



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 08:54 pm GMT

PDB ID : 6ZJ3
EMDB ID : EMD-11232
Title : Cryo-EM structure of the highly atypical cytoplasmic ribosome of *Euglena gracilis*
Authors : Matzov, D.; Halfon, H.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Gray, M.W.; Yonath, A.E.; Shalev-Benami, M.
Deposited on : 2020-06-27
Resolution : 3.15 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:

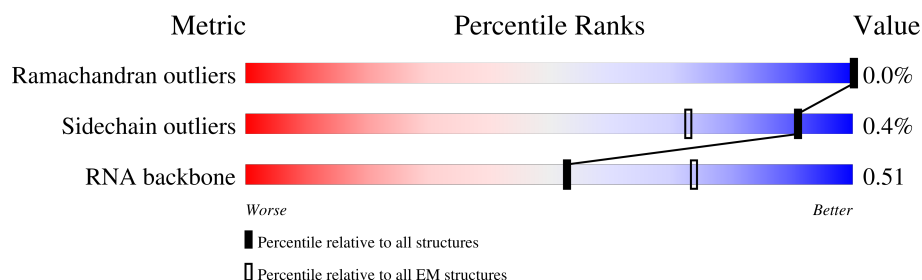
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.15 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.




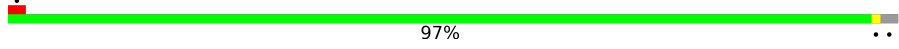


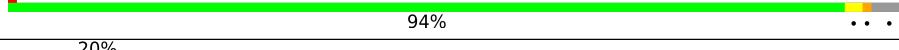
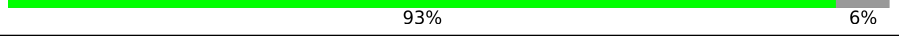
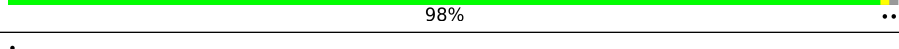
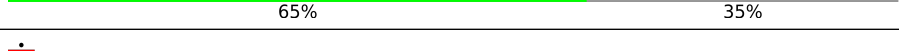
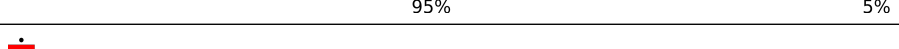
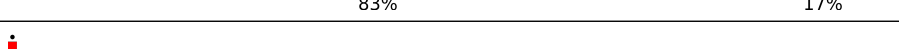
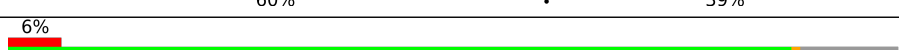

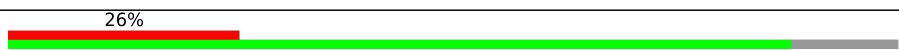
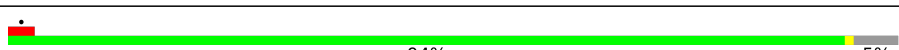
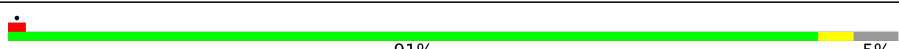

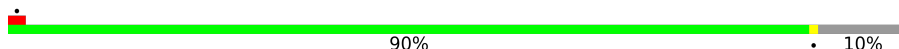


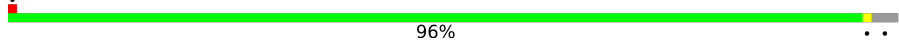
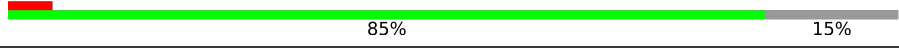
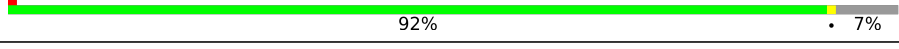



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S1	2315	
2	S2	76	
3	S3	76	
4	S4	76	
5	S5	12	
6	SA	249	
7	SB	261	
8	SC	220	

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Mol	Chain	Length	Quality of chain
9	SD	196	
10	SE	271	
11	SF	257	
12	SG	283	
13	SH	190	
14	SI	200	
15	SJ	130	
16	SK	304	
17	SL	151	
18	SM	121	
19	SN	152	
20	SO	152	
21	SP	143	
22	SQ	139	
23	SR	153	
24	SS	55	
25	ST	151	
26	SU	164	
27	SV	145	
28	SW	150	
29	SX	148	
30	SY	96	
31	SZ	137	
32	Sa	119	
33	Sb	120	

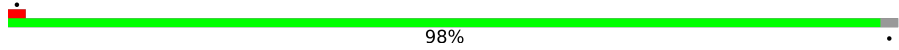
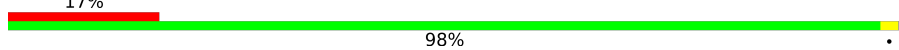

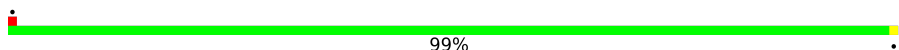
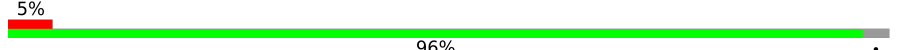
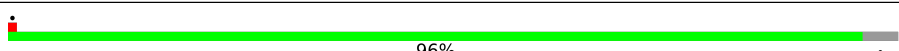
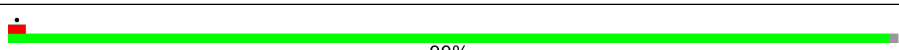

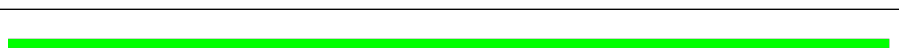
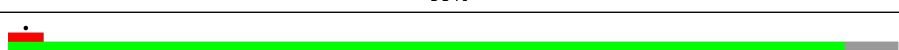
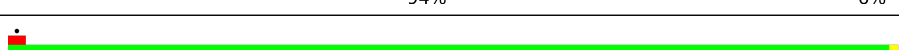
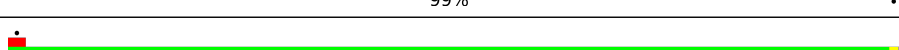
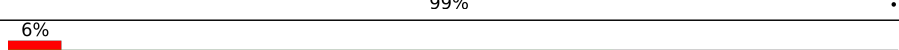
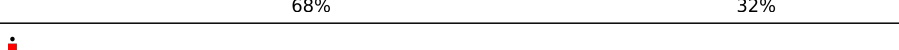
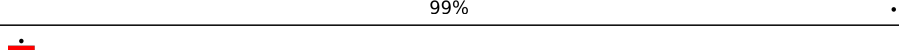
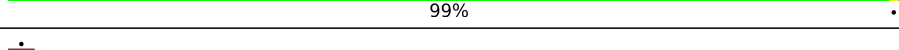
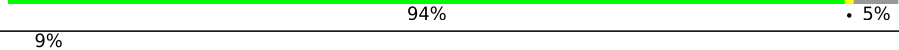




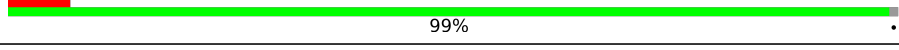
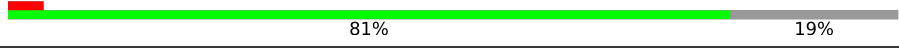
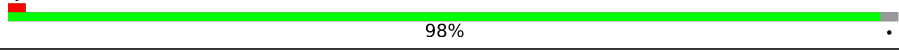

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Mol	Chain	Length	Quality of chain
34	Sc	86	
35	Sd	76	
36	Se	67	
37	Sf	157	
38	Sg	295	
39	Sh	317	
40	LA	163	
41	LB	133	
42	LC	350	
43	LD	116	
44	LE	698	
45	LF	527	
46	LG	234	
47	LH	744	
48	LI	617	
49	LJ	164	
50	LK	64	
51	LL	95	
52	LM	58	
53	LN	86	
54	LO	120	
55	LP	264	
56	LQ	410	
57	LR	375	
58	LS	191	



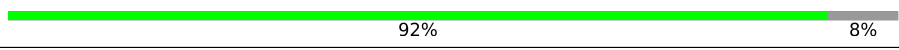
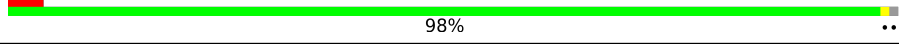

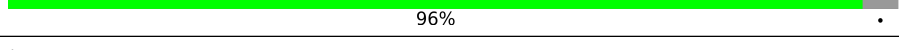
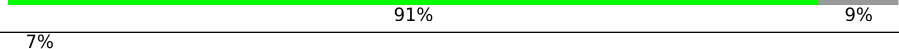
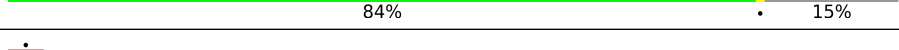
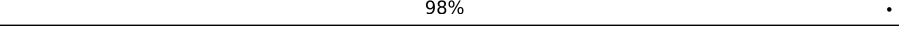
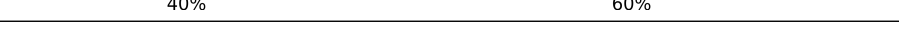
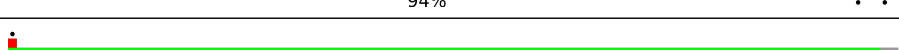
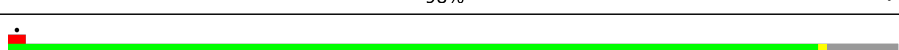


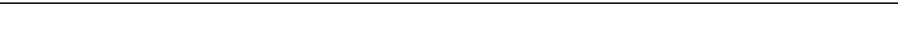
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Mol	Chain	Length	Quality of chain
59	LT	193	
60	LU	195	
61	LV	295	
62	LW	209	
63	LX	226	
64	LY	140	
65	LZ	219	
66	La	152	
67	Lb	204	
68	Lc	215	
69	Ld	260	
70	Le	193	
71	Lf	250	
72	Lg	182	
73	Lh	159	
74	Li	164	
75	Lj	170	
76	Lk	163	
77	Ll	146	
78	Lm	157	
79	Ln	134	
80	Lo	72	
81	Lp	123	
82	Lq	117	
83	Lr	242	

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Mol	Chain	Length	Quality of chain
84	Ls	109	
85	Lt	151	
86	Lu	139	
87	Lv	115	
88	Lw	128	
89	Lx	106	
90	Ly	117	
91	Lz	82	
92	L1	51	
93	L2	126	
94	L3	34	
95	L5	92	
96	L4	106	
97	L6	69	
98	L7	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	B8N	S1	1601	X	-	-	-

2 Entry composition [i](#)

There are 100 unique types of molecules in this entry. The entry contains 223607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S1	2024	Total	C	N	O	P	0	0
			43278	19338	7765	14151	2024		

- Molecule 2 is a RNA chain called A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	S2	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

- Molecule 3 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S3	76	Total	C	N	O	P	0	0
			1614	721	285	533	75		

- Molecule 4 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S4	76	Total	C	N	O	P	0	0
			1621	724	292	530	75		

- Molecule 5 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

- Molecule 6 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	221	Total	C	N	O	S	0	0
			1797	1133	331	323	10		

- Molecule 7 is a protein called Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SB	207	Total	C	N	O	S	0	0
			1657	1058	295	293	11		

- Molecule 8 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SC	212	Total	C	N	O	S	0	0
			1675	1061	310	296	8		

- Molecule 9 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SD	177	Total	C	N	O	S	0	0
			1436	913	277	240	6		

- Molecule 10 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SE	265	Total	C	N	O	S	0	0
			2125	1366	394	357	8		

- Molecule 11 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SF	221	Total	C	N	O	S	0	0
			1713	1105	301	300	7		

- Molecule 12 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SG	248	Total	C	N	O	S	0	0
			2016	1263	402	345	6		

- Molecule 13 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	182	Total	C	N	O	S	0	0
			1450	908	271	266	5		

- Molecule 14 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SI	187	Total	C	N	O	S	0	0
			1514	967	284	262	1		

- Molecule 15 is a protein called Ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SJ	129	Total	C	N	O	S	0	0
			1037	658	194	178	7		

- Molecule 16 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SK	199	Total	C	N	O	S	0	0
			1644	1038	338	264	4		

- Molecule 17 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SL	143	Total	C	N	O	S	0	0
			1144	725	220	194	5		

- Molecule 18 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SM	101	Total	C	N	O	S	0	0
			796	501	150	142	3		

- Molecule 19 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SN	92	Total	C	N	O	S	0	0
			775	509	130	133	3		

- Molecule 20 is a protein called Ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SO	135	Total	C	N	O	S	0	0
			1010	616	198	189	7		

- Molecule 21 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SP	141	Total	C	N	O	S	0	0
			1101	692	216	188	5		

- Molecule 22 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SQ	122	Total	C	N	O	S	0	0
			919	574	164	171	10		

- Molecule 23 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SR	146	Total	C	N	O	S	0	0
			1181	737	234	204	6		

- Molecule 24 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SS	52	Total	C	N	O	S	0	0
			433	267	95	68	3		

- Molecule 25 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	ST	148	Total	C	N	O	S	0	0
			1180	746	228	202	4		

- Molecule 26 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SU	148	Total	C	N	O	S	0	0
			1225	793	230	199	3		

- Molecule 27 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SV	125	Total	C	N	O	S	0	0
			998	625	183	183	7		

- Molecule 28 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SW	125	Total	C	N	O	S	0	0
			990	632	186	167	5		

- Molecule 29 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SX	143	Total	C	N	O	S	0	0
			1125	720	205	195	5		

- Molecule 30 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	82	Total	C	N	O	S	0	0
			624	391	111	119	3		

- Molecule 31 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	127	Total	C	N	O	S	0	0
			1052	668	205	174	5		

- Molecule 32 is a protein called Ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	78	Total	C	N	O	S	0	0
			633	405	118	108	2		

- Molecule 33 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	97	Total	C	N	O	S	0	0
			780	481	162	129	8		

- Molecule 34 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sc	84	Total	C	N	O	S	0	0
			649	414	115	114	6		

- Molecule 35 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sd	63	Total	C	N	O	S	0	0
			499	304	103	90	2		

- Molecule 36 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Se	64	Total	C	N	O		0	0
			484	305	101	78			

- Molecule 37 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Sf	64	Total	C	N	O	S	0	0
			508	322	95	85	6		

- Molecule 38 is a protein called Ribosomal protein eSEug1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Sg	199	Total	C	N	O	S	0	0
			1597	1022	301	267	7		

- Molecule 39 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Sh	311	Total	C	N	O	S	0	0
			2393	1516	407	454	16		

- Molecule 40 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LA	160	Total	C	N	O	P	0	0
			3423	1528	613	1122	160		

- Molecule 41 is a RNA chain called LSU rRNA chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LB	133	Total	C	N	O	P	0	0
			2847	1275	523	916	133		

- Molecule 42 is a RNA chain called LSU rRNA chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LC	350	Total	C	N	O	P	0	0
			7516	3355	1368	2443	350		

- Molecule 43 is a RNA chain called LSU rRNA chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LD	110	Total	C	N	O	P	0	0
			2342	1043	418	771	110		

- Molecule 44 is a RNA chain called LSU rRNA chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	652	Total	C	N	O	P	0	0
			13955	6233	2494	4576	652		

- Molecule 45 is a RNA chain called LSU rRNA chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LF	456	Total	C	N	O	P	0	0
			9702	4340	1740	3166	456		

- Molecule 46 is a RNA chain called LSU rRNA chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LG	207	Total	C	N	O	P	0	0
			4422	1975	789	1451	207		

- Molecule 47 is a RNA chain called LSU rRNA chain 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LH	559	Total	C	N	O	P	0	0
			11980	5366	2143	3912	559		

- Molecule 48 is a RNA chain called LSU rRNA chain 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LI	573	Total	C	N	O	P	0	0
			12233	5480	2170	4010	573		

- Molecule 49 is a RNA chain called LSU rRNA chain 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LJ	163	Total	C	N	O	P	0	0
			3486	1558	630	1135	163		

- Molecule 50 is a RNA chain called LSU rRNA chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LK	61	Total	C	N	O	P	0	0
			1301	581	237	422	61		

- Molecule 51 is a RNA chain called LSU rRNA chain 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LL	92	Total	C	N	O	P	0	0
			1983	882	366	643	92		

- Molecule 52 is a RNA chain called LSU rRNA chain 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LM	54	Total	C	N	O	P	0	0
			1158	517	214	373	54		

- Molecule 53 is a RNA chain called LSU rRNA chain 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	79	Total	C	N	O	P	0	0
			1696	753	307	557	79		

- Molecule 54 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LO	120	Total	C	N	O	P	0	0
			2559	1142	457	840	120		

- Molecule 55 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LP	249	Total	C	N	O	S	0	0
			1901	1193	380	317	11		

- Molecule 56 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	392	Total	C	N	O	S	1	0
			3118	1987	592	521	18		

- Molecule 57 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LR	365	Total	C	N	O	S	0	0
			2868	1807	572	482	7		

- Molecule 58 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LS	178	Total	C	N	O	S	0	0
			1437	912	273	248	4		

- Molecule 59 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	190	Total	C	N	O	S	0	0
			1521	959	283	269	10		

- Molecule 60 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LU	194	Total	C	N	O	S	0	0
			1580	1010	297	269	4		

- Molecule 61 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LV	238	Total	C	N	O	S	0	0
			1926	1236	365	321	4		

- Molecule 62 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LW	208	Total	C	N	O	S	0	0
			1713	1086	346	270	11		

- Molecule 63 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LX	219	Total	C	N	O	S	0	0
			1769	1115	357	292	5		

- Molecule 64 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LY	134	Total	C	N	O	S	0	0
			1001	634	187	173	7		

- Molecule 65 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	217	Total	C	N	O	S	0	0
			1780	1126	357	293	4		

- Molecule 66 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	La	151	Total	C	N	O	S	0	0
			1210	759	254	193	4		

- Molecule 67 is a protein called Ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lb	203	Total	C	N	O	S	0	0
			1711	1080	363	259	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lc	203	Total	C	N	O	S	0	0
			1643	1036	328	267	12		

- Molecule 69 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ld	260	Total	C	N	O	S	0	0
			2074	1313	384	367	10		

- Molecule 70 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Le	192	Total	C	N	O	S	0	0
			1526	963	313	241	9		

- Molecule 71 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lf	170	Total	C	N	O	S	0	0
			1392	874	291	219	8		

- Molecule 72 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lg	181	Total	C	N	O	S	0	0
			1494	961	278	246	9		

- Molecule 73 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lh	158	Total	C	N	O	S	0	0
			1279	814	254	209	2		

- Molecule 74 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Li	155	Total	C	N	O	S	0	0
			1255	785	250	213	7		

- Molecule 75 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lj	101	Total	C	N	O	S	0	0
			827	540	140	146	1		

- Molecule 76 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lk	131	Total	C	N	O	S	0	0
			1073	684	204	182	3		

- Molecule 77 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ll	124	Total	C	N	O	S	0	0
			1008	629	206	171	2		

- Molecule 78 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lm	66	Total	C	N	O	S	0	0
			549	355	108	84	2		

- Molecule 79 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ln	133	Total	C	N	O	S	0	0
			1084	695	213	172	4		

- Molecule 80 is a protein called Ribosomal protein eLEgr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Lo	58	Total	C	N	O	S	0	0
			459	291	86	80	2		

- Molecule 81 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lp	121	Total	C	N	O	S	0	0
			1010	645	198	164	3		

- Molecule 82 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Lq	91	Total	C	N	O	0	0
			767	478	164	125		

- Molecule 83 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Lr	218	Total	C	N	O	S	0	0
			1825	1184	346	285	10		

- Molecule 84 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ls	97	Total	C	N	O	S	0	0
			747	466	132	143	6		

- Molecule 85 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Lt	111	Total	C	N	O	S	0	0
			923	589	182	150	2		

- Molecule 86 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Lu	128	Total	C	N	O	S	0	0
			1068	680	219	167	2		

- Molecule 87 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Lv	114	Total	C	N	O	S	0	0
			915	589	182	140	4		

- Molecule 88 is a protein called Ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Lw	114	Total	C	N	O	S	0	0
			922	577	197	147	1		

- Molecule 89 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Lx	102	Total	C	N	O	S	0	0
			835	527	177	127	4		

- Molecule 90 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Ly	106	Total	C	N	O	S	0	0
			859	525	189	137	8		

- Molecule 91 is a protein called Ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Lz	70	Total	C	N	O	S	0	0
			570	367	103	98	2		

- Molecule 92 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	L1	50	Total	C	N	O	S	0	0
			447	287	93	65	2		

- Molecule 93 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	L2	51	Total	C	N	O	S	0	0
			415	255	83	67	10		

- Molecule 94 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	L3	33	Total	C	N	O	S	0	0
			302	180	81	38	3		

- Molecule 95 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	L5	90	Total	C	N	O	S	0	0
			719	449	147	117	6		

- Molecule 96 is a protein called Ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	L4	97	Total	C	N	O	S	0	0
			785	501	152	126	6		

- Molecule 97 is a protein called Ribosomal protein eLEgr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	L6	59	Total	C	N	O	S	0	0
			493	308	99	85	1		

- Molecule 98 is a protein called Ribosomal protein eLEgr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	L7	54	Total	C	N	O	S	0	0
			455	288	85	81	1		

- Molecule 99 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
99	Sb	1	Total	Zn	0
			1	1	
99	Ly	1	Total	Zn	0
			1	1	
99	L2	1	Total	Zn	0
			1	1	
99	L5	1	Total	Zn	0
			1	1	
99	L4	1	Total	Zn	0
			1	1	

- Molecule 100 is water.

Mol	Chain	Residues	Atoms		AltConf
100	S1	393	Total	O	0
			393	393	
100	S2	3	Total	O	0
			3	3	
100	S3	17	Total	O	0
			17	17	
100	S4	2	Total	O	0
			2	2	
100	S5	11	Total	O	0
			11	11	
100	SB	1	Total	O	0
			1	1	
100	SC	3	Total	O	0
			3	3	
100	SF	4	Total	O	0
			4	4	
100	SG	3	Total	O	0
			3	3	
100	SH	2	Total	O	0
			2	2	
100	SK	5	Total	O	0
			5	5	
100	SL	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
100	SM	1	Total 1	O 1	0
100	SO	1	Total 1	O 1	0
100	SP	4	Total 4	O 4	0
100	SR	1	Total 1	O 1	0
100	SS	2	Total 2	O 2	0
100	SU	1	Total 1	O 1	0
100	SX	2	Total 2	O 2	0
100	SZ	2	Total 2	O 2	0
100	Sb	1	Total 1	O 1	0
100	Sh	1	Total 1	O 1	0
100	LA	29	Total 29	O 29	0
100	LB	15	Total 15	O 15	0
100	LC	32	Total 32	O 32	0
100	LD	9	Total 9	O 9	0
100	LE	97	Total 97	O 97	0
100	LF	93	Total 93	O 93	0
100	LG	33	Total 33	O 33	0
100	LH	174	Total 174	O 174	0
100	LI	82	Total 82	O 82	0
100	LJ	46	Total 46	O 46	0
100	LK	3	Total 3	O 3	0

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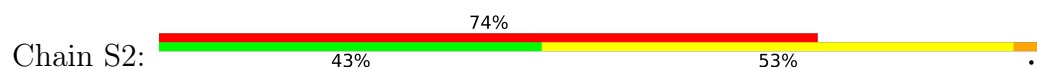
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Mol	Chain	Residues	Atoms		AltConf
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100	LM	11	Total 11	O 11	0
100	LN	12	Total 12	O 12	0
100	LO	15	Total 15	O 15	0
100	LP	2	Total 2	O 2	0
100	LQ	8	Total 8	O 8	0
100	LR	8	Total 8	O 8	0
100	LU	2	Total 2	O 2	0
100	LW	7	Total 7	O 7	0
100	LY	3	Total 3	O 3	0
100	La	2	Total 2	O 2	0
100	Lb	2	Total 2	O 2	0
100	Lc	2	Total 2	O 2	0
100	Ld	1	Total 1	O 1	0
100	Lf	1	Total 1	O 1	0
100	Li	2	Total 2	O 2	0
100	Lk	1	Total 1	O 1	0
100	Ll	1	Total 1	O 1	0
100	Lm	3	Total 3	O 3	0
100	Lp	1	Total 1	O 1	0
100	Lq	3	Total 3	O 3	0

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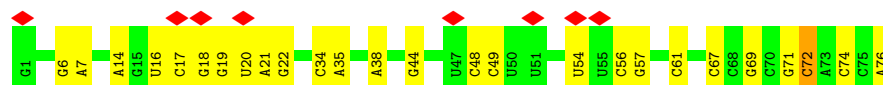
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100	Ls	1	Total 1	O 1	0
100	Lt	4	Total 4	O 4	0
100	Lu	1	Total 1	O 1	0
100	Lw	2	Total 2	O 2	0
100	Ly	2	Total 2	O 2	0
100	L2	3	Total 3	O 3	0
100	L3	10	Total 10	O 10	0
100	L5	2	Total 2	O 2	0
100	L4	1	Total 1	O 1	0
100	L7	1	Total 1	O 1	0

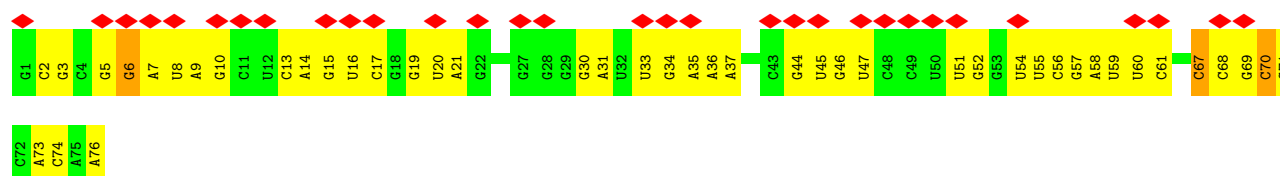




• Molecule 3: P-tRNA



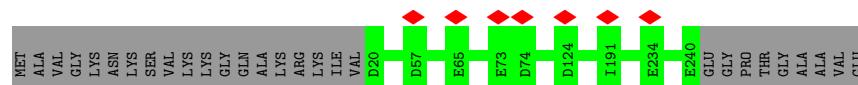
• Molecule 4: E-tRNA



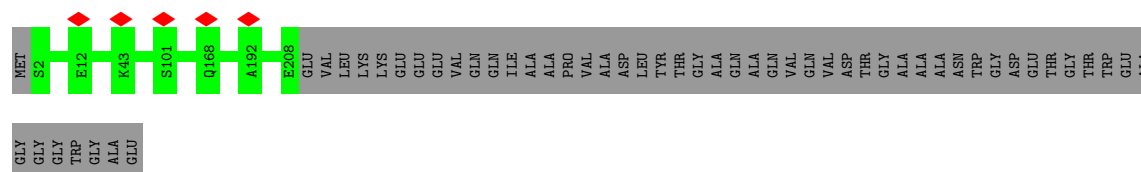
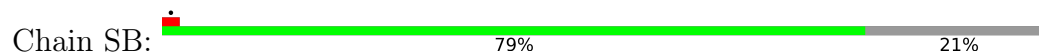
• Molecule 5: A-site tRNA



• Molecule 6: Ribosomal protein eS1



• Molecule 7: Ribosomal protein uS2



• Molecule 8: Ribosomal protein uS3

-
- | Amino Acid | Count | Red Diamond |
|------------|-------|-------------|
| V2 | 1 | No |
| D25 | 1 | Yes |
| E64 | 1 | Yes |
| E88 | 1 | Yes |
| D94 | 1 | Yes |
| D157 | 1 | Yes |
| G165 | 1 | Yes |
| A178 | 1 | No |
| ALA | 0 | No |
| GLU | 0 | No |
| SER | 0 | No |
| LYS | 0 | No |
| LYS | 0 | No |
| LYS | 0 | No |
| ASP | 0 | No |
| ASP | 0 | No |
| GLY | 0 | No |
| GLY | 0 | No |
| ASP | 0 | No |
| ASP | 0 | No |
| ASP | 0 | No |
| GLY | 0 | No |
| GLY | 0 | No |
| GLY | 0 | No |
| ASP | 0 | No |
| GLU | 0 | No |
| GLU | 0 | No |
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| ASP | 0 | No |

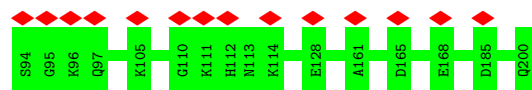
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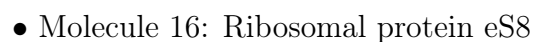
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- Diagram illustrating the structure of the 19S subunit of the 26S proteasome, showing residues and their corresponding amino acid types (ALA, LYS, GLY, PRO).
- | Residue | Amino Acid |
|---------|------------|
| M1 | ALA |
| D19 | GLY |
| D29 | ALA |
| S91 | LYS |
| E120 | LYS |
| E124 | LYS |
| D128 | LYS |
| D153 | LYS |
| A166 | ALA |
| K167 | LYS |
| D168 | GLY |
| N169 | LYS |
| K170 | LYS |
| K171 | LYS |
| R238 | LYS |
| R239 | LYS |
| E242 | LYS |
| L243 | LYS |
| D244 | LYS |
| V245 | LYS |
| I246 | LYS |
| N247 | LYS |
| K248 | LYS |
| G249 | LYS |
| ALA | ALA |
| LYS | LYS |
| LYS | LYS |
| ALA | ALA |
| ALA | ALA |
| ALA | ALA |
| ALA | ALA |
| ALA | ALA |
| ALA | ALA |
| ALA | ALA |
| LYS | LYS |
| LYS | LYS |
| LYS | LYS |
| PRO | PRO |
| ALA | ALA |

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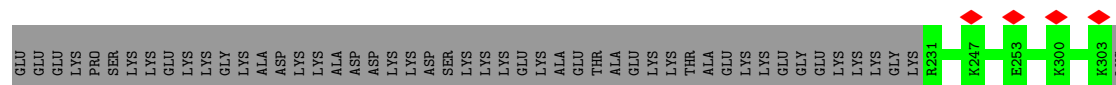
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- Chain SJ:  98%




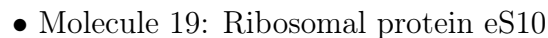
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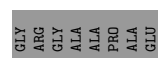
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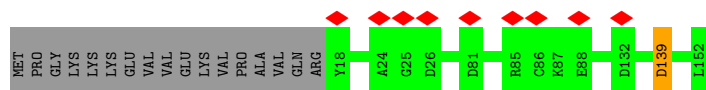
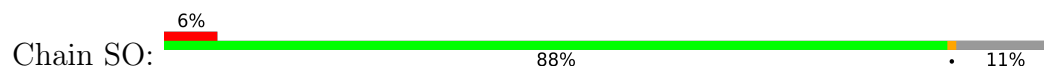
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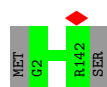
- Chain SN: 



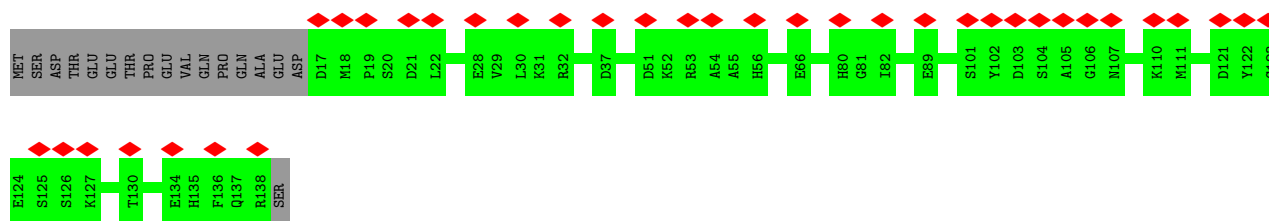
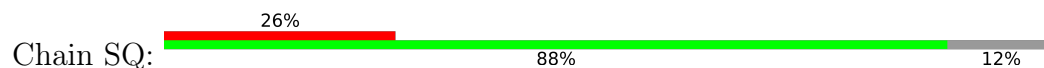
- Molecule 20: Ribosomal protein uS11



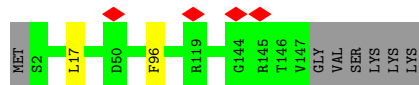
- Molecule 21: Ribosomal protein uS12



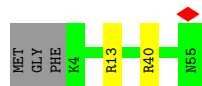
- Molecule 22: Ribosomal protein eS12



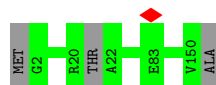
- Molecule 23: Ribosomal protein uS13



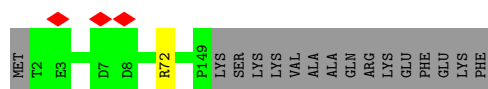
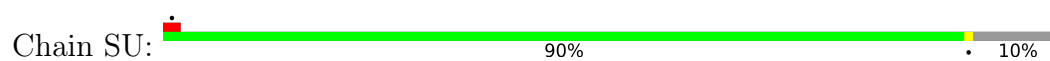
- Molecule 24: Ribosomal protein uS14



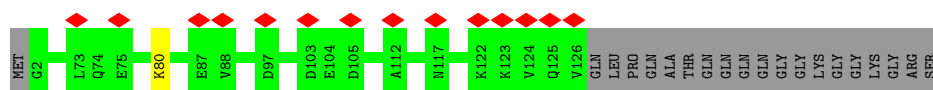
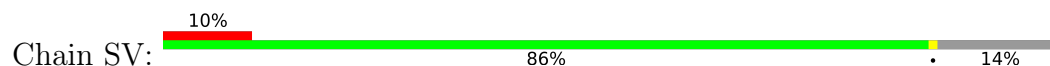
- Molecule 25: Ribosomal protein uS15



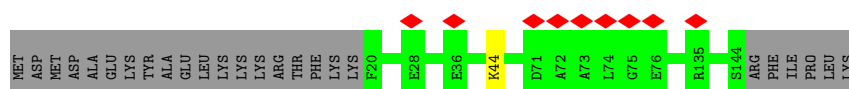
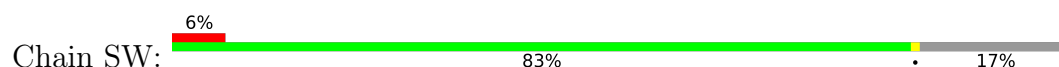
- Molecule 26: Ribosomal protein uS17



- Molecule 27: Ribosomal protein eS17



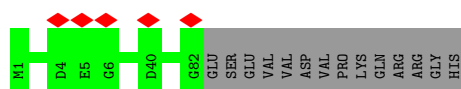
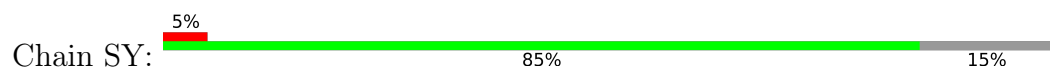
- Molecule 28: Ribosomal protein uS19



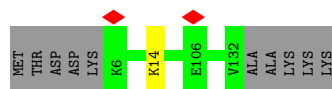
- Molecule 29: Ribosomal protein eS19



- Molecule 30: Ribosomal protein eS21

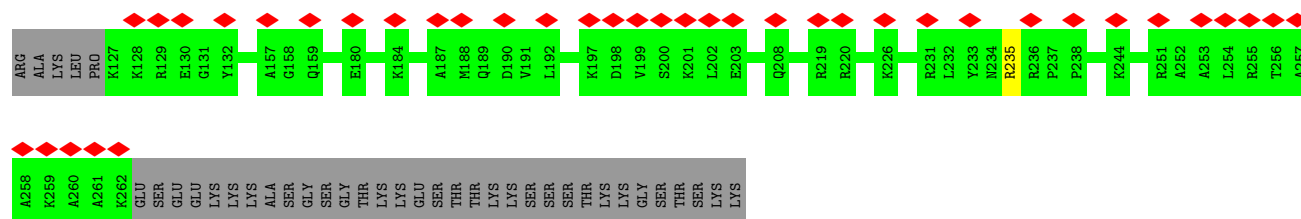


- Molecule 31: Ribosomal protein eS24

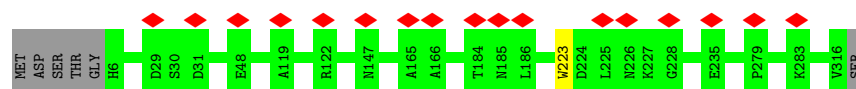


- Molecule 32: Ribosomal protein eS25

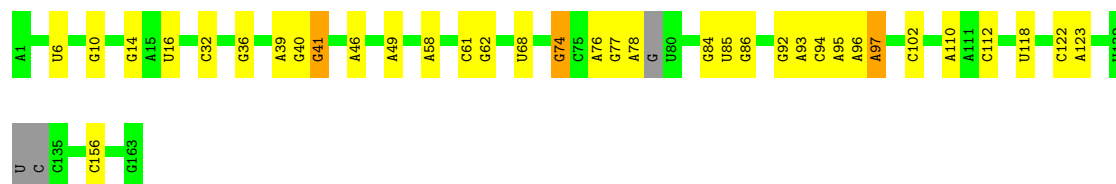
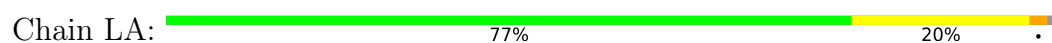




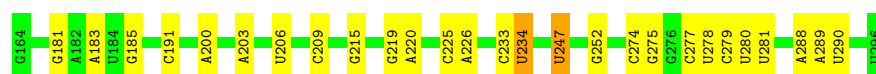
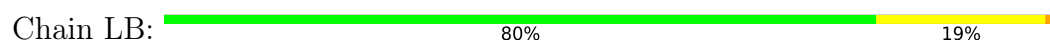
• Molecule 39: RACK1



