51	1.18	1.23
85	2	382	A2M	C8-N9	-2.50	1.33	1.37
2	3	13	OMU	O2-C2	-2.50	1.18	1.23
1	1	1107	OMU	O2-C2	-2.48	1.18	1.23
26	S1	668	A2M	O3'-C3'	-2.48	1.36	1.43
1	1	959[B]	OMG	C5-C6	2.48	1.53	1.44
1	1	1626	OMG	C4-N9	-2.47	1.31	1.38
1	1	407	A2M	C8-N9	-2.47	1.33	1.37
85	2	71	OMG	C5-C6	2.46	1.53	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	959[A]	OMG	C5-C6	2.46	1.53	1.44
1	1	1524	OMG	C5-C6	2.46	1.53	1.44
26	S1	2151	OMG	C4-N9	-2.45	1.31	1.38
6	7	75	OMG	C5-C6	2.44	1.53	1.44
1	1	959[A]	OMG	C6-N1	2.44	1.43	1.38
1	1	1190	OMG	C5-C6	2.44	1.53	1.44
26	S1	2021	A2M	C8-N9	-2.44	1.33	1.37
26	S1	479	A2M	O3'-C3'	-2.43	1.36	1.43
85	2	359	OMC	C5-C4	2.43	1.48	1.42
1	1	856	OMG	C5-C6	2.43	1.53	1.44
1	1	856	OMG	C4-N9	-2.42	1.31	1.38
1	1	1540	OMG	C5-C6	2.42	1.53	1.44
26	S1	1865	OMG	C4-N9	-2.41	1.31	1.38
26	S1	1879	OMG	C4-N9	-2.40	1.31	1.38
1	1	1626	OMG	C6-N1	2.40	1.43	1.38
26	S1	2151	OMG	C5-C6	2.39	1.53	1.44
26	S1	1550	OMG	C5-C6	2.39	1.53	1.44
26	S1	1623	OMG	C5-C6	2.39	1.53	1.44
1	1	858	A2M	C8-N9	-2.38	1.33	1.37
3	4	74	OMG	C5-C6	2.38	1.53	1.44
1	1	1626	OMG	C5-C6	2.38	1.53	1.44
26	S1	2184	MA6	C4-N9	-2.38	1.32	1.37
26	S1	1865	OMG	C5-C6	2.38	1.53	1.44
26	S1	1833	OMU	C5-C4	2.37	1.48	1.43
26	S1	1829	OMG	C4-N9	-2.36	1.32	1.38
6	7	75	OMG	C6-N1	2.36	1.43	1.38
1	1	959[B]	OMG	C6-N1	2.36	1.43	1.38
3	4	74	OMG	C6-N1	2.35	1.43	1.38
85	2	71	OMG	C4-N9	-2.35	1.32	1.38
26	S1	600	OMG	C4-N9	-2.35	1.32	1.38
26	S1	1829	OMG	C5-C6	2.35	1.53	1.44
26	S1	1879	OMG	C5-C6	2.34	1.53	1.44
1	1	1010	OMC	C5-C4	2.34	1.48	1.42
85	2	443	OMC	C5-C4	2.33	1.48	1.42
26	S1	600	OMG	C5-C6	2.33	1.53	1.44
1	1	1524	OMG	C6-N1	2.33	1.43	1.38
1	1	695	OMC	C5-C4	2.32	1.48	1.42
1	1	235	A2M	C8-N9	-2.32	1.33	1.37
1	1	1524	OMG	C4-N9	-2.32	1.32	1.38
6	7	75	OMG	C4-N9	-2.32	1.32	1.38
1	1	1107	OMU	C5-C4	2.31	1.48	1.43
1	1	959[A]	OMG	C4-N9	-2.31	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	1979	OMU	C5-C4	2.30	1.48	1.43
26	S1	1550	OMG	C4-N9	-2.30	1.32	1.38
26	S1	1621	OMU	C5-C4	2.30	1.48	1.43
85	2	56	OMU	C5-C4	2.30	1.48	1.43
2	3	13	OMU	C5-C4	2.30	1.48	1.43
1	1	1659	OMU	C5-C4	2.29	1.48	1.43
26	S1	1866	OMC	C5-C4	2.29	1.48	1.42
26	S1	1550	OMG	C6-N1	2.28	1.43	1.38
26	S1	1478	OMG	C5-C6	2.27	1.52	1.44
6	7	7	OMU	C5-C4	2.27	1.48	1.43
1	1	1190	OMG	C6-N1	2.27	1.43	1.38
26	S1	1647	OMG	C5-C6	2.27	1.52	1.44
26	S1	1879	OMG	C6-N1	2.27	1.43	1.38
1	1	856	OMG	C6-N1	2.26	1.43	1.38
26	S1	1623	OMG	C4-N9	-2.25	1.32	1.38
85	2	71	OMG	C6-N1	2.25	1.43	1.38
1	1	1011	PSU	O4'-C1'	-2.24	1.40	1.43
26	S1	1829	OMG	C6-N1	2.24	1.43	1.38
26	S1	2151	OMG	C6-N1	2.24	1.43	1.38
1	1	1540	OMG	C6-N1	2.24	1.43	1.38
26	S1	2140	OMC	C5-C4	2.24	1.48	1.42
1	1	1371	OMU	C5-C4	2.23	1.48	1.43
1	1	847	OMU	C5-C4	2.22	1.48	1.43
26	S1	38	OMC	C5-C4	2.22	1.48	1.42
85	2	73	OMU	C5-C4	2.21	1.48	1.43
26	S1	8	OMU	C5-C4	2.20	1.48	1.43
26	S1	1623	OMG	C6-N1	2.20	1.43	1.38
6	7	69	PSU	O4'-C1'	-2.20	1.40	1.43
1	1	1527	OMC	C5-C4	2.20	1.48	1.42
26	S1	1865	OMG	C6-N1	2.19	1.42	1.38
26	S1	1543	C4J	C31-C3	2.18	1.59	1.52
1	1	845	OMU	C5-C4	2.16	1.48	1.43
26	S1	29	OMU	C5-C4	2.14	1.48	1.43
26	S1	1478	OMG	C6-N1	2.13	1.42	1.38
26	S1	2184	MA6	C8-N9	-2.12	1.33	1.37
26	S1	33	PSU	O4'-C1'	-2.10	1.40	1.43
26	S1	2185	MA6	C8-N9	-2.09	1.34	1.37
26	S1	1566	PSU	C4-C5	2.07	1.50	1.44
26	S1	661	OMU	C5-C4	2.06	1.48	1.43
26	S1	600	OMG	C6-N1	2.06	1.42	1.38
6	7	69	PSU	C4-C5	2.05	1.50	1.44
26	S1	2202	PSU	O4'-C1'	-2.05	1.41	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	18	OMC	C5-C4	2.04	1.47	1.42
1	1	1181	PSU	C4-C5	2.01	1.49	1.44
26	S1	1192	PSU	O4'-C1'	-2.01	1.41	1.43
1	1	1011	PSU	C4-C5	2.00	1.49	1.44

