Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 03:06 am BST

PDB ID	:	8B2L
EMDB ID	:	EMD-15806
Title	:	Cryo-EM structure of the plant 80S ribosome
Authors	:	Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.; Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.
Deposited on	:	2022-09-14
Resolution	:	2.20 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:

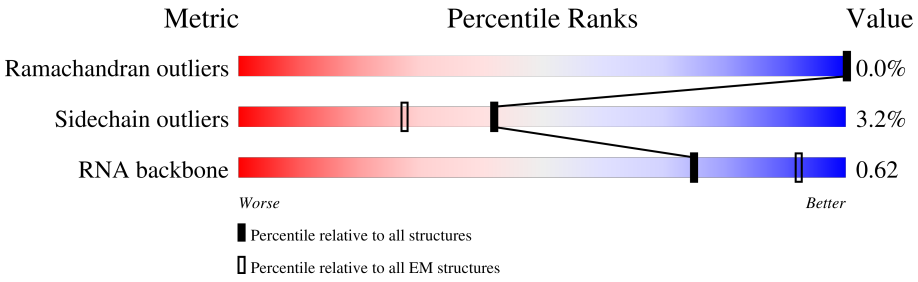
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	A1	264	95%
2	k1	249	21% 90% 8%
3	h1	1808	74% 15% 10%
4	l1	208	14% 43% 56%
5	C1	144	81% 78% 19%
6	D1	149	28% 74% 5% 20%
7	E1	143	6% 94% 5%
8	F1	261	80% 17%

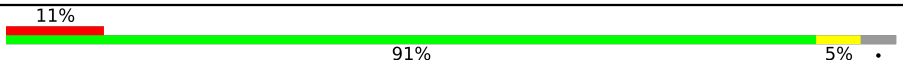
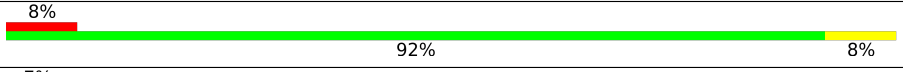
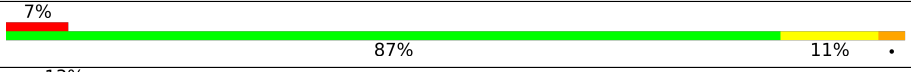
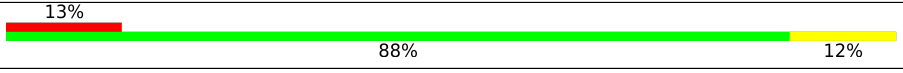
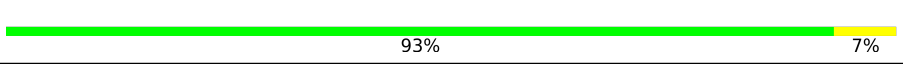
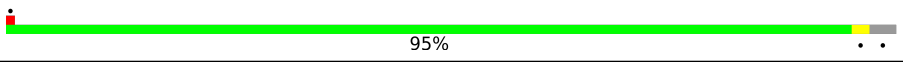
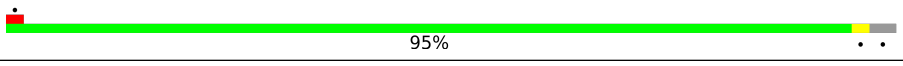
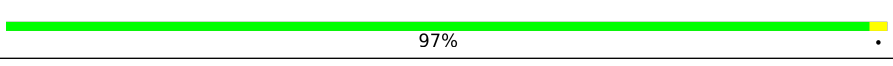
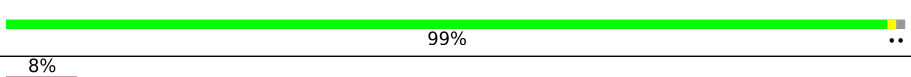
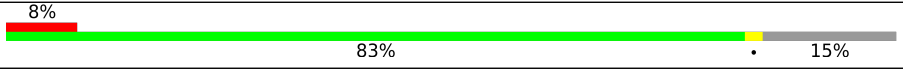
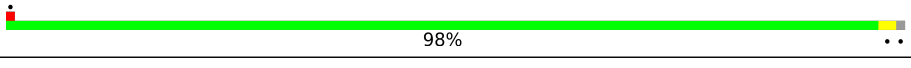
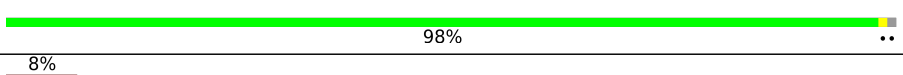
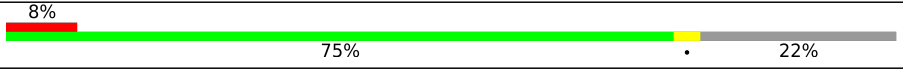
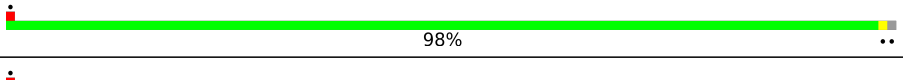
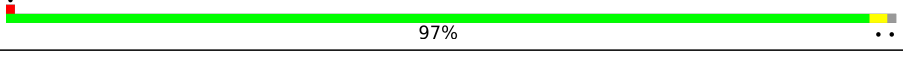
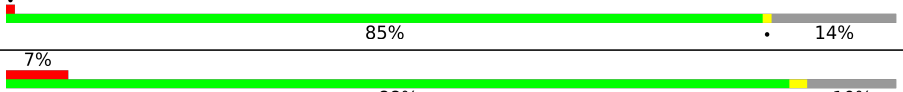
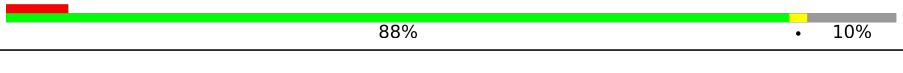
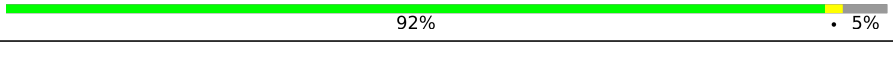
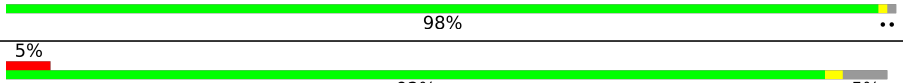
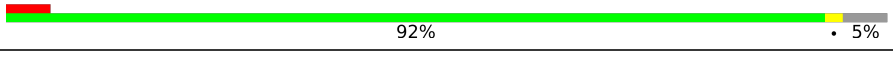
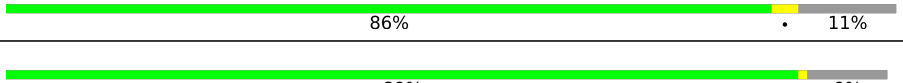
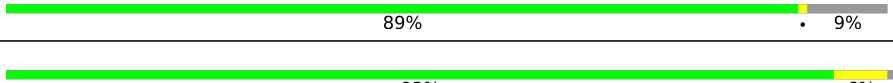
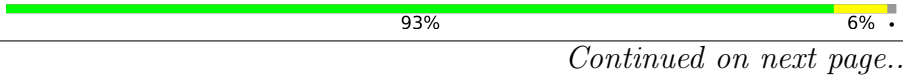
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	G1	83	6% 99%
10	H1	133	12% 92% 5%
11	I1	107	7% 66% 31%
12	J1	127	76% 23%
13	K1	86	10% 90% 8%
14	L1	65	12% 86% 8% 6%
15	M1	62	6% 84% 16%
16	N1	156	41% 43% 56%
17	O1	191	33% 94%
18	P1	224	7% 81% 17%
19	Q1	328	79% 88% 6% 6%
20	R1	122	34% 81% 16%
21	S1	150	84% 12%
22	T1	142	97%
23	U1	152	5% 91% 7%
24	V1	56	95%
25	W1	151	98%
26	X1	159	88% 9%
27	Y1	152	7% 85% 14%
28	Z1	336	59% 40%
29	a1	248	15% 82% 15%
30	b1	197	91% 7%
31	c1	280	75% 22%
32	d1	210	7% 90% 8%
33	e1	130	98%

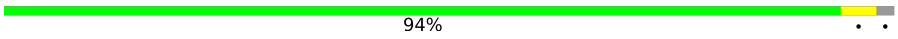
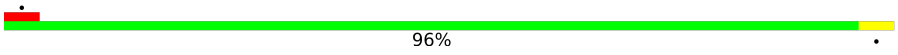
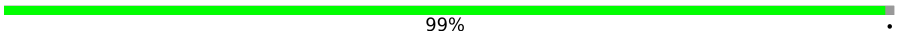
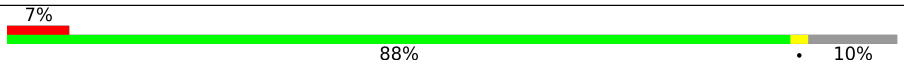
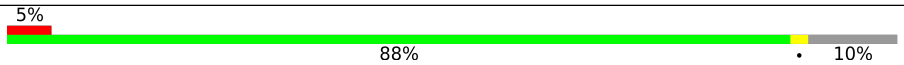
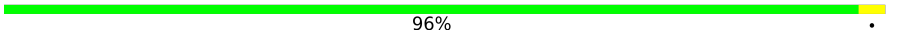
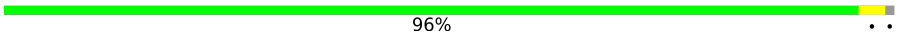
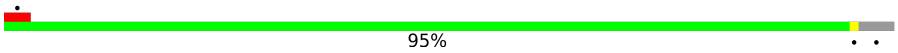
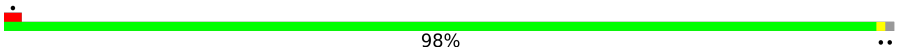
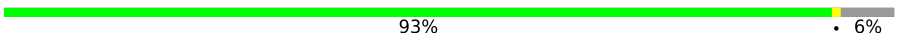
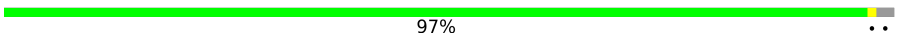
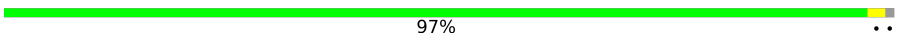
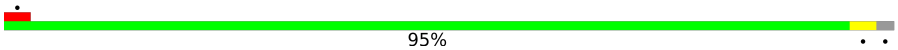
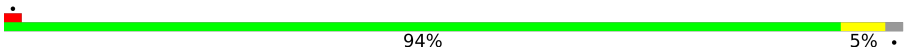
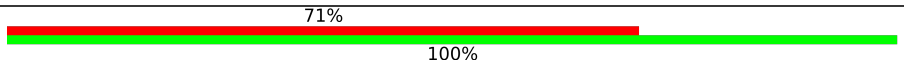
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f1	147	
35	B1	12	
36	W2	76	
36	i2	76	
37	C3	119	
38	D3	206	
39	E3	134	
40	F3	204	
41	G3	187	
42	H3	214	
43	I3	178	
44	J3	164	
45	K3	127	
46	L3	164	
47	M3	135	
48	N3	143	
49	O3	61	
50	P3	113	
51	Q3	120	
52	R3	133	
53	S3	112	
54	T3	120	
55	U3	110	
56	V3	95	
57	W3	69	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	X3	51	
59	Y3	128	
60	p3	25	
61	Z3	105	
62	a3	92	
63	b3	230	
64	c3	258	
65	d3	206	
66	e3	140	
67	f3	148	
68	g3	221	
69	h3	301	
70	j3	175	
71	k3	154	
72	m3	146	
73	n3	123	
74	o3	260	
75	q3	242	
76	r3	389	
77	s3	405	
78	t3	181	
79	u3	194	
80	l3	24	
81	A3	3390	
82	B3	163	

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 361205 atoms, of which 151371 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 protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A1	259	4254	1323	2180	387	357	7	0	0

- Molecule 2 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	k1	230	3816	1156	1965	361	326	8	0	0

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	h1	1626	52270	15549	17529	6195	11371	1626	0	0

- Molecule 4 is a protein called 40S ribosomal protein S10-1-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	l1	91	1549	508	776	125	136	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	C1	117	1778	553	900	153	165	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S17-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	D1	119	1989	604	1026	178	177	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S19-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	E1	136	Total	C	H	N	O	S	0	0
			2172	676	1091	211	190	4		

- Molecule 8 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	F1	216	Total	C	H	N	O	S	0	0
			3578	1118	1818	314	320	8		

- Molecule 9 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	G1	83	Total	C	H	N	O	S	0	0
			1295	404	643	120	125	3		

- Molecule 10 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	H1	127	Total	C	H	N	O	S	0	0
			2145	657	1111	200	174	3		

- Molecule 11 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I1	74	Total	C	H	N	O	S	0	0
			1204	365	621	109	106	3		

- Molecule 12 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J1	98	Total	C	H	N	O	S	0	0
			1610	491	818	161	132	8		

- Molecule 13 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K1	84	Total	C	H	N	O	S	0	0
			1307	404	656	122	118	7		

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L1	61	Total	C	H	N	O	S	0	0
			1018	303	525	102	86	2		

- Molecule 15 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	M1	52	Total	C	H	N	O	S	0	0
			851	249	442	94	65	1		

- Molecule 16 is a protein called ubiquitin-40S ribosomal protein S27a-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	N1	69	Total	C	H	N	O	S	0	0
			1143	360	581	103	94	5		

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	O1	188	Total	C	H	N	O	S	0	0
			3125	972	1591	281	279	2		

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	P1	186	Total	C	H	N	O	S	0	0
			3081	944	1570	300	263	4		

- Molecule 19 is a protein called guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Q1	309	Total	C	H	N	O	S	0	0
			4756	1512	2362	414	456	12		

- Molecule 20 is a protein called 40S ribosomal protein S20-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	R1	102	Total	C	H	N	O	S	0	0
			1668	505	864	151	145	3		

- Molecule 21 is a protein called 40S ribosomal protein S14-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	S1	132	Total	C	H	N	O	S	0	0
			2026	611	1028	197	185	5		

- Molecule 22 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	T1	141	Total	C	H	N	O	S	0	0
			2264	695	1164	215	187	3		

- Molecule 23 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	U1	142	Total	C	H	N	O	S	0	0
			2337	718	1184	227	202	6		

- Molecule 24 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	V1	55	Total	C	H	N	O	S	0	0
			871	274	430	90	71	6		

- Molecule 25 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	W1	149	Total	C	H	N	O	S	0	0
			2467	762	1278	223	202	2		

- Molecule 26 is a protein called 40S ribosomal protein S11-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X1	145	Total	C	H	N	O	S	0	0
			2362	734	1207	222	194	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Y1	131	Total	C	H	N	O	S	0	0
			2193	681	1132	199	176	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Z1	202	Total	C	H	N	O	S	0	0
			3233	1023	1623	289	288	10		

- Molecule 29 is a protein called 40S ribosomal protein S3-2-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	a1	211	Total	C	H	N	O	S	0	0
			3413	1052	1752	306	295	8		

- Molecule 30 is a protein called 40S ribosomal protein S9-2-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	b1	183	Total	C	H	N	O	S	0	0
			3118	964	1595	301	253	5		

- Molecule 31 is a protein called 40S ribosomal protein S2-3-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	c1	217	Total	C	H	N	O	S	0	0
			3472	1089	1786	300	289	8		

- Molecule 32 is a protein called 40S ribosomal protein S5-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	d1	194	Total	C	H	N	O	S	0	0
			3103	953	1572	290	280	8		

- Molecule 33 is a protein called 40S ribosomal protein S15a-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	e1	129	Total	C	H	N	O	S	0	0
			2100	659	1068	188	180	5		

- Molecule 34 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	f1	141	Total	C	H	N	O	S	0	0
			2332	722	1197	221	188	4		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	B1	12	Total	C	H	N	O	P	0	0
			360	108	120	24	96	12		

- Molecule 36 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	i2	76	Total	C	H	N	O	P	0	0
			2452	726	822	298	530	76		
36	W2	76	Total	C	H	N	O	P	0	0
			2451	726	822	298	529	76		

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	C3	119	Total	C	H	N	O	P	0	0
			3823	1133	1285	457	829	119		

- Molecule 38 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	D3	200	Total	C	H	N	O	S	0	0
			3296	1007	1691	324	270	4		

- Molecule 39 is a protein called 60S ribosomal protein L14-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	E3	130	Total	C	H	N	O	S	0	0
			2206	678	1150	196	179	3		

- Molecule 40 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	F3	203	Total	C	H	N	O	S	0	0
			3469	1071	1768	350	277	3		

- Molecule 41 is a protein called 60S ribosomal protein L18-2-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	G3	186	Total	C	H	N	O	S	0	0
			3042	931	1580	283	245	3		

- Molecule 42 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	H3	182	Total	C	H	N	O	S	0	0
			3181	946	1652	327	247	9		

- Molecule 43 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	I3	177	Total	C	H	N	O	S	0	0
			3061	969	1556	277	251	8		

- Molecule 44 is a protein called 60S ribosomal protein L21-1-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	J3	163	Total	C	H	N	O	S	0	0
			2672	823	1366	255	224	4		

- Molecule 45 is a protein called 60S ribosomal protein L22-2-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	K3	99	Total	C	H	N	O	S	0	0
			1653	515	845	141	150	2		

- Molecule 46 is a protein called 60S ribosomal protein L24-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	L3	62	Total	C	H	N	O	S	0	0
			1079	341	553	101	81	3		

- Molecule 47 is a protein called eL27 (60S ribosomal protein L27).

Mol	Chain	Residues	Atoms						AltConf	Trace
47	M3	134	Total	C	H	N	O	S	0	0
			2283	708	1184	206	183	2		

- Molecule 48 is a protein called eL28 (60S ribosomal protein L28).

Mol	Chain	Residues	Atoms						AltConf	Trace
48	N3	142	Total	C	H	N	O	S	0	0
			2298	701	1187	207	201	2		

- Molecule 49 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	O3	49	Total	C	H	N	O	S	0	0
			831	250	419	95	66	1		

- Molecule 50 is a protein called 60S ribosomal protein L30-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	P3	97	Total	C	H	N	O	S	0	0
			1526	475	781	130	135	5		

- Molecule 51 is a protein called eL31 (60S ribosomal protein L31).

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Q3	108	Total	C	H	N	O	S	0	0
			1809	549	934	168	156	2		

- Molecule 52 is a protein called 60S ribosomal protein L32-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	R3	126	Total	C	H	N	O	S	0	0
			2151	655	1115	207	169	5		

- Molecule 53 is a protein called eL33 (60S ribosomal protein L35a).

Mol	Chain	Residues	Atoms						AltConf	Trace
53	S3	111	Total	C	H	N	O	S	0	0
			1832	571	932	171	153	5		

- Molecule 54 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	T3	114	Total	C	H	N	O	S	0	0
			1939	579	1013	193	153	1		

- Molecule 55 is a protein called eL36 (60S ribosomal protein L36).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	U3	98	Total	C	H	N	O	S	0	0
			1650	489	868	162	129	2		

- Molecule 56 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	V3	86	Total	C	H	N	O	S	0	0
			1427	429	726	155	112	5		

- Molecule 57 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	W3	68	Total	C	H	N	O	S	0	0
			1160	358	602	99	98	3		

- Molecule 58 is a protein called 60S ribosomal protein L39-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	X3	50	Total	C	H	N	O	S	0	0
			928	286	480	96	64	2		

- Molecule 59 is a protein called ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Y3	51	Total	C	H	N	O	S	0	0
			881	262	460	88	65	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
60	p3	25	Total	C	H	N	O	S	0	0
			527	145	289	62	28	3		

- Molecule 61 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Z3	98	Total	C	H	N	O	S	0	0
			1629	494	842	157	131	5		

- Molecule 62 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	a3	91	Total	C	H	N	O	S	0	0
			1453	443	745	136	124	5		

- Molecule 63 is a protein called eL6 (60S ribosomal protein L6).

Mol	Chain	Residues	Atoms						AltConf	Trace
63	b3	208	Total	C	H	N	O	S	0	0
			3360	1046	1749	290	271	4		

- Molecule 64 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	c3	233	Total	C	H	N	O	S	0	0
			3907	1206	2028	347	319	7		

- Molecule 65 is a protein called uL13 (60S ribosomal protein L13a).

Mol	Chain	Residues	Atoms						AltConf	Trace
65	d3	205	Total	C	H	N	O	S	0	0
			3414	1046	1774	318	268	8		

- Molecule 66 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	e3	131	Total	C	H	N	O	S	0	0
			2029	623	1044	183	170	9		

- Molecule 67 is a protein called uL15 (60S ribosomal protein L27a).

Mol	Chain	Residues	Atoms						AltConf	Trace
67	f3	147	Total	C	H	N	O	S	0	0
			2361	740	1200	228	190	3		

- Molecule 68 is a protein called uL16 (60S ribosomal protein L10).

Mol	Chain	Residues	Atoms						AltConf	Trace
68	g3	209	Total	C	H	N	O	S	0	0
			3397	1058	1726	329	273	11		

- Molecule 69 is a protein called 60S ribosomal protein L5-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	h3	288	Total	C	H	N	O	S	0	0
			4715	1481	2374	426	429	5		

- Molecule 70 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	j3	154	Total	C	H	N	O	S	0	0
			2515	775	1270	246	219	5		

- Molecule 71 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	k3	117	Total	C	H	N	O	S	0	0
			1980	609	1030	170	169	2		

- Molecule 72 is a protein called uL24 (60S ribosomal protein L26).

Mol	Chain	Residues	Atoms						AltConf	Trace
72	m3	126	Total	C	H	N	O	S	0	0
			2124	634	1103	209	175	3		

- Molecule 73 is a protein called 60S ribosomal protein L35-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	n3	122	Total	C	H	N	O	S	0	0
			2140	642	1141	191	165	1		

- Molecule 74 is a protein called uL2 (60S ribosomal protein L8).

Mol	Chain	Residues	Atoms						AltConf	Trace
74	o3	245	Total	C	H	N	O	S	0	0
			3791	1174	1911	381	315	10		

- Molecule 75 is a protein called 60S ribosomal protein L7-4-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	q3	238	Total	C	H	N	O	S	0	0
			4016	1256	2058	359	339	4		

- Molecule 76 is a protein called uL3 (60S ribosomal protein L3).

Mol	Chain	Residues	Atoms						AltConf	Trace
76	r3	386	Total	C	H	N	O	S	0	0
			6327	1981	3223	578	530	15		

- Molecule 77 is a protein called uL4 (60S ribosomal protein L4).

Mol	Chain	Residues	Atoms						AltConf	Trace
77	s3	398	Total	C	H	N	O	S	0	0
			6324	1956	3227	583	548	10		

- Molecule 78 is a protein called uL5 (60S ribosomal protein L11).

Mol	Chain	Residues	Atoms						AltConf	Trace
78	t3	172	Total	C	H	N	O	S	0	0
			2836	882	1444	259	244	7		

- Molecule 79 is a protein called uL6 (60S ribosomal protein L9).

Mol	Chain	Residues	Atoms						AltConf	Trace
79	u3	191	Total	C	H	N	O	S	0	0
			3124	963	1604	276	276	5		

- Molecule 80 is a protein called nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	l3	24	Total	C	H	N	O	0	0
			169	72	49	24	24		

- Molecule 81 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	A3	3196	Total	C	H	N	O	P	0	0
			103169	30602	34651	12456	22264	3196		

- Molecule 82 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	B3	163	Total	C	H	N	O	P	0	0
			5243	1555	1763	627	1135	163		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	85	U	C	conflict	GB 1782605526

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	h1	73	Total Mg 73 73	0
83	S1	1	Total Mg 1 1	0
83	U1	1	Total Mg 1 1	0
83	B1	1	Total Mg 1 1	0
83	C3	4	Total Mg 4 4	0
83	V3	1	Total Mg 1 1	0
83	e3	1	Total Mg 1 1	0
83	j3	1	Total Mg 1 1	0
83	q3	1	Total Mg 1 1	0
83	r3	2	Total Mg 2 2	0
83	A3	49	Total Mg 49 49	0

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

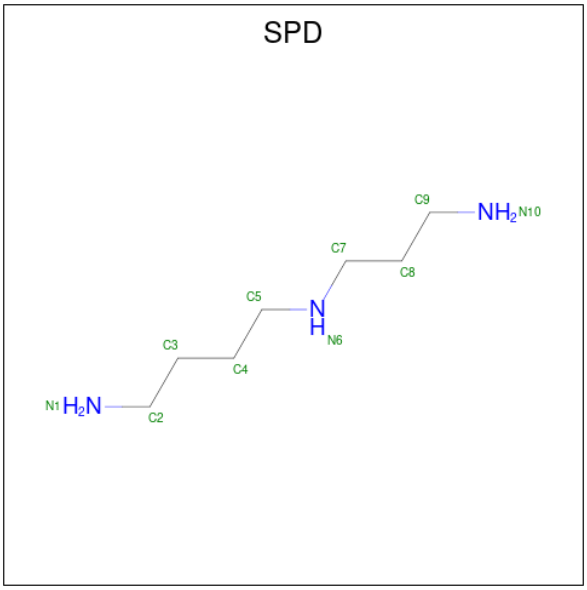
Mol	Chain	Residues	Atoms	AltConf
84	h1	42	Total K 42 42	0
84	S1	1	Total K 1 1	0
84	T1	1	Total K 1 1	0
84	U1	1	Total K 1 1	0
84	V1	1	Total K 1 1	0
84	W1	1	Total K 1 1	0
84	D3	1	Total K 1 1	0
84	R3	1	Total K 1 1	0
84	T3	1	Total K 1 1	0

Continued on next page...

Continued from previous page...

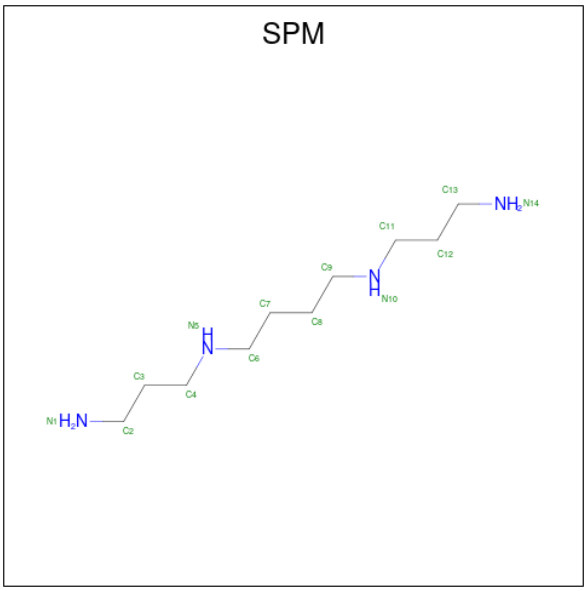
Mol	Chain	Residues	Atoms	AltConf
84	Z3	1	Total K 1 1	0
84	f3	2	Total K 2 2	0
84	g3	1	Total K 1 1	0
84	o3	2	Total K 2 2	0
84	r3	1	Total K 1 1	0
84	A3	83	Total K 83 83	0
84	B3	1	Total K 1 1	0

- Molecule 85 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
85	h1	1	Total C N 10 7 3	0
85	A3	1	Total C N 10 7 3	0

- Molecule 86 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
86	h1	1	Total C H N 40 10 26 4	0
86	h1	1	Total C H N 40 10 26 4	0
86	h1	1	Total C H N 40 10 26 4	0
86	A3	1	Total C H N 40 10 26 4	0
86	A3	1	Total C H N 40 10 26 4	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
87	J1	1	Total Zn 1 1	0
87	N1	1	Total Zn 1 1	0
87	V1	1	Total Zn 1 1	0
87	V3	1	Total Zn 1 1	0
87	Y3	1	Total Zn 1 1	0
87	Z3	1	Total Zn 1 1	0
87	a3	1	Total Zn 1 1	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms	AltConf
88	A1	7	Total O 7 7	0
88	k1	5	Total O 5 5	0
88	h1	2039	Total O 2039 2039	0
88	E1	12	Total O 12 12	0
88	F1	13	Total O 13 13	0
88	I1	1	Total O 1 1	0
88	J1	25	Total O 25 25	0
88	K1	6	Total O 6 6	0
88	M1	1	Total O 1 1	0
88	O1	1	Total O 1 1	0
88	P1	20	Total O 20 20	0
88	R1	12	Total O 12 12	0
88	S1	32	Total O 32 32	0
88	T1	43	Total O 43 43	0
88	U1	7	Total O 7 7	0
88	V1	4	Total O 4 4	0
88	W1	20	Total O 20 20	0
88	X1	21	Total O 21 21	0
88	Y1	6	Total O 6 6	0
88	Z1	1	Total O 1 1	0
88	b1	11	Total O 11 11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
88	c1	12	Total O 12 12	0
88	d1	12	Total O 12 12	0
88	e1	16	Total O 16 16	0
88	f1	10	Total O 10 10	0
88	B1	17	Total O 17 17	0
88	i2	7	Total O 7 7	0
88	W2	13	Total O 13 13	0
88	C3	91	Total O 91 91	0
88	D3	43	Total O 43 43	0
88	F3	105	Total O 105 105	0
88	G3	52	Total O 52 52	0
88	H3	10	Total O 10 10	0
88	I3	14	Total O 14 14	0
88	J3	27	Total O 27 27	0
88	M3	2	Total O 2 2	0
88	N3	10	Total O 10 10	0
88	O3	27	Total O 27 27	0
88	Q3	3	Total O 3 3	0
88	R3	42	Total O 42 42	0
88	S3	6	Total O 6 6	0
88	T3	14	Total O 14 14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
88	U3	4	Total O 4 4	0
88	V3	29	Total O 29 29	0
88	X3	7	Total O 7 7	0
88	Y3	2	Total O 2 2	0
88	p3	9	Total O 9 9	0
88	Z3	21	Total O 21 21	0
88	a3	6	Total O 6 6	0
88	b3	1	Total O 1 1	0
88	c3	10	Total O 10 10	0
88	d3	13	Total O 13 13	0
88	e3	12	Total O 12 12	0
88	f3	48	Total O 48 48	0
88	g3	16	Total O 16 16	0
88	h3	15	Total O 15 15	0
88	j3	16	Total O 16 16	0
88	k3	14	Total O 14 14	0
88	m3	9	Total O 9 9	0
88	n3	15	Total O 15 15	0
88	o3	56	Total O 56 56	0
88	q3	29	Total O 29 29	0
88	r3	27	Total O 27 27	0

Continued on next page...

Continued from previous page...

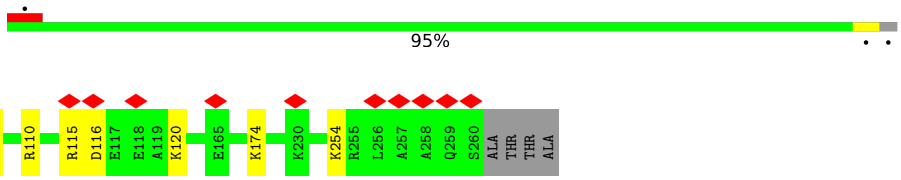
Mol	Chain	Residues	Atoms	AltConf
88	s3	65	Total O 65 65	0
88	t3	1	Total O 1 1	0
88	u3	2	Total O 2 2	0
88	A3	3383	Total O 3383 3383	0
88	B3	162	Total O 162 162	0

3 Residue-property plots (i)

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

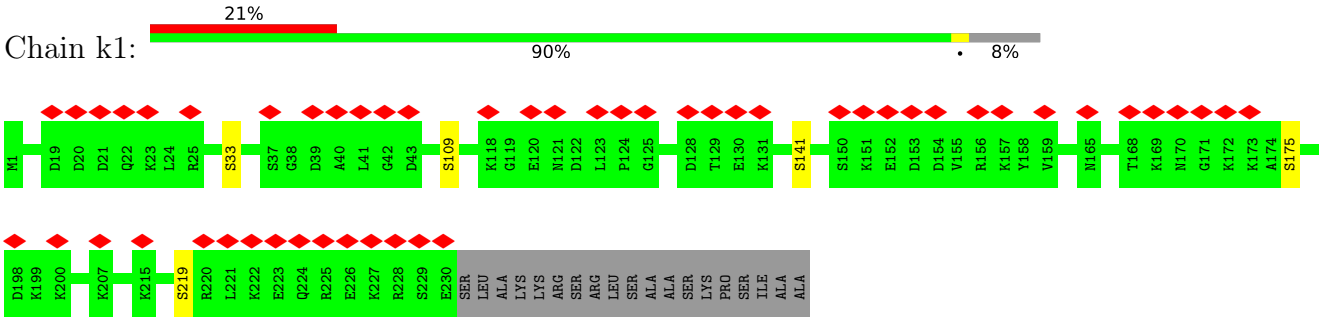
• Molecule 1: 40S ribosomal protein S4

Chain A1:



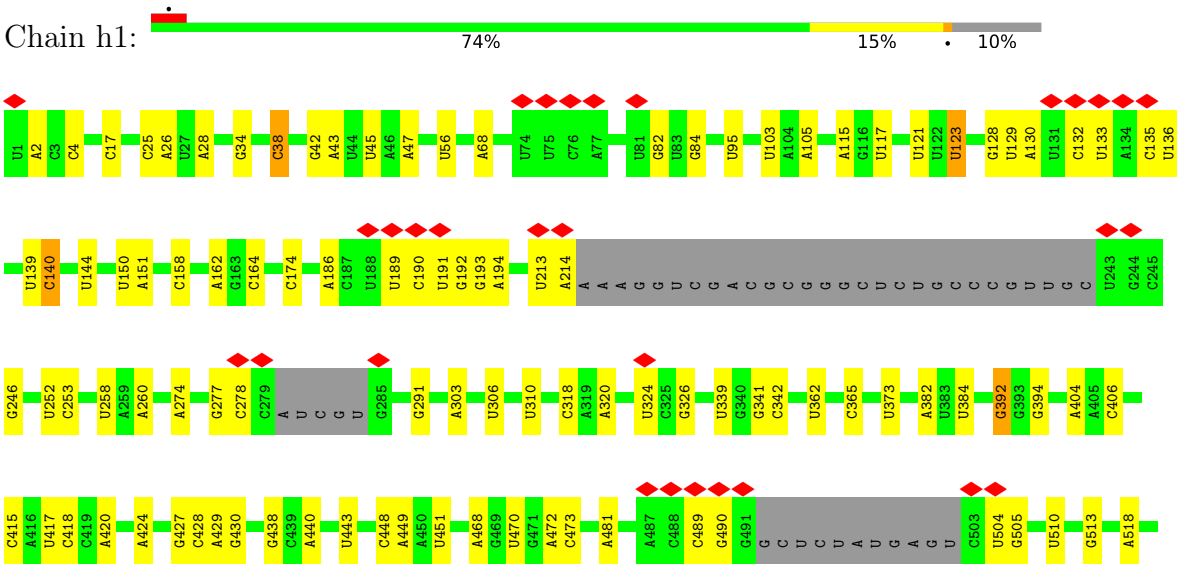
• Molecule 2: 40S ribosomal protein S6

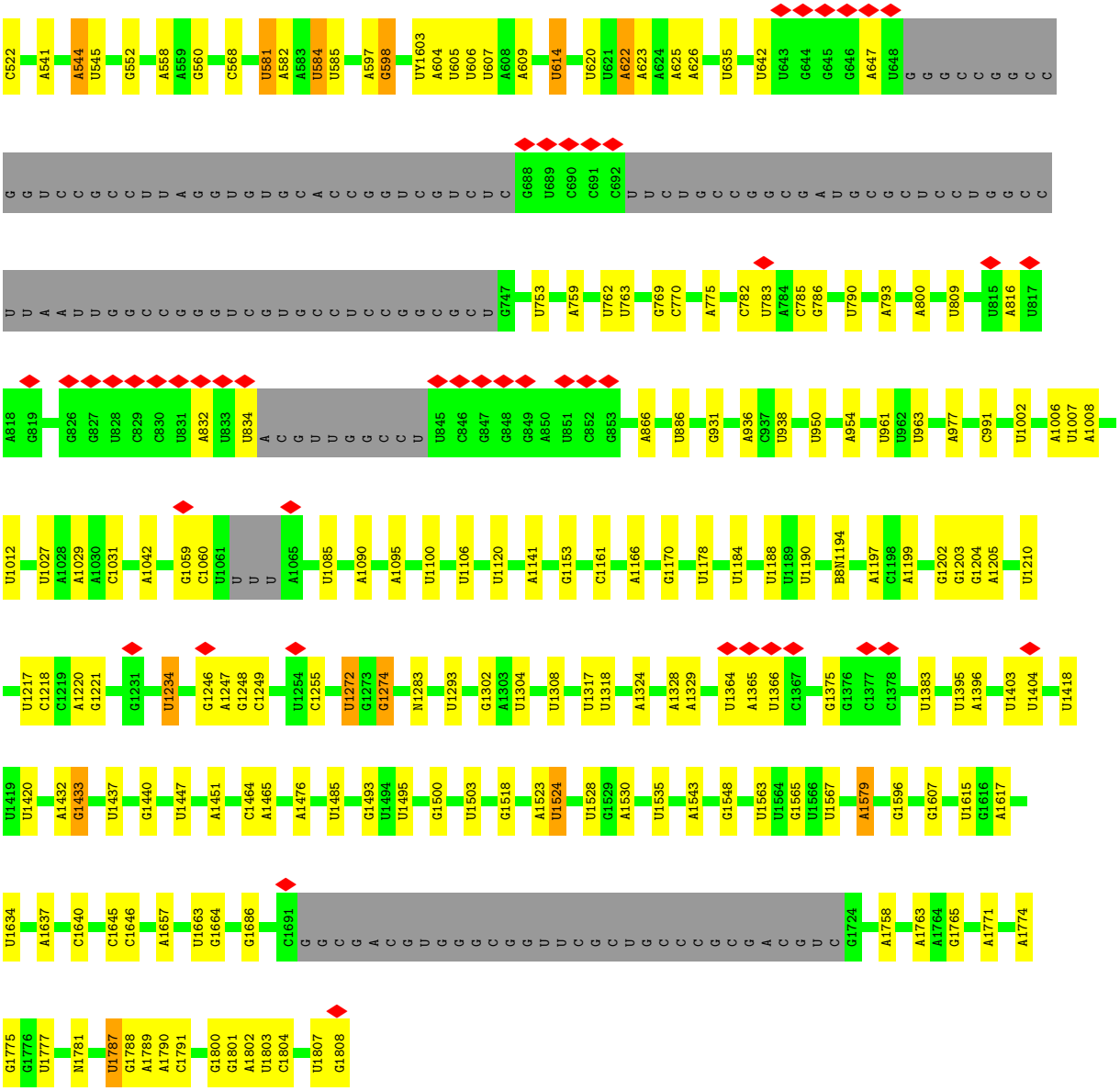
Chain k1:



• Molecule 3: 18S rRNA

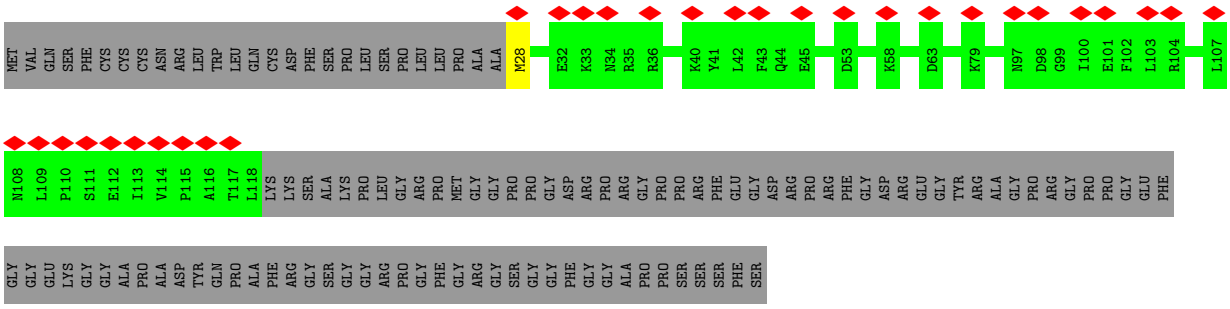
Chain h1:





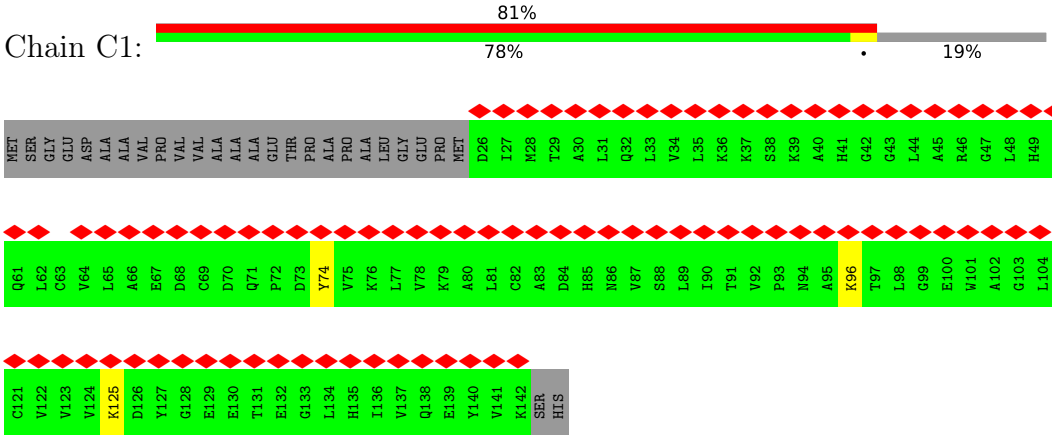
• Molecule 4: 40S ribosomal protein S10-1-like

Chain l1:



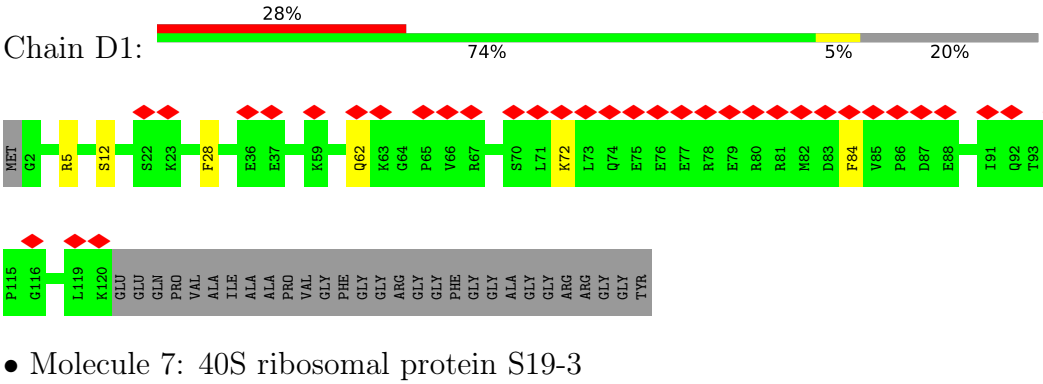
• Molecule 5: 40S ribosomal protein S12

Chain C1:



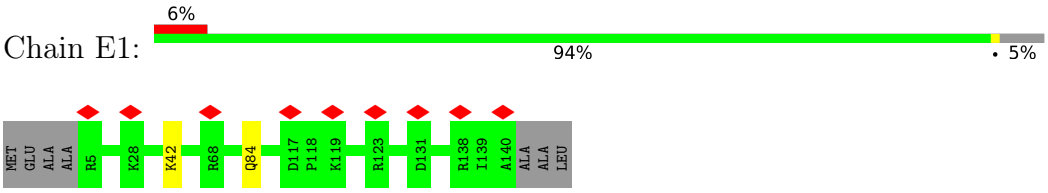
• Molecule 6: 40S ribosomal protein S17-like

Chain D1:



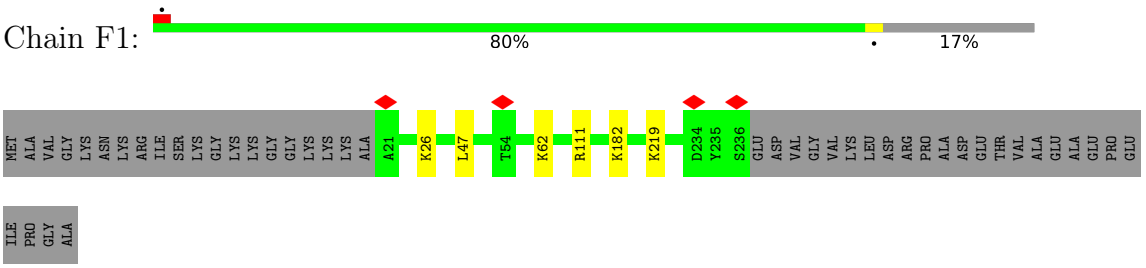
• Molecule 7: 40S ribosomal protein S19-3

Chain E1:



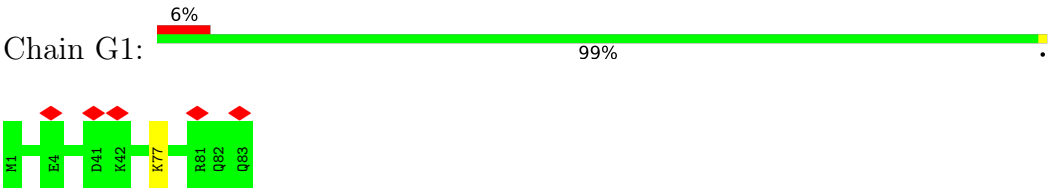
• Molecule 8: 40S ribosomal protein S3a

Chain F1:



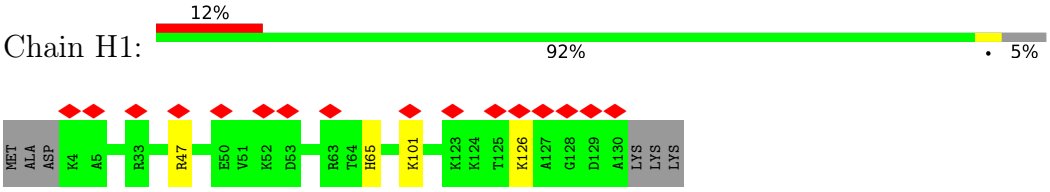
• Molecule 9: 40S ribosomal protein S21

Chain G1:



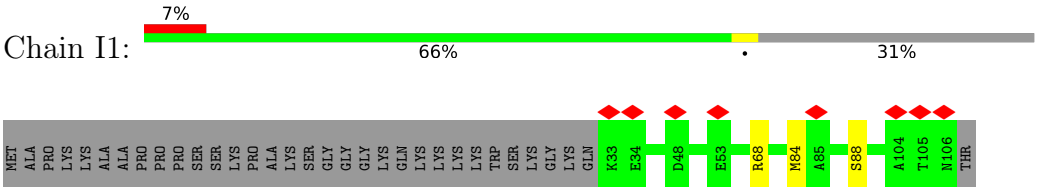
• Molecule 10: 40S ribosomal protein S24

Chain H1:



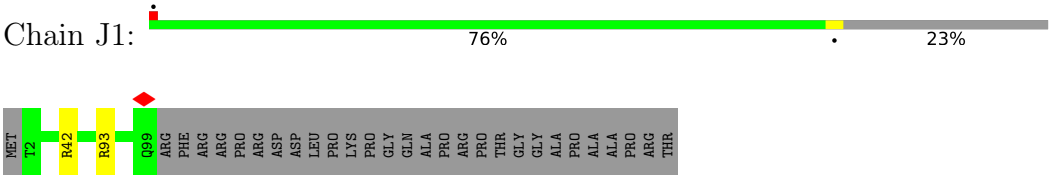
• Molecule 11: 40S ribosomal protein S25

Chain I1:



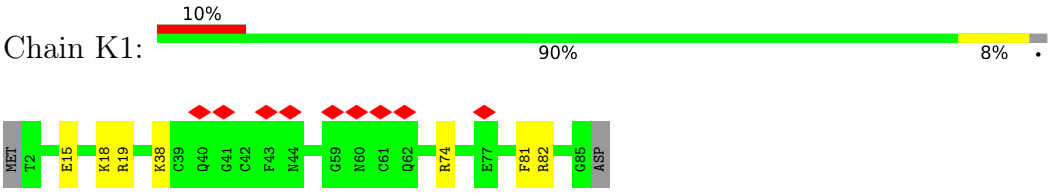
• Molecule 12: 40S ribosomal protein S26

Chain J1:



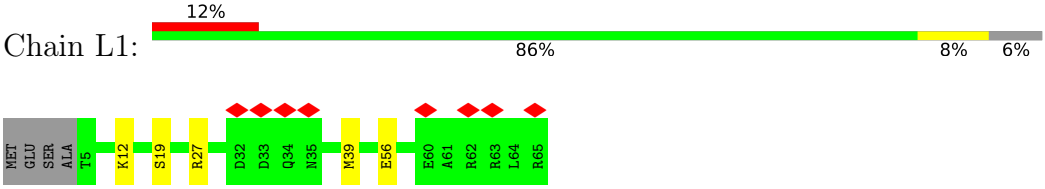
• Molecule 13: 40S ribosomal protein S27

Chain K1:



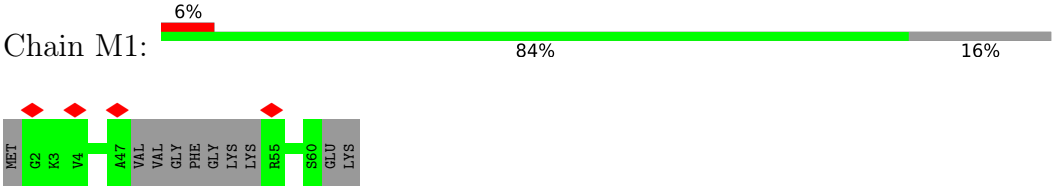
• Molecule 14: 40S ribosomal protein S28

Chain L1:



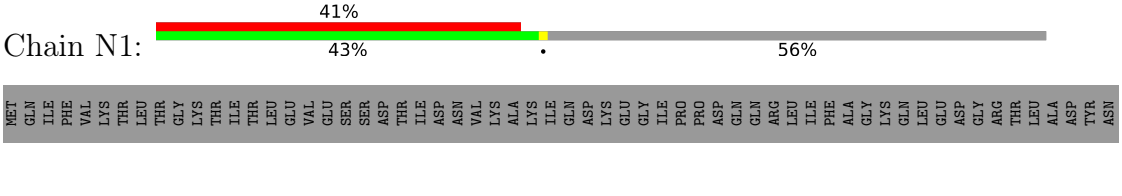
• Molecule 15: 40S ribosomal protein S30

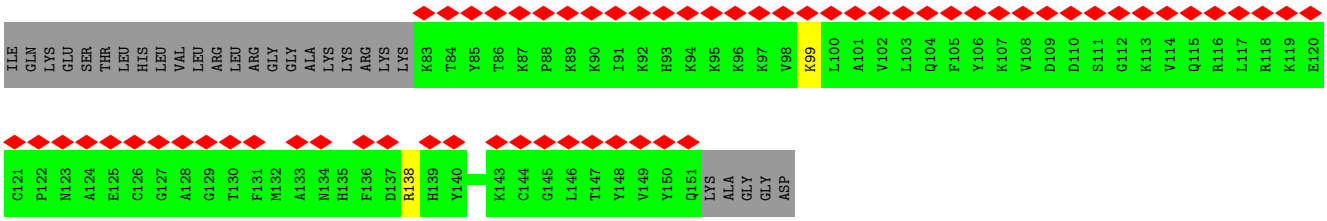
Chain M1:



• Molecule 16: ubiquitin-40S ribosomal protein S27a-like

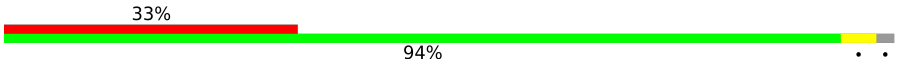
Chain N1:

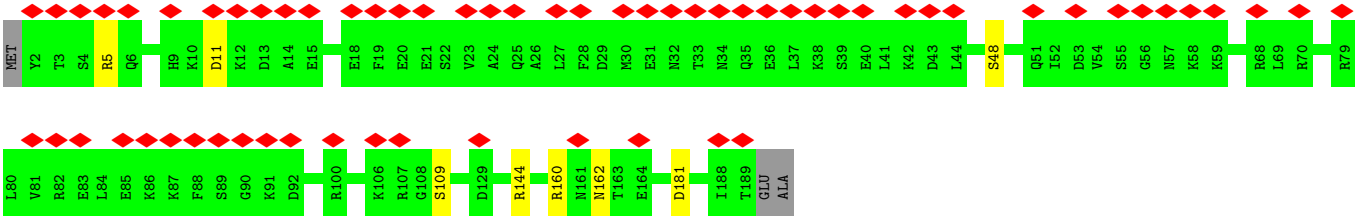




• Molecule 17: 40S ribosomal protein S7

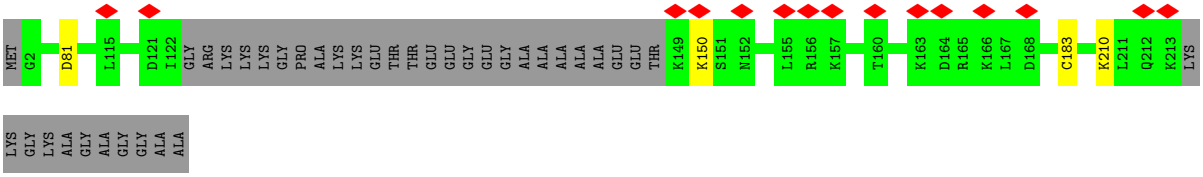
Chain O1:





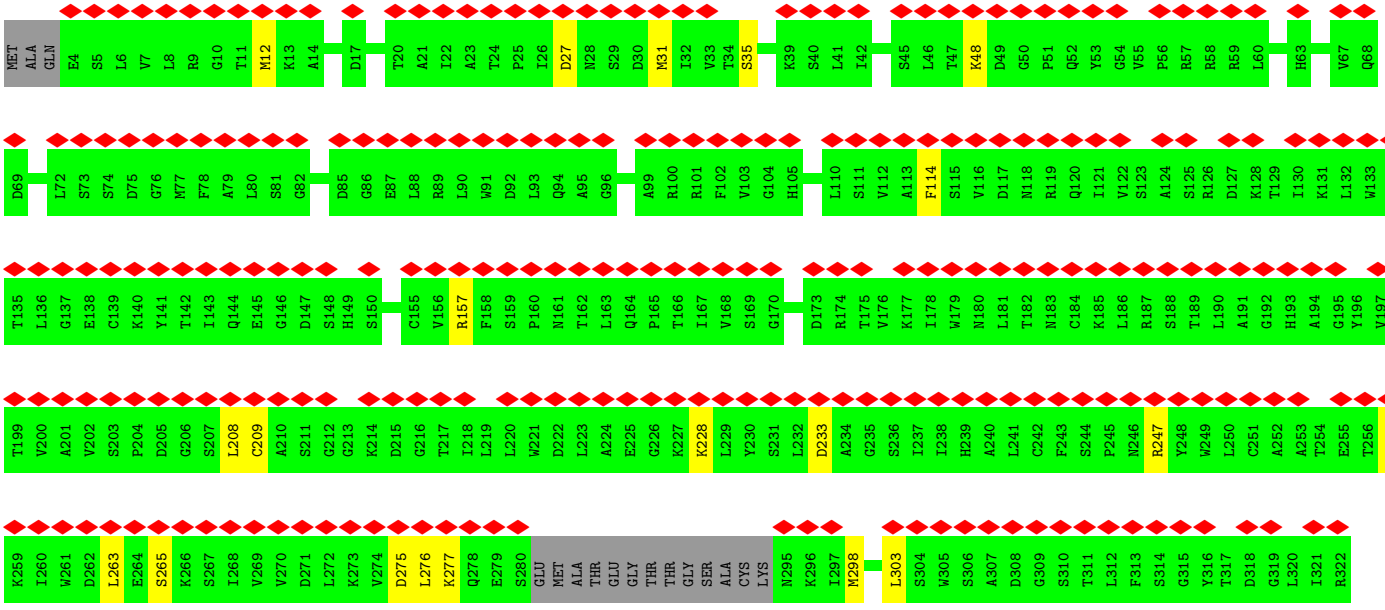
• Molecule 18: 40S ribosomal protein S8

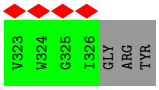
Chain P1:



• Molecule 19: guanine nucleotide-binding protein subunit beta-like protein

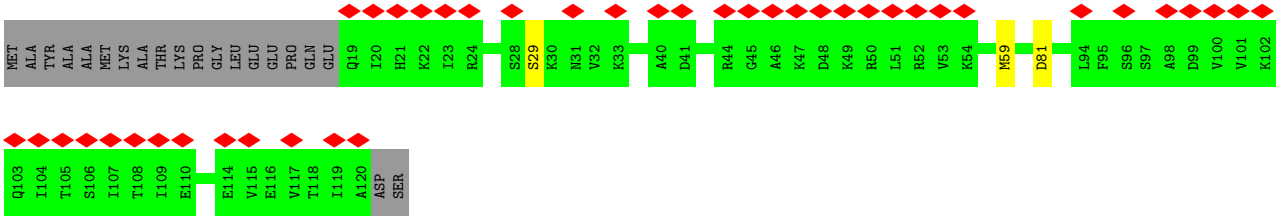
Chain Q1:





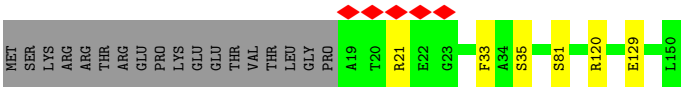
• Molecule 20: 40S ribosomal protein S20-2

Chain R1:



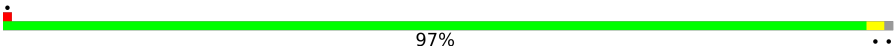
• Molecule 21: 40S ribosomal protein S14-2

Chain S1:



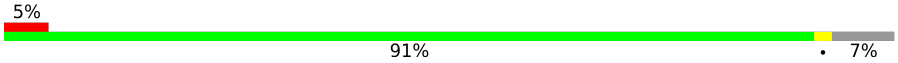
• Molecule 22: 40S ribosomal protein S23

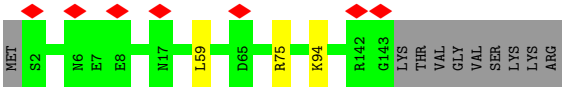
Chain T1:



• Molecule 23: 40S ribosomal protein S18

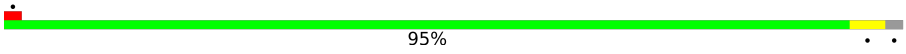
Chain U1:

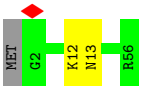




• Molecule 24: 40S ribosomal protein S29

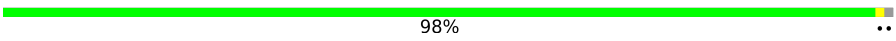
Chain V1:





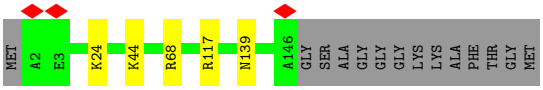
• Molecule 25: 30S ribosomal protein S15, chloroplastic

Chain W1:



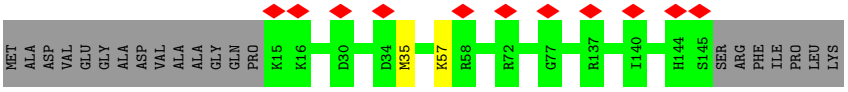
• Molecule 26: 40S ribosomal protein S11-like

Chain X1:



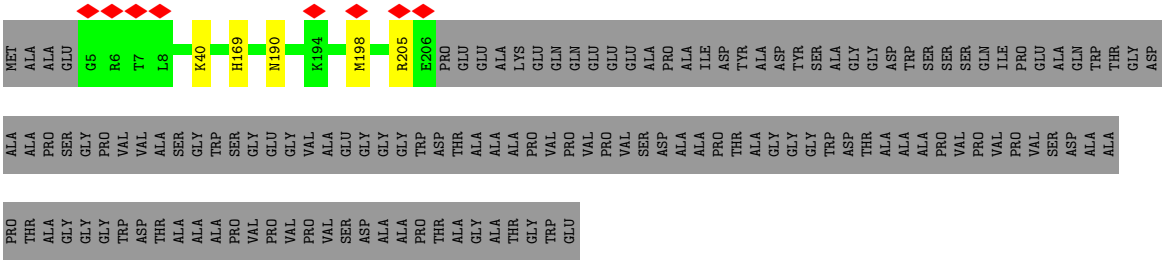
• Molecule 27: 40S ribosomal protein S15-like

Chain Y1:



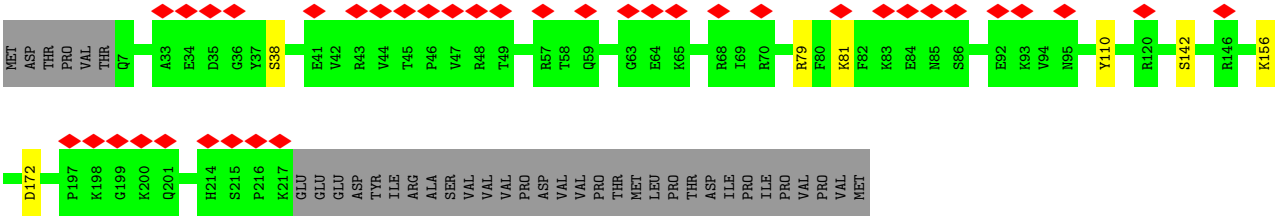
• Molecule 28: 40S ribosomal protein SA

Chain Z1:



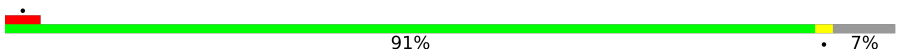
• Molecule 29: 40S ribosomal protein S3-2-like

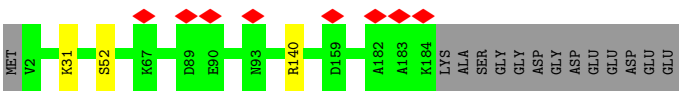
Chain a1:



• Molecule 30: 40S ribosomal protein S9-2-like

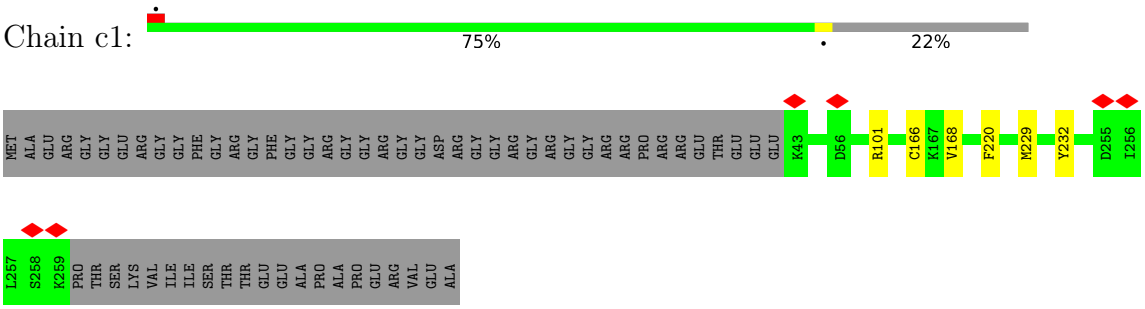
Chain b1:





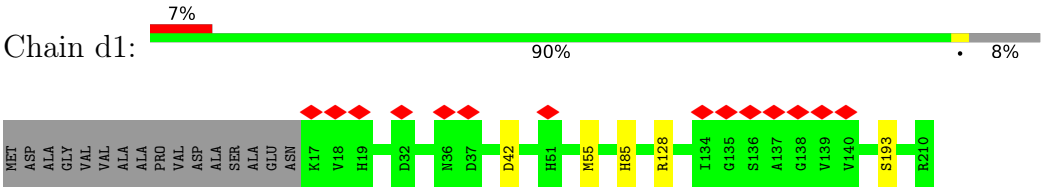
• Molecule 31: 40S ribosomal protein S2-3-like

Chain c1:



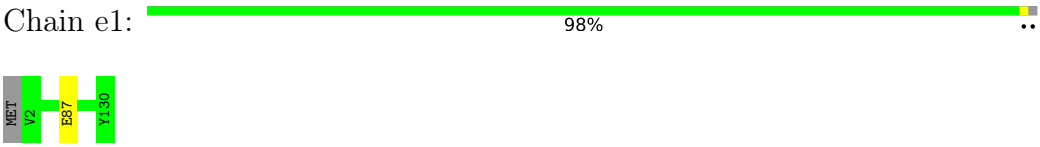
• Molecule 32: 40S ribosomal protein S5-like

Chain d1:



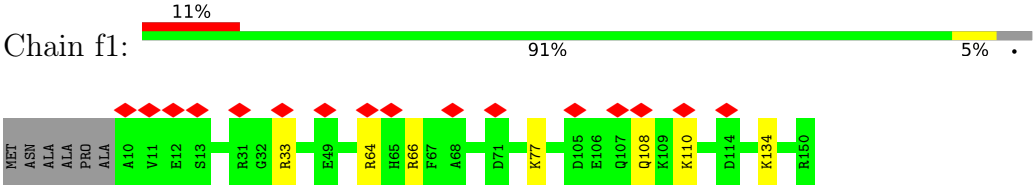
• Molecule 33: 40S ribosomal protein S15a-1

Chain e1:



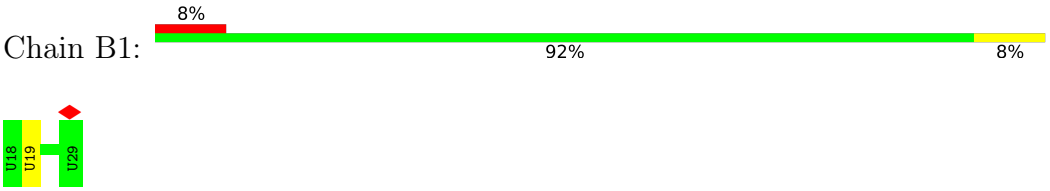
• Molecule 34: 40S ribosomal protein S16

Chain f1:



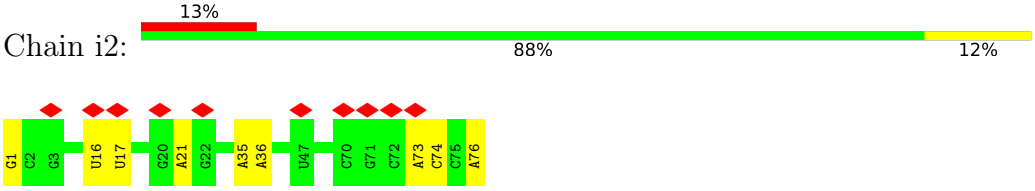
• Molecule 35: mRNA

Chain B1:



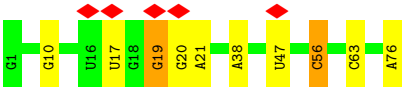
• Molecule 36: tRNA

Chain i2:



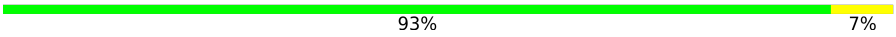
• Molecule 36: tRNA

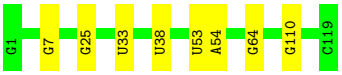
Chain W2:



• Molecule 37: 5S rRNA

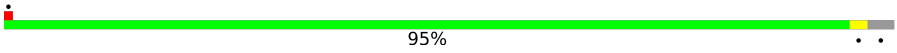
Chain C3:

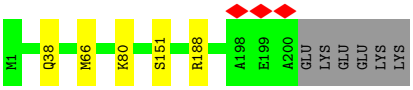




• Molecule 38: 60S ribosomal protein L13

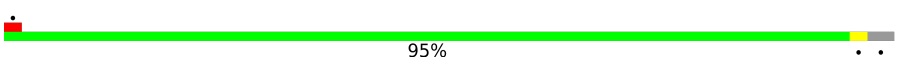
Chain D3:





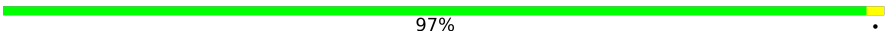
• Molecule 39: 60S ribosomal protein L14-1

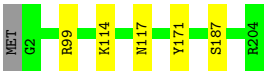
Chain E3:



• Molecule 40: Ribosomal protein L15

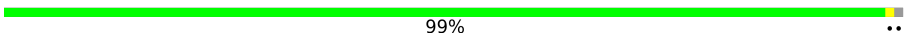
Chain F3:

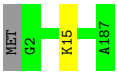




• Molecule 41: 60S ribosomal protein L18-2-like

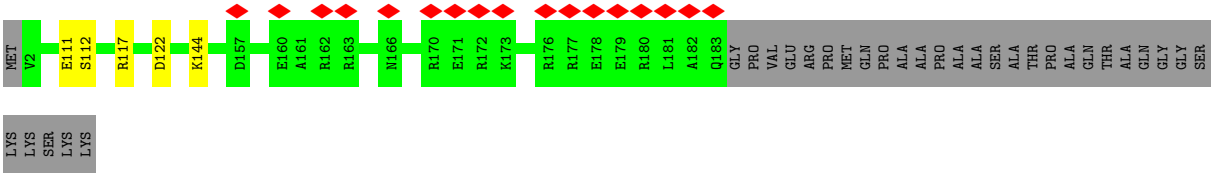
Chain G3:





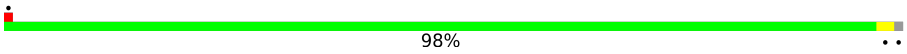
• Molecule 42: Ribosomal protein L19

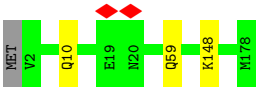
Chain H3:



• Molecule 43: 60S ribosomal protein L18a

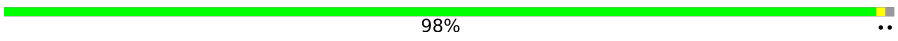
Chain I3:





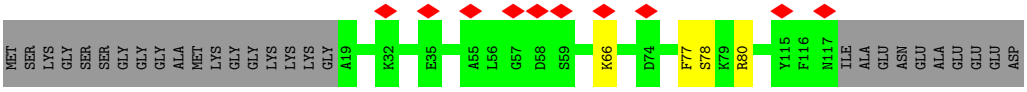
• Molecule 44: 60S ribosomal protein L21-1-like

Chain J3:



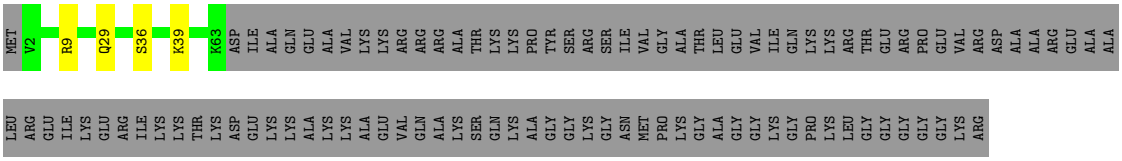
• Molecule 45: 60S ribosomal protein L22-2-like

Chain K3:



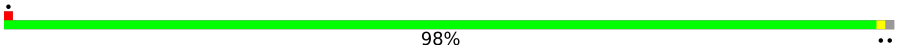
• Molecule 46: 60S ribosomal protein L24-like

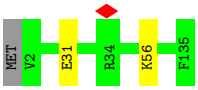
Chain L3:



• Molecule 47: eL27 (60S ribosomal protein L27)

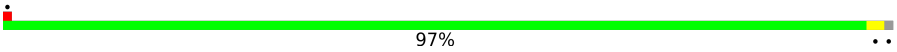
Chain M3:

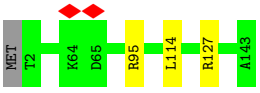




• Molecule 48: eL28 (60S ribosomal protein L28)

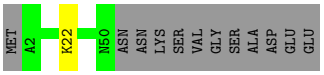
Chain N3:





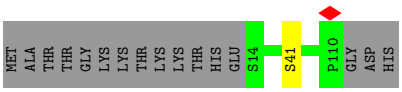
• Molecule 49: 60S ribosomal protein L29

Chain O3:



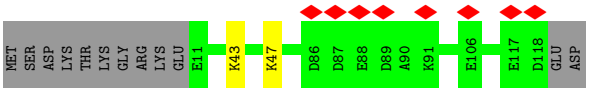
• Molecule 50: 60S ribosomal protein L30-like

Chain P3:



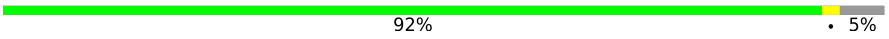
• Molecule 51: eL31 (60S ribosomal protein L31)

Chain Q3:



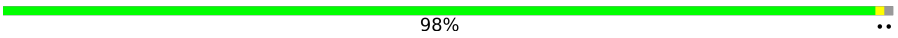
• Molecule 52: 60S ribosomal protein L32-1

Chain R3:



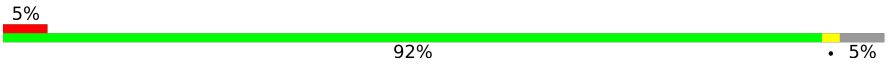
• Molecule 53: eL33 (60S ribosomal protein L35a)

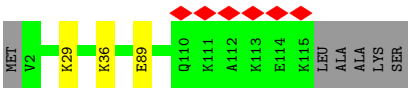
Chain S3:



• Molecule 54: 60S ribosomal protein L34

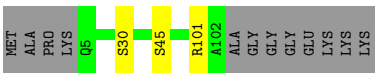
Chain T3:





• Molecule 55: eL36 (60S ribosomal protein L36)

Chain U3:

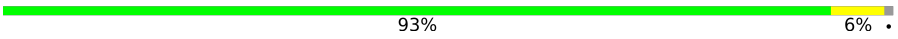


• Molecule 56: Ribosomal protein L37

Chain V3:

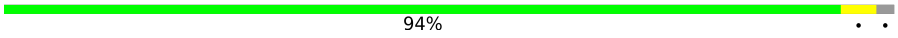
• Molecule 57: 60S ribosomal protein L38

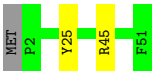
Chain W3:



• Molecule 58: 60S ribosomal protein L39-3

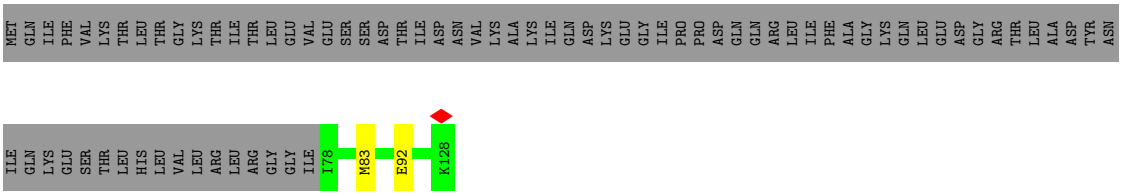
Chain X3:





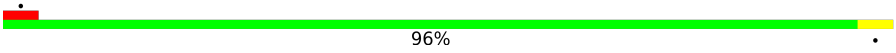
• Molecule 59: ubiquitin-60S ribosomal protein L40

Chain Y3:



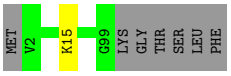
• Molecule 60: 60S ribosomal protein L41

Chain p3:



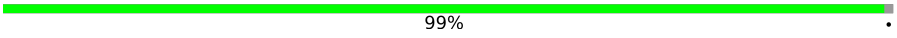
• Molecule 61: 60S ribosomal protein L44

Chain Z3:



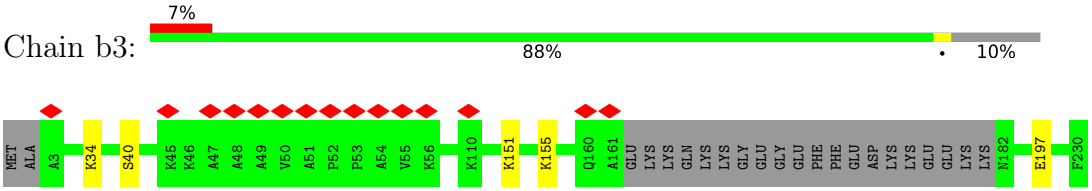
• Molecule 62: 60S ribosomal protein L37a

Chain a3:



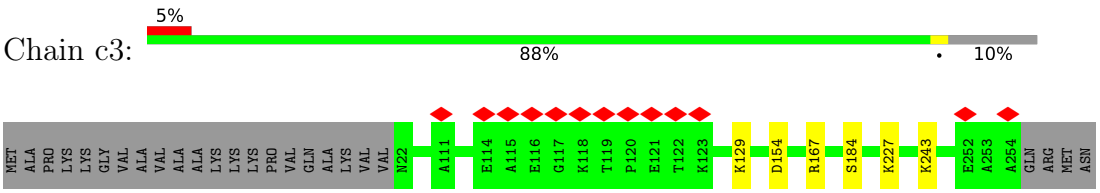
• Molecule 63: eL6 (60S ribosomal protein L6)

Chain b3:



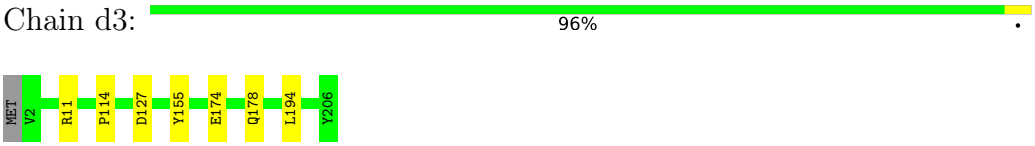
• Molecule 64: 60S ribosomal protein L7a

Chain c3:



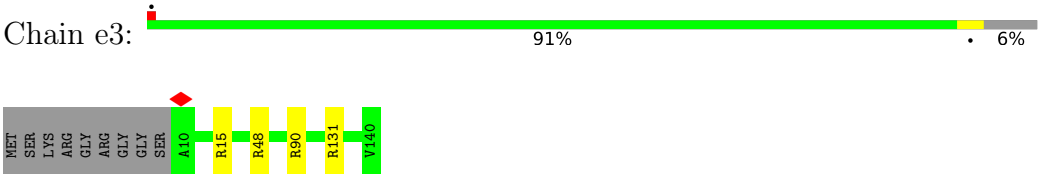
• Molecule 65: uL13 (60S ribosomal protein L13a)

Chain d3:



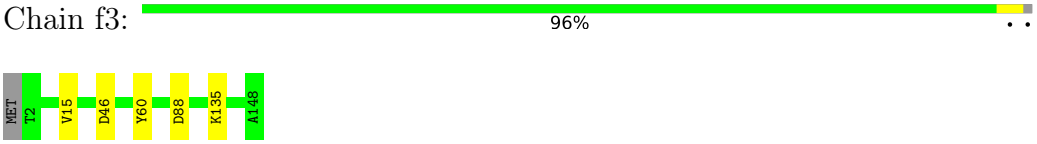
• Molecule 66: 60S ribosomal protein L23

Chain e3:



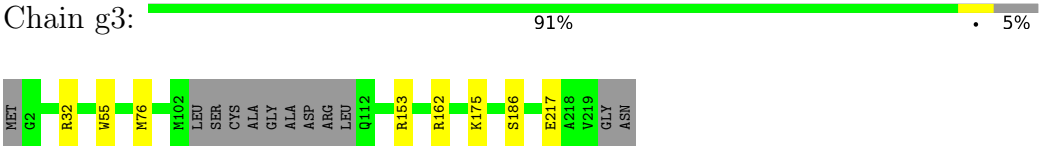
• Molecule 67: uL15 (60S ribosomal protein L27a)

Chain f3:



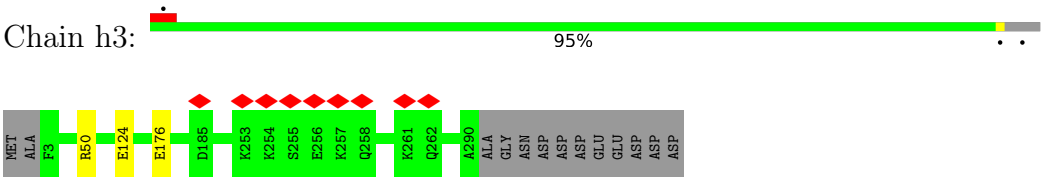
• Molecule 68: uL16 (60S ribosomal protein L10)

Chain g3:



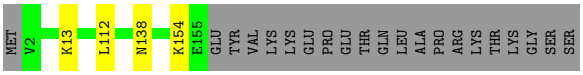
• Molecule 69: 60S ribosomal protein L5-like

Chain h3:



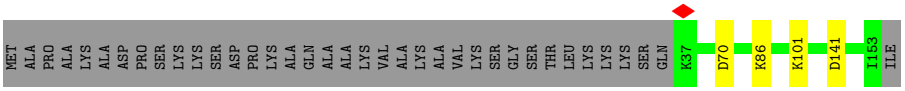
• Molecule 70: 50S ribosomal protein L22, chloroplastic

Chain j3:



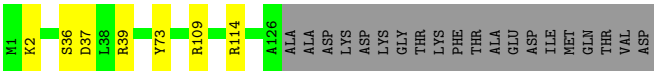
• Molecule 71: 60S ribosomal protein L23a

Chain k3:



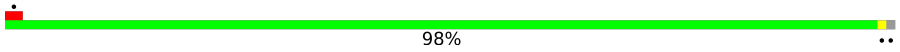
• Molecule 72: uL24 (60S ribosomal protein L26)

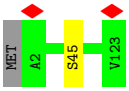
Chain m3:



• Molecule 73: 60S ribosomal protein L35-like

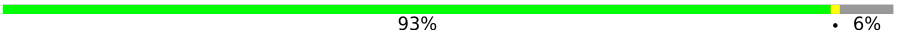
Chain n3:





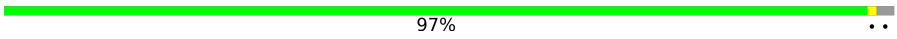
• Molecule 74: uL2 (60S ribosomal protein L8)

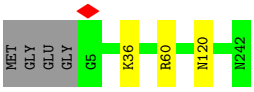
Chain o3:



• Molecule 75: 60S ribosomal protein L7-4-like

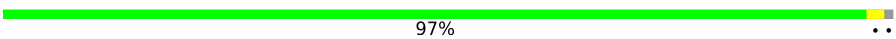
Chain q3:

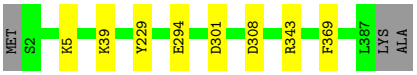




• Molecule 76: uL3 (60S ribosomal protein L3)

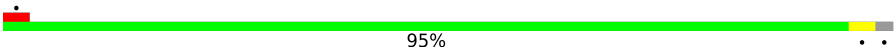
Chain r3:





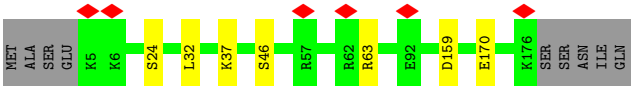
• Molecule 77: uL4 (60S ribosomal protein L4)

Chain s3:



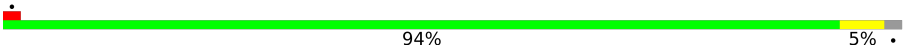
• Molecule 78: uL5 (60S ribosomal protein L11)

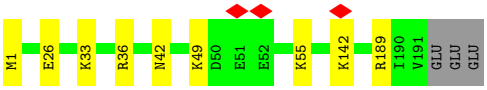
Chain t3:



• Molecule 79: uL6 (60S ribosomal protein L9)

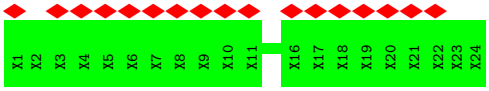
Chain u3:





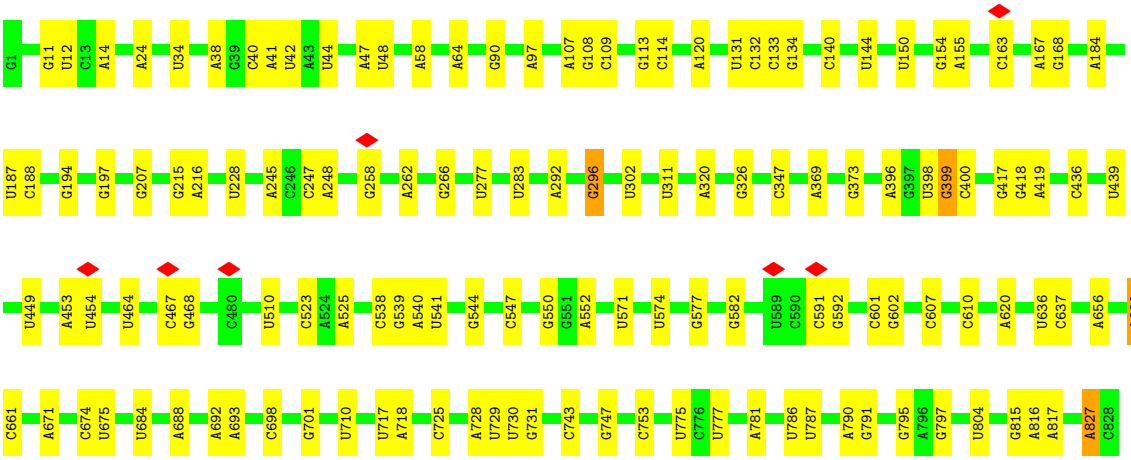
• Molecule 80: nascent chain

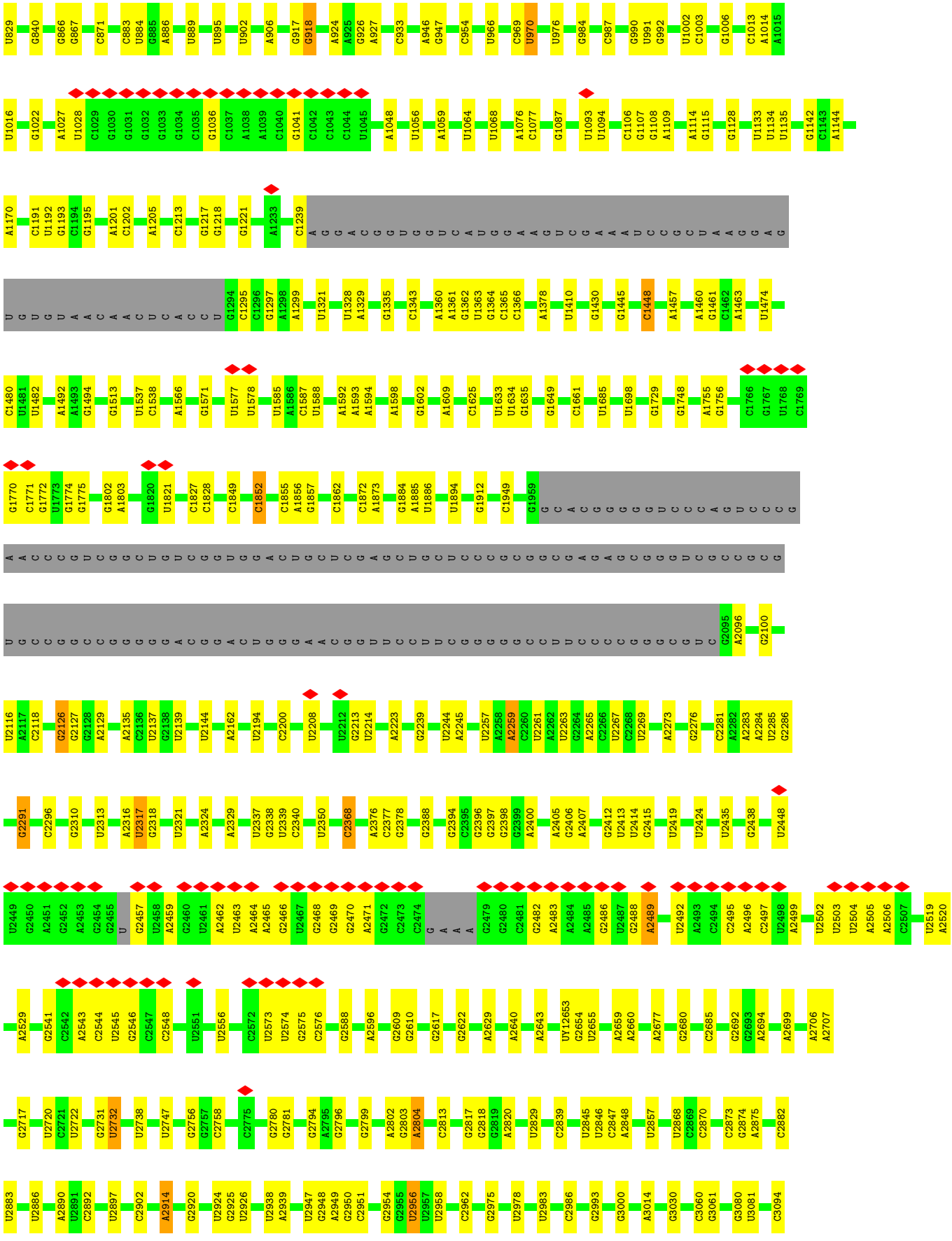
Chain l3:

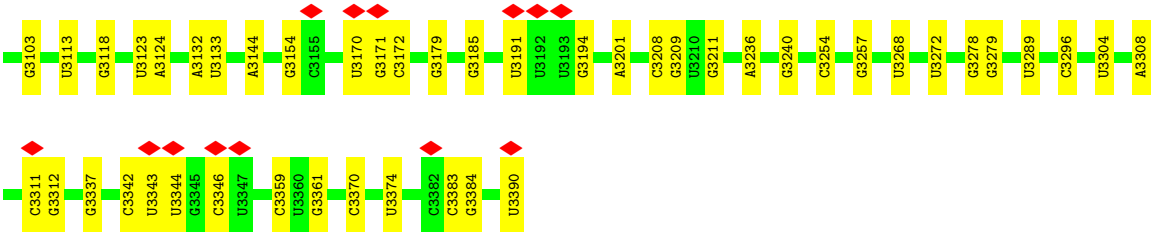


• Molecule 81: 25S rRNA

Chain A3:

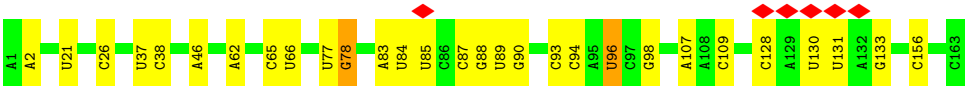






• Molecule 82: 5.8S rRNA

Chain B3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.499	Depositor
Minimum map value	-6.970	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.323	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	381.6, 381.6, 381.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

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

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	A1	0.25	0/2114	0.53	0/2837
2	k1	0.27	0/1875	0.57	0/2494
3	h1	0.17	0/36945	0.72	1/57563 (0.0%)
4	l1	0.25	0/794	0.44	0/1074
5	C1	0.25	0/889	0.52	0/1198
6	D1	0.26	0/973	0.55	0/1299
7	E1	0.25	0/1103	0.53	0/1480
8	F1	0.24	0/1790	0.51	0/2402
9	G1	0.25	0/662	0.50	0/891
10	H1	0.25	0/1049	0.54	0/1391
11	I1	0.24	0/589	0.54	0/789
12	J1	0.24	0/805	0.57	0/1076
13	K1	0.26	0/662	0.53	0/892
14	L1	0.24	0/496	0.62	0/661
15	M1	0.27	0/414	0.58	0/544
16	N1	0.27	0/574	0.50	0/763
17	O1	0.26	0/1560	0.56	0/2097
18	P1	0.25	0/1535	0.56	0/2050
19	Q1	0.25	0/2446	0.53	0/3324
20	R1	0.24	0/813	0.53	0/1095
21	S1	0.25	0/1010	0.59	0/1352
22	T1	0.25	0/1119	0.53	0/1487
23	U1	0.25	0/1170	0.55	0/1562
24	V1	0.26	0/453	0.52	0/605
25	W1	0.25	0/1214	0.50	0/1632
26	X1	0.26	0/1180	0.54	0/1579
27	Y1	0.26	0/1084	0.53	0/1450
28	Z1	0.26	0/1644	0.51	0/2223
29	a1	0.27	0/1684	0.56	0/2257
30	b1	0.24	0/1550	0.55	0/2073
31	c1	0.25	0/1721	0.51	0/2320

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	d1	0.24	0/1553	0.52	0/2095
33	e1	0.25	0/1050	0.53	0/1405
34	f1	0.25	0/1154	0.55	0/1542
35	B1	0.13	0/263	0.71	0/404
36	W2	0.20	0/1822	0.79	3/2840 (0.1%)
36	i2	0.30	1/1823 (0.1%)	0.75	0/2840
37	C3	0.17	0/2837	0.70	0/4420
38	D3	0.25	0/1635	0.55	0/2194
39	E3	0.24	0/1069	0.52	0/1427
40	F3	0.24	0/1740	0.60	0/2333
41	G3	0.25	0/1487	0.55	0/1989
42	H3	0.25	0/1548	0.59	0/2042
43	I3	0.25	0/1544	0.51	0/2071
44	J3	0.24	0/1331	0.54	0/1784
45	K3	0.24	0/819	0.51	0/1098
46	L3	0.26	0/539	0.51	0/716
47	M3	0.25	0/1118	0.52	0/1492
48	N3	0.25	0/1126	0.48	0/1508
49	O3	0.26	0/422	0.55	0/558
50	P3	0.26	0/757	0.48	0/1018
51	Q3	0.25	0/885	0.56	0/1184
52	R3	0.23	0/1053	0.55	0/1408
53	S3	0.26	0/920	0.53	0/1232
54	T3	0.24	0/939	0.57	0/1251
55	U3	0.25	0/791	0.56	0/1047
56	V3	0.26	0/714	0.64	0/949
57	W3	0.26	0/566	0.51	0/752
58	X3	0.22	0/460	0.57	0/611
59	Y3	0.24	0/427	0.54	0/562
60	p3	0.26	0/239	0.74	0/302
61	Z3	0.25	0/801	0.49	0/1058
62	a3	0.24	0/717	0.55	0/952
63	b3	0.27	0/1645	0.47	0/2210
64	c3	0.25	0/1912	0.50	0/2562
65	d3	0.25	0/1669	0.52	0/2235
66	e3	0.26	0/1001	0.55	0/1345
67	f3	0.26	0/1190	0.50	0/1591
68	g3	0.25	0/1707	0.56	0/2283
69	h3	0.26	0/2386	0.51	0/3200
70	j3	0.25	0/1270	0.54	0/1704
71	k3	0.25	0/965	0.49	0/1295
72	m3	0.24	0/1035	0.57	0/1383
73	n3	0.25	0/1009	0.51	0/1343

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	o3	0.25	0/1924	0.56	0/2585
75	q3	0.26	0/1992	0.49	0/2670
76	r3	0.25	0/3172	0.51	0/4249
77	s3	0.24	0/3159	0.51	0/4259
78	t3	0.26	0/1414	0.55	0/1890
79	u3	0.25	0/1539	0.51	0/2059
81	A3	0.20	0/73585	0.74	7/114781 (0.0%)
82	B3	0.19	0/3772	0.74	0/5878
All	All	0.22	1/212412 (0.0%)	0.66	11/311066 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	i2	1	G	OP3-P	-10.59	1.48	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2548	C	N3-C2-O2	-7.99	116.31	121.90
81	A3	2489	A	C6-N1-C2	-7.95	113.83	118.60
81	A3	2489	A	C5-C6-N1	7.53	121.47	117.70
3	h1	604	A	OP1-P-OP2	7.50	130.85	119.60
36	W2	56	C	C2-N3-C4	-6.84	116.48	119.90
81	A3	2489	A	N1-C6-N6	-6.74	114.56	118.60
36	W2	56	C	N3-C4-C5	6.46	124.48	121.90
81	A3	2541	G	C5-C6-O6	5.83	132.10	128.60
81	A3	710	U	C2-N1-C1'	5.55	124.36	117.70
81	A3	113	G	O4'-C1'-N9	5.55	112.64	108.20
36	W2	19	G	C5-C6-O6	5.26	131.76	128.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	257/264 (97%)	254 (99%)	3 (1%)	0	100	100
2	k1	228/249 (92%)	228 (100%)	0	0	100	100
4	l1	89/208 (43%)	87 (98%)	2 (2%)	0	100	100
5	C1	115/144 (80%)	114 (99%)	1 (1%)	0	100	100
6	D1	117/149 (78%)	115 (98%)	2 (2%)	0	100	100
7	E1	134/143 (94%)	132 (98%)	2 (2%)	0	100	100
8	F1	214/261 (82%)	213 (100%)	1 (0%)	0	100	100
9	G1	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
10	H1	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
11	I1	72/107 (67%)	70 (97%)	2 (3%)	0	100	100
12	J1	96/127 (76%)	96 (100%)	0	0	100	100
13	K1	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
14	L1	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
15	M1	48/62 (77%)	45 (94%)	3 (6%)	0	100	100
16	N1	67/156 (43%)	66 (98%)	1 (2%)	0	100	100
17	O1	186/191 (97%)	182 (98%)	4 (2%)	0	100	100
18	P1	182/224 (81%)	180 (99%)	2 (1%)	0	100	100
19	Q1	305/328 (93%)	297 (97%)	8 (3%)	0	100	100
20	R1	100/122 (82%)	98 (98%)	2 (2%)	0	100	100
21	S1	130/150 (87%)	129 (99%)	1 (1%)	0	100	100
22	T1	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
23	U1	140/152 (92%)	136 (97%)	4 (3%)	0	100	100
24	V1	53/56 (95%)	53 (100%)	0	0	100	100
25	W1	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
26	X1	143/159 (90%)	141 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Y1	129/152 (85%)	126 (98%)	3 (2%)	0	100	100
28	Z1	200/336 (60%)	197 (98%)	3 (2%)	0	100	100
29	a1	209/248 (84%)	201 (96%)	8 (4%)	0	100	100
30	b1	181/197 (92%)	176 (97%)	5 (3%)	0	100	100
31	c1	215/280 (77%)	210 (98%)	5 (2%)	0	100	100
32	d1	192/210 (91%)	184 (96%)	7 (4%)	1 (0%)	29	31
33	e1	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
34	f1	139/147 (95%)	138 (99%)	1 (1%)	0	100	100
38	D3	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
39	E3	128/134 (96%)	126 (98%)	2 (2%)	0	100	100
40	F3	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
41	G3	184/187 (98%)	182 (99%)	2 (1%)	0	100	100
42	H3	180/214 (84%)	179 (99%)	1 (1%)	0	100	100
43	I3	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
44	J3	161/164 (98%)	160 (99%)	1 (1%)	0	100	100
45	K3	97/127 (76%)	93 (96%)	4 (4%)	0	100	100
46	L3	60/164 (37%)	57 (95%)	3 (5%)	0	100	100
47	M3	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
48	N3	140/143 (98%)	136 (97%)	4 (3%)	0	100	100
49	O3	47/61 (77%)	46 (98%)	1 (2%)	0	100	100
50	P3	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
51	Q3	106/120 (88%)	106 (100%)	0	0	100	100
52	R3	124/133 (93%)	123 (99%)	1 (1%)	0	100	100
53	S3	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
54	T3	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
55	U3	96/110 (87%)	96 (100%)	0	0	100	100
56	V3	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
57	W3	66/69 (96%)	66 (100%)	0	0	100	100
58	X3	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
59	Y3	49/128 (38%)	49 (100%)	0	0	100	100
60	p3	23/25 (92%)	23 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	Z3	96/105 (91%)	95 (99%)	1 (1%)	0	100	100
62	a3	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
63	b3	204/230 (89%)	201 (98%)	3 (2%)	0	100	100
64	c3	231/258 (90%)	228 (99%)	3 (1%)	0	100	100
65	d3	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
66	e3	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
67	f3	145/148 (98%)	137 (94%)	7 (5%)	1 (1%)	22	22
68	g3	205/221 (93%)	202 (98%)	3 (2%)	0	100	100
69	h3	286/301 (95%)	278 (97%)	8 (3%)	0	100	100
70	j3	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
71	k3	115/154 (75%)	113 (98%)	2 (2%)	0	100	100
72	m3	124/146 (85%)	120 (97%)	4 (3%)	0	100	100
73	n3	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
74	o3	243/260 (94%)	234 (96%)	9 (4%)	0	100	100
75	q3	236/242 (98%)	231 (98%)	5 (2%)	0	100	100
76	r3	384/389 (99%)	380 (99%)	4 (1%)	0	100	100
77	s3	396/405 (98%)	390 (98%)	6 (2%)	0	100	100
78	t3	170/181 (94%)	168 (99%)	2 (1%)	0	100	100
79	u3	189/194 (97%)	188 (100%)	1 (0%)	0	100	100
All	All	11033/12575 (88%)	10841 (98%)	190 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	d1	85	HIS
67	f3	15	VAL