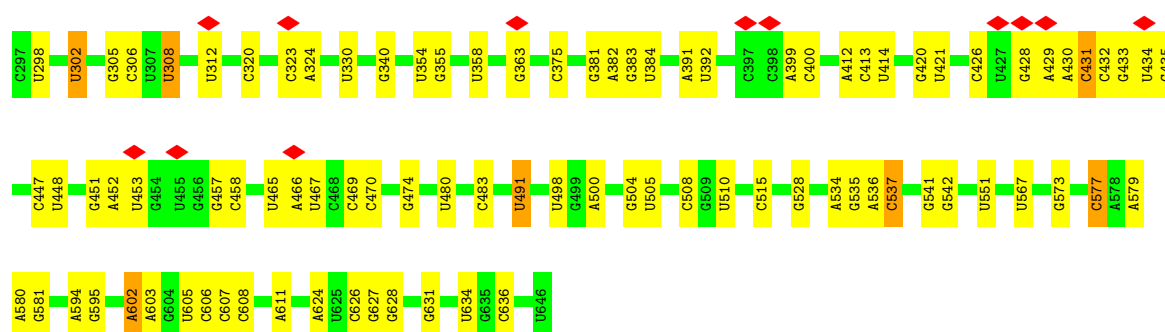
• Molecule 40: 5.8S rRNA



• Molecule 41: LSU rRNA chain 1



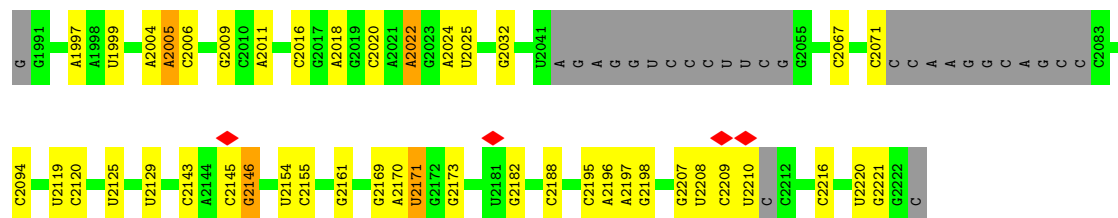
• Molecule 42: LSU rRNA chain 2



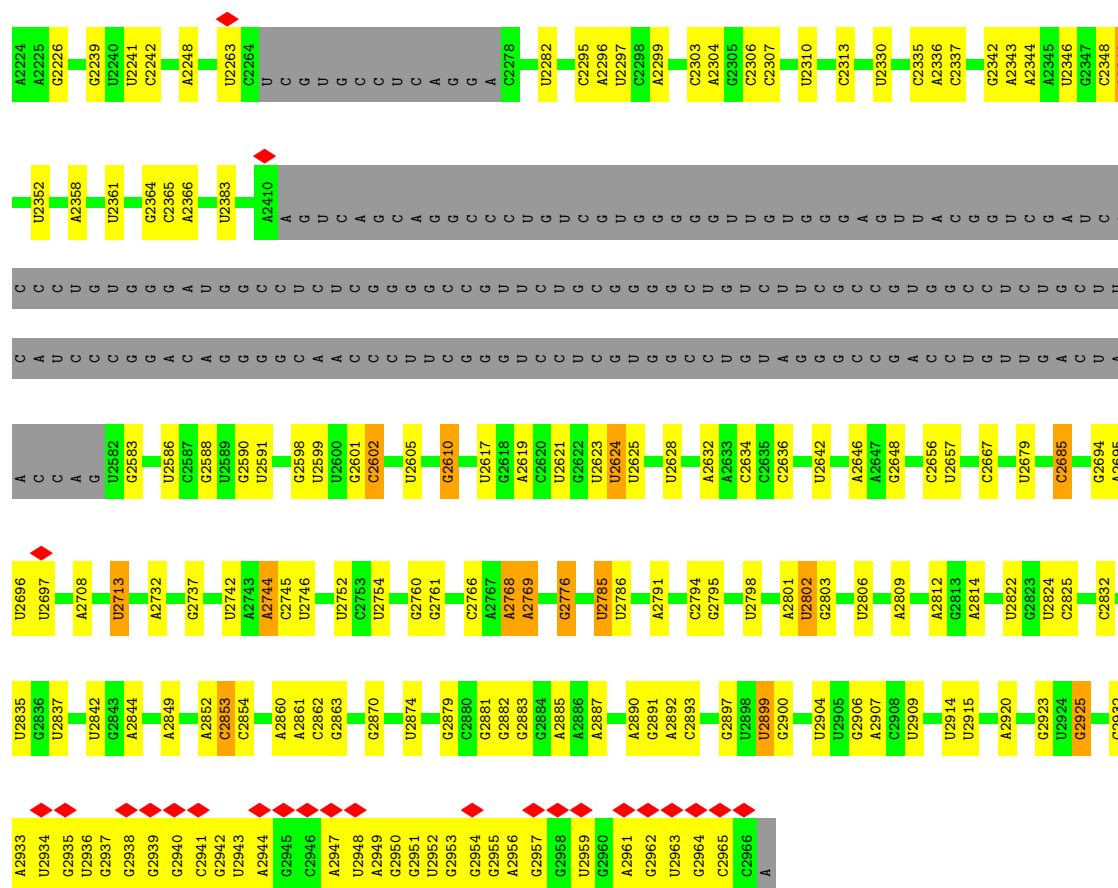
• Molecule 43: LSU rRNA chain 3



- Molecule 46: LSU rRNA chain 6

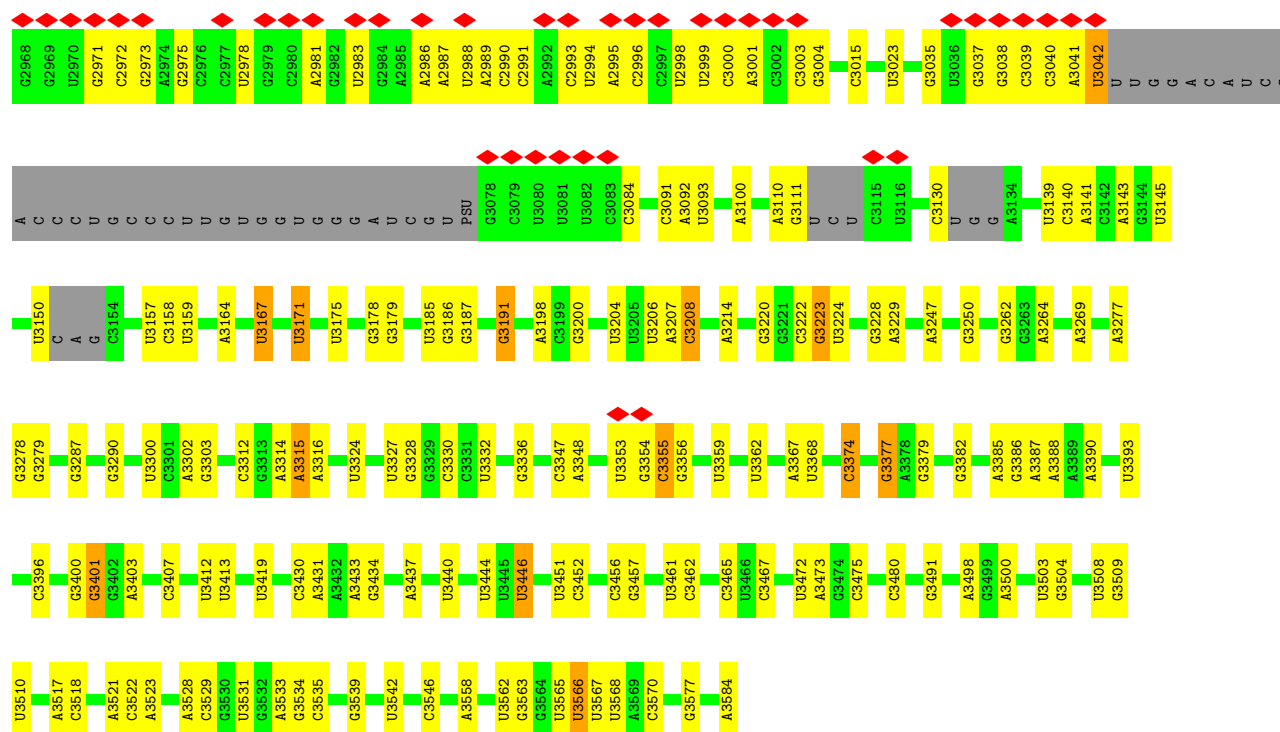


- Molecule 47: LSU rRNA chain 7

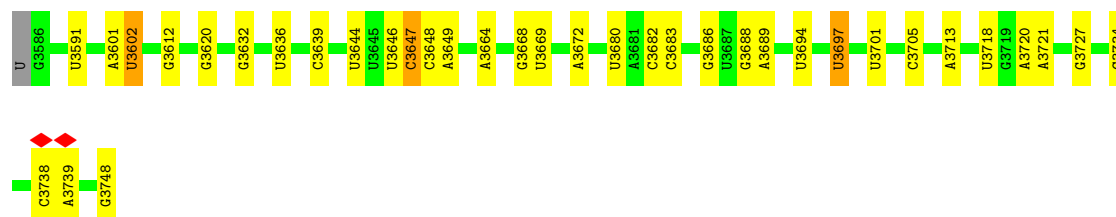
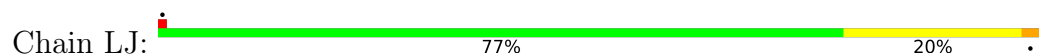


- Molecule 48: LSU rRNA chain 8





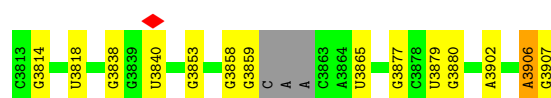
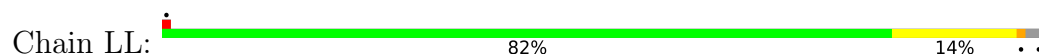
• Molecule 49: LSU rRNA chain 9



• Molecule 50: LSU rRNA chain 10

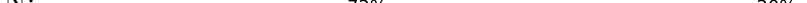


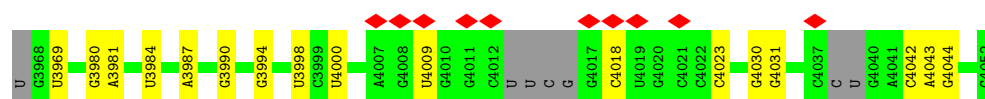
• Molecule 51: LSU rRNA chain 11



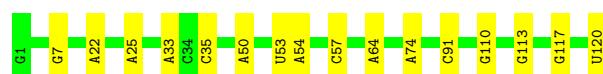
• Molecule 52: LSU rRNA chain 12

C C3910 A3911 C3921 C3922 C3927 G3944 A3951 G3952 U3953 G3954 U U C3957 G3961 G3962 U3963 U3964 A3965 U

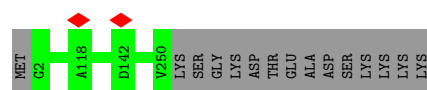
- Chain LN: 



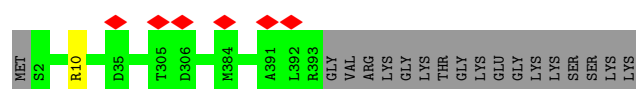
- Chain LO:  87% 13%



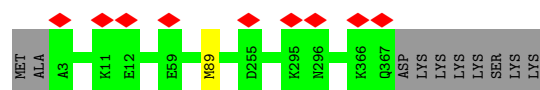
- Chain LP:  94% 6%



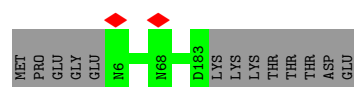
- Chain LQ: 95%



- Chain LR:

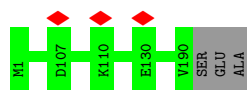


- Chain LS:  93% 7%



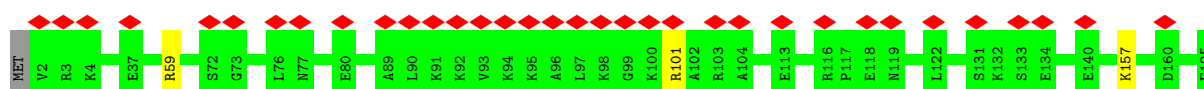
- Molecule 59: Ribosomal protein uL6

Chain LT:  98%




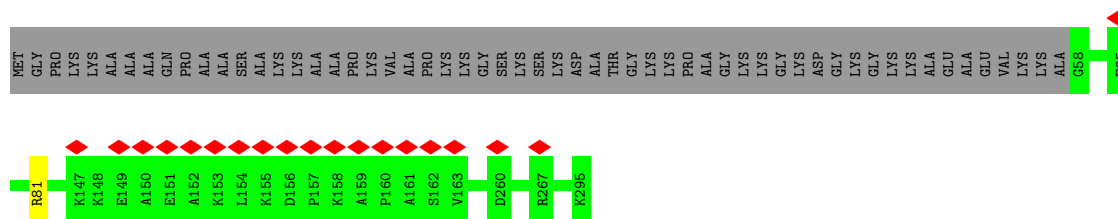
- Molecule 60: Ribosomal protein eL6

Chain LU:  98%



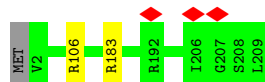
- Molecule 61: 60S ribosomal protein L7a

Chain LV:  80% 19%



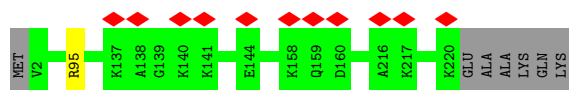
- Molecule 62: Ribosomal protein uL13

Chain LW:  99%



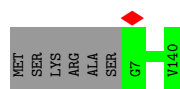
- Molecule 63: Ribosomal protein eL13

Chain LX:  96%

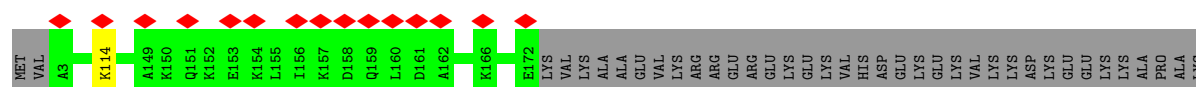
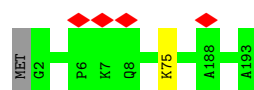
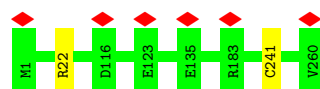
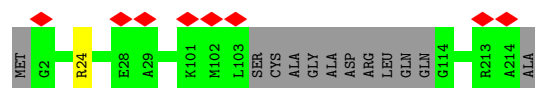
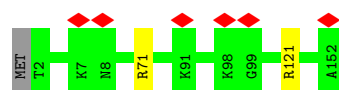


- Molecule 64: Ribosomal protein uL14

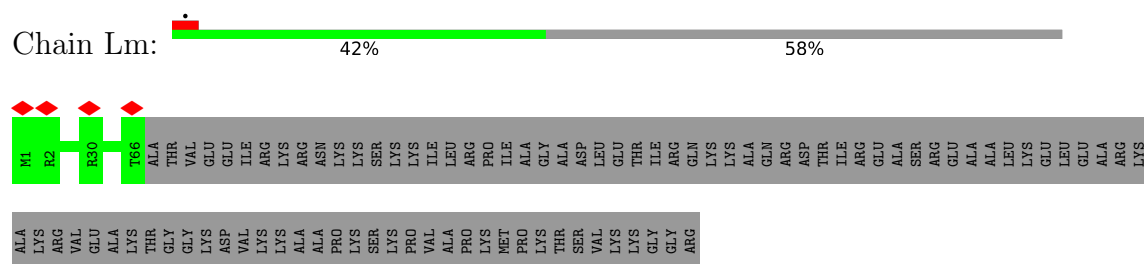
Chain LY:  96%



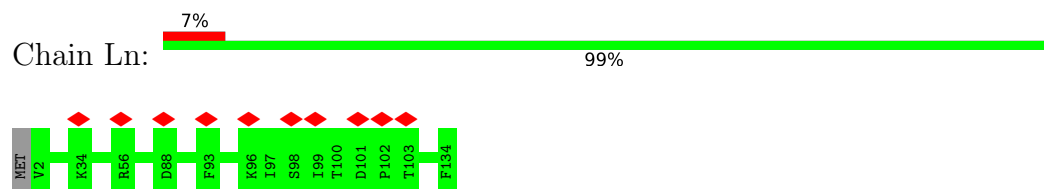
- Molecule 65: Ribosomal protein eL14



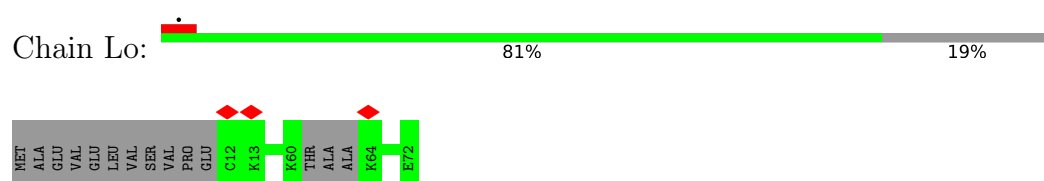
- Molecule 78: Ribosomal protein eL24



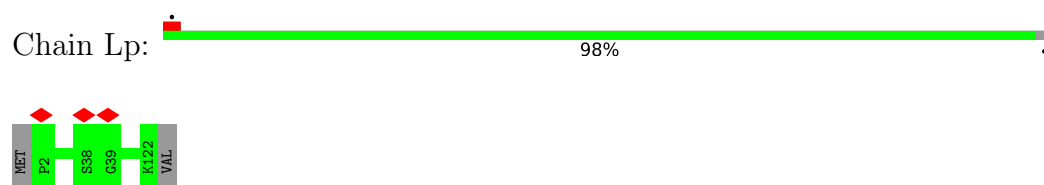
- Molecule 79: Ribosomal protein eL27



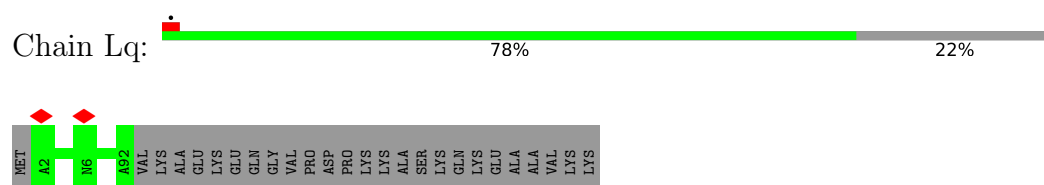
- Molecule 80: Ribosomal protein eLEgr1



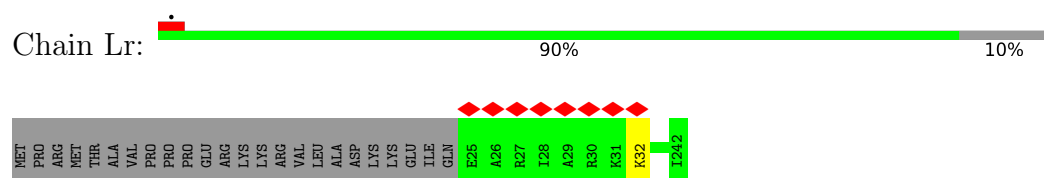
- Molecule 81: Ribosomal protein uL29



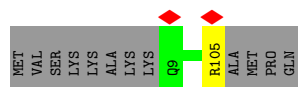
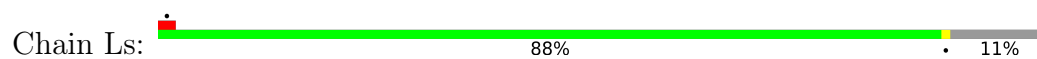
- Molecule 82: Ribosomal protein eL29



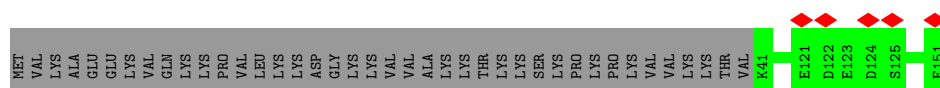
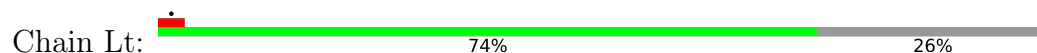
- Molecule 83: Ribosomal protein uL30



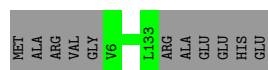
- Molecule 84: Ribosomal protein eL30



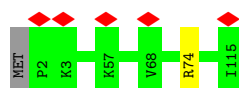
- Molecule 85: Ribosomal protein eL31



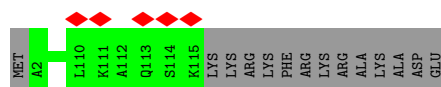
- Molecule 86: Ribosomal protein eL32



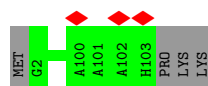
- Molecule 87: Ribosomal protein eL33



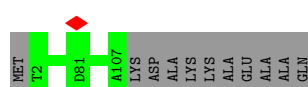
- Molecule 88: Ribosomal protein eL34

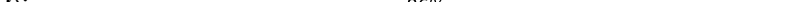


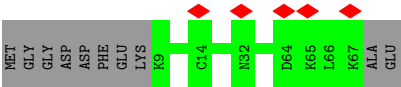
- Molecule 89: Ribosomal protein eL36



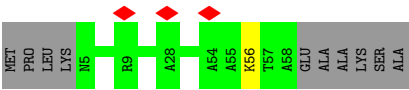
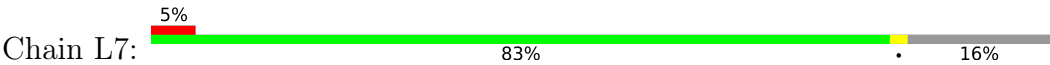
- Molecule 90: Ribosomal protein eL37



- Chain L6: 



• Molecule 98: Ribosomal protein eLEgr3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, A2M, B8H, 6MZ, 5MC, PSU, B8N, MIA, JMC, JMH, ZN, 1MA, OMC, 7MG, OMU, UR3, OMG

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	S1	0.57	0/46353	0.85	43/72230 (0.1%)
2	S2	0.35	0/1783	0.91	5/2776 (0.2%)
3	S3	0.52	0/1802	0.96	1/2807 (0.0%)
4	S4	0.38	0/1812	1.07	11/2824 (0.4%)
5	S5	0.87	0/279	0.95	0/431
6	SA	0.31	0/1828	0.51	0/2458
7	SB	0.31	0/1694	0.48	0/2301
8	SC	0.35	0/1701	0.48	0/2281
9	SD	0.32	0/1461	0.47	0/1955
10	SE	0.35	0/2169	0.51	0/2909
11	SF	0.36	0/1752	0.49	0/2371
12	SG	0.31	0/2036	0.48	0/2709
13	SH	0.53	2/1472 (0.1%)	0.65	3/1982 (0.2%)
14	SI	0.31	0/1538	0.49	0/2060
15	SJ	0.35	0/1056	0.49	0/1415
16	SK	0.35	0/1678	0.51	0/2240
17	SL	0.35	0/1162	0.47	0/1554
18	SM	0.31	0/808	0.49	0/1089
19	SN	0.36	0/796	0.51	1/1072 (0.1%)
20	SO	0.35	0/1024	0.55	1/1375 (0.1%)
21	SP	0.36	0/1119	0.52	0/1493
22	SQ	0.29	0/931	0.54	0/1252
23	SR	0.34	0/1198	0.56	1/1603 (0.1%)
24	SS	0.36	0/441	0.50	0/583
25	ST	0.32	0/1201	0.50	0/1608
26	SU	0.38	0/1259	0.47	0/1695
27	SV	0.32	0/1006	0.47	0/1344
28	SW	0.35	0/1008	0.47	0/1346
29	SX	0.37	0/1148	0.48	0/1543
30	SY	0.32	0/631	0.48	0/849
31	SZ	0.35	0/1070	0.47	0/1412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.35	0/642	0.50	0/862
33	Sb	0.36	0/791	0.51	0/1057
34	Sc	0.32	0/663	0.46	0/891
35	Sd	0.31	0/500	0.57	0/669
36	Se	0.32	0/490	0.51	0/646
37	Sf	0.33	0/519	0.54	1/691 (0.1%)
38	Sg	0.38	0/1623	0.56	0/2158
39	Sh	0.35	0/2454	0.56	0/3339
40	LA	0.59	0/3674	0.82	3/5722 (0.1%)
41	LB	0.61	0/3021	0.80	0/4708
42	LC	0.52	0/8081	0.81	4/12607 (0.0%)
43	LD	0.46	0/2613	0.83	2/4069 (0.0%)
44	LE	0.53	0/14709	0.79	3/22917 (0.0%)
45	LF	0.60	0/10013	0.83	9/15601 (0.1%)
46	LG	0.56	0/4698	0.83	0/7316
47	LH	0.64	0/12014	0.83	3/18729 (0.0%)
48	LI	0.55	0/12455	0.82	3/19402 (0.0%)
49	LJ	0.63	0/3692	0.86	6/5756 (0.1%)
50	LK	0.47	0/1453	0.82	1/2260 (0.0%)
51	LL	0.39	0/2170	0.79	0/3384
52	LM	0.60	0/1228	0.83	3/1914 (0.2%)
53	LN	0.45	0/1871	0.86	0/2914
54	LO	0.52	0/2860	0.78	1/4456 (0.0%)
55	LP	0.37	0/1941	0.49	0/2604
56	LQ	0.37	0/3177	0.49	0/4254
57	LR	0.34	0/2918	0.46	0/3918
58	LS	0.32	0/1456	0.50	0/1937
59	LT	0.33	0/1545	0.48	0/2068
60	LU	0.30	0/1606	0.48	0/2142
61	LV	0.31	0/1963	0.45	0/2627
62	LW	0.35	0/1745	0.49	0/2327
63	LX	0.33	0/1803	0.46	0/2404
64	LY	0.36	0/1017	0.50	0/1368
65	LZ	0.30	0/1809	0.45	0/2409
66	La	0.33	0/1238	0.47	0/1650
67	Lb	0.37	0/1757	0.49	1/2355 (0.0%)
68	Lc	0.33	0/1675	0.46	0/2237
69	Ld	0.33	0/2112	0.45	0/2838
70	Le	0.35	0/1554	0.49	0/2073
71	Lf	0.32	0/1410	0.45	0/1870
72	Lg	0.36	0/1532	0.49	0/2056
73	Lh	0.33	0/1306	0.47	0/1748
74	Li	0.39	0/1281	0.51	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.29	0/841	0.48	0/1125
76	Lk	0.34	0/1088	0.50	0/1455
77	Ll	0.31	0/1019	0.48	0/1350
78	Lm	0.33	0/562	0.49	0/756
79	Ln	0.32	0/1103	0.46	0/1470
80	Lo	0.34	0/470	0.45	0/631
81	Lp	0.31	0/1020	0.43	0/1352
82	Lq	0.29	0/780	0.41	0/1027
83	Lr	0.36	0/1867	0.46	0/2500
84	Ls	0.36	0/756	0.45	0/1014
85	Lt	0.36	0/941	0.50	0/1257
86	Lu	0.35	0/1093	0.45	0/1462
87	Lv	0.37	0/935	0.48	0/1247
88	Lw	0.34	0/937	0.50	0/1254
89	Lx	0.30	0/847	0.42	0/1122
90	Ly	0.35	0/872	0.52	0/1151
91	Lz	0.32	0/577	0.49	0/767
92	L1	0.32	0/457	0.46	0/603
93	L2	0.32	0/420	0.47	0/554
94	L3	0.50	0/304	0.63	0/390
95	L5	0.36	0/732	0.50	0/975
96	L4	0.36	0/798	0.46	0/1054
97	L6	0.29	0/500	0.45	0/665
98	L7	0.30	0/463	0.37	0/616
All	All	0.48	2/231677 (0.0%)	0.73	106/340038 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S1	1	0
45	LF	1	0
All	All	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	SH	60	ASN	C-O	9.43	1.41	1.23
13	SH	57	ARG	C-O	6.93	1.36	1.23

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	LI	3566	U	OP2-P-O3'	-11.41	80.11	105.20
13	SH	64	TYR	C-N-CA	9.75	146.07	121.70
4	S4	68	C	N3-C2-O2	-9.34	115.36	121.90
48	LI	3566	U	OP1-P-O3'	-8.56	86.36	105.20
45	LF	1704	C	N3-C2-O2	-8.25	116.12	121.90
1	S1	1245	C	N3-C2-O2	-8.12	116.22	121.90
45	LF	1704	C	N1-C2-O2	8.09	123.75	118.90
45	LF	1704	C	C2-N1-C1'	8.07	127.67	118.80
4	S4	60	U	C2-N1-C1'	8.05	127.36	117.70
1	S1	1245	C	N1-C2-O2	7.67	123.50	118.90
45	LF	1909	U	C2-N1-C1'	7.57	126.79	117.70
1	S1	983	G	N1-C6-O6	-7.57	115.36	119.90
4	S4	60	U	N1-C2-O2	7.46	128.02	122.80
1	S1	129	U	C2-N1-C1'	7.40	126.58	117.70
48	LI	3567	U	OP1-P-OP2	7.39	130.69	119.60
45	LF	1704	C	C6-N1-C2	-7.28	117.39	120.30
1	S1	66	C	C2-N1-C1'	7.23	126.75	118.80
4	S4	68	C	N1-C2-O2	7.12	123.17	118.90
2	S2	74	C	O4'-C1'-N1	7.02	113.82	108.20
19	SN	30	LYS	C-N-CA	-6.93	104.39	121.70
1	S1	66	C	N1-C2-O2	6.92	123.05	118.90
1	S1	129	U	N1-C2-O2	6.92	127.64	122.80
49	LJ	3648	C	N1-C2-O2	6.90	123.04	118.90
1	S1	983	G	C5-C6-O6	6.86	132.71	128.60
49	LJ	3648	C	C2-N1-C1'	6.67	126.14	118.80
1	S1	1362	C	C2-N1-C1'	6.58	126.04	118.80
1	S1	968	C	N3-C2-O2	-6.52	117.33	121.90
4	S4	60	U	N3-C2-O2	-6.50	117.65	122.20
4	S4	6	G	N1-C6-O6	-6.50	116.00	119.90
43	LD	686	G	O4'-C1'-N9	6.46	113.37	108.20
1	S1	2036	C	N3-C2-O2	-6.44	117.39	121.90
4	S4	6	G	C5-C6-O6	6.43	132.46	128.60
1	S1	1109	G	C4-N9-C1'	-6.26	118.36	126.50
23	SR	17	LEU	CA-CB-CG	6.26	129.71	115.30
1	S1	129	U	N3-C2-O2	-6.15	117.89	122.20
1	S1	862	C	N1-C2-O2	6.07	122.54	118.90
52	LM	3927	C	N1-C2-O2	6.06	122.53	118.90
1	S1	66	C	N3-C2-O2	-6.05	117.67	121.90
1	S1	1959	G	C4'-C3'-O3'	6.04	125.07	113.00
1	S1	1635	C	C2-N1-C1'	6.02	125.42	118.80
2	S2	60	U	C2-N1-C1'	6.00	124.90	117.70
1	S1	830	C	N3-C2-O2	-5.96	117.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	194	C	O5'-P-OP1	-5.89	100.40	105.70
42	LC	602	A	OP1-P-O3'	5.88	118.13	105.20
1	S1	1959	G	N9-C1'-C2'	-5.87	105.54	112.00
47	LH	2785	U	N1-C2-O2	5.83	126.88	122.80
1	S1	1943	G	N3-C4-N9	5.83	129.50	126.00
1	S1	1766	C	C2-N1-C1'	5.81	125.19	118.80
13	SH	64	TYR	CA-CB-CG	-5.80	102.37	113.40
49	LJ	3648	C	N3-C2-O2	-5.80	117.84	121.90
4	S4	5	G	N3-C4-N9	5.76	129.46	126.00
47	LH	2785	U	N3-C2-O2	-5.76	118.17	122.20
44	LE	1134	G	O4'-C1'-N9	5.74	112.79	108.20
2	S2	60	U	N1-C2-O2	5.73	126.81	122.80
47	LH	2785	U	C2-N1-C1'	5.72	124.57	117.70
50	LK	3791	C	C2-N1-C1'	5.70	125.07	118.80
20	SO	139	ASP	CB-CA-C	5.67	121.75	110.40
3	S3	72	C	C2-N1-C1'	5.67	125.04	118.80
45	LF	1697	G	O4'-C1'-N9	5.67	112.73	108.20
1	S1	1943	G	C4-N9-C1'	5.67	133.86	126.50
44	LE	1261	C	N1-C2-O2	5.65	122.29	118.90
52	LM	3927	C	C2-N1-C1'	5.63	124.99	118.80
1	S1	967	C	N1-C2-O2	5.63	122.28	118.90
1	S1	1400	A	O4'-C1'-N9	5.59	112.67	108.20
42	LC	431	C	C2-N1-C1'	5.55	124.91	118.80
1	S1	943	C	C2-N1-C1'	5.53	124.88	118.80
49	LJ	3647	C	N1-C2-O2	5.52	122.21	118.90
67	Lb	116	LEU	CA-CB-CG	5.47	127.88	115.30
45	LF	1909	U	N1-C2-O2	5.46	126.63	122.80
42	LC	602	A	P-O3'-C3'	5.46	126.25	119.70
4	S4	67	C	N1-C2-O2	5.46	122.17	118.90
1	S1	968	C	C6-N1-C1'	5.43	127.32	120.80
1	S1	550	G	C4-N9-C1'	5.43	133.56	126.50
13	SH	64	TYR	N-CA-C	5.42	125.64	111.00
1	S1	1109	G	C8-N9-C1'	5.42	134.04	127.00
1	S1	2137	C	N1-C2-O2	5.42	122.15	118.90
1	S1	1943	G	C8-N9-C1'	-5.41	119.97	127.00
45	LF	1910	C	C2-N1-C1'	5.40	124.74	118.80
1	S1	1109	G	N3-C4-N9	-5.36	122.78	126.00
44	LE	1261	C	C2-N1-C1'	5.34	124.68	118.80
1	S1	2137	C	C2-N1-C1'	5.34	124.67	118.80
4	S4	60	U	C6-N1-C1'	-5.33	113.74	121.20
42	LC	431	C	N1-C2-O2	5.33	122.10	118.90
1	S1	2036	C	N1-C2-O2	5.32	122.09	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	LJ	3602	U	N3-C2-O2	-5.29	118.50	122.20
40	LA	78	A	O4'-C1'-N9	5.27	112.42	108.20
2	S2	60	U	N3-C2-O2	-5.27	118.51	122.20
49	LJ	3647	C	N3-C2-O2	-5.21	118.25	121.90
40	LA	118	U	N1-C2-O2	5.21	126.44	122.80
1	S1	1109	G	C6-C5-N7	5.20	133.52	130.40
1	S1	943	C	N1-C2-O2	5.20	122.02	118.90
1	S1	774	G	N9-C4-C5	-5.16	103.34	105.40
37	Sf	126	ASP	CB-CG-OD2	5.15	122.94	118.30
54	LO	35	C	C2-N1-C1'	5.12	124.44	118.80
1	S1	448	U	C2-N1-C1'	5.12	123.84	117.70
4	S4	70	C	N1-C2-O2	5.10	121.96	118.90
43	LD	716	C	N3-C2-O2	-5.09	118.34	121.90
1	S1	1943	G	C6-C5-N7	-5.09	127.35	130.40
40	LA	118	U	N3-C2-O2	-5.05	118.67	122.20
1	S1	249	C	C2-N1-C1'	5.04	124.35	118.80
1	S1	650	C	C6-N1-C2	-5.04	118.28	120.30
1	S1	1109	G	N3-C4-C5	5.03	131.12	128.60
1	S1	1871	C	C2-N1-C1'	5.03	124.33	118.80
2	S2	66	U	N1-C2-O2	5.01	126.31	122.80
45	LF	1909	U	C6-N1-C1'	-5.00	114.19	121.20
52	LM	3927	C	N3-C2-O2	-5.00	118.40	121.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	S1	1601	B8N	C33
45	LF	1923	JMC	C4