All (732) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	2185	MA6	N1-C6-N6	-9.89	104.81	116.86
26	S1	2184	MA6	N1-C6-N6	-9.67	105.07	116.86
1	1	677	1MA	C1'-N9-C8	-9.42	99.97	126.73
1	1	677	1MA	C1'-N9-C4	9.19	153.63	126.49
26	S1	1623	OMG	C1'-N9-C8	-8.15	103.59	126.73
26	S1	1550	OMG	C1'-N9-C8	-8.05	103.87	126.73
26	S1	600	OMG	C1'-N9-C8	-7.95	104.16	126.73
26	S1	1879	OMG	C1'-N9-C8	-7.93	104.21	126.73
26	S1	1829	OMG	C1'-N9-C8	-7.89	104.31	126.73
1	1	959[A]	OMG	C1'-N9-C8	-7.82	104.52	126.73
6	7	75	OMG	C1'-N9-C8	-7.58	105.19	126.73
3	4	74	OMG	C1'-N9-C8	-7.56	105.27	126.73
1	1	1540	OMG	C1'-N9-C8	-7.48	105.49	126.73
1	1	1626	OMG	C1'-N9-C8	-7.47	105.51	126.73
26	S1	2151	OMG	C1'-N9-C8	-7.46	105.54	126.73
1	1	1524	OMG	C1'-N9-C8	-7.46	105.55	126.73
1	1	856	OMG	C1'-N9-C8	-7.44	105.58	126.73
26	S1	1865	OMG	C1'-N9-C8	-7.42	105.66	126.73
26	S1	1647	OMG	C1'-N9-C8	-7.36	105.81	126.73
1	1	678	A2M	O2'-C2'-C1'	7.35	122.94	108.99
85	2	71	OMG	C1'-N9-C8	-7.26	106.11	126.73
26	S1	1478	OMG	C1'-N9-C8	-7.21	106.26	126.73
26	S1	1623	OMG	C1'-N9-C4	7.01	147.19	126.49
1	1	1190	OMG	C1'-N9-C8	-6.87	107.20	126.73
26	S1	1550	OMG	C1'-N9-C4	6.87	146.77	126.49
26	S1	1829	OMG	C1'-N9-C4	6.78	146.51	126.49
26	S1	600	OMG	C1'-N9-C4	6.73	146.37	126.49
26	S1	1879	OMG	C1'-N9-C4	6.71	146.31	126.49
6	7	75	OMG	C1'-N9-C4	6.46	145.58	126.49
1	1	959[A]	OMG	C1'-N9-C4	6.45	145.54	126.49
1	1	959[B]	OMG	C1'-N9-C8	-6.43	108.47	126.73
3	4	74	OMG	C1'-N9-C4	6.34	145.20	126.49
26	S1	1865	OMG	C1'-N9-C4	6.32	145.16	126.49
1	1	856	OMG	C1'-N9-C4	6.32	145.16	126.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1626	OMG	C1'-N9-C4	6.29	145.07	126.49
26	S1	2185	MA6	C5-C6-N6	6.29	135.29	125.33
1	1	1524	OMG	C1'-N9-C4	6.28	145.04	126.49
26	S1	2151	OMG	C1'-N9-C4	6.27	145.00	126.49
1	1	1540	OMG	C1'-N9-C4	6.23	144.89	126.49
85	2	71	OMG	C1'-N9-C4	6.20	144.79	126.49
1	1	845	OMU	C4-N3-C2	-6.19	118.93	126.61
26	S1	1647	OMG	C1'-N9-C4	6.10	144.51	126.49
26	S1	2184	MA6	C5-C6-N6	6.09	134.98	125.33
26	S1	8	OMU	C4-N3-C2	-6.07	119.07	126.61
1	1	959[B]	OMG	C1'-N9-C4	6.04	144.32	126.49
26	S1	1478	OMG	C1'-N9-C4	6.04	144.31	126.49
26	S1	661	OMU	C4-N3-C2	-5.87	119.33	126.61
26	S1	1833	OMU	C4-N3-C2	-5.86	119.33	126.61
26	S1	29	OMU	C4-N3-C2	-5.85	119.35	126.61
85	2	56	OMU	C4-N3-C2	-5.83	119.37	126.61
1	1	235	A2M	N3-C2-N1	-5.78	119.84	128.58
1	1	847	OMU	C4-N3-C2	-5.77	119.45	126.61
1	1	1107	OMU	C4-N3-C2	-5.75	119.47	126.61
26	S1	1979	OMU	C4-N3-C2	-5.73	119.50	126.61
1	1	1659	OMU	C4-N3-C2	-5.70	119.54	126.61
2	3	13	OMU	C4-N3-C2	-5.69	119.54	126.61
6	7	7	OMU	C4-N3-C2	-5.69	119.55	126.61
26	S1	1621	OMU	C4-N3-C2	-5.65	119.60	126.61
1	1	1190	OMG	C1'-N9-C4	5.64	143.16	126.49
1	1	697	A2M	N3-C2-N1	-5.59	120.12	128.58
85	2	382	A2M	N3-C2-N1	-5.58	120.14	128.58
1	1	677	1MA	N1-C2-N3	-5.57	119.37	126.00
1	1	858	A2M	N3-C2-N1	-5.56	120.17	128.58
26	S1	668	A2M	N3-C2-N1	-5.56	120.17	128.58
85	2	73	OMU	C4-N3-C2	-5.55	119.72	126.61
26	S1	2185	MA6	N1-C2-N3	-5.55	120.19	128.58
26	S1	2184	MA6	N1-C2-N3	-5.54	120.19	128.58
6	7	162	A2M	N3-C2-N1	-5.54	120.20	128.58
26	S1	479	A2M	N3-C2-N1	-5.48	120.29	128.58
1	1	1539	A2M	N3-C2-N1	-5.47	120.30	128.58
1	1	681	A2M	C5-C4-N3	-5.47	119.19	126.72
1	1	305	A2M	C5-C4-N3	-5.46	119.20	126.72
26	S1	98	A2M	C5-C4-N3	-5.45	119.21	126.72
1	1	407	A2M	C5-C4-N3	-5.43	119.23	126.72
26	S1	2021	A2M	N3-C2-N1	-5.43	120.36	128.58
1	1	955	A2M	N3-C2-N1	-5.42	120.39	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	681	A2M	N3-C2-N1	-5.41	120.39	128.58
6	7	43	A2M	N3-C2-N1	-5.41	120.39	128.58
1	1	407	A2M	N3-C2-N1	-5.40	120.40	128.58
1	1	927	A2M	N3-C2-N1	-5.40	120.42	128.58
1	1	1371	OMU	C4-N3-C2	-5.39	119.92	126.61
1	1	927	A2M	C5-C4-N3	-5.38	119.31	126.72
26	S1	512	A2M	C5-C4-N3	-5.33	119.38	126.72
85	2	382	A2M	C5-C4-N3	-5.30	119.42	126.72
26	S1	98	A2M	N3-C2-N1	-5.29	120.57	128.58
1	1	235	A2M	C5-C4-N3	-5.28	119.44	126.72
26	S1	479	A2M	C5-C4-N3	-5.26	119.47	126.72
1	1	678	A2M	N3-C2-N1	-5.25	120.63	128.58
85	2	95	A2M	C5-C4-N3	-5.24	119.50	126.72
1	1	858	A2M	C5-C4-N3	-5.23	119.51	126.72
1	1	1539	A2M	C5-C4-N3	-5.23	119.52	126.72
26	S1	668	A2M	C5-C4-N3	-5.22	119.53	126.72
1	1	305	A2M	N3-C2-N1	-5.21	120.69	128.58
1	1	697	A2M	C5-C4-N3	-5.21	119.55	126.72
85	2	95	A2M	N3-C2-N1	-5.19	120.73	128.58
1	1	678	A2M	C5-C4-N3	-5.18	119.58	126.72
26	S1	2021	A2M	C5-C4-N3	-5.17	119.59	126.72
26	S1	668	A2M	N6-C6-N1	-5.17	106.86	118.38
26	S1	512	A2M	N3-C2-N1	-5.16	120.76	128.58
1	1	955	A2M	C5-C4-N3	-5.16	119.62	126.72
1	1	681	A2M	N6-C6-N1	-5.15	106.90	118.38
6	7	43	A2M	C5-C4-N3	-5.15	119.62	126.72
1	1	959[B]	OMG	C5-C4-N3	-5.15	120.19	128.39
26	S1	2046	PSU	C4-N3-C2	-5.13	119.30	126.37
1	1	858	A2M	N6-C6-N1	-5.13	106.95	118.38
26	S1	2021	A2M	N6-C6-N1	-5.07	107.07	118.38
26	S1	1995	7MG	C5-C6-N1	5.06	119.85	110.94
1	1	678	A2M	O4'-C1'-C2'	-5.06	97.87	106.59
6	7	162	A2M	C5-C4-N3	-5.04	119.78	126.72
1	1	870	PSU	C4-N3-C2	-5.03	119.44	126.37
26	S1	1657	PSU	C4-N3-C2	-5.03	119.44	126.37
1	1	927	A2M	N6-C6-N1	-5.03	107.18	118.38
6	7	162	A2M	N6-C6-N1	-5.01	107.22	118.38
85	2	382	A2M	N6-C6-N1	-5.01	107.23	118.38
26	S1	455	PSU	C4-N3-C2	-5.00	119.48	126.37
85	2	437	PSU	C4-N3-C2	-5.00	119.49	126.37
26	S1	1246	PSU	C4-N3-C2	-4.99	119.49	126.37
26	S1	1156	PSU	C4-N3-C2	-4.98	119.51	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	845	OMU	N3-C2-N1	4.96	121.35	114.89
1	1	305	A2M	N6-C6-N1	-4.96	107.34	118.38
1	1	677	1MA	C5-C4-N3	-4.95	119.98	127.27
1	1	1171	PSU	C4-N3-C2	-4.95	119.55	126.37
26	S1	609	PSU	C4-N3-C2	-4.94	119.57	126.37
26	S1	2048	PSU	C4-N3-C2	-4.93	119.58	126.37
26	S1	1841	PSU	N1-C2-N3	4.92	120.36	115.17
1	1	1533	PSU	C4-N3-C2	-4.90	119.62	126.37
85	2	78	PSU	C4-N3-C2	-4.89	119.64	126.37
26	S1	12	PSU	C4-N3-C2	-4.88	119.65	126.37
1	1	1039	PSU	C4-N3-C2	-4.86	119.68	126.37
1	1	672	PSU	C4-N3-C2	-4.84	119.70	126.37
26	S1	1623	OMG	C5-C4-N3	-4.84	120.69	128.39
26	S1	104	PSU	C4-N3-C2	-4.82	119.73	126.37
1	1	940	PSU	C4-N3-C2	-4.82	119.74	126.37
1	1	1017	PSU	C4-N3-C2	-4.80	119.75	126.37
26	S1	2046	PSU	N1-C2-N3	4.80	120.23	115.17
1	1	955	A2M	N6-C6-N1	-4.80	107.69	118.38
6	7	74	PSU	C4-N3-C2	-4.79	119.77	126.37
1	1	1528	PSU	C4-N3-C2	-4.78	119.79	126.37
1	1	239	PSU	C4-N3-C2	-4.77	119.80	126.37
1	1	1664	PSU	C4-N3-C2	-4.77	119.80	126.37
26	S1	1550	OMG	C5-C4-N3	-4.76	120.81	128.39
85	2	472	PSU	C4-N3-C2	-4.75	119.83	126.37
26	S1	455	PSU	N1-C2-N3	4.74	120.17	115.17
26	S1	479	A2M	N6-C6-N1	-4.74	107.82	118.38
85	2	95	A2M	N6-C6-N1	-4.73	107.84	118.38
26	S1	1246	PSU	N1-C2-N3	4.73	120.16	115.17
26	S1	1841	PSU	C4-N3-C2	-4.71	119.88	126.37
26	S1	600	OMG	C5-C4-N3	-4.71	120.90	128.39
26	S1	609	PSU	N1-C2-N3	4.71	120.13	115.17
26	S1	2184	MA6	C5-C4-N3	-4.70	120.24	126.72
26	S1	1533	PSU	C4-N3-C2	-4.70	119.90	126.37
1	1	697	A2M	N6-C6-N1	-4.69	107.92	118.38
26	S1	1539	PSU	C4-N3-C2	-4.69	119.92	126.37
6	7	43	A2M	N6-C6-N1	-4.68	107.94	118.38
26	S1	1829	OMG	C5-C4-N3	-4.68	120.94	128.39
26	S1	2048	PSU	N1-C2-N3	4.68	120.11	115.17
1	1	1533	PSU	N1-C2-N3	4.67	120.09	115.17
1	1	1181	PSU	C4-N3-C2	-4.67	119.94	126.37
26	S1	2202	PSU	C4-N3-C2	-4.66	119.95	126.37
26	S1	2185	MA6	C5-C4-N3	-4.65	120.31	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	422	PSU	C4-N3-C2	-4.64	119.98	126.37
6	7	69	PSU	C4-N3-C2	-4.64	119.98	126.37
85	2	472	PSU	N1-C2-N3	4.64	120.06	115.17
1	1	1524	OMG	C5-C4-N3	-4.63	121.02	128.39
1	1	959[B]	OMG	C2-N3-C4	4.61	120.25	112.30
26	S1	1156	PSU	N1-C2-N3	4.61	120.03	115.17
85	2	71	OMG	C5-C4-N3	-4.61	121.06	128.39
26	S1	1566	PSU	C4-N3-C2	-4.60	120.03	126.37
26	S1	607	PSU	C4-N3-C2	-4.60	120.03	126.37
26	S1	2151	OMG	C5-C4-N3	-4.60	121.07	128.39
1	1	1017	PSU	N1-C2-N3	4.60	120.02	115.17
26	S1	98	A2M	N6-C6-N1	-4.60	108.14	118.38
1	1	1011	PSU	C4-N3-C2	-4.59	120.05	126.37
26	S1	1879	OMG	C5-C4-N3	-4.58	121.10	128.39
6	7	75	OMG	C5-C4-N3	-4.58	121.10	128.39
26	S1	12	PSU	N1-C2-N3	4.57	119.99	115.17
26	S1	512	A2M	N6-C6-N1	-4.57	108.19	118.38
1	1	870	PSU	N1-C2-N3	4.57	119.99	115.17
1	1	678	A2M	N6-C6-N1	-4.57	108.20	118.38
1	1	1039	PSU	N1-C2-N3	4.57	119.98	115.17
26	S1	1657	PSU	N1-C2-N3	4.54	119.96	115.17
1	1	1539	A2M	N6-C6-N1	-4.54	108.26	118.38
26	S1	1865	OMG	C5-C4-N3	-4.54	121.16	128.39
26	S1	1539	PSU	N1-C2-N3	4.53	119.95	115.17
1	1	672	PSU	N1-C2-N3	4.53	119.94	115.17
1	1	1171	PSU	N1-C2-N3	4.52	119.94	115.17
85	2	437	PSU	N1-C2-N3	4.51	119.92	115.17
85	2	78	PSU	N1-C2-N3	4.51	119.92	115.17
26	S1	2151	OMG	C2-N3-C4	4.51	120.06	112.30
1	1	235	A2M	N6-C6-N1	-4.50	108.36	118.38
26	S1	1192	PSU	C4-N3-C2	-4.50	120.18	126.37
1	1	1664	PSU	N1-C2-N3	4.50	119.91	115.17
1	1	856	OMG	C5-C4-N3	-4.50	121.23	128.39
1	1	1528	PSU	N1-C2-N3	4.48	119.90	115.17
1	1	959[A]	OMG	C5-C4-N3	-4.48	121.26	128.39
26	S1	33	PSU	N1-C2-N3	4.48	119.89	115.17
26	S1	1995	7MG	C2-N3-C4	4.48	120.01	112.30
6	7	74	PSU	N1-C2-N3	4.47	119.89	115.17
26	S1	1647	OMG	C5-C4-N3	-4.47	121.27	128.39
1	1	407	A2M	N6-C6-N1	-4.46	108.43	118.38
1	1	678	A2M	N9-C8-N7	-4.45	107.62	113.94
26	S1	33	PSU	C4-N3-C2	-4.45	120.24	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	940	PSU	N1-C2-N3	4.44	119.86	115.17
1	1	239	PSU	N1-C2-N3	4.42	119.83	115.17
1	1	856	OMG	C2-N3-C4	4.41	119.90	112.30
6	7	75	OMG	C2-N3-C4	4.41	119.90	112.30
85	2	71	OMG	C2-N3-C4	4.41	119.89	112.30
26	S1	2184	MA6	N9-C8-N7	-4.41	107.68	113.94
26	S1	1623	OMG	C2-N3-C4	4.40	119.88	112.30
1	1	1011	PSU	N1-C2-N3	4.40	119.81	115.17
1	1	1626	OMG	C5-C4-N3	-4.39	121.39	128.39
26	S1	1879	OMG	C2-N3-C4	4.39	119.87	112.30
26	S1	1192	PSU	N1-C2-N3	4.38	119.79	115.17
1	1	1524	OMG	C2-N3-C4	4.37	119.83	112.30
1	1	1181	PSU	N1-C2-N3	4.37	119.77	115.17
26	S1	1550	OMG	C2-N3-C4	4.36	119.82	112.30
26	S1	1829	OMG	C2-N3-C4	4.36	119.81	112.30
1	1	1626	OMG	C2-N3-C4	4.36	119.81	112.30
1	1	1402	PSU	C4-N3-C2	-4.36	120.37	126.37
26	S1	600	OMG	C2-N3-C4	4.35	119.80	112.30
6	7	69	PSU	N1-C2-N3	4.35	119.75	115.17
26	S1	1533	PSU	N1-C2-N3	4.35	119.75	115.17
26	S1	1865	OMG	C2-N3-C4	4.32	119.74	112.30
1	1	1190	OMG	C2-N3-C4	4.32	119.73	112.30
26	S1	104	PSU	N1-C2-N3	4.31	119.72	115.17
26	S1	1478	OMG	C2-N3-C4	4.31	119.72	112.30
26	S1	1566	PSU	N1-C2-N3	4.30	119.71	115.17
1	1	959[A]	OMG	C2-N3-C4	4.30	119.71	112.30
3	4	74	OMG	C5-C4-N3	-4.30	121.55	128.39
26	S1	2185	MA6	N9-C8-N7	-4.30	107.84	113.94
26	S1	607	PSU	N1-C2-N3	4.30	119.70	115.17
3	4	74	OMG	C2-N3-C4	4.29	119.69	112.30
1	1	422	PSU	N1-C2-N3	4.28	119.69	115.17
26	S1	1647	OMG	C2-N3-C4	4.27	119.66	112.30
26	S1	8	OMU	N3-C2-N1	4.27	120.45	114.89
1	1	1402	PSU	N1-C2-N3	4.24	119.64	115.17
1	1	1540	OMG	C2-N3-C4	4.24	119.60	112.30
1	1	1190	OMG	C5-C4-N3	-4.20	121.71	128.39
26	S1	2202	PSU	N1-C2-N3	4.19	119.59	115.17
1	1	1540	OMG	C5-C4-N3	-4.17	121.75	128.39
26	S1	661	OMU	N3-C2-N1	4.16	120.31	114.89
26	S1	1833	OMU	N3-C2-N1	4.14	120.29	114.89
26	S1	1478	OMG	C5-C4-N3	-4.13	121.82	128.39