5.3.2 Protein sidechains (i)

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
1	A1	225/228 (99%)	216 (96%)	9 (4%)	31 40
2	k1	199/213 (93%)	194 (98%)	5 (2%)	47 60
4	l1	85/169 (50%)	84 (99%)	1 (1%)	71 83
5	C1	94/112 (84%)	90 (96%)	4 (4%)	29 36
6	D1	109/124 (88%)	101 (93%)	8 (7%)	14 15
7	E1	111/114 (97%)	109 (98%)	2 (2%)	59 72
8	F1	195/228 (86%)	189 (97%)	6 (3%)	40 51
9	G1	70/70 (100%)	69 (99%)	1 (1%)	67 80
10	H1	108/113 (96%)	104 (96%)	4 (4%)	34 43
11	I1	64/89 (72%)	61 (95%)	3 (5%)	26 33
12	J1	87/109 (80%)	85 (98%)	2 (2%)	50 63
13	K1	76/78 (97%)	69 (91%)	7 (9%)	9 9
14	L1	54/57 (95%)	49 (91%)	5 (9%)	9 8
15	M1	41/49 (84%)	41 (100%)	0	100 100
16	N1	60/134 (45%)	58 (97%)	2 (3%)	38 49
17	O1	169/171 (99%)	161 (95%)	8 (5%)	26 33
18	P1	158/178 (89%)	154 (98%)	4 (2%)	47 60
19	Q1	266/279 (95%)	246 (92%)	20 (8%)	13 14
20	R1	93/108 (86%)	90 (97%)	3 (3%)	39 50
21	S1	103/120 (86%)	97 (94%)	6 (6%)	20 23
22	T1	113/114 (99%)	110 (97%)	3 (3%)	44 57
23	U1	122/131 (93%)	119 (98%)	3 (2%)	47 60
24	V1	46/47 (98%)	44 (96%)	2 (4%)	29 36
25	W1	130/131 (99%)	129 (99%)	1 (1%)	81 90
26	X1	124/131 (95%)	119 (96%)	5 (4%)	31 40
27	Y1	115/130 (88%)	113 (98%)	2 (2%)	60 74
28	Z1	171/256 (67%)	166 (97%)	5 (3%)	42 54
29	a1	179/215 (83%)	172 (96%)	7 (4%)	32 41
30	b1	161/171 (94%)	158 (98%)	3 (2%)	57 71
31	c1	184/226 (81%)	178 (97%)	6 (3%)	38 49
32	d1	165/175 (94%)	161 (98%)	4 (2%)	49 62
33	e1	111/112 (99%)	110 (99%)	1 (1%)	78 88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	f1	116/120 (97%)	109 (94%)	7 (6%)	19	22
38	D3	165/171 (96%)	160 (97%)	5 (3%)	41	53
39	E3	114/117 (97%)	111 (97%)	3 (3%)	46	58
40	F3	176/177 (99%)	171 (97%)	5 (3%)	43	56
41	G3	154/155 (99%)	153 (99%)	1 (1%)	86	93
42	H3	160/182 (88%)	155 (97%)	5 (3%)	40	51
43	I3	163/164 (99%)	160 (98%)	3 (2%)	59	72
44	J3	140/141 (99%)	138 (99%)	2 (1%)	67	80
45	K3	91/109 (84%)	87 (96%)	4 (4%)	28	35
46	L3	57/133 (43%)	53 (93%)	4 (7%)	15	16
47	M3	117/118 (99%)	115 (98%)	2 (2%)	60	74
48	N3	123/124 (99%)	120 (98%)	3 (2%)	49	62
49	O3	43/53 (81%)	42 (98%)	1 (2%)	50	63
50	P3	85/98 (87%)	84 (99%)	1 (1%)	71	83
51	Q3	95/106 (90%)	93 (98%)	2 (2%)	53	67
52	R3	114/121 (94%)	111 (97%)	3 (3%)	46	58
53	S3	98/99 (99%)	97 (99%)	1 (1%)	76	86
54	T3	100/104 (96%)	97 (97%)	3 (3%)	41	53
55	U3	83/90 (92%)	80 (96%)	3 (4%)	35	45
56	V3	72/77 (94%)	71 (99%)	1 (1%)	67	80
57	W3	64/65 (98%)	60 (94%)	4 (6%)	18	20
58	X3	47/48 (98%)	45 (96%)	2 (4%)	29	36
59	Y3	46/114 (40%)	44 (96%)	2 (4%)	29	36
60	p3	24/24 (100%)	23 (96%)	1 (4%)	30	38
61	Z3	86/92 (94%)	85 (99%)	1 (1%)	71	83
62	a3	73/74 (99%)	73 (100%)	0	100	100
63	b3	175/194 (90%)	170 (97%)	5 (3%)	42	54
64	c3	202/221 (91%)	196 (97%)	6 (3%)	41	53
65	d3	173/174 (99%)	166 (96%)	7 (4%)	31	40
66	e3	103/109 (94%)	99 (96%)	4 (4%)	32	41
67	f3	119/120 (99%)	115 (97%)	4 (3%)	37	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
68	g3	173/181 (96%)	165 (95%)	8 (5%)	27 34
69	h3	244/254 (96%)	241 (99%)	3 (1%)	71 83
70	j3	135/154 (88%)	131 (97%)	4 (3%)	41 53
71	k3	106/134 (79%)	102 (96%)	4 (4%)	33 42
72	m3	115/131 (88%)	108 (94%)	7 (6%)	18 21
73	n3	109/110 (99%)	108 (99%)	1 (1%)	78 88
74	o3	190/197 (96%)	187 (98%)	3 (2%)	62 76
75	q3	207/209 (99%)	204 (99%)	3 (1%)	67 80
76	r3	330/332 (99%)	322 (98%)	8 (2%)	49 62
77	s3	326/329 (99%)	312 (96%)	14 (4%)	29 36
78	t3	149/157 (95%)	142 (95%)	7 (5%)	26 33
79	u3	167/170 (98%)	158 (95%)	9 (5%)	22 26
All	All	9617/10634 (90%)	9309 (97%)	308 (3%)	42 50

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	11	ARG
1	A1	66	MET
1	A1	71	MET
1	A1	110	ARG
1	A1	115	ARG
1	A1	116	ASP
1	A1	120	LYS
1	A1	174	LYS
1	A1	254	LYS
2	k1	33	SER
2	k1	109	SER
2	k1	141	SER
2	k1	175	SER
2	k1	219	SER
4	l1	28	MET
5	C1	74	TYR
5	C1	96	LYS
5	C1	112	LYS
5	C1	125	LYS
6	D1	5	ARG
6	D1	12	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D1	28	PHE
6	D1	62	GLN
6	D1	72	LYS
6	D1	84	PHE
6	D1	100	LYS
6	D1	113	GLU
7	E1	42	LYS
7	E1	84	GLN
8	F1	26	LYS
8	F1	47	LEU
8	F1	62	LYS
8	F1	111	ARG
8	F1	182	LYS
8	F1	219	LYS
9	G1	77	LYS
10	H1	47	ARG
10	H1	65	HIS
10	H1	101	LYS
10	H1	126	LYS
11	I1	68	ARG
11	I1	84	MET
11	I1	88	SER
12	J1	42	ARG
12	J1	93	ARG
13	K1	15	GLU
13	K1	18	LYS
13	K1	19	ARG
13	K1	38	LYS
13	K1	74	ARG
13	K1	81	PHE
13	K1	82	ARG
14	L1	12	LYS
14	L1	19	SER
14	L1	27	ARG
14	L1	39	MET
14	L1	56	GLU
16	N1	99	LYS
16	N1	138	ARG
17	O1	5	ARG
17	O1	11	ASP
17	O1	48	SER
17	O1	109	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	O1	144	ARG
17	O1	160	ARG
17	O1	162	ASN
17	O1	181	ASP
18	P1	81	ASP
18	P1	150	LYS
18	P1	183	CYS
18	P1	210	LYS
19	Q1	12	MET
19	Q1	27	ASP
19	Q1	31	MET
19	Q1	35	SER
19	Q1	48	LYS
19	Q1	114	PHE
19	Q1	157	ARG
19	Q1	208	LEU
19	Q1	209	CYS
19	Q1	228	LYS
19	Q1	233	ASP
19	Q1	247	ARG
19	Q1	257	SER
19	Q1	263	LEU
19	Q1	265	SER
19	Q1	275	ASP
19	Q1	276	LEU
19	Q1	277	LYS
19	Q1	298	MET
19	Q1	303	LEU
20	R1	29	SER
20	R1	59	MET
20	R1	81	ASP
21	S1	21	ARG
21	S1	33	PHE
21	S1	35	SER
21	S1	81	SER
21	S1	120	ARG
21	S1	129	GLU
22	T1	95	GLU
22	T1	104	PHE
22	T1	107	LYS
23	U1	59	LEU
23	U1	75	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U1	94	LYS
24	V1	12	LYS
24	V1	13	ASN
25	W1	39	LYS
26	X1	24	LYS
26	X1	44	LYS
26	X1	68	ARG
26	X1	117	ARG
26	X1	139	ASN
27	Y1	35	MET
27	Y1	57	LYS
28	Z1	40	LYS
28	Z1	169	HIS
28	Z1	190	ASN
28	Z1	198	MET
28	Z1	205	ARG
29	a1	38	SER
29	a1	79	ARG
29	a1	81	LYS
29	a1	110	TYR
29	a1	142	SER
29	a1	156	LYS
29	a1	172	ASP
30	b1	31	LYS
30	b1	52	SER
30	b1	140	ARG
31	c1	101	ARG
31	c1	166	CYS
31	c1	168	VAL
31	c1	220	PHE
31	c1	229	MET
31	c1	232	TYR
32	d1	42	ASP
32	d1	55	MET
32	d1	128	ARG
32	d1	193	SER
33	e1	87	GLU
34	f1	33	ARG
34	f1	64	ARG
34	f1	66	ARG
34	f1	77	LYS
34	f1	108	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	f1	110	LYS
34	f1	134	LYS
38	D3	38	GLN
38	D3	66	MET
38	D3	80	LYS
38	D3	151	SER
38	D3	188	ARG
39	E3	35	ARG
39	E3	69	LYS
39	E3	117	ARG
40	F3	99	ARG
40	F3	114	LYS
40	F3	117	ASN
40	F3	171	TYR
40	F3	187	SER
41	G3	15	LYS
42	H3	111	GLU
42	H3	112	SER
42	H3	117	ARG
42	H3	122	ASP
42	H3	144	LYS
43	I3	10	GLN
43	I3	59	GLN
43	I3	148	LYS
44	J3	96	VAL
44	J3	130	ARG
45	K3	66	LYS
45	K3	77	PHE
45	K3	78	SER
45	K3	80	ARG
46	L3	9	ARG
46	L3	29	GLN
46	L3	36	SER
46	L3	39	LYS
47	M3	31	GLU
47	M3	56	LYS
48	N3	95	ARG
48	N3	114	LEU
48	N3	127	ARG
49	O3	22	LYS
50	P3	41	SER
51	Q3	43	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	Q3	47	LYS
52	R3	9	LYS
52	R3	42	ARG
52	R3	84	GLU
53	S3	61	LYS
54	T3	29	LYS
54	T3	36	LYS
54	T3	89	GLU
55	U3	30	SER
55	U3	45	SER
55	U3	101	ARG
56	V3	33	ARG
57	W3	16	ARG
57	W3	17	ARG
57	W3	55	LYS
57	W3	67	GLN
58	X3	25	TYR
58	X3	45	ARG
59	Y3	83	MET
59	Y3	92	GLU
60	p3	1	MET
61	Z3	15	LYS
63	b3	34	LYS
63	b3	40	SER
63	b3	151	LYS
63	b3	155	LYS
63	b3	197	GLU
64	c3	129	LYS
64	c3	154	ASP
64	c3	167	ARG
64	c3	184	SER
64	c3	227	LYS
64	c3	243	LYS
65	d3	11	ARG
65	d3	114	PRO
65	d3	127	ASP
65	d3	155	TYR
65	d3	174	GLU
65	d3	178	GLN
65	d3	194	LEU
66	e3	15	ARG
66	e3	48	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	e3	90	ARG
66	e3	131	ARG
67	f3	46	ASP
67	f3	60	TYR
67	f3	88	ASP
67	f3	135	LYS
68	g3	32	ARG
68	g3	55	TRP
68	g3	76	MET
68	g3	153	ARG
68	g3	162	ARG
68	g3	175	LYS
68	g3	186	SER
68	g3	217	GLU
69	h3	50	ARG
69	h3	124	GLU
69	h3	176	GLU
70	j3	13	LYS
70	j3	112	LEU
70	j3	138	ASN
70	j3	154	LYS
71	k3	70	ASP
71	k3	86	LYS
71	k3	101	LYS
71	k3	141	ASP
72	m3	2	LYS
72	m3	36	SER
72	m3	37	ASP
72	m3	39	ARG
72	m3	73	TYR
72	m3	109	ARG
72	m3	114	ARG
73	n3	45	SER
74	o3	80	GLU
74	o3	179	MET
74	o3	208	GLU
75	q3	36	LYS
75	q3	60	ARG
75	q3	120	ASN
76	r3	5	LYS
76	r3	39	LYS
76	r3	229	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	r3	294	GLU
76	r3	301	ASP
76	r3	308	ASP
76	r3	343	ARG
76	r3	369	PHE
77	s3	19	MET
77	s3	31	MET
77	s3	60	LYS
77	s3	125	TYR
77	s3	148	GLU
77	s3	158	SER
77	s3	185	LYS
77	s3	265	ASP
77	s3	288	MET
77	s3	295	ARG
77	s3	300	ASP
77	s3	344	SER
77	s3	350	GLN
77	s3	390	ASP
78	t3	24	SER
78	t3	32	LEU
78	t3	37	LYS
78	t3	46	SER
78	t3	63	ARG
78	t3	159	ASP
78	t3	170	GLU
79	u3	1	MET
79	u3	26	GLU
79	u3	33	LYS
79	u3	36	ARG
79	u3	42	ASN
79	u3	49	LYS
79	u3	55	LYS
79	u3	142	LYS
79	u3	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
28	Z1	16	GLN
34	f1	65	HIS
43	I3	23	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	N3	86	ASN
79	u3	37	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	h1	1610/1808 (89%)	222 (13%)	0
35	B1	11/12 (91%)	1 (9%)	0
36	W2	75/76 (98%)	10 (13%)	0
36	i2	75/76 (98%)	8 (10%)	0
37	C3	118/119 (99%)	8 (6%)	0
81	A3	3190/3390 (94%)	414 (12%)	19 (0%)
82	B3	162/163 (99%)	26 (16%)	0
All	All	5241/5644 (92%)	689 (13%)	19 (0%)

All (689) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	h1	2	A
3	h1	4	C
3	h1	17	C
3	h1	25	C
3	h1	26	A
3	h1	34	G
3	h1	38	OMC
3	h1	42	G
3	h1	43	A
3	h1	45	U
3	h1	47	A
3	h1	56	U
3	h1	68	A
3	h1	82	G
3	h1	84	G
3	h1	105	A
3	h1	115	A
3	h1	117	U
3	h1	123	OMU
3	h1	128	G
3	h1	129	U
3	h1	130	A
3	h1	132	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	h1	133	U
3	h1	135	C
3	h1	136	U
3	h1	139	U
3	h1	140	OMC
3	h1	144	U
3	h1	150	U
3	h1	151	A
3	h1	158	C
3	h1	164	C
3	h1	174	C
3	h1	186	A
3	h1	189	U
3	h1	190	C
3	h1	191	U
3	h1	192	G
3	h1	193	G
3	h1	194	A
3	h1	213	U
3	h1	214	A
3	h1	252	U
3	h1	253	C
3	h1	260	A
3	h1	274	A
3	h1	277	G
3	h1	278	C
3	h1	291	G
3	h1	303	A
3	h1	318	C
3	h1	320	A
3	h1	324	U
3	h1	326	G
3	h1	341	G
3	h1	342	C
3	h1	365	C
3	h1	382	A
3	h1	384	U
3	h1	392	OMG
3	h1	394	G
3	h1	404	A
3	h1	406	C
3	h1	415	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	h1	420	A
3	h1	427	G
3	h1	428	C
3	h1	429	A
3	h1	430	G
3	h1	438	G
3	h1	443	U
3	h1	448	C
3	h1	449	A
3	h1	472	A
3	h1	481	A
3	h1	489	C
3	h1	490	G
3	h1	504	U
3	h1	505	G
3	h1	510	U
3	h1	513	G
3	h1	518	A
3	h1	522	C
3	h1	541	A
3	h1	544	A2M
3	h1	545	U
3	h1	552	G
3	h1	558	A
3	h1	560	G
3	h1	568	C
3	h1	581	OMU
3	h1	582	A
3	h1	584	PSU
3	h1	585	U
3	h1	597	A
3	h1	598	OMG
3	h1	609	A
3	h1	614	OMU
3	h1	620	U
3	h1	622	A2M
3	h1	623	A
3	h1	625	A
3	h1	626	A
3	h1	642	U
3	h1	647	A
3	h1	759	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	h1	769	G
3	h1	770	C
3	h1	775	A
3	h1	782	C
3	h1	783	U
3	h1	785	C
3	h1	786	G
3	h1	790	U
3	h1	793	A
3	h1	816	A
3	h1	832	A
3	h1	834	U
3	h1	866	A
3	h1	931	G
3	h1	936	A
3	h1	938	U
3	h1	954	A
3	h1	963	U
3	h1	991	C
3	h1	1006	A
3	h1	1007	U
3	h1	1008	A
3	h1	1029	A
3	h1	1031	C
3	h1	1042	A
3	h1	1059	G
3	h1	1060	C
3	h1	1085	U
3	h1	1090	A
3	h1	1095	A
3	h1	1100	U
3	h1	1141	A
3	h1	1153	G
3	h1	1161	C
3	h1	1166	A
3	h1	1170	G
3	h1	1188	U
3	h1	1197	A
3	h1	1199	A
3	h1	1202	G
3	h1	1203	G
3	h1	1204	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	h1	1205	A
3	h1	1220	A
3	h1	1221	G
3	h1	1234	OMU
3	h1	1246	G
3	h1	1247	A
3	h1	1248	G
3	h1	1249	C
3	h1	1255	C
3	h1	1272	OMU
3	h1	1274	OMG
3	h1	1302	G
3	h1	1317	U
3	h1	1318	U
3	h1	1324	A
3	h1	1328	A
3	h1	1364	U
3	h1	1365	A
3	h1	1366	U
3	h1	1375	G
3	h1	1395	U
3	h1	1396	A
3	h1	1403	U
3	h1	1404	U
3	h1	1418	U
3	h1	1420	U
3	h1	1432	A
3	h1	1433	OMG
3	h1	1437	U
3	h1	1440	G
3	h1	1451	A
3	h1	1464	C
3	h1	1465	A
3	h1	1476	A
3	h1	1493	G
3	h1	1495	U
3	h1	1500	G
3	h1	1503	U
3	h1	1518	G
3	h1	1523	A
3	h1	1524	PSU
3	h1	1528	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	h1	1530	A
3	h1	1543	A
3	h1	1548	G
3	h1	1563	U
3	h1	1565	G
3	h1	1579	A2M
3	h1	1596	G
3	h1	1607	G
3	h1	1617	A
3	h1	1637	A
3	h1	1640	C
3	h1	1646	C
3	h1	1657	A
3	h1	1663	U
3	h1	1664	G
3	h1	1686	G
3	h1	1763	A
3	h1	1765	G
3	h1	1774	A
3	h1	1775	G
3	h1	1777	U
3	h1	1787	PSU
3	h1	1788	G
3	h1	1791	C
3	h1	1800	G
3	h1	1801	G
3	h1	1802	A
3	h1	1803	U
3	h1	1804	C
3	h1	1807	U
3	h1	1808	G
35	B1	19	U
36	i2	16	U
36	i2	17	U
36	i2	21	A
36	i2	35	A
36	i2	36	A
36	i2	73	A
36	i2	74	C
36	i2	76	A
36	W2	10	G
36	W2	17	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	W2	19	G
36	W2	20	G
36	W2	21	A
36	W2	38	A
36	W2	47	U
36	W2	56	C
36	W2	63	C
36	W2	76	A
37	C3	7	G
37	C3	25	G
37	C3	33	U
37	C3	38	U
37	C3	53	U
37	C3	54	A
37	C3	64	G
37	C3	110	G
81	A3	11	G
81	A3	12	U
81	A3	14	A
81	A3	24	A
81	A3	38	A
81	A3	41	A
81	A3	47	A
81	A3	58	A
81	A3	64	A
81	A3	90	G
81	A3	97	A
81	A3	107	A
81	A3	108	G
81	A3	109	C
81	A3	114	C
81	A3	120	A
81	A3	131	U
81	A3	132	C
81	A3	133	C
81	A3	134	G
81	A3	140	C
81	A3	154	G
81	A3	155	A
81	A3	163	C
81	A3	167	A
81	A3	168	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	184	A
81	A3	187	U
81	A3	188	C
81	A3	194	G
81	A3	197	G
81	A3	207	G
81	A3	215	G
81	A3	216	A
81	A3	245	A
81	A3	247	C
81	A3	248	A
81	A3	258	G
81	A3	262	A
81	A3	266	G
81	A3	283	U
81	A3	292	A
81	A3	296	OMG
81	A3	302	U
81	A3	320	A
81	A3	326	G
81	A3	347	C
81	A3	373	G
81	A3	396	A
81	A3	398	U
81	A3	399	OMG
81	A3	400	C
81	A3	417	G
81	A3	418	G
81	A3	419	A
81	A3	436	C
81	A3	439	U
81	A3	449	U
81	A3	453	A
81	A3	454	U
81	A3	467	C
81	A3	468	G
81	A3	523	C
81	A3	525	A
81	A3	538	C
81	A3	539	G
81	A3	540	A
81	A3	541	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	544	G
81	A3	547	C
81	A3	550	G
81	A3	552	A
81	A3	571	U
81	A3	574	U
81	A3	577	G
81	A3	582	G
81	A3	591	C
81	A3	592	G
81	A3	602	G
81	A3	607	C
81	A3	610	C
81	A3	620	A
81	A3	636	U
81	A3	637	C
81	A3	660	A2M
81	A3	661	C
81	A3	671	A
81	A3	688	A
81	A3	693	A
81	A3	698	C
81	A3	701	G
81	A3	718	A
81	A3	725	C
81	A3	728	A
81	A3	729	U
81	A3	730	U
81	A3	731	G
81	A3	743	C
81	A3	747	G
81	A3	753	C
81	A3	775	U
81	A3	777	U
81	A3	781	A
81	A3	790	A
81	A3	791	G
81	A3	795	G
81	A3	797	G
81	A3	816	A
81	A3	827	A2M
81	A3	840	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	867	G
81	A3	871	C
81	A3	884	U
81	A3	889	U
81	A3	906	A
81	A3	917	G
81	A3	918	OMG
81	A3	924	A
81	A3	926	G
81	A3	927	A
81	A3	933	C
81	A3	947	G
81	A3	954	C
81	A3	969	C
81	A3	970	PSU
81	A3	984	G
81	A3	987	C
81	A3	991	U
81	A3	992	G
81	A3	1003	C
81	A3	1006	G
81	A3	1013	C
81	A3	1014	A
81	A3	1022	G
81	A3	1028	U
81	A3	1036	G
81	A3	1041	G
81	A3	1048	A
81	A3	1059	A
81	A3	1076	A
81	A3	1077	C
81	A3	1087	G
81	A3	1093	U
81	A3	1094	U
81	A3	1106	C
81	A3	1107	G
81	A3	1108	G
81	A3	1109	A
81	A3	1114	A
81	A3	1115	G
81	A3	1128	G
81	A3	1142	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	1170	A
81	A3	1191	C
81	A3	1192	U
81	A3	1193	G
81	A3	1195	G
81	A3	1201	A
81	A3	1202	C
81	A3	1205	A
81	A3	1213	C
81	A3	1217	G
81	A3	1218	G
81	A3	1221	G
81	A3	1239	C
81	A3	1295	C
81	A3	1297	G
81	A3	1299	A
81	A3	1321	U
81	A3	1328	U
81	A3	1329	A
81	A3	1335	G
81	A3	1343	C
81	A3	1360	A
81	A3	1361	A
81	A3	1362	G
81	A3	1363	U
81	A3	1364	G
81	A3	1365	C
81	A3	1366	C
81	A3	1410	U
81	A3	1430	G
81	A3	1445	G
81	A3	1448	OMC
81	A3	1457	A
81	A3	1463	A
81	A3	1492	A
81	A3	1494	G
81	A3	1513	G
81	A3	1538	C
81	A3	1566	A
81	A3	1571	G
81	A3	1577	U
81	A3	1578	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	1585	U
81	A3	1587	C
81	A3	1588	U
81	A3	1592	A
81	A3	1593	A
81	A3	1594	A
81	A3	1598	A
81	A3	1602	G
81	A3	1609	A
81	A3	1625	C
81	A3	1633	U
81	A3	1635	G
81	A3	1649	G
81	A3	1661	C
81	A3	1698	U
81	A3	1729	G
81	A3	1748	G
81	A3	1755	A
81	A3	1756	G
81	A3	1770	G
81	A3	1771	C
81	A3	1772	G
81	A3	1774	G
81	A3	1775	G
81	A3	1802	G
81	A3	1803	A
81	A3	1821	U
81	A3	1827	C
81	A3	1828	C
81	A3	1855	C
81	A3	1856	A
81	A3	1872	C
81	A3	1873	A
81	A3	1884	G
81	A3	1885	A
81	A3	1886	U
81	A3	1912	G
81	A3	1949	C
81	A3	2096	A
81	A3	2100	G
81	A3	2116	U
81	A3	2118	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	2126	OMG
81	A3	2135	A
81	A3	2144	U
81	A3	2162	A
81	A3	2208	U
81	A3	2213	G
81	A3	2244	U
81	A3	2245	A
81	A3	2259	A2M
81	A3	2265	A
81	A3	2273	A
81	A3	2276	G
81	A3	2283	A
81	A3	2285	U
81	A3	2286	G
81	A3	2291	OMG
81	A3	2310	G
81	A3	2313	U
81	A3	2316	A
81	A3	2317	PSU
81	A3	2318	G
81	A3	2337	U
81	A3	2338	G
81	A3	2339	U
81	A3	2368	OMC
81	A3	2376	A
81	A3	2377	C
81	A3	2378	G
81	A3	2388	G
81	A3	2396	G
81	A3	2397	G
81	A3	2400	A
81	A3	2405	A
81	A3	2406	G
81	A3	2407	A
81	A3	2414	U
81	A3	2415	G
81	A3	2438	G
81	A3	2448	U
81	A3	2457	G
81	A3	2459	A
81	A3	2462	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	2463	U
81	A3	2464	A
81	A3	2465	A
81	A3	2466	G
81	A3	2468	G
81	A3	2469	G
81	A3	2470	G
81	A3	2471	A
81	A3	2483	A
81	A3	2486	G
81	A3	2488	G
81	A3	2489	A
81	A3	2492	U
81	A3	2495	C
81	A3	2496	A
81	A3	2497	C
81	A3	2499	A
81	A3	2502	U
81	A3	2503	U
81	A3	2504	U
81	A3	2505	A
81	A3	2506	A
81	A3	2519	U
81	A3	2520	A
81	A3	2529	A
81	A3	2544	C
81	A3	2545	U
81	A3	2546	G
81	A3	2556	U
81	A3	2573	U
81	A3	2574	U
81	A3	2575	G
81	A3	2576	C
81	A3	2588	G
81	A3	2596	A
81	A3	2609	G
81	A3	2610	G
81	A3	2617	G
81	A3	2629	A
81	A3	2640	A
81	A3	2655	U
81	A3	2659	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	2660	A
81	A3	2677	A
81	A3	2680	G
81	A3	2692	G
81	A3	2694	A
81	A3	2699	A
81	A3	2706	A
81	A3	2707	A
81	A3	2717	G
81	A3	2722	U
81	A3	2731	G
81	A3	2732	OMU
81	A3	2756	G
81	A3	2758	C
81	A3	2780	G
81	A3	2781	G
81	A3	2799	G
81	A3	2802	A
81	A3	2803	G
81	A3	2804	A2M
81	A3	2813	C
81	A3	2817	G
81	A3	2820	A
81	A3	2845	U
81	A3	2846	U
81	A3	2847	C
81	A3	2848	A
81	A3	2870	C
81	A3	2874	G
81	A3	2875	A
81	A3	2890	A
81	A3	2892	C
81	A3	2902	C
81	A3	2914	A2M
81	A3	2938	U
81	A3	2939	A
81	A3	2948	G
81	A3	2950	G
81	A3	2954	G
81	A3	2956	UR3
81	A3	2975	G
81	A3	2983	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	2986	C
81	A3	2993	G
81	A3	3000	G
81	A3	3014	A
81	A3	3030	G
81	A3	3060	C
81	A3	3061	G
81	A3	3080	G
81	A3	3081	U
81	A3	3094	C
81	A3	3103	G
81	A3	3118	G
81	A3	3124	A
81	A3	3132	A
81	A3	3133	U
81	A3	3144	A
81	A3	3154	G
81	A3	3170	U
81	A3	3171	G
81	A3	3172	C
81	A3	3179	G
81	A3	3185	G
81	A3	3191	U
81	A3	3194	G
81	A3	3201	A
81	A3	3208	C
81	A3	3209	G
81	A3	3211	G
81	A3	3236	A
81	A3	3240	G
81	A3	3254	C
81	A3	3257	G
81	A3	3268	U
81	A3	3272	U
81	A3	3278	G
81	A3	3279	G
81	A3	3296	C
81	A3	3308	A
81	A3	3311	C
81	A3	3312	G
81	A3	3337	G
81	A3	3342	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	3343	U
81	A3	3344	U
81	A3	3346	C
81	A3	3359	C
81	A3	3361	G
81	A3	3370	C
81	A3	3374	U
81	A3	3383	C
81	A3	3384	G
81	A3	3390	U
82	B3	2	A
82	B3	26	C
82	B3	37	U
82	B3	38	C
82	B3	62	A
82	B3	65	C
82	B3	66	U
82	B3	78	OMG
82	B3	83	A
82	B3	84	U
82	B3	85	U
82	B3	87	C
82	B3	88	G
82	B3	89	U
82	B3	90	G
82	B3	93	C
82	B3	94	C
82	B3	96	PSU
82	B3	98	G
82	B3	107	A
82	B3	109	C
82	B3	128	C
82	B3	130	U
82	B3	131	U
82	B3	133	G
82	B3	156	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
81	A3	11	G
81	A3	398	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	A3	399	OMG
81	A3	540	A
81	A3	601	C
81	A3	692	A
81	A3	866	G
81	A3	883	C
81	A3	926	G
81	A3	990	G
81	A3	1027	A
81	A3	1634	U
81	A3	1852	OMC
81	A3	2468	G
81	A3	2482	G
81	A3	2496	A
81	A3	2503	U
81	A3	2543	A
81	A3	3123	U

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

216 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	$\#\|Z\| > 2$
81	A2M	A3	2914	81	18,25,26	4.15	7 (38%)	18,36,39	3.88	4 (22%)
81	OMC	A3	1480	81	19,22,23	3.30	8 (42%)	26,31,34	0.73	0
81	PSU	A3	2829	81	18,21,22	4.62	8 (44%)	22,30,33	1.90	6 (27%)
3	PSU	h1	470	3	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
3	A2M	h1	424	3	18,25,26	4.16	7 (38%)	18,36,39	3.86	4 (22%)
81	OMG	A3	296	81	18,26,27	2.84	8 (44%)	19,38,41	1.54	4 (21%)
81	PSU	A3	34	81	18,21,22	4.63	8 (44%)	22,30,33	1.87	5 (22%)
3	PSU	h1	1524	3	18,21,22	4.69	8 (44%)	22,30,33	1.75	5 (22%)
3	MA6	h1	1790	3	18,26,27	0.96	1 (5%)	19,38,41	2.68	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMU	h1	614	3	19,22,23	3.21	8 (42%)	26,31,34	1.65	5 (19%)
81	PSU	A3	1002	81	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
81	A2M	A3	369	81	18,25,26	4.12	7 (38%)	18,36,39	3.85	5 (27%)
81	OMU	A3	1068	81	19,22,23	3.20	8 (42%)	26,31,34	1.70	5 (19%)
81	OMC	A3	1862	81	19,22,23	3.26	8 (42%)	26,31,34	0.68	0
81	OMG	A3	2239	81	18,26,27	2.85	8 (44%)	19,38,41	1.52	4 (21%)
81	A2M	A3	2329	81	18,25,26	4.13	7 (38%)	18,36,39	3.82	5 (27%)
81	PSU	A3	2947	81,84	18,21,22	4.64	9 (50%)	22,30,33	1.85	6 (27%)
82	PSU	B3	77	82	18,21,22	4.65	8 (44%)	22,30,33	1.86	5 (22%)
3	PSU	h1	258	3	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
3	PSU	h1	1308	3	18,21,22	4.64	8 (44%)	22,30,33	1.78	5 (22%)
3	A2M	h1	1579	3	18,25,26	4.11	7 (38%)	18,36,39	3.88	5 (27%)
81	OMU	A3	787	81	19,22,23	3.21	8 (42%)	26,31,34	1.65	5 (19%)
3	PSU	h1	1002	3	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
81	OMG	A3	2818	81	18,26,27	2.81	8 (44%)	19,38,41	1.56	5 (26%)
81	PSU	A3	2269	81	18,21,22	4.68	8 (44%)	22,30,33	1.78	5 (22%)
3	OMU	h1	886	3	19,22,23	3.22	8 (42%)	26,31,34	1.80	5 (19%)
81	PSU	A3	3113	81	18,21,22	4.63	8 (44%)	22,30,33	1.77	5 (22%)
3	PSU	h1	362	3	18,21,22	4.62	8 (44%)	22,30,33	1.81	5 (22%)
81	PSU	A3	1474	81	18,21,22	4.64	8 (44%)	22,30,33	1.82	5 (22%)
81	OMG	A3	815	81	18,26,27	2.83	8 (44%)	19,38,41	1.56	5 (26%)
3	OMC	h1	38	3	19,22,23	3.32	8 (42%)	26,31,34	0.71	0
81	A2M	A3	817	81	18,25,26	4.14	7 (38%)	18,36,39	3.79	5 (27%)
81	OMC	A3	2296	81	19,22,23	3.29	8 (42%)	26,31,34	0.74	0
81	PSU	A3	970	81	18,21,22	4.66	9 (50%)	22,30,33	1.89	5 (22%)
81	PSU	A3	2263	81	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
3	OMU	h1	581	84,3	19,22,23	3.23	8 (42%)	26,31,34	1.67	4 (15%)
3	A2M	h1	28	3,83	18,25,26	4.14	7 (38%)	18,36,39	3.82	4 (22%)
81	PSU	A3	2883	81	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
3	OMU	h1	123	3	19,22,23	3.21	8 (42%)	26,31,34	1.66	5 (19%)
81	PSU	A3	895	81	18,21,22	4.61	8 (44%)	22,30,33	1.78	5 (22%)
81	OMU	A3	2350	81	19,22,23	3.23	8 (42%)	26,31,34	1.67	5 (19%)
3	PSU	h1	1293	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
3	PSU	h1	635	3	18,21,22	4.62	8 (44%)	22,30,33	1.79	5 (22%)
3	PSU	h1	1106	3	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	h1	1634	3	18,21,22	4.64	8 (44%)	22,30,33	1.80	5 (22%)
81	PSU	A3	684	81	18,21,22	4.64	8 (44%)	22,30,33	1.80	5 (22%)
3	PSU	h1	1567	3	18,21,22	4.67	8 (44%)	22,30,33	1.83	5 (22%)
81	PSU	A3	1133	81	18,21,22	4.63	8 (44%)	22,30,33	1.82	5 (22%)
81	A2M	A3	2259	81	18,25,26	4.17	7 (38%)	18,36,39	3.89	4 (22%)
81	A2M	A3	1144	81	18,25,26	4.13	7 (38%)	18,36,39	3.88	4 (22%)
81	A2M	A3	1378	81	18,25,26	4.13	7 (38%)	18,36,39	3.72	4 (22%)
81	OMU	A3	2738	81	19,22,23	3.21	8 (42%)	26,31,34	1.67	5 (19%)
81	PSU	A3	277	81	18,21,22	4.62	8 (44%)	22,30,33	1.83	5 (22%)
82	PSU	B3	21	81,82	18,21,22	4.62	8 (44%)	22,30,33	1.78	5 (22%)
3	PSU	h1	1615	3	18,21,22	4.63	8 (44%)	22,30,33	1.81	5 (22%)
3	PSU	h1	95	3	18,21,22	4.67	8 (44%)	22,30,33	1.80	5 (22%)
81	OMG	A3	2126	81	18,26,27	2.80	8 (44%)	19,38,41	1.56	5 (26%)
81	A2M	A3	2643	81	18,25,26	4.12	7 (38%)	18,36,39	3.75	4 (22%)
81	A2M	A3	660	81	18,25,26	4.14	7 (38%)	18,36,39	3.98	6 (33%)
81	5MC	A3	2281	81	18,22,23	4.01	7 (38%)	26,32,35	1.04	2 (7%)
3	PSU	h1	1120	3	18,21,22	4.64	8 (44%)	22,30,33	1.77	5 (22%)
81	OMU	A3	675	81	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
81	OMG	A3	2398	81	18,26,27	2.81	8 (44%)	19,38,41	1.60	5 (26%)
3	OMU	h1	1234	3	19,22,23	3.20	8 (42%)	26,31,34	1.65	4 (15%)
3	OMC	h1	473	3	19,22,23	3.30	8 (42%)	26,31,34	0.72	0
81	OMC	A3	2962	81	19,22,23	3.25	8 (42%)	26,31,34	0.77	0
3	A2M	h1	977	3	18,25,26	4.14	7 (38%)	18,36,39	3.73	4 (22%)
81	PSU	A3	228	81	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
81	PSU	A3	902	81,84,83	18,21,22	4.65	8 (44%)	22,30,33	1.81	5 (22%)
81	OMU	A3	1894	81	19,22,23	3.23	8 (42%)	26,31,34	1.71	5 (19%)
81	OMG	A3	2394	81	18,26,27	2.82	8 (44%)	19,38,41	1.59	5 (26%)
81	OMG	A3	2796	81	18,26,27	2.81	8 (44%)	19,38,41	1.52	5 (26%)
3	PSU	h1	1787	3	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
3	OMG	h1	392	3	18,26,27	2.86	8 (44%)	19,38,41	1.55	4 (21%)
81	OMC	A3	2368	81	19,22,23	3.27	8 (42%)	26,31,34	0.69	0
81	OMU	A3	3289	81	19,22,23	3.20	8 (42%)	26,31,34	1.63	4 (15%)
81	PSU	A3	311	81,84	18,21,22	4.66	8 (44%)	22,30,33	1.73	5 (22%)
81	OMG	A3	918	81,84	18,26,27	2.81	8 (44%)	19,38,41	1.50	4 (21%)
3	B8N	h1	1194	3	24,29,30	3.04	7 (29%)	29,42,45	1.73	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	h1	1217	3	18,21,22	4.68	8 (44%)	22,30,33	1.81	5 (22%)
3	PSU	h1	121	3,83	18,21,22	4.66	8 (44%)	22,30,33	1.80	5 (22%)
81	A2M	A3	2129	81	18,25,26	4.17	7 (38%)	18,36,39	3.84	4 (22%)
81	PSU	A3	2214	81	18,21,22	4.65	8 (44%)	22,30,33	1.87	5 (22%)
81	OMG	A3	2291	81	18,26,27	2.82	8 (44%)	19,38,41	1.52	4 (21%)
81	OMC	A3	1849	81	19,22,23	3.25	8 (42%)	26,31,34	0.70	0
81	1MA	A3	656	81	16,25,26	3.83	5 (31%)	18,37,40	1.70	3 (16%)
81	OMG	A3	2925	81	18,26,27	2.82	8 (44%)	19,38,41	1.52	4 (21%)
81	OMG	A3	2622	81,36	18,26,27	2.82	8 (44%)	19,38,41	1.49	4 (21%)
3	OMC	h1	1218	3	19,22,23	3.31	8 (42%)	26,31,34	0.71	0
3	OMU	h1	1012	3	19,22,23	3.20	8 (42%)	26,31,34	1.67	4 (15%)
81	PSU	A3	829	81	18,21,22	4.63	8 (44%)	22,30,33	1.86	5 (22%)
3	PSU	h1	417	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
3	OMU	h1	1272	3	19,22,23	3.23	8 (42%)	26,31,34	1.66	4 (15%)
81	OMU	A3	144	81	19,22,23	3.21	8 (42%)	26,31,34	1.65	4 (15%)
81	OMU	A3	804	81	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
81	OMU	A3	2720	81	19,22,23	3.20	8 (42%)	26,31,34	1.64	4 (15%)
81	5MC	A3	2873	81,84	18,22,23	4.02	7 (38%)	26,32,35	1.09	1 (3%)
81	OMG	A3	2654	81	18,26,27	2.81	8 (44%)	19,38,41	1.69	6 (31%)
81	PSU	A3	2897	81	18,21,22	4.64	8 (44%)	22,30,33	1.80	5 (22%)
3	6MZ	h1	1771	84,3,83	18,25,26	2.02	4 (22%)	16,36,39	2.33	4 (25%)
81	A2M	A3	2223	81	18,25,26	4.16	7 (38%)	18,36,39	3.77	4 (22%)
81	PSU	A3	1685	81	18,21,22	4.65	8 (44%)	22,30,33	1.87	6 (27%)
3	A2M	h1	622	3,83	18,25,26	4.10	7 (38%)	18,36,39	3.97	5 (27%)
81	PSU	A3	717	81	18,21,22	4.65	8 (44%)	22,30,33	1.86	5 (22%)
81	PSU	A3	976	81,84	18,21,22	4.67	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	h1	950	3	18,21,22	4.64	8 (44%)	22,30,33	1.79	5 (22%)
81	A2M	A3	1460	81	18,25,26	4.13	7 (38%)	18,36,39	3.81	4 (22%)
81	OMU	A3	2924	81,84	19,22,23	3.21	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	h1	1210	3	18,21,22	4.63	8 (44%)	22,30,33	1.83	5 (22%)
81	PSU	A3	1064	81	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
3	OMU	h1	1383	3,83	19,22,23	3.23	8 (42%)	26,31,34	1.67	4 (15%)
3	OMC	h1	1645	3	19,22,23	3.30	8 (42%)	26,31,34	0.71	0
81	PSU	A3	1135	81	18,21,22	4.64	8 (44%)	22,30,33	1.86	5 (22%)
81	OMC	A3	1448	81	19,22,23	3.29	8 (42%)	26,31,34	0.87	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	h1	606	3	18,21,22	4.61	8 (44%)	22,30,33	1.79	5 (22%)
3	A2M	h1	162	3	18,25,26	4.18	7 (38%)	18,36,39	3.84	4 (22%)
3	A2M	h1	1758	3	18,25,26	4.12	8 (44%)	18,36,39	3.75	4 (22%)
3	MA6	h1	1789	3	18,26,27	0.94	1 (5%)	19,38,41	2.64	3 (15%)
81	OMC	A3	674	81	19,22,23	3.25	8 (42%)	26,31,34	0.68	0
81	OMG	A3	2920	81	18,26,27	2.81	8 (44%)	19,38,41	1.54	5 (26%)
81	PSU	A3	510	81	18,21,22	4.65	8 (44%)	22,30,33	1.85	5 (22%)
3	PSU	h1	762	3	18,21,22	4.65	8 (44%)	22,30,33	1.80	5 (22%)
81	OMG	A3	2412	81,84	18,26,27	2.83	8 (44%)	19,38,41	1.59	5 (26%)
81	PSU	A3	2419	81	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
81	PSU	A3	2261	81	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	2257	81	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
3	A2M	h1	800	3	18,25,26	4.20	7 (38%)	18,36,39	3.77	5 (27%)
3	PSU	h1	1027	3	18,21,22	4.68	9 (50%)	22,30,33	1.81	5 (22%)
81	A2M	A3	827	81,84,83	18,25,26	4.18	7 (38%)	18,36,39	3.87	4 (22%)
81	PSU	A3	1016	81,84	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
81	OMU	A3	2732	81	19,22,23	3.20	8 (42%)	26,31,34	1.61	4 (15%)
81	PSU	A3	1134	81	18,21,22	4.60	8 (44%)	22,30,33	1.88	5 (22%)
3	4AC	h1	1781	3	21,24,25	3.26	11 (52%)	29,34,37	1.04	3 (10%)
81	OMG	A3	2794	81	18,26,27	2.80	8 (44%)	19,38,41	1.46	5 (26%)
3	PSU	h1	1304	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	966	81	18,21,22	4.61	8 (44%)	22,30,33	1.74	5 (22%)
3	A2M	h1	1329	3	18,25,26	4.16	7 (38%)	18,36,39	3.86	4 (22%)
81	OMC	A3	2839	81	19,22,23	3.28	8 (42%)	26,31,34	0.78	0
81	A2M	A3	2949	81	18,25,26	4.15	7 (38%)	18,36,39	3.77	4 (22%)
81	PSU	A3	2321	81,83	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
81	OMG	A3	2127	81	18,26,27	2.82	8 (44%)	19,38,41	1.62	5 (26%)
81	PSU	A3	2267	81	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
81	PSU	A3	786	81	18,21,22	4.66	8 (44%)	22,30,33	1.73	5 (22%)
81	OMC	A3	40	81	19,22,23	3.27	8 (42%)	26,31,34	0.89	1 (3%)
3	PSU	h1	1535	3	18,21,22	4.67	8 (44%)	22,30,33	1.80	5 (22%)
82	OMG	B3	78	82	18,26,27	2.81	8 (44%)	19,38,41	1.52	4 (21%)
81	PSU	A3	2978	81	18,21,22	4.65	8 (44%)	22,30,33	1.80	5 (22%)
82	A2M	B3	46	82	18,25,26	4.14	7 (38%)	18,36,39	3.82	4 (22%)
81	OMC	A3	2951	81	19,22,23	3.23	8 (42%)	26,31,34	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
81	PSU	A3	42	81,84	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
81	OMU	A3	2424	81	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
81	OMG	A3	1857	81	18,26,27	2.80	8 (44%)	19,38,41	1.51	5 (26%)
3	A2M	h1	468	3	18,25,26	4.17	7 (38%)	18,36,39	3.84	4 (22%)
81	PSU	A3	1482	81	18,21,22	4.62	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	h1	1184	3	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	h1	753	3	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
3	OMC	h1	418	3	19,22,23	3.30	8 (42%)	26,31,34	0.89	1 (3%)
3	PSU	h1	605	3	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
3	OMG	h1	1433	3,83	18,26,27	2.80	8 (44%)	19,38,41	1.47	5 (26%)
3	OMG	h1	1274	3	18,26,27	2.84	8 (44%)	19,38,41	1.52	4 (21%)
81	A2M	A3	2284	81	18,25,26	4.04	7 (38%)	18,36,39	3.99	4 (22%)
3	OMU	h1	1447	3	19,22,23	3.20	8 (42%)	26,31,34	1.61	4 (15%)
81	OMU	A3	3304	81	19,22,23	3.20	8 (42%)	26,31,34	1.64	4 (15%)
3	UY1	h1	603	3	19,22,23	4.17	7 (36%)	22,31,34	1.84	5 (22%)
81	PSU	A3	1056	81	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
3	PSU	h1	103	84,3	18,21,22	4.64	8 (44%)	22,30,33	1.84	5 (22%)
3	OMU	h1	373	3	19,22,23	3.22	8 (42%)	26,31,34	1.66	4 (15%)
81	PSU	A3	464	81	18,21,22	4.67	8 (44%)	22,30,33	1.80	6 (27%)
3	PSU	h1	1178	3	18,21,22	4.64	8 (44%)	22,30,33	1.82	5 (22%)
82	PSU	B3	96	84,82	18,21,22	4.66	8 (44%)	22,30,33	1.75	5 (22%)
81	UY1	A3	2653	81	19,22,23	4.20	7 (36%)	22,31,34	1.87	5 (22%)
81	OMU	A3	44	81,84	19,22,23	3.23	8 (42%)	26,31,34	1.63	4 (15%)
81	UR3	A3	2956	81	19,22,23	2.79	8 (42%)	26,32,35	1.31	2 (7%)
3	OMG	h1	598	3	18,26,27	2.83	8 (44%)	19,38,41	1.54	4 (21%)
81	PSU	A3	2139	81	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
3	PSU	h1	961	84,3	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
81	OMG	A3	1461	81	18,26,27	2.81	8 (44%)	19,38,41	1.52	4 (21%)
3	4AC	h1	1283	3	21,24,25	3.25	11 (52%)	29,34,37	0.98	2 (6%)
81	OMU	A3	48	81	19,22,23	3.19	8 (42%)	26,31,34	1.63	4 (15%)
81	A2M	A3	886	81	18,25,26	4.14	7 (38%)	18,36,39	3.81	6 (33%)
81	A2M	A3	2324	81	18,25,26	4.11	7 (38%)	18,36,39	3.82	4 (22%)
81	OMC	A3	2340	81	19,22,23	3.28	8 (42%)	26,31,34	0.68	0
81	OMC	A3	2685	81	19,22,23	3.28	8 (42%)	26,31,34	0.73	0
81	PSU	A3	2747	81	18,21,22	4.62	8 (44%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	h1	1190	3	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
81	PSU	A3	2857	81	18,21,22	4.64	8 (44%)	22,30,33	1.87	5 (22%)
81	OMU	A3	2886	81	19,22,23	3.21	8 (42%)	26,31,34	1.63	4 (15%)
3	PSU	h1	763	3	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
81	OMG	A3	399	81	18,26,27	2.86	8 (44%)	19,38,41	1.54	4 (21%)
81	PSU	A3	150	81,84	18,21,22	4.65	8 (44%)	22,30,33	1.85	5 (22%)
81	A2M	A3	946	81	18,25,26	4.14	8 (44%)	18,36,39	3.94	6 (33%)
81	OMU	A3	2413	81,84	19,22,23	3.17	8 (42%)	26,31,34	1.59	4 (15%)
81	PSU	A3	2926	81,84	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
3	A2M	h1	544	3	18,25,26	4.18	7 (38%)	18,36,39	3.66	4 (22%)
81	OMC	A3	2882	81	19,22,23	3.27	8 (42%)	26,31,34	0.75	0
81	PSU	A3	2958	81	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
81	PSU	A3	2317	81,84	18,21,22	4.65	8 (44%)	22,30,33	1.90	5 (22%)
81	OMU	A3	1537	81	19,22,23	3.21	8 (42%)	26,31,34	1.63	4 (15%)
81	OMC	A3	1852	81	19,22,23	3.31	8 (42%)	26,31,34	0.74	0
3	OMC	h1	140	3	19,22,23	3.31	8 (42%)	26,31,34	0.72	0
3	PSU	h1	310	3	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
81	PSU	A3	2137	81,84	18,21,22	4.65	8 (44%)	22,30,33	1.92	5 (22%)
3	OMG	h1	246	84,3	18,26,27	2.85	8 (44%)	19,38,41	1.50	4 (21%)
3	A2M	h1	440	3	18,25,26	4.15	7 (38%)	18,36,39	3.86	4 (22%)
3	PSU	h1	306	3	18,21,22	4.65	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	h1	339	84,3	18,21,22	4.66	8 (44%)	22,30,33	1.80	6 (27%)
3	PSU	h1	1485	3	18,21,22	4.67	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	h1	584	3	18,21,22	4.75	9 (50%)	22,30,33	1.79	5 (22%)
81	A2M	A3	2804	81	18,25,26	4.11	6 (33%)	18,36,39	4.11	6 (33%)
81	PSU	A3	2435	81	18,21,22	4.64	8 (44%)	22,30,33	1.90	6 (27%)
81	OMC	A3	2200	81,84	19,22,23	3.29	8 (42%)	26,31,34	0.80	0
3	PSU	h1	607	3	18,21,22	4.66	8 (44%)	22,30,33	1.86	6 (27%)
3	PSU	h1	809	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	2194	81,84	18,21,22	4.63	8 (44%)	22,30,33	1.80	5 (22%)
81	PSU	A3	2868	81	18,21,22	4.64	8 (44%)	22,30,33	1.90	6 (27%)
3	PSU	h1	451	84,3	18,21,22	4.67	8 (44%)	22,30,33	1.87	6 (27%)