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	
6	SA	219/249 (88%)	197 (90%)	22 (10%)	0	100	100
7	SB	205/261 (78%)	186 (91%)	19 (9%)	0	100	100
8	SC	210/220 (96%)	196 (93%)	14 (7%)	0	100	100
9	SD	175/196 (89%)	166 (95%)	9 (5%)	0	100	100
10	SE	263/271 (97%)	243 (92%)	20 (8%)	0	100	100
11	SF	219/257 (85%)	207 (94%)	12 (6%)	0	100	100
12	SG	246/283 (87%)	227 (92%)	19 (8%)	0	100	100
13	SH	178/190 (94%)	154 (86%)	23 (13%)	1 (1%)	25	62
14	SI	183/200 (92%)	168 (92%)	15 (8%)	0	100	100
15	SJ	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	SK	195/304 (64%)	182 (93%)	13 (7%)	0	100	100
17	SL	141/151 (93%)	132 (94%)	9 (6%)	0	100	100
18	SM	99/121 (82%)	96 (97%)	3 (3%)	0	100	100
19	SN	90/152 (59%)	86 (96%)	4 (4%)	0	100	100
20	SO	133/152 (88%)	125 (94%)	8 (6%)	0	100	100
21	SP	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
22	SQ	120/139 (86%)	100 (83%)	20 (17%)	0	100	100
23	SR	144/153 (94%)	132 (92%)	12 (8%)	0	100	100
24	SS	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
25	ST	144/151 (95%)	129 (90%)	15 (10%)	0	100	100
26	SU	146/164 (89%)	135 (92%)	11 (8%)	0	100	100
27	SV	123/145 (85%)	113 (92%)	10 (8%)	0	100	100
28	SW	123/150 (82%)	117 (95%)	6 (5%)	0	100	100
29	SX	141/148 (95%)	130 (92%)	11 (8%)	0	100	100
30	SY	80/96 (83%)	72 (90%)	8 (10%)	0	100	100
31	SZ	125/137 (91%)	116 (93%)	9 (7%)	0	100	100
32	Sa	74/119 (62%)	69 (93%)	5 (7%)	0	100	100
33	Sb	95/120 (79%)	89 (94%)	6 (6%)	0	100	100
34	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Sd	61/76 (80%)	50 (82%)	11 (18%)	0	100	100
36	Se	60/67 (90%)	53 (88%)	7 (12%)	0	100	100
37	Sf	62/157 (40%)	57 (92%)	5 (8%)	0	100	100
38	Sg	195/295 (66%)	164 (84%)	31 (16%)	0	100	100
39	Sh	309/317 (98%)	270 (87%)	39 (13%)	0	100	100
55	LP	247/264 (94%)	232 (94%)	15 (6%)	0	100	100
56	LQ	390/410 (95%)	365 (94%)	25 (6%)	0	100	100
57	LR	363/375 (97%)	338 (93%)	25 (7%)	0	100	100
58	LS	176/191 (92%)	166 (94%)	10 (6%)	0	100	100
59	LT	188/193 (97%)	177 (94%)	11 (6%)	0	100	100
60	LU	192/195 (98%)	171 (89%)	21 (11%)	0	100	100
61	LV	236/295 (80%)	228 (97%)	8 (3%)	0	100	100
62	LW	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
63	LX	217/226 (96%)	196 (90%)	21 (10%)	0	100	100
64	LY	132/140 (94%)	120 (91%)	12 (9%)	0	100	100
65	LZ	215/219 (98%)	198 (92%)	17 (8%)	0	100	100
66	La	149/152 (98%)	138 (93%)	11 (7%)	0	100	100
67	Lb	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
68	Lc	199/215 (93%)	183 (92%)	16 (8%)	0	100	100
69	Ld	258/260 (99%)	242 (94%)	16 (6%)	0	100	100
70	Le	190/193 (98%)	176 (93%)	14 (7%)	0	100	100
71	Lf	168/250 (67%)	157 (94%)	11 (6%)	0	100	100
72	Lg	179/182 (98%)	160 (89%)	19 (11%)	0	100	100
73	Lh	156/159 (98%)	141 (90%)	15 (10%)	0	100	100
74	Li	153/164 (93%)	147 (96%)	6 (4%)	0	100	100
75	Lj	99/170 (58%)	94 (95%)	5 (5%)	0	100	100
76	Lk	129/163 (79%)	114 (88%)	15 (12%)	0	100	100
77	Ll	122/146 (84%)	112 (92%)	10 (8%)	0	100	100
78	Lm	64/157 (41%)	62 (97%)	2 (3%)	0	100	100
79	Ln	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
80	Lo	54/72 (75%)	48 (89%)	6 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	Lp	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
82	Lq	89/117 (76%)	83 (93%)	6 (7%)	0	100	100
83	Lr	216/242 (89%)	208 (96%)	8 (4%)	0	100	100
84	Ls	95/109 (87%)	92 (97%)	3 (3%)	0	100	100
85	Lt	109/151 (72%)	98 (90%)	11 (10%)	0	100	100
86	Lu	126/139 (91%)	121 (96%)	5 (4%)	0	100	100
87	Lv	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
88	Lw	112/128 (88%)	99 (88%)	13 (12%)	0	100	100
89	Lx	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
90	Ly	104/117 (89%)	95 (91%)	9 (9%)	0	100	100
91	Lz	68/82 (83%)	66 (97%)	2 (3%)	0	100	100
92	L1	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
93	L2	49/126 (39%)	48 (98%)	1 (2%)	0	100	100
94	L3	31/34 (91%)	27 (87%)	4 (13%)	0	100	100
95	L5	88/92 (96%)	82 (93%)	6 (7%)	0	100	100
96	L4	95/106 (90%)	87 (92%)	8 (8%)	0	100	100
97	L6	57/69 (83%)	53 (93%)	4 (7%)	0	100	100
98	L7	52/64 (81%)	51 (98%)	1 (2%)	0	100	100
All	All	11440/13164 (87%)	10574 (92%)	865 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SH	64	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	SA	204/224 (91%)	204 (100%)	0	100	100
7	SB	179/215 (83%)	179 (100%)	0	100	100
8	SC	177/184 (96%)	177 (100%)	0	100	100
9	SD	155/169 (92%)	155 (100%)	0	100	100
10	SE	231/237 (98%)	229 (99%)	2 (1%)	78	91
11	SF	184/206 (89%)	184 (100%)	0	100	100
12	SG	217/231 (94%)	216 (100%)	1 (0%)	88	95
13	SH	160/166 (96%)	159 (99%)	1 (1%)	86	94
14	SI	165/176 (94%)	164 (99%)	1 (1%)	86	94
15	SJ	115/116 (99%)	114 (99%)	1 (1%)	78	91
16	SK	169/258 (66%)	168 (99%)	1 (1%)	86	94
17	SL	119/125 (95%)	119 (100%)	0	100	100
18	SM	91/104 (88%)	91 (100%)	0	100	100
19	SN	83/119 (70%)	83 (100%)	0	100	100
20	SO	104/119 (87%)	103 (99%)	1 (1%)	76	89
21	SP	118/120 (98%)	118 (100%)	0	100	100
22	SQ	97/113 (86%)	97 (100%)	0	100	100
23	SR	129/135 (96%)	128 (99%)	1 (1%)	81	92
24	SS	43/45 (96%)	41 (95%)	2 (5%)	26	60
25	ST	129/131 (98%)	129 (100%)	0	100	100
26	SU	132/146 (90%)	131 (99%)	1 (1%)	81	92
27	SV	111/125 (89%)	110 (99%)	1 (1%)	78	91
28	SW	104/127 (82%)	103 (99%)	1 (1%)	76	89
29	SX	114/117 (97%)	113 (99%)	1 (1%)	78	91
30	SY	63/76 (83%)	63 (100%)	0	100	100
31	SZ	113/121 (93%)	112 (99%)	1 (1%)	78	91
32	Sa	70/99 (71%)	70 (100%)	0	100	100
33	Sb	85/97 (88%)	85 (100%)	0	100	100
34	Sc	75/77 (97%)	75 (100%)	0	100	100
35	Sd	55/65 (85%)	55 (100%)	0	100	100
36	Se	48/50 (96%)	48 (100%)	0	100	100
37	Sf	55/136 (40%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Sg	169/241 (70%)	168 (99%)	1 (1%)	86	94
39	Sh	261/267 (98%)	260 (100%)	1 (0%)	91	96
55	LP	195/208 (94%)	195 (100%)	0	100	100
56	LQ	329/344 (96%)	328 (100%)	1 (0%)	92	97
57	LR	305/314 (97%)	304 (100%)	1 (0%)	92	97
58	LS	154/166 (93%)	154 (100%)	0	100	100
59	LT	166/168 (99%)	166 (100%)	0	100	100
60	LU	173/174 (99%)	170 (98%)	3 (2%)	60	82
61	LV	206/242 (85%)	205 (100%)	1 (0%)	88	95
62	LW	182/183 (100%)	180 (99%)	2 (1%)	73	88
63	LX	187/192 (97%)	186 (100%)	1 (0%)	88	95
64	LY	104/109 (95%)	104 (100%)	0	100	100
65	LZ	190/192 (99%)	190 (100%)	0	100	100
66	La	123/124 (99%)	121 (98%)	2 (2%)	62	83
67	Lb	174/175 (99%)	174 (100%)	0	100	100
68	Lc	167/175 (95%)	166 (99%)	1 (1%)	86	94
69	Ld	213/213 (100%)	211 (99%)	2 (1%)	78	91
70	Le	162/163 (99%)	161 (99%)	1 (1%)	86	94
71	Lf	142/208 (68%)	141 (99%)	1 (1%)	84	93
72	Lg	164/165 (99%)	164 (100%)	0	100	100
73	Lh	140/141 (99%)	139 (99%)	1 (1%)	84	93
74	Li	131/139 (94%)	130 (99%)	1 (1%)	81	92
75	Lj	90/144 (62%)	90 (100%)	0	100	100
76	Lk	117/139 (84%)	117 (100%)	0	100	100
77	Ll	110/129 (85%)	110 (100%)	0	100	100
78	Lm	62/135 (46%)	62 (100%)	0	100	100
79	Ln	116/117 (99%)	116 (100%)	0	100	100
80	Lo	48/59 (81%)	48 (100%)	0	100	100
81	Lp	111/113 (98%)	111 (100%)	0	100	100
82	Lq	81/102 (79%)	81 (100%)	0	100	100
83	Lr	193/215 (90%)	192 (100%)	1 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	Ls	84/94 (89%)	83 (99%)	1 (1%)	71	87
85	Lt	101/138 (73%)	101 (100%)	0	100	100
86	Lu	113/121 (93%)	113 (100%)	0	100	100
87	Lv	97/98 (99%)	96 (99%)	1 (1%)	76	89
88	Lw	101/113 (89%)	101 (100%)	0	100	100
89	Lx	86/90 (96%)	86 (100%)	0	100	100
90	Ly	89/96 (93%)	89 (100%)	0	100	100
91	Lz	67/76 (88%)	66 (98%)	1 (2%)	65	84
92	L1	47/48 (98%)	47 (100%)	0	100	100
93	L2	47/108 (44%)	47 (100%)	0	100	100
94	L3	31/32 (97%)	30 (97%)	1 (3%)	39	70
95	L5	74/76 (97%)	74 (100%)	0	100	100
96	L4	86/94 (92%)	85 (99%)	1 (1%)	71	87
97	L6	54/61 (88%)	54 (100%)	0	100	100
98	L7	46/53 (87%)	45 (98%)	1 (2%)	52	77
All	All	9982/11183 (89%)	9939 (100%)	43 (0%)	91	96

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	SE	69	TYR
10	SE	108	ARG
12	SG	239	ARG
13	SH	146	GLU
14	SI	74	PHE
15	SJ	118	LYS
16	SK	55	ARG
20	SO	139	ASP
23	SR	96	PHE
24	SS	13	ARG
24	SS	40	ARG
26	SU	72	ARG
27	SV	80	LYS
28	SW	44	LYS
29	SX	112	LYS
31	SZ	14	LYS
38	Sg	235	ARG

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Mol	Chain	Res	Type
39	Sh	223	TRP
56	LQ	10	ARG
57	LR	89	MET
60	LU	59	ARG
60	LU	101	ARG
60	LU	157	LYS
61	LV	81	ARG
62	LW	106	ARG
62	LW	183	ARG
63	LX	95	ARG
66	La	71	ARG
66	La	121	ARG
68	Lc	24	ARG
69	Ld	22	ARG
69	Ld	241	CYS
70	Le	75	LYS
71	Lf	114	LYS
73	Lh	10	ARG
74	Li	26	VAL
83	Lr	32	LYS
84	Ls	105	ARG
87	Lv	74	ARG
91	Lz	51	LYS
94	L3	8	ARG
96	L4	97	LYS
98	L7	56	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
7	SB	70	ASN
7	SB	164	ASN
10	SE	62	HIS
12	SG	204	GLN
12	SG	214	HIS
13	SH	25	GLN
13	SH	165	ASN
13	SH	189	ASN
14	SI	30	GLN
14	SI	47	GLN
14	SI	82	HIS
14	SI	97	GLN

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Mol	Chain	Res	Type
15	SJ	59	ASN
16	SK	246	GLN
17	SL	13	GLN
17	SL	40	ASN
17	SL	70	ASN
18	SM	94	HIS
21	SP	5	HIS
21	SP	61	GLN
22	SQ	135	HIS
23	SR	12	HIS
27	SV	94	GLN
28	SW	87	ASN
29	SX	70	ASN
35	Sd	34	GLN
35	Sd	43	ASN
35	Sd	52	ASN
36	Se	57	GLN
36	Se	61	GLN
37	Sf	124	HIS
38	Sg	106	ASN
38	Sg	153	HIS
38	Sg	189	GLN
55	LP	62	GLN
56	LQ	121	ASN
56	LQ	167	GLN
57	LR	224	ASN
58	LS	6	ASN
60	LU	156	GLN
65	LZ	47	ASN
65	LZ	150	ASN
66	La	56	HIS
67	Lb	196	ASN
68	Lc	79	ASN
68	Lc	143	GLN
69	Ld	240	ASN
73	Lh	22	HIS
73	Lh	158	ASN
75	Lj	86	GLN
75	Lj	150	ASN
76	Lk	100	ASN
79	Ln	86	ASN
80	Lo	27	ASN

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Mol	Chain	Res	Type
82	Lq	28	ASN
83	Lr	126	ASN
84	Ls	14	ASN
85	Lt	45	ASN
86	Lu	32	HIS
86	Lu	130	ASN
88	Lw	46	HIS
96	L4	73	GLN
96	L4	82	GLN
97	L6	50	ASN
97	L6	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S1	2001/2315 (86%)	483 (24%)	16 (0%)
2	S2	74/76 (97%)	41 (55%)	2 (2%)
3	S3	75/76 (98%)	25 (33%)	2 (2%)
4	S4	75/76 (98%)	41 (54%)	3 (4%)
40	LA	157/163 (96%)	30 (19%)	0
41	LB	132/133 (99%)	22 (16%)	1 (0%)
42	LC	349/350 (99%)	79 (22%)	5 (1%)
43	LD	108/116 (93%)	30 (27%)	1 (0%)
44	LE	641/698 (91%)	106 (16%)	4 (0%)
45	LF	447/527 (84%)	88 (19%)	1 (0%)
46	LG	203/234 (86%)	38 (18%)	0
47	LH	554/744 (74%)	119 (21%)	7 (1%)
48	LI	567/617 (91%)	136 (23%)	1 (0%)
49	LJ	162/164 (98%)	27 (16%)	0
5	S5	11/12 (91%)	1 (9%)	0
50	LK	59/64 (92%)	16 (27%)	0
51	LL	90/95 (94%)	13 (14%)	0
52	LM	52/58 (89%)	6 (11%)	0
53	LN	76/86 (88%)	16 (21%)	0
54	LO	119/120 (99%)	15 (12%)	0
All	All	5952/6724 (88%)	1332 (22%)	43 (0%)

All (1332) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S1	2	A

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Mol	Chain	Res	Type
1	S1	3	U
1	S1	4	C
1	S1	17	C
1	S1	34	U
1	S1	42	OMG
1	S1	45	U
1	S1	47	A
1	S1	50	C
1	S1	57	OMG
1	S1	69	A
1	S1	75	U
1	S1	76	G
1	S1	93	U
1	S1	103	OMC
1	S1	113	C
1	S1	114	A
1	S1	115	U
1	S1	122	G
1	S1	128	G
1	S1	131	U
1	S1	140	C
1	S1	141	A
1	S1	142	C
1	S1	144	U
1	S1	145	G
1	S1	149	G
1	S1	155	C
1	S1	156	A
1	S1	157	U
1	S1	161	A
1	S1	163	A
1	S1	169	C
1	S1	174	C
1	S1	176	PSU
1	S1	180	OMG
1	S1	185	A
1	S1	193	U
1	S1	194	C
1	S1	196	A
1	S1	200	A
1	S1	211	C
1	S1	213	A

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Mol	Chain	Res	Type
1	S1	217	U
1	S1	220	G
1	S1	222	A
1	S1	251	C
1	S1	257	G
1	S1	267	U
1	S1	268	A
1	S1	269	U
1	S1	280	PSU
1	S1	282	C
1	S1	283	G
1	S1	284	A
1	S1	287	A
1	S1	289	C
1	S1	291	G
1	S1	297	G
1	S1	299	A
1	S1	304	C
1	S1	305	A
1	S1	306	G
1	S1	308	G
1	S1	309	U
1	S1	318	G
1	S1	326	C
1	S1	327	A
1	S1	334	C
1	S1	335	C
1	S1	347	C
1	S1	348	A
1	S1	352	C
1	S1	353	U
1	S1	354	G
1	S1	362	U
1	S1	363	C
1	S1	365	U
1	S1	378	C
1	S1	381	G
1	S1	382	C
1	S1	384	C
1	S1	394	G
1	S1	398	G
1	S1	404	C

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Mol	Chain	Res	Type
1	S1	412	U
1	S1	413	C
1	S1	415	G
1	S1	419	G
1	S1	434	G
1	S1	435	A
1	S1	442	U
1	S1	456	A
1	S1	457	A
1	S1	458	C
1	S1	465	PSU
1	S1	477	U
1	S1	485	OMG
1	S1	487	G
1	S1	491	C
1	S1	497	G
1	S1	498	A
1	S1	499	C
1	S1	510	A
1	S1	514	A
1	S1	516	G
1	S1	518	G
1	S1	520	G
1	S1	521	C
1	S1	523	G
1	S1	525	A
1	S1	531	G
1	S1	536	U
1	S1	541	C
1	S1	542	C
1	S1	545	G
1	S1	549	A
1	S1	550	G
1	S1	551	A
1	S1	555	U
1	S1	565	A2M
1	S1	569	A
1	S1	570	C
1	S1	578	A
1	S1	582	A
1	S1	588	U
1	S1	594	U

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Mol	Chain	Res	Type
1	S1	600	G
1	S1	602	C
1	S1	605	U
1	S1	615	A
1	S1	621	OMC
1	S1	624	U
1	S1	625	A
1	S1	639	G
1	S1	641	OMG
1	S1	643	G
1	S1	646	U
1	S1	649	A2M
1	S1	653	G
1	S1	655	G
1	S1	661	G
1	S1	668	G
1	S1	669	C
1	S1	672	G
1	S1	681	G
1	S1	682	OMU
1	S1	683	A
1	S1	698	G
1	S1	714	G
1	S1	715	C
1	S1	723	A2M
1	S1	724	A
1	S1	725	A
1	S1	726	A
1	S1	727	C
1	S1	732	G
1	S1	743	A
1	S1	744	C
1	S1	745	G
1	S1	747	G
1	S1	750	G
1	S1	751	C
1	S1	755	U
1	S1	757	U
1	S1	759	C
1	S1	762	G
1	S1	763	G
1	S1	764	U

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Mol	Chain	Res	Type
1	S1	767	C
1	S1	769	G
1	S1	770	G
1	S1	771	U
1	S1	772	U
1	S1	773	U
1	S1	774	G
1	S1	776	U
1	S1	777	G
1	S1	778	U
1	S1	782	U
1	S1	784	U
1	S1	785	G
1	S1	786	G
1	S1	789	A
1	S1	812	U
1	S1	814	U
1	S1	815	G
1	S1	817	U
1	S1	819	G
1	S1	820	G
1	S1	823	G
1	S1	824	C
1	S1	826	A
1	S1	827	C
1	S1	830	C
1	S1	832	G
1	S1	833	G
1	S1	855	C
1	S1	857	C
1	S1	861	G
1	S1	862	C
1	S1	865	A
1	S1	883	A
1	S1	884	G
1	S1	905	U
1	S1	921	A
1	S1	924	G
1	S1	926	G
1	S1	929	U
1	S1	931	A
1	S1	932	U

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Mol	Chain	Res	Type
1	S1	934	C
1	S1	940	G
1	S1	941	C
1	S1	944	U
1	S1	945	G
1	S1	950	C
1	S1	951	G
1	S1	959	A
1	S1	961	A
1	S1	965	G
1	S1	966	A
1	S1	967	C
1	S1	968	C
1	S1	970	A
1	S1	978	G
1	S1	979	C
1	S1	980	U
1	S1	983	G
1	S1	984	U
1	S1	994	C
1	S1	996	G
1	S1	997	G
1	S1	1002	C
1	S1	1003	C
1	S1	1018	U
1	S1	1035	A
1	S1	1045	G
1	S1	1046	C
1	S1	1061	C
1	S1	1062	G
1	S1	1063	A2M
1	S1	1065	G
1	S1	1068	PSU
1	S1	1071	A
1	S1	1074	U
1	S1	1075	C
1	S1	1076	C
1	S1	1077	A
1	S1	1078	U
1	S1	1079	C
1	S1	1085	A
1	S1	1090	C

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Mol	Chain	Res	Type
1	S1	1093	G
1	S1	1096	A2M
1	S1	1098	C
1	S1	1101	C
1	S1	1104	A
1	S1	1106	U
1	S1	1109	G
1	S1	1110	G
1	S1	1112	A
1	S1	1113	U
1	S1	1114	U
1	S1	1115	G
1	S1	1116	G
1	S1	1117	A
1	S1	1122	U
1	S1	1126	G
1	S1	1129	C
1	S1	1130	U
1	S1	1134	G
1	S1	1135	G
1	S1	1136	C
1	S1	1139	A
1	S1	1140	C
1	S1	1141	U
1	S1	1142	C
1	S1	1144	G
1	S1	1145	G
1	S1	1148	A
1	S1	1149	A
1	S1	1151	C
1	S1	1152	U
1	S1	1153	G
1	S1	1159	G
1	S1	1244	C
1	S1	1246	A
1	S1	1247	U
1	S1	1248	C
1	S1	1249	G
1	S1	1250	A
1	S1	1251	U
1	S1	1252	C
1	S1	1253	G

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Mol	Chain	Res	Type
1	S1	1254	U
1	S1	1255	A
1	S1	1256	A
1	S1	1257	G
1	S1	1260	A
1	S1	1273	G
1	S1	1283	U
1	S1	1293	C
1	S1	1296	G
1	S1	1310	A
1	S1	1311	G
1	S1	1329	U
1	S1	1330	G
1	S1	1331	C
1	S1	1339	G
1	S1	1342	U
1	S1	1356	G
1	S1	1363	G
1	S1	1367	A
1	S1	1371	A2M
1	S1	1385	A
1	S1	1389	A
1	S1	1400	A
1	S1	1417	C
1	S1	1418	C
1	S1	1422	G
1	S1	1424	A
1	S1	1425	A
1	S1	1427	C
1	S1	1429	A
1	S1	1453	A
1	S1	1454	A
1	S1	1455	G
1	S1	1457	A
1	S1	1458	U
1	S1	1459	C
1	S1	1461	U
1	S1	1463	G
1	S1	1495	A
1	S1	1500	C
1	S1	1502	C
1	S1	1507	U

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Mol	Chain	Res	Type
1	S1	1508	G
1	S1	1510	G
1	S1	1524	G
1	S1	1536	OMG
1	S1	1548	A
1	S1	1549	A2M
1	S1	1560	G
1	S1	1568	C
1	S1	1595	U
1	S1	1604	A
1	S1	1606	G
1	S1	1609	G
1	S1	1610	G
1	S1	1611	G
1	S1	1612	A
1	S1	1614	U
1	S1	1624	PSU
1	S1	1627	G
1	S1	1628	G
1	S1	1638	G
1	S1	1639	G
1	S1	1651	G
1	S1	1653	G
1	S1	1654	A
1	S1	1655	G
1	S1	1656	C
1	S1	1662	C
1	S1	1665	G
1	S1	1680	G
1	S1	1683	G
1	S1	1694	C
1	S1	1696	U
1	S1	1698	A
1	S1	1711	PSU
1	S1	1724	U
1	S1	1725	U
1	S1	1726	C
1	S1	1731	A
1	S1	1735	A
1	S1	1755	C
1	S1	1756	U
1	S1	1757	A

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Mol	Chain	Res	Type
1	S1	1765	G
1	S1	1766	C
1	S1	1767	U
1	S1	1770	C
1	S1	1780	G
1	S1	1785	G
1	S1	1787	C
1	S1	1789	G
1	S1	1790	C
1	S1	1833	A
1	S1	1835	G
1	S1	1841	G
1	S1	1842	A
1	S1	1843	G
1	S1	1849	C
1	S1	1850	C
1	S1	1852	G
1	S1	1853	U
1	S1	1854	U
1	S1	1855	C
1	S1	1856	A
1	S1	1860	U
1	S1	1865	G
1	S1	1872	U
1	S1	1880	C
1	S1	1882	A
1	S1	1885	A
1	S1	1897	G
1	S1	1898	C
1	S1	1899	U
1	S1	1900	A2M
1	S1	1903	G
1	S1	1906	A
1	S1	1907	A
1	S1	1910	G
1	S1	1912	A
1	S1	1913	G
1	S1	1917	U
1	S1	1918	G
1	S1	1920	G
1	S1	1944	C
1	S1	1946	C

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Mol	Chain	Res	Type
1	S1	1956	A
1	S1	1957	U
1	S1	1958	U
1	S1	1959	G
1	S1	1960	PSU
1	S1	1975	C
1	S1	1977	A
1	S1	1978	C
1	S1	1979	A
1	S1	1992	U
1	S1	1993	G
1	S1	2007	A
1	S1	2009	A
1	S1	2011	G
1	S1	2019	A
1	S1	2023	U
1	S1	2024	G
1	S1	2026	A
1	S1	2030	C
1	S1	2031	U
1	S1	2039	A
1	S1	2040	C
1	S1	2045	G
1	S1	2052	G
1	S1	2060	C
1	S1	2062	G
1	S1	2075	OMG
1	S1	2076	U
1	S1	2078	7MG
1	S1	2085	U
1	S1	2093	C
1	S1	2101	PSU
1	S1	2102	C
1	S1	2103	A
1	S1	2104	G
1	S1	2110	A
1	S1	2119	G
1	S1	2124	U
1	S1	2138	A
1	S1	2144	5MC
1	S1	2181	G
1	S1	2182	G

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Mol	Chain	Res	Type
1	S1	2189	U
1	S1	2194	G
1	S1	2216	C
1	S1	2217	A
1	S1	2218	U
1	S1	2222	A
1	S1	2233	G
1	S1	2256	A
1	S1	2261	A
1	S1	2266	G
1	S1	2268	A
1	S1	2272	A
1	S1	2275	U
1	S1	2286	G
1	S1	2298	G
1	S1	2299	G
1	S1	2300	A
1	S1	2301	U
1	S1	2302	C
1	S1	2305	PSU
2	S2	3	G
2	S2	5	G
2	S2	8	U
2	S2	9	A
2	S2	10	G
2	S2	12	U
2	S2	14	A
2	S2	16	U
2	S2	17	C
2	S2	19	G
2	S2	20	U
2	S2	22	G
2	S2	27	G
2	S2	29	G
2	S2	34	G
2	S2	35	A
2	S2	36	A
2	S2	38	A
2	S2	43	C
2	S2	44	G
2	S2	45	U
2	S2	46	G

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Mol	Chain	Res	Type
2	S2	47	U
2	S2	49	C
2	S2	50	U
2	S2	51	U
2	S2	52	G
2	S2	54	U
2	S2	56	C
2	S2	57	G
2	S2	59	U
2	S2	60	U
2	S2	61	C
2	S2	64	A
2	S2	66	U
2	S2	71	G
2	S2	72	C
2	S2	73	A
2	S2	74	C
2	S2	75	C
2	S2	76	A
3	S3	7	A
3	S3	14	A
3	S3	16	U
3	S3	17	C
3	S3	18	G
3	S3	19	G
3	S3	20	U
3	S3	21	A
3	S3	22	G
3	S3	34	C
3	S3	35	A
3	S3	38	A
3	S3	44	G
3	S3	48	C
3	S3	49	C
3	S3	54	U
3	S3	56	C
3	S3	57	G
3	S3	61	C
3	S3	67	C
3	S3	69	G
3	S3	71	G
3	S3	72	C

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Mol	Chain	Res	Type
3	S3	74	C
3	S3	76	A
4	S4	2	C
4	S4	3	G
4	S4	6	G
4	S4	7	A
4	S4	8	U
4	S4	9	A
4	S4	10	G
4	S4	14	A
4	S4	15	G
4	S4	16	U
4	S4	17	C
4	S4	19	G
4	S4	20	U
4	S4	21	A
4	S4	30	G
4	S4	31	A
4	S4	33	U
4	S4	34	G
4	S4	35	A
4	S4	36	A
4	S4	37	A
4	S4	44	G
4	S4	45	U
4	S4	46	G
4	S4	47	U
4	S4	51	U
4	S4	52	G
4	S4	54	U
4	S4	55	U
4	S4	56	C
4	S4	57	G
4	S4	58	A
4	S4	59	U
4	S4	61	C
4	S4	67	C
4	S4	69	G
4	S4	70	C
4	S4	71	G
4	S4	73	A
4	S4	74	C

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Mol	Chain	Res	Type
4	S4	76	A
5	S5	5	A
40	LA	6	U
40	LA	10	G
40	LA	14	G
40	LA	32	C
40	LA	36	G
40	LA	40	G
40	LA	41	OMG
40	LA	46	A
40	LA	49	A
40	LA	58	A
40	LA	61	C
40	LA	62	G
40	LA	74	OMG
40	LA	76	A
40	LA	77	G
40	LA	84	G
40	LA	85	U
40	LA	86	G
40	LA	92	G
40	LA	93	A
40	LA	94	C
40	LA	95	A
40	LA	96	A
40	LA	97	A2M
40	LA	102	C
40	LA	110	A
40	LA	112	C
40	LA	122	C
40	LA	123	A
40	LA	156	C
41	LB	181	G
41	LB	185	G
41	LB	191	C
41	LB	200	A
41	LB	203	A
41	LB	209	C
41	LB	219	G
41	LB	220	A
41	LB	225	C
41	LB	226	A

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Mol	Chain	Res	Type
41	LB	233	C
41	LB	234	PSU
41	LB	247	OMU
41	LB	252	G
41	LB	274	C
41	LB	275	G
41	LB	277	C
41	LB	278	U
41	LB	279	C
41	LB	288	A
41	LB	289	A
41	LB	290	U
42	LC	298	U
42	LC	302	PSU
42	LC	305	G
42	LC	306	C
42	LC	308	PSU
42	LC	312	U
42	LC	320	C
42	LC	323	C
42	LC	324	A
42	LC	330	U
42	LC	340	G
42	LC	354	U
42	LC	355	G
42	LC	358	U
42	LC	363	G
42	LC	375	C
42	LC	381	G
42	LC	382	A
42	LC	383	G
42	LC	384	U
42	LC	391	A
42	LC	392	U
42	LC	399	A
42	LC	400	C
42	LC	412	A
42	LC	413	C
42	LC	414	U
42	LC	420	G
42	LC	426	C
42	LC	428	G

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Mol	Chain	Res	Type
42	LC	429	A
42	LC	430	A
42	LC	431	C
42	LC	432	C
42	LC	433	G
42	LC	434	U
42	LC	435	G
42	LC	448	U
42	LC	451	G
42	LC	452	A
42	LC	453	U
42	LC	457	G
42	LC	458	C
42	LC	466	A
42	LC	467	U
42	LC	469	C
42	LC	470	C
42	LC	474	G
42	LC	491	OMU
42	LC	500	A
42	LC	504	G
42	LC	505	U
42	LC	508	C
42	LC	510	U
42	LC	515	C
42	LC	528	G
42	LC	534	A
42	LC	535	G
42	LC	536	A
42	LC	537	OMC
42	LC	542	G
42	LC	551	U
42	LC	573	G
42	LC	577	OMC
42	LC	580	A
42	LC	581	G
42	LC	595	G
42	LC	602	A
42	LC	603	A
42	LC	605	U
42	LC	606	C
42	LC	607	C

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Mol	Chain	Res	Type
42	LC	608	C
42	LC	611	A
42	LC	624	A
42	LC	626	C
42	LC	627	G
42	LC	634	U
42	LC	636	C
43	LD	661	C
43	LD	668	A
43	LD	675	G
43	LD	679	G
43	LD	680	G
43	LD	686	G
43	LD	687	A
43	LD	688	G
43	LD	689	C
43	LD	697	U
43	LD	700	G
43	LD	701	G
43	LD	705	G
43	LD	709	U
43	LD	713	U
43	LD	715	U
43	LD	727	C
43	LD	730	G
43	LD	731	G
43	LD	733	G
43	LD	734	G
43	LD	736	A
43	LD	738	C
43	LD	742	G
43	LD	746	G
43	LD	747	C
43	LD	749	A
43	LD	750	G
43	LD	751	G
43	LD	756	G
44	LE	765	C
44	LE	771	U
44	LE	772	G
44	LE	776	G
44	LE	778	G

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Mol	Chain	Res	Type
44	LE	802	G
44	LE	805	C
44	LE	808	G
44	LE	809	G
44	LE	812	C
44	LE	813	U
44	LE	817	C
44	LE	826	C
44	LE	831	G
44	LE	841	U
44	LE	842	G
44	LE	846	G
44	LE	850	C
44	LE	851	G
44	LE	858	A
44	LE	878	U
44	LE	883	A
44	LE	884	G
44	LE	888	A
44	LE	889	G
44	LE	896	A
44	LE	911	G
44	LE	923	C
44	LE	933	A
44	LE	935	A2M
44	LE	936	OMC
44	LE	946	A
44	LE	963	A
44	LE	968	G
44	LE	969	A
44	LE	974	U
44	LE	1006	G
44	LE	1016	U
44	LE	1030	A
44	LE	1032	U
44	LE	1038	C
44	LE	1046	G
44	LE	1047	A
44	LE	1075	PSU
44	LE	1076	U
44	LE	1080	G
44	LE	1084	U

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Mol	Chain	Res	Type
44	LE	1098	G
44	LE	1101	C
44	LE	1104	OMG
44	LE	1111	G
44	LE	1114	G
44	LE	1116	A
44	LE	1129	A
44	LE	1160	C
44	LE	1170	U
44	LE	1173	U
44	LE	1178	U
44	LE	1179	G
44	LE	1188	G
44	LE	1195	G
44	LE	1196	A
44	LE	1207	G
44	LE	1208	OMG
44	LE	1209	G
44	LE	1214	A
44	LE	1216	G
44	LE	1217	OMG
44	LE	1221	A
44	LE	1223	C
44	LE	1224	G
44	LE	1225	A
44	LE	1237	G
44	LE	1244	C
44	LE	1259	C
44	LE	1260	PSU
44	LE	1261	C
44	LE	1277	C
44	LE	1297	G
44	LE	1298	U
44	LE	1299	G
44	LE	1300	A
44	LE	1301	C
44	LE	1314	G
44	LE	1325	C
44	LE	1326	A
44	LE	1356	C
44	LE	1357	U
44	LE	1361	C

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Mol	Chain	Res	Type
44	LE	1371	A
44	LE	1376	U
44	LE	1403	C
44	LE	1409	U
44	LE	1414	C
44	LE	1423	G
44	LE	1424	C
44	LE	1428	G
44	LE	1430	A
44	LE	1431	A
44	LE	1432	C
44	LE	1438	U
44	LE	1440	C
44	LE	1445	C
44	LE	1451	C
44	LE	1452	OMU
44	LE	1453	G
45	LF	1466	G
45	LF	1467	A
45	LF	1477	C
45	LF	1486	A
45	LF	1491	G
45	LF	1492	A
45	LF	1493	C
45	LF	1500	G
45	LF	1504	OMU
45	LF	1513	U
45	LF	1522	C
45	LF	1530	G
45	LF	1537	U
45	LF	1549	G
45	LF	1550	U
45	LF	1551	G
45	LF	1555	G
45	LF	1564	C
45	LF	1565	A
45	LF	1568	PSU
45	LF	1569	C
45	LF	1572	A
45	LF	1573	OMC
45	LF	1581	G
45	LF	1590	U

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Mol	Chain	Res	Type
45	LF	1662	OMG
45	LF	1664	G
45	LF	1665	C
45	LF	1666	A
45	LF	1667	OMG
45	LF	1674	A
45	LF	1677	U
45	LF	1679	G
45	LF	1681	OMU
45	LF	1685	G
45	LF	1689	A
45	LF	1698	U
45	LF	1699	G
45	LF	1702	U
45	LF	1703	C
45	LF	1704	C
45	LF	1708	A
45	LF	1710	A
45	LF	1727	G
45	LF	1730	G
45	LF	1738	A2M
45	LF	1740	A
45	LF	1757	A
45	LF	1771	A
45	LF	1772	G
45	LF	1802	A
45	LF	1804	G
45	LF	1813	A
45	LF	1819	OMG
45	LF	1822	OMC
45	LF	1827	U
45	LF	1831	A
45	LF	1835	OMG
45	LF	1840	U
45	LF	1852	A
45	LF	1853	G
45	LF	1854	A
45	LF	1856	OMG
45	LF	1857	A
45	LF	1858	G
45	LF	1862	C
45	LF	1874	G

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Mol	Chain	Res	Type
45	LF	1881	G
45	LF	1895	G
45	LF	1902	G
45	LF	1910	C
45	LF	1916	C
45	LF	1917	A
45	LF	1918	A
45	LF	1922	G
45	LF	1924	C
45	LF	1925	G
45	LF	1926	PSU
45	LF	1937	U
45	LF	1938	C
45	LF	1940	A
45	LF	1946	C
45	LF	1947	G
45	LF	1961	A
45	LF	1971	A
45	LF	1976	OMC
45	LF	1979	A
45	LF	1980	A
46	LG	1997	A
46	LG	2004	A
46	LG	2005	A2M
46	LG	2006	C
46	LG	2011	A
46	LG	2016	C
46	LG	2018	A
46	LG	2020	C
46	LG	2022	A2M
46	LG	2024	A
46	LG	2025	U
46	LG	2032	G
46	LG	2067	C
46	LG	2071	C
46	LG	2094	C
46	LG	2120	C
46	LG	2143	C
46	LG	2145	C
46	LG	2146	OMG
46	LG	2155	C
46	LG	2161	G

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Mol	Chain	Res	Type
46	LG	2169	G
46	LG	2170	A
46	LG	2171	PSU
46	LG	2173	G
46	LG	2182	G
46	LG	2188	C
46	LG	2195	C
46	LG	2196	A
46	LG	2197	A
46	LG	2198	G
46	LG	2207	G
46	LG	2208	U
46	LG	2209	C
46	LG	2210	U
46	LG	2216	C
46	LG	2220	U
46	LG	2221	G
47	LH	2226	G
47	LH	2239	G
47	LH	2241	U
47	LH	2248	A
47	LH	2263	U
47	LH	2282	U
47	LH	2295	C
47	LH	2296	A
47	LH	2297	U
47	LH	2299	A
47	LH	2303	C
47	LH	2304	A
47	LH	2306	C
47	LH	2307	C
47	LH	2310	U
47	LH	2335	C
47	LH	2336	A
47	LH	2337	C
47	LH	2343	A
47	LH	2344	A
47	LH	2349	A2M
47	LH	2352	U
47	LH	2364	G
47	LH	2365	C
47	LH	2366	A