26	S1	1995	7MG	C5-C4-N3	-4.12	120.39	128.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	1543	C4J	C4-N3-C2	-4.10	120.58	125.62
1	1	678	A2M	C3'-C2'-C1'	-4.09	94.97	102.81
1	1	847	OMU	N3-C2-N1	4.08	120.20	114.89
26	S1	29	OMU	N3-C2-N1	4.06	120.18	114.89
1	1	305	A2M	N9-C8-N7	-4.04	108.21	113.94
1	1	1659	OMU	N3-C2-N1	4.02	120.12	114.89
1	1	1371	OMU	N3-C2-N1	4.01	120.11	114.89
1	1	681	A2M	C5-C6-N6	3.99	133.18	123.29
26	S1	33	PSU	C6-N1-C2	-3.99	118.99	122.69
26	S1	1995	7MG	C4-C5-N7	3.98	110.08	105.38
85	2	56	OMU	N3-C2-N1	3.98	120.08	114.89
26	S1	1841	PSU	C6-N1-C2	-3.96	119.02	122.69
85	2	382	A2M	C5-C6-N6	3.96	133.08	123.29
26	S1	2021	A2M	N9-C8-N7	-3.95	108.33	113.94
26	S1	668	A2M	C5-C6-N6	3.93	133.01	123.29
1	1	1107	OMU	N3-C2-N1	3.93	120.00	114.89
26	S1	2184	MA6	C4-C5-C6	3.93	119.97	115.91
1	1	677	1MA	C2-N3-C4	3.91	120.21	112.53
1	1	927	A2M	C5-C6-N6	3.90	132.94	123.29
6	7	162	A2M	C5-C6-N6	3.88	132.88	123.29
26	S1	1979	OMU	N3-C2-N1	3.88	119.94	114.89
26	S1	2021	A2M	C5-C6-N6	3.86	132.85	123.29
1	1	858	A2M	C5-C6-N6	3.86	132.84	123.29
6	7	7	OMU	N3-C2-N1	3.85	119.90	114.89
26	S1	2185	MA6	C4-C5-C6	3.84	119.88	115.91
26	S1	1647	OMG	N9-C8-N7	-3.84	106.27	113.40
26	S1	668	A2M	N9-C8-N7	-3.83	108.51	113.94
26	S1	1621	OMU	N3-C2-N1	3.82	119.86	114.89
85	2	73	OMU	N3-C2-N1	3.81	119.86	114.89
1	1	305	A2M	C5-C6-N6	3.81	132.72	123.29
26	S1	8	OMU	C5-C4-N3	3.81	120.13	114.80
1	1	1190	OMG	N9-C8-N7	-3.80	106.36	113.40
2	3	13	OMU	N3-C2-N1	3.79	119.83	114.89
1	1	1371	OMU	C1'-N1-C2	3.79	124.41	117.59
26	S1	661	OMU	C5-C4-N3	3.79	120.11	114.80
1	1	959[A]	OMG	N9-C8-N7	-3.77	106.41	113.40
1	1	858	A2M	N9-C8-N7	-3.76	108.60	113.94
85	2	95	A2M	C5-C6-N6	3.75	132.57	123.29
1	1	955	A2M	C5-C6-N6	3.74	132.56	123.29
1	1	1540	OMG	N9-C8-N7	-3.72	106.50	113.40
6	7	7	OMU	C5-C4-N3	3.72	120.00	114.80
85	2	56	OMU	C5-C4-N3	3.71	119.99	114.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	13	OMU	C5-C4-N3	3.70	119.99	114.80
1	1	1107	OMU	C5-C4-N3	3.69	119.97	114.80
26	S1	29	OMU	C5-C4-N3	3.68	119.96	114.80
85	2	73	OMU	C5-C4-N3	3.68	119.95	114.80
26	S1	1979	OMU	C5-C4-N3	3.68	119.95	114.80
1	1	697	A2M	C5-C6-N6	3.67	132.37	123.29
26	S1	1621	OMU	C5-C4-N3	3.66	119.93	114.80
6	7	43	A2M	C5-C6-N6	3.66	132.34	123.29
26	S1	2151	OMG	N9-C8-N7	-3.66	106.62	113.40
26	S1	512	A2M	N9-C8-N7	-3.65	108.75	113.94
1	1	845	OMU	C1'-N1-C2	3.65	124.15	117.59
1	1	1524	OMG	N9-C8-N7	-3.65	106.63	113.40
3	4	74	OMG	N9-C8-N7	-3.63	106.67	113.40
1	1	1659	OMU	C5-C4-N3	3.63	119.88	114.80
1	1	1402	PSU	C6-N1-C2	-3.63	119.33	122.69
26	S1	1833	OMU	C5-C4-N3	3.62	119.88	114.80
26	S1	600	OMG	N9-C8-N7	-3.61	106.71	113.40
26	S1	1478	OMG	N9-C8-N7	-3.61	106.71	113.40
1	1	847	OMU	C5-C4-N3	3.61	119.85	114.80
26	S1	479	A2M	C5-C6-N6	3.61	132.22	123.29
26	S1	1879	OMG	N9-C8-N7	-3.60	106.73	113.40
6	7	162	A2M	N9-C8-N7	-3.59	108.84	113.94
1	1	1626	OMG	N9-C8-N7	-3.58	106.76	113.40
1	1	235	A2M	C2-N3-C4	3.58	120.58	111.83
1	1	681	A2M	C2-N3-C4	3.57	120.55	111.83
1	1	856	OMG	N9-C8-N7	-3.55	106.82	113.40
1	1	678	A2M	C5-C6-N6	3.54	132.06	123.29
1	1	407	A2M	N9-C8-N7	-3.54	108.91	113.94
26	S1	98	A2M	C5-C6-N6	3.54	132.05	123.29
1	1	1371	OMU	C5-C4-N3	3.54	119.75	114.80
26	S1	512	A2M	C5-C6-N6	3.54	132.04	123.29
6	7	43	A2M	N9-C8-N7	-3.53	108.92	113.94
26	S1	1865	OMG	N9-C8-N7	-3.53	106.86	113.40
1	1	858	A2M	C2-N3-C4	3.53	120.45	111.83
1	1	955	A2M	N9-C8-N7	-3.52	108.94	113.94
6	7	75	OMG	N9-C8-N7	-3.52	106.88	113.40
1	1	1539	A2M	C5-C6-N6	3.52	132.00	123.29
26	S1	1550	OMG	N9-C8-N7	-3.50	106.91	113.40
26	S1	668	A2M	C2-N3-C4	3.50	120.37	111.83
85	2	472	PSU	C6-N1-C2	-3.49	119.45	122.69
1	1	927	A2M	C2-N3-C4	3.49	120.34	111.83
85	2	382	A2M	C2-N3-C4	3.48	120.33	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	2	71	OMG	N9-C8-N7	-3.48	106.95	113.40
26	S1	1192	PSU	C6-N1-C2	-3.48	119.46	122.69
1	1	407	A2M	C2-N3-C4	3.47	120.31	111.83
26	S1	479	A2M	C2-N3-C4	3.46	120.29	111.83
1	1	697	A2M	C2-N3-C4	3.46	120.28	111.83
26	S1	1623	OMG	N9-C8-N7	-3.45	107.00	113.40
1	1	1539	A2M	C2-N3-C4	3.45	120.26	111.83
6	7	162	A2M	C2-N3-C4	3.44	120.23	111.83
26	S1	1829	OMG	N9-C8-N7	-3.44	107.02	113.40
26	S1	2048	PSU	C6-N1-C2	-3.41	119.52	122.69
26	S1	98	A2M	C2-N3-C4	3.40	120.14	111.83
1	1	305	A2M	C2-N3-C4	3.40	120.14	111.83
1	1	955	A2M	C2-N3-C4	3.40	120.13	111.83
6	7	43	A2M	C2-N3-C4	3.40	120.13	111.83
26	S1	1539	PSU	C6-N1-C2	-3.39	119.54	122.69
1	1	927	A2M	N9-C8-N7	-3.39	109.12	113.94
85	2	95	A2M	N9-C8-N7	-3.39	109.13	113.94
26	S1	609	PSU	C6-N1-C2	-3.38	119.55	122.69
1	1	235	A2M	N9-C8-N7	-3.38	109.14	113.94
26	S1	2021	A2M	C2-N3-C4	3.37	120.07	111.83
26	S1	1544	5MC	C5-C6-N1	-3.37	119.65	123.31
1	1	1533	PSU	C6-N1-C2	-3.36	119.57	122.69
1	1	1017	PSU	C6-N1-C2	-3.35	119.58	122.69
1	1	422	PSU	C6-N1-C2	-3.35	119.58	122.69
1	1	235	A2M	C5-C6-N6	3.34	131.56	123.29
1	1	1011	PSU	C6-N1-C2	-3.33	119.60	122.69
1	1	1039	PSU	C6-N1-C2	-3.33	119.60	122.69
26	S1	512	A2M	C2-N3-C4	3.33	119.97	111.83
26	S1	2185	MA6	C2-N1-C6	3.31	119.91	111.83
1	1	407	A2M	C5-C6-N6	3.31	131.47	123.29
85	2	95	A2M	C2-N3-C4	3.31	119.91	111.83
26	S1	2184	MA6	C2-N1-C6	3.29	119.87	111.83
1	1	697	A2M	N9-C8-N7	-3.28	109.29	113.94
1	1	1539	A2M	N9-C8-N7	-3.28	109.29	113.94
26	S1	1246	PSU	C6-C5-C4	3.27	120.38	118.17
1	1	681	A2M	N9-C8-N7	-3.27	109.30	113.94
1	1	1528	PSU	C6-N1-C2	-3.27	119.66	122.69
26	S1	2185	MA6	C2-N3-C4	3.27	119.81	111.83
26	S1	2046	PSU	C6-N1-C2	-3.26	119.67	122.69
1	1	672	PSU	C6-N1-C2	-3.26	119.67	122.69
26	S1	2184	MA6	C2-N3-C4	3.26	119.78	111.83
1	1	678	A2M	N3-C4-N9	3.24	132.68	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	455	PSU	C6-N1-C2	-3.24	119.68	122.69
1	1	678	A2M	C2-N3-C4	3.24	119.74	111.83
1	1	1664	PSU	C6-N1-C2	-3.23	119.69	122.69
6	7	74	PSU	C6-N1-C2	-3.23	119.70	122.69
1	1	678	A2M	C2'-C3'-C4'	-3.22	95.06	101.99
26	S1	1246	PSU	C6-N1-C2	-3.22	119.70	122.69
1	1	305	A2M	N3-C4-N9	3.22	132.64	127.17
1	1	407	A2M	C2'-C1'-N9	-3.22	108.46	113.75
26	S1	98	A2M	N9-C8-N7	-3.21	109.38	113.94
26	S1	12	PSU	C6-N1-C2	-3.20	119.72	122.69
1	1	235	A2M	N3-C4-N9	3.19	132.59	127.17
26	S1	1647	OMG	C2-N1-C6	-3.18	119.34	125.11
6	7	69	PSU	C6-N1-C2	-3.18	119.74	122.69
26	S1	1995	7MG	C5-C4-N9	3.17	110.40	106.33
1	1	940	PSU	C6-N1-C2	-3.17	119.75	122.69
1	1	845	OMU	C5-C4-N3	3.16	119.23	114.80
1	1	239	PSU	C6-N1-C2	-3.16	119.76	122.69
1	1	678	A2M	C5-N7-C8	3.16	108.41	103.45
26	S1	1156	PSU	C6-N1-C2	-3.16	119.76	122.69
1	1	1181	PSU	C6-N1-C2	-3.15	119.76	122.69
1	1	407	A2M	N3-C4-N9	3.15	132.53	127.17
26	S1	607	PSU	C6-N1-C2	-3.15	119.77	122.69
26	S1	1533	PSU	C6-N1-C2	-3.15	119.77	122.69
26	S1	1550	OMG	C2-N1-C6	-3.13	119.43	125.11
1	1	1533	PSU	C6-C5-C4	3.13	120.28	118.17
26	S1	479	A2M	N9-C8-N7	-3.13	109.50	113.94
26	S1	1623	OMG	C2-N1-C6	-3.11	119.47	125.11
26	S1	1841	PSU	C6-C5-C4	3.10	120.27	118.17
1	1	1171	PSU	C6-N1-C2	-3.10	119.82	122.69
85	2	437	PSU	C6-N1-C2	-3.09	119.82	122.69
26	S1	2151	OMG	C2-N1-C6	-3.08	119.52	125.11
1	1	305	A2M	C5-N7-C8	3.08	108.30	103.45
85	2	78	PSU	C6-N1-C2	-3.08	119.83	122.69
26	S1	2202	PSU	C6-N1-C2	-3.08	119.84	122.69
26	S1	29	OMU	O4-C4-C5	-3.07	119.86	125.16
1	1	858	A2M	N3-C4-N9	3.07	132.39	127.17
26	S1	1657	PSU	C6-N1-C2	-3.06	119.85	122.69
26	S1	600	OMG	C2-N1-C6	-3.06	119.56	125.11
1	1	1524	OMG	C2-N1-C6	-3.06	119.56	125.11
26	S1	1621	OMU	O4-C4-C5	-3.05	119.91	125.16
26	S1	455	PSU	C6-C5-C4	3.04	120.22	118.17
26	S1	1879	OMG	C2-N1-C6	-3.04	119.60	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	1829	OMG	C2-N1-C6	-3.04	119.61	125.11
26	S1	1995	7MG	C2-N1-C6	-3.03	119.62	125.11
26	S1	2021	A2M	N3-C4-N9	3.03	132.31	127.17
2	3	13	OMU	O4-C4-C5	-3.02	119.95	125.16
26	S1	98	A2M	N3-C4-N9	3.02	132.30	127.17
6	7	7	OMU	O4-C4-C5	-3.01	119.97	125.16
26	S1	1566	PSU	C6-N1-C2	-3.01	119.90	122.69
26	S1	1979	OMU	O4-C4-C5	-3.00	119.99	125.16
1	1	959[B]	OMG	C2-N1-C6	-3.00	119.68	125.11
26	S1	1865	OMG	C2-N1-C6	-2.99	119.68	125.11
26	S1	661	OMU	O4-C4-C5	-2.99	120.00	125.16
85	2	382	A2M	N9-C8-N7	-2.99	109.69	113.94
85	2	56	OMU	O4-C4-C5	-2.99	120.01	125.16
26	S1	1478	OMG	C2-N1-C6	-2.99	119.69	125.11
85	2	71	OMG	C2-N1-C6	-2.98	119.71	125.11
26	S1	668	A2M	C3'-C2'-C1'	2.97	108.49	102.81
6	7	75	OMG	C2-N1-C6	-2.96	119.74	125.11
1	1	1626	OMG	C2-N1-C6	-2.95	119.75	125.11
1	1	1107	OMU	O4-C4-C5	-2.94	120.08	125.16
1	1	1659	OMU	O4-C4-C5	-2.94	120.09	125.16
1	1	847	OMU	O4-C4-C5	-2.93	120.10	125.16
26	S1	1623	OMG	N9-C4-N3	2.93	131.82	125.95
85	2	73	OMU	O4-C4-C5	-2.93	120.11	125.16
1	1	927	A2M	N3-C4-N9	2.93	132.15	127.17
26	S1	609	PSU	O2-C2-N1	-2.92	119.78	122.79
1	1	856	OMG	C2-N1-C6	-2.92	119.82	125.11
26	S1	2061	5MC	C5-C6-N1	-2.91	120.15	123.31
26	S1	1550	OMG	N9-C4-N3	2.91	131.77	125.95
1	1	870	PSU	C6-N1-C2	-2.90	120.00	122.69
1	1	1190	OMG	C2-N1-C6	-2.89	119.86	125.11
26	S1	2184	MA6	C5-N7-C8	2.89	108.00	103.45
26	S1	668	A2M	N3-C4-N9	2.89	132.08	127.17
26	S1	104	PSU	C6-N1-C2	-2.89	120.01	122.69
26	S1	512	A2M	N3-C4-N9	2.89	132.08	127.17
1	1	1039	PSU	C6-C5-C4	2.89	120.12	118.17
1	1	1540	OMG	C2-N1-C6	-2.88	119.88	125.11
85	2	472	PSU	C6-C5-C4	2.88	120.12	118.17
1	1	1533	PSU	O2-C2-N1	-2.88	119.82	122.79
85	2	382	A2M	N3-C4-N9	2.87	132.06	127.17
85	2	78	PSU	C6-C5-C4	2.87	120.11	118.17
3	4	74	OMG	C2-N1-C6	-2.87	119.91	125.11
26	S1	1833	OMU	O4-C4-C5	-2.87	120.22	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	600	OMG	N9-C4-N3	2.86	131.68	125.95
26	S1	2184	MA6	N3-C4-N9	2.86	132.03	127.17
26	S1	1995	7MG	O6-C6-C5	-2.86	120.61	127.62
26	S1	2021	A2M	C5-N7-C8	2.85	107.93	103.45
26	S1	609	PSU	C6-C5-C4	2.85	120.10	118.17
1	1	697	A2M	N3-C4-N9	2.84	132.00	127.17
1	1	681	A2M	C5-C4-N9	2.84	108.91	105.81
26	S1	2151	OMG	C5-C6-N1	2.83	120.44	113.25
1	1	959[A]	OMG	C2-N1-C6	-2.82	119.99	125.11
1	1	1017	PSU	O2-C2-N1	-2.82	119.88	122.79
6	7	162	A2M	N3-C4-N9	2.82	131.96	127.17
26	S1	1841	PSU	O2-C2-N1	-2.82	119.89	122.79
1	1	940	PSU	C6-C5-C4	2.81	120.07	118.17
85	2	472	PSU	O2-C2-N1	-2.81	119.89	122.79
85	2	95	A2M	N3-C4-N9	2.80	131.92	127.17
26	S1	1478	OMG	C5-C6-N1	2.79	120.36	113.25
26	S1	600	OMG	C5-C6-N1	2.79	120.35	113.25
1	1	681	A2M	N3-C4-N9	2.79	131.91	127.17
26	S1	668	A2M	C5-N7-C8	2.78	107.82	103.45
26	S1	2185	MA6	C5-N7-C8	2.78	107.82	103.45
26	S1	1879	OMG	C5-C6-N1	2.78	120.33	113.25
1	1	955	A2M	N3-C4-N9	2.78	131.89	127.17
26	S1	1647	OMG	C5-C6-N1	2.77	120.31	113.25
1	1	1664	PSU	C6-C5-C4	2.77	120.04	118.17
26	S1	1829	OMG	N9-C4-N3	2.77	131.49	125.95
1	1	1539	A2M	N3-C4-N9	2.76	131.86	127.17
26	S1	479	A2M	C5-C4-N9	2.76	108.82	105.81
1	1	959[A]	OMG	N9-C4-N3	2.76	131.46	125.95
26	S1	1550	OMG	C5-C6-N1	2.75	120.26	113.25
1	1	870	PSU	C6-C5-C4	2.75	120.03	118.17
85	2	71	OMG	C5-C6-N1	2.75	120.26	113.25
26	S1	1879	OMG	N9-C4-N3	2.75	131.45	125.95
1	1	239	PSU	C6-C5-C4	2.75	120.03	118.17
1	1	1371	OMU	O4-C4-C5	-2.74	120.44	125.16