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
81	A2M	A3	2914	81	-	2/5/27/28	0/3/3/3
81	OMC	A3	1480	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	2829	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	470	3	-	0/7/25/26	0/2/2/2
3	A2M	h1	424	3	-	0/5/27/28	0/3/3/3
81	OMG	A3	296	81	-	2/5/27/28	0/3/3/3
81	PSU	A3	34	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1524	3	-	2/7/25/26	0/2/2/2
3	MA6	h1	1790	3	-	4/7/29/30	0/3/3/3
3	OMU	h1	614	3	-	3/9/27/28	0/2/2/2
81	PSU	A3	1002	81	-	2/7/25/26	0/2/2/2
81	A2M	A3	369	81	-	1/5/27/28	0/3/3/3
81	OMU	A3	1068	81	-	0/9/27/28	0/2/2/2
81	OMC	A3	1862	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	2239	81	-	0/5/27/28	0/3/3/3
81	A2M	A3	2329	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	2947	81,84	-	2/7/25/26	0/2/2/2
82	PSU	B3	77	82	-	0/7/25/26	0/2/2/2
3	PSU	h1	258	3	-	1/7/25/26	0/2/2/2
3	PSU	h1	1308	3	-	2/7/25/26	0/2/2/2
3	A2M	h1	1579	3	-	2/5/27/28	0/3/3/3
81	OMU	A3	787	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	1002	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	2818	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	2269	81	-	2/7/25/26	0/2/2/2
3	OMU	h1	886	3	-	3/9/27/28	0/2/2/2
81	PSU	A3	3113	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	362	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	1474	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	815	81	-	0/5/27/28	0/3/3/3
3	OMC	h1	38	3	-	2/9/27/28	0/2/2/2
81	A2M	A3	817	81	-	0/5/27/28	0/3/3/3
81	OMC	A3	2296	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	970	81	-	1/7/25/26	0/2/2/2
81	PSU	A3	2263	81	-	1/7/25/26	0/2/2/2
3	OMU	h1	581	84,3	-	2/9/27/28	0/2/2/2
3	A2M	h1	28	3,83	-	0/5/27/28	0/3/3/3
81	PSU	A3	2883	81	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	h1	123	3	-	2/9/27/28	0/2/2/2
81	PSU	A3	895	81	-	0/7/25/26	0/2/2/2
81	OMU	A3	2350	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	1293	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	635	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	1106	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	1634	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	684	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1567	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	1133	81	-	0/7/25/26	0/2/2/2
81	A2M	A3	2259	81	-	2/5/27/28	0/3/3/3
81	A2M	A3	1144	81	-	0/5/27/28	0/3/3/3
81	A2M	A3	1378	81	-	2/5/27/28	0/3/3/3
81	OMU	A3	2738	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	277	81	-	0/7/25/26	0/2/2/2
82	PSU	B3	21	81,82	-	0/7/25/26	0/2/2/2
3	PSU	h1	1615	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	95	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	2126	81	-	0/5/27/28	0/3/3/3
81	A2M	A3	2643	81	-	0/5/27/28	0/3/3/3
81	A2M	A3	660	81	-	2/5/27/28	0/3/3/3
81	5MC	A3	2281	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1120	3	-	0/7/25/26	0/2/2/2
81	OMU	A3	675	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	2398	81	-	0/5/27/28	0/3/3/3
3	OMU	h1	1234	3	-	2/9/27/28	0/2/2/2
3	OMC	h1	473	3	-	0/9/27/28	0/2/2/2
81	OMC	A3	2962	81	-	0/9/27/28	0/2/2/2
3	A2M	h1	977	3	-	0/5/27/28	0/3/3/3
81	PSU	A3	228	81	-	1/7/25/26	0/2/2/2
81	PSU	A3	902	81,84,83	-	0/7/25/26	0/2/2/2
81	OMU	A3	1894	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	2394	81	-	0/5/27/28	0/3/3/3
81	OMG	A3	2796	81	-	0/5/27/28	0/3/3/3
3	PSU	h1	1787	3	-	2/7/25/26	0/2/2/2
3	OMG	h1	392	3	-	2/5/27/28	0/3/3/3
81	OMC	A3	2368	81	-	3/9/27/28	0/2/2/2
81	OMU	A3	3289	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	311	81,84	-	0/7/25/26	0/2/2/2
81	OMG	A3	918	81,84	-	2/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B8N	h1	1194	3	-	3/16/34/35	0/2/2/2
3	PSU	h1	1217	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	121	3,83	-	0/7/25/26	0/2/2/2
81	A2M	A3	2129	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	2214	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	2291	81	-	2/5/27/28	0/3/3/3
81	OMC	A3	1849	81	-	0/9/27/28	0/2/2/2
81	1MA	A3	656	81	-	0/3/25/26	0/3/3/3
81	OMG	A3	2925	81	-	0/5/27/28	0/3/3/3
81	OMG	A3	2622	81,36	-	0/5/27/28	0/3/3/3
3	OMC	h1	1218	3	-	0/9/27/28	0/2/2/2
3	OMU	h1	1012	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	829	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	417	3	-	0/7/25/26	0/2/2/2
3	OMU	h1	1272	3	-	2/9/27/28	0/2/2/2
81	OMU	A3	144	81	-	1/9/27/28	0/2/2/2
81	OMU	A3	804	81	-	0/9/27/28	0/2/2/2
81	OMU	A3	2720	81	-	0/9/27/28	0/2/2/2
81	5MC	A3	2873	81,84	-	4/7/25/26	0/2/2/2
81	OMG	A3	2654	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	2897	81	-	0/7/25/26	0/2/2/2
3	6MZ	h1	1771	84,3,83	-	0/5/27/28	0/3/3/3
81	A2M	A3	2223	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	1685	81	-	0/7/25/26	0/2/2/2
3	A2M	h1	622	3,83	-	2/5/27/28	0/3/3/3
81	PSU	A3	717	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	976	81,84	-	0/7/25/26	0/2/2/2
3	PSU	h1	950	3	-	0/7/25/26	0/2/2/2
81	A2M	A3	1460	81	-	0/5/27/28	0/3/3/3
81	OMU	A3	2924	81,84	-	0/9/27/28	0/2/2/2
3	PSU	h1	1210	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	1064	81	-	0/7/25/26	0/2/2/2
3	OMU	h1	1383	3,83	-	0/9/27/28	0/2/2/2
3	OMC	h1	1645	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	1135	81	-	0/7/25/26	0/2/2/2
81	OMC	A3	1448	81	-	3/9/27/28	0/2/2/2
3	PSU	h1	606	3	-	0/7/25/26	0/2/2/2
3	A2M	h1	162	3	-	0/5/27/28	0/3/3/3
3	A2M	h1	1758	3	-	0/5/27/28	0/3/3/3
3	MA6	h1	1789	3	-	0/7/29/30	0/3/3/3
81	OMC	A3	674	81	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	OMG	A3	2920	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	510	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	762	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	2412	81,84	-	1/5/27/28	0/3/3/3
81	PSU	A3	2419	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2261	81	-	1/7/25/26	0/2/2/2
81	PSU	A3	2257	81	-	0/7/25/26	0/2/2/2
3	A2M	h1	800	3	-	0/5/27/28	0/3/3/3
3	PSU	h1	1027	3	-	1/7/25/26	0/2/2/2
81	A2M	A3	827	81,84,83	-	3/5/27/28	0/3/3/3
81	PSU	A3	1016	81,84	-	0/7/25/26	0/2/2/2
81	OMU	A3	2732	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	1134	81	-	0/7/25/26	0/2/2/2
3	4AC	h1	1781	3	-	0/11/29/30	0/2/2/2
81	OMG	A3	2794	81	-	0/5/27/28	0/3/3/3
3	PSU	h1	1304	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	966	81	-	0/7/25/26	0/2/2/2
3	A2M	h1	1329	3	-	0/5/27/28	0/3/3/3
81	OMC	A3	2839	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	2949	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	2321	81,83	-	2/7/25/26	0/2/2/2
81	OMG	A3	2127	81	-	0/5/27/28	0/3/3/3
81	PSU	A3	2267	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	786	81	-	3/7/25/26	0/2/2/2
81	OMC	A3	40	81	-	1/9/27/28	0/2/2/2
3	PSU	h1	1535	3	-	0/7/25/26	0/2/2/2
82	OMG	B3	78	82	-	2/5/27/28	0/3/3/3
81	PSU	A3	2978	81	-	0/7/25/26	0/2/2/2
82	A2M	B3	46	82	-	0/5/27/28	0/3/3/3
81	OMC	A3	2951	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	42	81,84	-	0/7/25/26	0/2/2/2
81	OMU	A3	2424	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	1857	81	-	0/5/27/28	0/3/3/3
3	A2M	h1	468	3	-	0/5/27/28	0/3/3/3
81	PSU	A3	1482	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1184	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	753	3	-	0/7/25/26	0/2/2/2
3	OMC	h1	418	3	-	2/9/27/28	0/2/2/2
3	PSU	h1	605	3	-	0/7/25/26	0/2/2/2
3	OMG	h1	1433	3,83	-	1/5/27/28	0/3/3/3
3	OMG	h1	1274	3	-	2/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	A2M	A3	2284	81	-	2/5/27/28	0/3/3/3
3	OMU	h1	1447	3	-	0/9/27/28	0/2/2/2
81	OMU	A3	3304	81	-	0/9/27/28	0/2/2/2
3	UY1	h1	603	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	1056	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	103	84,3	-	0/7/25/26	0/2/2/2
3	OMU	h1	373	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	464	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1178	3	-	0/7/25/26	0/2/2/2
82	PSU	B3	96	84,82	-	2/7/25/26	0/2/2/2
81	UY1	A3	2653	81	-	0/9/27/28	0/2/2/2
81	OMU	A3	44	81,84	-	0/9/27/28	0/2/2/2
81	UR3	A3	2956	81	-	2/7/25/26	0/2/2/2
3	OMG	h1	598	3	-	3/5/27/28	0/3/3/3
81	PSU	A3	2139	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	961	84,3	-	0/7/25/26	0/2/2/2
81	OMG	A3	1461	81	-	1/5/27/28	0/3/3/3
3	4AC	h1	1283	3	-	0/11/29/30	0/2/2/2
81	OMU	A3	48	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	886	81	-	0/5/27/28	0/3/3/3
81	A2M	A3	2324	81	-	0/5/27/28	0/3/3/3
81	OMC	A3	2340	81	-	0/9/27/28	0/2/2/2
81	OMC	A3	2685	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	2747	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1190	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	2857	81	-	0/7/25/26	0/2/2/2
81	OMU	A3	2886	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	763	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	399	81	-	2/5/27/28	0/3/3/3
81	PSU	A3	150	81,84	-	0/7/25/26	0/2/2/2
81	A2M	A3	946	81	-	2/5/27/28	0/3/3/3
81	OMU	A3	2413	81,84	-	2/9/27/28	0/2/2/2
81	PSU	A3	2926	81,84	-	3/7/25/26	0/2/2/2
3	A2M	h1	544	3	-	2/5/27/28	0/3/3/3
81	OMC	A3	2882	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	2958	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2317	81,84	-	3/7/25/26	0/2/2/2
81	OMU	A3	1537	81	-	0/9/27/28	0/2/2/2
81	OMC	A3	1852	81	-	0/9/27/28	0/2/2/2
3	OMC	h1	140	3	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	h1	310	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	2137	81,84	-	0/7/25/26	0/2/2/2
3	OMG	h1	246	84,3	-	0/5/27/28	0/3/3/3
3	A2M	h1	440	3	-	0/5/27/28	0/3/3/3
3	PSU	h1	306	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	339	84,3	-	0/7/25/26	0/2/2/2
3	PSU	h1	1485	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	584	3	-	6/7/25/26	0/2/2/2
81	A2M	A3	2804	81	-	2/5/27/28	0/3/3/3
81	PSU	A3	2435	81	-	0/7/25/26	0/2/2/2
81	OMC	A3	2200	81,84	-	4/9/27/28	0/2/2/2
3	PSU	h1	607	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	809	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	2194	81,84	-	0/7/25/26	0/2/2/2
81	PSU	A3	2868	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	451	84,3	-	0/7/25/26	0/2/2/2