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Mol	Chain	Res	Type
47	LH	2383	U
47	LH	2583	G
47	LH	2588	G
47	LH	2590	G
47	LH	2598	G
47	LH	2599	U
47	LH	2601	G
47	LH	2602	OMC
47	LH	2610	OMG
47	LH	2619	A
47	LH	2624	PSU
47	LH	2628	U
47	LH	2632	A
47	LH	2634	C
47	LH	2646	A
47	LH	2648	G
47	LH	2657	U
47	LH	2667	C
47	LH	2685	OMC
47	LH	2694	G
47	LH	2695	A
47	LH	2696	U
47	LH	2697	U
47	LH	2713	OMU
47	LH	2732	A
47	LH	2737	G
47	LH	2744	A2M
47	LH	2745	C
47	LH	2760	G
47	LH	2761	G
47	LH	2768	A2M
47	LH	2769	A2M
47	LH	2776	OMG
47	LH	2785	U
47	LH	2786	U
47	LH	2791	A
47	LH	2794	C
47	LH	2795	G
47	LH	2798	U
47	LH	2801	A
47	LH	2802	PSU
47	LH	2803	G

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Mol	Chain	Res	Type
47	LH	2822	U
47	LH	2824	U
47	LH	2844	A
47	LH	2852	A
47	LH	2853	OMC
47	LH	2854	C
47	LH	2860	A
47	LH	2861	A
47	LH	2862	C
47	LH	2863	G
47	LH	2881	G
47	LH	2882	G
47	LH	2885	A
47	LH	2890	A
47	LH	2891	G
47	LH	2892	A
47	LH	2893	C
47	LH	2899	PSU
47	LH	2900	G
47	LH	2906	G
47	LH	2907	A
47	LH	2923	G
47	LH	2925	OMG
47	LH	2932	C
47	LH	2933	A
47	LH	2934	U
47	LH	2935	G
47	LH	2936	U
47	LH	2937	G
47	LH	2938	G
47	LH	2939	G
47	LH	2940	G
47	LH	2941	C
47	LH	2942	G
47	LH	2943	U
47	LH	2944	A
47	LH	2947	A
47	LH	2948	U
47	LH	2949	A
47	LH	2950	G
47	LH	2951	G
47	LH	2952	U

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Mol	Chain	Res	Type
47	LH	2953	G
47	LH	2954	G
47	LH	2955	G
47	LH	2956	A
47	LH	2957	G
47	LH	2959	U
47	LH	2961	A
47	LH	2962	G
47	LH	2963	U
47	LH	2965	C
48	LI	2971	G
48	LI	2972	C
48	LI	2973	G
48	LI	2975	G
48	LI	2978	U
48	LI	2981	A
48	LI	2983	U
48	LI	2986	A
48	LI	2987	A
48	LI	2988	U
48	LI	2989	A
48	LI	2990	C
48	LI	2991	C
48	LI	2993	C
48	LI	2994	U
48	LI	2995	A
48	LI	2996	C
48	LI	2998	U
48	LI	3000	C
48	LI	3001	A
48	LI	3003	C
48	LI	3004	G
48	LI	3015	C
48	LI	3023	U
48	LI	3035	G
48	LI	3037	G
48	LI	3038	G
48	LI	3039	C
48	LI	3040	C
48	LI	3041	A
48	LI	3042	PSU
48	LI	3084	C

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Mol	Chain	Res	Type
48	LI	3091	C
48	LI	3092	A
48	LI	3093	U
48	LI	3100	A
48	LI	3110	A
48	LI	3111	G
48	LI	3130	C
48	LI	3139	U
48	LI	3140	C
48	LI	3141	A
48	LI	3143	A
48	LI	3150	U
48	LI	3157	U
48	LI	3158	C
48	LI	3164	A
48	LI	3167	PSU
48	LI	3171	OMU
48	LI	3178	G
48	LI	3179	G
48	LI	3186	G
48	LI	3191	OMG
48	LI	3198	A
48	LI	3200	G
48	LI	3207	A
48	LI	3208	OMC
48	LI	3220	G
48	LI	3223	OMG
48	LI	3224	U
48	LI	3228	G
48	LI	3229	A
48	LI	3247	A
48	LI	3250	G
48	LI	3262	G
48	LI	3264	A
48	LI	3269	A
48	LI	3277	A
48	LI	3278	G
48	LI	3279	G
48	LI	3287	G
48	LI	3290	G
48	LI	3302	A
48	LI	3303	G

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Mol	Chain	Res	Type
48	LI	3312	C
48	LI	3314	A
48	LI	3315	A2M
48	LI	3316	A
48	LI	3324	U
48	LI	3327	U
48	LI	3328	G
48	LI	3330	C
48	LI	3336	G
48	LI	3353	U
48	LI	3354	G
48	LI	3355	OMC
48	LI	3356	G
48	LI	3359	U
48	LI	3362	U
48	LI	3368	U
48	LI	3374	OMC
48	LI	3377	OMG
48	LI	3382	G
48	LI	3385	A
48	LI	3386	G
48	LI	3387	A
48	LI	3388	A
48	LI	3390	A
48	LI	3393	U
48	LI	3396	C
48	LI	3400	G
48	LI	3401	OMG
48	LI	3403	A
48	LI	3407	C
48	LI	3413	U
48	LI	3419	U
48	LI	3430	C
48	LI	3431	A
48	LI	3433	A
48	LI	3437	A
48	LI	3446	PSU
48	LI	3452	C
48	LI	3457	G
48	LI	3461	U
48	LI	3462	C
48	LI	3467	C

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Mol	Chain	Res	Type
48	LI	3472	U
48	LI	3473	A
48	LI	3475	C
48	LI	3480	C
48	LI	3491	G
48	LI	3498	A
48	LI	3517	A
48	LI	3522	C
48	LI	3523	A
48	LI	3528	A
48	LI	3529	C
48	LI	3534	G
48	LI	3539	G
48	LI	3558	A
48	LI	3563	G
48	LI	3565	U
48	LI	3566	U
48	LI	3570	C
48	LI	3577	G
48	LI	3584	A
49	LJ	3601	A
49	LJ	3602	U
49	LJ	3612	G
49	LJ	3620	G
49	LJ	3632	G
49	LJ	3639	C
49	LJ	3646	U
49	LJ	3647	C
49	LJ	3649	A
49	LJ	3664	A
49	LJ	3668	G
49	LJ	3669	U
49	LJ	3672	A
49	LJ	3682	C
49	LJ	3683	C
49	LJ	3686	G
49	LJ	3689	A
49	LJ	3697	PSU
49	LJ	3705	C
49	LJ	3713	A
49	LJ	3720	A
49	LJ	3721	A

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Mol	Chain	Res	Type
49	LJ	3727	G
49	LJ	3734	C
49	LJ	3738	C
49	LJ	3739	A
49	LJ	3748	G
50	LK	3753	C
50	LK	3754	A
50	LK	3757	G
50	LK	3761	C
50	LK	3762	A
50	LK	3764	A
50	LK	3770	A
50	LK	3774	U
50	LK	3776	C
50	LK	3783	U
50	LK	3786	G
50	LK	3795	A
50	LK	3805	G
50	LK	3808	C
50	LK	3809	U
50	LK	3810	G
51	LL	3814	G
51	LL	3818	U
51	LL	3838	G
51	LL	3840	U
51	LL	3853	G
51	LL	3858	G
51	LL	3859	G
51	LL	3877	G
51	LL	3879	U
51	LL	3880	G
51	LL	3902	A
51	LL	3906	A2M
51	LL	3907	G
52	LM	3911	A
52	LM	3921	C
52	LM	3922	C
52	LM	3944	G
52	LM	3951	A
52	LM	3961	G
53	LN	3980	G
53	LN	3981	A

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Mol	Chain	Res	Type
53	LN	3984	U
53	LN	3987	A
53	LN	3990	G
53	LN	3994	G
53	LN	3998	U
53	LN	4000	U
53	LN	4009	U
53	LN	4018	C
53	LN	4023	C
53	LN	4030	G
53	LN	4031	G
53	LN	4042	C
53	LN	4043	A
53	LN	4044	G
54	LO	7	G
54	LO	22	A
54	LO	25	A
54	LO	33	A
54	LO	50	A
54	LO	53	U
54	LO	54	A
54	LO	57	C
54	LO	64	A
54	LO	74	A
54	LO	91	C
54	LO	110	G
54	LO	113	G
54	LO	117	G
54	LO	120	U

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S1	143	C
1	S1	193	U
1	S1	267	U
1	S1	282	C
1	S1	303	C
1	S1	1243	C
1	S1	1245	C
1	S1	1247	U
1	S1	1249	G