1	1	672	PSU	O2-C2-N1	-2.74	119.96	122.79
26	S1	33	PSU	O2-C2-N1	-2.74	119.96	122.79
1	1	1626	OMG	C5-C6-N1	2.74	120.23	113.25
26	S1	512	A2M	C5-N7-C8	2.74	107.75	103.45
26	S1	1623	OMG	C5-C6-N1	2.74	120.22	113.25
1	1	1528	PSU	C6-C5-C4	2.74	120.02	118.17
1	1	858	A2M	C5-N7-C8	2.73	107.74	103.45
26	S1	1865	OMG	C5-C6-N1	2.72	120.19	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	8	OMU	O4-C4-C5	-2.72	120.46	125.16
1	1	1524	OMG	C5-C6-N1	2.72	120.18	113.25
26	S1	2046	PSU	O2-C2-N1	-2.72	119.99	122.79
6	7	75	OMG	C5-C6-N1	2.71	120.16	113.25
1	1	856	OMG	C5-C6-N1	2.71	120.15	113.25
1	1	672	PSU	C6-C5-C4	2.71	120.00	118.17
1	1	1190	OMG	C5-C6-N1	2.71	120.14	113.25
26	S1	1829	OMG	C5-C6-N1	2.70	120.14	113.25
1	1	1664	PSU	O2-C2-N1	-2.70	120.00	122.79
6	7	43	A2M	N3-C4-N9	2.70	131.76	127.17
1	1	422	PSU	O2-C2-N1	-2.69	120.02	122.79
1	1	1011	PSU	O2-C2-N1	-2.69	120.02	122.79
1	1	1540	OMG	C5-C6-N1	2.67	120.06	113.25
26	S1	1657	PSU	C6-C5-C4	2.67	119.98	118.17
26	S1	479	A2M	N3-C4-N9	2.67	131.71	127.17
6	7	74	PSU	C6-C5-C4	2.67	119.97	118.17
1	1	959[B]	OMG	N9-C4-N3	2.67	131.29	125.95
26	S1	1543	C4J	N3-C2-N1	2.67	119.97	116.72
1	1	959[B]	OMG	C5-C6-N1	2.66	120.02	113.25
26	S1	2185	MA6	N3-C4-N9	2.65	131.67	127.17
1	1	959[A]	OMG	C5-C6-N1	2.65	119.99	113.25
6	7	162	A2M	C5-N7-C8	2.65	107.61	103.45
26	S1	1246	PSU	O2-C2-N1	-2.65	120.06	122.79
26	S1	2046	PSU	C6-C5-C4	2.64	119.96	118.17
3	4	74	OMG	C5-C6-N1	2.64	119.97	113.25
26	S1	1539	PSU	O2-C2-N1	-2.64	120.07	122.79
6	7	43	A2M	C5-N7-C8	2.63	107.59	103.45
26	S1	512	A2M	C6-C5-C4	2.63	120.77	117.18
1	1	681	A2M	C5-N7-C8	2.63	107.58	103.45
1	1	1039	PSU	O2-C2-N1	-2.63	120.08	122.79
1	1	955	A2M	C5-N7-C8	2.63	107.58	103.45
1	1	678	A2M	C6-C5-C4	2.62	120.76	117.18
1	1	681	A2M	C4-C5-N7	-2.62	107.58	110.58
26	S1	1156	PSU	C6-C5-C4	2.62	119.94	118.17
26	S1	2151	OMG	N9-C4-N3	2.62	131.20	125.95
6	7	75	OMG	N9-C4-N3	2.62	131.19	125.95
6	7	74	PSU	O2-C2-N1	-2.62	120.09	122.79
1	1	927	A2M	C5-N7-C8	2.62	107.56	103.45
1	1	1524	OMG	N9-C4-N3	2.61	131.18	125.95
26	S1	1657	PSU	O2-C2-N1	-2.61	120.10	122.79
1	1	239	PSU	O2-C2-N1	-2.60	120.10	122.79
1	1	305	A2M	C4-C5-N7	-2.59	107.62	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	2184	MA6	C4-N9-C8	2.58	108.45	105.74
6	7	43	A2M	C5-C4-N9	2.58	108.62	105.81
26	S1	98	A2M	C6-C5-C4	2.58	120.70	117.18
1	1	1539	A2M	C5-C4-N9	2.57	108.62	105.81
1	1	1528	PSU	O2-C2-N1	-2.57	120.14	122.79
6	7	43	A2M	C2'-C1'-N9	-2.56	109.54	113.75
26	S1	1879	OMG	O6-C6-C5	-2.56	119.78	126.53
26	S1	1995	7MG	N9-C4-N3	2.56	129.21	125.46
85	2	95	A2M	C6-C5-C4	2.56	120.67	117.18
85	2	437	PSU	O2-C2-N1	-2.55	120.15	122.79
85	2	95	A2M	C5-N7-C8	2.55	107.46	103.45
1	1	407	A2M	C5-N7-C8	2.55	107.46	103.45
26	S1	1533	PSU	O2-C2-N1	-2.55	120.16	122.79
1	1	959[B]	OMG	N9-C8-N7	-2.55	108.68	113.40
1	1	677	1MA	N9-C8-N7	-2.54	108.69	113.40
26	S1	1865	OMG	N9-C4-N3	2.54	131.03	125.95
85	2	71	OMG	N9-C4-N3	2.54	131.02	125.95
26	S1	2048	PSU	O2-C2-N1	-2.53	120.17	122.79
85	2	95	A2M	C5-C4-N9	2.53	108.57	105.81
1	1	1527	OMC	O2-C2-N3	-2.53	118.34	122.33
1	1	1626	OMG	O6-C6-C5	-2.53	119.86	126.53
26	S1	8	OMU	O2-C2-N1	-2.53	119.51	122.80
26	S1	2202	PSU	O2-C2-N1	-2.53	120.18	122.79
1	1	1527	OMC	C1'-N1-C2	2.52	124.02	118.44
1	1	1402	PSU	O2-C2-N1	-2.52	120.19	122.79
26	S1	1156	PSU	O2-C2-N1	-2.52	120.19	122.79
1	1	940	PSU	O2-C2-N1	-2.52	120.19	122.79
1	1	305	A2M	C6-C5-C4	2.51	120.61	117.18
1	1	927	A2M	C5-C4-N9	2.51	108.54	105.81
26	S1	512	A2M	C5-C4-N9	2.50	108.54	105.81
1	1	1626	OMG	N9-C4-N3	2.50	130.96	125.95
26	S1	1550	OMG	O6-C6-C5	-2.50	119.94	126.53
1	1	1539	A2M	C5-N7-C8	2.50	107.37	103.45
26	S1	2048	PSU	C6-C5-C4	2.50	119.86	118.17
1	1	858	A2M	C4'-O4'-C1'	-2.49	103.96	109.47
85	2	382	A2M	C5-C4-N9	2.49	108.53	105.81
26	S1	1829	OMG	O6-C6-C5	-2.49	119.96	126.53
1	1	870	PSU	O2-C2-N1	-2.48	120.23	122.79
1	1	856	OMG	N9-C4-N3	2.48	130.92	125.95
85	2	78	PSU	O2-C2-N1	-2.48	120.23	122.79
1	1	697	A2M	C5-N7-C8	2.47	107.34	103.45
26	S1	1623	OMG	O6-C6-C5	-2.47	120.01	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	407	A2M	C6-C5-C4	2.47	120.55	117.18
26	S1	455	PSU	O2-C2-N1	-2.46	120.25	122.79
26	S1	98	A2M	C5-C4-N9	2.46	108.50	105.81
26	S1	1478	OMG	O6-C6-C5	-2.46	120.03	126.53
26	S1	12	PSU	O2-C2-N1	-2.46	120.25	122.79
26	S1	1192	PSU	O2-C2-N1	-2.46	120.25	122.79
26	S1	98	A2M	C5-N7-C8	2.46	107.32	103.45
26	S1	1647	OMG	C8-N7-C5	2.46	108.64	104.26
6	7	43	A2M	C4-C5-N7	-2.46	107.77	110.58
1	1	955	A2M	C5-C4-N9	2.46	108.49	105.81
3	4	74	OMG	O6-C6-C5	-2.46	120.05	126.53
26	S1	2151	OMG	O6-C6-C5	-2.45	120.06	126.53
26	S1	1647	OMG	N9-C4-N3	2.45	130.86	125.95
6	7	75	OMG	O6-C6-C5	-2.45	120.06	126.53
1	1	1017	PSU	C6-C5-C4	2.45	119.83	118.17
26	S1	1995	7MG	N9-C8-N7	2.45	106.83	103.37
26	S1	1647	OMG	O6-C6-C5	-2.45	120.08	126.53
1	1	959[A]	OMG	O6-C6-C5	-2.44	120.10	126.53
1	1	927	A2M	C4-C5-N7	-2.44	107.80	110.58
1	1	845	OMU	O4-C4-C5	-2.44	120.96	125.16
85	2	437	PSU	C6-C5-C4	2.43	119.82	118.17
1	1	955	A2M	C4-C5-N7	-2.43	107.80	110.58
1	1	1171	PSU	C6-C5-C4	2.43	119.81	118.17
1	1	1524	OMG	O6-C6-C5	-2.43	120.12	126.53
1	1	1190	OMG	C8-N7-C5	2.43	108.59	104.26
1	1	235	A2M	C5-N7-C8	2.43	107.26	103.45
26	S1	600	OMG	O6-C6-C5	-2.43	120.13	126.53
3	4	74	OMG	N9-C4-N3	2.42	130.80	125.95
1	1	697	A2M	C5-C4-N9	2.42	108.45	105.81
1	1	1524	OMG	C8-N7-C5	2.42	108.58	104.26
1	1	959[B]	OMG	O6-C6-C5	-2.42	120.14	126.53
1	1	1181	PSU	O2-C2-N1	-2.41	120.31	122.79
1	1	678	A2M	C4-N9-C8	2.41	108.26	105.74
1	1	1540	OMG	O6-C6-C5	-2.40	120.19	126.53
1	1	959[A]	OMG	C8-N7-C5	2.40	108.54	104.26
85	2	95	A2M	C4-C5-N7	-2.40	107.84	110.58
85	2	382	A2M	C5-N7-C8	2.39	107.21	103.45
6	7	162	A2M	C4-C5-N7	-2.39	107.85	110.58
26	S1	1865	OMG	O6-C6-C5	-2.39	120.22	126.53
1	1	847	OMU	O2-C2-N1	-2.39	119.69	122.80
26	S1	479	A2M	C5-N7-C8	2.38	107.19	103.45
26	S1	607	PSU	C6-C5-C4	2.38	119.78	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	12	PSU	C6-C5-C4	2.38	119.78	118.17
1	1	1539	A2M	C6-C5-C4	2.36	120.40	117.18
26	S1	668	A2M	C5-C4-N9	2.36	108.38	105.81
85	2	71	OMG	O6-C6-C5	-2.36	120.31	126.53
26	S1	600	OMG	C8-N7-C5	2.35	108.45	104.26
1	1	856	OMG	O6-C6-C5	-2.35	120.32	126.53
1	1	927	A2M	C6-C5-C4	2.35	120.38	117.18
26	S1	607	PSU	O2-C2-N1	-2.35	120.37	122.79
26	S1	2151	OMG	C8-N7-C5	2.34	108.44	104.26
26	S1	512	A2M	C4-C5-N7	-2.33	107.92	110.58
85	2	382	A2M	C6-C5-C4	2.33	120.36	117.18
26	S1	668	A2M	C4-C5-N7	-2.33	107.92	110.58
26	S1	479	A2M	C6-C5-C4	2.32	120.35	117.18
85	2	71	OMG	C8-N7-C5	2.32	108.40	104.26
1	1	1171	PSU	O2-C2-N1	-2.32	120.39	122.79
1	1	1540	OMG	C8-N7-C5	2.32	108.39	104.26
1	1	1107	OMU	O2-C2-N1	-2.32	119.78	122.80
1	1	235	A2M	C6-C5-C4	2.31	120.33	117.18
1	1	856	OMG	C8-N7-C5	2.31	108.37	104.26
26	S1	661	OMU	O2-C2-N1	-2.31	119.79	122.80
26	S1	2021	A2M	C6-C5-C4	2.30	120.33	117.18
6	7	75	OMG	C8-N7-C5	2.30	108.35	104.26
26	S1	1533	PSU	C6-C5-C4	2.30	119.72	118.17
26	S1	2185	MA6	C4-N9-C8	2.29	108.14	105.74
1	1	1190	OMG	O6-C6-C5	-2.29	120.48	126.53
1	1	697	A2M	C2'-C1'-N9	-2.29	109.98	113.75
26	S1	1566	PSU	O2-C2-N1	-2.29	120.42	122.79
26	S1	1623	OMG	C8-N7-C5	2.29	108.34	104.26
6	7	43	A2M	C6-C5-C4	2.29	120.30	117.18
1	1	678	A2M	C4-C5-N7	-2.29	107.97	110.58
26	S1	512	A2M	C2'-C1'-N9	-2.28	109.99	113.75
1	1	697	A2M	C6-C5-C4	2.28	120.30	117.18
26	S1	1879	OMG	C8-N7-C5	2.28	108.32	104.26
1	1	955	A2M	C6-C5-C4	2.28	120.29	117.18
1	1	681	A2M	C6-C5-C4	2.28	120.29	117.18
26	S1	1833	OMU	O2-C2-N1	-2.28	119.83	122.80
1	1	845	OMU	O2-C2-N3	-2.27	117.29	121.49
3	4	74	OMG	C8-N7-C5	2.27	108.31	104.26
26	S1	2021	A2M	C4-C5-N7	-2.27	107.99	110.58
1	1	1626	OMG	C8-N7-C5	2.26	108.29	104.26
26	S1	1550	OMG	C8-N7-C5	2.26	108.29	104.26
26	S1	1539	PSU	C6-C5-C4	2.26	119.70	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1540	OMG	N9-C4-N3	2.26	130.47	125.95
6	7	69	PSU	O4'-C1'-C2'	2.26	108.27	105.15
26	S1	104	PSU	C6-C5-C4	2.25	119.69	118.17
26	S1	1865	OMG	C8-N7-C5	2.25	108.27	104.26
1	1	1539	A2M	C4-C5-N7	-2.25	108.01	110.58
6	7	162	A2M	C5-C4-N9	2.24	108.26	105.81
26	S1	479	A2M	C4-C5-N7	-2.24	108.02	110.58
1	1	407	A2M	C5-C4-N9	2.23	108.24	105.81
26	S1	1478	OMG	N9-C4-N3	2.22	130.39	125.95
1	1	1190	OMG	C2'-C1'-N9	-2.22	110.03	114.24
26	S1	98	A2M	C4-C5-N7	-2.21	108.05	110.58
26	S1	1829	OMG	C8-N7-C5	2.21	108.20	104.26
85	2	73	OMU	O2-C2-N1	-2.21	119.92	122.80
1	1	697	A2M	C4-C5-N7	-2.20	108.06	110.58
1	1	407	A2M	C5'-C4'-C3'	-2.20	107.28	115.21
1	1	1664	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	1	1533	PSU	O4'-C1'-C2'	2.19	108.19	105.15
26	S1	29	OMU	O2-C2-N1	-2.19	119.95	122.80
6	7	7	OMU	O2-C2-N1	-2.19	119.95	122.80
26	S1	668	A2M	C6-C5-C4	2.18	120.16	117.18
1	1	1171	PSU	O4'-C1'-C2'	2.18	108.16	105.15
1	1	678	A2M	C2'-C1'-N9	2.17	117.33	113.75
1	1	1540	OMG	N2-C2-N1	2.17	121.34	116.76
26	S1	1478	OMG	C8-N7-C5	2.17	108.12	104.26
26	S1	104	PSU	O2-C2-N1	-2.17	120.55	122.79
1	1	858	A2M	C4-C5-N7	-2.16	108.11	110.58
1	1	1190	OMG	N9-C4-N3	2.15	130.26	125.95
1	1	305	A2M	C5-C4-N9	2.15	108.16	105.81
1	1	1190	OMG	N2-C2-N1	2.15	121.31	116.76
1	1	672	PSU	O4'-C1'-C2'	2.15	108.13	105.15
85	2	382	A2M	C4-C5-N7	-2.15	108.13	110.58
26	S1	1543	C4J	C5-C4-N3	2.14	120.04	116.15
6	7	69	PSU	O2-C2-N1	-2.14	120.58	122.79
26	S1	1478	OMG	N2-C2-N1	2.14	121.28	116.76
26	S1	2184	MA6	C4-C5-N7	-2.14	108.14	110.58
2	3	13	OMU	O2-C2-N1	-2.12	120.04	122.80
1	1	1659	OMU	O2-C2-N1	-2.11	120.05	122.80
26	S1	479	A2M	C5'-C4'-C3'	-2.11	107.62	115.21
26	S1	2185	MA6	C4-C5-N7	-2.11	108.17	110.58
1	1	858	A2M	C5-C4-N9	2.10	108.09	105.81
26	S1	2021	A2M	C5-C4-N9	2.10	108.09	105.81
85	2	71	OMG	C2'-C1'-N9	-2.09	110.27	114.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1011	PSU	O4'-C1'-C2'	2.09	108.04	105.15
26	S1	1192	PSU	C6-C5-C4	2.09	119.58	118.17
26	S1	2061	5MC	CM5-C5-C6	-2.08	120.03	122.85
1	1	1011	PSU	C6-C5-C4	2.08	119.58	118.17
26	S1	607	PSU	O4'-C1'-C2'	2.08	108.03	105.15
26	S1	1543	C4J	C31-C3-N3	-2.07	108.55	112.16
26	S1	479	A2M	C3'-C2'-C1'	2.06	106.75	102.81
6	7	162	A2M	C6-C5-C4	2.05	119.98	117.18
26	S1	2140	OMC	O2-C2-N3	-2.05	119.09	122.33
1	1	235	A2M	C5'-C4'-C3'	-2.05	107.84	115.21
1	1	959[A]	OMG	C8-N9-C4	2.05	109.86	106.03
1	1	407	A2M	C4-C5-N7	-2.05	108.24	110.58
26	S1	1621	OMU	O2-C2-N1	-2.05	120.13	122.80
1	1	1190	OMG	C4-C5-N7	-2.04	107.43	110.67
1	1	959[A]	OMG	C3'-C2'-C1'	-2.03	98.92	102.81
3	4	74	OMG	N2-C2-N1	2.03	121.05	116.76
26	S1	1979	OMU	O2-C2-N1	-2.03	120.15	122.80
1	1	858	A2M	C3'-C2'-C1'	2.03	106.69	102.81
26	S1	2185	MA6	C5-C4-N9	2.03	108.02	105.81
1	1	677	1MA	C2'-C1'-N9	2.02	118.88	113.25
26	S1	1647	OMG	C2'-C1'-N9	-2.02	110.40	114.24
1	1	1181	PSU	C6-C5-C4	2.02	119.54	118.17
1	1	1626	OMG	N2-C2-N1	2.02	121.03	116.76
1	1	1528	PSU	O4'-C1'-C2'	2.02	107.94	105.15
1	1	1371	OMU	O2-C2-N3	-2.01	117.79	121.49
1	1	422	PSU	O3'-C3'-C2'	2.00	118.24	111.82