All (1681) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	656	1MA	C2-N3	13.39	1.45	1.29
3	h1	1524	PSU	C6-C5	12.36	1.49	1.35
3	h1	584	PSU	C6-C5	12.34	1.49	1.35
81	A3	2137	PSU	C6-C5	12.29	1.49	1.35
81	A3	2269	PSU	C6-C5	12.27	1.49	1.35
3	h1	1217	PSU	C6-C5	12.25	1.49	1.35
81	A3	786	PSU	C6-C5	12.25	1.49	1.35
81	A3	311	PSU	C6-C5	12.23	1.49	1.35
3	h1	1027	PSU	C6-C5	12.23	1.49	1.35
3	h1	451	PSU	C6-C5	12.22	1.49	1.35
3	h1	1485	PSU	C6-C5	12.22	1.49	1.35
3	h1	961	PSU	C6-C5	12.20	1.49	1.35
81	A3	1685	PSU	C6-C5	12.20	1.49	1.35
81	A3	902	PSU	C6-C5	12.19	1.49	1.35
81	A3	1002	PSU	C6-C5	12.19	1.49	1.35
81	A3	2883	PSU	C6-C5	12.19	1.49	1.35
81	A3	3113	PSU	C6-C5	12.19	1.49	1.35
3	h1	306	PSU	C6-C5	12.18	1.49	1.35
3	h1	1567	PSU	C6-C5	12.18	1.49	1.35
3	h1	1304	PSU	C6-C5	12.18	1.49	1.35
81	A3	464	PSU	C6-C5	12.18	1.49	1.35
81	A3	717	PSU	C6-C5	12.18	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	510	PSU	C6-C5	12.17	1.49	1.35
3	h1	1535	PSU	C6-C5	12.17	1.49	1.35
3	h1	1184	PSU	C6-C5	12.17	1.49	1.35
3	h1	258	PSU	C6-C5	12.17	1.49	1.35
3	h1	95	PSU	C6-C5	12.17	1.49	1.35
3	h1	121	PSU	C6-C5	12.16	1.49	1.35
81	A3	976	PSU	C6-C5	12.16	1.49	1.35
81	A3	2958	PSU	C6-C5	12.16	1.49	1.35
3	h1	1106	PSU	C6-C5	12.16	1.49	1.35
3	h1	1293	PSU	C6-C5	12.16	1.49	1.35
3	h1	310	PSU	C6-C5	12.16	1.49	1.35
3	h1	362	PSU	C6-C5	12.15	1.49	1.35
3	h1	950	PSU	C6-C5	12.15	1.49	1.35
81	A3	2317	PSU	C6-C5	12.15	1.49	1.35
81	A3	970	PSU	C6-C5	12.15	1.49	1.35
81	A3	2978	PSU	C6-C5	12.15	1.49	1.35
3	h1	1190	PSU	C6-C5	12.15	1.49	1.35
81	A3	2261	PSU	C6-C5	12.15	1.49	1.35
81	A3	2926	PSU	C6-C5	12.15	1.49	1.35
81	A3	2214	PSU	C6-C5	12.14	1.49	1.35
82	B3	77	PSU	C6-C5	12.14	1.49	1.35
81	A3	150	PSU	C6-C5	12.14	1.49	1.35
81	A3	2139	PSU	C6-C5	12.14	1.49	1.35
3	h1	1634	PSU	C6-C5	12.14	1.49	1.35
3	h1	605	PSU	C6-C5	12.14	1.49	1.35
81	A3	1016	PSU	C6-C5	12.14	1.49	1.35
3	h1	1178	PSU	C6-C5	12.14	1.49	1.35
81	A3	2435	PSU	C6-C5	12.14	1.49	1.35
3	h1	1120	PSU	C6-C5	12.13	1.49	1.35
3	h1	1002	PSU	C6-C5	12.13	1.49	1.35
3	h1	1787	PSU	C6-C5	12.13	1.49	1.35
3	h1	470	PSU	C6-C5	12.13	1.49	1.35
3	h1	763	PSU	C6-C5	12.13	1.49	1.35
81	A3	228	PSU	C6-C5	12.12	1.49	1.35
81	A3	2419	PSU	C6-C5	12.12	1.49	1.35
3	h1	607	PSU	C6-C5	12.12	1.49	1.35
81	A3	2321	PSU	C6-C5	12.12	1.49	1.35
3	h1	417	PSU	C6-C5	12.12	1.49	1.35
81	A3	1056	PSU	C6-C5	12.12	1.49	1.35
81	A3	1474	PSU	C6-C5	12.12	1.49	1.35
81	A3	1064	PSU	C6-C5	12.12	1.49	1.35
81	A3	2947	PSU	C6-C5	12.12	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2263	PSU	C6-C5	12.11	1.49	1.35
81	A3	895	PSU	C6-C5	12.11	1.49	1.35
81	A3	2857	PSU	C6-C5	12.11	1.49	1.35
3	h1	809	PSU	C6-C5	12.10	1.49	1.35
81	A3	1133	PSU	C6-C5	12.10	1.49	1.35
81	A3	2267	PSU	C6-C5	12.10	1.49	1.35
82	B3	96	PSU	C6-C5	12.10	1.49	1.35
81	A3	829	PSU	C6-C5	12.10	1.49	1.35
3	h1	103	PSU	C6-C5	12.09	1.49	1.35
81	A3	42	PSU	C6-C5	12.09	1.49	1.35
3	h1	762	PSU	C6-C5	12.09	1.49	1.35
3	h1	635	PSU	C6-C5	12.09	1.49	1.35
3	h1	1615	PSU	C6-C5	12.09	1.49	1.35
81	A3	684	PSU	C6-C5	12.09	1.49	1.35
81	A3	1135	PSU	C6-C5	12.09	1.49	1.35
82	B3	21	PSU	C6-C5	12.08	1.49	1.35
81	A3	2897	PSU	C6-C5	12.08	1.49	1.35
3	h1	339	PSU	C6-C5	12.07	1.49	1.35
3	h1	753	PSU	C6-C5	12.07	1.49	1.35
81	A3	966	PSU	C6-C5	12.07	1.49	1.35
81	A3	2747	PSU	C6-C5	12.06	1.49	1.35
81	A3	2868	PSU	C6-C5	12.06	1.49	1.35
3	h1	1210	PSU	C6-C5	12.05	1.49	1.35
81	A3	2257	PSU	C6-C5	12.05	1.49	1.35
81	A3	2194	PSU	C6-C5	12.05	1.49	1.35
81	A3	1134	PSU	C6-C5	12.02	1.49	1.35
81	A3	34	PSU	C6-C5	12.01	1.49	1.35
81	A3	277	PSU	C6-C5	12.01	1.49	1.35
3	h1	1308	PSU	C6-C5	12.01	1.49	1.35
81	A3	1482	PSU	C6-C5	12.00	1.49	1.35
81	A3	2829	PSU	C6-C5	11.99	1.49	1.35
3	h1	606	PSU	C6-C5	11.91	1.49	1.35
81	A3	2653	UY1	C6-C5	11.23	1.48	1.35
3	h1	603	UY1	C6-C5	11.15	1.48	1.35
3	h1	800	A2M	O4'-C1'	11.06	1.56	1.41
3	h1	162	A2M	O4'-C1'	10.97	1.56	1.41
3	h1	424	A2M	O4'-C1'	10.87	1.56	1.41
3	h1	468	A2M	O4'-C1'	10.87	1.56	1.41
81	A3	827	A2M	O4'-C1'	10.85	1.56	1.41
3	h1	544	A2M	O4'-C1'	10.85	1.56	1.41
81	A3	2259	A2M	O4'-C1'	10.84	1.56	1.41
81	A3	2223	A2M	O4'-C1'	10.84	1.56	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2129	A2M	O4'-C1'	10.82	1.56	1.41
3	h1	1329	A2M	O4'-C1'	10.78	1.56	1.41
81	A3	886	A2M	O4'-C1'	10.76	1.56	1.41
81	A3	2949	A2M	O4'-C1'	10.75	1.56	1.41
81	A3	1144	A2M	O4'-C1'	10.75	1.56	1.41
81	A3	2914	A2M	O4'-C1'	10.74	1.56	1.41
82	B3	46	A2M	O4'-C1'	10.74	1.56	1.41
3	h1	977	A2M	O4'-C1'	10.72	1.56	1.41
3	h1	28	A2M	O4'-C1'	10.71	1.56	1.41
81	A3	2329	A2M	O4'-C1'	10.71	1.56	1.41
81	A3	1460	A2M	O4'-C1'	10.70	1.56	1.41
81	A3	1378	A2M	O4'-C1'	10.68	1.56	1.41
81	A3	660	A2M	O4'-C1'	10.65	1.55	1.41
3	h1	440	A2M	O4'-C1'	10.63	1.55	1.41
81	A3	2643	A2M	O4'-C1'	10.63	1.55	1.41
81	A3	369	A2M	O4'-C1'	10.63	1.55	1.41
81	A3	2324	A2M	O4'-C1'	10.63	1.55	1.41
3	h1	1758	A2M	O4'-C1'	10.58	1.55	1.41
81	A3	817	A2M	O4'-C1'	10.56	1.55	1.41
3	h1	1579	A2M	O4'-C1'	10.55	1.55	1.41
81	A3	946	A2M	O4'-C1'	10.52	1.55	1.41
3	h1	622	A2M	O4'-C1'	10.46	1.55	1.41
81	A3	2804	A2M	O4'-C1'	10.34	1.55	1.41
81	A3	2284	A2M	O4'-C1'	10.24	1.55	1.41
3	h1	544	A2M	C3'-C4'	-9.90	1.27	1.53
81	A3	817	A2M	C3'-C4'	-9.87	1.27	1.53
81	A3	827	A2M	C3'-C4'	-9.86	1.27	1.53
81	A3	946	A2M	C3'-C4'	-9.84	1.27	1.53
81	A3	2259	A2M	C3'-C4'	-9.84	1.27	1.53
81	A3	2914	A2M	C3'-C4'	-9.82	1.27	1.53
81	A3	2129	A2M	C3'-C4'	-9.82	1.27	1.53
3	h1	162	A2M	C3'-C4'	-9.81	1.27	1.53
3	h1	800	A2M	C3'-C4'	-9.80	1.28	1.53
3	h1	468	A2M	C3'-C4'	-9.80	1.28	1.53
3	h1	1329	A2M	C3'-C4'	-9.79	1.28	1.53
3	h1	28	A2M	C3'-C4'	-9.79	1.28	1.53
81	A3	1378	A2M	C3'-C4'	-9.78	1.28	1.53
3	h1	1758	A2M	C3'-C4'	-9.76	1.28	1.53
3	h1	424	A2M	C3'-C4'	-9.76	1.28	1.53
81	A3	2223	A2M	C3'-C4'	-9.74	1.28	1.53
81	A3	2804	A2M	C3'-C4'	-9.73	1.28	1.53
3	h1	977	A2M	C3'-C4'	-9.72	1.28	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	622	A2M	C3'-C4'	-9.71	1.28	1.53
81	A3	2949	A2M	C3'-C4'	-9.71	1.28	1.53
81	A3	2873	5MC	C6-C5	9.69	1.50	1.34
81	A3	886	A2M	C3'-C4'	-9.69	1.28	1.53
3	h1	440	A2M	C3'-C4'	-9.68	1.28	1.53
82	B3	46	A2M	C3'-C4'	-9.67	1.28	1.53
81	A3	2329	A2M	C3'-C4'	-9.66	1.28	1.53
81	A3	42	PSU	C2-N1	9.65	1.49	1.36
81	A3	660	A2M	C3'-C4'	-9.65	1.28	1.53
81	A3	2643	A2M	C3'-C4'	-9.64	1.28	1.53
3	h1	584	PSU	C2-N1	9.64	1.49	1.36
81	A3	2257	PSU	C2-N1	9.64	1.49	1.36
3	h1	1579	A2M	C3'-C4'	-9.64	1.28	1.53
81	A3	1144	A2M	C3'-C4'	-9.63	1.28	1.53
81	A3	2137	PSU	C2-N1	9.63	1.49	1.36
3	h1	95	PSU	C2-N1	9.62	1.49	1.36
81	A3	510	PSU	C2-N1	9.62	1.49	1.36
81	A3	976	PSU	C2-N1	9.62	1.49	1.36
81	A3	2653	UY1	C2-N1	9.61	1.49	1.36
81	A3	1460	A2M	C3'-C4'	-9.61	1.28	1.53
3	h1	1535	PSU	C2-N1	9.60	1.49	1.36
3	h1	1293	PSU	C2-N1	9.59	1.49	1.36
3	h1	121	PSU	C2-N1	9.59	1.49	1.36
81	A3	2281	5MC	C6-C5	9.59	1.50	1.34
81	A3	369	A2M	C3'-C4'	-9.58	1.28	1.53
3	h1	1485	PSU	C2-N1	9.58	1.49	1.36
81	A3	2321	PSU	C2-N1	9.58	1.49	1.36
3	h1	961	PSU	C2-N1	9.58	1.49	1.36
81	A3	1016	PSU	C2-N1	9.57	1.49	1.36
3	h1	763	PSU	C2-N1	9.57	1.49	1.36
81	A3	464	PSU	C2-N1	9.57	1.49	1.36
3	h1	1002	PSU	C2-N1	9.57	1.49	1.36
81	A3	970	PSU	C2-N1	9.57	1.49	1.36
82	B3	77	PSU	C2-N1	9.56	1.49	1.36
81	A3	2324	A2M	C3'-C4'	-9.55	1.28	1.53
81	A3	2269	PSU	C2-N1	9.55	1.49	1.36
3	h1	1184	PSU	C2-N1	9.55	1.49	1.36
3	h1	1308	PSU	C2-N1	9.55	1.49	1.36
3	h1	1524	PSU	C2-N1	9.55	1.49	1.36
3	h1	258	PSU	C2-N1	9.55	1.49	1.36
3	h1	1217	PSU	C2-N1	9.55	1.49	1.36
3	h1	809	PSU	C2-N1	9.55	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	34	PSU	C2-N1	9.55	1.49	1.36
81	A3	717	PSU	C2-N1	9.54	1.49	1.36
81	A3	2897	PSU	C2-N1	9.54	1.49	1.36
3	h1	1027	PSU	C2-N1	9.54	1.49	1.36
81	A3	684	PSU	C2-N1	9.54	1.49	1.36
81	A3	228	PSU	C2-N1	9.54	1.49	1.36
3	h1	603	UY1	C2-N1	9.54	1.49	1.36
3	h1	1106	PSU	C2-N1	9.54	1.49	1.36
3	h1	306	PSU	C2-N1	9.53	1.49	1.36
81	A3	2214	PSU	C2-N1	9.53	1.49	1.36
81	A3	1135	PSU	C2-N1	9.53	1.49	1.36
81	A3	2263	PSU	C2-N1	9.53	1.49	1.36
81	A3	2317	PSU	C2-N1	9.53	1.49	1.36
82	B3	96	PSU	C2-N1	9.53	1.49	1.36
3	h1	762	PSU	C2-N1	9.52	1.49	1.36
81	A3	2857	PSU	C2-N1	9.52	1.49	1.36
3	h1	1567	PSU	C2-N1	9.52	1.49	1.36
81	A3	2194	PSU	C2-N1	9.52	1.49	1.36
3	h1	753	PSU	C2-N1	9.52	1.49	1.36
3	h1	339	PSU	C2-N1	9.52	1.49	1.36
81	A3	1064	PSU	C2-N1	9.52	1.49	1.36
81	A3	150	PSU	C2-N1	9.51	1.49	1.36
81	A3	2978	PSU	C2-N1	9.51	1.49	1.36
81	A3	1002	PSU	C2-N1	9.51	1.49	1.36
81	A3	2261	PSU	C2-N1	9.51	1.49	1.36
3	h1	417	PSU	C2-N1	9.50	1.49	1.36
3	h1	470	PSU	C2-N1	9.50	1.49	1.36
3	h1	1190	PSU	C2-N1	9.50	1.49	1.36
81	A3	2435	PSU	C2-N1	9.50	1.49	1.36
81	A3	829	PSU	C2-N1	9.50	1.49	1.36
3	h1	1304	PSU	C2-N1	9.50	1.49	1.36
81	A3	1685	PSU	C2-N1	9.50	1.49	1.36
81	A3	2868	PSU	C2-N1	9.49	1.49	1.36
3	h1	451	PSU	C2-N1	9.49	1.49	1.36
3	h1	1787	PSU	C2-N1	9.48	1.49	1.36
81	A3	1474	PSU	C2-N1	9.48	1.49	1.36
3	h1	103	PSU	C2-N1	9.48	1.49	1.36
81	A3	2958	PSU	C2-N1	9.48	1.49	1.36
81	A3	2284	A2M	C3'-C4'	-9.48	1.28	1.53
3	h1	1615	PSU	C2-N1	9.48	1.49	1.36
3	h1	605	PSU	C2-N1	9.48	1.49	1.36
81	A3	1056	PSU	C2-N1	9.47	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2926	PSU	C2-N1	9.47	1.49	1.36
81	A3	2883	PSU	C2-N1	9.47	1.49	1.36
81	A3	2267	PSU	C2-N1	9.47	1.49	1.36
81	A3	277	PSU	C2-N1	9.47	1.49	1.36
81	A3	2829	PSU	C2-N1	9.47	1.49	1.36
81	A3	1133	PSU	C2-N1	9.47	1.49	1.36
3	h1	310	PSU	C2-N1	9.46	1.49	1.36
3	h1	606	PSU	C2-N1	9.46	1.49	1.36
81	A3	2419	PSU	C2-N1	9.46	1.49	1.36
81	A3	1482	PSU	C2-N1	9.46	1.49	1.36
3	h1	950	PSU	C2-N1	9.45	1.49	1.36
3	h1	362	PSU	C2-N1	9.45	1.49	1.36
3	h1	1210	PSU	C2-N1	9.45	1.49	1.36
81	A3	895	PSU	C2-N1	9.44	1.49	1.36
81	A3	2947	PSU	C2-N1	9.44	1.49	1.36
3	h1	1120	PSU	C2-N1	9.44	1.49	1.36
81	A3	3113	PSU	C2-N1	9.44	1.49	1.36
3	h1	1178	PSU	C2-N1	9.44	1.49	1.36
3	h1	607	PSU	C2-N1	9.44	1.49	1.36
3	h1	1634	PSU	C2-N1	9.43	1.49	1.36
81	A3	311	PSU	C2-N1	9.43	1.49	1.36
81	A3	1134	PSU	C2-N1	9.43	1.49	1.36
81	A3	902	PSU	C2-N1	9.43	1.49	1.36
81	A3	966	PSU	C2-N1	9.41	1.49	1.36
3	h1	635	PSU	C2-N1	9.40	1.49	1.36
81	A3	2139	PSU	C2-N1	9.40	1.49	1.36
82	B3	21	PSU	C2-N1	9.39	1.49	1.36
81	A3	786	PSU	C2-N1	9.39	1.49	1.36
81	A3	2747	PSU	C2-N1	9.35	1.49	1.36
3	h1	417	PSU	C2-N3	8.34	1.51	1.37
3	h1	339	PSU	C2-N3	8.33	1.51	1.37
81	A3	464	PSU	C2-N3	8.29	1.51	1.37
81	A3	2926	PSU	C2-N3	8.29	1.51	1.37
3	h1	451	PSU	C2-N3	8.29	1.51	1.37
3	h1	1567	PSU	C2-N3	8.28	1.51	1.37
3	h1	961	PSU	C2-N3	8.28	1.51	1.37
3	h1	584	PSU	C2-N3	8.27	1.51	1.37
3	h1	1217	PSU	C2-N3	8.27	1.51	1.37
81	A3	1135	PSU	C2-N3	8.27	1.51	1.37
81	A3	228	PSU	C2-N3	8.27	1.51	1.37
3	h1	607	PSU	C2-N3	8.27	1.51	1.37
81	A3	717	PSU	C2-N3	8.27	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	1178	PSU	C2-N3	8.27	1.51	1.37
3	h1	258	PSU	C2-N3	8.27	1.51	1.37
3	h1	1308	PSU	C2-N3	8.27	1.51	1.37
3	h1	1210	PSU	C2-N3	8.27	1.51	1.37
3	h1	809	PSU	C2-N3	8.27	1.51	1.37
3	h1	1190	PSU	C2-N3	8.26	1.51	1.37
81	A3	1685	PSU	C2-N3	8.26	1.51	1.37
3	h1	1485	PSU	C2-N3	8.26	1.51	1.37
81	A3	2267	PSU	C2-N3	8.25	1.51	1.37
81	A3	2958	PSU	C2-N3	8.25	1.51	1.37
3	h1	1787	PSU	C2-N3	8.25	1.51	1.37
3	h1	121	PSU	C2-N3	8.25	1.51	1.37
3	h1	762	PSU	C2-N3	8.25	1.51	1.37
3	h1	763	PSU	C2-N3	8.25	1.51	1.37
81	A3	150	PSU	C2-N3	8.24	1.51	1.37
3	h1	1524	PSU	C2-N3	8.24	1.51	1.37
3	h1	605	PSU	C2-N3	8.24	1.51	1.37
3	h1	103	PSU	C2-N3	8.24	1.51	1.37
81	A3	976	PSU	C2-N3	8.24	1.51	1.37
82	B3	77	PSU	C2-N3	8.24	1.51	1.37
3	h1	1535	PSU	C2-N3	8.24	1.51	1.37
81	A3	2317	PSU	C2-N3	8.24	1.51	1.37
81	A3	2419	PSU	C2-N3	8.23	1.51	1.37
81	A3	2139	PSU	C2-N3	8.23	1.51	1.37
82	B3	96	PSU	C2-N3	8.23	1.51	1.37
3	h1	1634	PSU	C2-N3	8.23	1.51	1.37
3	h1	1120	PSU	C2-N3	8.23	1.51	1.37
81	A3	902	PSU	C2-N3	8.23	1.51	1.37
81	A3	2263	PSU	C2-N3	8.23	1.51	1.37
81	A3	1002	PSU	C2-N3	8.22	1.51	1.37
81	A3	1056	PSU	C2-N3	8.22	1.51	1.37
3	h1	1615	PSU	C2-N3	8.22	1.51	1.37
3	h1	470	PSU	C2-N3	8.22	1.51	1.37
3	h1	95	PSU	C2-N3	8.22	1.51	1.37
81	A3	970	PSU	C2-N3	8.22	1.51	1.37
81	A3	2857	PSU	C2-N3	8.21	1.51	1.37
3	h1	753	PSU	C2-N3	8.21	1.51	1.37
81	A3	1474	PSU	C2-N3	8.21	1.51	1.37
3	h1	1293	PSU	C2-N3	8.21	1.51	1.37
81	A3	1482	PSU	C2-N3	8.21	1.51	1.37
3	h1	606	PSU	C2-N3	8.21	1.51	1.37
81	A3	277	PSU	C2-N3	8.21	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2868	PSU	C2-N3	8.21	1.51	1.37
3	h1	635	PSU	C2-N3	8.21	1.51	1.37
81	A3	2269	PSU	C2-N3	8.21	1.51	1.37
81	A3	34	PSU	C2-N3	8.21	1.51	1.37
81	A3	2214	PSU	C2-N3	8.21	1.51	1.37
3	h1	310	PSU	C2-N3	8.20	1.51	1.37
81	A3	1064	PSU	C2-N3	8.20	1.51	1.37
81	A3	2261	PSU	C2-N3	8.20	1.51	1.37
81	A3	2883	PSU	C2-N3	8.20	1.51	1.37
81	A3	1016	PSU	C2-N3	8.20	1.51	1.37
81	A3	2747	PSU	C2-N3	8.20	1.51	1.37
82	B3	21	PSU	C2-N3	8.20	1.51	1.37
3	h1	1002	PSU	C2-N3	8.19	1.51	1.37
81	A3	2435	PSU	C2-N3	8.19	1.51	1.37
3	h1	1304	PSU	C2-N3	8.19	1.51	1.37
3	h1	950	PSU	C2-N3	8.19	1.51	1.37
81	A3	2321	PSU	C2-N3	8.19	1.51	1.37
81	A3	2897	PSU	C2-N3	8.18	1.51	1.37
81	A3	2829	PSU	C2-N3	8.18	1.51	1.37
81	A3	2257	PSU	C2-N3	8.18	1.51	1.37
81	A3	311	PSU	C2-N3	8.18	1.51	1.37
81	A3	786	PSU	C2-N3	8.18	1.51	1.37
3	h1	1106	PSU	C2-N3	8.18	1.51	1.37
81	A3	2947	PSU	C2-N3	8.17	1.51	1.37
81	A3	2978	PSU	C2-N3	8.17	1.51	1.37
3	h1	1184	PSU	C2-N3	8.16	1.51	1.37
81	A3	684	PSU	C2-N3	8.16	1.51	1.37
3	h1	1027	PSU	C2-N3	8.16	1.51	1.37
81	A3	1133	PSU	C2-N3	8.15	1.51	1.37
3	h1	306	PSU	C2-N3	8.15	1.51	1.37
81	A3	829	PSU	C2-N3	8.14	1.51	1.37
81	A3	1134	PSU	C2-N3	8.13	1.51	1.37
81	A3	966	PSU	C2-N3	8.13	1.51	1.37
81	A3	510	PSU	C2-N3	8.13	1.51	1.37
3	h1	362	PSU	C2-N3	8.12	1.51	1.37
81	A3	895	PSU	C2-N3	8.12	1.51	1.37
81	A3	42	PSU	C2-N3	8.12	1.51	1.37
81	A3	2194	PSU	C2-N3	8.11	1.51	1.37
81	A3	3113	PSU	C2-N3	8.10	1.51	1.37
81	A3	2137	PSU	C2-N3	8.01	1.51	1.37
3	h1	1194	B8N	C4-N3	-7.94	1.25	1.40
3	h1	1194	B8N	C6-N1	7.60	1.55	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	603	UY1	C2-N3	7.44	1.50	1.37
81	A3	2653	UY1	C2-N3	7.43	1.50	1.37
81	A3	2956	UR3	C2-N1	7.23	1.48	1.38
81	A3	2281	5MC	C4-N3	7.21	1.46	1.34
81	A3	2873	5MC	C4-N3	7.10	1.46	1.34
3	h1	1771	6MZ	C6-N6	7.09	1.46	1.35
3	h1	140	OMC	C2-N3	7.05	1.50	1.36
3	h1	373	OMU	C2-N3	7.03	1.50	1.38
3	h1	1781	4AC	C4-N3	7.03	1.45	1.32
3	h1	1272	OMU	C2-N3	7.03	1.50	1.38
3	h1	1447	OMU	C2-N3	7.03	1.50	1.38
81	A3	44	OMU	C2-N3	7.02	1.50	1.38
81	A3	804	OMU	C2-N3	7.02	1.50	1.38
3	h1	581	OMU	C2-N3	7.01	1.50	1.38
3	h1	123	OMU	C2-N3	7.01	1.50	1.38
3	h1	1012	OMU	C2-N3	7.01	1.50	1.38
3	h1	1383	OMU	C2-N3	7.01	1.50	1.38
3	h1	38	OMC	C2-N3	7.01	1.50	1.36
81	A3	1852	OMC	C2-N3	7.00	1.50	1.36
81	A3	2281	5MC	C2-N3	7.00	1.50	1.36
81	A3	3289	OMU	C2-N3	7.00	1.50	1.38
81	A3	2350	OMU	C2-N3	6.99	1.50	1.38
81	A3	2720	OMU	C2-N3	6.99	1.50	1.38
81	A3	2839	OMC	C2-N3	6.99	1.50	1.36
81	A3	144	OMU	C2-N3	6.99	1.50	1.38
3	h1	1218	OMC	C2-N3	6.99	1.50	1.36
81	A3	2886	OMU	C2-N3	6.98	1.50	1.38
81	A3	2685	OMC	C2-N3	6.98	1.50	1.36
81	A3	2924	OMU	C2-N3	6.98	1.50	1.38
3	h1	418	OMC	C2-N3	6.97	1.50	1.36
3	h1	473	OMC	C2-N3	6.97	1.50	1.36
81	A3	2296	OMC	C2-N3	6.97	1.50	1.36
81	A3	2424	OMU	C2-N3	6.96	1.50	1.38
3	h1	886	OMU	C2-N3	6.95	1.50	1.38
81	A3	1894	OMU	C2-N3	6.95	1.50	1.38
81	A3	675	OMU	C2-N3	6.94	1.50	1.38
3	h1	1645	OMC	C2-N3	6.94	1.50	1.36
3	h1	614	OMU	C2-N3	6.93	1.50	1.38
81	A3	2738	OMU	C2-N3	6.93	1.50	1.38
81	A3	1480	OMC	C2-N3	6.92	1.50	1.36
81	A3	2882	OMC	C2-N3	6.92	1.50	1.36
3	h1	1283	4AC	C4-N3	6.92	1.44	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2340	OMC	C2-N3	6.91	1.50	1.36
81	A3	3304	OMU	C2-N3	6.90	1.50	1.38
81	A3	2873	5MC	C2-N3	6.90	1.50	1.36
3	h1	1234	OMU	C2-N3	6.89	1.50	1.38
81	A3	1537	OMU	C2-N3	6.89	1.50	1.38
81	A3	1068	OMU	C2-N3	6.89	1.50	1.38
81	A3	1448	OMC	C2-N3	6.88	1.50	1.36
81	A3	2962	OMC	C2-N3	6.87	1.50	1.36
81	A3	787	OMU	C2-N3	6.87	1.50	1.38
81	A3	2951	OMC	C2-N3	6.87	1.50	1.36
81	A3	1862	OMC	C2-N3	6.87	1.50	1.36
81	A3	2368	OMC	C2-N3	6.86	1.50	1.36
81	A3	2732	OMU	C2-N3	6.86	1.50	1.38
81	A3	2200	OMC	C2-N3	6.86	1.50	1.36
81	A3	40	OMC	C2-N3	6.86	1.50	1.36
81	A3	674	OMC	C2-N3	6.82	1.50	1.36
81	A3	2413	OMU	C2-N3	6.80	1.50	1.38
81	A3	48	OMU	C2-N3	6.78	1.50	1.38
81	A3	1849	OMC	C2-N3	6.71	1.50	1.36
3	h1	581	OMU	C2-N1	6.65	1.49	1.38
3	h1	614	OMU	C2-N1	6.63	1.49	1.38
3	h1	1383	OMU	C2-N1	6.63	1.49	1.38
3	h1	1272	OMU	C2-N1	6.63	1.49	1.38
81	A3	1537	OMU	C2-N1	6.62	1.49	1.38
81	A3	1894	OMU	C2-N1	6.59	1.49	1.38
3	h1	886	OMU	C2-N1	6.59	1.49	1.38
81	A3	144	OMU	C2-N1	6.58	1.49	1.38
81	A3	675	OMU	C2-N1	6.58	1.49	1.38
81	A3	44	OMU	C2-N1	6.57	1.49	1.38
81	A3	2350	OMU	C2-N1	6.56	1.49	1.38
81	A3	2886	OMU	C2-N1	6.56	1.49	1.38
81	A3	3289	OMU	C2-N1	6.55	1.49	1.38
3	h1	373	OMU	C2-N1	6.55	1.49	1.38
3	h1	1283	4AC	C6-C5	6.54	1.50	1.35
81	A3	2424	OMU	C2-N1	6.53	1.48	1.38
81	A3	48	OMU	C2-N1	6.52	1.48	1.38
81	A3	787	OMU	C2-N1	6.52	1.48	1.38
81	A3	1068	OMU	C2-N1	6.51	1.48	1.38
81	A3	2720	OMU	C2-N1	6.51	1.48	1.38
81	A3	804	OMU	C2-N1	6.51	1.48	1.38
3	h1	1447	OMU	C2-N1	6.51	1.48	1.38
3	h1	123	OMU	C2-N1	6.50	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	3304	OMU	C2-N1	6.49	1.48	1.38
3	h1	1012	OMU	C2-N1	6.48	1.48	1.38
81	A3	2738	OMU	C2-N1	6.48	1.48	1.38
81	A3	2924	OMU	C2-N1	6.47	1.48	1.38
81	A3	2413	OMU	C2-N1	6.45	1.48	1.38
3	h1	1234	OMU	C2-N1	6.44	1.48	1.38
81	A3	2732	OMU	C2-N1	6.43	1.48	1.38
3	h1	1781	4AC	C6-C5	6.39	1.49	1.35
81	A3	2804	A2M	C3'-C2'	6.38	1.67	1.52
3	h1	1645	OMC	C6-C5	6.20	1.49	1.35
81	A3	2956	UR3	C6-C5	6.19	1.49	1.35
3	h1	473	OMC	C6-C5	6.19	1.49	1.35
81	A3	2340	OMC	C6-C5	6.19	1.49	1.35
81	A3	817	A2M	C3'-C2'	6.18	1.66	1.52
81	A3	1852	OMC	C6-C5	6.18	1.49	1.35
3	h1	544	A2M	C3'-C2'	6.18	1.66	1.52
81	A3	1849	OMC	C6-C5	6.17	1.49	1.35
3	h1	1218	OMC	C6-C5	6.17	1.49	1.35
81	A3	2200	OMC	C6-C5	6.16	1.49	1.35
3	h1	38	OMC	C6-C5	6.16	1.49	1.35
81	A3	2685	OMC	C6-C5	6.16	1.49	1.35
3	h1	418	OMC	C6-C5	6.15	1.49	1.35
81	A3	2368	OMC	C6-C5	6.15	1.49	1.35
81	A3	1448	OMC	C6-C5	6.13	1.49	1.35
81	A3	1480	OMC	C6-C5	6.13	1.49	1.35
3	h1	140	OMC	C6-C5	6.12	1.49	1.35
81	A3	2296	OMC	C6-C5	6.12	1.49	1.35
81	A3	2882	OMC	C6-C5	6.10	1.49	1.35
81	A3	40	OMC	C6-C5	6.10	1.49	1.35
81	A3	674	OMC	C6-C5	6.10	1.49	1.35
3	h1	440	A2M	C3'-C2'	6.10	1.66	1.52
81	A3	1862	OMC	C6-C5	6.09	1.49	1.35
81	A3	2962	OMC	C6-C5	6.09	1.49	1.35
3	h1	622	A2M	C3'-C2'	6.06	1.66	1.52
3	h1	1781	4AC	C2-N3	6.04	1.48	1.36
81	A3	2951	OMC	C6-C5	6.03	1.49	1.35
81	A3	660	A2M	C3'-C2'	6.02	1.66	1.52
81	A3	2839	OMC	C6-C5	6.01	1.49	1.35
81	A3	946	A2M	C3'-C2'	6.01	1.66	1.52
3	h1	1579	A2M	C3'-C2'	6.00	1.66	1.52
81	A3	827	A2M	C3'-C2'	5.99	1.66	1.52
3	h1	1283	4AC	C2-N3	5.98	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	369	A2M	C3'-C2'	5.98	1.66	1.52
81	A3	2873	5MC	C6-N1	5.97	1.48	1.38
81	A3	2223	A2M	C3'-C2'	5.95	1.66	1.52
3	h1	1329	A2M	C3'-C2'	5.95	1.66	1.52
81	A3	1460	A2M	C3'-C2'	5.95	1.66	1.52
81	A3	2129	A2M	C3'-C2'	5.91	1.66	1.52
81	A3	399	OMG	C2-N3	5.91	1.47	1.33
3	h1	28	A2M	C3'-C2'	5.89	1.66	1.52
81	A3	2914	A2M	C3'-C2'	5.89	1.66	1.52
3	h1	977	A2M	C3'-C2'	5.89	1.66	1.52
81	A3	2259	A2M	C3'-C2'	5.89	1.66	1.52
3	h1	246	OMG	C2-N3	5.88	1.47	1.33
81	A3	886	A2M	C3'-C2'	5.87	1.66	1.52
3	h1	1293	PSU	C6-N1	5.87	1.46	1.36
3	h1	424	A2M	C3'-C2'	5.87	1.66	1.52
81	A3	2284	A2M	C3'-C2'	5.86	1.66	1.52
81	A3	2643	A2M	C3'-C2'	5.86	1.66	1.52
3	h1	95	PSU	C6-N1	5.85	1.45	1.36
81	A3	918	OMG	C2-N3	5.85	1.47	1.33
81	A3	1144	A2M	C3'-C2'	5.85	1.66	1.52
3	h1	584	PSU	C6-N1	5.84	1.45	1.36
3	h1	809	PSU	C6-N1	5.84	1.45	1.36
3	h1	1758	A2M	C3'-C2'	5.84	1.66	1.52
3	h1	1308	PSU	C6-N1	5.83	1.45	1.36
81	A3	510	PSU	C6-N1	5.83	1.45	1.36
81	A3	2949	A2M	C3'-C2'	5.83	1.65	1.52
3	h1	1524	PSU	C6-N1	5.83	1.45	1.36
81	A3	1056	PSU	C6-N1	5.83	1.45	1.36
3	h1	417	PSU	C6-N1	5.83	1.45	1.36
3	h1	763	PSU	C6-N1	5.82	1.45	1.36
81	A3	228	PSU	C6-N1	5.82	1.45	1.36
3	h1	1274	OMG	C2-N3	5.82	1.47	1.33
3	h1	258	PSU	C6-N1	5.82	1.45	1.36
81	A3	2239	OMG	C2-N3	5.81	1.47	1.33
81	A3	2257	PSU	C6-N1	5.81	1.45	1.36
3	h1	1027	PSU	C6-N1	5.81	1.45	1.36
3	h1	1184	PSU	C6-N1	5.81	1.45	1.36
3	h1	1190	PSU	C6-N1	5.81	1.45	1.36
3	h1	762	PSU	C6-N1	5.81	1.45	1.36
3	h1	1535	PSU	C6-N1	5.80	1.45	1.36
3	h1	1634	PSU	C6-N1	5.80	1.45	1.36
81	A3	2269	PSU	C6-N1	5.80	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	1002	PSU	C6-N1	5.80	1.45	1.36
3	h1	468	A2M	C3'-C2'	5.80	1.65	1.52
81	A3	2137	PSU	C6-N1	5.80	1.45	1.36
81	A3	684	PSU	C6-N1	5.79	1.45	1.36
82	B3	96	PSU	C6-N1	5.79	1.45	1.36
3	h1	1304	PSU	C6-N1	5.79	1.45	1.36
81	A3	2324	A2M	C3'-C2'	5.79	1.65	1.52
3	h1	961	PSU	C6-N1	5.79	1.45	1.36
3	h1	1787	PSU	C6-N1	5.79	1.45	1.36
81	A3	976	PSU	C6-N1	5.79	1.45	1.36
3	h1	306	PSU	C6-N1	5.79	1.45	1.36
81	A3	42	PSU	C6-N1	5.79	1.45	1.36
81	A3	34	PSU	C6-N1	5.78	1.45	1.36
81	A3	2958	PSU	C6-N1	5.78	1.45	1.36
81	A3	2868	PSU	C6-N1	5.78	1.45	1.36
81	A3	2978	PSU	C6-N1	5.78	1.45	1.36
81	A3	2281	5MC	C6-N1	5.78	1.47	1.38
3	h1	1217	PSU	C6-N1	5.78	1.45	1.36
3	h1	598	OMG	C2-N3	5.78	1.47	1.33
81	A3	1133	PSU	C6-N1	5.78	1.45	1.36
81	A3	2194	PSU	C6-N1	5.78	1.45	1.36
3	h1	950	PSU	C6-N1	5.78	1.45	1.36
81	A3	2263	PSU	C6-N1	5.78	1.45	1.36
3	h1	1567	PSU	C6-N1	5.78	1.45	1.36
81	A3	970	PSU	C6-N1	5.78	1.45	1.36
3	h1	121	PSU	C6-N1	5.78	1.45	1.36
3	h1	1485	PSU	C6-N1	5.77	1.45	1.36
81	A3	902	PSU	C6-N1	5.77	1.45	1.36
3	h1	607	PSU	C6-N1	5.77	1.45	1.36
81	A3	2261	PSU	C6-N1	5.77	1.45	1.36
81	A3	2622	OMG	C2-N3	5.77	1.47	1.33
3	h1	1615	PSU	C6-N1	5.77	1.45	1.36
81	A3	1002	PSU	C6-N1	5.77	1.45	1.36
81	A3	2267	PSU	C6-N1	5.77	1.45	1.36
81	A3	1016	PSU	C6-N1	5.77	1.45	1.36
3	h1	310	PSU	C6-N1	5.77	1.45	1.36
81	A3	2329	A2M	C3'-C2'	5.76	1.65	1.52
81	A3	2419	PSU	C6-N1	5.76	1.45	1.36
3	h1	470	PSU	C6-N1	5.76	1.45	1.36
81	A3	2317	PSU	C6-N1	5.76	1.45	1.36
81	A3	2926	PSU	C6-N1	5.76	1.45	1.36
81	A3	311	PSU	C6-N1	5.75	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	1064	PSU	C6-N1	5.75	1.45	1.36
3	h1	162	A2M	C3'-C2'	5.75	1.65	1.52
82	B3	46	A2M	C3'-C2'	5.75	1.65	1.52
81	A3	2214	PSU	C6-N1	5.75	1.45	1.36
81	A3	2281	5MC	C4-N4	5.75	1.49	1.34
3	h1	605	PSU	C6-N1	5.75	1.45	1.36
81	A3	1134	PSU	C6-N1	5.75	1.45	1.36
3	h1	1106	PSU	C6-N1	5.75	1.45	1.36
81	A3	2857	PSU	C6-N1	5.75	1.45	1.36
3	h1	753	PSU	C6-N1	5.74	1.45	1.36
81	A3	2291	OMG	C2-N3	5.74	1.47	1.33
82	B3	78	OMG	C2-N3	5.74	1.47	1.33
81	A3	717	PSU	C6-N1	5.74	1.45	1.36
3	h1	339	PSU	C6-N1	5.74	1.45	1.36
81	A3	150	PSU	C6-N1	5.74	1.45	1.36
81	A3	3113	PSU	C6-N1	5.74	1.45	1.36
3	h1	451	PSU	C6-N1	5.73	1.45	1.36
81	A3	464	PSU	C6-N1	5.73	1.45	1.36
81	A3	786	PSU	C6-N1	5.73	1.45	1.36
3	h1	392	OMG	C2-N3	5.73	1.47	1.33
3	h1	1433	OMG	C2-N3	5.73	1.47	1.33
81	A3	1685	PSU	C6-N1	5.73	1.45	1.36
81	A3	2947	PSU	C6-N1	5.72	1.45	1.36
81	A3	1378	A2M	C3'-C2'	5.72	1.65	1.52
3	h1	606	PSU	C6-N1	5.72	1.45	1.36
3	h1	1178	PSU	C6-N1	5.72	1.45	1.36
81	A3	2321	PSU	C6-N1	5.72	1.45	1.36
81	A3	2925	OMG	C2-N3	5.72	1.47	1.33
82	B3	77	PSU	C6-N1	5.72	1.45	1.36
81	A3	1135	PSU	C6-N1	5.72	1.45	1.36
81	A3	815	OMG	C2-N3	5.72	1.47	1.33
81	A3	1482	PSU	C6-N1	5.71	1.45	1.36
81	A3	296	OMG	C2-N3	5.71	1.47	1.33
3	h1	1120	PSU	C6-N1	5.71	1.45	1.36
81	A3	2747	PSU	C6-N1	5.71	1.45	1.36
81	A3	2139	PSU	C6-N1	5.71	1.45	1.36
81	A3	895	PSU	C6-N1	5.71	1.45	1.36
81	A3	2897	PSU	C6-N1	5.70	1.45	1.36
3	h1	103	PSU	C6-N1	5.70	1.45	1.36
81	A3	2829	PSU	C6-N1	5.70	1.45	1.36
81	A3	2435	PSU	C6-N1	5.70	1.45	1.36
3	h1	635	PSU	C6-N1	5.70	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2883	PSU	C6-N1	5.70	1.45	1.36
81	A3	2796	OMG	C2-N3	5.70	1.47	1.33
3	h1	362	PSU	C6-N1	5.69	1.45	1.36
81	A3	966	PSU	C6-N1	5.69	1.45	1.36
81	A3	1461	OMG	C2-N3	5.69	1.47	1.33
82	B3	21	PSU	C6-N1	5.69	1.45	1.36
81	A3	2794	OMG	C2-N3	5.68	1.47	1.33
81	A3	2920	OMG	C2-N3	5.68	1.47	1.33
3	h1	800	A2M	C3'-C2'	5.68	1.65	1.52
3	h1	1210	PSU	C6-N1	5.67	1.45	1.36
81	A3	2873	5MC	C4-N4	5.67	1.48	1.34
81	A3	1857	OMG	C2-N3	5.65	1.46	1.33
81	A3	1474	PSU	C6-N1	5.65	1.45	1.36
81	A3	277	PSU	C6-N1	5.65	1.45	1.36
3	h1	140	OMC	C4-N3	5.65	1.45	1.34
81	A3	2412	OMG	C2-N3	5.64	1.46	1.33
3	h1	38	OMC	C4-N3	5.62	1.45	1.34
3	h1	1194	B8N	C2-N1	5.62	1.55	1.39
81	A3	829	PSU	C6-N1	5.61	1.45	1.36
81	A3	2839	OMC	C4-N3	5.59	1.45	1.34
3	h1	1218	OMC	C4-N3	5.58	1.45	1.34
81	A3	674	OMC	C4-N3	5.57	1.45	1.34
3	h1	473	OMC	C4-N3	5.56	1.45	1.34
81	A3	2126	OMG	C2-N3	5.56	1.46	1.33
3	h1	373	OMU	C6-C5	5.55	1.48	1.35
3	h1	1645	OMC	C4-N3	5.55	1.45	1.34
3	h1	886	OMU	C6-C5	5.54	1.47	1.35
81	A3	2738	OMU	C6-C5	5.54	1.47	1.35
81	A3	675	OMU	C6-C5	5.54	1.47	1.35
81	A3	1894	OMU	C6-C5	5.54	1.47	1.35
81	A3	1480	OMC	C4-N3	5.53	1.45	1.34
3	h1	418	OMC	C4-N3	5.53	1.45	1.34
3	h1	1234	OMU	C6-C5	5.53	1.47	1.35
81	A3	1068	OMU	C6-C5	5.52	1.47	1.35
81	A3	3304	OMU	C6-C5	5.52	1.47	1.35
81	A3	2818	OMG	C2-N3	5.51	1.46	1.33
81	A3	2413	OMU	C6-C5	5.51	1.47	1.35
81	A3	804	OMU	C6-C5	5.51	1.47	1.35
81	A3	2368	OMC	C4-N3	5.51	1.45	1.34
81	A3	2685	OMC	C4-N3	5.51	1.45	1.34
81	A3	787	OMU	C6-C5	5.51	1.47	1.35
81	A3	2350	OMU	C6-C5	5.51	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2127	OMG	C2-N3	5.51	1.46	1.33
3	h1	123	OMU	C6-C5	5.50	1.47	1.35
81	A3	2424	OMU	C6-C5	5.50	1.47	1.35
3	h1	1383	OMU	C6-C5	5.50	1.47	1.35
81	A3	2924	OMU	C6-C5	5.50	1.47	1.35
81	A3	48	OMU	C6-C5	5.50	1.47	1.35
81	A3	2732	OMU	C6-C5	5.49	1.47	1.35
3	h1	1272	OMU	C6-C5	5.49	1.47	1.35
81	A3	44	OMU	C6-C5	5.48	1.47	1.35
81	A3	1862	OMC	C4-N3	5.48	1.45	1.34
81	A3	1537	OMU	C6-C5	5.48	1.47	1.35
81	A3	2296	OMC	C4-N3	5.48	1.45	1.34
3	h1	614	OMU	C6-C5	5.48	1.47	1.35
81	A3	2882	OMC	C4-N3	5.48	1.45	1.34
81	A3	2394	OMG	C2-N3	5.48	1.46	1.33
3	h1	581	OMU	C6-C5	5.47	1.47	1.35
3	h1	1012	OMU	C6-C5	5.47	1.47	1.35
81	A3	2398	OMG	C2-N3	5.47	1.46	1.33
81	A3	2962	OMC	C4-N3	5.47	1.45	1.34
81	A3	2200	OMC	C4-N3	5.47	1.45	1.34
81	A3	1852	OMC	C4-N3	5.47	1.45	1.34
81	A3	2239	OMG	C2-N2	5.46	1.47	1.34
81	A3	1448	OMC	C4-N3	5.45	1.45	1.34
81	A3	40	OMC	C4-N3	5.45	1.45	1.34
81	A3	3289	OMU	C6-C5	5.45	1.47	1.35
81	A3	2340	OMC	C4-N3	5.44	1.45	1.34
81	A3	2720	OMU	C6-C5	5.44	1.47	1.35
81	A3	399	OMG	C2-N2	5.44	1.47	1.34
3	h1	392	OMG	C2-N2	5.43	1.47	1.34
3	h1	1274	OMG	C2-N2	5.43	1.47	1.34
3	h1	1447	OMU	C6-C5	5.43	1.47	1.35
3	h1	1194	B8N	C6-C5	5.43	1.42	1.34
3	h1	246	OMG	C2-N2	5.40	1.47	1.34
81	A3	296	OMG	C2-N2	5.40	1.47	1.34
81	A3	2925	OMG	C2-N2	5.40	1.47	1.34
81	A3	2886	OMU	C6-C5	5.40	1.47	1.35
81	A3	144	OMU	C6-C5	5.40	1.47	1.35
81	A3	2951	OMC	C4-N3	5.40	1.45	1.34
81	A3	2794	OMG	C2-N2	5.39	1.47	1.34
81	A3	1849	OMC	C4-N3	5.39	1.45	1.34
81	A3	2654	OMG	C2-N2	5.39	1.47	1.34
81	A3	2622	OMG	C2-N2	5.38	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	598	OMG	C2-N2	5.38	1.47	1.34
3	h1	1433	OMG	C2-N2	5.38	1.47	1.34
81	A3	2394	OMG	C2-N2	5.38	1.47	1.34
81	A3	918	OMG	C2-N2	5.37	1.47	1.34
82	B3	78	OMG	C2-N2	5.37	1.46	1.34
81	A3	2818	OMG	C2-N2	5.36	1.46	1.34
81	A3	815	OMG	C2-N2	5.36	1.46	1.34
81	A3	2796	OMG	C2-N2	5.36	1.46	1.34
81	A3	2412	OMG	C2-N2	5.35	1.46	1.34
81	A3	2654	OMG	C2-N3	5.34	1.46	1.33
81	A3	2126	OMG	C2-N2	5.33	1.46	1.34
81	A3	1461	OMG	C2-N2	5.33	1.46	1.34
81	A3	2291	OMG	C2-N2	5.33	1.46	1.34
81	A3	2920	OMG	C2-N2	5.32	1.46	1.34
81	A3	1857	OMG	C2-N2	5.31	1.46	1.34
81	A3	2398	OMG	C2-N2	5.31	1.46	1.34
81	A3	2127	OMG	C2-N2	5.28	1.46	1.34
3	h1	1218	OMC	C4-N4	5.25	1.46	1.33
81	A3	2653	UY1	C6-N1	5.24	1.44	1.36
3	h1	246	OMG	C4-N3	5.23	1.50	1.37
3	h1	140	OMC	C4-N4	5.22	1.46	1.33
3	h1	38	OMC	C4-N4	5.22	1.46	1.33
3	h1	418	OMC	C4-N4	5.22	1.46	1.33
81	A3	1448	OMC	C4-N4	5.21	1.46	1.33
81	A3	399	OMG	C4-N3	5.20	1.50	1.37
3	h1	800	A2M	O4'-C4'	5.20	1.56	1.45
81	A3	2296	OMC	C4-N4	5.20	1.46	1.33
81	A3	2962	OMC	C4-N4	5.20	1.46	1.33
3	h1	603	UY1	C6-N1	5.19	1.44	1.36
81	A3	2685	OMC	C4-N4	5.19	1.46	1.33
81	A3	2956	UR3	C2-N3	5.19	1.49	1.39
81	A3	2368	OMC	C4-N4	5.19	1.46	1.33
81	A3	40	OMC	C4-N4	5.18	1.46	1.33
81	A3	2622	OMG	C4-N3	5.17	1.49	1.37
3	h1	1645	OMC	C4-N4	5.16	1.46	1.33
3	h1	392	OMG	C4-N3	5.16	1.49	1.37
82	B3	46	A2M	O4'-C4'	5.16	1.56	1.45
3	h1	1274	OMG	C4-N3	5.16	1.49	1.37
81	A3	1480	OMC	C4-N4	5.16	1.46	1.33
81	A3	1852	OMC	C4-N4	5.16	1.46	1.33
81	A3	674	OMC	C4-N4	5.16	1.46	1.33
81	A3	2239	OMG	C4-N3	5.15	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	473	OMC	C4-N4	5.15	1.46	1.33
81	A3	2951	OMC	C4-N4	5.15	1.46	1.33
3	h1	468	A2M	O4'-C4'	5.15	1.56	1.45
81	A3	2839	OMC	C4-N4	5.15	1.46	1.33
81	A3	1862	OMC	C4-N4	5.14	1.46	1.33
81	A3	2340	OMC	C4-N4	5.14	1.46	1.33
81	A3	918	OMG	C4-N3	5.14	1.49	1.37
81	A3	2324	A2M	O4'-C4'	5.13	1.56	1.45
81	A3	2329	A2M	O4'-C4'	5.13	1.56	1.45
81	A3	1849	OMC	C4-N4	5.13	1.46	1.33
81	A3	296	OMG	C4-N3	5.12	1.49	1.37
81	A3	2882	OMC	C4-N4	5.12	1.46	1.33
3	h1	598	OMG	C4-N3	5.12	1.49	1.37
81	A3	2200	OMC	C4-N4	5.11	1.46	1.33
81	A3	2925	OMG	C4-N3	5.10	1.49	1.37
81	A3	2949	A2M	O4'-C4'	5.10	1.56	1.45
82	B3	78	OMG	C4-N3	5.10	1.49	1.37
81	A3	2291	OMG	C4-N3	5.09	1.49	1.37
81	A3	2129	A2M	O4'-C4'	5.08	1.56	1.45
81	A3	2284	A2M	O4'-C4'	5.07	1.56	1.45
81	A3	2794	OMG	C4-N3	5.07	1.49	1.37
81	A3	1378	A2M	O4'-C4'	5.07	1.56	1.45
3	h1	162	A2M	O4'-C4'	5.07	1.56	1.45
3	h1	977	A2M	O4'-C4'	5.06	1.56	1.45
81	A3	815	OMG	C4-N3	5.05	1.49	1.37
3	h1	440	A2M	O4'-C4'	5.05	1.56	1.45
81	A3	2796	OMG	C4-N3	5.05	1.49	1.37
81	A3	2259	A2M	O4'-C4'	5.04	1.56	1.45
3	h1	1433	OMG	C4-N3	5.04	1.49	1.37
3	h1	424	A2M	O4'-C4'	5.03	1.56	1.45
81	A3	886	A2M	O4'-C4'	5.02	1.56	1.45
81	A3	660	A2M	O4'-C4'	5.02	1.56	1.45
81	A3	2643	A2M	O4'-C4'	5.01	1.56	1.45
81	A3	1144	A2M	O4'-C4'	5.01	1.56	1.45
81	A3	1460	A2M	O4'-C4'	5.01	1.56	1.45
81	A3	2412	OMG	C4-N3	5.00	1.49	1.37
3	h1	1579	A2M	O4'-C4'	5.00	1.56	1.45
81	A3	1461	OMG	C4-N3	4.99	1.49	1.37
3	h1	1758	A2M	O4'-C4'	4.99	1.56	1.45
81	A3	369	A2M	O4'-C4'	4.99	1.56	1.45
81	A3	2920	OMG	C4-N3	4.96	1.49	1.37
81	A3	946	A2M	O4'-C4'	4.96	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2223	A2M	O4'-C4'	4.96	1.56	1.45
81	A3	1857	OMG	C4-N3	4.96	1.49	1.37
81	A3	2126	OMG	C4-N3	4.95	1.49	1.37
3	h1	28	A2M	O4'-C4'	4.95	1.56	1.45
81	A3	2127	OMG	C4-N3	4.95	1.49	1.37
81	A3	827	A2M	O4'-C4'	4.93	1.56	1.45
81	A3	2914	A2M	O4'-C4'	4.92	1.56	1.45
3	h1	1329	A2M	O4'-C4'	4.91	1.56	1.45
81	A3	656	1MA	C2-N1	4.91	1.45	1.35
81	A3	2818	OMG	C4-N3	4.89	1.49	1.37
81	A3	2394	OMG	C4-N3	4.84	1.49	1.37
81	A3	2398	OMG	C4-N3	4.84	1.49	1.37
81	A3	817	A2M	O4'-C4'	4.80	1.55	1.45
81	A3	2654	OMG	C4-N3	4.75	1.48	1.37
3	h1	544	A2M	O4'-C4'	4.75	1.55	1.45
3	h1	622	A2M	O4'-C4'	4.74	1.55	1.45
81	A3	2873	5MC	C2-N1	4.71	1.50	1.40
81	A3	2804	A2M	O4'-C4'	4.69	1.55	1.45
3	h1	1234	OMU	C4-N3	4.68	1.46	1.38
81	A3	44	OMU	C4-N3	4.66	1.46	1.38
3	h1	581	OMU	C4-N3	4.65	1.46	1.38
81	A3	2281	5MC	C2-N1	4.64	1.50	1.40
3	h1	1383	OMU	C4-N3	4.63	1.46	1.38
3	h1	373	OMU	C4-N3	4.63	1.46	1.38
3	h1	886	OMU	C4-N3	4.63	1.46	1.38
81	A3	2924	OMU	C4-N3	4.61	1.46	1.38
81	A3	144	OMU	C4-N3	4.61	1.46	1.38
3	h1	123	OMU	C4-N3	4.61	1.46	1.38
81	A3	2350	OMU	C4-N3	4.60	1.46	1.38
81	A3	2738	OMU	C4-N3	4.60	1.46	1.38
3	h1	1272	OMU	C4-N3	4.60	1.46	1.38
3	h1	1012	OMU	C4-N3	4.60	1.46	1.38
81	A3	804	OMU	C4-N3	4.59	1.46	1.38
81	A3	3304	OMU	C4-N3	4.59	1.46	1.38
81	A3	2424	OMU	O4-C4	-4.58	1.15	1.24
81	A3	2886	OMU	C4-N3	4.58	1.46	1.38
81	A3	1537	OMU	C4-N3	4.57	1.46	1.38
3	h1	1447	OMU	C4-N3	4.56	1.46	1.38
81	A3	787	OMU	O4-C4	-4.55	1.15	1.24
81	A3	1448	OMC	C2-N1	4.55	1.49	1.40
81	A3	2732	OMU	O4-C4	-4.55	1.15	1.24
81	A3	1068	OMU	C4-N3	4.54	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2424	OMU	C4-N3	4.54	1.46	1.38
81	A3	1480	OMC	C2-N1	4.54	1.49	1.40
81	A3	1894	OMU	C4-N3	4.54	1.46	1.38
81	A3	1852	OMC	C2-N1	4.53	1.49	1.40
3	h1	614	OMU	C4-N3	4.52	1.46	1.38
81	A3	675	OMU	C4-N3	4.52	1.46	1.38
81	A3	787	OMU	C4-N3	4.52	1.46	1.38
81	A3	48	OMU	O4-C4	-4.52	1.15	1.24
81	A3	2200	OMC	C2-N1	4.52	1.49	1.40
81	A3	44	OMU	O4-C4	-4.52	1.15	1.24
81	A3	804	OMU	O4-C4	-4.52	1.15	1.24
81	A3	2350	OMU	O4-C4	-4.51	1.15	1.24
81	A3	2886	OMU	O4-C4	-4.51	1.15	1.24
81	A3	3289	OMU	O4-C4	-4.51	1.15	1.24
81	A3	2720	OMU	C4-N3	4.51	1.46	1.38
81	A3	2738	OMU	O4-C4	-4.51	1.15	1.24
81	A3	1894	OMU	O4-C4	-4.50	1.15	1.24
81	A3	2413	OMU	O4-C4	-4.50	1.15	1.24
81	A3	3289	OMU	C4-N3	4.50	1.46	1.38
3	h1	473	OMC	C2-N1	4.50	1.49	1.40
81	A3	144	OMU	O4-C4	-4.50	1.15	1.24
81	A3	1537	OMU	O4-C4	-4.50	1.15	1.24
3	h1	38	OMC	C2-N1	4.50	1.49	1.40
3	h1	140	OMC	C2-N1	4.49	1.49	1.40
81	A3	2296	OMC	C2-N1	4.49	1.49	1.40
3	h1	418	OMC	C2-N1	4.48	1.49	1.40
81	A3	2882	OMC	C2-N1	4.48	1.49	1.40
3	h1	1218	OMC	C2-N1	4.48	1.49	1.40
81	A3	1068	OMU	O4-C4	-4.48	1.15	1.24
81	A3	3304	OMU	O4-C4	-4.47	1.15	1.24
3	h1	607	PSU	C4-N3	4.47	1.47	1.38
3	h1	1194	B8N	C1'-C5	-4.47	1.40	1.50
81	A3	2732	OMU	C4-N3	4.46	1.46	1.38
3	h1	1524	PSU	C4-N3	4.46	1.47	1.38
81	A3	40	OMC	C2-N1	4.46	1.49	1.40
81	A3	2720	OMU	O4-C4	-4.46	1.15	1.24
81	A3	2839	OMC	C2-N1	4.45	1.49	1.40
81	A3	2924	OMU	O4-C4	-4.45	1.15	1.24
3	h1	581	OMU	O4-C4	-4.45	1.15	1.24
81	A3	675	OMU	O4-C4	-4.45	1.15	1.24
3	h1	753	PSU	C4-N3	4.45	1.47	1.38
3	h1	1645	OMC	C2-N1	4.45	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	1272	OMU	O4-C4	-4.45	1.15	1.24
81	A3	48	OMU	C4-N3	4.44	1.46	1.38
81	A3	2413	OMU	C4-N3	4.44	1.46	1.38
3	h1	614	OMU	O4-C4	-4.43	1.15	1.24
3	h1	886	OMU	O4-C4	-4.43	1.15	1.24
3	h1	1217	PSU	C4-N3	4.43	1.47	1.38
81	A3	464	PSU	C4-N3	4.43	1.47	1.38
3	h1	1447	OMU	O4-C4	-4.43	1.15	1.24
3	h1	1535	PSU	C4-N3	4.43	1.47	1.38
3	h1	1567	PSU	C4-N3	4.42	1.47	1.38
3	h1	1012	OMU	O4-C4	-4.42	1.15	1.24
3	h1	123	OMU	O4-C4	-4.42	1.15	1.24
3	h1	1383	OMU	O4-C4	-4.42	1.15	1.24
3	h1	950	PSU	C4-N3	4.42	1.47	1.38
3	h1	373	OMU	O4-C4	-4.42	1.15	1.24
81	A3	2747	PSU	C4-N3	4.42	1.47	1.38
3	h1	339	PSU	C4-N3	4.42	1.47	1.38
81	A3	1002	PSU	C4-N3	4.42	1.47	1.38
3	h1	763	PSU	C4-N3	4.41	1.47	1.38
82	B3	96	PSU	C4-N3	4.41	1.47	1.38
81	A3	2654	OMG	C6-N1	4.41	1.44	1.37
3	h1	1210	PSU	C4-N3	4.41	1.47	1.38
81	A3	2269	PSU	C4-N3	4.41	1.47	1.38
82	B3	77	PSU	C4-N3	4.41	1.47	1.38
3	h1	451	PSU	C4-N3	4.40	1.47	1.38
81	A3	2340	OMC	C2-N1	4.40	1.49	1.40
3	h1	103	PSU	C4-N3	4.40	1.47	1.38
81	A3	2685	OMC	C2-N1	4.40	1.49	1.40
3	h1	809	PSU	C4-N3	4.39	1.47	1.38
3	h1	1485	PSU	C4-N3	4.39	1.47	1.38
3	h1	1787	PSU	C4-N3	4.39	1.47	1.38
3	h1	417	PSU	C4-N3	4.39	1.47	1.38
3	h1	1106	PSU	C4-N3	4.39	1.47	1.38
3	h1	95	PSU	C4-N3	4.39	1.47	1.38
3	h1	1304	PSU	C4-N3	4.39	1.47	1.38
3	h1	258	PSU	C4-N3	4.39	1.47	1.38
3	h1	1190	PSU	C4-N3	4.38	1.47	1.38
3	h1	121	PSU	C4-N3	4.38	1.47	1.38
3	h1	1293	PSU	C4-N3	4.38	1.47	1.38
3	h1	762	PSU	C4-N3	4.38	1.47	1.38
81	A3	2261	PSU	C4-N3	4.38	1.47	1.38
3	h1	1634	PSU	C4-N3	4.38	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	584	PSU	C4-N3	4.37	1.47	1.38
3	h1	606	PSU	C4-N3	4.37	1.47	1.38
3	h1	1178	PSU	C4-N3	4.37	1.47	1.38
3	h1	1120	PSU	C4-N3	4.37	1.46	1.38
81	A3	1482	PSU	C4-N3	4.37	1.46	1.38
81	A3	150	PSU	C4-N3	4.37	1.46	1.38
81	A3	2263	PSU	C4-N3	4.37	1.46	1.38
81	A3	786	PSU	C4-N3	4.37	1.46	1.38
81	A3	1064	PSU	C4-N3	4.37	1.46	1.38
3	h1	961	PSU	C4-N3	4.36	1.46	1.38
81	A3	311	PSU	C4-N3	4.36	1.46	1.38
81	A3	976	PSU	C4-N3	4.36	1.46	1.38
81	A3	2926	PSU	C4-N3	4.36	1.46	1.38
81	A3	2194	PSU	C4-N3	4.36	1.46	1.38
81	A3	1016	PSU	C4-N3	4.36	1.46	1.38
81	A3	2435	PSU	C4-N3	4.36	1.46	1.38
81	A3	2317	PSU	C4-N3	4.36	1.46	1.38
3	h1	1234	OMU	O4-C4	-4.35	1.16	1.24
3	h1	1002	PSU	C4-N3	4.35	1.46	1.38
81	A3	228	PSU	C4-N3	4.35	1.46	1.38
3	h1	1615	PSU	C4-N3	4.35	1.46	1.38
81	A3	829	PSU	C4-N3	4.35	1.46	1.38
81	A3	1474	PSU	C4-N3	4.35	1.46	1.38
3	h1	306	PSU	C4-N3	4.35	1.46	1.38
3	h1	470	PSU	C4-N3	4.34	1.46	1.38
3	h1	1308	PSU	C4-N3	4.34	1.46	1.38
81	A3	1685	PSU	C4-N3	4.34	1.46	1.38
3	h1	1184	PSU	C4-N3	4.34	1.46	1.38
81	A3	2214	PSU	C4-N3	4.34	1.46	1.38
3	h1	635	PSU	C4-N3	4.33	1.46	1.38
81	A3	277	PSU	C4-N3	4.33	1.46	1.38
81	A3	2419	PSU	C4-N3	4.33	1.46	1.38
81	A3	2267	PSU	C4-N3	4.33	1.46	1.38
81	A3	1849	OMC	C2-N1	4.33	1.49	1.40
81	A3	2897	PSU	C4-N3	4.33	1.46	1.38
81	A3	2951	OMC	C2-N1	4.33	1.49	1.40
3	h1	1027	PSU	C4-N3	4.33	1.46	1.38
81	A3	2139	PSU	C4-N3	4.33	1.46	1.38
81	A3	2368	OMC	C2-N1	4.33	1.49	1.40
81	A3	1056	PSU	C4-N3	4.33	1.46	1.38
81	A3	2978	PSU	C4-N3	4.33	1.46	1.38
3	h1	310	PSU	C4-N3	4.32	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	605	PSU	C4-N3	4.32	1.46	1.38
81	A3	902	PSU	C4-N3	4.32	1.46	1.38
81	A3	2857	PSU	C4-N3	4.32	1.46	1.38
81	A3	1133	PSU	C4-N3	4.32	1.46	1.38
81	A3	40	OMC	O2-C2	-4.32	1.15	1.23
81	A3	2394	OMG	C6-N1	4.32	1.44	1.37
81	A3	2958	PSU	C4-N3	4.31	1.46	1.38
81	A3	1862	OMC	C2-N1	4.31	1.49	1.40
81	A3	717	PSU	C4-N3	4.30	1.46	1.38
81	A3	2829	PSU	C4-N3	4.30	1.46	1.38
81	A3	2257	PSU	C4-N3	4.30	1.46	1.38
81	A3	2883	PSU	C4-N3	4.30	1.46	1.38
81	A3	2947	PSU	C4-N3	4.30	1.46	1.38
81	A3	970	PSU	C4-N3	4.30	1.46	1.38
81	A3	2868	PSU	C4-N3	4.29	1.46	1.38
82	B3	21	PSU	C4-N3	4.29	1.46	1.38
81	A3	966	PSU	C4-N3	4.29	1.46	1.38
81	A3	1849	OMC	O2-C2	-4.28	1.15	1.23
81	A3	2962	OMC	C2-N1	4.28	1.49	1.40
81	A3	1135	PSU	C4-N3	4.28	1.46	1.38
81	A3	2951	OMC	O2-C2	-4.27	1.15	1.23
81	A3	2321	PSU	C4-N3	4.26	1.46	1.38
81	A3	2398	OMG	C6-N1	4.26	1.44	1.37
81	A3	2412	OMG	C6-N1	4.26	1.44	1.37
81	A3	1862	OMC	O2-C2	-4.25	1.15	1.23
81	A3	2368	OMC	O2-C2	-4.25	1.15	1.23
3	h1	1645	OMC	O2-C2	-4.25	1.15	1.23
81	A3	674	OMC	O2-C2	-4.25	1.15	1.23
81	A3	510	PSU	C4-N3	4.25	1.46	1.38
81	A3	1448	OMC	O2-C2	-4.24	1.15	1.23
81	A3	2127	OMG	C6-N1	4.24	1.44	1.37
3	h1	1283	4AC	C5-C4	4.24	1.49	1.40
81	A3	2818	OMG	C6-N1	4.23	1.44	1.37
81	A3	2200	OMC	O2-C2	-4.23	1.15	1.23
81	A3	684	PSU	C4-N3	4.23	1.46	1.38
81	A3	2962	OMC	O2-C2	-4.22	1.15	1.23
81	A3	895	PSU	C4-N3	4.22	1.46	1.38
81	A3	1852	OMC	O2-C2	-4.22	1.15	1.23
81	A3	34	PSU	C4-N3	4.22	1.46	1.38
81	A3	2839	OMC	O2-C2	-4.22	1.15	1.23
81	A3	674	OMC	C2-N1	4.22	1.49	1.40
81	A3	2340	OMC	O2-C2	-4.22	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	362	PSU	C4-N3	4.21	1.46	1.38
81	A3	2296	OMC	O2-C2	-4.21	1.15	1.23
3	h1	38	OMC	O2-C2	-4.20	1.15	1.23
81	A3	1480	OMC	O2-C2	-4.20	1.15	1.23
81	A3	42	PSU	C4-N3	4.20	1.46	1.38
81	A3	2882	OMC	O2-C2	-4.20	1.15	1.23
81	A3	3113	PSU	C4-N3	4.20	1.46	1.38
3	h1	392	OMG	C6-N1	4.19	1.44	1.37
81	A3	2126	OMG	C6-N1	4.19	1.44	1.37
3	h1	473	OMC	O2-C2	-4.18	1.16	1.23
3	h1	418	OMC	O2-C2	-4.18	1.16	1.23
3	h1	1781	4AC	C5-C4	4.17	1.49	1.40
81	A3	1134	PSU	C4-N3	4.17	1.46	1.38
3	h1	140	OMC	O2-C2	-4.17	1.16	1.23
3	h1	1218	OMC	O2-C2	-4.16	1.16	1.23
81	A3	2685	OMC	O2-C2	-4.16	1.16	1.23
81	A3	2137	PSU	C4-N3	4.15	1.46	1.38
81	A3	2920	OMG	C6-N1	4.15	1.44	1.37
81	A3	815	OMG	C6-N1	4.15	1.44	1.37
81	A3	296	OMG	C6-N1	4.14	1.44	1.37
3	h1	1781	4AC	C7-N4	4.11	1.44	1.37
82	B3	78	OMG	C6-N1	4.11	1.44	1.37
81	A3	399	OMG	C6-N1	4.10	1.44	1.37
81	A3	2239	OMG	C6-N1	4.08	1.43	1.37
3	h1	1274	OMG	C6-N1	4.08	1.43	1.37
3	h1	246	OMG	C6-N1	4.07	1.43	1.37
3	h1	598	OMG	C6-N1	4.07	1.43	1.37
81	A3	2925	OMG	C6-N1	4.07	1.43	1.37
81	A3	2291	OMG	C6-N1	4.07	1.43	1.37
81	A3	1857	OMG	C6-N1	4.05	1.43	1.37
3	h1	1283	4AC	C7-N4	4.05	1.44	1.37
81	A3	2398	OMG	C5-C6	4.05	1.55	1.47
3	h1	1781	4AC	C2-N1	4.03	1.48	1.40
81	A3	2796	OMG	C6-N1	4.03	1.43	1.37
81	A3	1461	OMG	C6-N1	4.03	1.43	1.37
81	A3	2127	OMG	C5-C6	4.03	1.55	1.47
81	A3	2200	OMC	C6-N1	4.00	1.47	1.38
81	A3	2394	OMG	C5-C6	4.00	1.55	1.47
81	A3	2412	OMG	C5-C6	4.00	1.55	1.47
81	A3	2654	OMG	C5-C6	4.00	1.55	1.47
3	h1	1433	OMG	C6-N1	4.00	1.43	1.37
81	A3	656	1MA	C4-N3	3.98	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2794	OMG	C6-N1	3.95	1.43	1.37
81	A3	2622	OMG	C6-N1	3.95	1.43	1.37
81	A3	1448	OMC	C6-N1	3.94	1.47	1.38
81	A3	815	OMG	C5-C6	3.94	1.55	1.47
81	A3	2818	OMG	C5-C6	3.93	1.55	1.47
81	A3	1461	OMG	C5-C6	3.93	1.55	1.47
81	A3	1480	OMC	C6-N1	3.91	1.47	1.38
81	A3	918	OMG	C6-N1	3.91	1.43	1.37
3	h1	392	OMG	C5-C6	3.90	1.55	1.47
81	A3	1849	OMC	C6-N1	3.90	1.47	1.38
3	h1	1645	OMC	C6-N1	3.90	1.47	1.38
81	A3	2340	OMC	C6-N1	3.89	1.47	1.38
81	A3	296	OMG	C5-C6	3.89	1.55	1.47
3	h1	473	OMC	C6-N1	3.89	1.47	1.38
81	A3	2291	OMG	C5-C6	3.88	1.55	1.47
81	A3	2920	OMG	C5-C6	3.88	1.55	1.47
3	h1	603	UY1	C4-N3	3.87	1.46	1.38
3	h1	598	OMG	C5-C6	3.87	1.55	1.47
81	A3	1852	OMC	C6-N1	3.87	1.47	1.38
81	A3	2239	OMG	C5-C6	3.86	1.55	1.47
3	h1	38	OMC	C6-N1	3.86	1.47	1.38
3	h1	1283	4AC	C2-N1	3.86	1.48	1.40
81	A3	399	OMG	C5-C6	3.85	1.55	1.47
81	A3	2796	OMG	C5-C6	3.85	1.55	1.47
81	A3	2126	OMG	C5-C6	3.85	1.55	1.47
81	A3	2296	OMC	C6-N1	3.85	1.47	1.38
3	h1	1274	OMG	C5-C6	3.84	1.55	1.47
81	A3	2685	OMC	C6-N1	3.84	1.47	1.38
81	A3	1857	OMG	C5-C6	3.84	1.55	1.47
3	h1	418	OMC	C6-N1	3.83	1.47	1.38
81	A3	2653	UY1	C4-N3	3.82	1.45	1.38
81	A3	2368	OMC	C6-N1	3.82	1.47	1.38
3	h1	1218	OMC	C6-N1	3.81	1.47	1.38
81	A3	1862	OMC	C6-N1	3.81	1.47	1.38
3	h1	246	OMG	C5-C6	3.80	1.55	1.47
81	A3	2622	OMG	C5-C6	3.80	1.55	1.47
3	h1	140	OMC	C6-N1	3.79	1.47	1.38
81	A3	674	OMC	C6-N1	3.79	1.47	1.38
81	A3	2882	OMC	C6-N1	3.78	1.47	1.38
81	A3	40	OMC	C6-N1	3.77	1.47	1.38
82	B3	78	OMG	C5-C6	3.77	1.55	1.47
81	A3	48	OMU	C6-N1	3.77	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2951	OMC	C6-N1	3.77	1.47	1.38
81	A3	2925	OMG	C5-C6	3.76	1.55	1.47
81	A3	2839	OMC	C6-N1	3.76	1.47	1.38
81	A3	2886	OMU	C6-N1	3.75	1.47	1.38
81	A3	2794	OMG	C5-C6	3.75	1.55	1.47
3	h1	1272	OMU	C6-N1	3.75	1.47	1.38
3	h1	614	OMU	C6-N1	3.74	1.47	1.38
81	A3	2732	OMU	C6-N1	3.74	1.47	1.38
81	A3	918	OMG	C5-C6	3.73	1.55	1.47
81	A3	2962	OMC	C6-N1	3.73	1.47	1.38
81	A3	144	OMU	C6-N1	3.73	1.47	1.38
81	A3	44	OMU	C6-N1	3.73	1.47	1.38
3	h1	581	OMU	C6-N1	3.72	1.47	1.38
3	h1	1433	OMG	C5-C6	3.72	1.55	1.47
81	A3	2738	OMU	C6-N1	3.72	1.47	1.38
3	h1	886	OMU	C6-N1	3.71	1.47	1.38
3	h1	373	OMU	C6-N1	3.71	1.47	1.38
3	h1	1383	OMU	C6-N1	3.71	1.47	1.38
81	A3	675	OMU	C6-N1	3.70	1.46	1.38
81	A3	1894	OMU	C6-N1	3.70	1.46	1.38
3	h1	1234	OMU	C6-N1	3.70	1.46	1.38
81	A3	804	OMU	C6-N1	3.70	1.46	1.38
81	A3	1537	OMU	C6-N1	3.69	1.46	1.38
81	A3	3304	OMU	C6-N1	3.69	1.46	1.38
81	A3	2924	OMU	C6-N1	3.68	1.46	1.38
81	A3	2424	OMU	C6-N1	3.68	1.46	1.38
81	A3	787	OMU	C6-N1	3.68	1.46	1.38
81	A3	2732	OMU	O2-C2	-3.68	1.16	1.23
3	h1	1781	4AC	C4-N4	3.67	1.45	1.39
3	h1	1447	OMU	C6-N1	3.67	1.46	1.38
81	A3	1068	OMU	C6-N1	3.67	1.46	1.38
3	h1	1012	OMU	C6-N1	3.67	1.46	1.38
81	A3	2350	OMU	C6-N1	3.66	1.46	1.38
81	A3	675	OMU	O2-C2	-3.66	1.16	1.23
81	A3	2413	OMU	C6-N1	3.65	1.46	1.38
81	A3	2720	OMU	C6-N1	3.65	1.46	1.38
3	h1	123	OMU	C6-N1	3.65	1.46	1.38
81	A3	2350	OMU	O2-C2	-3.64	1.16	1.23
81	A3	804	OMU	O2-C2	-3.64	1.16	1.23
81	A3	3289	OMU	C6-N1	3.64	1.46	1.38
81	A3	2720	OMU	O2-C2	-3.63	1.16	1.23
81	A3	2886	OMU	O2-C2	-3.62	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	48	OMU	O2-C2	-3.62	1.16	1.23
81	A3	44	OMU	O2-C2	-3.61	1.16	1.23
81	A3	1068	OMU	O2-C2	-3.61	1.16	1.23
81	A3	2924	OMU	O2-C2	-3.60	1.16	1.23
81	A3	787	OMU	O2-C2	-3.60	1.16	1.23
81	A3	2424	OMU	O2-C2	-3.60	1.16	1.23
81	A3	144	OMU	O2-C2	-3.60	1.16	1.23
81	A3	1894	OMU	O2-C2	-3.59	1.16	1.23
3	h1	1283	4AC	C4-N4	3.59	1.44	1.39
3	h1	581	OMU	O2-C2	-3.58	1.16	1.23
3	h1	1383	OMU	O2-C2	-3.58	1.16	1.23
81	A3	1537	OMU	O2-C2	-3.57	1.16	1.23
3	h1	1234	OMU	O2-C2	-3.57	1.16	1.23
3	h1	1012	OMU	O2-C2	-3.56	1.16	1.23
81	A3	3289	OMU	O2-C2	-3.56	1.16	1.23
81	A3	2738	OMU	O2-C2	-3.55	1.16	1.23
3	h1	614	OMU	O2-C2	-3.55	1.16	1.23
3	h1	1272	OMU	O2-C2	-3.55	1.16	1.23
81	A3	2413	OMU	O2-C2	-3.54	1.16	1.23
81	A3	3304	OMU	O2-C2	-3.54	1.16	1.23
3	h1	1447	OMU	O2-C2	-3.53	1.16	1.23
3	h1	123	OMU	O2-C2	-3.50	1.16	1.23
3	h1	886	OMU	O2-C2	-3.50	1.16	1.23
3	h1	373	OMU	O2-C2	-3.50	1.16	1.23
3	h1	1781	4AC	O2-C2	-3.40	1.17	1.23
3	h1	1283	4AC	O2-C2	-3.40	1.17	1.23
3	h1	1283	4AC	C6-N1	3.32	1.46	1.38
81	A3	786	PSU	O4-C4	-3.32	1.17	1.23
81	A3	829	PSU	O4-C4	-3.31	1.17	1.23
81	A3	684	PSU	O4-C4	-3.29	1.17	1.23
81	A3	2958	PSU	O4-C4	-3.29	1.17	1.23
81	A3	277	PSU	O4-C4	-3.27	1.17	1.23
81	A3	42	PSU	O4-C4	-3.27	1.17	1.23
3	h1	1106	PSU	O4-C4	-3.26	1.17	1.23
81	A3	1135	PSU	O4-C4	-3.26	1.17	1.23
81	A3	976	PSU	O4-C4	-3.25	1.17	1.23
81	A3	2139	PSU	O4-C4	-3.25	1.17	1.23
81	A3	2978	PSU	O4-C4	-3.25	1.17	1.23
3	h1	362	PSU	O4-C4	-3.24	1.17	1.23
81	A3	2947	PSU	O4-C4	-3.24	1.17	1.23
82	B3	96	PSU	O4-C4	-3.24	1.17	1.23
3	h1	306	PSU	O4-C4	-3.24	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2897	PSU	O4-C4	-3.24	1.17	1.23
82	B3	21	PSU	O4-C4	-3.24	1.17	1.23
81	A3	2829	PSU	O4-C4	-3.24	1.17	1.23
81	A3	902	PSU	O4-C4	-3.23	1.17	1.23
81	A3	1482	PSU	O4-C4	-3.23	1.17	1.23
81	A3	2435	PSU	O4-C4	-3.23	1.17	1.23
81	A3	2214	PSU	O4-C4	-3.23	1.17	1.23
81	A3	311	PSU	O4-C4	-3.22	1.17	1.23
3	h1	606	PSU	O4-C4	-3.22	1.17	1.23
81	A3	895	PSU	O4-C4	-3.22	1.17	1.23
81	A3	510	PSU	O4-C4	-3.22	1.17	1.23
3	h1	1304	PSU	O4-C4	-3.22	1.17	1.23
81	A3	1134	PSU	O4-C4	-3.22	1.17	1.23
3	h1	1120	PSU	O4-C4	-3.22	1.17	1.23
81	A3	2194	PSU	O4-C4	-3.22	1.17	1.23
81	A3	1002	PSU	O4-C4	-3.22	1.17	1.23
81	A3	2883	PSU	O4-C4	-3.21	1.17	1.23
3	h1	1781	4AC	C6-N1	3.20	1.45	1.38
81	A3	2263	PSU	O4-C4	-3.20	1.17	1.23
81	A3	1064	PSU	O4-C4	-3.20	1.17	1.23
81	A3	2137	PSU	O4-C4	-3.20	1.17	1.23
81	A3	3113	PSU	O4-C4	-3.20	1.17	1.23
81	A3	2419	PSU	O4-C4	-3.20	1.17	1.23
81	A3	2926	PSU	O4-C4	-3.20	1.17	1.23
81	A3	1474	PSU	O4-C4	-3.20	1.17	1.23
81	A3	966	PSU	O4-C4	-3.20	1.17	1.23
81	A3	1056	PSU	O4-C4	-3.20	1.17	1.23
3	h1	763	PSU	O4-C4	-3.20	1.17	1.23
81	A3	2269	PSU	O4-C4	-3.20	1.17	1.23
82	B3	77	PSU	O4-C4	-3.19	1.17	1.23
3	h1	635	PSU	O4-C4	-3.19	1.17	1.23
81	A3	2857	PSU	O4-C4	-3.19	1.17	1.23
81	A3	2747	PSU	O4-C4	-3.19	1.17	1.23
3	h1	1027	PSU	O4-C4	-3.19	1.17	1.23
3	h1	424	A2M	C6-N6	3.19	1.45	1.34
3	h1	809	PSU	O4-C4	-3.19	1.17	1.23
81	A3	2321	PSU	O4-C4	-3.19	1.17	1.23
81	A3	2868	PSU	O4-C4	-3.19	1.17	1.23
3	h1	1002	PSU	O4-C4	-3.19	1.17	1.23
81	A3	970	PSU	O4-C4	-3.19	1.17	1.23
3	h1	451	PSU	O4-C4	-3.19	1.17	1.23
3	h1	162	A2M	C6-N6	3.19	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	1685	PSU	O4-C4	-3.18	1.17	1.23
3	h1	1293	PSU	O4-C4	-3.18	1.17	1.23
3	h1	1178	PSU	O4-C4	-3.18	1.17	1.23
3	h1	544	A2M	C6-N6	3.18	1.45	1.34
3	h1	103	PSU	O4-C4	-3.18	1.17	1.23
81	A3	1133	PSU	O4-C4	-3.18	1.17	1.23
81	A3	2317	PSU	O4-C4	-3.18	1.17	1.23
3	h1	1190	PSU	O4-C4	-3.17	1.17	1.23
81	A3	34	PSU	O4-C4	-3.17	1.17	1.23
3	h1	95	PSU	O4-C4	-3.17	1.17	1.23
81	A3	2257	PSU	O4-C4	-3.17	1.17	1.23
3	h1	1634	PSU	O4-C4	-3.17	1.17	1.23
3	h1	339	PSU	O4-C4	-3.17	1.17	1.23
3	h1	417	PSU	O4-C4	-3.17	1.17	1.23
3	h1	753	PSU	O4-C4	-3.17	1.17	1.23
3	h1	1787	PSU	O4-C4	-3.17	1.17	1.23
81	A3	717	PSU	O4-C4	-3.17	1.17	1.23
3	h1	1615	PSU	O4-C4	-3.16	1.17	1.23
3	h1	607	PSU	O4-C4	-3.16	1.17	1.23
3	h1	1567	PSU	O4-C4	-3.16	1.17	1.23
3	h1	1329	A2M	C6-N6	3.16	1.45	1.34
3	h1	950	PSU	O4-C4	-3.16	1.17	1.23
3	h1	1579	A2M	C6-N6	3.16	1.45	1.34
81	A3	464	PSU	O4-C4	-3.16	1.17	1.23
81	A3	150	PSU	O4-C4	-3.16	1.17	1.23
3	h1	440	A2M	C6-N6	3.16	1.45	1.34
81	A3	946	A2M	C6-N6	3.16	1.45	1.34
81	A3	2267	PSU	O4-C4	-3.16	1.17	1.23
3	h1	1210	PSU	O4-C4	-3.15	1.17	1.23
81	A3	2643	A2M	C6-N6	3.15	1.45	1.34
81	A3	2129	A2M	C6-N6	3.15	1.45	1.34
3	h1	1184	PSU	O4-C4	-3.15	1.17	1.23
3	h1	1485	PSU	O4-C4	-3.15	1.17	1.23
3	h1	468	A2M	C6-N6	3.15	1.45	1.34
81	A3	2324	A2M	C6-N6	3.15	1.45	1.34
3	h1	28	A2M	C6-N6	3.15	1.45	1.34
81	A3	228	PSU	O4-C4	-3.15	1.17	1.23
81	A3	2261	PSU	O4-C4	-3.15	1.17	1.23
81	A3	2914	A2M	C6-N6	3.15	1.45	1.34
3	h1	800	A2M	C6-N6	3.14	1.45	1.34
3	h1	1524	PSU	O4-C4	-3.14	1.17	1.23
3	h1	1535	PSU	O4-C4	-3.14	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	121	PSU	O4-C4	-3.14	1.17	1.23
3	h1	762	PSU	O4-C4	-3.14	1.17	1.23
3	h1	1217	PSU	O4-C4	-3.14	1.17	1.23
81	A3	1460	A2M	C6-N6	3.14	1.45	1.34
3	h1	1758	A2M	C6-N6	3.14	1.45	1.34
3	h1	622	A2M	C6-N6	3.14	1.45	1.34
81	A3	2223	A2M	C6-N6	3.14	1.45	1.34
81	A3	2949	A2M	C6-N6	3.14	1.45	1.34
81	A3	369	A2M	C6-N6	3.14	1.45	1.34
81	A3	1016	PSU	O4-C4	-3.14	1.17	1.23
81	A3	2654	OMG	C2-N1	3.14	1.45	1.37
3	h1	310	PSU	O4-C4	-3.13	1.17	1.23
3	h1	961	PSU	O4-C4	-3.13	1.17	1.23
81	A3	886	A2M	C6-N6	3.13	1.45	1.34
81	A3	2259	A2M	C6-N6	3.13	1.45	1.34
81	A3	827	A2M	C6-N6	3.13	1.45	1.34
3	h1	1308	PSU	O4-C4	-3.13	1.17	1.23
81	A3	1144	A2M	C6-N6	3.13	1.45	1.34
3	h1	470	PSU	O4-C4	-3.13	1.17	1.23
82	B3	46	A2M	C6-N6	3.13	1.45	1.34
81	A3	1378	A2M	C6-N6	3.13	1.45	1.34
81	A3	2804	A2M	C6-N6	3.13	1.45	1.34
81	A3	2329	A2M	C6-N6	3.12	1.45	1.34
81	A3	2394	OMG	C2-N1	3.12	1.45	1.37
3	h1	258	PSU	O4-C4	-3.12	1.17	1.23
3	h1	977	A2M	C6-N6	3.11	1.45	1.34
81	A3	817	A2M	C6-N6	3.11	1.45	1.34
3	h1	605	PSU	O4-C4	-3.11	1.17	1.23
3	h1	584	PSU	O4-C4	-3.11	1.17	1.23
81	A3	2956	UR3	C6-N1	3.09	1.45	1.38
81	A3	660	A2M	C6-N6	3.07	1.45	1.34
81	A3	2127	OMG	C2-N1	3.06	1.45	1.37
81	A3	2818	OMG	C2-N1	3.05	1.45	1.37
3	h1	392	OMG	C2-N1	3.05	1.45	1.37
81	A3	2398	OMG	C2-N1	3.05	1.45	1.37
81	A3	296	OMG	C2-N1	3.04	1.45	1.37
81	A3	2920	OMG	C2-N1	3.04	1.45	1.37
3	h1	598	OMG	C2-N1	3.04	1.45	1.37
81	A3	399	OMG	C2-N1	3.04	1.45	1.37
81	A3	2622	OMG	C2-N1	3.04	1.45	1.37
81	A3	2412	OMG	C2-N1	3.03	1.45	1.37
3	h1	1433	OMG	C2-N1	3.03	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2126	OMG	C2-N1	3.02	1.45	1.37
3	h1	1274	OMG	C2-N1	3.02	1.45	1.37
81	A3	1857	OMG	C2-N1	3.01	1.45	1.37
81	A3	1461	OMG	C2-N1	3.01	1.45	1.37
3	h1	246	OMG	C2-N1	3.01	1.45	1.37
3	h1	584	PSU	C1'-C5	3.01	1.57	1.50
81	A3	786	PSU	C1'-C5	3.01	1.57	1.50
81	A3	2796	OMG	C2-N1	3.00	1.45	1.37
81	A3	918	OMG	C2-N1	3.00	1.45	1.37
81	A3	815	OMG	C2-N1	3.00	1.45	1.37
81	A3	2291	OMG	C2-N1	3.00	1.45	1.37
82	B3	78	OMG	C2-N1	2.99	1.45	1.37
81	A3	2284	A2M	C6-N6	2.99	1.44	1.34
81	A3	2925	OMG	C2-N1	2.99	1.45	1.37
3	h1	584	PSU	O4'-C1'	-2.98	1.39	1.43
81	A3	2239	OMG	C2-N1	2.97	1.45	1.37
82	B3	96	PSU	C1'-C5	2.95	1.57	1.50
81	A3	311	PSU	C1'-C5	2.95	1.57	1.50
3	h1	1524	PSU	C1'-C5	2.92	1.56	1.50
81	A3	2794	OMG	C2-N1	2.91	1.44	1.37
81	A3	2194	PSU	C1'-C5	2.90	1.56	1.50
81	A3	1480	OMC	C5-C4	2.89	1.49	1.42
81	A3	2269	PSU	C1'-C5	2.88	1.56	1.50
81	A3	2263	PSU	C1'-C5	2.88	1.56	1.50
3	h1	1218	OMC	C5-C4	2.88	1.49	1.42
81	A3	2296	OMC	C5-C4	2.88	1.49	1.42
3	h1	339	PSU	C1'-C5	2.87	1.56	1.50
3	h1	1535	PSU	C1'-C5	2.87	1.56	1.50
3	h1	38	OMC	C5-C4	2.87	1.49	1.42
81	A3	2747	PSU	C1'-C5	2.87	1.56	1.50
3	h1	418	OMC	C5-C4	2.87	1.49	1.42
3	h1	1027	PSU	C1'-C5	2.87	1.56	1.50
3	h1	473	OMC	C5-C4	2.87	1.49	1.42
81	A3	2200	OMC	C5-C4	2.86	1.49	1.42
81	A3	464	PSU	C1'-C5	2.86	1.56	1.50
81	A3	1474	PSU	C1'-C5	2.86	1.56	1.50
81	A3	1849	OMC	C5-C4	2.85	1.49	1.42
81	A3	40	OMC	C5-C4	2.85	1.49	1.42
81	A3	1852	OMC	C5-C4	2.84	1.49	1.42
3	h1	1217	PSU	C1'-C5	2.84	1.56	1.50
3	h1	606	PSU	C1'-C5	2.84	1.56	1.50
81	A3	2261	PSU	C1'-C5	2.84	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2321	PSU	C1'-C5	2.84	1.56	1.50
81	A3	2340	OMC	C5-C4	2.83	1.49	1.42
81	A3	2419	PSU	C1'-C5	2.83	1.56	1.50
3	h1	306	PSU	C1'-C5	2.82	1.56	1.50
81	A3	2368	OMC	C5-C4	2.82	1.49	1.42
3	h1	1645	OMC	C5-C4	2.82	1.49	1.42
3	h1	1120	PSU	C1'-C5	2.82	1.56	1.50
3	h1	950	PSU	C1'-C5	2.82	1.56	1.50
3	h1	121	PSU	C1'-C5	2.82	1.56	1.50
3	h1	605	PSU	C1'-C5	2.81	1.56	1.50
81	A3	966	PSU	C1'-C5	2.81	1.56	1.50
81	A3	2958	PSU	C1'-C5	2.81	1.56	1.50
3	h1	607	PSU	C1'-C5	2.80	1.56	1.50
81	A3	1056	PSU	C1'-C5	2.80	1.56	1.50
3	h1	1790	MA6	C5-C4	-2.80	1.33	1.40
3	h1	310	PSU	C1'-C5	2.80	1.56	1.50
3	h1	753	PSU	C1'-C5	2.80	1.56	1.50
81	A3	2654	OMG	C5-C4	-2.80	1.35	1.43
81	A3	150	PSU	C1'-C5	2.80	1.56	1.50
81	A3	2883	PSU	C1'-C5	2.79	1.56	1.50
81	A3	1002	PSU	C1'-C5	2.79	1.56	1.50
81	A3	902	PSU	C1'-C5	2.79	1.56	1.50
81	A3	2214	PSU	C1'-C5	2.79	1.56	1.50
3	h1	258	PSU	C1'-C5	2.79	1.56	1.50
3	h1	1178	PSU	C1'-C5	2.79	1.56	1.50
3	h1	140	OMC	C5-C4	2.79	1.49	1.42
3	h1	451	PSU	C1'-C5	2.78	1.56	1.50
81	A3	1064	PSU	C1'-C5	2.78	1.56	1.50
3	h1	1308	PSU	C1'-C5	2.78	1.56	1.50
81	A3	2137	PSU	O2-C2	-2.78	1.17	1.23
81	A3	2685	OMC	C5-C4	2.78	1.49	1.42
3	h1	635	PSU	C1'-C5	2.77	1.56	1.50
81	A3	2897	PSU	C1'-C5	2.77	1.56	1.50
81	A3	1862	OMC	C5-C4	2.77	1.49	1.42
82	B3	21	PSU	C1'-C5	2.77	1.56	1.50
3	h1	1634	PSU	C1'-C5	2.77	1.56	1.50
3	h1	763	PSU	C1'-C5	2.77	1.56	1.50
81	A3	970	PSU	C1'-C5	2.77	1.56	1.50
3	h1	1567	PSU	C1'-C5	2.77	1.56	1.50
81	A3	1482	PSU	C1'-C5	2.77	1.56	1.50
81	A3	2868	PSU	C1'-C5	2.77	1.56	1.50
3	h1	809	PSU	C1'-C5	2.77	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	277	PSU	C1'-C5	2.76	1.56	1.50
3	h1	1002	PSU	C1'-C5	2.76	1.56	1.50
81	A3	2139	PSU	C1'-C5	2.76	1.56	1.50
81	A3	2882	OMC	C5-C4	2.76	1.49	1.42
81	A3	1448	OMC	C5-C4	2.76	1.49	1.42
81	A3	684	PSU	C1'-C5	2.76	1.56	1.50
3	h1	1787	PSU	C1'-C5	2.76	1.56	1.50
81	A3	2978	PSU	C1'-C5	2.76	1.56	1.50
3	h1	1293	PSU	C1'-C5	2.76	1.56	1.50
81	A3	2284	A2M	C5-C4	-2.76	1.33	1.40
81	A3	2962	OMC	C5-C4	2.75	1.49	1.42
3	h1	1190	PSU	C1'-C5	2.75	1.56	1.50
81	A3	1133	PSU	C1'-C5	2.75	1.56	1.50
81	A3	2829	PSU	C1'-C5	2.75	1.56	1.50
81	A3	3113	PSU	C1'-C5	2.75	1.56	1.50
3	h1	762	PSU	C1'-C5	2.74	1.56	1.50
3	h1	1106	PSU	C1'-C5	2.74	1.56	1.50
3	h1	1485	PSU	C1'-C5	2.74	1.56	1.50
81	A3	2127	OMG	C5-C4	-2.74	1.36	1.43
3	h1	1304	PSU	C1'-C5	2.74	1.56	1.50
3	h1	1184	PSU	C1'-C5	2.74	1.56	1.50
81	A3	1016	PSU	C1'-C5	2.74	1.56	1.50
81	A3	976	PSU	C1'-C5	2.74	1.56	1.50
81	A3	674	OMC	C5-C4	2.74	1.49	1.42
81	A3	1685	PSU	C1'-C5	2.74	1.56	1.50
81	A3	2139	PSU	O2-C2	-2.74	1.17	1.23
81	A3	829	PSU	O2-C2	-2.73	1.17	1.23
3	h1	1615	PSU	C1'-C5	2.73	1.56	1.50
3	h1	470	PSU	C1'-C5	2.73	1.56	1.50
81	A3	2883	PSU	O2-C2	-2.73	1.17	1.23
81	A3	660	A2M	C5-C4	-2.73	1.33	1.40
81	A3	2949	A2M	C5-C4	-2.73	1.33	1.40
81	A3	2804	A2M	C5-C4	-2.73	1.33	1.40
3	h1	622	A2M	C5-C4	-2.73	1.33	1.40
3	h1	103	PSU	C1'-C5	2.72	1.56	1.50
3	h1	1789	MA6	C5-C4	-2.72	1.33	1.40
81	A3	228	PSU	C1'-C5	2.72	1.56	1.50
81	A3	2926	PSU	C1'-C5	2.72	1.56	1.50
81	A3	2435	PSU	C1'-C5	2.72	1.56	1.50
3	h1	961	PSU	C1'-C5	2.71	1.56	1.50
81	A3	2267	PSU	C1'-C5	2.71	1.56	1.50
81	A3	2324	A2M	C5-C4	-2.71	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2257	PSU	C1'-C5	2.71	1.56	1.50
81	A3	34	PSU	C1'-C5	2.71	1.56	1.50
82	B3	77	PSU	C1'-C5	2.71	1.56	1.50
82	B3	46	A2M	C5-C4	-2.71	1.33	1.40
3	h1	95	PSU	C1'-C5	2.70	1.56	1.50
81	A3	2398	OMG	C5-C4	-2.70	1.36	1.43
81	A3	2839	OMC	C5-C4	2.70	1.49	1.42
81	A3	2978	PSU	O2-C2	-2.70	1.17	1.23
81	A3	1144	A2M	C5-C4	-2.70	1.33	1.40
81	A3	2394	OMG	C5-C4	-2.69	1.36	1.43
81	A3	827	A2M	C5-C4	-2.69	1.33	1.40
81	A3	277	PSU	O2-C2	-2.69	1.17	1.23
3	h1	417	PSU	C1'-C5	2.69	1.56	1.50
81	A3	2321	PSU	O2-C2	-2.69	1.17	1.23
81	A3	966	PSU	O2-C2	-2.69	1.17	1.23
81	A3	2419	PSU	O2-C2	-2.69	1.17	1.23
81	A3	1134	PSU	C1'-C5	2.68	1.56	1.50
81	A3	817	A2M	C5-C4	-2.68	1.33	1.40
81	A3	1134	PSU	O2-C2	-2.67	1.17	1.23
81	A3	2829	PSU	O2-C2	-2.67	1.17	1.23
81	A3	2329	A2M	C5-C4	-2.67	1.33	1.40
81	A3	2643	A2M	C5-C4	-2.67	1.33	1.40
81	A3	34	PSU	O2-C2	-2.67	1.17	1.23
81	A3	1016	PSU	O2-C2	-2.67	1.17	1.23
81	A3	684	PSU	O2-C2	-2.67	1.17	1.23
81	A3	2897	PSU	O2-C2	-2.67	1.17	1.23
81	A3	1460	A2M	C5-C4	-2.67	1.33	1.40
3	h1	103	PSU	O2-C2	-2.67	1.17	1.23
81	A3	886	A2M	C5-C4	-2.67	1.33	1.40
3	h1	1329	A2M	C5-C4	-2.66	1.33	1.40
81	A3	1135	PSU	O2-C2	-2.66	1.17	1.23
81	A3	2947	PSU	O2-C2	-2.66	1.17	1.23
81	A3	2435	PSU	O2-C2	-2.66	1.17	1.23
81	A3	2914	A2M	C5-C4	-2.66	1.33	1.40
81	A3	2129	A2M	C5-C4	-2.66	1.33	1.40
81	A3	510	PSU	O2-C2	-2.66	1.17	1.23
81	A3	2126	OMG	C5-C4	-2.66	1.36	1.43
81	A3	1378	A2M	C5-C4	-2.65	1.33	1.40
81	A3	2958	PSU	O2-C2	-2.65	1.17	1.23
82	B3	96	PSU	O2-C2	-2.65	1.17	1.23
81	A3	2818	OMG	C5-C4	-2.65	1.36	1.43
3	h1	1210	PSU	O2-C2	-2.65	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2263	PSU	O2-C2	-2.65	1.17	1.23
81	A3	2259	A2M	C5-C4	-2.65	1.33	1.40
81	A3	369	A2M	C5-C4	-2.65	1.33	1.40
81	A3	2194	PSU	O2-C2	-2.65	1.17	1.23
81	A3	2857	PSU	O2-C2	-2.65	1.17	1.23
81	A3	1482	PSU	O2-C2	-2.64	1.17	1.23
3	h1	635	PSU	O2-C2	-2.64	1.17	1.23
81	A3	311	PSU	O2-C2	-2.64	1.17	1.23
3	h1	977	A2M	C5-C4	-2.64	1.33	1.40
81	A3	1064	PSU	O2-C2	-2.64	1.17	1.23
81	A3	2947	PSU	C1'-C5	2.64	1.56	1.50
81	A3	2857	PSU	C1'-C5	2.64	1.56	1.50
81	A3	902	PSU	O2-C2	-2.64	1.17	1.23
81	A3	976	PSU	O2-C2	-2.64	1.17	1.23
3	h1	440	A2M	C5-C4	-2.64	1.33	1.40
3	h1	28	A2M	C5-C4	-2.64	1.33	1.40
81	A3	2317	PSU	C1'-C5	2.64	1.56	1.50
81	A3	42	PSU	O2-C2	-2.64	1.17	1.23
81	A3	895	PSU	O2-C2	-2.64	1.17	1.23
3	h1	162	A2M	C5-C4	-2.63	1.34	1.40
3	h1	1579	A2M	C5-C4	-2.63	1.34	1.40
81	A3	829	PSU	C1'-C5	2.63	1.56	1.50
3	h1	1210	PSU	C1'-C5	2.63	1.56	1.50
3	h1	362	PSU	O2-C2	-2.63	1.17	1.23
81	A3	228	PSU	O2-C2	-2.63	1.17	1.23
81	A3	1056	PSU	O2-C2	-2.63	1.17	1.23
81	A3	2868	PSU	O2-C2	-2.63	1.17	1.23
82	B3	21	PSU	O2-C2	-2.63	1.17	1.23
3	h1	763	PSU	O2-C2	-2.63	1.17	1.23
81	A3	1857	OMG	C5-C4	-2.63	1.36	1.43
81	A3	42	PSU	C1'-C5	2.63	1.56	1.50
3	h1	607	PSU	O2-C2	-2.63	1.17	1.23
81	A3	2261	PSU	O2-C2	-2.63	1.17	1.23
81	A3	510	PSU	C1'-C5	2.63	1.56	1.50
3	h1	424	A2M	C5-C4	-2.63	1.34	1.40
81	A3	296	OMG	C5-C4	-2.63	1.36	1.43
3	h1	362	PSU	C1'-C5	2.63	1.56	1.50
81	A3	2920	OMG	C5-C4	-2.62	1.36	1.43
81	A3	1002	PSU	O2-C2	-2.62	1.17	1.23
81	A3	3113	PSU	O2-C2	-2.62	1.17	1.23
3	h1	1634	PSU	O2-C2	-2.62	1.17	1.23
3	h1	800	A2M	C5-C4	-2.62	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	717	PSU	C1'-C5	2.62	1.56	1.50
81	A3	1135	PSU	C1'-C5	2.62	1.56	1.50
3	h1	809	PSU	O2-C2	-2.62	1.17	1.23
3	h1	1787	PSU	O2-C2	-2.62	1.17	1.23
3	h1	468	A2M	C5-C4	-2.62	1.34	1.40
81	A3	2223	A2M	C5-C4	-2.62	1.34	1.40
81	A3	1133	PSU	O2-C2	-2.62	1.17	1.23
3	h1	1758	A2M	C5-C4	-2.62	1.34	1.40
3	h1	1120	PSU	O2-C2	-2.61	1.17	1.23
3	h1	762	PSU	O2-C2	-2.61	1.17	1.23
3	h1	1304	PSU	O2-C2	-2.61	1.17	1.23
3	h1	1106	PSU	O2-C2	-2.61	1.17	1.23
3	h1	1178	PSU	O2-C2	-2.61	1.17	1.23
81	A3	895	PSU	C1'-C5	2.61	1.56	1.50
81	A3	2794	OMG	C5-C4	-2.61	1.36	1.43
3	h1	605	PSU	O2-C2	-2.61	1.17	1.23
81	A3	1474	PSU	O2-C2	-2.61	1.17	1.23
81	A3	2269	PSU	O2-C2	-2.61	1.17	1.23
3	h1	961	PSU	O2-C2	-2.61	1.17	1.23
81	A3	786	PSU	O2-C2	-2.61	1.17	1.23
3	h1	753	PSU	O2-C2	-2.60	1.17	1.23
3	h1	392	OMG	C5-C4	-2.60	1.36	1.43
82	B3	77	PSU	O2-C2	-2.60	1.17	1.23
81	A3	2267	PSU	O2-C2	-2.60	1.17	1.23
81	A3	2951	OMC	C5-C4	2.60	1.48	1.42
3	h1	306	PSU	O2-C2	-2.60	1.17	1.23
81	A3	2317	PSU	O2-C2	-2.60	1.17	1.23
81	A3	2622	OMG	C5-C4	-2.60	1.36	1.43
81	A3	2137	PSU	C1'-C5	2.60	1.56	1.50
81	A3	2747	PSU	O2-C2	-2.60	1.17	1.23
3	h1	470	PSU	O2-C2	-2.60	1.17	1.23
3	h1	1308	PSU	O2-C2	-2.60	1.17	1.23
3	h1	1615	PSU	O2-C2	-2.60	1.17	1.23
81	A3	150	PSU	O2-C2	-2.60	1.17	1.23
81	A3	656	1MA	CM1-N1	2.60	1.52	1.46
81	A3	970	PSU	O2-C2	-2.59	1.18	1.23
81	A3	2926	PSU	O2-C2	-2.59	1.18	1.23
3	h1	1002	PSU	O2-C2	-2.59	1.18	1.23
81	A3	815	OMG	C5-C4	-2.59	1.36	1.43
81	A3	2214	PSU	O2-C2	-2.59	1.18	1.23
81	A3	946	A2M	C5-C4	-2.59	1.34	1.40
3	h1	451	PSU	O2-C2	-2.59	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2257	PSU	O2-C2	-2.59	1.18	1.23
3	h1	950	PSU	O2-C2	-2.59	1.18	1.23
3	h1	1184	PSU	O2-C2	-2.59	1.18	1.23
3	h1	1190	PSU	O2-C2	-2.59	1.18	1.23
81	A3	2925	OMG	C5-C4	-2.58	1.36	1.43
3	h1	310	PSU	O2-C2	-2.58	1.18	1.23
81	A3	2291	OMG	C5-C4	-2.58	1.36	1.43
81	A3	464	PSU	O2-C2	-2.58	1.18	1.23
81	A3	2796	OMG	C5-C4	-2.58	1.36	1.43
3	h1	95	PSU	O2-C2	-2.57	1.18	1.23
3	h1	606	PSU	O2-C2	-2.57	1.18	1.23
81	A3	2239	OMG	C5-C4	-2.57	1.36	1.43
81	A3	2412	OMG	C5-C4	-2.57	1.36	1.43
3	h1	598	OMG	C5-C4	-2.57	1.36	1.43
3	h1	121	PSU	O2-C2	-2.57	1.18	1.23
3	h1	1293	PSU	O2-C2	-2.57	1.18	1.23
3	h1	1535	PSU	O2-C2	-2.57	1.18	1.23
81	A3	1461	OMG	C5-C4	-2.57	1.36	1.43
3	h1	258	PSU	O2-C2	-2.57	1.18	1.23
3	h1	417	PSU	O2-C2	-2.56	1.18	1.23
3	h1	584	PSU	O2-C2	-2.56	1.18	1.23
81	A3	717	PSU	O2-C2	-2.56	1.18	1.23
82	B3	78	OMG	C5-C4	-2.56	1.36	1.43
3	h1	1485	PSU	O2-C2	-2.56	1.18	1.23
81	A3	1685	PSU	O2-C2	-2.56	1.18	1.23
3	h1	1217	PSU	O2-C2	-2.55	1.18	1.23
81	A3	2653	UY1	O4-C4	-2.55	1.18	1.23
81	A3	2818	OMG	O6-C6	-2.55	1.18	1.23
3	h1	1567	PSU	O2-C2	-2.55	1.18	1.23
3	h1	1274	OMG	C5-C4	-2.55	1.36	1.43
3	h1	1433	OMG	C5-C4	-2.55	1.36	1.43
3	h1	544	A2M	C5-C4	-2.54	1.34	1.40
3	h1	1524	PSU	O2-C2	-2.54	1.18	1.23
3	h1	339	PSU	O2-C2	-2.54	1.18	1.23
3	h1	1027	PSU	O2-C2	-2.54	1.18	1.23
81	A3	2291	OMG	O6-C6	-2.54	1.18	1.23
81	A3	815	OMG	O6-C6	-2.53	1.18	1.23
3	h1	603	UY1	O4-C4	-2.52	1.18	1.23
81	A3	1857	OMG	O6-C6	-2.52	1.18	1.23
3	h1	246	OMG	C5-C4	-2.52	1.36	1.43
81	A3	399	OMG	C5-C4	-2.51	1.36	1.43
81	A3	918	OMG	C5-C4	-2.50	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2412	OMG	O6-C6	-2.50	1.18	1.23
81	A3	2794	OMG	O6-C6	-2.49	1.18	1.23
81	A3	2398	OMG	O6-C6	-2.49	1.18	1.23
81	A3	2126	OMG	O6-C6	-2.48	1.18	1.23
81	A3	2920	OMG	O6-C6	-2.48	1.18	1.23
81	A3	1461	OMG	O6-C6	-2.47	1.18	1.23
81	A3	2239	OMG	O6-C6	-2.47	1.18	1.23
3	h1	392	OMG	O6-C6	-2.46	1.18	1.23
81	A3	2127	OMG	O6-C6	-2.46	1.18	1.23
81	A3	2796	OMG	O6-C6	-2.45	1.18	1.23
81	A3	2622	OMG	O6-C6	-2.45	1.18	1.23
81	A3	2925	OMG	O6-C6	-2.44	1.18	1.23
81	A3	2873	5MC	O2-C2	-2.44	1.19	1.23
81	A3	918	OMG	O6-C6	-2.43	1.18	1.23
3	h1	1433	OMG	O6-C6	-2.43	1.18	1.23
82	B3	78	OMG	O6-C6	-2.43	1.18	1.23
81	A3	2654	OMG	O6-C6	-2.42	1.18	1.23
3	h1	1274	OMG	O6-C6	-2.42	1.18	1.23
3	h1	246	OMG	O6-C6	-2.42	1.18	1.23
81	A3	1894	OMU	C5-C4	2.42	1.49	1.43
81	A3	296	OMG	O6-C6	-2.41	1.18	1.23
81	A3	787	OMU	C5-C4	2.41	1.49	1.43
3	h1	373	OMU	C5-C4	2.41	1.49	1.43
81	A3	2394	OMG	O6-C6	-2.41	1.18	1.23
3	h1	598	OMG	O6-C6	-2.41	1.18	1.23
81	A3	656	1MA	C5-C4	-2.41	1.36	1.43
81	A3	2424	OMU	C5-C4	2.40	1.49	1.43
3	h1	1383	OMU	C5-C4	2.40	1.48	1.43
81	A3	399	OMG	O6-C6	-2.39	1.18	1.23
81	A3	1068	OMU	C5-C4	2.38	1.48	1.43
81	A3	2732	OMU	C5-C4	2.38	1.48	1.43
81	A3	44	OMU	C5-C4	2.38	1.48	1.43
3	h1	1234	OMU	C5-C4	2.38	1.48	1.43
81	A3	2281	5MC	O2-C2	-2.37	1.19	1.23
3	h1	1012	OMU	C5-C4	2.36	1.48	1.43
81	A3	48	OMU	C5-C4	2.34	1.48	1.43
81	A3	2924	OMU	C5-C4	2.34	1.48	1.43
3	h1	886	OMU	C5-C4	2.34	1.48	1.43
81	A3	1537	OMU	C5-C4	2.34	1.48	1.43
3	h1	1272	OMU	C5-C4	2.33	1.48	1.43
3	h1	123	OMU	C5-C4	2.33	1.48	1.43
81	A3	2413	OMU	C5-C4	2.33	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2738	OMU	C5-C4	2.33	1.48	1.43
81	A3	675	OMU	C5-C4	2.32	1.48	1.43
81	A3	2350	OMU	C5-C4	2.32	1.48	1.43
3	h1	581	OMU	C5-C4	2.32	1.48	1.43
81	A3	804	OMU	C5-C4	2.32	1.48	1.43
81	A3	3304	OMU	C5-C4	2.31	1.48	1.43
81	A3	2947	PSU	O4'-C1'	-2.31	1.40	1.43
81	A3	946	A2M	O5'-C5'	-2.30	1.39	1.44
3	h1	614	OMU	C5-C4	2.30	1.48	1.43
3	h1	1771	6MZ	C5-C4	-2.28	1.34	1.40
81	A3	2956	UR3	C5-C4	2.28	1.49	1.43
81	A3	144	OMU	C5-C4	2.28	1.48	1.43
81	A3	2720	OMU	C5-C4	2.26	1.48	1.43
3	h1	1329	A2M	C2-N3	2.26	1.35	1.32
3	h1	440	A2M	C2-N3	2.25	1.35	1.32
3	h1	1447	OMU	C5-C4	2.25	1.48	1.43
3	h1	1283	4AC	CM7-C7	2.24	1.55	1.50
81	A3	3289	OMU	C5-C4	2.23	1.48	1.43
3	h1	1758	A2M	C2-N3	2.23	1.35	1.32
81	A3	2949	A2M	C2-N3	2.23	1.35	1.32
81	A3	2956	UR3	C4-N3	2.23	1.45	1.40
81	A3	2643	A2M	C2-N3	2.22	1.35	1.32
81	A3	2653	UY1	O2-C2	-2.22	1.18	1.23
81	A3	660	A2M	C2-N3	2.21	1.35	1.32
81	A3	369	A2M	C2-N3	2.21	1.35	1.32
3	h1	1781	4AC	CM7-C7	2.21	1.55	1.50
3	h1	603	UY1	O2-C2	-2.20	1.18	1.23
81	A3	2223	A2M	C2-N3	2.20	1.35	1.32
3	h1	468	A2M	C2-N3	2.19	1.35	1.32
3	h1	544	A2M	C2-N3	2.19	1.35	1.32
81	A3	1378	A2M	C2-N3	2.19	1.35	1.32
81	A3	2886	OMU	C5-C4	2.19	1.48	1.43
3	h1	1579	A2M	C2-N3	2.19	1.35	1.32
3	h1	800	A2M	C2-N3	2.19	1.35	1.32
81	A3	946	A2M	C2-N3	2.18	1.35	1.32
81	A3	1460	A2M	C2-N3	2.18	1.35	1.32
3	h1	162	A2M	C2-N3	2.18	1.35	1.32
81	A3	827	A2M	C2-N3	2.18	1.35	1.32
81	A3	2259	A2M	C2-N3	2.17	1.35	1.32
81	A3	2329	A2M	C2-N3	2.16	1.35	1.32
3	h1	1194	B8N	O4-C4	-2.16	1.18	1.23
81	A3	2956	UR3	O4-C4	-2.15	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	2914	A2M	C2-N3	2.14	1.35	1.32
81	A3	2284	A2M	C2-N3	2.14	1.35	1.32
3	h1	977	A2M	C2-N3	2.14	1.35	1.32
3	h1	424	A2M	C2-N3	2.12	1.35	1.32
82	B3	46	A2M	C2-N3	2.12	1.35	1.32
81	A3	817	A2M	C2-N3	2.12	1.35	1.32
3	h1	1027	PSU	O4'-C1'	-2.11	1.40	1.43
3	h1	28	A2M	C2-N3	2.11	1.35	1.32
3	h1	1283	4AC	O7-C7	-2.11	1.18	1.23
3	h1	1781	4AC	O7-C7	-2.10	1.18	1.23
81	A3	2129	A2M	C2-N3	2.10	1.35	1.32
3	h1	622	A2M	C2-N3	2.09	1.35	1.32
81	A3	2324	A2M	C2-N3	2.09	1.35	1.32
3	h1	1194	B8N	O2-C2	-2.08	1.18	1.22
3	h1	1771	6MZ	C2-N3	2.07	1.35	1.32
81	A3	2956	UR3	O2-C2	-2.05	1.18	1.22
3	h1	1771	6MZ	C2-N1	2.04	1.37	1.33
3	h1	1758	A2M	O5'-C5'	-2.04	1.39	1.44
81	A3	886	A2M	C2-N3	2.03	1.35	1.32
81	A3	1144	A2M	C2-N3	2.02	1.35	1.32
81	A3	970	PSU	O4'-C1'	-2.02	1.41	1.43