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Mol	Chain	Res	Type
1	S1	1454	A
1	S1	1458	U
1	S1	1912	A
1	S1	1919	U
1	S1	1957	U
1	S1	1958	U
1	S1	1976	G
2	S2	13	C
2	S2	34	G
3	S3	6	G
3	S3	34	C
4	S4	13	C
4	S4	19	G
4	S4	34	G
41	LB	278	U
42	LC	447	C
42	LC	465	U
42	LC	466	A
42	LC	579	A
42	LC	602	A
43	LD	726	C
44	LE	1075	PSU
44	LE	1208	OMG
44	LE	1224	G
44	LE	1431	A
45	LF	1856	OMG
47	LH	2342	G
47	LH	2656	C
47	LH	2768	A2M
47	LH	2937	G
47	LH	2938	G
47	LH	2939	G
47	LH	2964	G
48	LI	2994	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	S1	1901	1	18,26,27	1.31	2 (11%)	19,38,41	1.53	5 (26%)
47	PSU	LH	2842	45,47	18,21,22	4.02	8 (44%)	22,30,33	1.80	6 (27%)
1	OMC	S1	38	1	19,22,23	1.01	1 (5%)	26,31,34	1.13	3 (11%)
1	A2M	S1	407	1	18,25,26	4.24	8 (44%)	18,36,39	2.99	4 (22%)
47	PSU	LH	2621	44,47	18,21,22	4.15	7 (38%)	22,30,33	1.75	5 (22%)
47	PSU	LH	2914	48,47	18,21,22	4.15	7 (38%)	22,30,33	1.89	5 (22%)
47	OMU	LH	2346	47	19,22,23	0.63	0	26,31,34	1.06	2 (7%)
48	OMG	LI	3509	48,2	18,26,27	1.31	2 (11%)	19,38,41	1.49	3 (15%)
47	PSU	LH	2899	48,47	18,21,22	4.11	7 (38%)	22,30,33	1.86	5 (22%)
1	UR3	S1	1597	1	19,22,23	0.78	1 (5%)	26,32,35	0.58	0
47	PSU	LH	2754	47	18,21,22	4.05	7 (38%)	22,30,33	1.96	5 (22%)
48	UR3	LI	3540	48	19,22,23	0.73	0	26,32,35	0.60	0
47	A2M	LH	2349	47	18,25,26	4.23	7 (38%)	18,36,39	3.00	3 (16%)
1	PSU	S1	2116	1	18,21,22	4.10	7 (38%)	22,30,33	1.71	4 (18%)
44	OMU	LE	1081	44	19,22,23	0.51	0	26,31,34	0.88	2 (7%)
1	A2M	S1	40	1	18,25,26	4.17	7 (38%)	18,36,39	2.96	3 (16%)
44	PSU	LE	1171	44	18,21,22	4.15	7 (38%)	22,30,33	1.88	5 (22%)
47	A2M	LH	2744	47	18,25,26	4.13	7 (38%)	18,36,39	3.14	5 (27%)
1	PSU	S1	1068	1	18,21,22	4.20	7 (38%)	22,30,33	1.81	5 (22%)
48	OMU	LI	3508	48	19,22,23	0.56	0	26,31,34	0.95	2 (7%)
45	OMC	LF	1822	44,45	19,22,23	0.87	1 (5%)	26,31,34	1.06	2 (7%)
48	OMG	LI	3434	48	18,26,27	1.31	2 (11%)	19,38,41	1.54	6 (31%)
1	OMG	S1	1536	1,94	18,26,27	1.31	2 (11%)	19,38,41	1.63	4 (21%)
45	PSU	LF	1582	45	18,21,22	4.11	7 (38%)	22,30,33	1.89	5 (22%)
1	PSU	S1	1591	1	18,21,22	3.97	7 (38%)	22,30,33	1.83	6 (27%)
47	PSU	LH	2623	47	18,21,22	4.09	7 (38%)	22,30,33	1.95	5 (22%)
44	OMG	LE	1104	44	18,26,27	1.34	2 (11%)	19,38,41	1.54	4 (21%)
47	A2M	LH	2358	47	18,25,26	4.13	7 (38%)	18,36,39	3.16	4 (22%)
48	OMU	LI	3300	48	19,22,23	0.53	0	26,31,34	1.00	2 (7%)
1	PSU	S1	1711	1	18,21,22	4.00	7 (38%)	22,30,33	1.95	5 (22%)
1	OMU	S1	2041	1	19,22,23	0.55	0	26,31,34	0.76	1 (3%)
47	PSU	LH	2874	48,47	18,21,22	4.19	7 (38%)	22,30,33	1.98	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	S1	1679	1	19,22,23	0.58	0	26,31,34	0.96	2 (7%)
45	OMU	LF	1824	44,45,42	19,22,23	0.50	0	26,31,34	1.01	2 (7%)
1	PSU	S1	2305	1	18,21,22	4.15	7 (38%)	22,30,33	1.72	5 (22%)
47	OMU	LH	2713	47	19,22,23	0.68	0	26,31,34	0.88	2 (7%)
47	PSU	LH	2802	47	18,21,22	4.17	7 (38%)	22,30,33	1.81	5 (22%)
47	OMG	LH	2883	48,47	18,26,27	1.37	2 (11%)	19,38,41	1.50	4 (21%)
45	OMG	LF	1662	45	18,26,27	1.35	3 (16%)	19,38,41	1.50	5 (26%)
53	PSU	LN	3969	53,52	18,21,22	4.30	7 (38%)	22,30,33	1.73	5 (22%)
1	OMG	S1	57	1	18,26,27	1.27	2 (11%)	19,38,41	1.61	5 (26%)
1	PSU	S1	640	1	18,21,22	4.16	7 (38%)	22,30,33	1.67	4 (18%)
1	OMU	S1	1966	1,29	19,22,23	0.53	0	26,31,34	0.83	2 (7%)
1	PSU	S1	2131	1	18,21,22	4.14	7 (38%)	22,30,33	1.91	5 (22%)
52	OMC	LM	3957	53,52	19,22,23	0.95	2 (10%)	26,31,34	1.02	2 (7%)
49	PSU	LJ	3701	49	18,21,22	4.10	7 (38%)	22,30,33	1.90	5 (22%)
44	PSU	LE	1198	44	18,21,22	4.11	7 (38%)	22,30,33	1.92	5 (22%)
48	OMC	LI	3355	48,44	19,22,23	0.97	1 (5%)	26,31,34	1.08	3 (11%)
1	OMG	S1	42	1	18,26,27	1.36	3 (16%)	19,38,41	1.60	5 (26%)
47	A2M	LH	2887	48,47	18,25,26	4.26	7 (38%)	18,36,39	3.10	3 (16%)
52	PSU	LM	3953	53,52	18,21,22	4.18	7 (38%)	22,30,33	1.83	5 (22%)
1	PSU	S1	280	1	18,21,22	4.19	7 (38%)	22,30,33	1.90	5 (22%)
44	PSU	LE	1407	44	18,21,22	4.11	7 (38%)	22,30,33	1.87	5 (22%)
48	6MZ	LI	3214	48,45	18,25,26	0.83	1 (5%)	16,36,39	2.14	4 (25%)
1	PSU	S1	105	1	18,21,22	4.21	7 (38%)	22,30,33	1.85	5 (22%)
48	OMC	LI	3222	48	19,22,23	0.91	1 (5%)	26,31,34	1.17	4 (15%)
47	JMH	LH	2636	47	18,22,23	1.11	1 (5%)	21,32,35	1.51	5 (23%)
42	OMU	LC	491	42	19,22,23	0.66	0	26,31,34	0.94	2 (7%)
1	PSU	S1	32	1	18,21,22	4.12	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	S1	403	1	18,21,22	4.20	7 (38%)	22,30,33	1.69	4 (18%)
47	OMC	LH	2685	47	19,22,23	1.26	1 (5%)	26,31,34	1.42	4 (15%)
44	PSU	LE	1184	44	18,21,22	4.13	7 (38%)	22,30,33	1.79	5 (22%)
41	PSU	LB	234	41	18,21,22	4.15	7 (38%)	22,30,33	1.79	5 (22%)
1	A2M	S1	1096	1	18,25,26	4.24	7 (38%)	18,36,39	2.92	3 (16%)
48	PSU	LI	3568	48,47	18,21,22	4.05	7 (38%)	22,30,33	1.83	6 (27%)
1	PSU	S1	1715	1	18,21,22	4.14	7 (38%)	22,30,33	1.77	5 (22%)
42	PSU	LC	302	42	18,21,22	4.20	7 (38%)	22,30,33	1.92	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMG	LF	1883	45	18,26,27	1.33	3 (16%)	19,38,41	1.48	4 (21%)
45	OMU	LF	1828	45,47	19,22,23	0.50	0	26,31,34	0.87	0
48	PSU	LI	3562	48	18,21,22	4.05	7 (38%)	22,30,33	1.97	5 (22%)
45	OMG	LF	1956	45	18,26,27	1.33	2 (11%)	19,38,41	1.51	4 (21%)
47	PSU	LH	2586	47	18,21,22	4.21	7 (38%)	22,30,33	1.80	5 (22%)
44	OMC	LE	936	44	19,22,23	0.81	0	26,31,34	1.09	3 (11%)
1	PSU	S1	2065	1	18,21,22	4.16	7 (38%)	22,30,33	1.88	5 (22%)
47	PSU	LH	2915	48,47	18,21,22	4.13	7 (38%)	22,30,33	1.81	5 (22%)
1	MA6	S1	2288	1	19,26,27	1.08	1 (5%)	18,38,41	3.76	2 (11%)
42	PSU	LC	308	42	18,21,22	4.22	7 (38%)	22,30,33	1.89	5 (22%)
1	OMG	S1	390	1	18,26,27	1.36	2 (11%)	19,38,41	1.53	5 (26%)
1	A2M	S1	649	1	18,25,26	4.11	7 (38%)	18,36,39	3.05	3 (16%)
44	OMG	LE	1324	44	18,26,27	1.35	3 (16%)	19,38,41	1.45	3 (15%)
47	PSU	LH	2624	47	18,21,22	4.10	8 (44%)	22,30,33	1.75	4 (18%)
48	A2M	LI	3367	48,42	18,25,26	4.23	7 (38%)	18,36,39	2.99	3 (16%)
1	A2M	S1	565	1	18,25,26	4.21	7 (38%)	18,36,39	3.09	4 (22%)
48	A2M	LI	3348	48	18,25,26	4.21	7 (38%)	18,36,39	3.01	3 (16%)
47	OMG	LH	2870	47	18,26,27	1.30	2 (11%)	19,38,41	1.53	5 (26%)
40	PSU	LA	68	40	18,21,22	4.13	8 (44%)	22,30,33	2.07	6 (27%)
41	OMU	LB	247	41	19,22,23	0.70	0	26,31,34	0.92	2 (7%)
47	OMC	LH	2832	47	19,22,23	0.81	0	26,31,34	1.10	3 (11%)
49	OMU	LJ	3694	49	19,22,23	0.55	0	26,31,34	0.94	2 (7%)
45	OMG	LF	1667	45	18,26,27	1.32	2 (11%)	19,38,41	1.56	4 (21%)
48	PSU	LI	3204	48	18,21,22	4.09	7 (38%)	22,30,33	1.82	5 (22%)
1	PSU	S1	89	1	18,21,22	4.12	7 (38%)	22,30,33	1.87	5 (22%)
1	PSU	S1	544	1	18,21,22	4.09	7 (38%)	22,30,33	1.95	5 (22%)
1	A2M	S1	110	1	18,25,26	4.17	7 (38%)	18,36,39	3.08	3 (16%)
1	OMU	S1	682	1	19,22,23	0.48	0	26,31,34	1.06	2 (7%)
47	PSU	LH	2591	47	18,21,22	4.15	7 (38%)	22,30,33	1.82	5 (22%)
44	PSU	LE	1075	44,48	18,21,22	4.07	8 (44%)	22,30,33	1.79	5 (22%)
1	A2M	S1	645	1	18,25,26	4.16	7 (38%)	18,36,39	3.06	4 (22%)
46	PSU	LG	2171	46	18,21,22	4.23	8 (44%)	22,30,33	1.78	4 (18%)
46	A2M	LG	2005	45,46	18,25,26	4.15	7 (38%)	18,36,39	3.15	3 (16%)
47	OMC	LH	2853	47	19,22,23	0.88	1 (5%)	26,31,34	1.12	3 (11%)
48	OMU	LI	3171	48,47	19,22,23	0.58	0	26,31,34	0.90	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S1	27	1	18,21,22	4.08	7 (38%)	22,30,33	1.84	5 (22%)
45	OMC	LF	1976	45	19,22,23	0.87	1 (5%)	26,31,34	1.16	3 (11%)
2	MIA	S2	37	2	24,31,32	2.48	4 (16%)	26,44,47	2.81	8 (30%)
48	5MC	LI	3518	48,64	18,22,23	1.53	4 (22%)	26,32,35	1.31	5 (19%)
1	OMC	S1	1625	1	19,22,23	0.77	0	26,31,34	0.98	3 (11%)
1	PSU	S1	2101	1	18,21,22	4.12	8 (44%)	22,30,33	1.75	4 (18%)
1	OMU	S1	1616	1	19,22,23	0.58	0	26,31,34	0.85	2 (7%)
44	OMG	LE	1201	44	18,26,27	1.34	2 (11%)	19,38,41	1.49	2 (10%)
48	PSU	LI	3503	48	18,21,22	4.10	7 (38%)	22,30,33	1.93	5 (22%)
1	A2M	S1	723	1	18,25,26	4.09	7 (38%)	18,36,39	3.04	4 (22%)
42	OMC	LC	483	42	19,22,23	0.93	1 (5%)	26,31,34	1.04	3 (11%)
47	OMU	LH	2605	47,49	19,22,23	0.56	0	26,31,34	0.82	1 (3%)
45	OMU	LF	1957	45	19,22,23	0.55	0	26,31,34	0.99	2 (7%)
1	PSU	S1	1396	1	18,21,22	4.17	7 (38%)	22,30,33	1.95	5 (22%)
44	OMG	LE	1208	44	18,26,27	1.04	1 (5%)	19,38,41	1.31	3 (15%)
47	OMC	LH	2825	47	19,22,23	0.79	0	26,31,34	1.07	4 (15%)
1	PSU	S1	1393	1	18,21,22	4.11	7 (38%)	22,30,33	1.94	5 (22%)
41	PSU	LB	280	41	18,21,22	4.15	7 (38%)	22,30,33	1.81	5 (22%)
40	OMG	LA	74	40	18,26,27	1.34	2 (11%)	19,38,41	1.43	3 (15%)
45	PSU	LF	1876	45	18,21,22	4.17	7 (38%)	22,30,33	1.88	5 (22%)
49	PSU	LJ	3644	49	18,21,22	3.97	7 (38%)	22,30,33	1.97	6 (27%)
45	PSU	LF	1859	45	18,21,22	4.13	7 (38%)	22,30,33	1.88	5 (22%)
42	OMG	LC	631	44,42	18,26,27	1.35	3 (16%)	19,38,41	1.53	4 (21%)
47	PSU	LH	2742	47	18,21,22	4.18	7 (38%)	22,30,33	1.79	4 (18%)
45	A2M	LF	1815	45	18,25,26	4.21	7 (38%)	18,36,39	2.96	3 (16%)
1	OMU	S1	1641	1	19,22,23	0.65	0	26,31,34	0.99	2 (7%)
45	OMU	LF	1504	45	19,22,23	0.57	0	26,31,34	0.98	2 (7%)
40	A2M	LA	39	40	18,25,26	4.27	7 (38%)	18,36,39	2.89	4 (22%)
44	PSU	LE	1363	44	18,21,22	4.14	7 (38%)	22,30,33	1.89	5 (22%)
44	A2M	LE	935	44	18,25,26	4.17	7 (38%)	18,36,39	3.02	3 (16%)
44	OMC	LE	1165	44	19,22,23	1.08	1 (5%)	26,31,34	1.28	4 (15%)
47	5MC	LH	2766	47	18,22,23	1.58	3 (16%)	26,32,35	1.21	3 (11%)
1	OMC	S1	2123	1	19,22,23	0.87	1 (5%)	26,31,34	1.01	3 (11%)
51	PSU	LL	3865	51	18,21,22	4.23	7 (38%)	22,30,33	1.93	5 (22%)
1	OMC	S1	1037	1	19,22,23	0.92	1 (5%)	26,31,34	1.14	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMG	LF	1826	44,45	18,26,27	1.33	2 (11%)	19,38,41	1.51	4 (21%)
47	A2M	LH	2708	47	18,25,26	4.27	7 (38%)	18,36,39	2.92	3 (16%)
1	PSU	S1	1624	1	18,21,22	4.14	7 (38%)	22,30,33	1.80	5 (22%)
48	PSU	LI	3185	48	18,21,22	4.11	7 (38%)	22,30,33	1.88	5 (22%)
48	OMC	LI	3546	48	19,22,23	0.82	0	26,31,34	1.21	4 (15%)
1	OMU	S1	8	1	19,22,23	0.43	0	26,31,34	1.02	2 (7%)
44	PSU	LE	1118	44	18,21,22	4.12	7 (38%)	22,30,33	1.86	4 (18%)
44	OMU	LE	1222	44	19,22,23	1.37	4 (21%)	26,31,34	1.93	7 (26%)
47	OMG	LH	2897	48,47	18,26,27	1.33	2 (11%)	19,38,41	1.61	5 (26%)
48	A2M	LI	3521	48	18,25,26	4.17	6 (33%)	18,36,39	3.06	3 (16%)
48	OMC	LI	3374	48	19,22,23	0.85	1 (5%)	26,31,34	1.09	3 (11%)
41	A2M	LB	183	41	18,25,26	4.15	7 (38%)	18,36,39	2.95	3 (16%)
49	PSU	LJ	3680	49	18,21,22	4.13	8 (44%)	22,30,33	2.11	6 (27%)
46	OMU	LG	2129	46	19,22,23	0.59	0	26,31,34	0.87	1 (3%)
47	OMC	LH	2313	45,47	19,22,23	0.83	1 (5%)	26,31,34	1.09	4 (15%)
42	OMC	LC	577	42	19,22,23	0.90	1 (5%)	26,31,34	1.00	2 (7%)
1	A2M	S1	1549	1	18,25,26	4.25	7 (38%)	18,36,39	3.13	4 (22%)
48	OMC	LI	3465	48	19,22,23	0.88	1 (5%)	26,31,34	1.04	3 (11%)
42	OMG	LC	541	40,42	18,26,27	1.30	2 (11%)	19,38,41	1.59	4 (21%)
46	PSU	LG	2119	46	18,21,22	4.20	7 (38%)	22,30,33	1.97	5 (22%)
44	A2M	LE	1121	44	18,25,26	4.25	8 (44%)	18,36,39	2.99	3 (16%)
42	OMC	LC	537	40,42	19,22,23	0.98	1 (5%)	26,31,34	1.11	4 (15%)
1	B8N	S1	1601	1	24,29,30	0.98	2 (8%)	29,42,45	2.20	8 (27%)
1	A2M	S1	1063	1	18,25,26	4.23	7 (38%)	18,36,39	2.94	3 (16%)
44	A2M	LE	1106	44	18,25,26	4.17	7 (38%)	18,36,39	3.01	4 (22%)
44	PSU	LE	1365	44	18,21,22	4.15	7 (38%)	22,30,33	1.88	5 (22%)
45	PSU	LF	1692	45	18,21,22	4.10	7 (38%)	22,30,33	1.89	5 (22%)
44	7MG	LE	938	44	22,26,27	1.71	2 (9%)	29,39,42	1.15	3 (10%)
1	OMC	S1	2142	1	19,22,23	0.78	0	26,31,34	1.06	3 (11%)
1	OMC	S1	99	1	19,22,23	0.85	1 (5%)	26,31,34	1.12	4 (15%)
47	OMG	LH	2610	47	18,26,27	1.33	2 (11%)	19,38,41	1.60	6 (31%)
45	A2M	LF	1888	45	18,25,26	4.25	7 (38%)	18,36,39	2.93	3 (16%)
48	PSU	LI	3206	48	18,21,22	4.11	7 (38%)	22,30,33	1.96	6 (27%)
48	OMG	LI	3191	48,3	18,26,27	1.32	2 (11%)	19,38,41	1.43	4 (21%)
1	PSU	S1	2129	1	18,21,22	4.10	7 (38%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	S1	180	1	18,26,27	1.31	2 (11%)	19,38,41	1.47	3 (15%)
44	OMC	LE	1312	44	19,22,23	0.84	1 (5%)	26,31,34	1.07	3 (11%)
1	OMG	S1	485	1	18,26,27	1.32	2 (11%)	19,38,41	1.44	3 (15%)
47	A2M	LH	2920	48,47	18,25,26	4.26	7 (38%)	18,36,39	2.93	3 (16%)
48	A2M	LI	3533	48,47	18,25,26	4.21	7 (38%)	18,36,39	2.95	3 (16%)
46	PSU	LG	2154	46	18,21,22	4.09	7 (38%)	22,30,33	1.85	6 (27%)
1	OMC	S1	393	1	19,22,23	0.86	0	26,31,34	1.05	2 (7%)
45	PSU	LF	1926	45	18,21,22	4.19	8 (44%)	22,30,33	1.72	4 (18%)
48	OMC	LI	3347	48	19,22,23	0.94	1 (5%)	26,31,34	1.03	3 (11%)
49	OMU	LJ	3718	49	19,22,23	0.59	0	26,31,34	0.75	1 (3%)
48	PSU	LI	3542	48,47	18,21,22	4.16	7 (38%)	22,30,33	1.88	5 (22%)
45	OMG	LF	1683	45	18,26,27	1.29	2 (11%)	19,38,41	1.48	4 (21%)
1	A2M	S1	28	1	18,25,26	4.22	7 (38%)	18,36,39	2.98	3 (16%)
47	OMU	LH	2909	48,47	19,22,23	0.56	0	26,31,34	0.95	2 (7%)
48	OMG	LI	3504	48	18,26,27	1.32	2 (11%)	19,38,41	1.47	4 (21%)
45	OMU	LF	1681	45	19,22,23	0.55	0	26,31,34	0.99	2 (7%)
48	OMC	LI	3535	48	19,22,23	0.91	1 (5%)	26,31,34	0.98	3 (11%)
1	OMG	S1	2075	1	18,26,27	1.36	2 (11%)	19,38,41	1.52	4 (21%)
1	OMG	S1	1705	1	18,26,27	1.34	2 (11%)	19,38,41	1.61	4 (21%)
48	PSU	LI	2999	48,47	18,21,22	4.33	7 (38%)	22,30,33	1.96	5 (22%)
45	PSU	LF	1568	45,54	18,21,22	4.34	7 (38%)	22,30,33	1.74	5 (22%)
47	A2M	LH	2812	47	18,25,26	4.22	7 (38%)	18,36,39	2.97	3 (16%)
47	B8H	LH	2904	48,47	19,22,23	1.35	3 (15%)	22,32,35	1.97	3 (13%)
44	PSU	LE	1266	44	18,21,22	4.07	7 (38%)	22,30,33	1.93	5 (22%)
48	OMG	LI	3401	48,47	18,26,27	1.24	2 (11%)	19,38,41	1.58	5 (26%)
44	OMC	LE	1218	44	19,22,23	0.84	0	26,31,34	1.15	4 (15%)
48	OMC	LI	3208	48	19,22,23	0.85	0	26,31,34	1.17	4 (15%)
48	PSU	LI	3444	48	18,21,22	4.14	8 (44%)	22,30,33	1.97	6 (27%)
44	A2M	LE	1204	44	18,25,26	4.27	7 (38%)	18,36,39	3.01	3 (16%)
47	PSU	LH	2837	47	18,21,22	4.16	7 (38%)	22,30,33	1.84	5 (22%)
44	PSU	LE	1235	44	18,21,22	4.15	7 (38%)	22,30,33	1.85	5 (22%)
47	OMU	LH	2806	47	19,22,23	0.63	0	26,31,34	0.89	2 (7%)
1	A2M	S1	1900	1,27	18,25,26	4.18	6 (33%)	18,36,39	2.91	3 (16%)
48	PSU	LI	3145	48	18,21,22	4.31	8 (44%)	22,30,33	1.95	5 (22%)
1	A2M	S1	1371	1	18,25,26	4.32	7 (38%)	18,36,39	3.11	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	LI	3451	48	18,21,22	4.16	8 (44%)	22,30,33	1.96	6 (27%)
40	PSU	LA	16	40,42	18,21,22	4.11	7 (38%)	22,30,33	1.86	5 (22%)
1	PSU	S1	1554	1	18,21,22	3.97	7 (38%)	22,30,33	1.76	4 (18%)
1	OMC	S1	621	1	19,22,23	0.90	1 (5%)	26,31,34	1.20	4 (15%)
49	PSU	LJ	3591	49	18,21,22	4.11	7 (38%)	22,30,33	1.90	5 (22%)
46	OMG	LG	2146	46	18,26,27	1.31	3 (16%)	19,38,41	1.49	3 (15%)
1	A2M	S1	2046	1	18,25,26	4.19	7 (38%)	18,36,39	3.10	3 (16%)
47	PSU	LH	2746	47	18,21,22	4.09	7 (38%)	22,30,33	2.14	5 (22%)
48	PSU	LI	3042	48	18,21,22	4.32	7 (38%)	22,30,33	1.83	5 (22%)
44	OMU	LE	1189	44	19,22,23	0.47	0	26,31,34	0.94	2 (7%)
44	PSU	LE	1023	44	18,21,22	4.15	7 (38%)	22,30,33	1.90	5 (22%)
47	OMU	LH	2835	47	19,22,23	0.69	1 (5%)	26,31,34	0.86	1 (3%)
1	PSU	S1	176	1	18,21,22	4.16	7 (38%)	22,30,33	1.87	5 (22%)
45	A2M	LF	1502	45	18,25,26	4.21	7 (38%)	18,36,39	3.08	3 (16%)
45	A2M	LF	1738	45	18,25,26	4.15	7 (38%)	18,36,39	3.02	3 (16%)
47	PSU	LH	2679	47	18,21,22	4.08	7 (38%)	22,30,33	1.83	5 (22%)
44	OMU	LE	1315	44	19,22,23	0.56	0	26,31,34	0.89	2 (7%)
1	PSU	S1	465	1	18,21,22	4.12	7 (38%)	22,30,33	1.94	5 (22%)
1	OMU	S1	179	1	19,22,23	0.64	0	26,31,34	0.93	2 (7%)
1	5MC	S1	2144	1	18,22,23	1.57	4 (22%)	26,32,35	1.20	4 (15%)
44	A2M	LE	1039	44	18,25,26	4.23	6 (33%)	18,36,39	2.96	3 (16%)
48	OMG	LI	3223	48	18,26,27	1.37	3 (16%)	19,38,41	1.46	4 (21%)
46	OMG	LG	2009	46	18,26,27	1.33	2 (11%)	19,38,41	1.49	5 (26%)
47	PSU	LH	2617	47	18,21,22	4.15	7 (38%)	22,30,33	1.95	5 (22%)
47	PSU	LH	2642	47	18,21,22	4.11	7 (38%)	22,30,33	1.88	5 (22%)
45	OMU	LF	1553	45	19,22,23	0.58	0	26,31,34	0.94	2 (7%)
1	OMC	S1	103	1	19,22,23	1.05	1 (5%)	26,31,34	1.13	3 (11%)
45	A2M	LF	1891	45,47	18,25,26	4.21	7 (38%)	18,36,39	2.96	3 (16%)
1	OMU	S1	1744	1	19,22,23	0.55	0	26,31,34	0.85	1 (3%)
44	1MA	LE	931	44	16,25,26	1.45	2 (12%)	18,37,40	1.05	3 (16%)
41	OMU	LB	206	41	19,22,23	0.57	0	26,31,34	0.83	1 (3%)
47	A2M	LH	2809	47	18,25,26	4.19	7 (38%)	18,36,39	3.10	3 (16%)
45	OMG	LF	1835	45,47	18,26,27	1.29	2 (11%)	19,38,41	1.57	4 (21%)
47	OMC	LH	2242	46,47	19,22,23	0.83	0	26,31,34	0.99	3 (11%)
1	PSU	S1	1660	1	18,21,22	4.25	7 (38%)	22,30,33	1.90	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMG	LI	3377	48	18,26,27	1.29	2 (11%)	19,38,41	1.59	5 (26%)
1	A2M	S1	2180	1	18,25,26	1.00	1 (5%)	18,36,39	1.21	2 (11%)
1	OMU	S1	186	1	19,22,23	0.52	0	26,31,34	1.08	2 (7%)
49	OMG	LJ	3688	49	18,26,27	1.34	2 (11%)	19,38,41	1.62	3 (15%)
49	PSU	LJ	3697	49	18,21,22	4.15	7 (38%)	22,30,33	1.90	5 (22%)
1	MA6	S1	2287	1	19,26,27	1.15	1 (5%)	18,38,41	3.55	2 (11%)
44	OMU	LE	1270	44,45	19,22,23	0.60	0	26,31,34	1.06	2 (7%)
44	PSU	LE	1126	44	18,21,22	4.09	7 (38%)	22,30,33	1.89	5 (22%)
48	PSU	LI	3531	48	18,21,22	4.19	7 (38%)	22,30,33	1.92	5 (22%)
48	PSU	LI	3440	48	18,21,22	4.12	7 (38%)	22,30,33	1.89	5 (22%)
41	PSU	LB	281	41	18,21,22	4.13	7 (38%)	22,30,33	1.72	4 (18%)
1	PSU	S1	121	1	18,21,22	1.41	4 (22%)	22,30,33	1.92	4 (18%)
42	PSU	LC	567	42	18,21,22	4.06	7 (38%)	22,30,33	1.86	5 (22%)
44	PSU	LE	1260	44,48	18,21,22	4.28	8 (44%)	22,30,33	2.09	6 (27%)
45	OMG	LF	1819	44,45	18,26,27	1.31	2 (11%)	19,38,41	1.58	5 (26%)
42	PSU	LC	498	42	18,21,22	4.14	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	S1	2081	1	18,21,22	4.17	7 (38%)	22,30,33	1.95	5 (22%)
44	OMU	LE	1185	44	19,22,23	0.58	0	26,31,34	0.83	1 (3%)
42	A2M	LC	594	42	18,25,26	4.23	7 (38%)	18,36,39	2.87	3 (16%)
46	PSU	LG	2125	46	18,21,22	4.12	7 (38%)	22,30,33	1.89	6 (27%)
48	OMG	LI	3379	48	18,26,27	1.31	2 (11%)	19,38,41	1.52	5 (26%)
52	PSU	LM	3963	53,52	18,21,22	4.24	7 (38%)	22,30,33	1.84	5 (22%)
1	PSU	S1	1592	1	18,21,22	4.11	7 (38%)	22,30,33	1.91	5 (22%)
48	OMG	LI	3187	48	18,26,27	1.33	2 (11%)	19,38,41	1.47	4 (21%)
40	A2M	LA	97	40	18,25,26	4.14	6 (33%)	18,36,39	3.12	4 (22%)
48	PSU	LI	3332	48	18,21,22	4.10	7 (38%)	22,30,33	1.91	5 (22%)
49	OMU	LJ	3636	49	19,22,23	0.56	0	26,31,34	0.87	1 (3%)
1	OMG	S1	1681	1	18,26,27	1.33	2 (11%)	19,38,41	1.46	4 (21%)
45	OMC	LF	1573	45	19,22,23	1.16	1 (5%)	26,31,34	1.21	4 (15%)
47	OMG	LH	2879	48,47	18,26,27	1.30	2 (11%)	19,38,41	1.48	5 (26%)
48	A2M	LI	3315	48	18,25,26	4.27	7 (38%)	18,36,39	3.01	4 (22%)
1	OMU	S1	702	1	19,22,23	0.57	0	26,31,34	0.91	2 (7%)
1	A2M	S1	533	1	18,25,26	4.21	7 (38%)	18,36,39	2.82	3 (16%)
47	A2M	LH	2769	47	18,25,26	4.06	7 (38%)	18,36,39	3.03	3 (16%)
44	OMG	LE	1217	44	18,26,27	1.31	2 (11%)	19,38,41	1.54	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMC	LF	1836	45,47	19,22,23	0.82	1 (5%)	26,31,34	1.17	3 (11%)
44	OMC	LE	949	44	19,22,23	0.78	0	26,31,34	1.02	2 (7%)
47	OMC	LH	2348	47	19,22,23	0.89	1 (5%)	26,31,34	1.06	3 (11%)
1	OMU	S1	704	1	19,22,23	0.52	0	26,31,34	0.93	2 (7%)
40	OMG	LA	41	40	18,26,27	1.34	2 (11%)	19,38,41	1.43	3 (15%)
46	A2M	LG	2022	45,46	18,25,26	4.23	7 (38%)	18,36,39	2.93	3 (16%)
42	PSU	LC	421	42	18,21,22	4.15	7 (38%)	22,30,33	1.76	4 (18%)
47	OMC	LH	2602	47	19,22,23	0.84	0	26,31,34	1.15	2 (7%)
45	PSU	LF	1586	45	18,21,22	4.17	7 (38%)	22,30,33	1.93	5 (22%)
47	A2M	LH	2768	47	18,25,26	4.18	8 (44%)	18,36,39	3.03	4 (22%)
45	A2M	LF	1929	45	18,25,26	4.17	7 (38%)	18,36,39	2.97	3 (16%)
41	OMG	LB	215	41	18,26,27	1.33	2 (11%)	19,38,41	1.54	3 (15%)
47	PSU	LH	2361	47	18,21,22	4.05	7 (38%)	22,30,33	1.87	5 (22%)
48	A2M	LI	3500	48	18,25,26	4.24	7 (38%)	18,36,39	2.92	3 (16%)
45	OMU	LF	1898	45,47	19,22,23	0.62	0	26,31,34	0.98	2 (7%)
51	A2M	LL	3906	60,51	18,25,26	4.25	7 (38%)	18,36,39	2.84	3 (16%)
47	PSU	LH	2330	45,47	18,21,22	4.05	7 (38%)	22,30,33	1.77	5 (22%)
48	PSU	LI	3175	48,47	18,21,22	4.15	7 (38%)	22,30,33	1.95	5 (22%)
47	A2M	LH	2814	47	18,25,26	4.23	7 (38%)	18,36,39	3.07	3 (16%)
47	OMG	LH	2925	48,47	18,26,27	1.34	2 (11%)	19,38,41	1.49	3 (15%)
47	OMG	LH	2776	47	18,26,27	1.32	3 (16%)	19,38,41	1.49	5 (26%)
42	PSU	LC	480	42	18,21,22	4.16	7 (38%)	22,30,33	1.97	5 (22%)
48	PSU	LI	3510	48,2	18,21,22	4.19	7 (38%)	22,30,33	1.92	5 (22%)
1	OMG	S1	641	1	18,26,27	1.35	3 (16%)	19,38,41	1.56	4 (21%)
1	PSU	S1	1378	1	18,21,22	4.04	7 (38%)	22,30,33	1.92	5 (22%)
48	PSU	LI	3446	48	18,21,22	4.27	7 (38%)	22,30,33	1.77	4 (18%)
42	OMG	LC	628	42	18,26,27	1.33	2 (11%)	19,38,41	1.49	5 (26%)
48	PSU	LI	3167	48	18,21,22	4.22	7 (38%)	22,30,33	1.84	5 (22%)
48	PSU	LI	3412	48	18,21,22	4.08	8 (44%)	22,30,33	1.99	6 (27%)
47	OMU	LH	2625	47	19,22,23	0.56	0	26,31,34	1.10	2 (7%)
47	A2M	LH	2849	47	18,25,26	4.18	7 (38%)	18,36,39	3.01	3 (16%)
1	7MG	S1	2078	3,1	22,26,27	1.73	2 (9%)	29,39,42	1.23	5 (17%)
44	OMU	LE	1452	44	19,22,23	0.65	0	26,31,34	0.88	2 (7%)
48	5MC	LI	3456	48,47	18,22,23	1.62	4 (22%)	26,32,35	1.23	3 (11%)
47	PSU	LH	2752	47	18,21,22	4.14	7 (38%)	22,30,33	1.89	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMU	LG	1999	45,46	19,22,23	0.60	0	26,31,34	0.89	2 (7%)
45	OMG	LF	1856	45	18,26,27	1.35	3 (16%)	19,38,41	1.52	3 (15%)
1	PSU	S1	1960	1	18,21,22	4.08	7 (38%)	22,30,33	1.86	5 (22%)
48	OMU	LI	3159	48	19,22,23	0.60	0	26,31,34	0.97	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S1	1901	1	-	0/5/27/28	0/3/3/3
47	PSU	LH	2842	45,47	-	0/7/25/26	0/2/2/2
1	OMC	S1	38	1	-	0/9/27/28	0/2/2/2
1	A2M	S1	407	1	-	0/5/27/28	0/3/3/3
47	PSU	LH	2621	44,47	-	0/7/25/26	0/2/2/2
47	PSU	LH	2914	48,47	-	0/7/25/26	0/2/2/2
47	OMU	LH	2346	47	-	0/9/27/28	0/2/2/2
48	OMG	LI	3509	48,2	-	0/5/27/28	0/3/3/3
47	PSU	LH	2899	48,47	-	2/7/25/26	0/2/2/2
1	UR3	S1	1597	1	-	0/7/25/26	0/2/2/2
47	PSU	LH	2754	47	-	0/7/25/26	0/2/2/2
48	UR3	LI	3540	48	-	0/7/25/26	0/2/2/2
47	A2M	LH	2349	47	-	2/5/27/28	0/3/3/3
1	PSU	S1	2116	1	-	2/7/25/26	0/2/2/2
44	OMU	LE	1081	44	-	1/9/27/28	0/2/2/2
1	A2M	S1	40	1	-	0/5/27/28	0/3/3/3
44	PSU	LE	1171	44	-	0/7/25/26	0/2/2/2
47	A2M	LH	2744	47	-	2/5/27/28	0/3/3/3
1	PSU	S1	1068	1	-	3/7/25/26	0/2/2/2
48	OMU	LI	3508	48	-	0/9/27/28	0/2/2/2
45	OMC	LF	1822	44,45	-	2/9/27/28	0/2/2/2
48	OMG	LI	3434	48	-	0/5/27/28	0/3/3/3
1	OMG	S1	1536	1,94	-	2/5/27/28	0/3/3/3
45	PSU	LF	1582	45	-	0/7/25/26	0/2/2/2
1	PSU	S1	1591	1	-	0/7/25/26	0/2/2/2
47	PSU	LH	2623	47	-	0/7/25/26	0/2/2/2
44	OMG	LE	1104	44	-	0/5/27/28	0/3/3/3
47	A2M	LH	2358	47	-	1/5/27/28	0/3/3/3
48	OMU	LI	3300	48	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S1	1711	1	-	2/7/25/26	0/2/2/2
1	OMU	S1	2041	1	-	1/9/27/28	0/2/2/2
47	PSU	LH	2874	48,47	-	0/7/25/26	0/2/2/2
1	OMU	S1	1679	1	-	0/9/27/28	0/2/2/2
45	OMU	LF	1824	44,45,42	-	0/9/27/28	0/2/2/2
1	PSU	S1	2305	1	-	3/7/25/26	0/2/2/2
47	OMU	LH	2713	47	-	3/9/27/28	0/2/2/2
47	PSU	LH	2802	47	-	4/7/25/26	0/2/2/2
47	OMG	LH	2883	48,47	-	0/5/27/28	0/3/3/3
45	OMG	LF	1662	45	-	2/5/27/28	0/3/3/3
53	PSU	LN	3969	53,52	-	0/7/25/26	0/2/2/2
1	OMG	S1	57	1	-	3/5/27/28	0/3/3/3
1	PSU	S1	640	1	-	3/7/25/26	0/2/2/2
1	OMU	S1	1966	1,29	-	1/9/27/28	0/2/2/2
1	PSU	S1	2131	1	-	0/7/25/26	0/2/2/2
52	OMC	LM	3957	53,52	-	2/9/27/28	0/2/2/2
49	PSU	LJ	3701	49	-	0/7/25/26	0/2/2/2
44	PSU	LE	1198	44	-	0/7/25/26	0/2/2/2
48	OMC	LI	3355	48,44	-	1/9/27/28	0/2/2/2
1	OMG	S1	42	1	-	0/5/27/28	0/3/3/3
47	A2M	LH	2887	48,47	-	1/5/27/28	0/3/3/3
52	PSU	LM	3953	53,52	-	0/7/25/26	0/2/2/2
1	PSU	S1	280	1	-	4/7/25/26	0/2/2/2
44	PSU	LE	1407	44	-	0/7/25/26	0/2/2/2
48	6MZ	LI	3214	48,45	-	4/5/27/28	0/3/3/3
1	PSU	S1	105	1	-	0/7/25/26	0/2/2/2
48	OMC	LI	3222	48	-	0/9/27/28	0/2/2/2
47	JMH	LH	2636	47	-	2/7/25/26	0/2/2/2
42	OMU	LC	491	42	-	2/9/27/28	0/2/2/2
1	PSU	S1	32	1	-	0/7/25/26	0/2/2/2
1	PSU	S1	403	1	-	3/7/25/26	0/2/2/2
47	OMC	LH	2685	47	-	5/9/27/28	0/2/2/2
44	PSU	LE	1184	44	-	0/7/25/26	0/2/2/2
41	PSU	LB	234	41	-	1/7/25/26	0/2/2/2
1	A2M	S1	1096	1	-	3/5/27/28	0/3/3/3
48	PSU	LI	3568	48,47	-	0/7/25/26	0/2/2/2
1	PSU	S1	1715	1	-	1/7/25/26	0/2/2/2
42	PSU	LC	302	42	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMG	LF	1883	45	-	0/5/27/28	0/3/3/3
45	OMU	LF	1828	45,47	-	0/9/27/28	0/2/2/2
48	PSU	LI	3562	48	-	0/7/25/26	0/2/2/2
45	OMG	LF	1956	45	-	0/5/27/28	0/3/3/3
47	PSU	LH	2586	47	-	1/7/25/26	0/2/2/2
44	OMC	LE	936	44	-	2/9/27/28	0/2/2/2
1	PSU	S1	2065	1	-	0/7/25/26	0/2/2/2
47	PSU	LH	2915	48,47	-	0/7/25/26	0/2/2/2
1	MA6	S1	2288	1	-	2/7/29/30	0/3/3/3
42	PSU	LC	308	42	-	2/7/25/26	0/2/2/2
1	OMG	S1	390	1	-	2/5/27/28	0/3/3/3
1	A2M	S1	649	1	-	2/5/27/28	0/3/3/3
44	OMG	LE	1324	44	-	0/5/27/28	0/3/3/3
47	PSU	LH	2624	47	-	0/7/25/26	0/2/2/2
48	A2M	LI	3367	48,42	-	1/5/27/28	0/3/3/3
1	A2M	S1	565	1	-	2/5/27/28	0/3/3/3
48	A2M	LI	3348	48	-	0/5/27/28	0/3/3/3
47	OMG	LH	2870	47	-	0/5/27/28	0/3/3/3
40	PSU	LA	68	40	-	0/7/25/26	0/2/2/2
41	OMU	LB	247	41	-	5/9/27/28	0/2/2/2
47	OMC	LH	2832	47	-	0/9/27/28	0/2/2/2
49	OMU	LJ	3694	49	-	2/9/27/28	0/2/2/2
45	OMG	LF	1667	45	-	3/5/27/28	0/3/3/3
48	PSU	LI	3204	48	-	0/7/25/26	0/2/2/2
1	PSU	S1	89	1	-	0/7/25/26	0/2/2/2
1	PSU	S1	544	1	-	0/7/25/26	0/2/2/2
1	A2M	S1	110	1	-	2/5/27/28	0/3/3/3
1	OMU	S1	682	1	-	2/9/27/28	0/2/2/2
47	PSU	LH	2591	47	-	0/7/25/26	0/2/2/2
44	PSU	LE	1075	44,48	-	4/7/25/26	0/2/2/2
1	A2M	S1	645	1	-	1/5/27/28	0/3/3/3
46	PSU	LG	2171	46	-	2/7/25/26	0/2/2/2
46	A2M	LG	2005	45,46	-	2/5/27/28	0/3/3/3
47	OMC	LH	2853	47	-	2/9/27/28	0/2/2/2
48	OMU	LI	3171	48,47	-	2/9/27/28	0/2/2/2
1	PSU	S1	27	1	-	0/7/25/26	0/2/2/2
45	OMC	LF	1976	45	-	2/9/27/28	0/2/2/2
2	MIA	S2	37	2	-	4/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	5MC	LI	3518	48,64	-	0/7/25/26	0/2/2/2
1	OMC	S1	1625	1	-	1/9/27/28	0/2/2/2
1	PSU	S1	2101	1	-	2/7/25/26	0/2/2/2
1	OMU	S1	1616	1	-	0/9/27/28	0/2/2/2
44	OMG	LE	1201	44	-	0/5/27/28	0/3/3/3
48	PSU	LI	3503	48	-	0/7/25/26	0/2/2/2
1	A2M	S1	723	1	-	2/5/27/28	0/3/3/3
42	OMC	LC	483	42	-	3/9/27/28	0/2/2/2
47	OMU	LH	2605	47,49	-	0/9/27/28	0/2/2/2
45	OMU	LF	1957	45	-	2/9/27/28	0/2/2/2
1	PSU	S1	1396	1	-	0/7/25/26	0/2/2/2
44	OMG	LE	1208	44	-	0/5/27/28	0/3/3/3
47	OMC	LH	2825	47	-	0/9/27/28	0/2/2/2
1	PSU	S1	1393	1	-	0/7/25/26	0/2/2/2
41	PSU	LB	280	41	-	2/7/25/26	0/2/2/2
40	OMG	LA	74	40	-	3/5/27/28	0/3/3/3
45	PSU	LF	1876	45	-	0/7/25/26	0/2/2/2
49	PSU	LJ	3644	49	-	0/7/25/26	0/2/2/2
45	PSU	LF	1859	45	-	0/7/25/26	0/2/2/2
42	OMG	LC	631	44,42	-	0/5/27/28	0/3/3/3
47	PSU	LH	2742	47	-	2/7/25/26	0/2/2/2
45	A2M	LF	1815	45	-	0/5/27/28	0/3/3/3
1	OMU	S1	1641	1	-	0/9/27/28	0/2/2/2
45	OMU	LF	1504	45	-	2/9/27/28	0/2/2/2
40	A2M	LA	39	40	-	0/5/27/28	0/3/3/3
44	PSU	LE	1363	44	-	0/7/25/26	0/2/2/2
44	A2M	LE	935	44	-	2/5/27/28	0/3/3/3
44	OMC	LE	1165	44	-	2/9/27/28	0/2/2/2
47	5MC	LH	2766	47	-	1/7/25/26	0/2/2/2
1	OMC	S1	2123	1	-	0/9/27/28	0/2/2/2
51	PSU	LL	3865	51	-	0/7/25/26	0/2/2/2
1	OMC	S1	1037	1	-	0/9/27/28	0/2/2/2
45	OMG	LF	1826	44,45	-	0/5/27/28	0/3/3/3
47	A2M	LH	2708	47	-	0/5/27/28	0/3/3/3
1	PSU	S1	1624	1	-	2/7/25/26	0/2/2/2
48	PSU	LI	3185	48	-	0/7/25/26	0/2/2/2
48	OMC	LI	3546	48	-	0/9/27/28	0/2/2/2
1	OMU	S1	8	1	-	6/9/27/28	0/2/2/2
44	PSU	LE	1118	44	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	OMU	LE	1222	44	-	4/9/27/28	0/2/2/2
47	OMG	LH	2897	48,47	-	0/5/27/28	0/3/3/3
48	A2M	LI	3521	48	-	0/5/27/28	0/3/3/3
48	OMC	LI	3374	48	-	0/9/27/28	0/2/2/2
41	A2M	LB	183	41	-	0/5/27/28	0/3/3/3
49	PSU	LJ	3680	49	-	1/7/25/26	0/2/2/2
46	OMU	LG	2129	46	-	1/9/27/28	0/2/2/2
47	OMC	LH	2313	45,47	-	0/9/27/28	0/2/2/2
42	OMC	LC	577	42	-	3/9/27/28	0/2/2/2
1	A2M	S1	1549	1	-	2/5/27/28	0/3/3/3
48	OMC	LI	3465	48	-	0/9/27/28	0/2/2/2
42	OMG	LC	541	40,42	-	1/5/27/28	0/3/3/3
46	PSU	LG	2119	46	-	0/7/25/26	0/2/2/2
44	A2M	LE	1121	44	-	0/5/27/28	0/3/3/3
42	OMC	LC	537	40,42	-	2/9/27/28	0/2/2/2
1	B8N	S1	1601	1	1/1/7/7	3/16/34/35	0/2/2/2
1	A2M	S1	1063	1	-	2/5/27/28	0/3/3/3
44	A2M	LE	1106	44	-	1/5/27/28	0/3/3/3
44	PSU	LE	1365	44	-	0/7/25/26	0/2/2/2
45	PSU	LF	1692	45	-	0/7/25/26	0/2/2/2
44	7MG	LE	938	44	-	0/7/37/38	0/3/3/3
1	OMC	S1	2142	1	-	2/9/27/28	0/2/2/2
1	OMC	S1	99	1	-	1/9/27/28	0/2/2/2
47	OMG	LH	2610	47	-	1/5/27/28	0/3/3/3
45	A2M	LF	1888	45	-	0/5/27/28	0/3/3/3
48	PSU	LI	3206	48	-	1/7/25/26	0/2/2/2
48	OMG	LI	3191	48,3	-	3/5/27/28	0/3/3/3
1	PSU	S1	2129	1	-	0/7/25/26	0/2/2/2
1	OMG	S1	180	1	-	3/5/27/28	0/3/3/3
44	OMC	LE	1312	44	-	0/9/27/28	0/2/2/2
1	OMG	S1	485	1	-	2/5/27/28	0/3/3/3
47	A2M	LH	2920	48,47	-	1/5/27/28	0/3/3/3
48	A2M	LI	3533	48,47	-	0/5/27/28	0/3/3/3
46	PSU	LG	2154	46	-	0/7/25/26	0/2/2/2
1	OMC	S1	393	1	-	0/9/27/28	0/2/2/2
45	PSU	LF	1926	45	-	2/7/25/26	0/2/2/2
48	OMC	LI	3347	48	-	0/9/27/28	0/2/2/2
49	OMU	LJ	3718	49	-	1/9/27/28	0/2/2/2
48	PSU	LI	3542	48,47	-	0/7/25/26	0/2/2/2
45	OMG	LF	1683	45	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S1	28	1	-	0/5/27/28	0/3/3/3
47	OMU	LH	2909	48,47	-	0/9/27/28	0/2/2/2
48	OMG	LI	3504	48	-	1/5/27/28	0/3/3/3
45	OMU	LF	1681	45	-	2/9/27/28	0/2/2/2
48	OMC	LI	3535	48	-	0/9/27/28	0/2/2/2
1	OMG	S1	2075	1	-	2/5/27/28	0/3/3/3
1	OMG	S1	1705	1	-	2/5/27/28	0/3/3/3
48	PSU	LI	2999	48,47	-	1/7/25/26	0/2/2/2
45	PSU	LF	1568	45,54	-	1/7/25/26	0/2/2/2
47	A2M	LH	2812	47	-	1/5/27/28	0/3/3/3
47	B8H	LH	2904	48,47	-	0/7/25/26	0/2/2/2
44	PSU	LE	1266	44	-	0/7/25/26	0/2/2/2
48	OMG	LI	3401	48,47	-	0/5/27/28	0/3/3/3
44	OMC	LE	1218	44	-	0/9/27/28	0/2/2/2
48	OMC	LI	3208	48	-	4/9/27/28	0/2/2/2
48	PSU	LI	3444	48	-	0/7/25/26	0/2/2/2
44	A2M	LE	1204	44	-	0/5/27/28	0/3/3/3
47	PSU	LH	2837	47	-	0/7/25/26	0/2/2/2
44	PSU	LE	1235	44	-	0/7/25/26	0/2/2/2
47	OMU	LH	2806	47	-	0/9/27/28	0/2/2/2
1	A2M	S1	1900	1,27	-	2/5/27/28	0/3/3/3
48	PSU	LI	3145	48	-	0/7/25/26	0/2/2/2
1	A2M	S1	1371	1	-	3/5/27/28	0/3/3/3
48	PSU	LI	3451	48	-	0/7/25/26	0/2/2/2
40	PSU	LA	16	40,42	-	0/7/25/26	0/2/2/2
1	PSU	S1	1554	1	-	2/7/25/26	0/2/2/2
1	OMC	S1	621	1	-	2/9/27/28	0/2/2/2
49	PSU	LJ	3591	49	-	0/7/25/26	0/2/2/2
46	OMG	LG	2146	46	-	2/5/27/28	0/3/3/3
1	A2M	S1	2046	1	-	0/5/27/28	0/3/3/3
47	PSU	LH	2746	47	-	3/7/25/26	0/2/2/2
48	PSU	LI	3042	48	-	3/7/25/26	0/2/2/2
44	OMU	LE	1189	44	-	0/9/27/28	0/2/2/2
44	PSU	LE	1023	44	-	0/7/25/26	0/2/2/2
47	OMU	LH	2835	47	-	3/9/27/28	0/2/2/2
1	PSU	S1	176	1	-	2/7/25/26	0/2/2/2
45	A2M	LF	1502	45	-	0/5/27/28	0/3/3/3
45	A2M	LF	1738	45	-	0/5/27/28	0/3/3/3
47	PSU	LH	2679	47	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	OMU	LE	1315	44	-	0/9/27/28	0/2/2/2
1	PSU	S1	465	1	-	0/7/25/26	0/2/2/2
1	OMU	S1	179	1	-	0/9/27/28	0/2/2/2
1	5MC	S1	2144	1	-	0/7/25/26	0/2/2/2
44	A2M	LE	1039	44	-	0/5/27/28	0/3/3/3
48	OMG	LI	3223	48	-	1/5/27/28	0/3/3/3
46	OMG	LG	2009	46	-	1/5/27/28	0/3/3/3
47	PSU	LH	2617	47	-	0/7/25/26	0/2/2/2
47	PSU	LH	2642	47	-	0/7/25/26	0/2/2/2
45	OMU	LF	1553	45	-	0/9/27/28	0/2/2/2
1	OMC	S1	103	1	-	3/9/27/28	0/2/2/2
45	A2M	LF	1891	45,47	-	0/5/27/28	0/3/3/3
1	OMU	S1	1744	1	-	0/9/27/28	0/2/2/2
44	1MA	LE	931	44	-	0/3/25/26	0/3/3/3
41	OMU	LB	206	41	-	0/9/27/28	0/2/2/2
47	A2M	LH	2809	47	-	0/5/27/28	0/3/3/3
45	OMG	LF	1835	45,47	-	2/5/27/28	0/3/3/3
47	OMC	LH	2242	46,47	-	3/9/27/28	0/2/2/2
1	PSU	S1	1660	1	-	0/7/25/26	0/2/2/2
48	OMG	LI	3377	48	-	2/5/27/28	0/3/3/3
1	A2M	S1	2180	1	-	0/5/27/28	0/3/3/3
1	OMU	S1	186	1	-	1/9/27/28	0/2/2/2
49	OMG	LJ	3688	49	-	2/5/27/28	0/3/3/3
49	PSU	LJ	3697	49	-	2/7/25/26	0/2/2/2
1	MA6	S1	2287	1	-	0/7/29/30	0/3/3/3
44	OMU	LE	1270	44,45	-	0/9/27/28	0/2/2/2
44	PSU	LE	1126	44	-	3/7/25/26	0/2/2/2
48	PSU	LI	3531	48	-	1/7/25/26	0/2/2/2
48	PSU	LI	3440	48	-	0/7/25/26	0/2/2/2
41	PSU	LB	281	41	-	3/7/25/26	0/2/2/2
1	PSU	S1	121	1	-	0/7/25/26	0/2/2/2
42	PSU	LC	567	42	-	1/7/25/26	0/2/2/2
44	PSU	LE	1260	44,48	-	3/7/25/26	0/2/2/2
45	OMG	LF	1819	44,45	-	5/5/27/28	0/3/3/3
42	PSU	LC	498	42	-	0/7/25/26	0/2/2/2
1	PSU	S1	2081	1	-	0/7/25/26	0/2/2/2
44	OMU	LE	1185	44	-	1/9/27/28	0/2/2/2
42	A2M	LC	594	42	-	0/5/27/28	0/3/3/3
46	PSU	LG	2125	46	-	1/7/25/26	0/2/2/2
48	OMG	LI	3379	48	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	LM	3963	53,52	-	0/7/25/26	0/2/2/2
1	PSU	S1	1592	1	-	0/7/25/26	0/2/2/2
48	OMG	LI	3187	48	-	0/5/27/28	0/3/3/3
40	A2M	LA	97	40	-	2/5/27/28	0/3/3/3
48	PSU	LI	3332	48	-	0/7/25/26	0/2/2/2
49	OMU	LJ	3636	49	-	1/9/27/28	0/2/2/2
1	OMG	S1	1681	1	-	0/5/27/28	0/3/3/3
45	OMC	LF	1573	45	-	5/9/27/28	0/2/2/2
47	OMG	LH	2879	48,47	-	1/5/27/28	0/3/3/3
48	A2M	LI	3315	48	-	2/5/27/28	0/3/3/3
1	OMU	S1	702	1	-	0/9/27/28	0/2/2/2
1	A2M	S1	533	1	-	0/5/27/28	0/3/3/3
47	A2M	LH	2769	47	-	3/5/27/28	0/3/3/3
44	OMG	LE	1217	44	-	0/5/27/28	0/3/3/3
45	OMC	LF	1836	45,47	-	0/9/27/28	0/2/2/2
44	OMC	LE	949	44	-	1/9/27/28	0/2/2/2
47	OMC	LH	2348	47	-	0/9/27/28	0/2/2/2
1	OMU	S1	704	1	-	1/9/27/28	0/2/2/2
40	OMG	LA	41	40	-	0/5/27/28	0/3/3/3
46	A2M	LG	2022	45,46	-	3/5/27/28	0/3/3/3
42	PSU	LC	421	42	-	0/7/25/26	0/2/2/2
47	OMC	LH	2602	47	-	5/9/27/28	0/2/2/2
45	PSU	LF	1586	45	-	0/7/25/26	0/2/2/2
47	A2M	LH	2768	47	-	2/5/27/28	0/3/3/3
45	A2M	LF	1929	45	-	2/5/27/28	0/3/3/3
41	OMG	LB	215	41	-	1/5/27/28	0/3/3/3
47	PSU	LH	2361	47	-	0/7/25/26	0/2/2/2
48	A2M	LI	3500	48	-	2/5/27/28	0/3/3/3
45	OMU	LF	1898	45,47	-	0/9/27/28	0/2/2/2
51	A2M	LL	3906	60,51	-	2/5/27/28	0/3/3/3
47	PSU	LH	2330	45,47	-	0/7/25/26	0/2/2/2
48	PSU	LI	3175	48,47	-	0/7/25/26	0/2/2/2
47	A2M	LH	2814	47	-	0/5/27/28	0/3/3/3
47	OMG	LH	2925	48,47	-	3/5/27/28	0/3/3/3
47	OMG	LH	2776	47	-	3/5/27/28	0/3/3/3
42	PSU	LC	480	42	-	0/7/25/26	0/2/2/2
48	PSU	LI	3510	48,2	-	1/7/25/26	0/2/2/2
1	OMG	S1	641	1	-	2/5/27/28	0/3/3/3
1	PSU	S1	1378	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	LI	3446	48	-	3/7/25/26	0/2/2/2
42	OMG	LC	628	42	-	0/5/27/28	0/3/3/3
48	PSU	LI	3167	48	-	5/7/25/26	0/2/2/2
48	PSU	LI	3412	48	-	0/7/25/26	0/2/2/2
47	OMU	LH	2625	47	-	0/9/27/28	0/2/2/2
47	A2M	LH	2849	47	-	1/5/27/28	0/3/3/3
1	7MG	S1	2078	3,1	-	2/7/37/38	0/3/3/3
44	OMU	LE	1452	44	-	0/9/27/28	0/2/2/2
48	5MC	LI	3456	48,47	-	4/7/25/26	0/2/2/2
47	PSU	LH	2752	47	-	0/7/25/26	0/2/2/2
46	OMU	LG	1999	45,46	-	0/9/27/28	0/2/2/2
45	OMG	LF	1856	45	-	2/5/27/28	0/3/3/3
1	PSU	S1	1960	1	-	0/7/25/26	0/2/2/2
48	OMU	LI	3159	48	-	0/9/27/28	0/2/2/2