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	407	A2M	O4'-C4'-C5'-O5'
1	1	678	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	O4'-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	959[A]	OMG	O4'-C4'-C5'-O5'
1	1	959[A]	OMG	C3'-C4'-C5'-O5'
1	1	1010	OMC	C1'-C2'-O2'-CM2
1	1	1107	OMU	O4'-C4'-C5'-O5'
1	1	1181	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	1181	PSU	O4'-C1'-C5-C6
1	1	1371	OMU	O4'-C1'-N1-C2
1	1	1371	OMU	O4'-C1'-N1-C6
1	1	1540	OMG	O4'-C4'-C5'-O5'
6	7	7	OMU	C1'-C2'-O2'-CM2
6	7	69	PSU	O4'-C1'-C5-C4
6	7	69	PSU	O4'-C1'-C5-C6
6	7	75	OMG	O4'-C4'-C5'-O5'
6	7	162	A2M	C1'-C2'-O2'-CM'
26	S1	104	PSU	C3'-C4'-C5'-O5'
26	S1	104	PSU	O4'-C4'-C5'-O5'
26	S1	479	A2M	O4'-C4'-C5'-O5'
26	S1	600	OMG	O4'-C4'-C5'-O5'
26	S1	607	PSU	O4'-C1'-C5-C4
26	S1	607	PSU	O4'-C1'-C5-C6
26	S1	1543	C4J	N33-C32-C34-O36
26	S1	1566	PSU	O4'-C4'-C5'-O5'
26	S1	1623	OMG	C1'-C2'-O2'-CM2
26	S1	1879	OMG	C1'-C2'-O2'-CM2
26	S1	2021	A2M	C1'-C2'-O2'-CM'
26	S1	2202	PSU	O4'-C1'-C5-C6
85	2	382	A2M	C1'-C2'-O2'-CM'
1	1	407	A2M	C3'-C4'-C5'-O5'
1	1	1107	OMU	C3'-C4'-C5'-O5'
1	1	1371	OMU	C3'-C4'-C5'-O5'
1	1	1540	OMG	C3'-C4'-C5'-O5'
6	7	74	PSU	C3'-C4'-C5'-O5'
6	7	74	PSU	O4'-C4'-C5'-O5'
6	7	75	OMG	C3'-C4'-C5'-O5'
26	S1	33	PSU	C3'-C4'-C5'-O5'
26	S1	479	A2M	C3'-C4'-C5'-O5'
26	S1	512	A2M	O4'-C4'-C5'-O5'
26	S1	512	A2M	C3'-C4'-C5'-O5'
26	S1	2140	OMC	C3'-C4'-C5'-O5'
26	S1	2140	OMC	O4'-C4'-C5'-O5'
1	1	1371	OMU	O4'-C4'-C5'-O5'
26	S1	33	PSU	O4'-C4'-C5'-O5'
26	S1	98	A2M	O4'-C4'-C5'-O5'
26	S1	668	A2M	O4'-C4'-C5'-O5'
26	S1	1550	OMG	O4'-C4'-C5'-O5'
26	S1	1550	OMG	C3'-C4'-C5'-O5'
85	2	443	OMC	C2'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	678	A2M	C3'-C4'-C5'-O5'
1	1	681	A2M	C3'-C4'-C5'-O5'
1	1	1402	PSU	O4'-C4'-C5'-O5'
26	S1	600	OMG	C3'-C4'-C5'-O5'
26	S1	668	A2M	C3'-C4'-C5'-O5'
26	S1	1566	PSU	C3'-C4'-C5'-O5'
1	1	1181	PSU	C3'-C4'-C5'-O5'
26	S1	1533	PSU	C3'-C4'-C5'-O5'
85	2	443	OMC	C2'-C1'-N1-C2
1	1	1181	PSU	O4'-C4'-C5'-O5'
26	S1	1995	7MG	O4'-C4'-C5'-O5'
26	S1	1543	C4J	C31-C32-C34-O35
1	1	678	A2M	C3'-C2'-O2'-CM'
26	S1	1543	C4J	N33-C32-C34-O35
26	S1	8	OMU	C2'-C1'-N1-C6
26	S1	1543	C4J	C31-C32-C34-O36
1	1	305	A2M	O4'-C4'-C5'-O5'
26	S1	1533	PSU	O4'-C4'-C5'-O5'
26	S1	1995	7MG	C3'-C4'-C5'-O5'
1	1	927	A2M	C1'-C2'-O2'-CM'
26	S1	98	A2M	C3'-C4'-C5'-O5'
26	S1	1539	PSU	C3'-C4'-C5'-O5'
26	S1	668	A2M	C2'-C1'-N9-C8
85	2	443	OMC	O4'-C1'-N1-C2
1	1	1402	PSU	C3'-C4'-C5'-O5'
26	S1	8	OMU	O4'-C1'-N1-C6
85	2	443	OMC	O4'-C1'-N1-C6
1	1	407	A2M	C3'-C2'-O2'-CM'
1	1	1107	OMU	C3'-C2'-O2'-CM2
1	1	681	A2M	C4'-C5'-O5'-P
26	S1	1543	C4J	C4'-C5'-O5'-P
26	S1	1657	PSU	O4'-C1'-C5-C4
26	S1	2185	MA6	C4'-C5'-O5'-P
26	S1	1841	PSU	O4'-C4'-C5'-O5'
26	S1	8	OMU	C3'-C2'-O2'-CM2
26	S1	1550	OMG	C3'-C2'-O2'-CM2
26	S1	1539	PSU	O4'-C4'-C5'-O5'
26	S1	1623	OMG	O4'-C4'-C5'-O5'
1	1	1527	OMC	C2'-C1'-N1-C6
26	S1	2021	A2M	C3'-C4'-C5'-O5'
26	S1	1657	PSU	O4'-C1'-C5-C6
1	1	1524	OMG	C3'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	S1	8	OMU	O4'-C1'-N1-C2
6	7	69	PSU	O4'-C4'-C5'-O5'
1	1	858	A2M	O4'-C1'-N9-C8
26	S1	8	OMU	C2'-C1'-N1-C2
26	S1	668	A2M	O4'-C1'-N9-C8
26	S1	1833	OMU	C4'-C5'-O5'-P
1	1	305	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1010	OMC	1	0
1	1	845	OMU	3	0
6	7	162	A2M	1	0
1	1	422	PSU	1	0
26	S1	1539	PSU	1	0
85	2	95	A2M	2	0
26	S1	2185	MA6	1	0
1	1	955	A2M	2	0
85	2	382	A2M	1	0
1	1	235	A2M	1	0
26	S1	2021	A2M	1	0
1	1	959[A]	OMG	1	0
26	S1	2202	PSU	1	0
26	S1	29	OMU	1	0
26	S1	661	OMU	1	0
1	1	1524	OMG	1	0
1	1	695	OMC	1	0
26	S1	479	A2M	1	0
1	1	677	1MA	1	0
26	S1	1550	OMG	1	0
26	S1	668	A2M	1	0
1	1	1181	PSU	1	0
1	1	847	OMU	1	0
1	1	678	A2M	1	0
1	1	1527	OMC	1	0
26	S1	1879	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 367 ligands modelled in this entry, 367 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
27	S4	1
31	SD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S4	6:G	O3'	63:G	P	19.63
1	SD	163:PHE	C	164:GLY	N	4.10