All (914) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2284	A2M	C5-C6-N6	10.86	136.85	120.35
81	A3	2804	A2M	C5-C6-N6	10.80	136.77	120.35
81	A3	946	A2M	C5-C6-N6	10.79	136.75	120.35
81	A3	2259	A2M	C5-C6-N6	10.71	136.63	120.35
81	A3	827	A2M	C5-C6-N6	10.70	136.61	120.35
3	h1	424	A2M	C5-C6-N6	10.70	136.61	120.35
81	A3	1144	A2M	C5-C6-N6	10.68	136.58	120.35
3	h1	162	A2M	C5-C6-N6	10.67	136.56	120.35
81	A3	2914	A2M	C5-C6-N6	10.66	136.55	120.35
81	A3	2129	A2M	C5-C6-N6	10.65	136.53	120.35
3	h1	1579	A2M	C5-C6-N6	10.64	136.53	120.35
81	A3	660	A2M	C5-C6-N6	10.63	136.51	120.35
81	A3	886	A2M	C5-C6-N6	10.63	136.50	120.35
3	h1	468	A2M	C5-C6-N6	10.61	136.48	120.35
81	A3	817	A2M	C5-C6-N6	10.61	136.47	120.35
82	B3	46	A2M	C5-C6-N6	10.61	136.47	120.35
3	h1	622	A2M	C5-C6-N6	10.60	136.47	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	1460	A2M	C5-C6-N6	10.60	136.46	120.35
81	A3	2329	A2M	C5-C6-N6	10.59	136.45	120.35
3	h1	1329	A2M	C5-C6-N6	10.59	136.44	120.35
3	h1	800	A2M	C5-C6-N6	10.59	136.44	120.35
3	h1	440	A2M	C5-C6-N6	10.58	136.43	120.35
3	h1	28	A2M	C5-C6-N6	10.57	136.41	120.35
3	h1	544	A2M	C5-C6-N6	10.53	136.36	120.35
81	A3	2324	A2M	C5-C6-N6	10.53	136.36	120.35
81	A3	369	A2M	C5-C6-N6	10.49	136.30	120.35
3	h1	977	A2M	C5-C6-N6	10.48	136.28	120.35
81	A3	1378	A2M	C5-C6-N6	10.47	136.27	120.35
81	A3	2643	A2M	C5-C6-N6	10.42	136.19	120.35
3	h1	1758	A2M	C5-C6-N6	10.42	136.18	120.35
81	A3	2223	A2M	C5-C6-N6	10.39	136.14	120.35
81	A3	2949	A2M	C5-C6-N6	10.38	136.12	120.35
3	h1	1790	MA6	N1-C6-N6	-8.96	107.62	117.06
81	A3	2804	A2M	C1'-N9-C4	-8.93	110.95	126.64
3	h1	1789	MA6	N1-C6-N6	-8.71	107.89	117.06
3	h1	622	A2M	C1'-N9-C4	-8.66	111.43	126.64
81	A3	2284	A2M	C1'-N9-C4	-8.32	112.03	126.64
81	A3	1144	A2M	C1'-N9-C4	-8.30	112.07	126.64
81	A3	2914	A2M	C1'-N9-C4	-8.17	112.28	126.64
81	A3	660	A2M	C1'-N9-C4	-8.09	112.42	126.64
81	A3	827	A2M	C1'-N9-C4	-8.03	112.52	126.64
81	A3	2259	A2M	C1'-N9-C4	-8.03	112.54	126.64
81	A3	2324	A2M	C1'-N9-C4	-7.99	112.60	126.64
3	h1	424	A2M	C1'-N9-C4	-7.90	112.76	126.64
3	h1	468	A2M	C1'-N9-C4	-7.90	112.77	126.64
3	h1	440	A2M	C1'-N9-C4	-7.89	112.78	126.64
81	A3	369	A2M	C1'-N9-C4	-7.89	112.78	126.64
3	h1	1579	A2M	C1'-N9-C4	-7.87	112.81	126.64
3	h1	28	A2M	C1'-N9-C4	-7.87	112.81	126.64
81	A3	2129	A2M	C1'-N9-C4	-7.86	112.84	126.64
3	h1	1329	A2M	C1'-N9-C4	-7.82	112.90	126.64
3	h1	162	A2M	C1'-N9-C4	-7.81	112.93	126.64
81	A3	2949	A2M	C1'-N9-C4	-7.81	112.93	126.64
81	A3	2329	A2M	C1'-N9-C4	-7.73	113.06	126.64
81	A3	946	A2M	C1'-N9-C4	-7.72	113.07	126.64
82	B3	46	A2M	C1'-N9-C4	-7.70	113.12	126.64
81	A3	2284	A2M	N6-C6-N1	-7.61	102.77	118.57
81	A3	2223	A2M	C1'-N9-C4	-7.59	113.31	126.64
81	A3	1460	A2M	C1'-N9-C4	-7.52	113.42	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2643	A2M	C1'-N9-C4	-7.42	113.60	126.64
81	A3	946	A2M	N6-C6-N1	-7.41	103.20	118.57
81	A3	2804	A2M	N6-C6-N1	-7.35	103.32	118.57
3	h1	424	A2M	N6-C6-N1	-7.33	103.36	118.57
81	A3	2259	A2M	N6-C6-N1	-7.33	103.36	118.57
81	A3	817	A2M	N6-C6-N1	-7.32	103.38	118.57
81	A3	660	A2M	N6-C6-N1	-7.32	103.39	118.57
3	h1	162	A2M	N6-C6-N1	-7.31	103.39	118.57
3	h1	1579	A2M	N6-C6-N1	-7.30	103.43	118.57
3	h1	977	A2M	C1'-N9-C4	-7.29	113.83	126.64
81	A3	827	A2M	N6-C6-N1	-7.27	103.49	118.57
81	A3	2914	A2M	N6-C6-N1	-7.26	103.51	118.57
3	h1	800	A2M	N6-C6-N1	-7.25	103.52	118.57
3	h1	440	A2M	N6-C6-N1	-7.24	103.55	118.57
3	h1	1329	A2M	N6-C6-N1	-7.24	103.55	118.57
81	A3	2329	A2M	N6-C6-N1	-7.24	103.55	118.57
3	h1	622	A2M	N6-C6-N1	-7.24	103.55	118.57
3	h1	544	A2M	N6-C6-N1	-7.24	103.55	118.57
3	h1	468	A2M	N6-C6-N1	-7.22	103.59	118.57
82	B3	46	A2M	N6-C6-N1	-7.21	103.61	118.57
81	A3	2129	A2M	N6-C6-N1	-7.21	103.61	118.57
81	A3	886	A2M	C1'-N9-C4	-7.19	114.00	126.64
81	A3	1460	A2M	N6-C6-N1	-7.19	103.64	118.57
3	h1	800	A2M	C1'-N9-C4	-7.18	114.03	126.64
3	h1	1758	A2M	C1'-N9-C4	-7.17	114.05	126.64
3	h1	28	A2M	N6-C6-N1	-7.14	103.75	118.57
81	A3	886	A2M	N6-C6-N1	-7.14	103.76	118.57
81	A3	2324	A2M	N6-C6-N1	-7.14	103.76	118.57
81	A3	2949	A2M	N6-C6-N1	-7.13	103.77	118.57
81	A3	1378	A2M	N6-C6-N1	-7.13	103.77	118.57
81	A3	369	A2M	N6-C6-N1	-7.13	103.77	118.57
3	h1	977	A2M	N6-C6-N1	-7.10	103.83	118.57
3	h1	1758	A2M	N6-C6-N1	-7.10	103.83	118.57
81	A3	1144	A2M	N6-C6-N1	-7.09	103.86	118.57
81	A3	2643	A2M	N6-C6-N1	-7.07	103.89	118.57
81	A3	2223	A2M	N6-C6-N1	-7.04	103.97	118.57
81	A3	817	A2M	C1'-N9-C4	-6.99	114.36	126.64
81	A3	1378	A2M	C1'-N9-C4	-6.97	114.40	126.64
3	h1	544	A2M	C1'-N9-C4	-6.07	115.97	126.64
81	A3	2804	A2M	N3-C2-N1	-5.65	119.85	128.68
81	A3	1144	A2M	N3-C2-N1	-5.62	119.89	128.68
3	h1	1790	MA6	N3-C2-N1	-5.61	119.91	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B3	46	A2M	N3-C2-N1	-5.60	119.93	128.68
3	h1	622	A2M	N3-C2-N1	-5.59	119.94	128.68
81	A3	660	A2M	N3-C2-N1	-5.56	119.98	128.68
81	A3	886	A2M	N3-C2-N1	-5.56	119.99	128.68
81	A3	2259	A2M	N3-C2-N1	-5.54	120.01	128.68
81	A3	2329	A2M	N3-C2-N1	-5.54	120.01	128.68
3	h1	468	A2M	N3-C2-N1	-5.52	120.04	128.68
3	h1	1789	MA6	N3-C2-N1	-5.52	120.05	128.68
3	h1	424	A2M	N3-C2-N1	-5.50	120.07	128.68
3	h1	1771	6MZ	N3-C2-N1	-5.50	120.08	128.68
81	A3	827	A2M	N3-C2-N1	-5.50	120.09	128.68
3	h1	800	A2M	N3-C2-N1	-5.49	120.09	128.68
3	h1	28	A2M	N3-C2-N1	-5.48	120.12	128.68
81	A3	946	A2M	N3-C2-N1	-5.48	120.12	128.68
3	h1	1579	A2M	N3-C2-N1	-5.47	120.12	128.68
3	h1	162	A2M	N3-C2-N1	-5.47	120.13	128.68
81	A3	2284	A2M	N3-C2-N1	-5.47	120.14	128.68
3	h1	1329	A2M	N3-C2-N1	-5.46	120.14	128.68
81	A3	2914	A2M	N3-C2-N1	-5.45	120.16	128.68
81	A3	2129	A2M	N3-C2-N1	-5.45	120.16	128.68
81	A3	2949	A2M	N3-C2-N1	-5.45	120.16	128.68
3	h1	1758	A2M	N3-C2-N1	-5.44	120.18	128.68
3	h1	440	A2M	N3-C2-N1	-5.43	120.19	128.68
3	h1	544	A2M	N3-C2-N1	-5.43	120.19	128.68
81	A3	2223	A2M	N3-C2-N1	-5.42	120.21	128.68
81	A3	369	A2M	N3-C2-N1	-5.40	120.23	128.68
3	h1	977	A2M	N3-C2-N1	-5.40	120.24	128.68
81	A3	817	A2M	N3-C2-N1	-5.38	120.27	128.68
81	A3	1460	A2M	N3-C2-N1	-5.36	120.30	128.68
81	A3	2643	A2M	N3-C2-N1	-5.33	120.34	128.68
81	A3	2324	A2M	N3-C2-N1	-5.31	120.38	128.68
81	A3	1378	A2M	N3-C2-N1	-5.29	120.41	128.68
81	A3	1894	OMU	C4-N3-C2	-5.26	119.64	126.58
81	A3	1068	OMU	C4-N3-C2	-5.19	119.73	126.58
81	A3	2924	OMU	C4-N3-C2	-5.17	119.75	126.58
81	A3	2350	OMU	C4-N3-C2	-5.16	119.77	126.58
3	h1	1771	6MZ	C1'-N9-C4	-5.15	117.60	126.64
81	A3	2424	OMU	C4-N3-C2	-5.14	119.80	126.58
3	h1	1234	OMU	C4-N3-C2	-5.13	119.82	126.58
3	h1	581	OMU	C4-N3-C2	-5.11	119.83	126.58
3	h1	1383	OMU	C4-N3-C2	-5.11	119.83	126.58
3	h1	1012	OMU	C4-N3-C2	-5.11	119.84	126.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	886	OMU	C4-N3-C2	-5.10	119.85	126.58
3	h1	373	OMU	C4-N3-C2	-5.10	119.86	126.58
81	A3	2738	OMU	C4-N3-C2	-5.09	119.86	126.58
81	A3	656	1MA	N1-C2-N3	-5.08	120.09	126.02
81	A3	144	OMU	C4-N3-C2	-5.08	119.88	126.58
81	A3	804	OMU	C4-N3-C2	-5.07	119.89	126.58
3	h1	1194	B8N	C5-C4-N3	5.06	125.54	116.17
3	h1	1272	OMU	C4-N3-C2	-5.06	119.91	126.58
3	h1	123	OMU	C4-N3-C2	-5.05	119.92	126.58
81	A3	675	OMU	C4-N3-C2	-5.04	119.93	126.58
81	A3	3304	OMU	C4-N3-C2	-5.01	119.97	126.58
81	A3	48	OMU	C4-N3-C2	-5.01	119.97	126.58
81	A3	1537	OMU	C4-N3-C2	-5.00	119.98	126.58
81	A3	787	OMU	C4-N3-C2	-5.00	119.99	126.58
81	A3	44	OMU	C4-N3-C2	-4.97	120.02	126.58
81	A3	2720	OMU	C4-N3-C2	-4.97	120.02	126.58
3	h1	614	OMU	C4-N3-C2	-4.93	120.08	126.58
81	A3	2732	OMU	C4-N3-C2	-4.91	120.10	126.58
81	A3	2413	OMU	C4-N3-C2	-4.91	120.11	126.58
81	A3	3289	OMU	C4-N3-C2	-4.85	120.19	126.58
81	A3	2956	UR3	C4-N3-C2	-4.82	120.02	124.56
3	h1	1447	OMU	C4-N3-C2	-4.82	120.23	126.58
81	A3	2886	OMU	C4-N3-C2	-4.78	120.27	126.58
81	A3	2137	PSU	C4-N3-C2	-4.76	119.47	126.34
81	A3	970	PSU	C4-N3-C2	-4.68	119.60	126.34
81	A3	2926	PSU	C4-N3-C2	-4.67	119.61	126.34
81	A3	2958	PSU	C4-N3-C2	-4.67	119.61	126.34
81	A3	1135	PSU	C4-N3-C2	-4.66	119.62	126.34
81	A3	2257	PSU	C4-N3-C2	-4.64	119.65	126.34
81	A3	1056	PSU	C4-N3-C2	-4.64	119.65	126.34
81	A3	2857	PSU	C4-N3-C2	-4.64	119.66	126.34
81	A3	1064	PSU	C4-N3-C2	-4.64	119.66	126.34
81	A3	2653	UY1	C4-N3-C2	-4.62	119.68	126.34
81	A3	2214	PSU	C4-N3-C2	-4.62	119.69	126.34
3	h1	103	PSU	C4-N3-C2	-4.62	119.69	126.34
81	A3	34	PSU	C4-N3-C2	-4.61	119.69	126.34
81	A3	2868	PSU	C4-N3-C2	-4.61	119.69	126.34
81	A3	717	PSU	C4-N3-C2	-4.61	119.69	126.34
81	A3	1685	PSU	C4-N3-C2	-4.61	119.69	126.34
82	B3	77	PSU	C4-N3-C2	-4.61	119.70	126.34
81	A3	2321	PSU	C4-N3-C2	-4.61	119.70	126.34
3	h1	1210	PSU	C4-N3-C2	-4.61	119.70	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	961	PSU	C4-N3-C2	-4.60	119.72	126.34
3	h1	1217	PSU	C4-N3-C2	-4.60	119.72	126.34
3	h1	95	PSU	C4-N3-C2	-4.59	119.72	126.34
3	h1	1567	PSU	C4-N3-C2	-4.59	119.72	126.34
81	A3	2829	PSU	C4-N3-C2	-4.59	119.72	126.34
81	A3	42	PSU	C4-N3-C2	-4.59	119.73	126.34
3	h1	1184	PSU	C4-N3-C2	-4.59	119.73	126.34
3	h1	1787	PSU	C4-N3-C2	-4.59	119.73	126.34
3	h1	1535	PSU	C4-N3-C2	-4.58	119.74	126.34
81	A3	976	PSU	C4-N3-C2	-4.58	119.74	126.34
81	A3	1016	PSU	C4-N3-C2	-4.58	119.74	126.34
81	A3	2317	PSU	C4-N3-C2	-4.58	119.74	126.34
81	A3	1002	PSU	C4-N3-C2	-4.58	119.74	126.34
3	h1	1293	PSU	C4-N3-C2	-4.58	119.75	126.34
81	A3	2435	PSU	C4-N3-C2	-4.58	119.75	126.34
3	h1	584	PSU	C4-N3-C2	-4.58	119.75	126.34
3	h1	1304	PSU	C4-N3-C2	-4.57	119.75	126.34
81	A3	2261	PSU	C4-N3-C2	-4.57	119.75	126.34
3	h1	763	PSU	C4-N3-C2	-4.57	119.76	126.34
81	A3	228	PSU	C4-N3-C2	-4.57	119.76	126.34
81	A3	1134	PSU	C4-N3-C2	-4.57	119.76	126.34
81	A3	150	PSU	C4-N3-C2	-4.56	119.76	126.34
3	h1	1190	PSU	C4-N3-C2	-4.56	119.77	126.34
81	A3	1133	PSU	C4-N3-C2	-4.56	119.77	126.34
81	A3	829	PSU	C4-N3-C2	-4.56	119.77	126.34
3	h1	603	UY1	C4-N3-C2	-4.55	119.78	126.34
3	h1	1178	PSU	C4-N3-C2	-4.55	119.78	126.34
3	h1	762	PSU	C4-N3-C2	-4.55	119.78	126.34
81	A3	2263	PSU	C4-N3-C2	-4.55	119.79	126.34
3	h1	258	PSU	C4-N3-C2	-4.54	119.80	126.34
3	h1	1106	PSU	C4-N3-C2	-4.54	119.80	126.34
3	h1	1308	PSU	C4-N3-C2	-4.53	119.81	126.34
81	A3	2883	PSU	C4-N3-C2	-4.53	119.81	126.34
3	h1	1524	PSU	C4-N3-C2	-4.53	119.81	126.34
3	h1	1789	MA6	C1'-N9-C4	4.53	134.60	126.64
3	h1	1485	PSU	C4-N3-C2	-4.53	119.81	126.34
81	A3	2267	PSU	C4-N3-C2	-4.53	119.81	126.34
3	h1	753	PSU	C4-N3-C2	-4.53	119.82	126.34
3	h1	809	PSU	C4-N3-C2	-4.52	119.82	126.34
81	A3	464	PSU	C4-N3-C2	-4.52	119.82	126.34
81	A3	786	PSU	C4-N3-C2	-4.52	119.83	126.34
82	B3	21	PSU	C4-N3-C2	-4.52	119.83	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2897	PSU	C4-N3-C2	-4.52	119.83	126.34
3	h1	605	PSU	C4-N3-C2	-4.52	119.83	126.34
3	h1	1002	PSU	C4-N3-C2	-4.52	119.83	126.34
81	A3	2194	PSU	C4-N3-C2	-4.51	119.83	126.34
3	h1	1027	PSU	C4-N3-C2	-4.51	119.83	126.34
81	A3	2419	PSU	C4-N3-C2	-4.51	119.83	126.34
3	h1	950	PSU	C4-N3-C2	-4.50	119.86	126.34
3	h1	470	PSU	C4-N3-C2	-4.50	119.86	126.34
3	h1	607	PSU	C4-N3-C2	-4.50	119.86	126.34
81	A3	2947	PSU	C4-N3-C2	-4.49	119.86	126.34
3	h1	1634	PSU	C4-N3-C2	-4.49	119.87	126.34
81	A3	684	PSU	C4-N3-C2	-4.49	119.87	126.34
3	h1	121	PSU	C4-N3-C2	-4.49	119.87	126.34
81	A3	2978	PSU	C4-N3-C2	-4.49	119.87	126.34
3	h1	417	PSU	C4-N3-C2	-4.49	119.87	126.34
3	h1	310	PSU	C4-N3-C2	-4.49	119.88	126.34
81	A3	1474	PSU	C4-N3-C2	-4.48	119.88	126.34
82	B3	96	PSU	C4-N3-C2	-4.48	119.89	126.34
81	A3	510	PSU	C4-N3-C2	-4.47	119.89	126.34
81	A3	902	PSU	C4-N3-C2	-4.47	119.90	126.34
81	A3	2269	PSU	C4-N3-C2	-4.47	119.91	126.34
3	h1	1120	PSU	C4-N3-C2	-4.46	119.91	126.34
81	A3	277	PSU	C4-N3-C2	-4.46	119.91	126.34
81	A3	2137	PSU	N1-C2-N3	4.46	120.18	115.13
3	h1	1615	PSU	C4-N3-C2	-4.46	119.92	126.34
81	A3	2747	PSU	C4-N3-C2	-4.44	119.94	126.34
3	h1	451	PSU	C4-N3-C2	-4.44	119.94	126.34
3	h1	339	PSU	C4-N3-C2	-4.44	119.95	126.34
3	h1	306	PSU	C4-N3-C2	-4.41	119.99	126.34
3	h1	635	PSU	C4-N3-C2	-4.41	119.99	126.34
3	h1	606	PSU	C4-N3-C2	-4.41	119.99	126.34
81	A3	2139	PSU	C4-N3-C2	-4.41	119.99	126.34
81	A3	1482	PSU	C4-N3-C2	-4.39	120.01	126.34
3	h1	362	PSU	C4-N3-C2	-4.37	120.04	126.34
81	A3	311	PSU	C4-N3-C2	-4.36	120.06	126.34
81	A3	2926	PSU	N1-C2-N3	4.28	119.97	115.13
81	A3	2435	PSU	N1-C2-N3	4.27	119.97	115.13
81	A3	3113	PSU	C4-N3-C2	-4.27	120.18	126.34
81	A3	2317	PSU	N1-C2-N3	4.24	119.94	115.13
81	A3	2868	PSU	N1-C2-N3	4.24	119.93	115.13
81	A3	2214	PSU	N1-C2-N3	4.24	119.93	115.13
81	A3	1134	PSU	N1-C2-N3	4.23	119.93	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2958	PSU	N1-C2-N3	4.23	119.92	115.13
81	A3	2829	PSU	N1-C2-N3	4.22	119.92	115.13
81	A3	829	PSU	N1-C2-N3	4.21	119.90	115.13
81	A3	1056	PSU	N1-C2-N3	4.21	119.90	115.13
3	h1	1210	PSU	N1-C2-N3	4.21	119.90	115.13
81	A3	277	PSU	N1-C2-N3	4.21	119.89	115.13
81	A3	1685	PSU	N1-C2-N3	4.20	119.89	115.13
81	A3	2857	PSU	N1-C2-N3	4.20	119.89	115.13
81	A3	2653	UY1	N1-C2-N3	4.20	119.89	115.13
81	A3	970	PSU	N1-C2-N3	4.19	119.88	115.13
81	A3	966	PSU	C4-N3-C2	-4.19	120.30	126.34
81	A3	1016	PSU	N1-C2-N3	4.19	119.88	115.13
81	A3	2257	PSU	N1-C2-N3	4.19	119.88	115.13
81	A3	895	PSU	C4-N3-C2	-4.18	120.31	126.34
81	A3	717	PSU	N1-C2-N3	4.18	119.87	115.13
81	A3	1002	PSU	N1-C2-N3	4.18	119.87	115.13
81	A3	228	PSU	N1-C2-N3	4.18	119.86	115.13
3	h1	1787	PSU	N1-C2-N3	4.17	119.86	115.13
3	h1	603	UY1	N1-C2-N3	4.17	119.86	115.13
81	A3	1135	PSU	N1-C2-N3	4.17	119.86	115.13
81	A3	34	PSU	N1-C2-N3	4.17	119.85	115.13
81	A3	1064	PSU	N1-C2-N3	4.17	119.85	115.13
3	h1	103	PSU	N1-C2-N3	4.16	119.84	115.13
82	B3	77	PSU	N1-C2-N3	4.16	119.84	115.13
3	h1	961	PSU	N1-C2-N3	4.15	119.84	115.13
81	A3	150	PSU	N1-C2-N3	4.15	119.84	115.13
81	A3	510	PSU	N1-C2-N3	4.15	119.84	115.13
81	A3	2883	PSU	N1-C2-N3	4.15	119.83	115.13
3	h1	1184	PSU	N1-C2-N3	4.15	119.83	115.13
81	A3	2321	PSU	N1-C2-N3	4.15	119.83	115.13
3	h1	1304	PSU	N1-C2-N3	4.14	119.83	115.13
81	A3	2261	PSU	N1-C2-N3	4.14	119.83	115.13
3	h1	1194	B8N	C4-N3-C2	-4.14	120.23	125.46
3	h1	1190	PSU	N1-C2-N3	4.13	119.81	115.13
81	A3	976	PSU	N1-C2-N3	4.13	119.81	115.13
3	h1	607	PSU	N1-C2-N3	4.12	119.80	115.13
81	A3	2978	PSU	N1-C2-N3	4.12	119.80	115.13
3	h1	451	PSU	N1-C2-N3	4.12	119.80	115.13
3	h1	1790	MA6	C1'-N9-C4	4.12	133.88	126.64
3	h1	1217	PSU	N1-C2-N3	4.12	119.80	115.13
81	A3	2263	PSU	N1-C2-N3	4.11	119.79	115.13
3	h1	1485	PSU	N1-C2-N3	4.11	119.79	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	1002	PSU	N1-C2-N3	4.11	119.78	115.13
81	A3	2267	PSU	N1-C2-N3	4.11	119.78	115.13
3	h1	470	PSU	N1-C2-N3	4.11	119.78	115.13
3	h1	605	PSU	N1-C2-N3	4.11	119.78	115.13
3	h1	1178	PSU	N1-C2-N3	4.11	119.78	115.13
3	h1	1567	PSU	N1-C2-N3	4.10	119.78	115.13
3	h1	258	PSU	N1-C2-N3	4.10	119.78	115.13
3	h1	1293	PSU	N1-C2-N3	4.10	119.77	115.13
3	h1	1106	PSU	N1-C2-N3	4.10	119.77	115.13
81	A3	2139	PSU	N1-C2-N3	4.09	119.77	115.13
81	A3	42	PSU	N1-C2-N3	4.09	119.77	115.13
3	h1	362	PSU	N1-C2-N3	4.09	119.76	115.13
81	A3	2947	PSU	N1-C2-N3	4.09	119.76	115.13
3	h1	809	PSU	N1-C2-N3	4.09	119.76	115.13
81	A3	1133	PSU	N1-C2-N3	4.09	119.76	115.13
3	h1	763	PSU	N1-C2-N3	4.09	119.76	115.13
81	A3	2194	PSU	N1-C2-N3	4.08	119.76	115.13
81	A3	1474	PSU	N1-C2-N3	4.08	119.75	115.13
81	A3	2897	PSU	N1-C2-N3	4.08	119.75	115.13
3	h1	1634	PSU	N1-C2-N3	4.08	119.75	115.13
3	h1	950	PSU	N1-C2-N3	4.08	119.75	115.13
81	A3	902	PSU	N1-C2-N3	4.08	119.75	115.13
81	A3	2269	PSU	N1-C2-N3	4.08	119.75	115.13
81	A3	2747	PSU	N1-C2-N3	4.07	119.74	115.13
81	A3	2419	PSU	N1-C2-N3	4.07	119.74	115.13
82	B3	21	PSU	N1-C2-N3	4.07	119.74	115.13
3	h1	1308	PSU	N1-C2-N3	4.06	119.73	115.13
3	h1	95	PSU	N1-C2-N3	4.06	119.72	115.13
3	h1	1524	PSU	N1-C2-N3	4.06	119.72	115.13
3	h1	753	PSU	N1-C2-N3	4.05	119.72	115.13
3	h1	635	PSU	N1-C2-N3	4.05	119.72	115.13
3	h1	121	PSU	N1-C2-N3	4.05	119.71	115.13
3	h1	310	PSU	N1-C2-N3	4.05	119.71	115.13
3	h1	1615	PSU	N1-C2-N3	4.04	119.71	115.13
3	h1	1027	PSU	N1-C2-N3	4.04	119.71	115.13
3	h1	762	PSU	N1-C2-N3	4.04	119.71	115.13
81	A3	684	PSU	N1-C2-N3	4.04	119.71	115.13
3	h1	417	PSU	N1-C2-N3	4.03	119.70	115.13
3	h1	606	PSU	N1-C2-N3	4.02	119.68	115.13
3	h1	1535	PSU	N1-C2-N3	4.01	119.68	115.13
81	A3	464	PSU	N1-C2-N3	4.01	119.67	115.13
3	h1	584	PSU	N1-C2-N3	4.01	119.67	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	3113	PSU	N1-C2-N3	4.00	119.66	115.13
3	h1	339	PSU	N1-C2-N3	3.98	119.64	115.13
81	A3	895	PSU	N1-C2-N3	3.98	119.64	115.13
3	h1	1120	PSU	N1-C2-N3	3.97	119.63	115.13
3	h1	306	PSU	N1-C2-N3	3.96	119.62	115.13
81	A3	1482	PSU	N1-C2-N3	3.94	119.59	115.13
82	B3	96	PSU	N1-C2-N3	3.94	119.59	115.13
81	A3	311	PSU	N1-C2-N3	3.94	119.59	115.13
81	A3	966	PSU	N1-C2-N3	3.91	119.56	115.13
81	A3	786	PSU	N1-C2-N3	3.88	119.53	115.13
81	A3	656	1MA	C5-C6-N1	3.88	119.68	113.90
3	h1	1771	6MZ	C2-N1-C6	3.87	119.91	116.59
81	A3	675	OMU	N3-C2-N1	3.85	120.00	114.89
81	A3	1068	OMU	N3-C2-N1	3.84	119.99	114.89
81	A3	804	OMU	N3-C2-N1	3.81	119.95	114.89
81	A3	1894	OMU	N3-C2-N1	3.80	119.93	114.89
81	A3	2924	OMU	N3-C2-N1	3.80	119.93	114.89
81	A3	2738	OMU	N3-C2-N1	3.79	119.93	114.89
81	A3	2350	OMU	N3-C2-N1	3.79	119.92	114.89
3	h1	581	OMU	N3-C2-N1	3.78	119.91	114.89
81	A3	2886	OMU	N3-C2-N1	3.78	119.91	114.89
3	h1	1383	OMU	N3-C2-N1	3.75	119.87	114.89
3	h1	886	OMU	N3-C2-N1	3.75	119.86	114.89
81	A3	3304	OMU	N3-C2-N1	3.73	119.84	114.89
81	A3	2424	OMU	N3-C2-N1	3.73	119.84	114.89
3	h1	123	OMU	N3-C2-N1	3.72	119.83	114.89
3	h1	1012	OMU	N3-C2-N1	3.71	119.82	114.89
3	h1	1272	OMU	N3-C2-N1	3.71	119.82	114.89
81	A3	48	OMU	N3-C2-N1	3.71	119.81	114.89
81	A3	144	OMU	N3-C2-N1	3.70	119.81	114.89
3	h1	1234	OMU	N3-C2-N1	3.70	119.80	114.89
81	A3	787	OMU	N3-C2-N1	3.69	119.79	114.89
3	h1	373	OMU	N3-C2-N1	3.68	119.78	114.89
81	A3	1537	OMU	N3-C2-N1	3.68	119.77	114.89
81	A3	44	OMU	N3-C2-N1	3.62	119.70	114.89
81	A3	2732	OMU	N3-C2-N1	3.62	119.69	114.89
3	h1	1447	OMU	N3-C2-N1	3.60	119.67	114.89
81	A3	2720	OMU	N3-C2-N1	3.60	119.66	114.89
81	A3	2317	PSU	C6-C5-C4	3.59	120.71	118.20
3	h1	614	OMU	N3-C2-N1	3.57	119.64	114.89
81	A3	3289	OMU	N3-C2-N1	3.57	119.63	114.89
81	A3	2413	OMU	N3-C2-N1	3.57	119.63	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	1771	6MZ	C9-N6-C6	-3.55	119.81	122.87
81	A3	815	OMG	C5-C6-N1	3.49	120.12	113.95
81	A3	2291	OMG	C5-C6-N1	3.44	120.03	113.95
81	A3	2412	OMG	C5-C6-N1	3.43	120.00	113.95
3	h1	392	OMG	C5-C6-N1	3.43	120.00	113.95
81	A3	399	OMG	C5-C6-N1	3.43	120.00	113.95
3	h1	1274	OMG	C5-C6-N1	3.42	119.99	113.95
81	A3	2127	OMG	C5-C6-N1	3.41	119.98	113.95
81	A3	1894	OMU	C5-C4-N3	3.41	119.94	114.84
81	A3	2925	OMG	C5-C6-N1	3.41	119.97	113.95
3	h1	598	OMG	C5-C6-N1	3.40	119.96	113.95
81	A3	296	OMG	C5-C6-N1	3.40	119.96	113.95
81	A3	2622	OMG	C5-C6-N1	3.40	119.96	113.95
82	B3	78	OMG	C5-C6-N1	3.39	119.94	113.95
81	A3	2818	OMG	C5-C6-N1	3.39	119.94	113.95
81	A3	1461	OMG	C5-C6-N1	3.39	119.94	113.95
81	A3	918	OMG	C5-C6-N1	3.39	119.93	113.95
81	A3	2796	OMG	C5-C6-N1	3.39	119.93	113.95
81	A3	2281	5MC	C5-C6-N1	-3.37	119.87	123.34
3	h1	246	OMG	C5-C6-N1	3.37	119.91	113.95
81	A3	48	OMU	C5-C4-N3	3.37	119.88	114.84
81	A3	1857	OMG	C5-C6-N1	3.37	119.90	113.95
81	A3	2239	OMG	C5-C6-N1	3.35	119.87	113.95
81	A3	2920	OMG	C5-C6-N1	3.35	119.86	113.95
81	A3	2424	OMU	C5-C4-N3	3.35	119.85	114.84
81	A3	2398	OMG	C5-C6-N1	3.34	119.85	113.95
81	A3	34	PSU	C6-C5-C4	3.33	120.53	118.20
81	A3	2924	OMU	C5-C4-N3	3.33	119.82	114.84
81	A3	2394	OMG	C5-C6-N1	3.33	119.83	113.95
3	h1	373	OMU	C5-C4-N3	3.33	119.82	114.84
81	A3	2126	OMG	C5-C6-N1	3.33	119.82	113.95
3	h1	1234	OMU	C5-C4-N3	3.32	119.81	114.84
81	A3	829	PSU	C6-C5-C4	3.32	120.52	118.20
3	h1	614	OMU	C5-C4-N3	3.32	119.80	114.84
81	A3	1068	OMU	C5-C4-N3	3.32	119.80	114.84
81	A3	144	OMU	C5-C4-N3	3.31	119.80	114.84
3	h1	886	OMU	C5-C4-N3	3.31	119.79	114.84
81	A3	1537	OMU	C5-C4-N3	3.31	119.79	114.84
81	A3	2413	OMU	C5-C4-N3	3.31	119.79	114.84
3	h1	1272	OMU	C5-C4-N3	3.31	119.78	114.84
81	A3	2829	PSU	C6-C5-C4	3.30	120.51	118.20
3	h1	1383	OMU	C5-C4-N3	3.30	119.78	114.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2653	UY1	C6-C5-C4	3.30	120.51	118.20
3	h1	1012	OMU	C5-C4-N3	3.30	119.77	114.84
81	A3	2738	OMU	C5-C4-N3	3.29	119.77	114.84
81	A3	510	PSU	C6-C5-C4	3.29	120.50	118.20
81	A3	2435	PSU	C6-C5-C4	3.28	120.49	118.20
81	A3	2350	OMU	C5-C4-N3	3.28	119.75	114.84
3	h1	581	OMU	C5-C4-N3	3.28	119.75	114.84
81	A3	1134	PSU	C6-C5-C4	3.28	120.49	118.20
81	A3	2732	OMU	C5-C4-N3	3.28	119.74	114.84
81	A3	787	OMU	C5-C4-N3	3.27	119.74	114.84
81	A3	2654	OMG	C5-C6-N1	3.27	119.73	113.95
81	A3	1135	PSU	C6-C5-C4	3.27	120.48	118.20
3	h1	123	OMU	C5-C4-N3	3.26	119.72	114.84
81	A3	804	OMU	C5-C4-N3	3.26	119.72	114.84
81	A3	3289	OMU	C5-C4-N3	3.25	119.71	114.84
81	A3	2794	OMG	C5-C6-N1	3.25	119.69	113.95
81	A3	2868	PSU	C6-C5-C4	3.25	120.47	118.20
81	A3	3304	OMU	C5-C4-N3	3.25	119.70	114.84
81	A3	44	OMU	C5-C4-N3	3.25	119.70	114.84
81	A3	2857	PSU	C6-C5-C4	3.24	120.46	118.20
81	A3	717	PSU	C6-C5-C4	3.24	120.46	118.20
81	A3	2137	PSU	C6-C5-C4	3.23	120.46	118.20
3	h1	1433	OMG	C5-C6-N1	3.23	119.66	113.95
81	A3	2720	OMU	C5-C4-N3	3.22	119.66	114.84
81	A3	675	OMU	C5-C4-N3	3.21	119.65	114.84
81	A3	895	PSU	C6-C5-C4	3.20	120.44	118.20
81	A3	970	PSU	C6-C5-C4	3.19	120.43	118.20
3	h1	362	PSU	C6-C5-C4	3.18	120.42	118.20
81	A3	2654	OMG	N2-C2-N1	3.18	123.47	116.71
3	h1	961	PSU	C6-C5-C4	3.17	120.42	118.20
82	B3	77	PSU	C6-C5-C4	3.17	120.41	118.20
3	h1	1210	PSU	C6-C5-C4	3.17	120.41	118.20
81	A3	2926	PSU	C6-C5-C4	3.17	120.41	118.20
3	h1	763	PSU	C6-C5-C4	3.16	120.41	118.20
3	h1	886	OMU	CM2-O2'-C2'	3.16	122.82	114.52
3	h1	470	PSU	C6-C5-C4	3.16	120.41	118.20
81	A3	277	PSU	C6-N1-C2	-3.15	119.46	122.68
81	A3	966	PSU	C6-N1-C2	-3.15	119.46	122.68
3	h1	1447	OMU	C5-C4-N3	3.15	119.56	114.84
81	A3	2257	PSU	C6-C5-C4	3.14	120.39	118.20
3	h1	1002	PSU	C6-C5-C4	3.13	120.39	118.20
3	h1	1485	PSU	C6-C5-C4	3.13	120.38	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2139	PSU	C6-C5-C4	3.13	120.38	118.20
81	A3	2214	PSU	C6-C5-C4	3.12	120.38	118.20
3	h1	417	PSU	C6-C5-C4	3.12	120.38	118.20
81	A3	1685	PSU	C6-C5-C4	3.12	120.38	118.20
81	A3	2267	PSU	C6-C5-C4	3.12	120.38	118.20
3	h1	451	PSU	C6-C5-C4	3.11	120.37	118.20
81	A3	2947	PSU	C6-C5-C4	3.09	120.36	118.20
81	A3	228	PSU	C6-C5-C4	3.09	120.36	118.20
81	A3	2873	5MC	C5-C6-N1	-3.09	120.16	123.34
81	A3	1002	PSU	C6-C5-C4	3.08	120.35	118.20
3	h1	606	PSU	C6-N1-C2	-3.08	119.54	122.68
81	A3	2886	OMU	C5-C4-N3	3.08	119.44	114.84
81	A3	895	PSU	C6-N1-C2	-3.07	119.54	122.68
81	A3	1064	PSU	C6-C5-C4	3.07	120.34	118.20
81	A3	2897	PSU	C6-C5-C4	3.07	120.34	118.20
81	A3	2883	PSU	C6-C5-C4	3.07	120.34	118.20
3	h1	1304	PSU	C6-C5-C4	3.06	120.34	118.20
81	A3	42	PSU	C6-C5-C4	3.06	120.34	118.20
81	A3	3113	PSU	C6-N1-C2	-3.06	119.56	122.68
3	h1	1787	PSU	C6-C5-C4	3.05	120.33	118.20
81	A3	2263	PSU	C6-C5-C4	3.04	120.32	118.20
81	A3	2978	PSU	C6-N1-C2	-3.03	119.58	122.68
81	A3	150	PSU	C6-C5-C4	3.02	120.31	118.20
81	A3	2398	OMG	C8-N7-C5	3.02	108.74	102.99
3	h1	603	UY1	C6-N1-C2	-3.01	119.60	122.68
3	h1	1106	PSU	C6-C5-C4	3.01	120.30	118.20
81	A3	2127	OMG	C8-N7-C5	3.01	108.73	102.99
3	h1	607	PSU	C6-N1-C2	-3.01	119.60	122.68
3	h1	451	PSU	C6-N1-C2	-3.00	119.61	122.68
3	h1	1567	PSU	C6-C5-C4	3.00	120.30	118.20
81	A3	2321	PSU	C6-C5-C4	3.00	120.30	118.20
81	A3	2747	PSU	C6-N1-C2	-3.00	119.62	122.68
3	h1	1184	PSU	C6-C5-C4	3.00	120.29	118.20
3	h1	1308	PSU	C6-C5-C4	3.00	120.29	118.20
81	A3	1482	PSU	C6-N1-C2	-2.99	119.62	122.68
81	A3	2435	PSU	C6-N1-C2	-2.99	119.62	122.68
3	h1	635	PSU	C6-N1-C2	-2.99	119.62	122.68
3	h1	103	PSU	C6-C5-C4	2.99	120.29	118.20
81	A3	976	PSU	C6-C5-C4	2.99	120.29	118.20
3	h1	1615	PSU	C6-C5-C4	2.98	120.28	118.20
81	A3	296	OMG	C8-N7-C5	2.98	108.67	102.99
3	h1	1190	PSU	C6-C5-C4	2.97	120.28	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	362	PSU	C6-N1-C2	-2.97	119.64	122.68
3	h1	950	PSU	C6-N1-C2	-2.97	119.65	122.68
81	A3	510	PSU	C6-N1-C2	-2.97	119.65	122.68
3	h1	809	PSU	C6-C5-C4	2.97	120.27	118.20
81	A3	902	PSU	C6-N1-C2	-2.96	119.65	122.68
81	A3	2214	PSU	C6-N1-C2	-2.96	119.65	122.68
81	A3	2139	PSU	C6-N1-C2	-2.96	119.65	122.68
3	h1	607	PSU	C6-C5-C4	2.96	120.27	118.20
3	h1	1210	PSU	C6-N1-C2	-2.96	119.66	122.68
81	A3	2419	PSU	C6-C5-C4	2.95	120.26	118.20
3	h1	1274	OMG	C2-N1-C6	-2.95	119.66	125.10
81	A3	1474	PSU	C6-N1-C2	-2.95	119.66	122.68
3	h1	598	OMG	C8-N7-C5	2.95	108.62	102.99
3	h1	310	PSU	C6-N1-C2	-2.95	119.67	122.68
3	h1	1634	PSU	C6-C5-C4	2.95	120.26	118.20
81	A3	1016	PSU	C6-C5-C4	2.95	120.26	118.20
81	A3	2829	PSU	C6-N1-C2	-2.94	119.67	122.68
81	A3	1016	PSU	C6-N1-C2	-2.94	119.68	122.68
3	h1	1274	OMG	C8-N7-C5	2.94	108.59	102.99
3	h1	605	PSU	C6-N1-C2	-2.94	119.68	122.68
81	A3	277	PSU	C6-C5-C4	2.94	120.25	118.20
81	A3	2394	OMG	C8-N7-C5	2.94	108.59	102.99
3	h1	392	OMG	C8-N7-C5	2.94	108.58	102.99
81	A3	1461	OMG	C2-N1-C6	-2.94	119.69	125.10
81	A3	2958	PSU	C6-C5-C4	2.93	120.25	118.20
3	h1	258	PSU	C6-N1-C2	-2.93	119.68	122.68
81	A3	150	PSU	C6-N1-C2	-2.93	119.68	122.68
81	A3	1134	PSU	C6-N1-C2	-2.93	119.68	122.68
3	h1	339	PSU	C6-N1-C2	-2.93	119.69	122.68
81	A3	1056	PSU	C6-C5-C4	2.93	120.25	118.20
81	A3	399	OMG	C2-N1-C6	-2.93	119.70	125.10
81	A3	2926	PSU	C6-N1-C2	-2.93	119.69	122.68
81	A3	228	PSU	C6-N1-C2	-2.93	119.69	122.68
81	A3	918	OMG	C2-N1-C6	-2.93	119.71	125.10
81	A3	1002	PSU	C6-N1-C2	-2.92	119.69	122.68
81	A3	2269	PSU	C6-N1-C2	-2.92	119.69	122.68
3	h1	886	OMU	O4-C4-C5	-2.92	120.02	125.16
81	A3	2317	PSU	C6-N1-C2	-2.92	119.69	122.68
3	h1	1787	PSU	C6-N1-C2	-2.92	119.70	122.68
81	A3	804	OMU	O4-C4-C5	-2.92	120.03	125.16
81	A3	2194	PSU	C6-N1-C2	-2.92	119.70	122.68
3	h1	1194	B8N	N3-C2-N1	2.92	120.88	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	392	OMG	C2-N1-C6	-2.92	119.73	125.10
3	h1	809	PSU	C6-N1-C2	-2.92	119.70	122.68
3	h1	1002	PSU	C6-N1-C2	-2.91	119.70	122.68
81	A3	2920	OMG	C2-N1-C6	-2.91	119.73	125.10
3	h1	1178	PSU	C6-C5-C4	2.91	120.23	118.20
3	h1	1615	PSU	C6-N1-C2	-2.91	119.71	122.68
81	A3	1461	OMG	C8-N7-C5	2.91	108.53	102.99
81	A3	1857	OMG	C8-N7-C5	2.91	108.53	102.99
81	A3	1133	PSU	C6-C5-C4	2.91	120.23	118.20
3	h1	306	PSU	C6-N1-C2	-2.91	119.71	122.68
3	h1	1308	PSU	C6-N1-C2	-2.90	119.71	122.68
81	A3	2925	OMG	C8-N7-C5	2.90	108.52	102.99
81	A3	2291	OMG	C8-N7-C5	2.90	108.52	102.99
3	h1	762	PSU	C6-C5-C4	2.90	120.23	118.20
81	A3	684	PSU	C6-N1-C2	-2.90	119.72	122.68
81	A3	2261	PSU	C6-C5-C4	2.90	120.23	118.20
3	h1	246	OMG	C2-N1-C6	-2.90	119.76	125.10
3	h1	598	OMG	C2-N1-C6	-2.90	119.76	125.10
3	h1	246	OMG	C8-N7-C5	2.90	108.51	102.99
3	h1	1190	PSU	C6-N1-C2	-2.89	119.72	122.68
81	A3	2137	PSU	C6-N1-C2	-2.89	119.72	122.68
81	A3	2622	OMG	C8-N7-C5	2.89	108.50	102.99
3	h1	1524	PSU	C6-N1-C2	-2.89	119.72	122.68
82	B3	78	OMG	C2-N1-C6	-2.89	119.77	125.10
3	h1	1178	PSU	C6-N1-C2	-2.89	119.73	122.68
81	A3	2868	PSU	C6-N1-C2	-2.89	119.73	122.68
3	h1	1293	PSU	C6-C5-C4	2.89	120.22	118.20
81	A3	918	OMG	C8-N7-C5	2.89	108.50	102.99
3	h1	603	UY1	C6-C5-C4	2.89	120.22	118.20
3	h1	753	PSU	C6-C5-C4	2.89	120.22	118.20
81	A3	2291	OMG	C2-N1-C6	-2.89	119.78	125.10
81	A3	815	OMG	C2-N1-C6	-2.89	119.78	125.10
81	A3	311	PSU	C6-N1-C2	-2.89	119.73	122.68
3	h1	1293	PSU	C6-N1-C2	-2.89	119.73	122.68
81	A3	1685	PSU	C6-N1-C2	-2.89	119.73	122.68
81	A3	2126	OMG	C8-N7-C5	2.89	108.49	102.99
81	A3	1056	PSU	C6-N1-C2	-2.89	119.73	122.68
82	B3	78	OMG	C8-N7-C5	2.89	108.49	102.99
81	A3	684	PSU	C6-C5-C4	2.88	120.22	118.20
3	h1	470	PSU	C6-N1-C2	-2.88	119.73	122.68
81	A3	2654	OMG	C8-N7-C5	2.88	108.48	102.99
3	h1	121	PSU	C6-N1-C2	-2.88	119.73	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2267	PSU	C6-N1-C2	-2.88	119.73	122.68
3	h1	614	OMU	O4-C4-C5	-2.88	120.09	125.16
3	h1	1383	OMU	O4-C4-C5	-2.88	120.09	125.16
81	A3	2239	OMG	C8-N7-C5	2.88	108.48	102.99
81	A3	2794	OMG	C8-N7-C5	2.88	108.48	102.99
81	A3	2818	OMG	C8-N7-C5	2.88	108.48	102.99
81	A3	2920	OMG	C8-N7-C5	2.88	108.48	102.99
81	A3	3113	PSU	C6-C5-C4	2.88	120.21	118.20
81	A3	1857	OMG	C2-N1-C6	-2.88	119.79	125.10
3	h1	635	PSU	C6-C5-C4	2.88	120.21	118.20
3	h1	103	PSU	C6-N1-C2	-2.88	119.74	122.68
81	A3	2622	OMG	C2-N1-C6	-2.88	119.80	125.10
81	A3	2897	PSU	C6-N1-C2	-2.88	119.74	122.68
3	h1	1194	B8N	O4-C4-N3	-2.87	115.10	119.98
82	B3	77	PSU	C6-N1-C2	-2.87	119.74	122.68
3	h1	961	PSU	C6-N1-C2	-2.87	119.74	122.68
3	h1	1184	PSU	C6-N1-C2	-2.87	119.74	122.68
3	h1	1304	PSU	C6-N1-C2	-2.87	119.74	122.68
81	A3	2261	PSU	C6-N1-C2	-2.87	119.74	122.68
3	h1	417	PSU	C6-N1-C2	-2.87	119.75	122.68
81	A3	2412	OMG	C2-N1-C6	-2.87	119.81	125.10
3	h1	1272	OMU	O4-C4-C5	-2.87	120.11	125.16
81	A3	3289	OMU	O4-C4-C5	-2.87	120.12	125.16
81	A3	902	PSU	C6-C5-C4	2.87	120.20	118.20
81	A3	976	PSU	C6-N1-C2	-2.87	119.75	122.68
81	A3	2883	PSU	C6-N1-C2	-2.86	119.75	122.68
3	h1	1634	PSU	C6-N1-C2	-2.86	119.75	122.68
81	A3	829	PSU	C6-N1-C2	-2.86	119.75	122.68
81	A3	296	OMG	C2-N1-C6	-2.86	119.83	125.10
81	A3	2925	OMG	C2-N1-C6	-2.86	119.83	125.10
3	h1	753	PSU	C6-N1-C2	-2.86	119.76	122.68
81	A3	464	PSU	C6-N1-C2	-2.86	119.76	122.68
3	h1	373	OMU	O4-C4-C5	-2.86	120.13	125.16
3	h1	1485	PSU	C6-N1-C2	-2.86	119.76	122.68
81	A3	2263	PSU	C6-N1-C2	-2.86	119.76	122.68
81	A3	2412	OMG	C8-N7-C5	2.86	108.43	102.99
3	h1	310	PSU	C6-C5-C4	2.86	120.19	118.20
81	A3	2857	PSU	C6-N1-C2	-2.86	119.76	122.68
81	A3	815	OMG	C8-N7-C5	2.85	108.43	102.99
81	A3	717	PSU	C6-N1-C2	-2.85	119.77	122.68
81	A3	2257	PSU	C6-N1-C2	-2.85	119.77	122.68
3	h1	1217	PSU	C6-C5-C4	2.85	120.19	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	2947	PSU	C6-N1-C2	-2.85	119.77	122.68
81	A3	2958	PSU	C6-N1-C2	-2.85	119.77	122.68
81	A3	2239	OMG	C2-N1-C6	-2.85	119.85	125.10
81	A3	2818	OMG	C2-N1-C6	-2.85	119.85	125.10
82	B3	96	PSU	C6-N1-C2	-2.85	119.77	122.68
81	A3	1133	PSU	C6-N1-C2	-2.85	119.77	122.68
81	A3	2653	UY1	C6-N1-C2	-2.85	119.77	122.68
3	h1	95	PSU	C6-C5-C4	2.84	120.18	118.20
81	A3	2738	OMU	O4-C4-C5	-2.84	120.17	125.16
3	h1	1234	OMU	O4-C4-C5	-2.84	120.17	125.16
3	h1	1106	PSU	C6-N1-C2	-2.84	119.78	122.68
81	A3	42	PSU	C6-N1-C2	-2.84	119.78	122.68
81	A3	2796	OMG	C8-N7-C5	2.84	108.39	102.99
3	h1	121	PSU	C6-C5-C4	2.83	120.18	118.20
3	h1	339	PSU	C6-C5-C4	2.83	120.18	118.20
3	h1	1012	OMU	O4-C4-C5	-2.83	120.18	125.16
3	h1	1217	PSU	C6-N1-C2	-2.83	119.79	122.68
81	A3	2398	OMG	C2-N1-C6	-2.83	119.89	125.10
3	h1	584	PSU	C6-N1-C2	-2.83	119.79	122.68
81	A3	2720	OMU	O4-C4-C5	-2.82	120.19	125.16
81	A3	2394	OMG	C2-N1-C6	-2.82	119.90	125.10
3	h1	605	PSU	C6-C5-C4	2.82	120.17	118.20
81	A3	399	OMG	C8-N7-C5	2.82	108.36	102.99
81	A3	2419	PSU	C6-N1-C2	-2.82	119.80	122.68
81	A3	2126	OMG	C2-N1-C6	-2.81	119.92	125.10
3	h1	1567	PSU	C6-N1-C2	-2.81	119.81	122.68
3	h1	1535	PSU	C6-N1-C2	-2.81	119.81	122.68
81	A3	2350	OMU	O4-C4-C5	-2.81	120.22	125.16
81	A3	2127	OMG	C2-N1-C6	-2.81	119.93	125.10
3	h1	1120	PSU	C6-N1-C2	-2.80	119.81	122.68
81	A3	34	PSU	C6-N1-C2	-2.80	119.82	122.68
81	A3	3304	OMU	O4-C4-C5	-2.80	120.23	125.16
3	h1	762	PSU	C6-N1-C2	-2.80	119.82	122.68
3	h1	1027	PSU	C6-N1-C2	-2.80	119.82	122.68
81	A3	2924	OMU	O4-C4-C5	-2.80	120.23	125.16
3	h1	581	OMU	O4-C4-C5	-2.80	120.23	125.16
81	A3	464	PSU	C6-C5-C4	2.80	120.16	118.20
81	A3	1064	PSU	C6-N1-C2	-2.80	119.82	122.68
82	B3	21	PSU	C6-N1-C2	-2.80	119.82	122.68
81	A3	2796	OMG	C2-N1-C6	-2.80	119.95	125.10
81	A3	144	OMU	O4-C4-C5	-2.79	120.25	125.16
81	A3	1537	OMU	O4-C4-C5	-2.79	120.25	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	258	PSU	C6-C5-C4	2.79	120.15	118.20
81	A3	970	PSU	C6-N1-C2	-2.78	119.84	122.68
3	h1	1447	OMU	O4-C4-C5	-2.78	120.27	125.16
81	A3	1474	PSU	C6-C5-C4	2.78	120.14	118.20
3	h1	1433	OMG	C8-N7-C5	2.78	108.28	102.99
81	A3	660	A2M	C2'-C3'-C4'	2.78	108.03	101.99
81	A3	44	OMU	O4-C4-C5	-2.78	120.28	125.16
81	A3	2804	A2M	C3'-C2'-C1'	2.78	108.11	102.89
3	h1	763	PSU	C6-N1-C2	-2.77	119.85	122.68
81	A3	2321	PSU	C6-N1-C2	-2.77	119.85	122.68
3	h1	95	PSU	C6-N1-C2	-2.77	119.85	122.68
81	A3	2424	OMU	O4-C4-C5	-2.77	120.29	125.16
81	A3	2978	PSU	C6-C5-C4	2.76	120.13	118.20
3	h1	123	OMU	O4-C4-C5	-2.76	120.31	125.16
3	h1	1535	PSU	C6-C5-C4	2.75	120.12	118.20
81	A3	1068	OMU	O4-C4-C5	-2.75	120.32	125.16
3	h1	606	PSU	C6-C5-C4	2.74	120.11	118.20
81	A3	1135	PSU	C6-N1-C2	-2.73	119.89	122.68
81	A3	787	OMU	O4-C4-C5	-2.73	120.36	125.16
82	B3	21	PSU	C6-C5-C4	2.73	120.10	118.20
81	A3	1894	OMU	O4-C4-C5	-2.72	120.38	125.16
81	A3	2747	PSU	C6-C5-C4	2.72	120.10	118.20
3	h1	1027	PSU	C6-C5-C4	2.71	120.10	118.20
81	A3	2886	OMU	O4-C4-C5	-2.71	120.39	125.16
81	A3	675	OMU	O4-C4-C5	-2.70	120.41	125.16
3	h1	1210	PSU	O2-C2-N1	-2.70	119.82	122.79
81	A3	2194	PSU	C6-C5-C4	2.69	120.08	118.20
81	A3	2269	PSU	C6-C5-C4	2.69	120.08	118.20
3	h1	1433	OMG	C2-N1-C6	-2.69	120.14	125.10
81	A3	966	PSU	C6-C5-C4	2.69	120.08	118.20
3	h1	306	PSU	C6-C5-C4	2.68	120.07	118.20
81	A3	2732	OMU	O4-C4-C5	-2.68	120.44	125.16
81	A3	48	OMU	O4-C4-C5	-2.68	120.45	125.16
81	A3	2654	OMG	C2-N1-C6	-2.67	120.18	125.10
81	A3	2394	OMG	N2-C2-N1	2.67	122.40	116.71
81	A3	656	1MA	C8-N7-C5	2.66	108.07	102.99
3	h1	1120	PSU	C6-C5-C4	2.66	120.06	118.20
3	h1	607	PSU	O2-C2-N1	-2.66	119.86	122.79
81	A3	2435	PSU	O2-C2-N1	-2.64	119.88	122.79
81	A3	2747	PSU	O2-C2-N1	-2.63	119.89	122.79
81	A3	1482	PSU	C6-C5-C4	2.63	120.04	118.20
3	h1	451	PSU	O2-C2-N1	-2.63	119.90	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	1474	PSU	O2-C2-N1	-2.63	119.90	122.79
81	A3	150	PSU	O2-C2-N1	-2.62	119.90	122.79
3	h1	950	PSU	C6-C5-C4	2.62	120.03	118.20
81	A3	2883	PSU	O2-C2-N1	-2.61	119.91	122.79
3	h1	103	PSU	O2-C2-N1	-2.61	119.92	122.79
81	A3	2413	OMU	O4-C4-C5	-2.60	120.59	125.16
82	B3	77	PSU	O2-C2-N1	-2.60	119.93	122.79
81	A3	2868	PSU	O2-C2-N1	-2.58	119.95	122.79
3	h1	603	UY1	O2-C2-N1	-2.57	119.96	122.79
3	h1	1787	PSU	O2-C2-N1	-2.57	119.96	122.79
81	A3	2926	PSU	O2-C2-N1	-2.57	119.96	122.79
81	A3	2829	PSU	O2-C2-N1	-2.57	119.96	122.79
81	A3	2419	PSU	O2-C2-N1	-2.56	119.97	122.79
81	A3	786	PSU	C6-N1-C2	-2.54	120.08	122.68
82	B3	21	PSU	O2-C2-N1	-2.54	120.00	122.79
3	h1	622	A2M	C3'-C2'-C1'	2.53	107.65	102.89
81	A3	277	PSU	O2-C2-N1	-2.52	120.01	122.79
81	A3	1685	PSU	O2-C2-N1	-2.52	120.02	122.79
3	h1	417	PSU	O2-C2-N1	-2.52	120.02	122.79
81	A3	2794	OMG	C2-N1-C6	-2.52	120.46	125.10
81	A3	2857	PSU	O2-C2-N1	-2.52	120.02	122.79
3	h1	1524	PSU	C6-C5-C4	2.52	119.96	118.20
81	A3	2214	PSU	O2-C2-N1	-2.51	120.03	122.79
81	A3	2127	OMG	N2-C2-N1	2.50	122.04	116.71
81	A3	970	PSU	O2-C2-N1	-2.50	120.04	122.79
3	h1	1106	PSU	O2-C2-N1	-2.50	120.04	122.79
81	A3	717	PSU	O2-C2-N1	-2.50	120.04	122.79
81	A3	2263	PSU	O2-C2-N1	-2.50	120.04	122.79
81	A3	2398	OMG	N2-C2-N1	2.49	122.02	116.71
3	h1	605	PSU	O2-C2-N1	-2.49	120.05	122.79
3	h1	1120	PSU	O2-C2-N1	-2.49	120.05	122.79
81	A3	2261	PSU	O2-C2-N1	-2.49	120.05	122.79
3	h1	1567	PSU	O2-C2-N1	-2.49	120.05	122.79
81	A3	829	PSU	O2-C2-N1	-2.48	120.06	122.79
3	h1	1190	PSU	O2-C2-N1	-2.48	120.06	122.79
81	A3	464	PSU	O2-C2-N1	-2.48	120.06	122.79
81	A3	1135	PSU	O2-C2-N1	-2.47	120.07	122.79
3	h1	809	PSU	O2-C2-N1	-2.47	120.07	122.79
3	h1	753	PSU	O2-C2-N1	-2.47	120.07	122.79
3	h1	1308	PSU	O2-C2-N1	-2.47	120.07	122.79
81	A3	2804	A2M	C2'-C3'-C4'	2.47	107.36	101.99
3	h1	961	PSU	O2-C2-N1	-2.47	120.08	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B3	96	PSU	C6-C5-C4	2.46	119.92	118.20
81	A3	1016	PSU	O2-C2-N1	-2.46	120.08	122.79
3	h1	1178	PSU	O2-C2-N1	-2.46	120.08	122.79
81	A3	2281	5MC	CM5-C5-C6	-2.46	119.56	122.85
3	h1	1524	PSU	O2-C2-N1	-2.46	120.08	122.79
3	h1	418	OMC	CM2-O2'-C2'	2.46	120.97	114.52
3	h1	763	PSU	O2-C2-N1	-2.46	120.09	122.79
81	A3	2958	PSU	O2-C2-N1	-2.45	120.09	122.79
81	A3	1134	PSU	O2-C2-N1	-2.45	120.09	122.79
81	A3	2317	PSU	O2-C2-N1	-2.45	120.09	122.79
3	h1	1485	PSU	O2-C2-N1	-2.45	120.10	122.79
81	A3	2269	PSU	O2-C2-N1	-2.44	120.10	122.79
3	h1	635	PSU	O2-C2-N1	-2.44	120.10	122.79
81	A3	2818	OMG	N2-C2-N1	2.44	121.91	116.71
3	h1	584	PSU	C6-C5-C4	2.44	119.90	118.20
3	h1	339	PSU	O2-C2-N1	-2.44	120.11	122.79
81	A3	2194	PSU	O2-C2-N1	-2.44	120.11	122.79
81	A3	1002	PSU	O2-C2-N1	-2.44	120.11	122.79
3	h1	1781	4AC	C5-C4-N3	-2.44	118.67	122.59
3	h1	121	PSU	O2-C2-N1	-2.43	120.11	122.79
3	h1	1615	PSU	O2-C2-N1	-2.43	120.12	122.79
3	h1	1634	PSU	O2-C2-N1	-2.43	120.12	122.79
3	h1	258	PSU	O2-C2-N1	-2.42	120.12	122.79
3	h1	606	PSU	O2-C2-N1	-2.42	120.12	122.79
81	A3	1482	PSU	O2-C2-N1	-2.42	120.13	122.79
3	h1	1217	PSU	O2-C2-N1	-2.42	120.13	122.79
3	h1	584	PSU	O2-C2-N1	-2.42	120.13	122.79
81	A3	228	PSU	O2-C2-N1	-2.42	120.13	122.79
81	A3	976	PSU	O2-C2-N1	-2.41	120.13	122.79
81	A3	1056	PSU	O2-C2-N1	-2.41	120.14	122.79
81	A3	2139	PSU	O2-C2-N1	-2.41	120.14	122.79
81	A3	2126	OMG	N2-C2-N1	2.41	121.84	116.71
81	A3	311	PSU	O2-C2-N1	-2.41	120.14	122.79
81	A3	786	PSU	O2-C2-N1	-2.41	120.14	122.79
81	A3	2267	PSU	O2-C2-N1	-2.41	120.14	122.79
81	A3	2321	PSU	O2-C2-N1	-2.41	120.14	122.79
81	A3	311	PSU	C6-C5-C4	2.40	119.88	118.20
3	h1	1293	PSU	O2-C2-N1	-2.40	120.15	122.79
3	h1	1535	PSU	O2-C2-N1	-2.40	120.15	122.79
3	h1	1304	PSU	O2-C2-N1	-2.39	120.16	122.79
81	A3	1133	PSU	O2-C2-N1	-2.39	120.16	122.79
3	h1	950	PSU	O2-C2-N1	-2.39	120.16	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	1027	PSU	O2-C2-N1	-2.39	120.16	122.79
3	h1	470	PSU	O2-C2-N1	-2.38	120.17	122.79
3	h1	762	PSU	O2-C2-N1	-2.38	120.17	122.79
81	A3	817	A2M	C3'-C2'-C1'	2.38	107.37	102.89
81	A3	1064	PSU	O2-C2-N1	-2.38	120.17	122.79
3	h1	1781	4AC	N4-C4-N3	2.37	117.84	113.85
3	h1	1184	PSU	O2-C2-N1	-2.37	120.18	122.79
3	h1	310	PSU	O2-C2-N1	-2.37	120.19	122.79
81	A3	2653	UY1	O2-C2-N1	-2.36	120.19	122.79
81	A3	895	PSU	O2-C2-N1	-2.36	120.19	122.79
3	h1	1002	PSU	O2-C2-N1	-2.35	120.21	122.79
81	A3	2897	PSU	O2-C2-N1	-2.35	120.21	122.79
81	A3	34	PSU	O2-C2-N1	-2.34	120.21	122.79
3	h1	1283	4AC	C6-C5-C4	2.34	119.82	116.96
81	A3	510	PSU	O2-C2-N1	-2.33	120.22	122.79
82	B3	96	PSU	O2-C2-N1	-2.33	120.22	122.79
81	A3	902	PSU	O2-C2-N1	-2.33	120.23	122.79
3	h1	362	PSU	O2-C2-N1	-2.32	120.23	122.79
81	A3	40	OMC	CM2-O2'-C2'	2.32	120.62	114.52
81	A3	966	PSU	O2-C2-N1	-2.32	120.23	122.79
81	A3	2947	PSU	O2-C2-N1	-2.32	120.23	122.79
81	A3	3113	PSU	O2-C2-N1	-2.32	120.24	122.79
3	h1	95	PSU	O2-C2-N1	-2.31	120.25	122.79
81	A3	2257	PSU	O2-C2-N1	-2.30	120.26	122.79
81	A3	946	A2M	C3'-C2'-C1'	2.29	107.20	102.89
3	h1	1781	4AC	C6-C5-C4	2.29	119.76	116.96
3	h1	451	PSU	O4'-C1'-C2'	2.27	108.35	105.14
81	A3	684	PSU	O2-C2-N1	-2.25	120.31	122.79
81	A3	369	A2M	C2'-C3'-C4'	2.25	106.88	101.99
3	h1	306	PSU	O2-C2-N1	-2.24	120.33	122.79
3	h1	1283	4AC	C5-C4-N3	-2.24	119.00	122.59
81	A3	2920	OMG	O6-C6-C5	-2.23	120.02	124.37
81	A3	2978	PSU	O2-C2-N1	-2.23	120.34	122.79
81	A3	815	OMG	O6-C6-C5	-2.23	120.02	124.37
81	A3	399	OMG	O6-C6-C5	-2.23	120.03	124.37
81	A3	2239	OMG	O6-C6-C5	-2.22	120.05	124.37
81	A3	946	A2M	C2'-C3'-C4'	2.21	106.80	101.99
82	B3	78	OMG	O6-C6-C5	-2.21	120.05	124.37
81	A3	2920	OMG	N2-C2-N1	2.20	121.41	116.71
81	A3	2622	OMG	O6-C6-C5	-2.20	120.08	124.37
3	h1	1194	B8N	O4'-C1'-C2'	2.20	108.24	105.14
3	h1	392	OMG	O6-C6-C5	-2.19	120.09	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h1	246	OMG	O6-C6-C5	-2.19	120.09	124.37
81	A3	2412	OMG	N2-C2-N1	2.19	121.37	116.71
3	h1	1274	OMG	O6-C6-C5	-2.18	120.11	124.37
81	A3	2947	PSU	O4'-C1'-C2'	2.18	108.22	105.14
81	A3	2925	OMG	O6-C6-C5	-2.18	120.12	124.37
3	h1	598	OMG	O6-C6-C5	-2.17	120.13	124.37
81	A3	918	OMG	O6-C6-C5	-2.17	120.13	124.37
81	A3	296	OMG	O6-C6-C5	-2.17	120.14	124.37
81	A3	2394	OMG	O6-C6-C5	-2.16	120.15	124.37
81	A3	2883	PSU	O4'-C1'-C2'	2.16	108.19	105.14
81	A3	42	PSU	O2-C2-N1	-2.16	120.42	122.79
3	h1	607	PSU	O4'-C1'-C2'	2.16	108.18	105.14
81	A3	2818	OMG	O6-C6-C5	-2.16	120.16	124.37
81	A3	1857	OMG	O6-C6-C5	-2.15	120.18	124.37
81	A3	786	PSU	C6-C5-C4	2.14	119.70	118.20
81	A3	2412	OMG	O6-C6-C5	-2.14	120.20	124.37
3	h1	1579	A2M	C2'-C3'-C4'	2.13	106.63	101.99
81	A3	1068	OMU	O2-C2-N1	-2.12	119.96	122.79
81	A3	2829	PSU	O4'-C1'-C2'	2.12	108.14	105.14
81	A3	2654	OMG	O6-C6-C5	-2.12	120.24	124.37
81	A3	2796	OMG	O6-C6-C5	-2.10	120.26	124.37
81	A3	1894	OMU	O2-C2-N1	-2.10	119.99	122.79
81	A3	2868	PSU	O4'-C1'-C2'	2.10	108.11	105.14
81	A3	886	A2M	C3'-C2'-C1'	2.10	106.83	102.89
81	A3	2435	PSU	O4'-C1'-C2'	2.09	108.10	105.14
81	A3	2654	OMG	N1-C2-N3	-2.09	119.42	123.32
81	A3	2291	OMG	O6-C6-C5	-2.09	120.29	124.37
81	A3	2126	OMG	O6-C6-C5	-2.09	120.30	124.37
81	A3	2738	OMU	O2-C2-N1	-2.08	120.02	122.79
81	A3	2956	UR3	C6-N1-C2	-2.08	119.93	121.79
3	h1	339	PSU	O4'-C1'-C2'	2.08	108.08	105.14
3	h1	1433	OMG	O6-C6-C5	-2.07	120.33	124.37
81	A3	2424	OMU	O2-C2-N1	-2.07	120.04	122.79
3	h1	1194	B8N	C31-N3-C4	2.06	120.35	117.31
81	A3	2127	OMG	O6-C6-C5	-2.06	120.36	124.37
81	A3	2350	OMU	O2-C2-N1	-2.05	120.06	122.79
81	A3	464	PSU	O4'-C1'-C2'	2.05	108.03	105.14
3	h1	1433	OMG	N2-C2-N1	2.05	121.08	116.71
3	h1	123	OMU	O2-C2-N1	-2.05	120.06	122.79
3	h1	614	OMU	C1'-N1-C2	2.05	121.28	117.57
81	A3	804	OMU	O2-C2-N1	-2.05	120.06	122.79
81	A3	660	A2M	C3'-C2'-C1'	2.05	106.73	102.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A3	815	OMG	N2-C2-N1	2.04	121.06	116.71
81	A3	1685	PSU	O4'-C1'-C2'	2.04	108.02	105.14
81	A3	886	A2M	C2'-C3'-C4'	2.04	106.42	101.99
81	A3	2398	OMG	O6-C6-C5	-2.03	120.40	124.37
3	h1	800	A2M	O4'-C1'-C2'	-2.03	103.07	106.59
81	A3	2794	OMG	N1-C2-N3	-2.03	119.54	123.32
81	A3	2137	PSU	O2-C2-N1	-2.02	120.57	122.79
81	A3	787	OMU	O2-C2-N1	-2.02	120.10	122.79
81	A3	2329	A2M	O4'-C1'-C2'	-2.02	103.09	106.59
81	A3	2796	OMG	N2-C2-N1	2.02	121.00	116.71
81	A3	675	OMU	O2-C2-N1	-2.01	120.12	122.79
81	A3	2794	OMG	O6-C6-C5	-2.00	120.46	124.37
81	A3	1461	OMG	N2-C2-N1	2.00	120.98	116.71
81	A3	1448	OMC	O2-C2-N3	-2.00	119.07	122.33
81	A3	1857	OMG	N2-C2-N1	2.00	120.97	116.71