All (1348) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	1371	A2M	O4'-C1'	15.42	1.62	1.41
47	LH	2708	A2M	O4'-C1'	15.36	1.62	1.41
40	LA	39	A2M	O4'-C1'	15.36	1.62	1.41
51	LL	3906	A2M	O4'-C1'	15.29	1.62	1.41
48	LI	3315	A2M	O4'-C1'	15.29	1.62	1.41
44	LE	1204	A2M	O4'-C1'	15.22	1.62	1.41
44	LE	1121	A2M	O4'-C1'	15.20	1.62	1.41
48	LI	3500	A2M	O4'-C1'	15.19	1.62	1.41
45	LF	1888	A2M	O4'-C1'	15.18	1.62	1.41
47	LH	2887	A2M	O4'-C1'	15.18	1.62	1.41
44	LE	1039	A2M	O4'-C1'	15.17	1.62	1.41
48	LI	3367	A2M	O4'-C1'	15.13	1.62	1.41
47	LH	2920	A2M	O4'-C1'	15.13	1.62	1.41
47	LH	2349	A2M	O4'-C1'	15.13	1.62	1.41
1	S1	1549	A2M	O4'-C1'	15.12	1.62	1.41
48	LI	3348	A2M	O4'-C1'	15.12	1.62	1.41
1	S1	1096	A2M	O4'-C1'	15.09	1.62	1.41
1	S1	407	A2M	O4'-C1'	15.07	1.62	1.41
46	LG	2022	A2M	O4'-C1'	15.06	1.62	1.41
47	LH	2814	A2M	O4'-C1'	15.04	1.62	1.41
47	LH	2812	A2M	O4'-C1'	15.03	1.62	1.41
1	S1	28	A2M	O4'-C1'	15.02	1.62	1.41
1	S1	565	A2M	O4'-C1'	15.02	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	533	A2M	O4'-C1'	14.98	1.62	1.41
1	S1	1900	A2M	O4'-C1'	14.96	1.62	1.41
42	LC	594	A2M	O4'-C1'	14.96	1.61	1.41
45	LF	1891	A2M	O4'-C1'	14.95	1.61	1.41
1	S1	1063	A2M	O4'-C1'	14.94	1.61	1.41
47	LH	2809	A2M	O4'-C1'	14.93	1.61	1.41
45	LF	1502	A2M	O4'-C1'	14.92	1.61	1.41
45	LF	1815	A2M	O4'-C1'	14.92	1.61	1.41
47	LH	2768	A2M	O4'-C1'	14.86	1.61	1.41
45	LF	1929	A2M	O4'-C1'	14.85	1.61	1.41
48	LI	3533	A2M	O4'-C1'	14.85	1.61	1.41
1	S1	2046	A2M	O4'-C1'	14.84	1.61	1.41
44	LE	935	A2M	O4'-C1'	14.82	1.61	1.41
44	LE	1106	A2M	O4'-C1'	14.80	1.61	1.41
46	LG	2005	A2M	O4'-C1'	14.80	1.61	1.41
1	S1	110	A2M	O4'-C1'	14.78	1.61	1.41
1	S1	645	A2M	O4'-C1'	14.77	1.61	1.41
1	S1	40	A2M	O4'-C1'	14.76	1.61	1.41
48	LI	3521	A2M	O4'-C1'	14.76	1.61	1.41
41	LB	183	A2M	O4'-C1'	14.74	1.61	1.41
45	LF	1738	A2M	O4'-C1'	14.71	1.61	1.41
40	LA	97	A2M	O4'-C1'	14.65	1.61	1.41
47	LH	2849	A2M	O4'-C1'	14.59	1.61	1.41
47	LH	2744	A2M	O4'-C1'	14.52	1.61	1.41
1	S1	649	A2M	O4'-C1'	14.45	1.61	1.41
47	LH	2358	A2M	O4'-C1'	14.40	1.61	1.41
47	LH	2769	A2M	O4'-C1'	14.32	1.61	1.41
1	S1	723	A2M	O4'-C1'	14.10	1.60	1.41
48	LI	2999	PSU	C6-C5	11.41	1.48	1.35
45	LF	1568	PSU	C6-C5	11.40	1.48	1.35
48	LI	3042	PSU	C6-C5	11.34	1.48	1.35
53	LN	3969	PSU	C6-C5	11.24	1.48	1.35
1	S1	1660	PSU	C6-C5	11.24	1.48	1.35
44	LE	1260	PSU	C6-C5	11.19	1.48	1.35
48	LI	3446	PSU	C6-C5	11.15	1.48	1.35
48	LI	3145	PSU	C6-C5	11.13	1.48	1.35
46	LG	2171	PSU	C6-C5	11.07	1.48	1.35
42	LC	308	PSU	C6-C5	11.07	1.48	1.35
47	LH	2874	PSU	C6-C5	11.02	1.48	1.35
1	S1	105	PSU	C6-C5	11.00	1.48	1.35
46	LG	2119	PSU	C6-C5	10.99	1.48	1.35
48	LI	3167	PSU	C6-C5	10.99	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	LI	3510	PSU	C6-C5	10.98	1.48	1.35
51	LL	3865	PSU	C6-C5	10.96	1.48	1.35
52	LM	3963	PSU	C6-C5	10.95	1.48	1.35
1	S1	1068	PSU	C6-C5	10.93	1.48	1.35
1	S1	2065	PSU	C6-C5	10.92	1.48	1.35
42	LC	302	PSU	C6-C5	10.91	1.48	1.35
42	LC	480	PSU	C6-C5	10.90	1.48	1.35
45	LF	1926	PSU	C6-C5	10.90	1.48	1.35
40	LA	68	PSU	C6-C5	10.88	1.48	1.35
44	LE	1023	PSU	C6-C5	10.88	1.48	1.35
48	LI	3531	PSU	C6-C5	10.88	1.48	1.35
1	S1	2081	PSU	C6-C5	10.88	1.48	1.35
47	LH	2586	PSU	C6-C5	10.87	1.48	1.35
41	LB	281	PSU	C6-C5	10.87	1.48	1.35
52	LM	3953	PSU	C6-C5	10.86	1.48	1.35
47	LH	2746	PSU	C6-C5	10.86	1.48	1.35
47	LH	2752	PSU	C6-C5	10.86	1.48	1.35
47	LH	2915	PSU	C6-C5	10.85	1.47	1.35
1	S1	1715	PSU	C6-C5	10.85	1.47	1.35
1	S1	176	PSU	C6-C5	10.83	1.47	1.35
1	S1	403	PSU	C6-C5	10.83	1.47	1.35
49	LJ	3697	PSU	C6-C5	10.83	1.47	1.35
44	LE	1365	PSU	C6-C5	10.83	1.47	1.35
1	S1	640	PSU	C6-C5	10.82	1.47	1.35
1	S1	280	PSU	C6-C5	10.82	1.47	1.35
1	S1	89	PSU	C6-C5	10.82	1.47	1.35
47	LH	2742	PSU	C6-C5	10.81	1.47	1.35
47	LH	2914	PSU	C6-C5	10.80	1.47	1.35
46	LG	2125	PSU	C6-C5	10.80	1.47	1.35
47	LH	2591	PSU	C6-C5	10.80	1.47	1.35
44	LE	1184	PSU	C6-C5	10.80	1.47	1.35
1	S1	2131	PSU	C6-C5	10.80	1.47	1.35
41	LB	234	PSU	C6-C5	10.79	1.47	1.35
41	LB	280	PSU	C6-C5	10.79	1.47	1.35
1	S1	2305	PSU	C6-C5	10.79	1.47	1.35
45	LF	1586	PSU	C6-C5	10.78	1.47	1.35
47	LH	2617	PSU	C6-C5	10.78	1.47	1.35
47	LH	2837	PSU	C6-C5	10.78	1.47	1.35
40	LA	16	PSU	C6-C5	10.78	1.47	1.35
44	LE	1171	PSU	C6-C5	10.76	1.47	1.35
44	LE	1118	PSU	C6-C5	10.76	1.47	1.35
49	LJ	3680	PSU	C6-C5	10.76	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	LF	1582	PSU	C6-C5	10.75	1.47	1.35
1	S1	27	PSU	C6-C5	10.75	1.47	1.35
44	LE	1198	PSU	C6-C5	10.75	1.47	1.35
48	LI	3542	PSU	C6-C5	10.74	1.47	1.35
44	LE	1126	PSU	C6-C5	10.74	1.47	1.35
1	S1	465	PSU	C6-C5	10.73	1.47	1.35
1	S1	1393	PSU	C6-C5	10.73	1.47	1.35
1	S1	1396	PSU	C6-C5	10.70	1.47	1.35
1	S1	32	PSU	C6-C5	10.70	1.47	1.35
1	S1	544	PSU	C6-C5	10.69	1.47	1.35
1	S1	2116	PSU	C6-C5	10.69	1.47	1.35
48	LI	3444	PSU	C6-C5	10.69	1.47	1.35
1	S1	1624	PSU	C6-C5	10.69	1.47	1.35
48	LI	3175	PSU	C6-C5	10.68	1.47	1.35
44	LE	1363	PSU	C6-C5	10.67	1.47	1.35
49	LJ	3701	PSU	C6-C5	10.66	1.47	1.35
47	LH	2361	PSU	C6-C5	10.66	1.47	1.35
1	S1	1592	PSU	C6-C5	10.66	1.47	1.35
44	LE	1235	PSU	C6-C5	10.66	1.47	1.35
48	LI	3412	PSU	C6-C5	10.66	1.47	1.35
45	LF	1876	PSU	C6-C5	10.66	1.47	1.35
42	LC	421	PSU	C6-C5	10.66	1.47	1.35
47	LH	2623	PSU	C6-C5	10.65	1.47	1.35
49	LJ	3591	PSU	C6-C5	10.65	1.47	1.35
45	LF	1859	PSU	C6-C5	10.65	1.47	1.35
47	LH	2802	PSU	C6-C5	10.65	1.47	1.35
1	S1	2101	PSU	C6-C5	10.65	1.47	1.35
47	LH	2621	PSU	C6-C5	10.65	1.47	1.35
48	LI	3185	PSU	C6-C5	10.64	1.47	1.35
48	LI	3204	PSU	C6-C5	10.64	1.47	1.35
48	LI	3451	PSU	C6-C5	10.63	1.47	1.35
44	LE	1075	PSU	C6-C5	10.63	1.47	1.35
46	LG	2154	PSU	C6-C5	10.63	1.47	1.35
42	LC	498	PSU	C6-C5	10.63	1.47	1.35
48	LI	3562	PSU	C6-C5	10.62	1.47	1.35
48	LI	3503	PSU	C6-C5	10.61	1.47	1.35
47	LH	2899	PSU	C6-C5	10.61	1.47	1.35
48	LI	3440	PSU	C6-C5	10.61	1.47	1.35
44	LE	1407	PSU	C6-C5	10.61	1.47	1.35
48	LI	3332	PSU	C6-C5	10.60	1.47	1.35
47	LH	2679	PSU	C6-C5	10.60	1.47	1.35
42	LC	567	PSU	C6-C5	10.59	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	2129	PSU	C6-C5	10.59	1.47	1.35
1	S1	1960	PSU	C6-C5	10.58	1.47	1.35
47	LH	2642	PSU	C6-C5	10.55	1.47	1.35
48	LI	3206	PSU	C6-C5	10.55	1.47	1.35
47	LH	2330	PSU	C6-C5	10.53	1.47	1.35
45	LF	1692	PSU	C6-C5	10.51	1.47	1.35
47	LH	2624	PSU	C6-C5	10.47	1.47	1.35
44	LE	1266	PSU	C6-C5	10.46	1.47	1.35
47	LH	2754	PSU	C6-C5	10.45	1.47	1.35
47	LH	2842	PSU	C6-C5	10.43	1.47	1.35
48	LI	3568	PSU	C6-C5	10.40	1.47	1.35
1	S1	1378	PSU	C6-C5	10.38	1.47	1.35
1	S1	1711	PSU	C6-C5	10.28	1.47	1.35
49	LJ	3644	PSU	C6-C5	10.25	1.47	1.35
1	S1	1591	PSU	C6-C5	10.25	1.47	1.35
1	S1	1554	PSU	C6-C5	10.08	1.47	1.35
48	LI	2999	PSU	C2-N1	9.61	1.49	1.36
48	LI	3145	PSU	C2-N1	9.60	1.49	1.36
45	LF	1568	PSU	C2-N1	9.59	1.49	1.36
48	LI	3446	PSU	C2-N1	9.58	1.49	1.36
48	LI	3042	PSU	C2-N1	9.56	1.49	1.36
47	LH	2742	PSU	C2-N1	9.55	1.49	1.36
47	LH	2621	PSU	C2-N1	9.52	1.49	1.36
53	LN	3969	PSU	C2-N1	9.50	1.49	1.36
52	LM	3963	PSU	C2-N1	9.49	1.49	1.36
44	LE	1260	PSU	C2-N1	9.45	1.49	1.36
51	LL	3865	PSU	C2-N1	9.45	1.49	1.36
48	LI	3531	PSU	C2-N1	9.43	1.49	1.36
1	S1	403	PSU	C2-N1	9.43	1.49	1.36
48	LI	3451	PSU	C2-N1	9.42	1.49	1.36
1	S1	105	PSU	C2-N1	9.41	1.49	1.36
47	LH	2586	PSU	C2-N1	9.41	1.49	1.36
45	LF	1876	PSU	C2-N1	9.40	1.49	1.36
46	LG	2119	PSU	C2-N1	9.40	1.49	1.36
1	S1	1396	PSU	C2-N1	9.39	1.49	1.36
48	LI	3542	PSU	C2-N1	9.38	1.49	1.36
52	LM	3953	PSU	C2-N1	9.38	1.49	1.36
47	LH	2802	PSU	C2-N1	9.38	1.49	1.36
44	LE	1118	PSU	C2-N1	9.37	1.49	1.36
1	S1	1660	PSU	C2-N1	9.37	1.49	1.36
47	LH	2617	PSU	C2-N1	9.35	1.49	1.36
1	S1	1068	PSU	C2-N1	9.34	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	LC	302	PSU	C2-N1	9.34	1.49	1.36
48	LI	3175	PSU	C2-N1	9.34	1.49	1.36
1	S1	2081	PSU	C2-N1	9.33	1.49	1.36
44	LE	1171	PSU	C2-N1	9.33	1.49	1.36
47	LH	2837	PSU	C2-N1	9.32	1.49	1.36
47	LH	2874	PSU	C2-N1	9.32	1.49	1.36
44	LE	1235	PSU	C2-N1	9.32	1.49	1.36
47	LH	2642	PSU	C2-N1	9.32	1.49	1.36
47	LH	2914	PSU	C2-N1	9.31	1.49	1.36
46	LG	2171	PSU	C2-N1	9.30	1.49	1.36
1	S1	2065	PSU	C2-N1	9.30	1.49	1.36
48	LI	3167	PSU	C2-N1	9.30	1.49	1.36
1	S1	32	PSU	C2-N1	9.30	1.49	1.36
1	S1	280	PSU	C2-N1	9.30	1.49	1.36
41	LB	280	PSU	C2-N1	9.29	1.49	1.36
42	LC	308	PSU	C2-N1	9.29	1.49	1.36
47	LH	2624	PSU	C2-N1	9.28	1.49	1.36
1	S1	1592	PSU	C2-N1	9.27	1.49	1.36
1	S1	640	PSU	C2-N1	9.26	1.49	1.36
45	LF	1586	PSU	C2-N1	9.26	1.49	1.36
45	LF	1692	PSU	C2-N1	9.25	1.49	1.36
42	LC	498	PSU	C2-N1	9.24	1.49	1.36
45	LF	1926	PSU	C2-N1	9.24	1.49	1.36
47	LH	2591	PSU	C2-N1	9.24	1.49	1.36
1	S1	176	PSU	C2-N1	9.24	1.49	1.36
48	LI	3510	PSU	C2-N1	9.23	1.49	1.36
1	S1	2129	PSU	C2-N1	9.22	1.49	1.36
48	LI	3440	PSU	C2-N1	9.22	1.49	1.36
48	LI	3185	PSU	C2-N1	9.21	1.49	1.36
44	LE	1407	PSU	C2-N1	9.21	1.49	1.36
49	LJ	3591	PSU	C2-N1	9.20	1.49	1.36
44	LE	1198	PSU	C2-N1	9.19	1.49	1.36
45	LF	1859	PSU	C2-N1	9.19	1.49	1.36
42	LC	480	PSU	C2-N1	9.19	1.49	1.36
48	LI	3332	PSU	C2-N1	9.19	1.49	1.36
44	LE	1363	PSU	C2-N1	9.18	1.49	1.36
49	LJ	3680	PSU	C2-N1	9.18	1.49	1.36
1	S1	2131	PSU	C2-N1	9.18	1.49	1.36
44	LE	1365	PSU	C2-N1	9.17	1.49	1.36
48	LI	3444	PSU	C2-N1	9.17	1.49	1.36
47	LH	2915	PSU	C2-N1	9.17	1.49	1.36
49	LJ	3697	PSU	C2-N1	9.16	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	LB	234	PSU	C2-N1	9.16	1.49	1.36
1	S1	2305	PSU	C2-N1	9.15	1.49	1.36
1	S1	1624	PSU	C2-N1	9.15	1.49	1.36
47	LH	2899	PSU	C2-N1	9.15	1.49	1.36
1	S1	465	PSU	C2-N1	9.14	1.49	1.36
48	LI	3206	PSU	C2-N1	9.14	1.49	1.36
47	LH	2623	PSU	C2-N1	9.13	1.49	1.36
47	LH	2746	PSU	C2-N1	9.13	1.49	1.36
40	LA	16	PSU	C2-N1	9.12	1.49	1.36
1	S1	544	PSU	C2-N1	9.11	1.49	1.36
1	S1	89	PSU	C2-N1	9.10	1.49	1.36
47	LH	2679	PSU	C2-N1	9.10	1.49	1.36
47	LH	2752	PSU	C2-N1	9.10	1.49	1.36
44	LE	1266	PSU	C2-N1	9.10	1.49	1.36
48	LI	3503	PSU	C2-N1	9.09	1.49	1.36
1	S1	1715	PSU	C2-N1	9.09	1.49	1.36
41	LB	281	PSU	C2-N1	9.09	1.49	1.36
47	LH	2330	PSU	C2-N1	9.09	1.49	1.36
1	S1	1554	PSU	C2-N1	9.09	1.49	1.36
44	LE	1126	PSU	C2-N1	9.08	1.49	1.36
49	LJ	3701	PSU	C2-N1	9.08	1.49	1.36
44	LE	1023	PSU	C2-N1	9.07	1.49	1.36
46	LG	2154	PSU	C2-N1	9.07	1.49	1.36
48	LI	3412	PSU	C2-N1	9.06	1.49	1.36
48	LI	3562	PSU	C2-N1	9.05	1.49	1.36
40	LA	68	PSU	C2-N1	9.05	1.49	1.36
1	S1	2116	PSU	C2-N1	9.04	1.49	1.36
42	LC	421	PSU	C2-N1	9.04	1.49	1.36
44	LE	1184	PSU	C2-N1	9.03	1.48	1.36
1	S1	1393	PSU	C2-N1	9.02	1.48	1.36
1	S1	27	PSU	C2-N1	9.02	1.48	1.36
1	S1	1378	PSU	C2-N1	9.01	1.48	1.36
48	LI	3568	PSU	C2-N1	9.00	1.48	1.36
1	S1	1960	PSU	C2-N1	8.99	1.48	1.36
42	LC	567	PSU	C2-N1	8.99	1.48	1.36
48	LI	3204	PSU	C2-N1	8.99	1.48	1.36
47	LH	2361	PSU	C2-N1	8.98	1.48	1.36
46	LG	2125	PSU	C2-N1	8.97	1.48	1.36
45	LF	1582	PSU	C2-N1	8.95	1.48	1.36
44	LE	1075	PSU	C2-N1	8.94	1.48	1.36
47	LH	2754	PSU	C2-N1	8.93	1.48	1.36
1	S1	2101	PSU	C2-N1	8.91	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	1591	PSU	C2-N1	8.85	1.48	1.36
49	LJ	3644	PSU	C2-N1	8.79	1.48	1.36
47	LH	2842	PSU	C2-N1	8.77	1.48	1.36
1	S1	1711	PSU	C2-N1	8.62	1.48	1.36
48	LI	3042	PSU	C2-N3	7.50	1.50	1.37
48	LI	2999	PSU	C2-N3	7.47	1.50	1.37
53	LN	3969	PSU	C2-N3	7.46	1.50	1.37
48	LI	3167	PSU	C2-N3	7.37	1.50	1.37
42	LC	308	PSU	C2-N3	7.36	1.50	1.37
52	LM	3963	PSU	C2-N3	7.35	1.50	1.37
48	LI	3510	PSU	C2-N3	7.33	1.50	1.37
51	LL	3865	PSU	C2-N3	7.32	1.50	1.37
1	S1	280	PSU	C2-N3	7.32	1.50	1.37
45	LF	1568	PSU	C2-N3	7.32	1.50	1.37
2	S2	37	MIA	C13-C14	7.28	1.53	1.32
1	S1	1624	PSU	C2-N3	7.27	1.50	1.37
42	LC	421	PSU	C2-N3	7.27	1.50	1.37
45	LF	1586	PSU	C2-N3	7.26	1.49	1.37
44	LE	1235	PSU	C2-N3	7.26	1.49	1.37
47	LH	2586	PSU	C2-N3	7.25	1.49	1.37
48	LI	3145	PSU	C2-N3	7.25	1.49	1.37
46	LG	2171	PSU	C2-N3	7.23	1.49	1.37
42	LC	498	PSU	C2-N3	7.23	1.49	1.37
1	S1	2081	PSU	C2-N3	7.22	1.49	1.37
1	S1	1396	PSU	C2-N3	7.22	1.49	1.37
47	LH	2802	PSU	C2-N3	7.21	1.49	1.37
44	LE	1363	PSU	C2-N3	7.21	1.49	1.37
46	LG	2125	PSU	C2-N3	7.21	1.49	1.37
1	S1	1068	PSU	C2-N3	7.21	1.49	1.37
48	LI	3206	PSU	C2-N3	7.20	1.49	1.37
42	LC	302	PSU	C2-N3	7.20	1.49	1.37
48	LI	3440	PSU	C2-N3	7.20	1.49	1.37
48	LI	3175	PSU	C2-N3	7.20	1.49	1.37
1	S1	2101	PSU	C2-N3	7.18	1.49	1.37
45	LF	1859	PSU	C2-N3	7.18	1.49	1.37
1	S1	1660	PSU	C2-N3	7.18	1.49	1.37
1	S1	1393	PSU	C2-N3	7.18	1.49	1.37
47	LH	2842	PSU	C2-N3	7.17	1.49	1.37
49	LJ	3697	PSU	C2-N3	7.17	1.49	1.37
44	LE	1260	PSU	C2-N3	7.17	1.49	1.37
44	LE	1023	PSU	C2-N3	7.16	1.49	1.37
48	LI	3568	PSU	C2-N3	7.16	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	LH	2591	PSU	C2-N3	7.16	1.49	1.37
48	LI	3444	PSU	C2-N3	7.15	1.49	1.37
1	S1	176	PSU	C2-N3	7.14	1.49	1.37
48	LI	3446	PSU	C2-N3	7.14	1.49	1.37
47	LH	2874	PSU	C2-N3	7.14	1.49	1.37
42	LC	480	PSU	C2-N3	7.14	1.49	1.37
49	LJ	3680	PSU	C2-N3	7.14	1.49	1.37
44	LE	1171	PSU	C2-N3	7.13	1.49	1.37
47	LH	2617	PSU	C2-N3	7.13	1.49	1.37
1	S1	1711	PSU	C2-N3	7.13	1.49	1.37
47	LH	2899	PSU	C2-N3	7.12	1.49	1.37
1	S1	2065	PSU	C2-N3	7.12	1.49	1.37
44	LE	1266	PSU	C2-N3	7.12	1.49	1.37
47	LH	2752	PSU	C2-N3	7.11	1.49	1.37
45	LF	1876	PSU	C2-N3	7.10	1.49	1.37
52	LM	3953	PSU	C2-N3	7.10	1.49	1.37
1	S1	2305	PSU	C2-N3	7.10	1.49	1.37
46	LG	2154	PSU	C2-N3	7.10	1.49	1.37
1	S1	105	PSU	C2-N3	7.10	1.49	1.37
1	S1	1960	PSU	C2-N3	7.09	1.49	1.37
44	LE	1365	PSU	C2-N3	7.09	1.49	1.37
44	LE	1184	PSU	C2-N3	7.09	1.49	1.37
45	LF	1582	PSU	C2-N3	7.09	1.49	1.37
48	LI	3531	PSU	C2-N3	7.08	1.49	1.37
1	S1	1715	PSU	C2-N3	7.08	1.49	1.37
47	LH	2837	PSU	C2-N3	7.08	1.49	1.37
48	LI	3451	PSU	C2-N3	7.08	1.49	1.37
1	S1	2131	PSU	C2-N3	7.08	1.49	1.37
48	LI	3503	PSU	C2-N3	7.08	1.49	1.37
46	LG	2119	PSU	C2-N3	7.08	1.49	1.37
44	LE	1407	PSU	C2-N3	7.07	1.49	1.37
47	LH	2754	PSU	C2-N3	7.07	1.49	1.37
45	LF	1692	PSU	C2-N3	7.06	1.49	1.37
1	S1	465	PSU	C2-N3	7.05	1.49	1.37
41	LB	234	PSU	C2-N3	7.05	1.49	1.37
1	S1	403	PSU	C2-N3	7.05	1.49	1.37
1	S1	723	A2M	O4'-C4'	-7.04	1.29	1.45
49	LJ	3701	PSU	C2-N3	7.04	1.49	1.37
1	S1	640	PSU	C2-N3	7.03	1.49	1.37
1	S1	2129	PSU	C2-N3	7.03	1.49	1.37
47	LH	2914	PSU	C2-N3	7.03	1.49	1.37
1	S1	1378	PSU	C2-N3	7.03	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	LB	281	PSU	C2-N3	7.03	1.49	1.37
45	LF	1926	PSU	C2-N3	7.02	1.49	1.37
47	LH	2624	PSU	C2-N3	7.01	1.49	1.37
48	LI	3542	PSU	C2-N3	7.01	1.49	1.37
49	LJ	3591	PSU	C2-N3	7.01	1.49	1.37
48	LI	3204	PSU	C2-N3	7.00	1.49	1.37
41	LB	280	PSU	C2-N3	6.99	1.49	1.37
40	LA	68	PSU	C2-N3	6.99	1.49	1.37
47	LH	2642	PSU	C2-N3	6.99	1.49	1.37
48	LI	3332	PSU	C2-N3	6.98	1.49	1.37
1	S1	89	PSU	C2-N3	6.97	1.49	1.37
47	LH	2621	PSU	C2-N3	6.97	1.49	1.37
47	LH	2330	PSU	C2-N3	6.96	1.49	1.37
47	LH	2742	PSU	C2-N3	6.95	1.49	1.37
47	LH	2915	PSU	C2-N3	6.94	1.49	1.37
1	S1	32	PSU	C2-N3	6.94	1.49	1.37
1	S1	544	PSU	C2-N3	6.93	1.49	1.37
44	LE	1198	PSU	C2-N3	6.92	1.49	1.37
1	S1	27	PSU	C2-N3	6.92	1.49	1.37
40	LA	16	PSU	C2-N3	6.91	1.49	1.37
47	LH	2623	PSU	C2-N3	6.90	1.49	1.37
1	S1	2116	PSU	C2-N3	6.89	1.49	1.37
44	LE	1126	PSU	C2-N3	6.89	1.49	1.37
47	LH	2679	PSU	C2-N3	6.88	1.49	1.37
42	LC	567	PSU	C2-N3	6.87	1.49	1.37
48	LI	3412	PSU	C2-N3	6.87	1.49	1.37
48	LI	3185	PSU	C2-N3	6.86	1.49	1.37
48	LI	3562	PSU	C2-N3	6.86	1.49	1.37
47	LH	2361	PSU	C2-N3	6.83	1.49	1.37
44	LE	1075	PSU	C2-N3	6.81	1.49	1.37
49	LJ	3644	PSU	C2-N3	6.78	1.49	1.37
1	S1	1592	PSU	C2-N3	6.78	1.49	1.37
1	S1	1591	PSU	C2-N3	6.74	1.49	1.37
47	LH	2849	A2M	O4'-C4'	-6.74	1.29	1.45
47	LH	2920	A2M	O4'-C4'	-6.72	1.30	1.45
45	LF	1502	A2M	O4'-C4'	-6.70	1.30	1.45
42	LC	594	A2M	O4'-C4'	-6.68	1.30	1.45
1	S1	1554	PSU	C2-N3	6.68	1.48	1.37
47	LH	2887	A2M	O4'-C4'	-6.66	1.30	1.45
1	S1	2046	A2M	O4'-C4'	-6.65	1.30	1.45
48	LI	3533	A2M	O4'-C4'	-6.63	1.30	1.45
1	S1	1063	A2M	O4'-C4'	-6.61	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	40	A2M	O4'-C4'	-6.60	1.30	1.45
1	S1	110	A2M	O4'-C4'	-6.59	1.30	1.45
44	LE	1106	A2M	O4'-C4'	-6.59	1.30	1.45
48	LI	3521	A2M	O4'-C4'	-6.59	1.30	1.45
47	LH	2744	A2M	O4'-C4'	-6.56	1.30	1.45
1	S1	1096	A2M	O4'-C4'	-6.55	1.30	1.45
44	LE	1204	A2M	O4'-C4'	-6.55	1.30	1.45
1	S1	1371	A2M	O4'-C4'	-6.55	1.30	1.45
46	LG	2022	A2M	O4'-C4'	-6.55	1.30	1.45
1	S1	645	A2M	O4'-C4'	-6.54	1.30	1.45
47	LH	2768	A2M	O4'-C4'	-6.54	1.30	1.45
47	LH	2358	A2M	O4'-C4'	-6.54	1.30	1.45
1	S1	407	A2M	O4'-C4'	-6.53	1.30	1.45
44	LE	1118	PSU	C2-N3	6.50	1.48	1.37
47	LH	2809	A2M	O4'-C4'	-6.50	1.30	1.45
45	LF	1891	A2M	O4'-C4'	-6.49	1.30	1.45
41	LB	183	A2M	O4'-C4'	-6.48	1.30	1.45
1	S1	649	A2M	O4'-C4'	-6.48	1.30	1.45
1	S1	28	A2M	O4'-C4'	-6.48	1.30	1.45
48	LI	3315	A2M	O4'-C4'	-6.48	1.30	1.45
45	LF	1815	A2M	O4'-C4'	-6.47	1.30	1.45
47	LH	2814	A2M	O4'-C4'	-6.47	1.30	1.45
1	S1	1549	A2M	O4'-C4'	-6.47	1.30	1.45
48	LI	3367	A2M	O4'-C4'	-6.45	1.30	1.45
47	LH	2812	A2M	O4'-C4'	-6.45	1.30	1.45
44	LE	1121	A2M	O4'-C4'	-6.42	1.30	1.45
45	LF	1888	A2M	O4'-C4'	-6.41	1.30	1.45
1	S1	533	A2M	O4'-C4'	-6.41	1.30	1.45
46	LG	2005	A2M	O4'-C4'	-6.41	1.30	1.45
40	LA	39	A2M	O4'-C4'	-6.39	1.30	1.45
44	LE	1039	A2M	O4'-C4'	-6.39	1.30	1.45
47	LH	2746	PSU	C2-N3	6.38	1.48	1.37
45	LF	1929	A2M	O4'-C4'	-6.35	1.30	1.45
1	S1	1900	A2M	O4'-C4'	-6.35	1.30	1.45
44	LE	935	A2M	O4'-C4'	-6.35	1.30	1.45
45	LF	1738	A2M	O4'-C4'	-6.34	1.30	1.45
47	LH	2349	A2M	O4'-C4'	-6.34	1.30	1.45
1	S1	565	A2M	O4'-C4'	-6.33	1.30	1.45
47	LH	2769	A2M	O4'-C4'	-6.33	1.30	1.45
47	LH	2708	A2M	O4'-C4'	-6.32	1.30	1.45
48	LI	3348	A2M	O4'-C4'	-6.31	1.30	1.45
48	LI	3500	A2M	O4'-C4'	-6.26	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	LA	97	A2M	O4'-C4'	-6.22	1.31	1.45
2	S2	37	MIA	C2-S10	6.15	1.80	1.75
51	LL	3906	A2M	O4'-C4'	-6.15	1.31	1.45
2	S2	37	MIA	C6-N6	5.85	1.45	1.34
1	S1	2078	7MG	C8-N9	5.53	1.49	1.46
53	LN	3969	PSU	C6-N1	5.31	1.45	1.36
48	LI	3042	PSU	C6-N1	5.30	1.45	1.36
45	LF	1568	PSU	C6-N1	5.27	1.45	1.36
47	LH	2802	PSU	C6-N1	5.22	1.44	1.36
48	LI	3446	PSU	C6-N1	5.22	1.44	1.36
44	LE	938	7MG	C8-N9	5.21	1.48	1.46
1	S1	403	PSU	C6-N1	5.19	1.44	1.36
48	LI	2999	PSU	C6-N1	5.17	1.44	1.36
45	LF	1876	PSU	C6-N1	5.17	1.44	1.36
1	S1	105	PSU	C6-N1	5.17	1.44	1.36
48	LI	3185	PSU	C6-N1	5.16	1.44	1.36
1	S1	280	PSU	C6-N1	5.15	1.44	1.36
48	LI	3145	PSU	C6-N1	5.15	1.44	1.36
1	S1	1660	PSU	C6-N1	5.14	1.44	1.36
47	LH	2586	PSU	C6-N1	5.14	1.44	1.36
52	LM	3953	PSU	C6-N1	5.13	1.44	1.36
52	LM	3963	PSU	C6-N1	5.12	1.44	1.36
45	LF	1926	PSU	C6-N1	5.12	1.44	1.36
1	S1	2305	PSU	C6-N1	5.11	1.44	1.36
41	LB	280	PSU	C6-N1	5.11	1.44	1.36
51	LL	3865	PSU	C6-N1	5.10	1.44	1.36
42	LC	302	PSU	C6-N1	5.10	1.44	1.36
1	S1	2101	PSU	C6-N1	5.09	1.44	1.36
44	LE	1260	PSU	C6-N1	5.09	1.44	1.36
1	S1	640	PSU	C6-N1	5.08	1.44	1.36
47	LH	2742	PSU	C6-N1	5.07	1.44	1.36
1	S1	1592	PSU	C6-N1	5.06	1.44	1.36
1	S1	1068	PSU	C6-N1	5.06	1.44	1.36
48	LI	3542	PSU	C6-N1	5.05	1.44	1.36
44	LE	1363	PSU	C6-N1	5.05	1.44	1.36
45	LF	1586	PSU	C6-N1	5.04	1.44	1.36
44	LE	1118	PSU	C6-N1	5.03	1.44	1.36
47	LH	2591	PSU	C6-N1	5.03	1.44	1.36
47	LH	2899	PSU	C6-N1	5.03	1.44	1.36
47	LH	2621	PSU	C6-N1	5.03	1.44	1.36
47	LH	2837	PSU	C6-N1	5.03	1.44	1.36
48	LI	3451	PSU	C6-N1	5.03	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	LG	2119	PSU	C6-N1	5.02	1.44	1.36
1	S1	32	PSU	C6-N1	5.02	1.44	1.36
47	LH	2874	PSU	C6-N1	5.02	1.44	1.36
49	LJ	3591	PSU	C6-N1	5.02	1.44	1.36
41	LB	234	PSU	C6-N1	5.01	1.44	1.36
44	LE	1184	PSU	C6-N1	5.01	1.44	1.36
42	LC	421	PSU	C6-N1	5.01	1.44	1.36
48	LI	3167	PSU	C6-N1	5.01	1.44	1.36
48	LI	3204	PSU	C6-N1	5.00	1.44	1.36
48	LI	3531	PSU	C6-N1	5.00	1.44	1.36
44	LE	1365	PSU	C6-N1	4.99	1.44	1.36
42	LC	308	PSU	C6-N1	4.99	1.44	1.36
44	LE	1171	PSU	C6-N1	4.99	1.44	1.36
48	LI	3440	PSU	C6-N1	4.99	1.44	1.36
1	S1	1715	PSU	C6-N1	4.99	1.44	1.36
44	LE	1407	PSU	C6-N1	4.99	1.44	1.36
47	LH	2915	PSU	C6-N1	4.98	1.44	1.36
1	S1	1624	PSU	C6-N1	4.98	1.44	1.36
45	LF	1859	PSU	C6-N1	4.98	1.44	1.36
40	LA	16	PSU	C6-N1	4.97	1.44	1.36
47	LH	2624	PSU	C6-N1	4.97	1.44	1.36
47	LH	2914	PSU	C6-N1	4.97	1.44	1.36
42	LC	480	PSU	C6-N1	4.97	1.44	1.36
1	S1	2116	PSU	C6-N1	4.97	1.44	1.36
48	LI	3332	PSU	C6-N1	4.97	1.44	1.36
45	LF	1582	PSU	C6-N1	4.97	1.44	1.36
1	S1	2131	PSU	C6-N1	4.96	1.44	1.36
1	S1	1396	PSU	C6-N1	4.96	1.44	1.36
1	S1	2065	PSU	C6-N1	4.96	1.44	1.36
46	LG	2171	PSU	C6-N1	4.96	1.44	1.36
48	LI	3503	PSU	C6-N1	4.95	1.44	1.36
1	S1	89	PSU	C6-N1	4.95	1.44	1.36
48	LI	3510	PSU	C6-N1	4.95	1.44	1.36
1	S1	176	PSU	C6-N1	4.94	1.44	1.36
49	LJ	3697	PSU	C6-N1	4.94	1.44	1.36
42	LC	498	PSU	C6-N1	4.93	1.44	1.36
44	LE	1198	PSU	C6-N1	4.93	1.44	1.36
1	S1	27	PSU	C6-N1	4.93	1.44	1.36
1	S1	2129	PSU	C6-N1	4.93	1.44	1.36
49	LJ	3680	PSU	C6-N1	4.92	1.44	1.36
40	LA	68	PSU	C6-N1	4.92	1.44	1.36
44	LE	938	7MG	C5-N7	4.91	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	LG	2154	PSU	C6-N1	4.90	1.44	1.36
41	LB	281	PSU	C6-N1	4.90	1.44	1.36
1	S1	1711	PSU	C6-N1	4.90	1.44	1.36
44	LE	1235	PSU	C6-N1	4.90	1.44	1.36
45	LF	1692	PSU	C6-N1	4.90	1.44	1.36
48	LI	3206	PSU	C6-N1	4.89	1.44	1.36
1	S1	2081	PSU	C6-N1	4.89	1.44	1.36
48	LI	3444	PSU	C6-N1	4.89	1.44	1.36
44	LE	1126	PSU	C6-N1	4.88	1.44	1.36
47	LH	2679	PSU	C6-N1	4.88	1.44	1.36
46	LG	2125	PSU	C6-N1	4.87	1.44	1.36
48	LI	3175	PSU	C6-N1	4.87	1.44	1.36
47	LH	2617	PSU	C6-N1	4.86	1.44	1.36
1	S1	465	PSU	C6-N1	4.86	1.44	1.36
47	LH	2642	PSU	C6-N1	4.86	1.44	1.36
42	LC	567	PSU	C6-N1	4.84	1.44	1.36
47	LH	2752	PSU	C6-N1	4.84	1.44	1.36
1	S1	544	PSU	C6-N1	4.84	1.44	1.36
1	S1	1960	PSU	C6-N1	4.84	1.44	1.36
47	LH	2623	PSU	C6-N1	4.82	1.44	1.36
1	S1	1554	PSU	C6-N1	4.82	1.44	1.36
49	LJ	3701	PSU	C6-N1	4.81	1.44	1.36
1	S1	1591	PSU	C6-N1	4.81	1.44	1.36
48	LI	3568	PSU	C6-N1	4.81	1.44	1.36
1	S1	1393	PSU	C6-N1	4.81	1.44	1.36
44	LE	1023	PSU	C6-N1	4.80	1.44	1.36
44	LE	1266	PSU	C6-N1	4.79	1.44	1.36
47	LH	2330	PSU	C6-N1	4.79	1.44	1.36
1	S1	1378	PSU	C6-N1	4.78	1.44	1.36
47	LH	2746	PSU	C6-N1	4.77	1.44	1.36
47	LH	2754	PSU	C6-N1	4.77	1.44	1.36
44	LE	1075	PSU	C6-N1	4.75	1.44	1.36
48	LI	3562	PSU	C6-N1	4.70	1.44	1.36
49	LJ	3644	PSU	C6-N1	4.66	1.44	1.36
48	LI	3412	PSU	C6-N1	4.65	1.43	1.36
47	LH	2361	PSU	C6-N1	4.63	1.43	1.36
47	LH	2842	PSU	C6-N1	4.62	1.43	1.36
1	S1	2078	7MG	C5-N7	4.58	1.40	1.35
47	LH	2685	OMC	C2-N1	4.44	1.49	1.40
45	LF	1856	OMG	C6-N1	4.28	1.44	1.37
44	LE	931	1MA	C2-N3	4.27	1.34	1.29
1	S1	180	OMG	C6-N1	4.24	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	LH	2925	OMG	C6-N1	4.13	1.44	1.37
44	LE	1324	OMG	C6-N1	4.10	1.44	1.37
1	S1	641	OMG	C6-N1	4.09	1.44	1.37
1	S1	390	OMG	C6-N1	4.09	1.44	1.37
1	S1	2075	OMG	C6-N1	4.08	1.43	1.37
47	LH	2883	OMG	C6-N1	4.05	1.43	1.37
1	S1	42	OMG	C6-N1	4.05	1.43	1.37
40	LA	74	OMG	C6-N1	4.01	1.43	1.37
48	LI	3509	OMG	C6-N1	4.01	1.43	1.37
48	LI	3042	PSU	C4-N3	4.01	1.46	1.38
42	LC	628	OMG	C6-N1	4.00	1.43	1.37
48	LI	3223	OMG	C6-N1	3.99	1.43	1.37
49	LJ	3688	OMG	C6-N1	3.98	1.43	1.37
1	S1	1681	OMG	C6-N1	3.98	1.43	1.37
45	LF	1826	OMG	C6-N1	3.98	1.43	1.37
42	LC	631	OMG	C6-N1	3.96	1.43	1.37
46	LG	2009	OMG	C6-N1	3.96	1.43	1.37
41	LB	215	OMG	C6-N1	3.96	1.43	1.37
45	LF	1662	OMG	C6-N1	3.96	1.43	1.37
47	LH	2897	OMG	C6-N1	3.96	1.43	1.37
47	LH	2879	OMG	C6-N1	3.94	1.43	1.37
44	LE	1201	OMG	C6-N1	3.94	1.43	1.37
45	LF	1883	OMG	C6-N1	3.93	1.43	1.37
48	LI	3187	OMG	C6-N1	3.93	1.43	1.37
45	LF	1573	OMC	C2-N1	3.93	1.48	1.40
1	S1	1705	OMG	C6-N1	3.90	1.43	1.37
40	LA	41	OMG	C6-N1	3.90	1.43	1.37
47	LH	2870	OMG	C6-N1	3.90	1.43	1.37
48	LI	3434	OMG	C6-N1	3.90	1.43	1.37
1	S1	1536	OMG	C6-N1	3.88	1.43	1.37
1	S1	1901	OMG	C6-N1	3.88	1.43	1.37
44	LE	1217	OMG	C6-N1	3.88	1.43	1.37
45	LF	1819	OMG	C6-N1	3.88	1.43	1.37
48	LI	3191	OMG	C6-N1	3.87	1.43	1.37
45	LF	1568	PSU	C4-N3	3.87	1.46	1.38
46	LG	2146	OMG	C6-N1	3.86	1.43	1.37
1	S1	485	OMG	C6-N1	3.86	1.43	1.37
48	LI	3504	OMG	C6-N1	3.85	1.43	1.37
47	LH	2776	OMG	C6-N1	3.84	1.43	1.37
47	LH	2610	OMG	C6-N1	3.83	1.43	1.37
48	LI	2999	PSU	C4-N3	3.83	1.45	1.38
48	LI	3379	OMG	C6-N1	3.82	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	LI	3446	PSU	C4-N3	3.82	1.45	1.38
45	LF	1835	OMG	C6-N1	3.82	1.43	1.37
48	LI	3377	OMG	C6-N1	3.82	1.43	1.37
45	LF	1667	OMG	C6-N1	3.81	1.43	1.37
53	LN	3969	PSU	C4-N3	3.80	1.45	1.38
52	LM	3963	PSU	C4-N3	3.80	1.45	1.38
1	S1	280	PSU	C4-N3	3.80	1.45	1.38
42	LC	541	OMG	C6-N1	3.80	1.43	1.37
45	LF	1956	OMG	C6-N1	3.78	1.43	1.37
42	LC	421	PSU	C4-N3	3.78	1.45	1.38
47	LH	2766	5MC	C2-N1	3.78	1.48	1.40
48	LI	3145	PSU	C4-N3	3.77	1.45	1.38
46	LG	2125	PSU	C4-N3	3.76	1.45	1.38
44	LE	1104	OMG	C6-N1	3.75	1.43	1.37
42	LC	308	PSU	C4-N3	3.75	1.45	1.38
41	LB	281	PSU	C4-N3	3.74	1.45	1.38
47	LH	2586	PSU	C4-N3	3.74	1.45	1.38
51	LL	3865	PSU	C4-N3	3.73	1.45	1.38
45	LF	1683	OMG	C6-N1	3.73	1.43	1.37
44	LE	1023	PSU	C4-N3	3.71	1.45	1.38
48	LI	3510	PSU	C4-N3	3.71	1.45	1.38
1	S1	57	OMG	C6-N1	3.71	1.43	1.37
48	LI	3542	PSU	C4-N3	3.70	1.45	1.38
45	LF	1586	PSU	C4-N3	3.70	1.45	1.38
1	S1	1660	PSU	C4-N3	3.68	1.45	1.38
42	LC	302	PSU	C4-N3	3.68	1.45	1.38
45	LF	1926	PSU	C4-N3	3.67	1.45	1.38
1	S1	640	PSU	C4-N3	3.67	1.45	1.38
1	S1	1068	PSU	C4-N3	3.66	1.45	1.38
1	S1	1715	PSU	C4-N3	3.66	1.45	1.38
1	S1	176	PSU	C4-N3	3.66	1.45	1.38
48	LI	3175	PSU	C4-N3	3.66	1.45	1.38
48	LI	3444	PSU	C4-N3	3.65	1.45	1.38
47	LH	2802	PSU	C4-N3	3.65	1.45	1.38
1	S1	465	PSU	C4-N3	3.65	1.45	1.38
45	LF	1859	PSU	C4-N3	3.65	1.45	1.38
1	S1	1393	PSU	C4-N3	3.64	1.45	1.38
48	LI	3440	PSU	C4-N3	3.64	1.45	1.38
49	LJ	3701	PSU	C4-N3	3.64	1.45	1.38
47	LH	2842	PSU	C4-N3	3.64	1.45	1.38
47	LH	2752	PSU	C4-N3	3.64	1.45	1.38
48	LI	3332	PSU	C4-N3	3.64	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	LB	234	PSU	C4-N3	3.64	1.45	1.38
52	LM	3953	PSU	C4-N3	3.63	1.45	1.38
1	S1	1624	PSU	C4-N3	3.63	1.45	1.38
1	S1	2101	PSU	C4-N3	3.63	1.45	1.38
41	LB	280	PSU	C4-N3	3.63	1.45	1.38
1	S1	1960	PSU	C4-N3	3.63	1.45	1.38
42	LC	498	PSU	C4-N3	3.63	1.45	1.38
47	LH	2642	PSU	C4-N3	3.62	1.45	1.38
44	LE	1365	PSU	C4-N3	3.62	1.45	1.38
1	S1	2305	PSU	C4-N3	3.62	1.45	1.38
1	S1	1378	PSU	C4-N3	3.62	1.45	1.38
45	LF	1876	PSU	C4-N3	3.62	1.45	1.38
44	LE	1363	PSU	C4-N3	3.61	1.45	1.38
48	LI	3167	PSU	C4-N3	3.61	1.45	1.38
45	LF	1582	PSU	C4-N3	3.60	1.45	1.38
44	LE	1407	PSU	C4-N3	3.60	1.45	1.38
45	LF	1692	PSU	C4-N3	3.59	1.45	1.38
44	LE	1184	PSU	C4-N3	3.58	1.45	1.38
1	S1	2081	PSU	C4-N3	3.58	1.45	1.38
47	LH	2679	PSU	C4-N3	3.58	1.45	1.38
44	LE	1235	PSU	C4-N3	3.58	1.45	1.38
47	LH	2621	PSU	C4-N3	3.57	1.45	1.38
47	LH	2617	PSU	C4-N3	3.57	1.45	1.38
47	LH	2837	PSU	C4-N3	3.56	1.45	1.38
1	S1	403	PSU	C4-N3	3.55	1.45	1.38