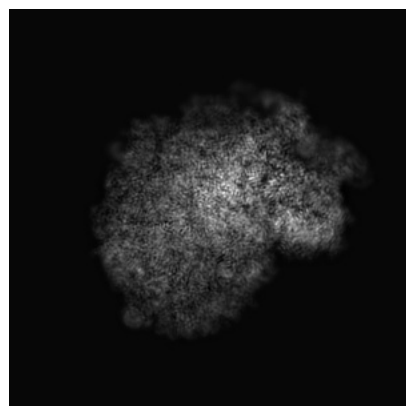
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17216. These allow visual inspection of the internal detail of the map and identification of artifacts.

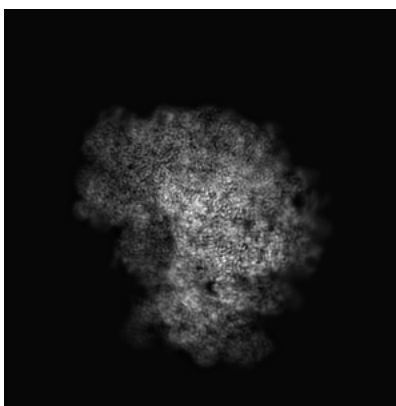
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

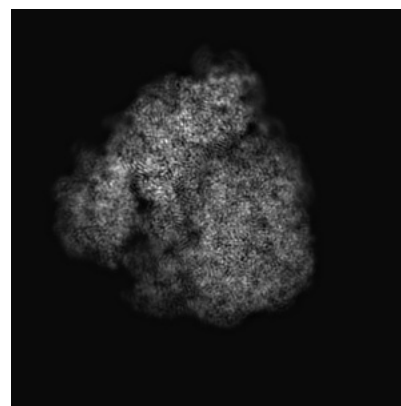
6.1.1 Primary map



X

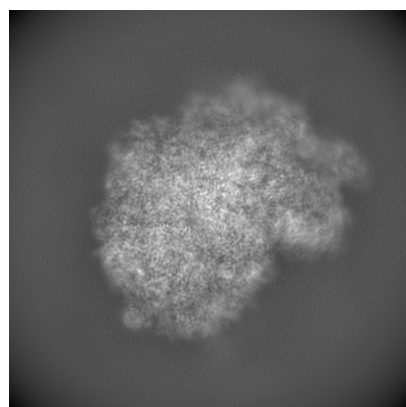


Y

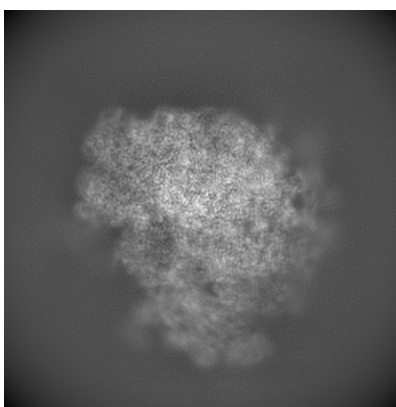


Z

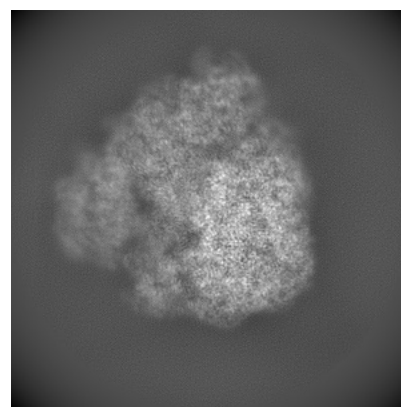
6.1.2 Raw map



X



Y

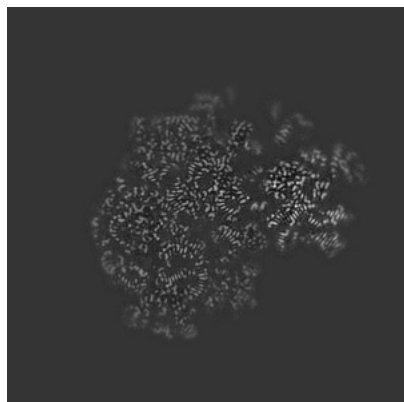


Z

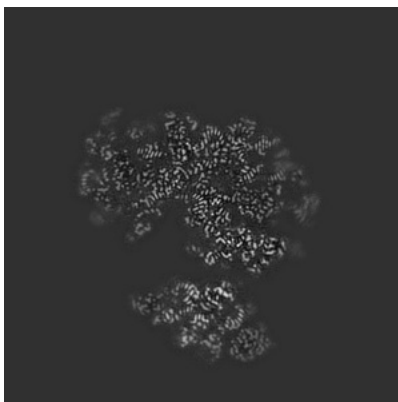
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

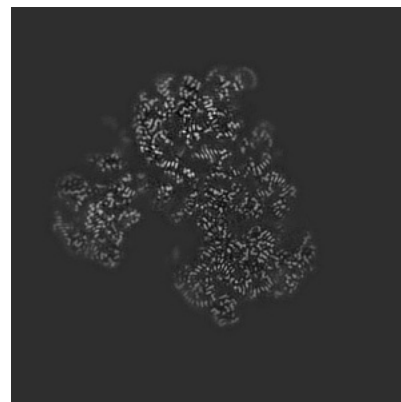
6.2.1 Primary map



X Index: 240

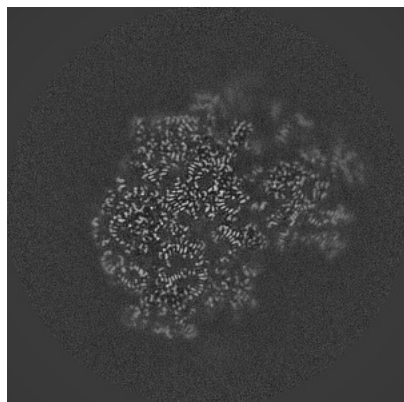


Y Index: 240

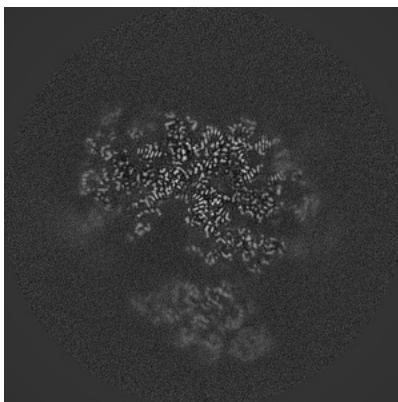


Z Index: 240

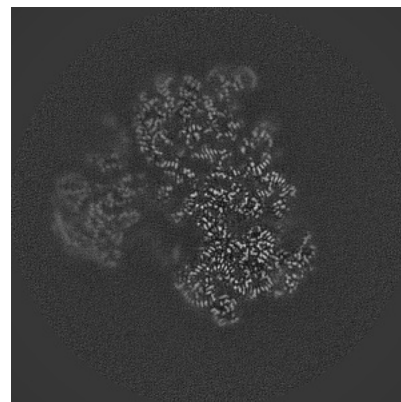
6.2.2 Raw map



X Index: 240



Y Index: 240

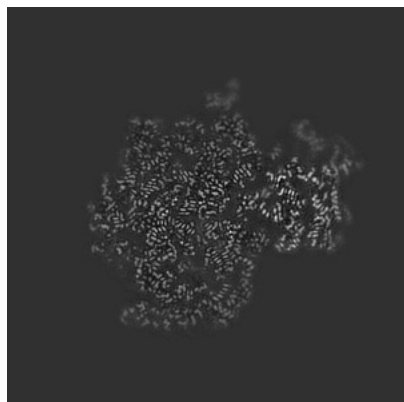


Z Index: 240

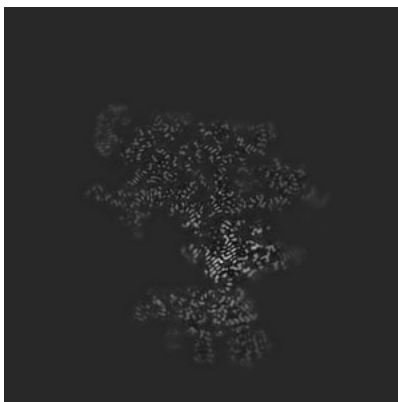
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

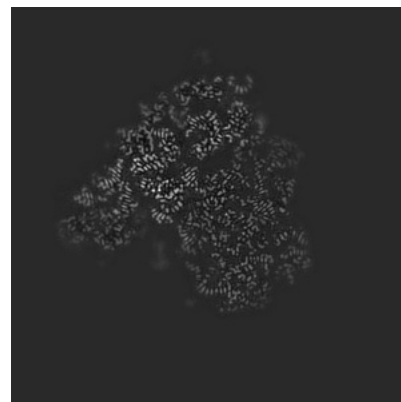
6.3.1 Primary map



X Index: 252

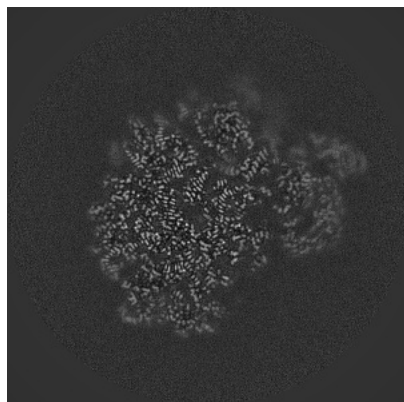


Y Index: 265

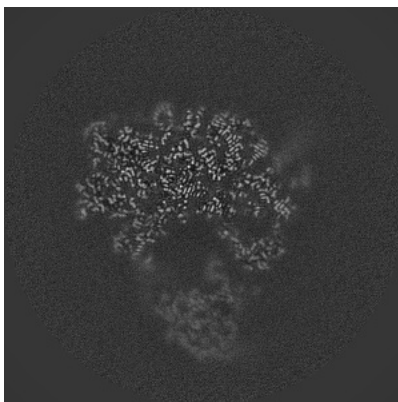


Z Index: 264

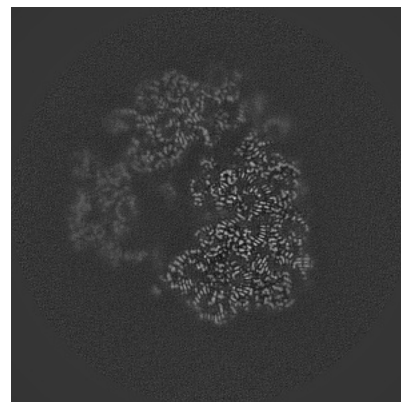
6.3.2 Raw map



X Index: 267



Y Index: 207

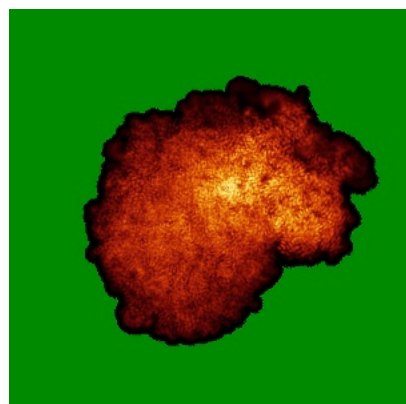


Z Index: 216

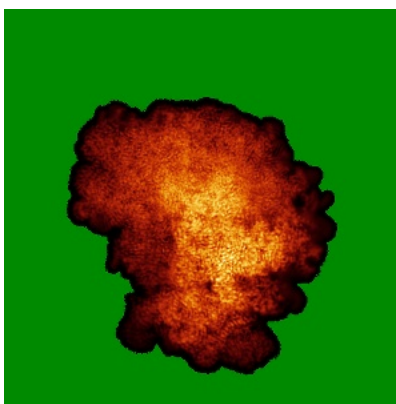
The images above show the largest variance slices of the map in three orthogonal directions.