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	B3	78	OMG	O4'-C4'-C5'-O5'
82	B3	78	OMG	C3'-C4'-C5'-O5'
82	B3	96	PSU	C3'-C4'-C5'-O5'
82	B3	96	PSU	O4'-C4'-C5'-O5'
3	h1	38	OMC	C3'-C4'-C5'-O5'
3	h1	123	OMU	O4'-C4'-C5'-O5'
3	h1	140	OMC	C3'-C4'-C5'-O5'
3	h1	140	OMC	O4'-C4'-C5'-O5'
3	h1	392	OMG	O4'-C4'-C5'-O5'
3	h1	418	OMC	C1'-C2'-O2'-CM2
3	h1	418	OMC	C3'-C2'-O2'-CM2
3	h1	584	PSU	C2'-C1'-C5-C4
3	h1	584	PSU	C2'-C1'-C5-C6
3	h1	584	PSU	C3'-C4'-C5'-O5'
3	h1	598	OMG	O4'-C4'-C5'-O5'
3	h1	614	OMU	O4'-C4'-C5'-O5'
3	h1	886	OMU	C1'-C2'-O2'-CM2
3	h1	1194	B8N	N34-C33-C34-O35
3	h1	1234	OMU	O4'-C4'-C5'-O5'
3	h1	1274	OMG	O4'-C4'-C5'-O5'
3	h1	1274	OMG	C3'-C4'-C5'-O5'
3	h1	1308	PSU	C2'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	h1	1579	A2M	O4'-C4'-C5'-O5'
3	h1	1787	PSU	C3'-C4'-C5'-O5'
3	h1	1787	PSU	O4'-C4'-C5'-O5'
3	h1	1790	MA6	O4'-C4'-C5'-O5'
3	h1	1790	MA6	C3'-C4'-C5'-O5'
81	A3	40	OMC	C3'-C2'-O2'-CM2
81	A3	296	OMG	O4'-C4'-C5'-O5'
81	A3	296	OMG	C3'-C4'-C5'-O5'
81	A3	660	A2M	C1'-C2'-O2'-CM'
81	A3	786	PSU	C2'-C1'-C5-C4
81	A3	918	OMG	O4'-C4'-C5'-O5'
81	A3	918	OMG	C3'-C4'-C5'-O5'
81	A3	2200	OMC	C2'-C1'-N1-C6
81	A3	2259	A2M	O4'-C4'-C5'-O5'
81	A3	2259	A2M	C3'-C4'-C5'-O5'
81	A3	2284	A2M	O4'-C4'-C5'-O5'
81	A3	2291	OMG	O4'-C4'-C5'-O5'
81	A3	2291	OMG	C3'-C4'-C5'-O5'
81	A3	2317	PSU	O4'-C4'-C5'-O5'
81	A3	2368	OMC	C3'-C4'-C5'-O5'
81	A3	2368	OMC	O4'-C4'-C5'-O5'
81	A3	2804	A2M	C1'-C2'-O2'-CM'
81	A3	2956	UR3	O4'-C4'-C5'-O5'
81	A3	2956	UR3	C3'-C4'-C5'-O5'
81	A3	2200	OMC	C2'-C1'-N1-C2
3	h1	38	OMC	O4'-C4'-C5'-O5'
3	h1	123	OMU	C3'-C4'-C5'-O5'
3	h1	392	OMG	C3'-C4'-C5'-O5'
3	h1	581	OMU	O4'-C4'-C5'-O5'
3	h1	598	OMG	C3'-C4'-C5'-O5'
3	h1	614	OMU	C3'-C4'-C5'-O5'
3	h1	622	A2M	O4'-C4'-C5'-O5'
3	h1	622	A2M	C3'-C4'-C5'-O5'
3	h1	886	OMU	C3'-C4'-C5'-O5'
3	h1	1234	OMU	C3'-C4'-C5'-O5'
3	h1	1272	OMU	O4'-C4'-C5'-O5'
3	h1	1579	A2M	C3'-C4'-C5'-O5'
81	A3	399	OMG	O4'-C4'-C5'-O5'
81	A3	399	OMG	C3'-C4'-C5'-O5'
81	A3	1002	PSU	C3'-C4'-C5'-O5'
81	A3	2914	A2M	C3'-C4'-C5'-O5'
3	h1	584	PSU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	h1	886	OMU	O4'-C4'-C5'-O5'
81	A3	1002	PSU	O4'-C4'-C5'-O5'
81	A3	2284	A2M	C3'-C4'-C5'-O5'
81	A3	2317	PSU	C3'-C4'-C5'-O5'
81	A3	2914	A2M	O4'-C4'-C5'-O5'
81	A3	827	A2M	C3'-C2'-O2'-CM'
3	h1	1194	B8N	N34-C33-C34-O36
81	A3	1378	A2M	O4'-C4'-C5'-O5'
81	A3	2873	5MC	C2'-C1'-N1-C6
81	A3	786	PSU	O4'-C4'-C5'-O5'
81	A3	2269	PSU	C3'-C4'-C5'-O5'
3	h1	1790	MA6	C5-C6-N6-C10
81	A3	2321	PSU	O4'-C4'-C5'-O5'
3	h1	581	OMU	C3'-C4'-C5'-O5'
81	A3	2413	OMU	C1'-C2'-O2'-CM2
3	h1	1790	MA6	C4'-C5'-O5'-P
3	h1	544	A2M	C3'-C4'-C5'-O5'
81	A3	2200	OMC	O4'-C1'-N1-C2
81	A3	2368	OMC	C3'-C2'-O2'-CM2
81	A3	2413	OMU	C3'-C2'-O2'-CM2
81	A3	2200	OMC	O4'-C1'-N1-C6
81	A3	2873	5MC	O4'-C1'-N1-C6
3	h1	1433	OMG	C4'-C5'-O5'-P
81	A3	228	PSU	C3'-C4'-C5'-O5'
81	A3	946	A2M	C3'-C4'-C5'-O5'
81	A3	2926	PSU	C3'-C4'-C5'-O5'
3	h1	598	OMG	C4'-C5'-O5'-P
81	A3	2317	PSU	C4'-C5'-O5'-P
81	A3	2873	5MC	O4'-C1'-N1-C2
81	A3	2926	PSU	C4'-C5'-O5'-P
81	A3	2269	PSU	O4'-C4'-C5'-O5'
81	A3	2873	5MC	C2'-C1'-N1-C2
81	A3	827	A2M	C4'-C5'-O5'-P
81	A3	144	OMU	O4'-C4'-C5'-O5'
81	A3	1448	OMC	C2'-C1'-N1-C6
81	A3	1461	OMG	C4'-C5'-O5'-P
81	A3	2804	A2M	C4'-C5'-O5'-P
81	A3	1378	A2M	C3'-C4'-C5'-O5'
3	h1	584	PSU	O4'-C1'-C5-C4
3	h1	1194	B8N	O4'-C1'-C5-C4
3	h1	1308	PSU	O4'-C1'-C5-C4
81	A3	2947	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
81	A3	2412	OMG	C3'-C2'-O2'-CM2
81	A3	1448	OMC	C2'-C1'-N1-C2
3	h1	258	PSU	O4'-C4'-C5'-O5'
81	A3	2261	PSU	O4'-C4'-C5'-O5'
81	A3	2263	PSU	O4'-C4'-C5'-O5'
81	A3	786	PSU	C3'-C4'-C5'-O5'
81	A3	2321	PSU	C3'-C4'-C5'-O5'
81	A3	369	A2M	C1'-C2'-O2'-CM'
81	A3	946	A2M	O4'-C4'-C5'-O5'
81	A3	2926	PSU	O4'-C4'-C5'-O5'
3	h1	584	PSU	O4'-C1'-C5-C6
3	h1	1524	PSU	O4'-C1'-C5-C6
81	A3	970	PSU	O4'-C1'-C5-C6
81	A3	2947	PSU	O4'-C1'-C5-C6
81	A3	827	A2M	O4'-C4'-C5'-O5'
3	h1	1524	PSU	O4'-C4'-C5'-O5'
81	A3	1448	OMC	O4'-C4'-C5'-O5'
3	h1	614	OMU	C2'-C1'-N1-C2
3	h1	544	A2M	C4'-C5'-O5'-P
3	h1	1027	PSU	C4'-C5'-O5'-P
3	h1	1272	OMU	C4'-C5'-O5'-P
81	A3	660	A2M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 290 ligands modelled in this entry, 283 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	SPD	h1	2016	-	9,9,9	0.33	0	8,8,8	0.66	0
86	SPM	h1	2017	-	13,13,13	0.47	0	12,12,12	0.95	0
86	SPM	A3	3451	-	13,13,13	0.35	0	12,12,12	1.05	0
85	SPD	A3	3450	-	9,9,9	0.31	0	8,8,8	0.51	0
86	SPM	h1	2018	-	13,13,13	0.38	0	12,12,12	1.01	0
86	SPM	h1	2019	-	13,13,13	0.42	0	12,12,12	1.03	0
86	SPM	A3	3452	-	13,13,13	0.37	0	12,12,12	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	h1	2016	-	-	4/7/7/7	-
86	SPM	h1	2017	-	-	5/11/11/11	-
86	SPM	A3	3451	-	-	5/11/11/11	-
85	SPD	A3	3450	-	-	2/7/7/7	-
86	SPM	h1	2018	-	-	3/11/11/11	-
86	SPM	h1	2019	-	-	2/11/11/11	-
86	SPM	A3	3452	-	-	7/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	A3	3452	SPM	N10-C11-C12-C13
86	A3	3452	SPM	C7-C8-C9-N10
86	h1	2017	SPM	C7-C8-C9-N10
85	h1	2016	SPD	C3-C4-C5-N6
85	h1	2016	SPD	N6-C7-C8-C9
86	h1	2017	SPM	N10-C11-C12-C13
85	h1	2016	SPD	C4-C5-N6-C7
86	A3	3452	SPM	N5-C6-C7-C8
86	h1	2019	SPM	N5-C6-C7-C8
85	h1	2016	SPD	C8-C7-N6-C5
86	h1	2017	SPM	C8-C9-N10-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
86	A3	3451	SPM	C3-C4-N5-C6
86	h1	2017	SPM	C11-C12-C13-N14
86	A3	3451	SPM	N10-C11-C12-C13
85	A3	3450	SPD	C2-C3-C4-C5
86	h1	2018	SPM	C6-C7-C8-C9
86	A3	3451	SPM	C7-C8-C9-N10
86	A3	3452	SPM	C7-C6-N5-C4
86	A3	3451	SPM	C8-C9-N10-C11
86	h1	2019	SPM	C11-C12-C13-N14
86	A3	3452	SPM	C2-C3-C4-N5
86	h1	2017	SPM	C7-C6-N5-C4
86	h1	2018	SPM	C7-C6-N5-C4
86	A3	3452	SPM	C8-C9-N10-C11
86	A3	3451	SPM	C11-C12-C13-N14
86	A3	3452	SPM	C11-C12-C13-N14
86	h1	2018	SPM	C8-C9-N10-C11
85	A3	3450	SPD	C3-C4-C5-N6