46	LG	2154	PSU	C4-N3	3.54	1.45	1.38
1	S1	105	PSU	C4-N3	3.54	1.45	1.38
49	LJ	3697	PSU	C4-N3	3.54	1.45	1.38
47	LH	2914	PSU	C4-N3	3.54	1.45	1.38
47	LH	2915	PSU	C4-N3	3.54	1.45	1.38
48	LI	3401	OMG	C6-N1	3.53	1.43	1.37
48	LI	3185	PSU	C4-N3	3.53	1.45	1.38
1	S1	27	PSU	C4-N3	3.53	1.45	1.38
47	LH	2874	PSU	C4-N3	3.52	1.45	1.38
1	S1	1396	PSU	C4-N3	3.51	1.45	1.38
46	LG	2171	PSU	C4-N3	3.51	1.45	1.38
40	LA	68	PSU	C4-N3	3.51	1.45	1.38
44	LE	1260	PSU	C4-N3	3.51	1.45	1.38
48	LI	3451	PSU	C4-N3	3.51	1.45	1.38
44	LE	1266	PSU	C4-N3	3.51	1.45	1.38
1	S1	2131	PSU	C4-N3	3.50	1.45	1.38
48	LI	3206	PSU	C4-N3	3.50	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	LH	2754	PSU	C4-N3	3.50	1.45	1.38
48	LI	3503	PSU	C4-N3	3.50	1.45	1.38
1	S1	2065	PSU	C4-N3	3.49	1.45	1.38
49	LJ	3644	PSU	C4-N3	3.49	1.45	1.38
49	LJ	3591	PSU	C4-N3	3.49	1.45	1.38
48	LI	3412	PSU	C4-N3	3.49	1.45	1.38
44	LE	1198	PSU	C4-N3	3.49	1.45	1.38
42	LC	480	PSU	C4-N3	3.49	1.45	1.38
44	LE	1075	PSU	C4-N3	3.48	1.45	1.38
47	LH	2591	PSU	C4-N3	3.48	1.45	1.38
47	LH	2330	PSU	C4-N3	3.48	1.45	1.38
46	LG	2119	PSU	C4-N3	3.48	1.45	1.38
48	LI	3204	PSU	C4-N3	3.47	1.45	1.38
42	LC	567	PSU	C4-N3	3.47	1.45	1.38
48	LI	3456	5MC	C2-N1	3.47	1.47	1.40
48	LI	3568	PSU	C4-N3	3.47	1.45	1.38
47	LH	2623	PSU	C4-N3	3.47	1.45	1.38
44	LE	1171	PSU	C4-N3	3.47	1.45	1.38
47	LH	2899	PSU	C4-N3	3.46	1.45	1.38
1	S1	2116	PSU	C4-N3	3.46	1.45	1.38
1	S1	1711	PSU	C4-N3	3.46	1.45	1.38
1	S1	2129	PSU	C4-N3	3.44	1.45	1.38
44	LE	1165	OMC	C2-N1	3.43	1.47	1.40
48	LI	3531	PSU	C4-N3	3.41	1.45	1.38
47	LH	2624	PSU	C4-N3	3.40	1.45	1.38
1	S1	544	PSU	C4-N3	3.39	1.45	1.38
1	S1	1591	PSU	C4-N3	3.38	1.45	1.38
40	LA	16	PSU	C4-N3	3.38	1.45	1.38
40	LA	97	A2M	O3'-C3'	-3.38	1.35	1.43
1	S1	103	OMC	C2-N1	3.35	1.47	1.40
48	LI	3518	5MC	C2-N1	3.35	1.47	1.40
1	S1	89	PSU	C4-N3	3.34	1.45	1.38
1	S1	32	PSU	C4-N3	3.34	1.45	1.38
47	LH	2742	PSU	C4-N3	3.34	1.45	1.38
49	LJ	3680	PSU	C4-N3	3.32	1.45	1.38
1	S1	1371	A2M	O3'-C3'	-3.31	1.35	1.43
47	LH	2358	A2M	O2'-C2'	3.30	1.51	1.42
1	S1	1592	PSU	C4-N3	3.30	1.45	1.38
44	LE	1126	PSU	C4-N3	3.29	1.44	1.38
47	LH	2361	PSU	C4-N3	3.29	1.44	1.38
45	LF	1815	A2M	O3'-C3'	-3.27	1.35	1.43
1	S1	407	A2M	O3'-C3'	-3.24	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	1554	PSU	C4-N3	3.24	1.44	1.38
44	LE	1118	PSU	C4-N3	3.23	1.44	1.38
1	S1	565	A2M	O3'-C3'	-3.23	1.35	1.43
44	LE	1121	A2M	O3'-C3'	-3.23	1.35	1.43
48	LI	3562	PSU	C4-N3	3.23	1.44	1.38
1	S1	2144	5MC	C2-N1	3.21	1.47	1.40
48	LI	3315	A2M	O3'-C3'	-3.21	1.35	1.43
47	LH	2887	A2M	O3'-C3'	-3.21	1.35	1.43
48	LI	3533	A2M	O3'-C3'	-3.20	1.35	1.43
42	LC	594	A2M	O3'-C3'	-3.20	1.35	1.43
51	LL	3906	A2M	O3'-C3'	-3.19	1.35	1.43
47	LH	2744	A2M	C5-C4	-3.19	1.32	1.40
47	LH	2814	A2M	O3'-C3'	-3.19	1.35	1.43
45	LF	1888	A2M	O3'-C3'	-3.18	1.35	1.43
1	S1	1549	A2M	O3'-C3'	-3.17	1.35	1.43
45	LF	1502	A2M	O3'-C3'	-3.17	1.35	1.43
47	LH	2746	PSU	O4-C4	-3.17	1.17	1.23
1	S1	28	A2M	O3'-C3'	-3.16	1.35	1.43
44	LE	1204	A2M	O3'-C3'	-3.15	1.35	1.43
45	LF	1891	A2M	C5-C4	-3.15	1.32	1.40
44	LE	1118	PSU	O4-C4	-3.15	1.17	1.23
47	LH	2349	A2M	O3'-C3'	-3.15	1.35	1.43
47	LH	2849	A2M	O2'-C2'	3.13	1.50	1.42
40	LA	39	A2M	O3'-C3'	-3.13	1.35	1.43
1	S1	1592	PSU	O4-C4	-3.13	1.17	1.23
1	S1	723	A2M	O3'-C3'	-3.11	1.35	1.43
40	LA	97	A2M	C6-N6	3.11	1.45	1.34
45	LF	1929	A2M	O3'-C3'	-3.11	1.35	1.43
45	LF	1929	A2M	C6-N6	3.10	1.45	1.34
48	LI	3315	A2M	C6-N6	3.10	1.45	1.34
47	LH	2708	A2M	O3'-C3'	-3.09	1.35	1.43
48	LI	3500	A2M	C6-N6	3.09	1.45	1.34
45	LF	1738	A2M	O3'-C3'	-3.09	1.35	1.43
47	LH	2746	PSU	C4-N3	3.09	1.44	1.38
1	S1	1063	A2M	C6-N6	3.09	1.45	1.34
1	S1	1096	A2M	C6-N6	3.09	1.45	1.34
44	LE	1039	A2M	O3'-C3'	-3.08	1.35	1.43
1	S1	40	A2M	O3'-C3'	-3.08	1.35	1.43
1	S1	1063	A2M	O3'-C3'	-3.08	1.35	1.43
48	LI	3533	A2M	C5-C4	-3.07	1.32	1.40
47	LH	2920	A2M	C6-N6	3.07	1.45	1.34
1	S1	2287	MA6	C5-C4	-3.07	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	407	A2M	C6-N6	3.07	1.45	1.34
47	LH	2358	A2M	O3'-C3'	-3.07	1.35	1.43
44	LE	935	A2M	O3'-C3'	-3.07	1.35	1.43
1	S1	645	A2M	C6-N6	3.07	1.45	1.34
1	S1	1063	A2M	O2'-C2'	3.06	1.50	1.42
1	S1	1549	A2M	C6-N6	3.06	1.45	1.34
41	LB	183	A2M	O3'-C3'	-3.06	1.35	1.43
46	LG	2022	A2M	C6-N6	3.06	1.45	1.34
41	LB	183	A2M	C6-N6	3.06	1.45	1.34
44	LE	1106	A2M	C6-N6	3.06	1.45	1.34
48	LI	3500	A2M	O3'-C3'	-3.06	1.35	1.43
44	LE	1121	A2M	C6-N6	3.06	1.45	1.34
45	LF	1891	A2M	C6-N6	3.05	1.45	1.34
1	S1	533	A2M	C6-N6	3.05	1.45	1.34
47	LH	2809	A2M	C5-C4	-3.05	1.32	1.40
46	LG	2005	A2M	C6-N6	3.05	1.45	1.34
1	S1	649	A2M	C6-N6	3.05	1.45	1.34
47	LH	2769	A2M	C5-C4	-3.05	1.32	1.40
42	LC	594	A2M	C6-N6	3.05	1.45	1.34
1	S1	565	A2M	C6-N6	3.05	1.45	1.34
47	LH	2349	A2M	C6-N6	3.05	1.45	1.34
48	LI	3521	A2M	O3'-C3'	-3.04	1.35	1.43
2	S2	37	MIA	C5-C4	-3.04	1.32	1.40
48	LI	3348	A2M	C6-N6	3.04	1.45	1.34
45	LF	1815	A2M	C6-N6	3.04	1.45	1.34
48	LI	3521	A2M	C6-N6	3.04	1.45	1.34
1	S1	110	A2M	C6-N6	3.03	1.45	1.34
44	LE	931	1MA	C6-N6	3.03	1.35	1.27
44	LE	1106	A2M	O3'-C3'	-3.03	1.35	1.43
1	S1	2046	A2M	C6-N6	3.03	1.45	1.34
1	S1	1900	A2M	C6-N6	3.03	1.45	1.34
47	LH	2708	A2M	C6-N6	3.03	1.45	1.34
45	LF	1502	A2M	C6-N6	3.03	1.45	1.34
45	LF	1891	A2M	O3'-C3'	-3.03	1.35	1.43
45	LF	1738	A2M	C6-N6	3.02	1.45	1.34
1	S1	723	A2M	C6-N6	3.02	1.45	1.34
47	LH	2358	A2M	C5-C4	-3.02	1.32	1.40
51	LL	3906	A2M	C6-N6	3.02	1.45	1.34
1	S1	2046	A2M	O3'-C3'	-3.02	1.35	1.43
47	LH	2809	A2M	C6-N6	3.02	1.45	1.34
47	LH	2887	A2M	C6-N6	3.02	1.45	1.34
47	LH	2746	PSU	O2-C2	-3.02	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	LH	2744	A2M	C6-N6	3.02	1.45	1.34
48	LI	3533	A2M	C6-N6	3.01	1.45	1.34
1	S1	533	A2M	O3'-C3'	-3.01	1.35	1.43
44	LE	1204	A2M	C6-N6	3.01	1.45	1.34
47	LH	2814	A2M	C6-N6	3.01	1.45	1.34
45	LF	1888	A2M	C6-N6	3.01	1.45	1.34
47	LH	2904	B8H	C4-N3	-3.01	1.33	1.38
47	LH	2349	A2M	C5-C4	-3.01	1.33	1.40
47	LH	2812	A2M	C6-N6	3.01	1.45	1.34
1	S1	1371	A2M	C6-N6	3.01	1.45	1.34
44	LE	935	A2M	C5-C4	-3.01	1.33	1.40
47	LH	2768	A2M	O3'-C3'	-3.00	1.35	1.43
47	LH	2849	A2M	C6-N6	3.00	1.45	1.34
1	S1	110	A2M	O3'-C3'	-3.00	1.35	1.43
1	S1	1096	A2M	O3'-C3'	-3.00	1.35	1.43
48	LI	3145	PSU	O4'-C1'	-3.00	1.39	1.43
1	S1	28	A2M	C5-C4	-2.99	1.33	1.40
1	S1	2288	MA6	C5-C4	-2.99	1.33	1.40
47	LH	2887	A2M	C5-C4	-2.99	1.33	1.40
47	LH	2809	A2M	O3'-C3'	-2.99	1.35	1.43
1	S1	28	A2M	C6-N6	2.99	1.45	1.34
47	LH	2768	A2M	C6-N6	2.99	1.45	1.34
48	LI	3367	A2M	C5-C4	-2.99	1.33	1.40
47	LH	2812	A2M	O3'-C3'	-2.99	1.35	1.43
48	LI	3367	A2M	C6-N6	2.98	1.44	1.34
44	LE	1039	A2M	C6-N6	2.98	1.44	1.34
47	LH	2358	A2M	C6-N6	2.98	1.44	1.34
1	S1	110	A2M	C5-C4	-2.98	1.33	1.40
46	LG	2005	A2M	O3'-C3'	-2.98	1.36	1.43
45	LF	1502	A2M	C5-C4	-2.97	1.33	1.40
1	S1	2046	A2M	C5-C4	-2.97	1.33	1.40
45	LF	1738	A2M	C5-C4	-2.97	1.33	1.40
47	LH	2766	5MC	C2-N3	2.97	1.42	1.36
47	LH	2812	A2M	O2'-C2'	2.97	1.50	1.42
1	S1	645	A2M	O3'-C3'	-2.96	1.36	1.43
1	S1	40	A2M	C6-N6	2.96	1.44	1.34
44	LE	935	A2M	C6-N6	2.96	1.44	1.34
40	LA	39	A2M	C6-N6	2.95	1.44	1.34
1	S1	723	A2M	C5-C4	-2.95	1.33	1.40
48	LI	3521	A2M	C5-C4	-2.95	1.33	1.40
47	LH	2849	A2M	O3'-C3'	-2.95	1.36	1.43
47	LH	2742	PSU	O4-C4	-2.95	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	LI	3367	A2M	O3'-C3'	-2.95	1.36	1.43
1	S1	1371	A2M	C5-C4	-2.94	1.33	1.40
42	LC	421	PSU	O4-C4	-2.94	1.18	1.23
47	LH	2920	A2M	C5-C4	-2.94	1.33	1.40
47	LH	2920	A2M	O3'-C3'	-2.94	1.36	1.43
47	LH	2769	A2M	C6-N6	2.94	1.44	1.34
1	S1	40	A2M	C5-C4	-2.92	1.33	1.40
1	S1	2144	5MC	C6-N1	-2.92	1.33	1.38
1	S1	649	A2M	O3'-C3'	-2.92	1.36	1.43
40	LA	97	A2M	C5-C4	-2.92	1.33	1.40
48	LI	3348	A2M	C5-C4	-2.92	1.33	1.40
48	LI	3500	A2M	C5-C4	-2.92	1.33	1.40
1	S1	649	A2M	C5-C4	-2.91	1.33	1.40
1	S1	1900	A2M	O3'-C3'	-2.91	1.36	1.43
48	LI	3355	OMC	C2-N1	2.91	1.46	1.40
1	S1	38	OMC	C2-N1	2.90	1.46	1.40
48	LI	3348	A2M	O3'-C3'	-2.90	1.36	1.43
1	S1	1549	A2M	C5-C4	-2.90	1.33	1.40
1	S1	1396	PSU	O4-C4	-2.89	1.18	1.23
45	LF	1888	A2M	C5-C4	-2.89	1.33	1.40
46	LG	2022	A2M	O3'-C3'	-2.89	1.36	1.43
44	LE	1106	A2M	C5-C4	-2.89	1.33	1.40
47	LH	2812	A2M	C5-C4	-2.89	1.33	1.40
47	LH	2769	A2M	O3'-C3'	-2.89	1.36	1.43
42	LC	594	A2M	C5-C4	-2.88	1.33	1.40
47	LH	2849	A2M	C5-C4	-2.88	1.33	1.40
44	LE	1204	A2M	C5-C4	-2.88	1.33	1.40
48	LI	3531	PSU	O4-C4	-2.88	1.18	1.23
40	LA	39	A2M	C5-C4	-2.88	1.33	1.40
45	LF	1815	A2M	C5-C4	-2.87	1.33	1.40
1	S1	403	PSU	O4-C4	-2.87	1.18	1.23
44	LE	1104	OMG	C5-C6	-2.87	1.41	1.47
45	LF	1956	OMG	C5-C6	-2.87	1.41	1.47
46	LG	2005	A2M	C5-C4	-2.86	1.33	1.40
1	S1	121	PSU	C6-C5	2.86	1.38	1.35
45	LF	1929	A2M	C5-C4	-2.86	1.33	1.40
44	LE	1039	A2M	C5-C4	-2.85	1.33	1.40
1	S1	32	PSU	O4-C4	-2.85	1.18	1.23
48	LI	3191	OMG	C5-C6	-2.85	1.41	1.47
47	LH	2814	A2M	C5-C4	-2.85	1.33	1.40
47	LH	2814	A2M	O2'-C2'	2.85	1.49	1.42
41	LB	183	A2M	C5-C4	-2.84	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	LI	3315	A2M	C5-C4	-2.84	1.33	1.40
45	LF	1926	PSU	O4-C4	-2.84	1.18	1.23
1	S1	565	A2M	C5-C4	-2.84	1.33	1.40
47	LH	2708	A2M	C5-C4	-2.84	1.33	1.40
47	LH	2361	PSU	O4-C4	-2.84	1.18	1.23
47	LH	2744	A2M	O2'-C2'	2.84	1.49	1.42
48	LI	3456	5MC	C6-N1	-2.84	1.33	1.38
1	S1	1900	A2M	C5-C4	-2.84	1.33	1.40
1	S1	533	A2M	C5-C4	-2.83	1.33	1.40
1	S1	121	PSU	C4-N3	-2.82	1.33	1.38
47	LH	2768	A2M	C5-C4	-2.82	1.33	1.40
46	LG	2022	A2M	C5-C4	-2.82	1.33	1.40
44	LE	1260	PSU	O4-C4	-2.82	1.18	1.23
44	LE	1126	PSU	O4-C4	-2.81	1.18	1.23
1	S1	723	A2M	O2'-C2'	2.81	1.49	1.42
47	LH	2920	A2M	O2'-C2'	2.80	1.49	1.42
1	S1	1096	A2M	O2'-C2'	2.80	1.49	1.42
45	LF	1815	A2M	O2'-C2'	2.80	1.49	1.42
47	LH	2766	5MC	C6-N1	-2.79	1.33	1.38
1	S1	2101	PSU	O4-C4	-2.79	1.18	1.23
1	S1	1096	A2M	C5-C4	-2.79	1.33	1.40
1	S1	1591	PSU	O4-C4	-2.79	1.18	1.23
42	LC	498	PSU	O4-C4	-2.79	1.18	1.23
44	LE	1204	A2M	O2'-C2'	2.79	1.49	1.42
1	S1	1554	PSU	O4-C4	-2.78	1.18	1.23
47	LH	2591	PSU	O4-C4	-2.78	1.18	1.23
1	S1	2131	PSU	O4-C4	-2.78	1.18	1.23
1	S1	649	A2M	O2'-C2'	2.77	1.49	1.42
48	LI	3206	PSU	O4-C4	-2.77	1.18	1.23
1	S1	89	PSU	O4-C4	-2.77	1.18	1.23
45	LF	1876	PSU	O4-C4	-2.77	1.18	1.23
44	LE	1260	PSU	O4'-C1'	-2.76	1.40	1.43
1	S1	110	A2M	O2'-C2'	2.76	1.49	1.42
44	LE	1222	OMU	C2-N1	2.76	1.42	1.38
40	LA	97	A2M	O2'-C2'	2.76	1.49	1.42
42	LC	594	A2M	O2'-C2'	2.75	1.49	1.42
1	S1	2116	PSU	O4-C4	-2.75	1.18	1.23
42	LC	480	PSU	O4-C4	-2.75	1.18	1.23
1	S1	2129	PSU	O4-C4	-2.75	1.18	1.23
45	LF	1738	A2M	O2'-C2'	2.75	1.49	1.42
44	LE	1121	A2M	C5-C4	-2.75	1.33	1.40
47	LH	2623	PSU	O4-C4	-2.75	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	LI	3185	PSU	O4-C4	-2.75	1.18	1.23
48	LI	3533	A2M	O2'-C2'	2.74	1.49	1.42
48	LI	3562	PSU	O4-C4	-2.74	1.18	1.23
1	S1	1900	A2M	O2'-C2'	2.74	1.49	1.42
1	S1	407	A2M	C5-C4	-2.74	1.33	1.40
47	LH	2914	PSU	O4-C4	-2.74	1.18	1.23
44	LE	1222	OMU	C4-N3	-2.74	1.33	1.38
44	LE	1235	PSU	O4-C4	-2.74	1.18	1.23
47	LH	2642	PSU	O4-C4	-2.73	1.18	1.23
51	LL	3906	A2M	O2'-C2'	2.73	1.49	1.42
48	LI	3412	PSU	O4-C4	-2.73	1.18	1.23
44	LE	1171	PSU	O4-C4	-2.73	1.18	1.23
47	LH	2621	PSU	O4-C4	-2.73	1.18	1.23
46	LG	2119	PSU	O4-C4	-2.73	1.18	1.23
1	S1	105	PSU	O4-C4	-2.73	1.18	1.23
47	LH	2837	PSU	O4-C4	-2.73	1.18	1.23
1	S1	1063	A2M	C5-C4	-2.72	1.33	1.40
47	LH	2915	PSU	O4-C4	-2.72	1.18	1.23
47	LH	2708	A2M	O2'-C2'	2.72	1.49	1.42
1	S1	1624	PSU	O4-C4	-2.72	1.18	1.23
48	LI	3521	A2M	O2'-C2'	2.71	1.49	1.42
48	LI	3223	OMG	C5-C6	-2.71	1.41	1.47
40	LA	41	OMG	C5-C6	-2.71	1.41	1.47
1	S1	40	A2M	O2'-C2'	2.71	1.49	1.42
47	LH	2330	PSU	O4-C4	-2.71	1.18	1.23
47	LH	2624	PSU	O4-C4	-2.71	1.18	1.23
41	LB	234	PSU	O4-C4	-2.71	1.18	1.23
47	LH	2809	A2M	O2'-C2'	2.70	1.49	1.42
1	S1	1068	PSU	O4-C4	-2.70	1.18	1.23
40	LA	16	PSU	O4-C4	-2.70	1.18	1.23
44	LE	1039	A2M	O2'-C2'	2.70	1.49	1.42
48	LI	3503	PSU	O4-C4	-2.70	1.18	1.23
48	LI	3518	5MC	C2-N3	2.70	1.41	1.36
48	LI	3167	PSU	O4-C4	-2.70	1.18	1.23
47	LH	2768	A2M	O2'-C2'	2.69	1.49	1.42
44	LE	1184	PSU	O4-C4	-2.69	1.18	1.23
51	LL	3906	A2M	C5-C4	-2.69	1.33	1.40
1	S1	645	A2M	C5-C4	-2.69	1.33	1.40
44	LE	935	A2M	O2'-C2'	2.69	1.49	1.42
47	LH	2754	PSU	O4-C4	-2.69	1.18	1.23
48	LI	3204	PSU	O4-C4	-2.69	1.18	1.23
1	S1	645	A2M	O2'-C2'	2.69	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	LI	3315	A2M	O2'-C2'	2.69	1.49	1.42
48	LI	3440	PSU	O4-C4	-2.69	1.18	1.23
1	S1	1711	PSU	O4-C4	-2.69	1.18	1.23
47	LH	2769	A2M	O2'-C2'	2.69	1.49	1.42
47	LH	2897	OMG	C5-C6	-2.68	1.42	1.47
42	LC	537	OMC	C2-N1	2.68	1.45	1.40
45	LF	1888	A2M	O2'-C2'	2.68	1.49	1.42
48	LI	3348	A2M	O2'-C2'	2.68	1.49	1.42
1	S1	407	A2M	O2'-C2'	2.68	1.49	1.42
44	LE	1075	PSU	O4-C4	-2.68	1.18	1.23
47	LH	2874	PSU	O4-C4	-2.68	1.18	1.23
1	S1	1597	UR3	C3U-N3	-2.68	1.42	1.47
48	LI	3444	PSU	O4-C4	-2.68	1.18	1.23
48	LI	3518	5MC	C6-N1	-2.68	1.33	1.38
1	S1	544	PSU	O4-C4	-2.68	1.18	1.23
46	LG	2171	PSU	O4-C4	-2.68	1.18	1.23
46	LG	2022	A2M	O2'-C2'	2.68	1.49	1.42
52	LM	3963	PSU	O4-C4	-2.68	1.18	1.23
1	S1	1660	PSU	O4-C4	-2.67	1.18	1.23
49	LJ	3697	PSU	O4-C4	-2.67	1.18	1.23
48	LI	3187	OMG	C5-C6	-2.67	1.42	1.47
47	LH	2883	OMG	C5-C6	-2.67	1.42	1.47
48	LI	3451	PSU	O4-C4	-2.67	1.18	1.23
48	LI	3367	A2M	O2'-C2'	2.67	1.49	1.42
1	S1	1681	OMG	C5-C6	-2.67	1.42	1.47
1	S1	2065	PSU	O4-C4	-2.67	1.18	1.23
48	LI	3568	PSU	O4-C4	-2.67	1.18	1.23
48	LI	3401	OMG	C5-C6	-2.66	1.42	1.47
44	LE	1121	A2M	O2'-C2'	2.66	1.49	1.42
45	LF	1502	A2M	O2'-C2'	2.66	1.49	1.42
1	S1	533	A2M	O2'-C2'	2.65	1.49	1.42
1	S1	2046	A2M	O2'-C2'	2.65	1.49	1.42
45	LF	1692	PSU	O4-C4	-2.65	1.18	1.23
52	LM	3953	PSU	O4-C4	-2.65	1.18	1.23
48	LI	3332	PSU	O4-C4	-2.65	1.18	1.23
49	LJ	3680	PSU	O4-C4	-2.65	1.18	1.23
45	LF	1667	OMG	C5-C6	-2.65	1.42	1.47
48	LI	3504	OMG	C5-C6	-2.64	1.42	1.47
1	S1	1378	PSU	O4-C4	-2.64	1.18	1.23
45	LF	1859	PSU	O4-C4	-2.64	1.18	1.23
48	LI	3446	PSU	O4-C4	-2.64	1.18	1.23
1	S1	1371	A2M	O2'-C2'	2.64	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	LJ	3591	PSU	O4-C4	-2.63	1.18	1.23
44	LE	1201	OMG	C5-C6	-2.63	1.42	1.47
1	S1	1393	PSU	O4-C4	-2.63	1.18	1.23
47	LH	2752	PSU	O4-C4	-2.63	1.18	1.23
44	LE	1363	PSU	O4-C4	-2.63	1.18	1.23
47	LH	2349	A2M	O2'-C2'	2.63	1.49	1.42
45	LF	1568	PSU	O4-C4	-2.63	1.18	1.23
45	LF	1662	OMG	C5-C6	-2.63	1.42	1.47
1	S1	42	OMG	C5-C6	-2.63	1.42	1.47
1	S1	1901	OMG	C5-C6	-2.63	1.42	1.47
48	LI	3510	PSU	O4-C4	-2.62	1.18	1.23
45	LF	1891	A2M	O2'-C2'	2.62	1.49	1.42
47	LH	2899	PSU	O4-C4	-2.62	1.18	1.23
49	LJ	3701	PSU	O4-C4	-2.62	1.18	1.23
47	LH	2617	PSU	O4-C4	-2.61	1.18	1.23
1	S1	2144	5MC	C2-N3	2.61	1.41	1.36
44	LE	1198	PSU	O4-C4	-2.61	1.18	1.23
47	LH	2842	PSU	O4-C4	-2.61	1.18	1.23
1	S1	2081	PSU	O4-C4	-2.61	1.18	1.23
40	LA	68	PSU	O4-C4	-2.61	1.18	1.23
45	LF	1683	OMG	C5-C6	-2.61	1.42	1.47
47	LH	2887	A2M	O2'-C2'	2.61	1.49	1.42
45	LF	1586	PSU	O4-C4	-2.61	1.18	1.23
48	LI	3500	A2M	O2'-C2'	2.61	1.49	1.42
45	LF	1929	A2M	O2'-C2'	2.61	1.49	1.42
46	LG	2009	OMG	C5-C6	-2.61	1.42	1.47
42	LC	308	PSU	O4-C4	-2.60	1.18	1.23
42	LC	631	OMG	C5-C6	-2.60	1.42	1.47
45	LF	1582	PSU	O4-C4	-2.60	1.18	1.23
46	LG	2146	OMG	C5-C6	-2.60	1.42	1.47
42	LC	567	PSU	O4-C4	-2.60	1.18	1.23
48	LI	3175	PSU	O4-C4	-2.60	1.18	1.23
1	S1	1960	PSU	O4-C4	-2.60	1.18	1.23
1	S1	485	OMG	C5-C6	-2.60	1.42	1.47
47	LH	2679	PSU	O4-C4	-2.60	1.18	1.23
45	LF	1826	OMG	C5-C6	-2.60	1.42	1.47
48	LI	3347	OMC	C2-N1	2.59	1.45	1.40
46	LG	2154	PSU	O4-C4	-2.59	1.18	1.23
1	S1	390	OMG	C5-C6	-2.59	1.42	1.47
44	LE	1266	PSU	O4-C4	-2.58	1.18	1.23
47	LH	2802	PSU	O4-C4	-2.58	1.18	1.23
41	LB	183	A2M	O2'-C2'	2.58	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	LJ	3644	PSU	O4-C4	-2.58	1.18	1.23
1	S1	27	PSU	O4-C4	-2.58	1.18	1.23
40	LA	39	A2M	O2'-C2'	2.58	1.49	1.42
44	LE	1365	PSU	O4-C4	-2.58	1.18	1.23
47	LH	2904	B8H	C2-N3	-2.58	1.33	1.38
47	LH	2610	OMG	C5-C6	-2.58	1.42	1.47
44	LE	1407	PSU	O4-C4	-2.58	1.18	1.23
46	LG	2005	A2M	O2'-C2'	2.58	1.49	1.42
1	S1	2305	PSU	O4-C4	-2.57	1.18	1.23
47	LH	2586	PSU	O4-C4	-2.57	1.18	1.23
1	S1	1715	PSU	O4-C4	-2.57	1.18	1.23
42	LC	302	PSU	O4-C4	-2.57	1.18	1.23
52	LM	3957	OMC	C2-N1	2.57	1.45	1.40
48	LI	3456	5MC	O2-C2	-2.57	1.19	1.23
48	LI	3145	PSU	O4-C4	-2.56	1.18	1.23
44	LE	1208	OMG	C6-N1	-2.56	1.34	1.37
48	LI	3379	OMG	C5-C6	-2.56	1.42	1.47
1	S1	640	PSU	O4-C4	-2.56	1.18	1.23
1	S1	565	A2M	O2'-C2'	2.55	1.49	1.42
44	LE	1118	PSU	O2-C2	-2.55	1.18	1.23
1	S1	280	PSU	O4-C4	-2.55	1.18	1.23
1	S1	28	A2M	O2'-C2'	2.55	1.49	1.42
1	S1	176	PSU	O4-C4	-2.55	1.18	1.23
1	S1	2144	5MC	O2-C2	-2.54	1.19	1.23
53	LN	3969	PSU	O4-C4	-2.53	1.18	1.23
44	LE	1023	PSU	O4-C4	-2.53	1.18	1.23
41	LB	281	PSU	O4-C4	-2.53	1.18	1.23
41	LB	280	PSU	O4-C4	-2.52	1.18	1.23
42	LC	577	OMC	C2-N1	2.52	1.45	1.40
45	LF	1835	OMG	C5-C6	-2.52	1.42	1.47
47	LH	2879	OMG	C5-C6	-2.52	1.42	1.47
48	LI	3542	PSU	O4-C4	-2.52	1.18	1.23
40	LA	74	OMG	C5-C6	-2.51	1.42	1.47
1	S1	1037	OMC	C2-N1	2.51	1.45	1.40
44	LE	1106	A2M	O2'-C2'	2.51	1.49	1.42
48	LI	3412	PSU	O4'-C1'	-2.51	1.40	1.43
47	LH	2776	OMG	C5-C6	-2.50	1.42	1.47
45	LF	1819	OMG	C5-C6	-2.50	1.42	1.47
49	LJ	3644	PSU	O2-C2	-2.50	1.18	1.23
48	LI	3456	5MC	C2-N3	2.49	1.41	1.36
40	LA	68	PSU	O2-C2	-2.49	1.18	1.23
1	S1	641	OMG	C5-C6	-2.49	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	465	PSU	O4-C4	-2.49	1.18	1.23
1	S1	57	OMG	C5-C6	-2.49	1.42	1.47
42	LC	628	OMG	C5-C6	-2.49	1.42	1.47
48	LI	3222	OMC	C2-N1	2.48	1.45	1.40
1	S1	1592	PSU	O2-C2	-2.48	1.18	1.23
1	S1	1549	A2M	O2'-C2'	2.48	1.49	1.42
1	S1	1601	B8N	C6-C5	2.47	1.38	1.34
47	LH	2623	PSU	O2-C2	-2.47	1.18	1.23
45	LF	1883	OMG	C5-C6	-2.47	1.42	1.47
44	LE	1324	OMG	C5-C6	-2.47	1.42	1.47
1	S1	1549	A2M	O5'-C5'	-2.47	1.38	1.44
49	LJ	3701	PSU	O2-C2	-2.46	1.18	1.23
42	LC	483	OMC	C2-N1	2.46	1.45	1.40
48	LI	3434	OMG	C5-C6	-2.46	1.42	1.47
48	LI	2999	PSU	O4-C4	-2.46	1.18	1.23
48	LI	3509	OMG	C5-C6	-2.46	1.42	1.47
44	LE	1217	OMG	C5-C6	-2.46	1.42	1.47
46	LG	2119	PSU	O2-C2	-2.45	1.18	1.23
42	LC	541	OMG	C5-C6	-2.45	1.42	1.47
51	LL	3865	PSU	O4-C4	-2.45	1.18	1.23
47	LH	2870	OMG	C5-C6	-2.45	1.42	1.47
1	S1	1711	PSU	O2-C2	-2.44	1.18	1.23
47	LH	2361	PSU	O2-C2	-2.44	1.18	1.23
48	LI	3377	OMG	C5-C6	-2.43	1.42	1.47
44	LE	1365	PSU	O2-C2	-2.42	1.18	1.23
1	S1	1705	OMG	C5-C6	-2.42	1.42	1.47
48	LI	3042	PSU	O4-C4	-2.42	1.19	1.23
48	LI	3204	PSU	O2-C2	-2.42	1.18	1.23
42	LC	421	PSU	O2-C2	-2.42	1.18	1.23
48	LI	3444	PSU	O2-C2	-2.42	1.18	1.23
46	LG	2125	PSU	O4-C4	-2.42	1.19	1.23
41	LB	215	OMG	C5-C6	-2.42	1.42	1.47
45	LF	1582	PSU	O2-C2	-2.42	1.18	1.23
47	LH	2679	PSU	O2-C2	-2.41	1.18	1.23
49	LJ	3680	PSU	O2-C2	-2.41	1.18	1.23
1	S1	1536	OMG	C5-C6	-2.41	1.42	1.47
46	LG	2125	PSU	O2-C2	-2.40	1.18	1.23
1	S1	2180	A2M	C5-C4	2.40	1.47	1.40
44	LE	1266	PSU	O2-C2	-2.40	1.18	1.23
47	LH	2899	PSU	O2-C2	-2.40	1.18	1.23
1	S1	1371	A2M	O5'-C5'	-2.40	1.38	1.44
49	LJ	3591	PSU	O2-C2	-2.40	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	LH	2904	B8H	C6-C5	2.39	1.38	1.34
44	LE	1126	PSU	O2-C2	-2.39	1.18	1.23
47	LH	2624	PSU	O4'-C1'	-2.39	1.40	1.43
48	LI	3332	PSU	O2-C2	-2.39	1.18	1.23
47	LH	2617	PSU	O2-C2	-2.38	1.18	1.23
46	LG	2171	PSU	O4'-C1'	-2.38	1.40	1.43
44	LE	1075	PSU	O4'-C1'	-2.38	1.40	1.43
1	S1	1378	PSU	O2-C2	-2.38	1.18	1.23
41	LB	234	PSU	O2-C2	-2.38	1.18	1.23
42	LC	480	PSU	O2-C2	-2.38	1.18	1.23
49	LJ	3688	OMG	C5-C6	-2.38	1.42	1.47
1	S1	544	PSU	O2-C2	-2.37	1.18	1.23
47	LH	2914	PSU	O2-C2	-2.37	1.18	1.23
1	S1	1591	PSU	O2-C2	-2.37	1.18	1.23
44	LE	1075	PSU	O2-C2	-2.37	1.18	1.23
47	LH	2754	PSU	O2-C2	-2.37	1.18	1.23
48	LI	3562	PSU	O2-C2	-2.37	1.18	1.23
1	S1	465	PSU	O2-C2	-2.36	1.18	1.23
1	S1	2075	OMG	C5-C6	-2.36	1.42	1.47
44	LE	1260	PSU	O2-C2	-2.36	1.18	1.23
48	LI	3503	PSU	O2-C2	-2.36	1.18	1.23
1	S1	2305	PSU	O2-C2	-2.36	1.18	1.23
48	LI	3206	PSU	O2-C2	-2.36	1.18	1.23
1	S1	1660	PSU	O2-C2	-2.36	1.18	1.23
47	LH	2925	OMG	C5-C6	-2.36	1.42	1.47
45	LF	1876	PSU	O2-C2	-2.36	1.18	1.23
47	LH	2349	A2M	O5'-C5'	-2.35	1.39	1.44
1	S1	27	PSU	O2-C2	-2.35	1.18	1.23
44	LE	1235	PSU	O2-C2	-2.35	1.18	1.23
45	LF	1692	PSU	O2-C2	-2.35	1.18	1.23
44	LE	1184	PSU	O2-C2	-2.35	1.18	1.23
47	LH	2752	PSU	O2-C2	-2.35	1.18	1.23
44	LE	1198	PSU	O2-C2	-2.35	1.18	1.23
47	LH	2814	A2M	O5'-C5'	-2.35	1.39	1.44
47	LH	2915	PSU	O2-C2	-2.35	1.18	1.23
42	LC	567	PSU	O2-C2	-2.34	1.18	1.23
47	LH	2874	PSU	O2-C2	-2.34	1.18	1.23
48	LI	3451	PSU	O2-C2	-2.34	1.18	1.23
1	S1	2131	PSU	O2-C2	-2.34	1.18	1.23
48	LI	3412	PSU	O2-C2	-2.34	1.18	1.23
1	S1	407	A2M	O5'-C5'	-2.34	1.39	1.44
44	LE	1023	PSU	O2-C2	-2.34	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	89	PSU	O2-C2	-2.34	1.18	1.23
1	S1	2101	PSU	O2-C2	-2.33	1.18	1.23
44	LE	1407	PSU	O2-C2	-2.33	1.18	1.23
48	LI	3531	PSU	O2-C2	-2.33	1.18	1.23
1	S1	1393	PSU	O2-C2	-2.33	1.18	1.23
47	LH	2837	PSU	O2-C2	-2.33	1.18	1.23
44	LE	1363	PSU	O2-C2	-2.32	1.18	1.23
1	S1	2129	PSU	O2-C2	-2.32	1.18	1.23
45	LF	1859	PSU	O2-C2	-2.32	1.18	1.23
47	LH	2642	PSU	O2-C2	-2.32	1.18	1.23
42	LC	498	PSU	O2-C2	-2.32	1.18	1.23
44	LE	1222	OMU	C2-N3	-2.32	1.33	1.38
51	LL	3865	PSU	O2-C2	-2.32	1.18	1.23
1	S1	2116	PSU	O2-C2	-2.31	1.18	1.23
48	LI	3175	PSU	O2-C2	-2.31	1.18	1.23
49	LJ	3697	PSU	O2-C2	-2.31	1.18	1.23
1	S1	1960	PSU	O2-C2	-2.31	1.18	1.23
1	S1	1554	PSU	O2-C2	-2.30	1.18	1.23
41	LB	280	PSU	O2-C2	-2.30	1.18	1.23
46	LG	2154	PSU	O2-C2	-2.30	1.18	1.23
44	LE	1222	OMU	C5-C4	-2.30	1.38	1.43
48	LI	3542	PSU	O2-C2	-2.30	1.18	1.23
48	LI	3185	PSU	O2-C2	-2.30	1.18	1.23
45	LF	1568	PSU	O2-C2	-2.30	1.18	1.23
1	S1	2081	PSU	O2-C2	-2.30	1.18	1.23
47	LH	2744	A2M	O3'-C3'	-2.29	1.37	1.43
47	LH	2849	A2M	O5'-C5'	-2.29	1.39	1.44
40	LA	16	PSU	O2-C2	-2.29	1.18	1.23
45	LF	1586	PSU	O2-C2	-2.29	1.18	1.23
47	LH	2586	PSU	O2-C2	-2.29	1.18	1.23
48	LI	3518	5MC	O2-C2	-2.29	1.19	1.23
48	LI	3568	PSU	O2-C2	-2.28	1.18	1.23
47	LH	2742	PSU	O2-C2	-2.28	1.18	1.23
48	LI	3214	6MZ	C5-C4	2.28	1.47	1.40
45	LF	1976	OMC	C2-N1	2.28	1.44	1.40
48	LI	3535	OMC	C2-N1	2.28	1.44	1.40
1	S1	176	PSU	O2-C2	-2.27	1.18	1.23
1	S1	1715	PSU	O2-C2	-2.27	1.18	1.23
48	LI	3315	A2M	O5'-C5'	-2.27	1.39	1.44
47	LH	2842	PSU	O2-C2	-2.27	1.18	1.23
41	LB	281	PSU	O2-C2	-2.27	1.18	1.23
1	S1	105	PSU	O2-C2	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	LE	1171	PSU	O2-C2	-2.27	1.18	1.23
45	LF	1926	PSU	O2-C2	-2.27	1.18	1.23
42	LC	302	PSU	O2-C2	-2.27	1.18	1.23
1	S1	32	PSU	O2-C2	-2.26	1.18	1.23
47	LH	2330	PSU	O2-C2	-2.26	1.18	1.23
1	S1	621	OMC	C2-N1	2.26	1.44	1.40
48	LI	3440	PSU	O2-C2	-2.26	1.18	1.23
47	LH	2636	JMH	C2-N1	2.25	1.41	1.38
45	LF	1815	A2M	O5'-C5'	-2.25	1.39	1.44
1	S1	403	PSU	O2-C2	-2.25	1.18	1.23
1	S1	2065	PSU	O2-C2	-2.25	1.18	1.23
1	S1	280	PSU	O2-C2	-2.24	1.18	1.23
1	S1	1396	PSU	O2-C2	-2.24	1.18	1.23
48	LI	3446	PSU	O2-C2	-2.23	1.18	1.23
47	LH	2348	OMC	C2-N1	2.23	1.44	1.40
1	S1	1068	PSU	O2-C2	-2.23	1.18	1.23
47	LH	2802	PSU	O2-C2	-2.23	1.18	1.23
48	LI	3167	PSU	O2-C2	-2.23	1.18	1.23
1	S1	565	A2M	O5'-C5'	-2.23	1.39	1.44
1	S1	640	PSU	O2-C2	-2.22	1.18	1.23
48	LI	3510	PSU	O2-C2	-2.22	1.18	1.23
1	S1	723	A2M	O5'-C5'	-2.22	1.39	1.44
49	LJ	3680	PSU	O4'-C1'	-2.22	1.40	1.43
48	LI	3145	PSU	O2-C2	-2.22	1.18	1.23
47	LH	2591	PSU	O2-C2	-2.21	1.18	1.23
52	LM	3953	PSU	O2-C2	-2.21	1.18	1.23
1	S1	649	A2M	O5'-C5'	-2.21	1.39	1.44
1	S1	2046	A2M	O5'-C5'	-2.20	1.39	1.44
42	LC	308	PSU	O2-C2	-2.20	1.18	1.23
45	LF	1822	OMC	C2-N1	2.19	1.44	1.40
45	LF	1929	A2M	O5'-C5'	-2.19	1.39	1.44
44	LE	1204	A2M	O5'-C5'	-2.18	1.39	1.44
48	LI	3042	PSU	O2-C2	-2.18	1.18	1.23
47	LH	2853	OMC	C2-N1	2.18	1.44	1.40
1	S1	1624	PSU	O2-C2	-2.18	1.18	1.23
48	LI	2999	PSU	O2-C2	-2.18	1.18	1.23
47	LH	2358	A2M	O5'-C5'	-2.18	1.39	1.44
1	S1	40	A2M	O5'-C5'	-2.17	1.39	1.44
1	S1	28	A2M	O5'-C5'	-2.17	1.39	1.44
52	LM	3963	PSU	O2-C2	-2.17	1.18	1.23
46	LG	2171	PSU	O2-C2	-2.17	1.18	1.23
47	LH	2624	PSU	O2-C2	-2.17	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	LH	2835	OMU	C2-N1	2.16	1.41	1.38
53	LN	3969	PSU	O2-C2	-2.16	1.18	1.23
47	LH	2809	A2M	O5'-C5'	-2.15	1.39	1.44
42	LC	594	A2M	O5'-C5'	-2.15	1.39	1.44
45	LF	1926	PSU	O4'-C1'	-2.14	1.40	1.43
1	S1	2123	OMC	C2-N1	2.14	1.44	1.40
44	LE	935	A2M	O5'-C5'	-2.14	1.39	1.44
51	LL	3906	A2M	C2-N3	2.14	1.35	1.32
47	LH	2744	A2M	O5'-C5'	-2.14	1.39	1.44
46	LG	2005	A2M	O5'-C5'	-2.13	1.39	1.44
1	S1	1601	B8N	O4'-C1'	-2.13	1.40	1.43
47	LH	2769	A2M	O5'-C5'	-2.12	1.39	1.44
44	LE	1121	A2M	O5'-C5'	-2.12	1.39	1.44
48	LI	3500	A2M	O5'-C5'	-2.12	1.39	1.44
45	LF	1856	OMG	C5-C6	-2.12	1.43	1.47
46	LG	2022	A2M	O5'-C5'	-2.12	1.39	1.44
1	S1	121	PSU	C2-N3	-2.12	1.33	1.37
45	LF	1662	OMG	C2-N2	2.12	1.39	1.34
1	S1	1063	A2M	C2-N3	2.11	1.35	1.32
47	LH	2887	A2M	O5'-C5'	-2.11	1.39	1.44
48	LI	3444	PSU	O4'-C1'	-2.11	1.40	1.43
47	LH	2776	OMG	C2-N2	2.10	1.39	1.34
48	LI	3465	OMC	C2-N1	2.10	1.44	1.40
47	LH	2920	A2M	O5'-C5'	-2.10	1.39	1.44
48	LI	3223	OMG	C2-N2	2.10	1.39	1.34
41	LB	183	A2M	O5'-C5'	-2.10	1.39	1.44
47	LH	2621	PSU	O2-C2	-2.09	1.19	1.23
47	LH	2768	A2M	O5'-C5'	-2.08	1.39	1.44
47	LH	2708	A2M	C2-N3	2.08	1.35	1.32
1	S1	533	A2M	O5'-C5'	-2.08	1.39	1.44
47	LH	2313	OMC	C2-N1	2.08	1.44	1.40
45	LF	1738	A2M	O5'-C5'	-2.08	1.39	1.44
45	LF	1502	A2M	O5'-C5'	-2.07	1.39	1.44
1	S1	645	A2M	C2-N3	2.07	1.35	1.32
40	LA	39	A2M	O5'-C5'	-2.07	1.39	1.44
45	LF	1891	A2M	O5'-C5'	-2.07	1.39	1.44
1	S1	110	A2M	O5'-C5'	-2.06	1.39	1.44
1	S1	641	OMG	C2-N2	2.06	1.39	1.34
40	LA	68	PSU	O4'-C1'	-2.06	1.41	1.43
47	LH	2842	PSU	O4'-C1'	-2.05	1.41	1.43
45	LF	1836	OMC	C2-N1	2.05	1.44	1.40
44	LE	1121	A2M	C2-N3	2.05	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	LE	1106	A2M	O5'-C5'	-2.05	1.39	1.44
1	S1	1096	A2M	C2-N3	2.05	1.35	1.32
1	S1	99	OMC	C2-N1	2.04	1.44	1.40
44	LE	1324	OMG	C2-N2	2.04	1.39	1.34
46	LG	2146	OMG	C2-N2	2.04	1.39	1.34
42	LC	631	OMG	C2-N2	2.04	1.39	1.34
52	LM	3957	OMC	C2-N3	2.04	1.40	1.36
48	LI	3367	A2M	O5'-C5'	-2.04	1.39	1.44
1	S1	42	OMG	C2-N2	2.03	1.39	1.34
48	LI	3533	A2M	O5'-C5'	-2.03	1.39	1.44
1	S1	407	A2M	C2-N3	2.03	1.35	1.32
1	S1	2101	PSU	O4'-C1'	-2.02	1.41	1.43
47	LH	2812	A2M	O5'-C5'	-2.02	1.39	1.44
48	LI	3348	A2M	O5'-C5'	-2.02	1.39	1.44
1	S1	180	OMG	C2-N2	2.02	1.39	1.34
44	LE	1312	OMC	C2-N1	2.02	1.44	1.40
48	LI	3451	PSU	O4'-C1'	-2.02	1.41	1.43
48	LI	3374	OMC	C2-N1	2.02	1.44	1.40
47	LH	2768	A2M	C2-N3	2.02	1.35	1.32
45	LF	1883	OMG	C2-N2	2.01	1.39	1.34
1	S1	121	PSU	C2-N1	-2.00	1.34	1.36
45	LF	1856	OMG	C2-N2	2.00	1.39	1.34
45	LF	1888	A2M	C2-N3	2.00	1.35	1.32