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

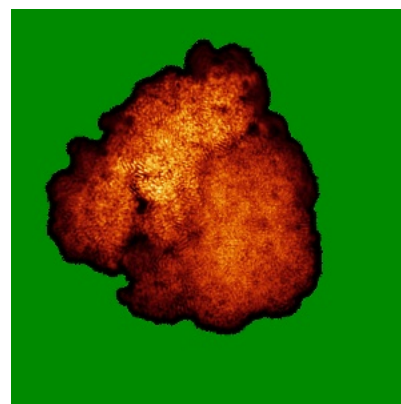
6.4.1 Primary map



X

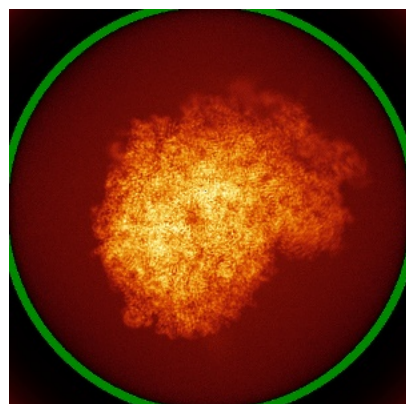


Y

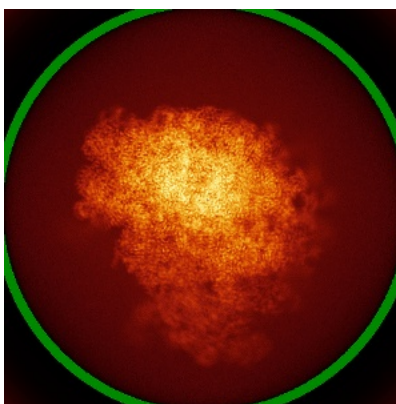


Z

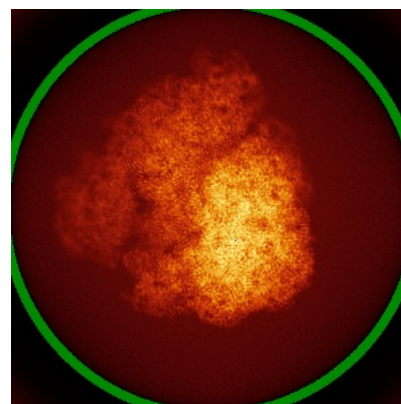
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

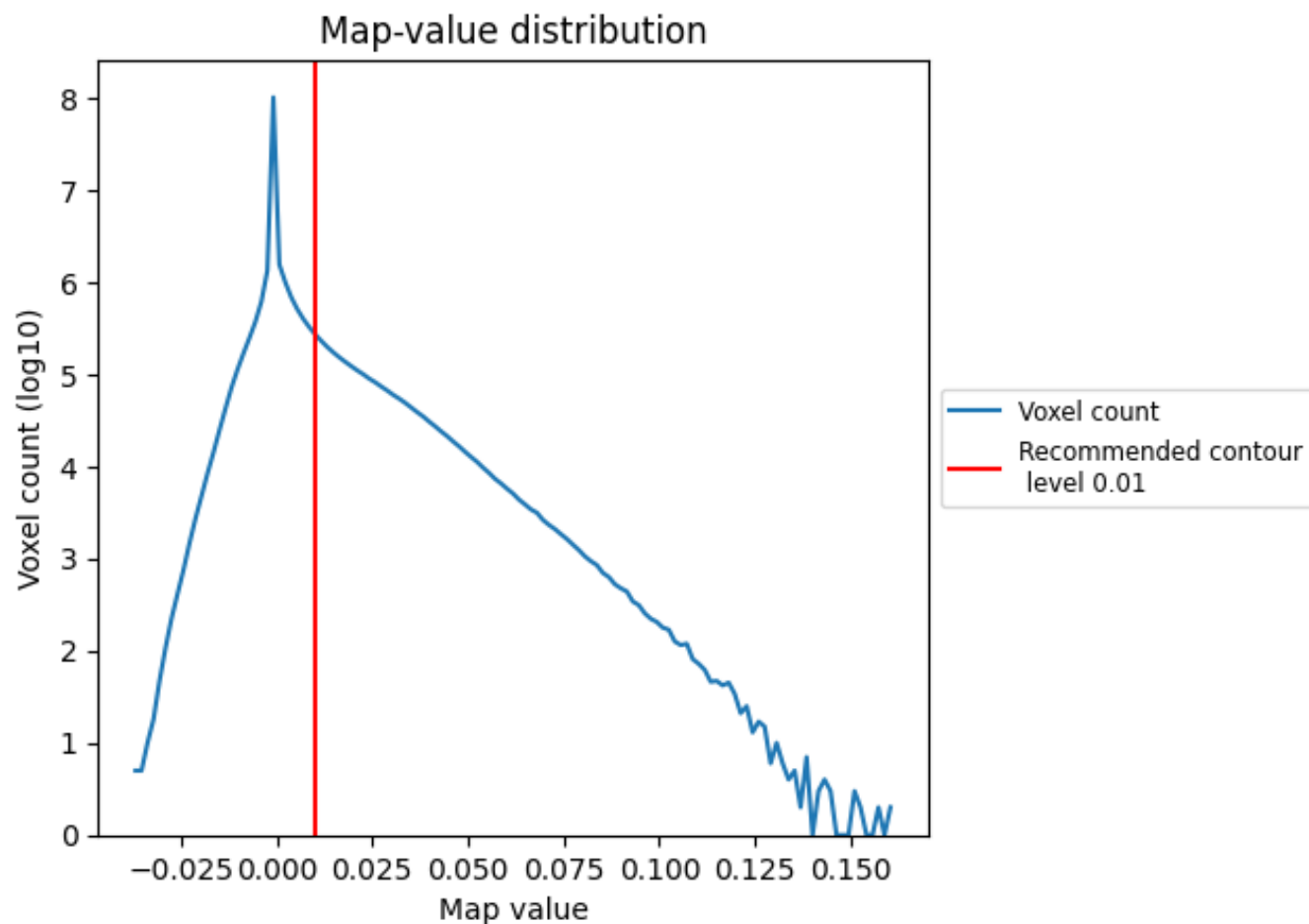
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

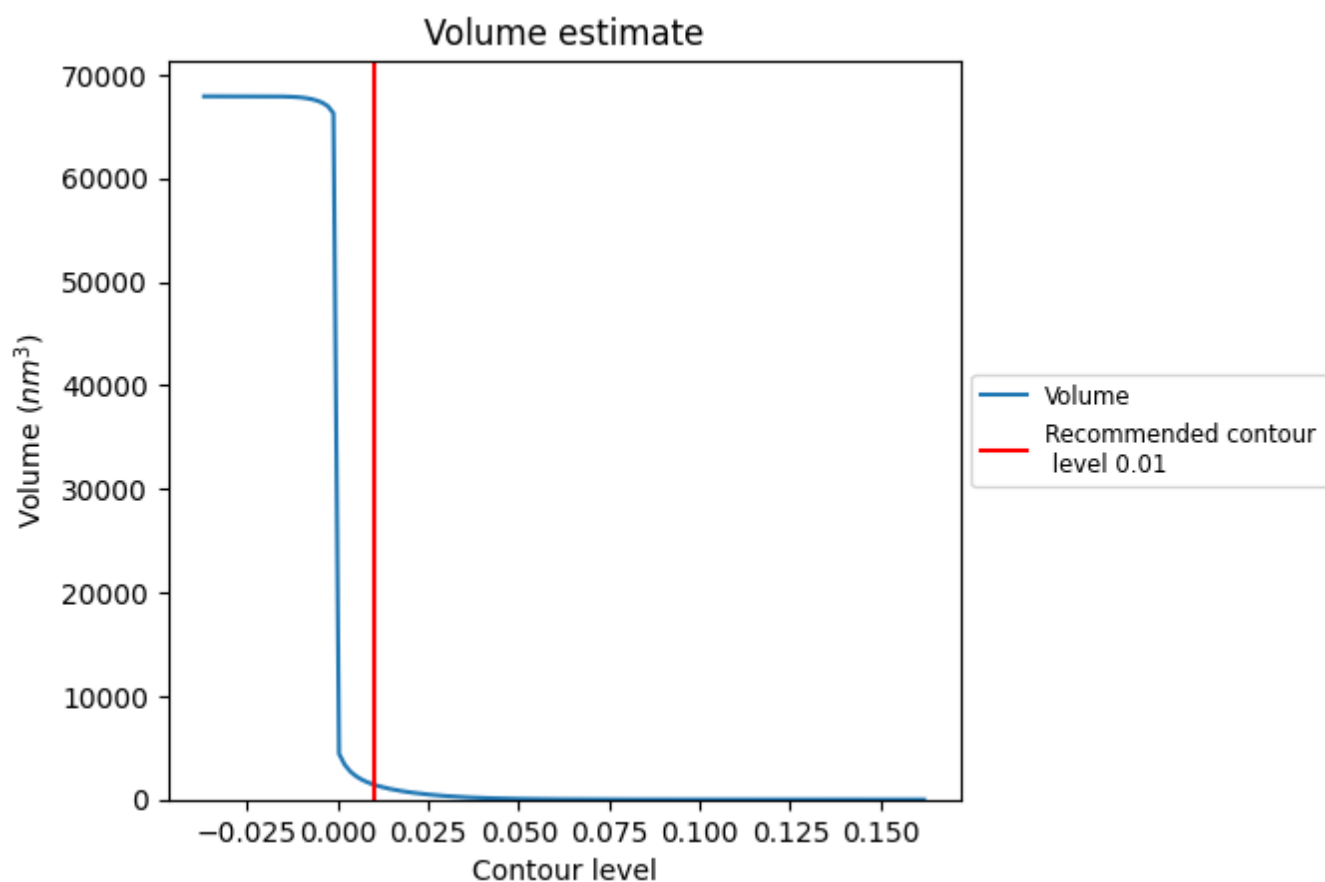
This section contains the results of statistical analysis of the map.

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.

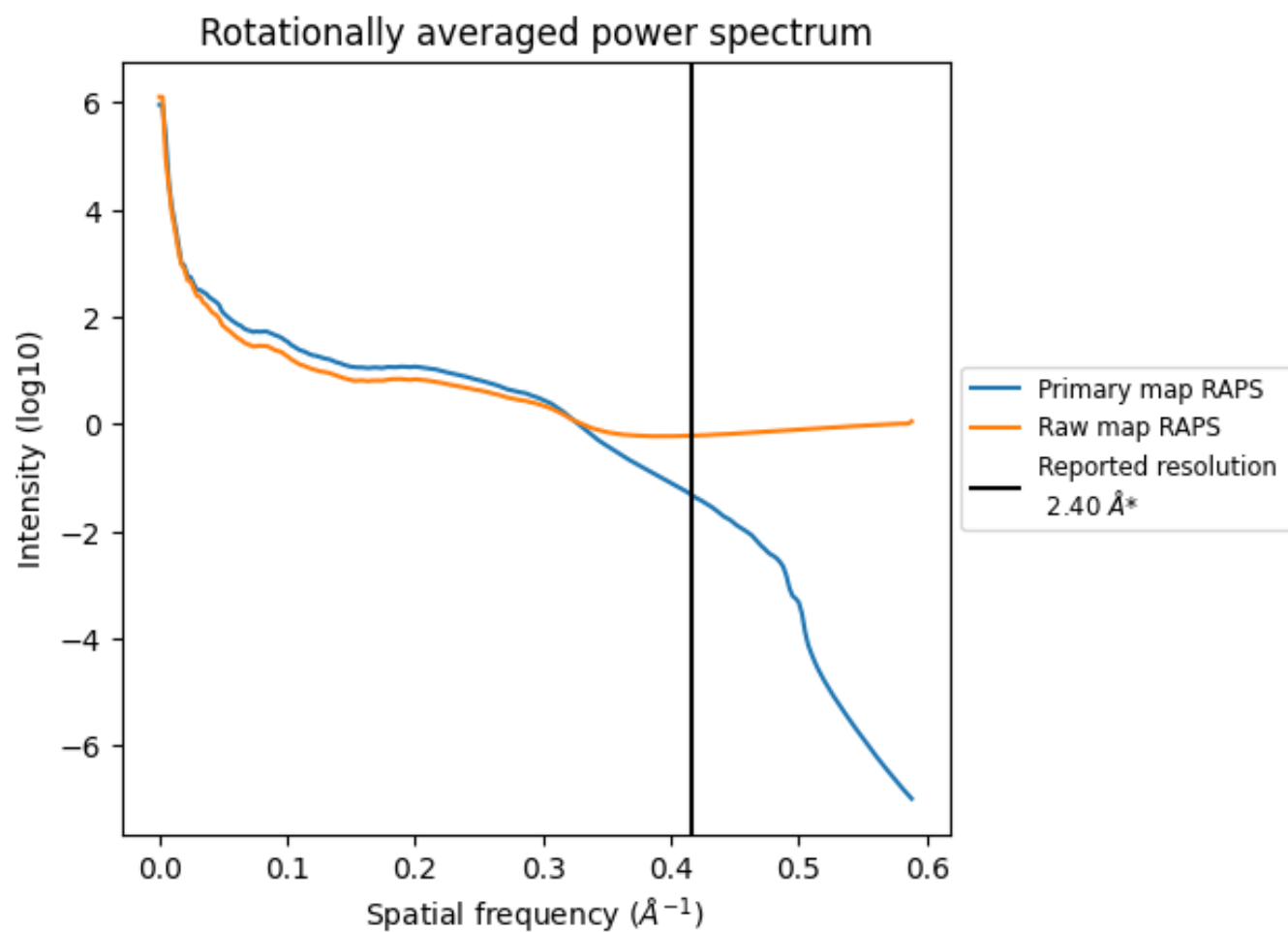
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1449 nm^3 ; this corresponds to an approximate mass of 1309 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 ⓘ