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
81	A3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A3	2973:C	O3'	2974:A	P	4.08

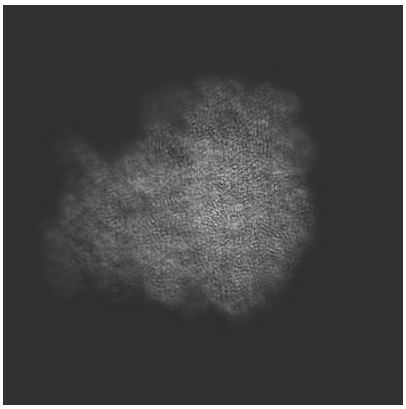
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15806. These allow visual inspection of the internal detail of the map and identification of artifacts.

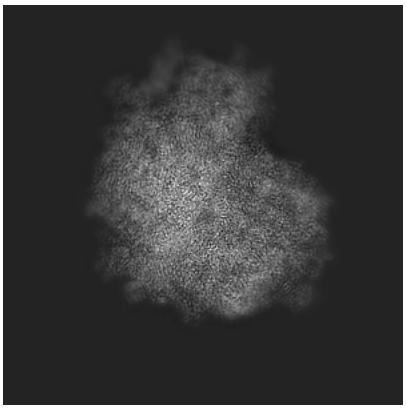
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

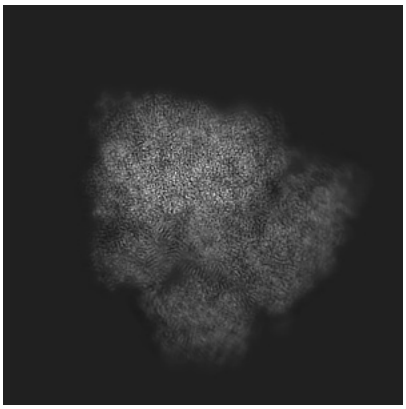
6.1.1 Primary map



X

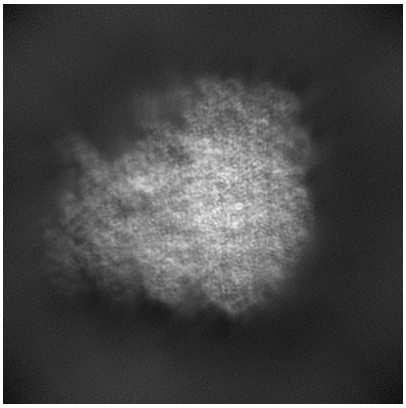


Y

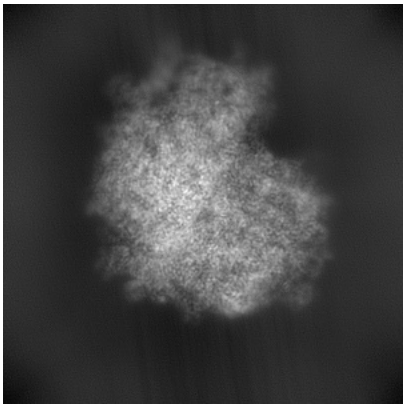


Z

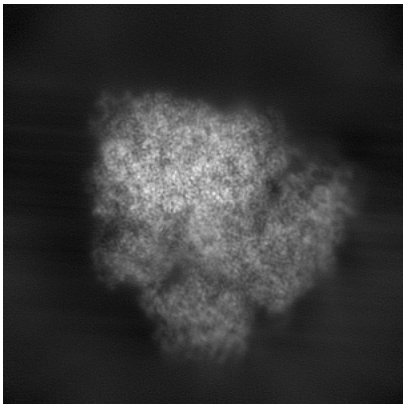
6.1.2 Raw map



X



Y

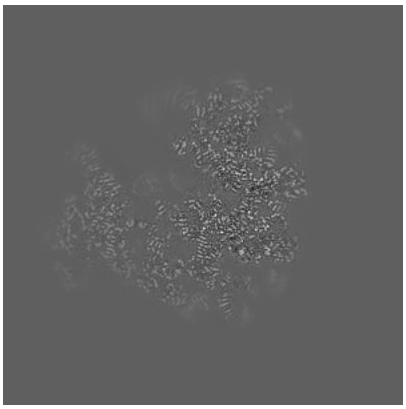


Z

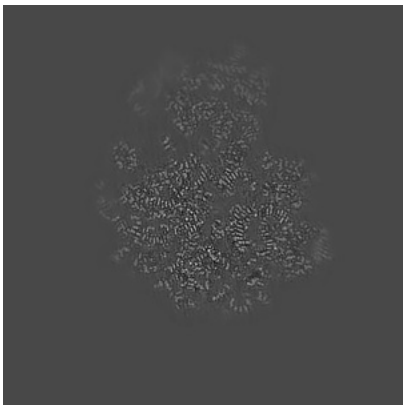
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

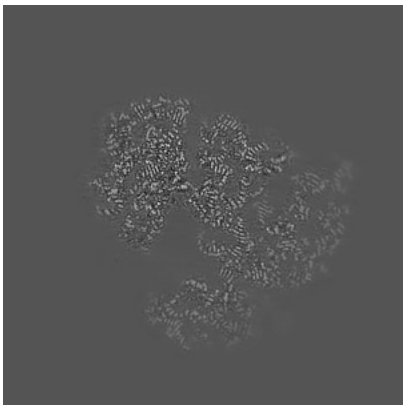
6.2.1 Primary map



X Index: 225

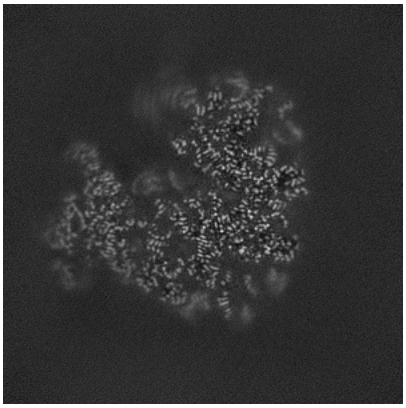


Y Index: 225

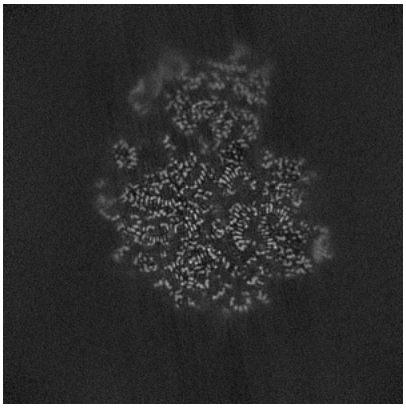


Z Index: 225

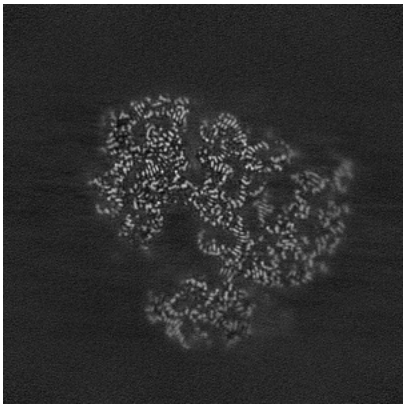
6.2.2 Raw map



X Index: 225



Y Index: 225

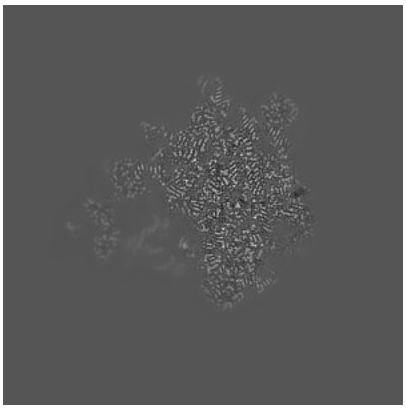


Z Index: 225

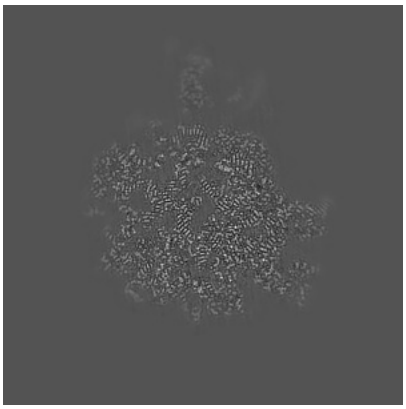
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

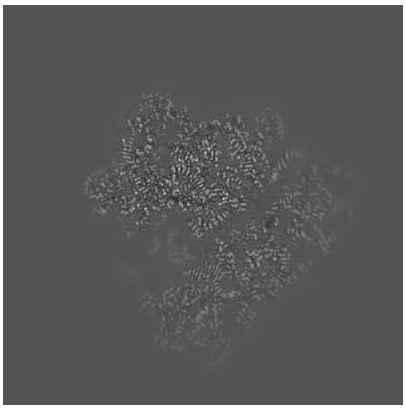
6.3.1 Primary map



X Index: 169

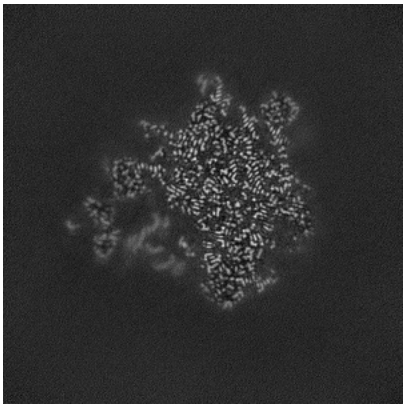


Y Index: 262

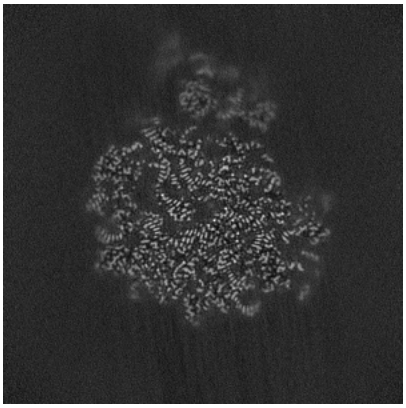


Z Index: 206

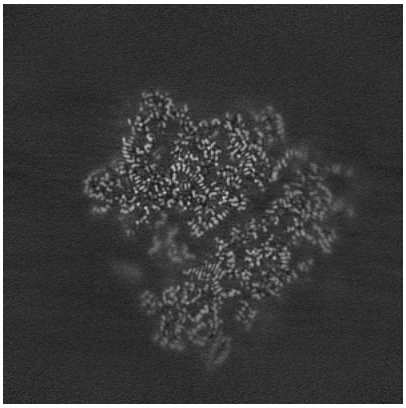
6.3.2 Raw map



X Index: 169



Y Index: 254

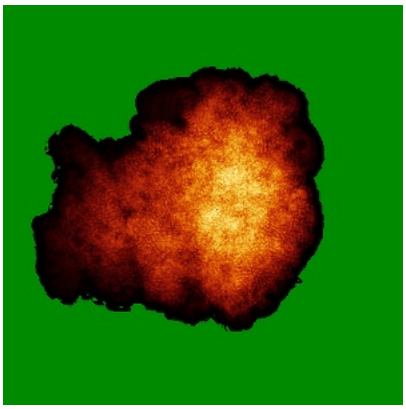


Z Index: 206

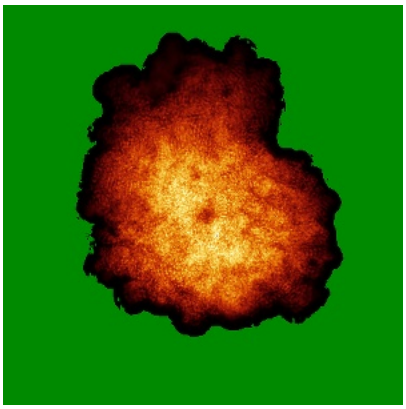
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

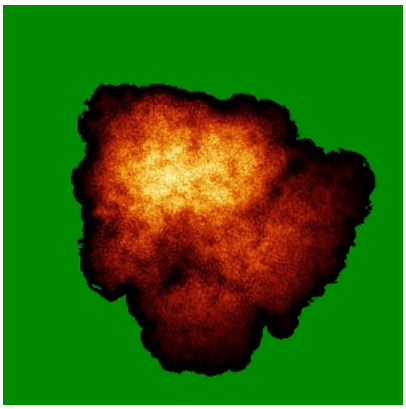
6.4.1 Primary map



X

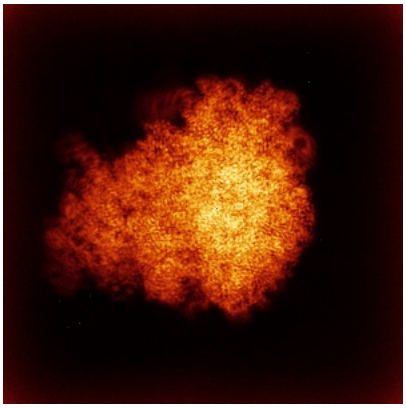


Y

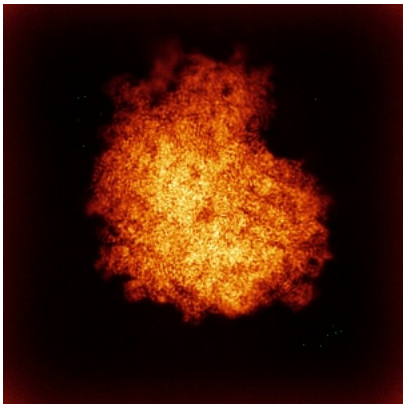


Z

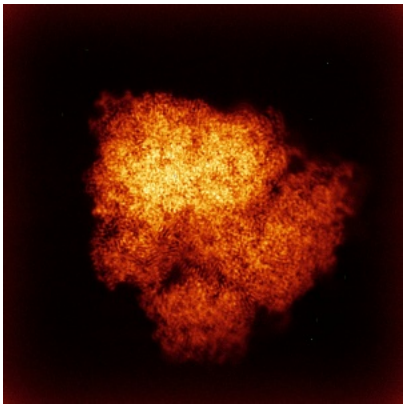
6.4.2 Raw map



X



Y

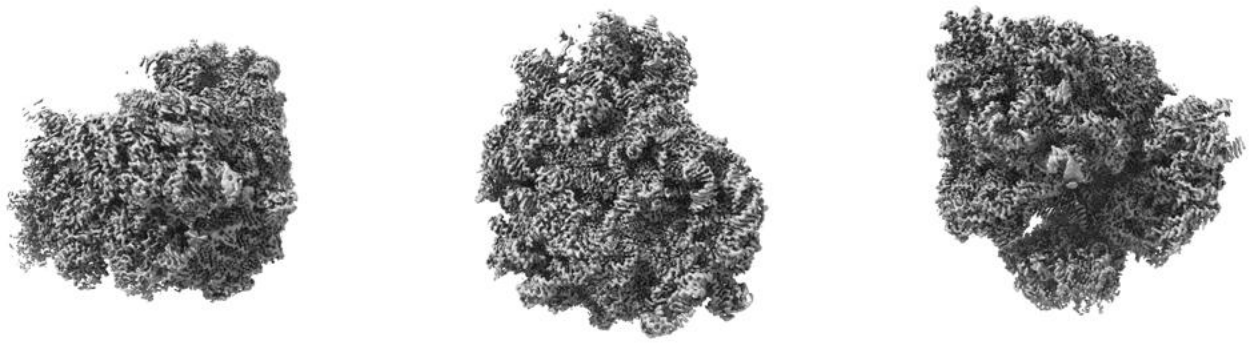


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

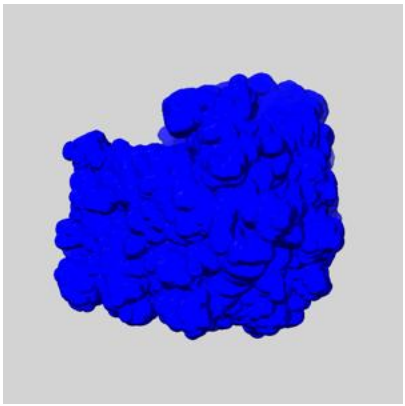
6.6 Mask visualisation (i)

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

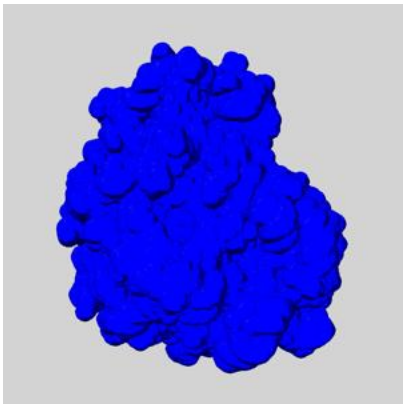
A mask typically either:

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

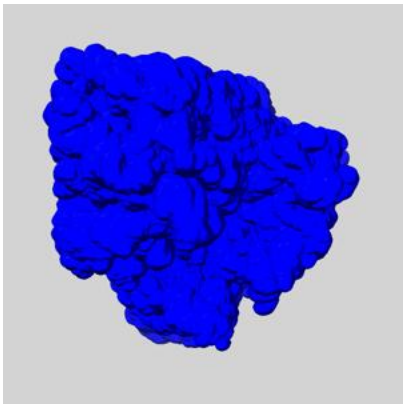
6.6.1 emd_15806_msk_1.map (i)



X



Y

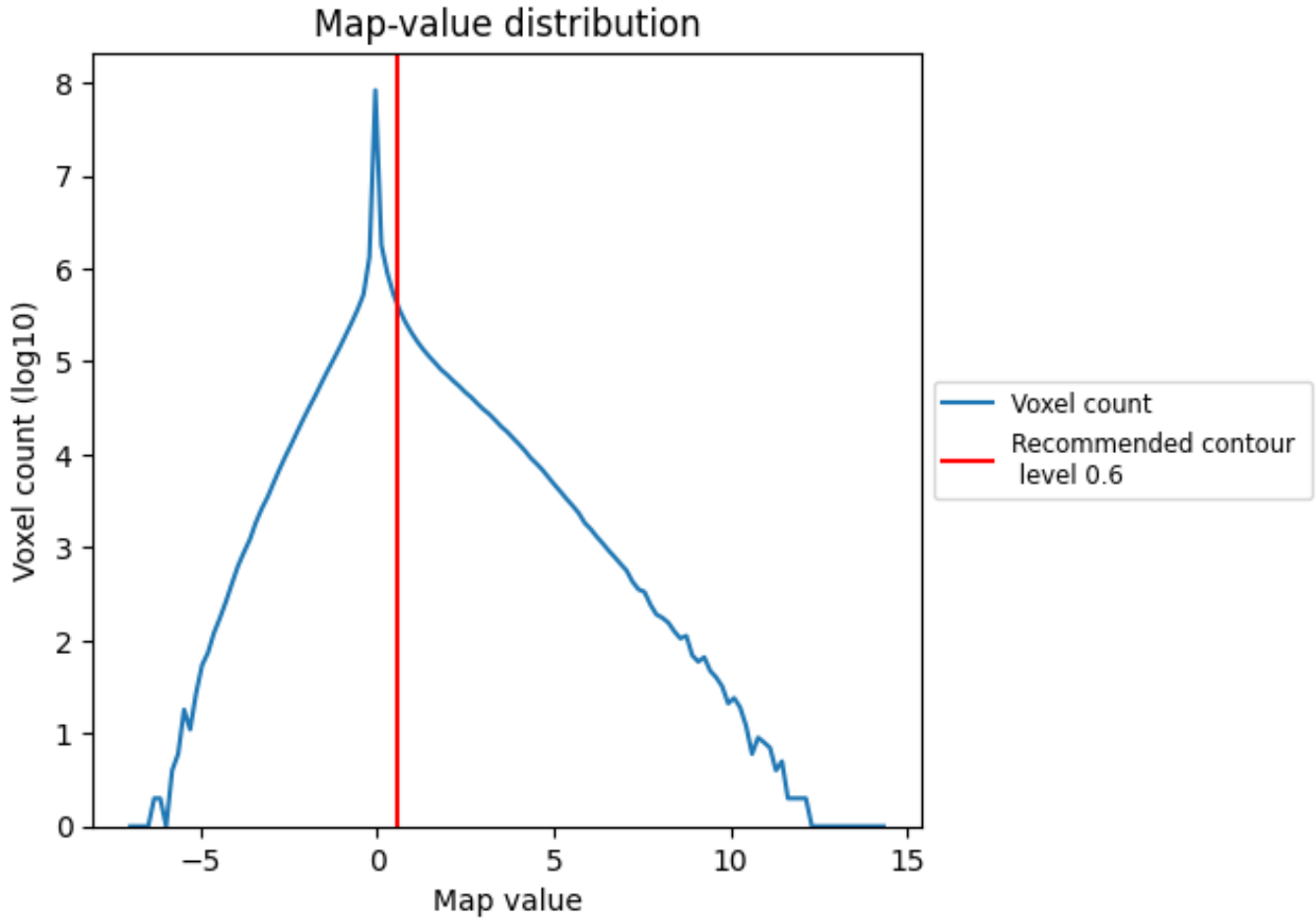


Z

7 Map analysis

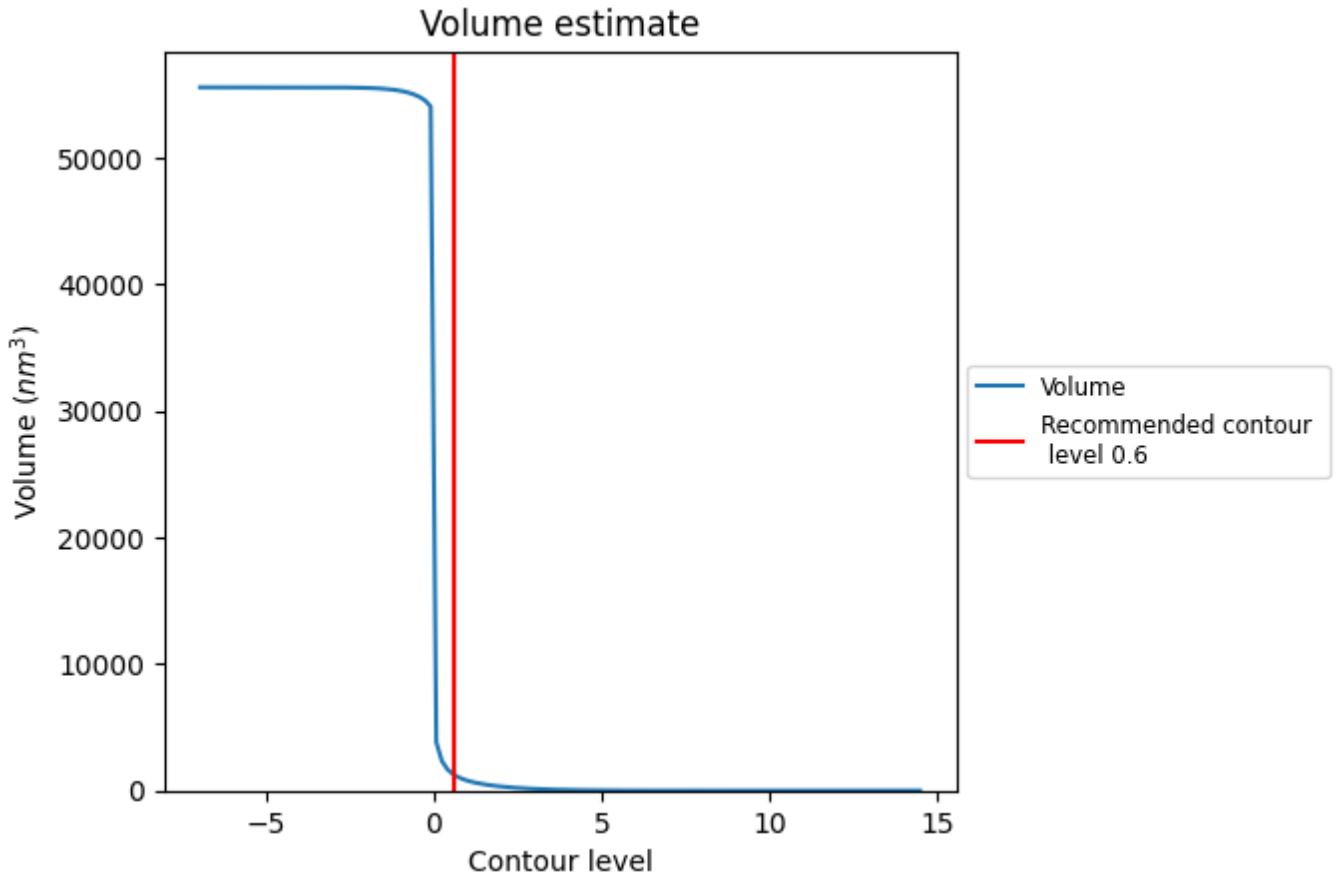
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

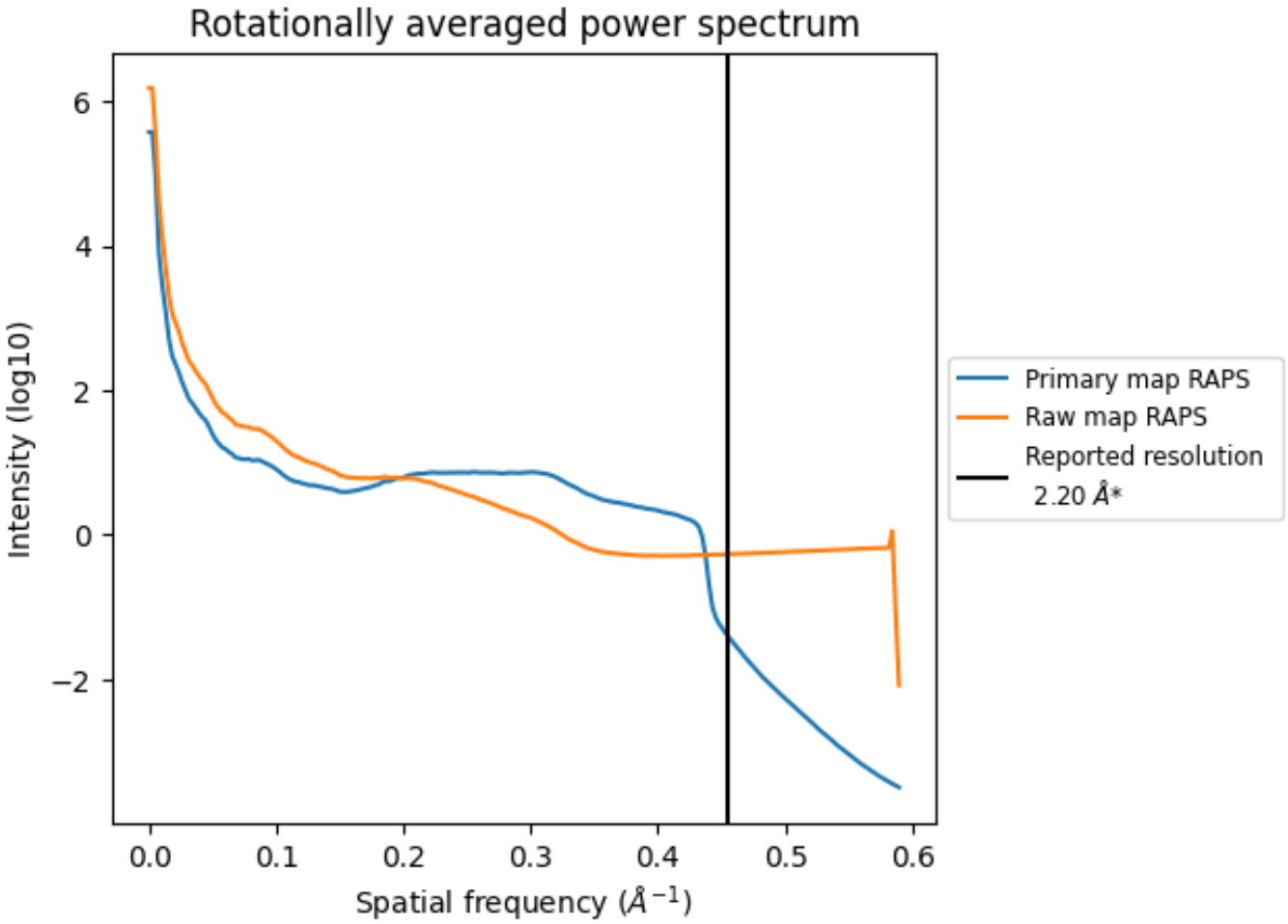
7.2 Volume estimate



The volume at the recommended contour level is 1255 nm^3; this corresponds to an approximate mass of 1133 kDa.

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

7.3 Rotationally averaged power spectrum (i)

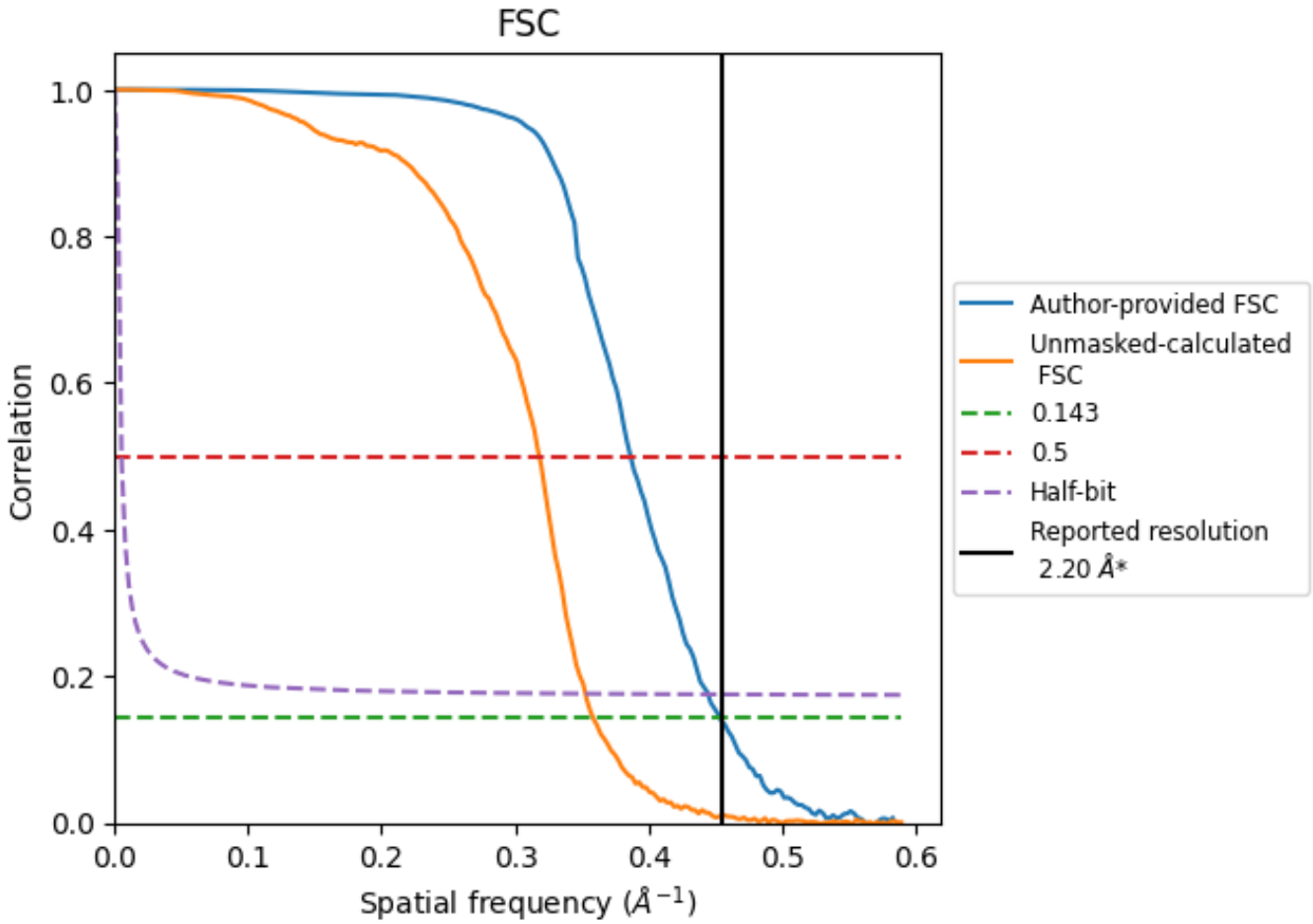


*Reported resolution corresponds to spatial frequency of 0.455 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.455 $Å^{-1}$

8.2 Resolution estimates (i)

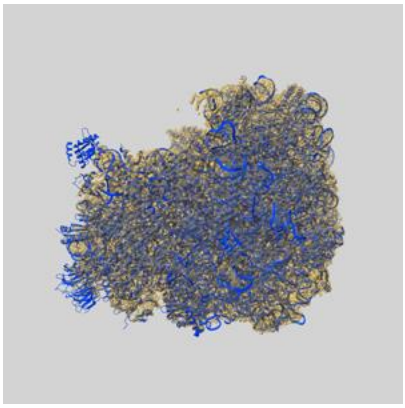
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.59	2.25
Unmasked-calculated*	2.79	3.14	2.83

*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 2.79 differs from the reported value 2.2 by more than 10 %

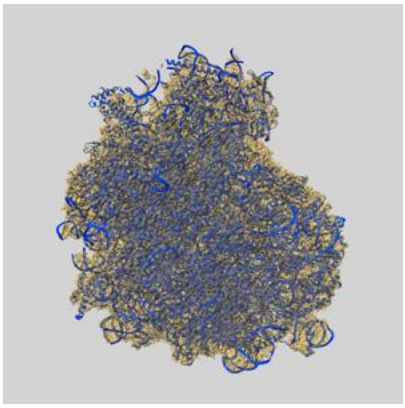
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15806 and PDB model 8B2L. Per-residue inclusion information can be found in section 3 on page 25.

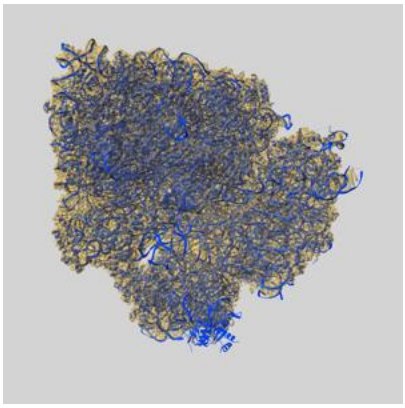
9.1 Map-model overlay



X



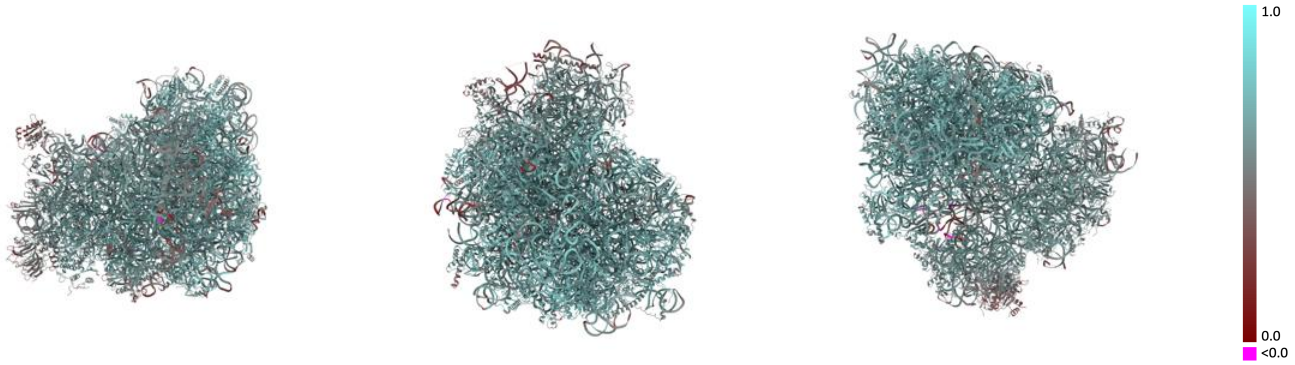
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

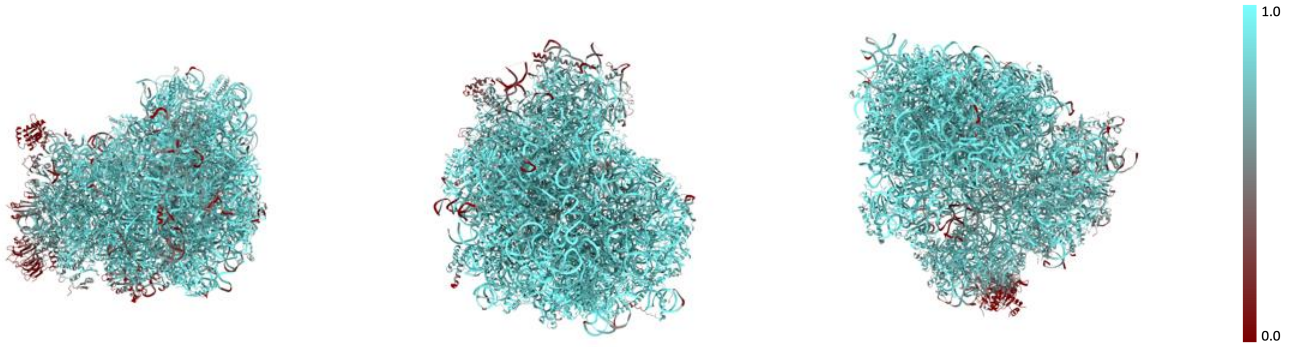
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

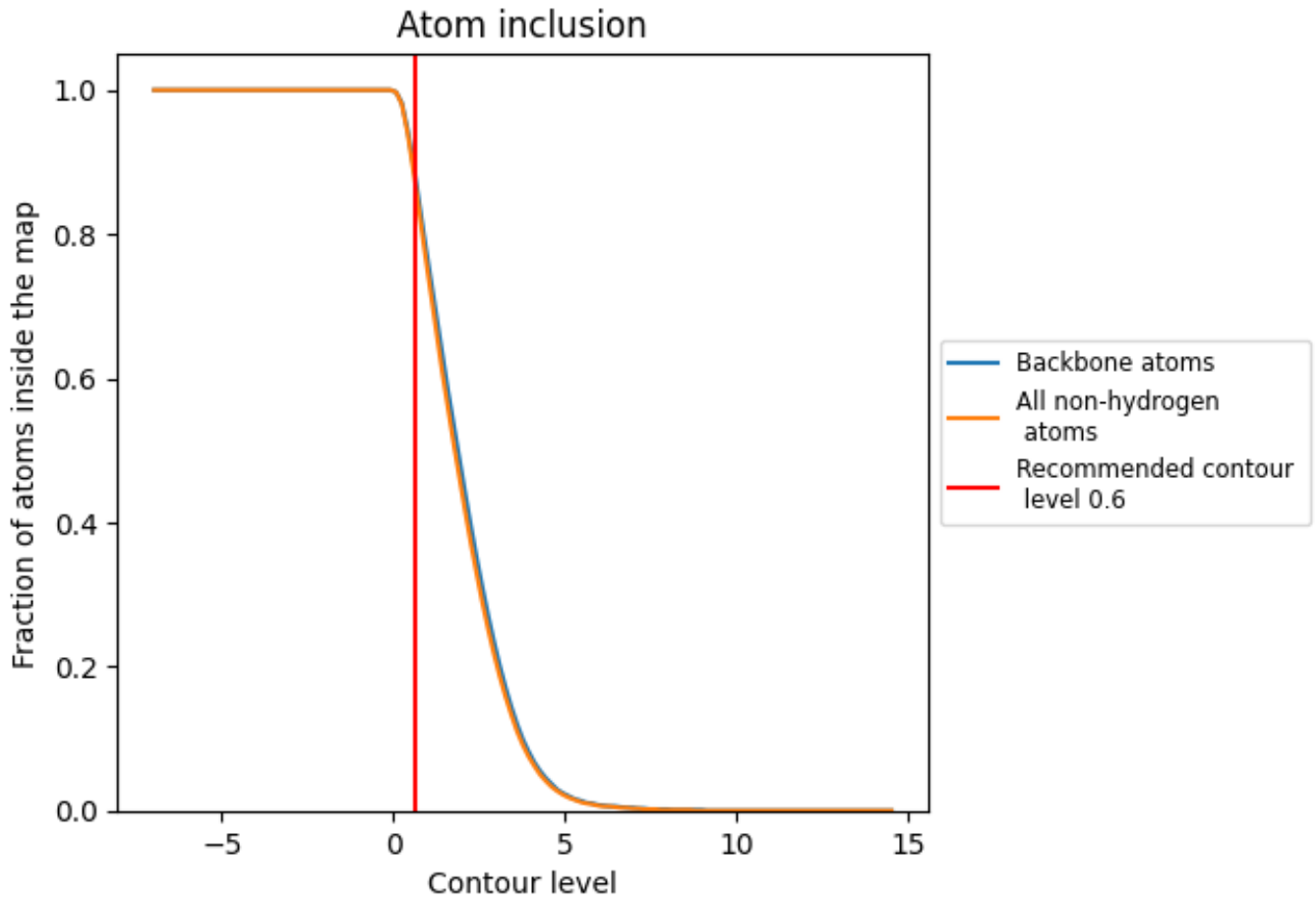
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.6390
A1	0.8190	0.5960
A3	0.9420	0.6580
B1	0.8630	0.5920
B3	0.9250	0.6540
C1	0.0330	0.3580
C3	0.9920	0.6690
D1	0.5440	0.5170
D3	0.9470	0.6870
E1	0.7930	0.5800
E3	0.9330	0.6720
F1	0.8900	0.6410
F3	0.9950	0.7280
G1	0.8220	0.6030
G3	0.9850	0.7180
H1	0.6990	0.5590
H3	0.8540	0.6410
I1	0.6890	0.5490
I3	0.9690	0.6980
J1	0.9250	0.6660
J3	0.9700	0.6940
K1	0.7610	0.5970
K3	0.7590	0.5600
L1	0.7270	0.5640
L3	0.9570	0.6940
M1	0.7750	0.6010
M3	0.9300	0.6620
N1	0.1380	0.4170
N3	0.9490	0.6890
O1	0.5500	0.5350
O3	0.9770	0.7160
P1	0.8080	0.5880
P3	0.9180	0.6510
Q1	0.1780	0.4430
Q3	0.8990	0.6680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
R1	0.5160	0.5290
R3	0.9800	0.7230
S1	0.9260	0.6540
S3	0.9820	0.7150
T1	0.9500	0.6840
T3	0.9280	0.6820
U1	0.8230	0.6030
U3	0.9420	0.6640
V1	0.8900	0.6270
V3	0.9940	0.7270
W1	0.8970	0.6440
W2	0.7580	0.4970
W3	0.8320	0.6110
X1	0.8990	0.6400
X3	0.9840	0.7200
Y1	0.7710	0.5880
Y3	0.9610	0.6930
Z1	0.8330	0.6130
Z3	0.9730	0.7140
a1	0.6660	0.5540
a3	0.9650	0.7040
b1	0.8110	0.5990
b3	0.8580	0.6320
c1	0.8940	0.6520
c3	0.8650	0.6390
d1	0.7620	0.5730
d3	0.9680	0.7060
e1	0.9660	0.6780
e3	0.9690	0.7020
f1	0.7230	0.5770
f3	0.9620	0.7020
g3	0.9640	0.6900
h1	0.9020	0.6130
h3	0.8880	0.6410
i2	0.6690	0.5070
j3	0.9670	0.7050
k1	0.6380	0.5290
k3	0.9520	0.6830
l1	0.5510	0.5210
l3	0.3670	0.3350
m3	0.9560	0.6860
n3	0.9210	0.6620

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
o3	0.9910	0.7270
p3	0.9360	0.6640
q3	0.9460	0.6940
r3	0.9710	0.7100
s3	0.9290	0.6870
t3	0.8750	0.6240
u3	0.9090	0.6590