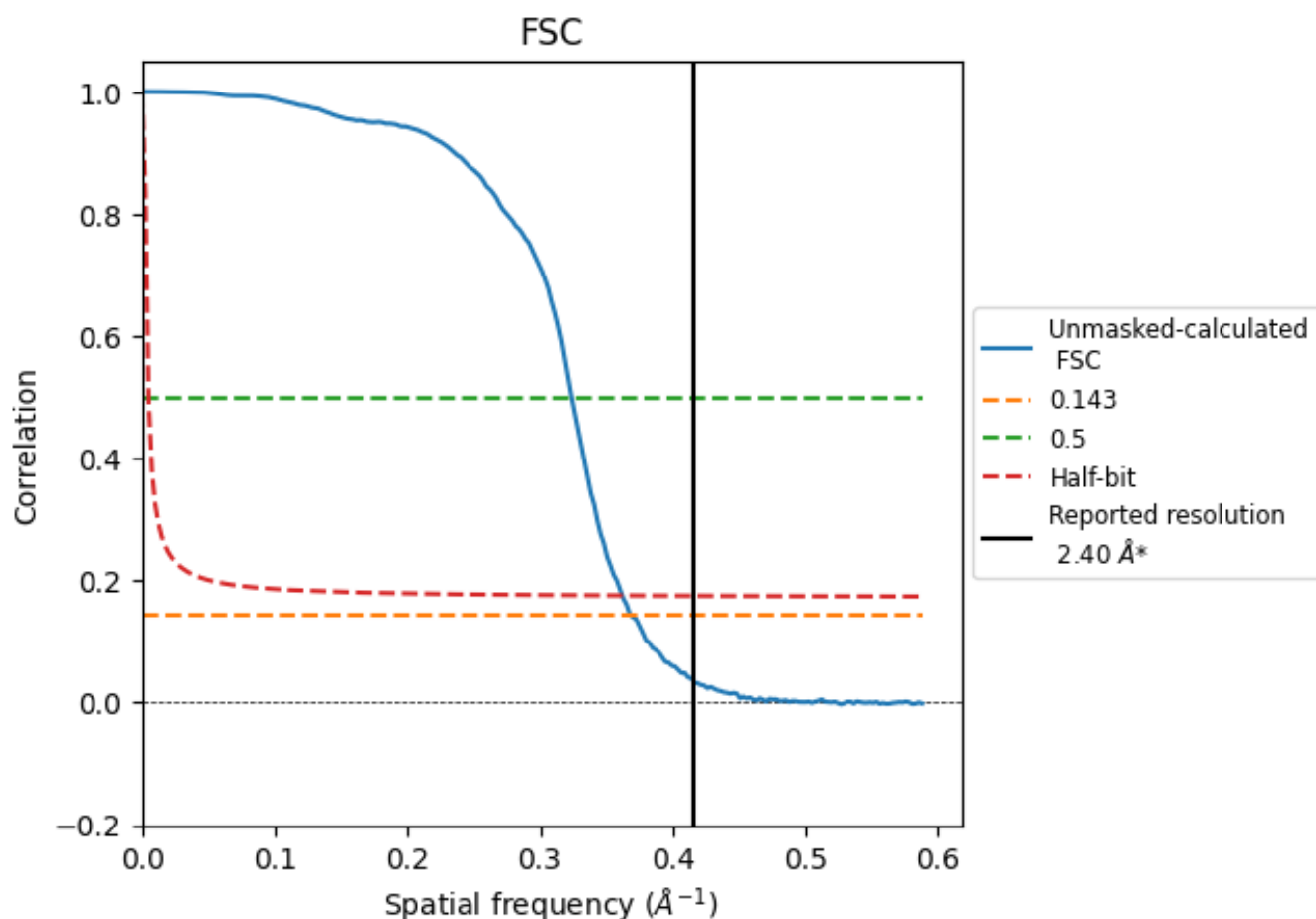


*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.71	3.09	2.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.71 differs from the reported value 2.4 by more than 10 %

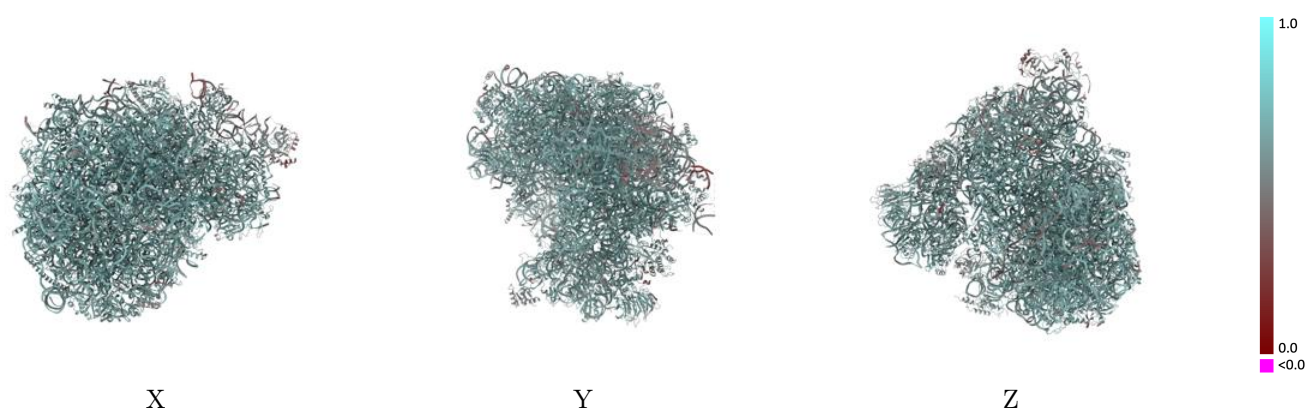
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17216 and PDB model 8OVJ. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)

This section was not generated.

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

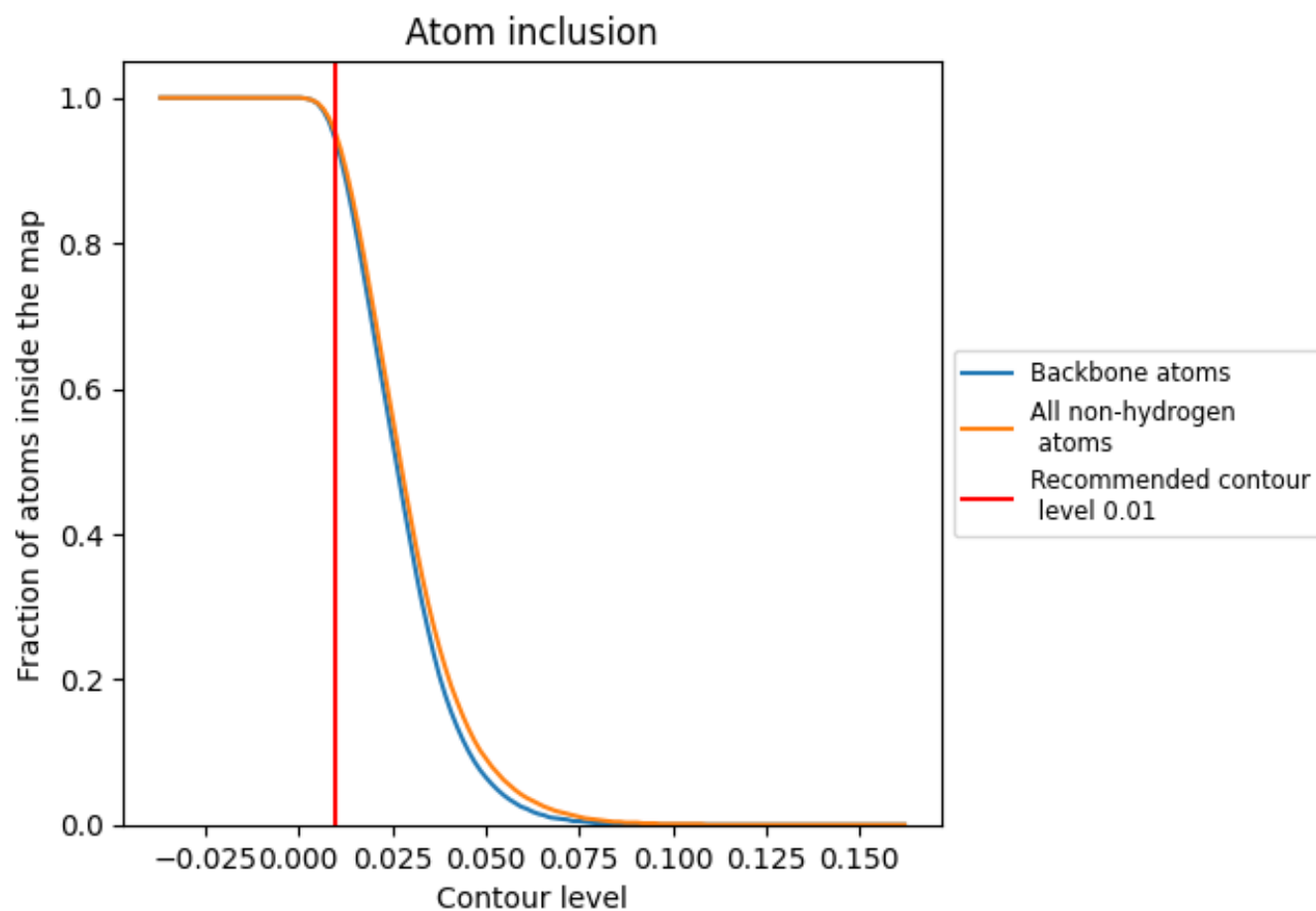


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.6300
1	 0.9760	 0.6460
2	 0.9730	 0.6410
3	 0.9530	 0.6210
4	 0.9780	 0.6420
5	 0.9610	 0.6280
6	 0.9320	 0.5920
7	 0.9750	 0.6410
8	 0.9880	 0.6130
A	 0.9740	 0.6870
B	 0.9720	 0.6620
C	 0.9710	 0.6600
D	 0.8890	 0.5650
E	 0.9170	 0.6220
F	 0.9300	 0.6190
G	 0.9510	 0.6370
H	 0.9740	 0.6590
I	 0.9360	 0.6530
J	 0.9310	 0.6600
K	 0.9080	 0.6100
L	 0.9720	 0.6820
M	 0.9870	 0.6890
N	 0.8480	 0.6160
O	 0.9190	 0.6020
P	 0.9680	 0.6760
Q	 0.9550	 0.6320
R	 0.9640	 0.6550
S	 0.9290	 0.6460
S1	 0.9800	 0.6180
S4	 0.7190	 0.5120
SA	 0.9690	 0.6230
SB	 0.9180	 0.5410
SC	 0.8590	 0.5970
SD	 0.9630	 0.6070
SE	 0.9530	 0.6210



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SF	 0.9700	 0.6120
SG	 0.9400	 0.5980
SH	 0.9370	 0.6230
SI	 0.9780	 0.5940
SJ	 0.9780	 0.6440
SK	 0.9520	 0.6260
SL	 0.9500	 0.6350
SM	 0.8380	 0.6040
SN	 0.8430	 0.6080
SO	 0.9830	 0.6400
SP	 0.9720	 0.6380
SQ	 0.3390	 0.4980
SR	 0.8580	 0.6170
SS	 0.9690	 0.6400
ST	 0.9710	 0.6440
SU	 0.9630	 0.6440
SV	 0.8560	 0.5720
SW	 0.8410	 0.6140
SX	 0.9520	 0.6330
SY	 0.9430	 0.5800
SZ	 0.9670	 0.6030
Sa	 0.9190	 0.6070
Sb	 0.9900	 0.6450
Sc	 0.9450	 0.6090
Sd	 0.9380	 0.6000
Se	 0.9470	 0.5860
Sg	 0.8060	 0.5900
Sh	 0.5700	 0.4520
T	 0.9670	 0.6780
U	 0.6730	 0.5720
V	 0.9380	 0.6530
W	 0.9390	 0.6420
X	 0.9400	 0.6510
Y	 0.9190	 0.6200
Z	 0.9370	 0.6470
a	 0.9160	 0.6270
b	 0.9320	 0.6620
c	 0.9450	 0.6620
d	 0.8940	 0.6260
e	 0.8630	 0.6180
f	 0.9530	 0.6730
g	 0.9270	 0.6550

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.8590	 0.6190
i	 0.8860	 0.6240
j	 0.9890	 0.6850
k	 0.8240	 0.6040
l	 0.9580	 0.6720
m	 0.8210	 0.6060
n	 0.9630	 0.6610
o	 0.9470	 0.6630
p	 0.9050	 0.6450