All (1210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2288	MA6	N1-C6-N6	-14.51	101.79	117.06
1	S1	2287	MA6	N1-C6-N6	-13.76	102.57	117.06
1	S1	110	A2M	C5-C6-N6	9.57	134.90	120.35
1	S1	565	A2M	C5-C6-N6	9.45	134.72	120.35
47	LH	2809	A2M	C5-C6-N6	9.42	134.66	120.35
46	LG	2005	A2M	C5-C6-N6	9.41	134.66	120.35
48	LI	3521	A2M	C5-C6-N6	9.40	134.64	120.35
1	S1	2046	A2M	C5-C6-N6	9.39	134.62	120.35
47	LH	2814	A2M	C5-C6-N6	9.38	134.61	120.35
45	LF	1502	A2M	C5-C6-N6	9.38	134.61	120.35
1	S1	1549	A2M	C5-C6-N6	9.38	134.60	120.35
47	LH	2358	A2M	C5-C6-N6	9.31	134.50	120.35
47	LH	2887	A2M	C5-C6-N6	9.30	134.49	120.35
40	LA	97	A2M	C5-C6-N6	9.27	134.44	120.35
1	S1	649	A2M	C5-C6-N6	9.26	134.42	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	LI	3348	A2M	C5-C6-N6	9.25	134.41	120.35
1	S1	645	A2M	C5-C6-N6	9.23	134.37	120.35
47	LH	2744	A2M	C5-C6-N6	9.22	134.36	120.35
48	LI	3315	A2M	C5-C6-N6	9.19	134.32	120.35
44	LE	1121	A2M	C5-C6-N6	9.14	134.24	120.35
1	S1	1371	A2M	C5-C6-N6	9.12	134.22	120.35
44	LE	935	A2M	C5-C6-N6	9.11	134.20	120.35
1	S1	28	A2M	C5-C6-N6	9.10	134.18	120.35
44	LE	1204	A2M	C5-C6-N6	9.10	134.18	120.35
47	LH	2769	A2M	C5-C6-N6	9.08	134.15	120.35
45	LF	1738	A2M	C5-C6-N6	9.07	134.14	120.35
47	LH	2849	A2M	C5-C6-N6	9.05	134.10	120.35
48	LI	3367	A2M	C5-C6-N6	9.04	134.10	120.35
47	LH	2768	A2M	C5-C6-N6	9.03	134.08	120.35
45	LF	1815	A2M	C5-C6-N6	9.03	134.08	120.35
1	S1	1063	A2M	C5-C6-N6	9.03	134.07	120.35
44	LE	1039	A2M	C5-C6-N6	9.03	134.07	120.35
1	S1	40	A2M	C5-C6-N6	9.03	134.07	120.35
2	S2	37	MIA	C12-C13-C14	-9.01	109.61	127.14
44	LE	1106	A2M	C5-C6-N6	9.01	134.04	120.35
47	LH	2349	A2M	C5-C6-N6	8.99	134.02	120.35
1	S1	723	A2M	C5-C6-N6	8.96	133.97	120.35
46	LG	2022	A2M	C5-C6-N6	8.95	133.96	120.35
48	LI	3533	A2M	C5-C6-N6	8.95	133.95	120.35
41	LB	183	A2M	C5-C6-N6	8.95	133.95	120.35
1	S1	1900	A2M	C5-C6-N6	8.94	133.94	120.35
47	LH	2708	A2M	C5-C6-N6	8.94	133.93	120.35
45	LF	1929	A2M	C5-C6-N6	8.92	133.91	120.35
45	LF	1891	A2M	C5-C6-N6	8.89	133.85	120.35
47	LH	2812	A2M	C5-C6-N6	8.87	133.83	120.35
45	LF	1888	A2M	C5-C6-N6	8.85	133.79	120.35
47	LH	2920	A2M	C5-C6-N6	8.84	133.78	120.35
42	LC	594	A2M	C5-C6-N6	8.81	133.75	120.35
1	S1	407	A2M	C5-C6-N6	8.81	133.74	120.35
1	S1	1096	A2M	C5-C6-N6	8.80	133.73	120.35
48	LI	3500	A2M	C5-C6-N6	8.79	133.71	120.35
1	S1	533	A2M	C5-C6-N6	8.67	133.53	120.35
40	LA	39	A2M	C5-C6-N6	8.65	133.49	120.35
51	LL	3906	A2M	C5-C6-N6	8.63	133.47	120.35
1	S1	1601	B8N	C31-N3-C4	6.99	127.61	117.31
2	S2	37	MIA	C11-S10-C2	6.68	107.26	102.27
46	LG	2005	A2M	N6-C6-N1	-6.59	104.90	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	LH	2358	A2M	N6-C6-N1	-6.58	104.92	118.57
1	S1	110	A2M	N6-C6-N1	-6.56	104.95	118.57
1	S1	2046	A2M	N6-C6-N1	-6.56	104.97	118.57
47	LH	2769	A2M	N6-C6-N1	-6.53	105.02	118.57
47	LH	2809	A2M	N6-C6-N1	-6.51	105.06	118.57
44	LE	935	A2M	N6-C6-N1	-6.47	105.14	118.57
47	LH	2814	A2M	N6-C6-N1	-6.45	105.18	118.57
48	LI	3348	A2M	N6-C6-N1	-6.44	105.20	118.57
1	S1	1549	A2M	N6-C6-N1	-6.40	105.29	118.57
48	LI	3521	A2M	N6-C6-N1	-6.39	105.30	118.57
45	LF	1502	A2M	N6-C6-N1	-6.39	105.32	118.57
1	S1	645	A2M	N6-C6-N1	-6.38	105.32	118.57
1	S1	1371	A2M	N6-C6-N1	-6.37	105.36	118.57
47	LH	2744	A2M	N6-C6-N1	-6.35	105.38	118.57
1	S1	565	A2M	N6-C6-N1	-6.33	105.43	118.57
48	LI	3315	A2M	N6-C6-N1	-6.33	105.43	118.57
45	LF	1738	A2M	N6-C6-N1	-6.33	105.44	118.57
44	LE	1039	A2M	N6-C6-N1	-6.31	105.48	118.57
44	LE	1121	A2M	N6-C6-N1	-6.30	105.49	118.57
44	LE	1204	A2M	N6-C6-N1	-6.29	105.52	118.57
40	LA	39	A2M	N6-C6-N1	-6.27	105.56	118.57
1	S1	28	A2M	N6-C6-N1	-6.26	105.58	118.57
1	S1	649	A2M	N6-C6-N1	-6.26	105.59	118.57
1	S1	40	A2M	N6-C6-N1	-6.25	105.60	118.57
40	LA	97	A2M	N6-C6-N1	-6.24	105.61	118.57
47	LH	2349	A2M	N6-C6-N1	-6.22	105.66	118.57
47	LH	2768	A2M	N6-C6-N1	-6.22	105.67	118.57
1	S1	407	A2M	N6-C6-N1	-6.20	105.70	118.57
47	LH	2887	A2M	N6-C6-N1	-6.20	105.70	118.57
48	LI	3367	A2M	N6-C6-N1	-6.19	105.72	118.57
47	LH	2920	A2M	N6-C6-N1	-6.18	105.75	118.57
1	S1	1900	A2M	N6-C6-N1	-6.16	105.79	118.57
41	LB	183	A2M	N6-C6-N1	-6.16	105.79	118.57
47	LH	2849	A2M	N6-C6-N1	-6.14	105.83	118.57
47	LH	2708	A2M	N6-C6-N1	-6.12	105.86	118.57
46	LG	2022	A2M	N6-C6-N1	-6.12	105.87	118.57
47	LH	2812	A2M	N6-C6-N1	-6.11	105.88	118.57
45	LF	1891	A2M	N6-C6-N1	-6.11	105.89	118.57
45	LF	1815	A2M	N6-C6-N1	-6.10	105.91	118.57
45	LF	1888	A2M	N6-C6-N1	-6.10	105.92	118.57
1	S1	723	A2M	N6-C6-N1	-6.10	105.92	118.57
48	LI	3533	A2M	N6-C6-N1	-6.08	105.96	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	LE	1106	A2M	N6-C6-N1	-6.07	105.98	118.57
1	S1	1063	A2M	N6-C6-N1	-6.05	106.02	118.57
45	LF	1929	A2M	N6-C6-N1	-6.04	106.04	118.57
47	LH	2887	A2M	N3-C2-N1	-6.01	119.28	128.68
1	S1	1096	A2M	N6-C6-N1	-6.00	106.11	118.57
45	LF	1891	A2M	N3-C2-N1	-5.99	119.32	128.68
1	S1	121	PSU	N1-C2-N3	5.94	121.86	115.13
1	S1	1601	B8N	C4-N3-C2	-5.92	117.97	125.46
48	LI	3500	A2M	N6-C6-N1	-5.90	106.33	118.57
1	S1	2288	MA6	N3-C2-N1	-5.89	119.48	128.68
51	LL	3906	A2M	N6-C6-N1	-5.88	106.36	118.57
1	S1	533	A2M	N6-C6-N1	-5.87	106.39	118.57
42	LC	594	A2M	N6-C6-N1	-5.86	106.42	118.57
44	LE	935	A2M	N3-C2-N1	-5.85	119.53	128.68
45	LF	1502	A2M	N3-C2-N1	-5.83	119.57	128.68
47	LH	2904	B8H	N3-C2-N1	5.81	121.42	115.14
1	S1	2046	A2M	N3-C2-N1	-5.81	119.60	128.68
47	LH	2809	A2M	N3-C2-N1	-5.81	119.60	128.68
47	LH	2744	A2M	N3-C2-N1	-5.77	119.66	128.68
40	LA	97	A2M	N3-C2-N1	-5.76	119.67	128.68
1	S1	1371	A2M	N3-C2-N1	-5.76	119.67	128.68
47	LH	2349	A2M	N3-C2-N1	-5.74	119.70	128.68
48	LI	3367	A2M	N3-C2-N1	-5.71	119.75	128.68
1	S1	723	A2M	N3-C2-N1	-5.71	119.76	128.68
46	LG	2005	A2M	N3-C2-N1	-5.71	119.76	128.68
1	S1	407	A2M	N3-C2-N1	-5.71	119.76	128.68
47	LH	2358	A2M	N3-C2-N1	-5.70	119.78	128.68
1	S1	28	A2M	N3-C2-N1	-5.69	119.79	128.68
48	LI	3500	A2M	N3-C2-N1	-5.69	119.79	128.68
1	S1	645	A2M	N3-C2-N1	-5.68	119.80	128.68
44	LE	1204	A2M	N3-C2-N1	-5.66	119.83	128.68
1	S1	565	A2M	N3-C2-N1	-5.66	119.83	128.68
48	LI	3533	A2M	N3-C2-N1	-5.66	119.83	128.68
44	LE	1039	A2M	N3-C2-N1	-5.63	119.87	128.68
45	LF	1738	A2M	N3-C2-N1	-5.63	119.88	128.68
45	LF	1888	A2M	N3-C2-N1	-5.63	119.88	128.68
1	S1	649	A2M	N3-C2-N1	-5.61	119.90	128.68
1	S1	2287	MA6	N3-C2-N1	-5.60	119.92	128.68
1	S1	1096	A2M	N3-C2-N1	-5.59	119.94	128.68
45	LF	1929	A2M	N3-C2-N1	-5.58	119.95	128.68
44	LE	1121	A2M	N3-C2-N1	-5.58	119.95	128.68
41	LB	183	A2M	N3-C2-N1	-5.57	119.98	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	LH	2920	A2M	N3-C2-N1	-5.56	119.99	128.68
47	LH	2849	A2M	N3-C2-N1	-5.55	120.00	128.68
1	S1	40	A2M	N3-C2-N1	-5.55	120.00	128.68
48	LI	3315	A2M	N3-C2-N1	-5.54	120.02	128.68
1	S1	1900	A2M	N3-C2-N1	-5.52	120.04	128.68
42	LC	594	A2M	N3-C2-N1	-5.52	120.05	128.68
45	LF	1815	A2M	N3-C2-N1	-5.51	120.07	128.68
47	LH	2812	A2M	N3-C2-N1	-5.50	120.08	128.68
47	LH	2708	A2M	N3-C2-N1	-5.49	120.10	128.68
47	LH	2814	A2M	N3-C2-N1	-5.48	120.12	128.68
51	LL	3906	A2M	N3-C2-N1	-5.47	120.12	128.68
48	LI	3521	A2M	N3-C2-N1	-5.47	120.13	128.68
47	LH	2746	PSU	N1-C2-N3	5.47	121.32	115.13
48	LI	3214	6MZ	C2-N1-C6	5.45	121.26	116.59
1	S1	110	A2M	N3-C2-N1	-5.43	120.19	128.68
47	LH	2746	PSU	C4-N3-C2	-5.41	118.55	126.34
46	LG	2022	A2M	N3-C2-N1	-5.40	120.24	128.68
47	LH	2768	A2M	N3-C2-N1	-5.38	120.27	128.68
44	LE	1106	A2M	N3-C2-N1	-5.38	120.28	128.68
48	LI	3348	A2M	N3-C2-N1	-5.36	120.30	128.68
47	LH	2769	A2M	N3-C2-N1	-5.33	120.34	128.68
1	S1	1549	A2M	N3-C2-N1	-5.33	120.34	128.68
1	S1	1063	A2M	N3-C2-N1	-5.32	120.37	128.68
40	LA	39	A2M	N3-C2-N1	-5.25	120.47	128.68
1	S1	533	A2M	N3-C2-N1	-5.22	120.51	128.68
47	LH	2904	B8H	C4-N3-C2	-5.15	120.68	127.35
44	LE	1118	PSU	C4-N3-C2	-5.08	119.03	126.34
1	S1	1592	PSU	C4-N3-C2	-5.00	119.13	126.34
44	LE	1222	OMU	C1'-N1-C2	5.00	126.62	117.57
48	LI	3214	6MZ	C9-N6-C6	-4.94	118.61	122.87
46	LG	2119	PSU	C4-N3-C2	-4.93	119.23	126.34
1	S1	2131	PSU	C4-N3-C2	-4.92	119.25	126.34
40	LA	68	PSU	N1-C2-N3	4.87	120.64	115.13
47	LH	2642	PSU	C4-N3-C2	-4.87	119.33	126.34
48	LI	3332	PSU	C4-N3-C2	-4.85	119.35	126.34
49	LJ	3644	PSU	C4-N3-C2	-4.85	119.35	126.34
45	LF	1876	PSU	C4-N3-C2	-4.83	119.38	126.34
48	LI	3206	PSU	C4-N3-C2	-4.81	119.41	126.34
44	LE	1260	PSU	C4-N3-C2	-4.81	119.42	126.34
47	LH	2874	PSU	C4-N3-C2	-4.79	119.44	126.34
48	LI	3451	PSU	C4-N3-C2	-4.79	119.44	126.34
51	LL	3865	PSU	C4-N3-C2	-4.78	119.45	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	LJ	3680	PSU	N1-C2-N3	4.78	120.55	115.13
48	LI	3444	PSU	C4-N3-C2	-4.78	119.46	126.34
48	LI	3145	PSU	C4-N3-C2	-4.77	119.46	126.34
47	LH	2617	PSU	C4-N3-C2	-4.77	119.47	126.34
48	LI	3185	PSU	C4-N3-C2	-4.76	119.47	126.34
47	LH	2742	PSU	C4-N3-C2	-4.76	119.48	126.34
48	LI	3175	PSU	C4-N3-C2	-4.75	119.49	126.34
42	LC	480	PSU	C4-N3-C2	-4.74	119.52	126.34
48	LI	3542	PSU	C4-N3-C2	-4.73	119.52	126.34
1	S1	544	PSU	C4-N3-C2	-4.73	119.53	126.34
47	LH	2837	PSU	C4-N3-C2	-4.73	119.53	126.34
1	S1	1660	PSU	C4-N3-C2	-4.73	119.53	126.34
47	LH	2621	PSU	C4-N3-C2	-4.72	119.53	126.34
44	LE	1407	PSU	C4-N3-C2	-4.72	119.54	126.34
49	LJ	3591	PSU	C4-N3-C2	-4.71	119.56	126.34
1	S1	105	PSU	C4-N3-C2	-4.70	119.56	126.34
1	S1	1396	PSU	C4-N3-C2	-4.70	119.57	126.34
40	LA	16	PSU	C4-N3-C2	-4.70	119.57	126.34
1	S1	1393	PSU	C4-N3-C2	-4.69	119.58	126.34
42	LC	308	PSU	C4-N3-C2	-4.68	119.59	126.34
48	LI	2999	PSU	C4-N3-C2	-4.68	119.60	126.34
44	LE	1260	PSU	N1-C2-N3	4.68	120.43	115.13
42	LC	498	PSU	C4-N3-C2	-4.68	119.60	126.34
48	LI	3510	PSU	C4-N3-C2	-4.67	119.61	126.34
48	LI	3446	PSU	C4-N3-C2	-4.67	119.61	126.34
42	LC	302	PSU	C4-N3-C2	-4.67	119.61	126.34
47	LH	2899	PSU	C4-N3-C2	-4.67	119.61	126.34
48	LI	3503	PSU	C4-N3-C2	-4.67	119.62	126.34
52	LM	3963	PSU	C4-N3-C2	-4.67	119.62	126.34
47	LH	2914	PSU	C4-N3-C2	-4.66	119.62	126.34
47	LH	2679	PSU	C4-N3-C2	-4.64	119.65	126.34
1	S1	1378	PSU	C4-N3-C2	-4.64	119.65	126.34
48	LI	3531	PSU	C4-N3-C2	-4.64	119.65	126.34
47	LH	2330	PSU	C4-N3-C2	-4.64	119.66	126.34
49	LJ	3701	PSU	C4-N3-C2	-4.64	119.66	126.34
48	LI	3412	PSU	C4-N3-C2	-4.63	119.67	126.34
49	LJ	3697	PSU	C4-N3-C2	-4.63	119.67	126.34
44	LE	1365	PSU	C4-N3-C2	-4.63	119.67	126.34
49	LJ	3680	PSU	C4-N3-C2	-4.63	119.67	126.34
45	LF	1586	PSU	C4-N3-C2	-4.63	119.67	126.34
1	S1	544	PSU	N1-C2-N3	4.62	120.37	115.13
48	LI	3562	PSU	N1-C2-N3	4.62	120.36	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	LH	2623	PSU	C4-N3-C2	-4.62	119.68	126.34
44	LE	1126	PSU	C4-N3-C2	-4.62	119.68	126.34
45	LF	1582	PSU	C4-N3-C2	-4.62	119.68	126.34
45	LF	1692	PSU	C4-N3-C2	-4.62	119.69	126.34
48	LI	3412	PSU	N1-C2-N3	4.61	120.36	115.13
40	LA	68	PSU	C4-N3-C2	-4.61	119.70	126.34
49	LJ	3644	PSU	N1-C2-N3	4.60	120.35	115.13
1	S1	2065	PSU	C4-N3-C2	-4.60	119.71	126.34
47	LH	2754	PSU	C4-N3-C2	-4.60	119.71	126.34
1	S1	2129	PSU	C4-N3-C2	-4.60	119.71	126.34
46	LG	2119	PSU	N1-C2-N3	4.60	120.34	115.13
1	S1	280	PSU	C4-N3-C2	-4.59	119.72	126.34
1	S1	1591	PSU	C4-N3-C2	-4.59	119.73	126.34
1	S1	2081	PSU	C4-N3-C2	-4.59	119.73	126.34
47	LH	2874	PSU	N1-C2-N3	4.59	120.33	115.13
45	LF	1859	PSU	C4-N3-C2	-4.59	119.73	126.34
47	LH	2802	PSU	C4-N3-C2	-4.59	119.73	126.34
1	S1	176	PSU	C4-N3-C2	-4.59	119.73	126.34
47	LH	2636	JMH	C1'-N1-C2	4.58	124.72	116.99
46	LG	2154	PSU	C4-N3-C2	-4.58	119.75	126.34
47	LH	2361	PSU	C4-N3-C2	-4.57	119.75	126.34
47	LH	2586	PSU	C4-N3-C2	-4.56	119.76	126.34
1	S1	465	PSU	N1-C2-N3	4.56	120.30	115.13
1	S1	32	PSU	C4-N3-C2	-4.56	119.77	126.34
1	S1	1554	PSU	C4-N3-C2	-4.56	119.77	126.34
47	LH	2624	PSU	C4-N3-C2	-4.56	119.77	126.34
48	LI	3042	PSU	C4-N3-C2	-4.56	119.77	126.34
1	S1	1960	PSU	C4-N3-C2	-4.56	119.78	126.34
52	LM	3953	PSU	C4-N3-C2	-4.55	119.78	126.34
47	LH	2915	PSU	C4-N3-C2	-4.55	119.78	126.34
42	LC	480	PSU	N1-C2-N3	4.55	120.29	115.13
46	LG	2125	PSU	C4-N3-C2	-4.55	119.78	126.34
48	LI	3562	PSU	C4-N3-C2	-4.55	119.79	126.34
47	LH	2623	PSU	N1-C2-N3	4.55	120.28	115.13
1	S1	403	PSU	C4-N3-C2	-4.54	119.80	126.34
48	LI	3440	PSU	C4-N3-C2	-4.54	119.80	126.34
1	S1	1068	PSU	C4-N3-C2	-4.54	119.80	126.34
47	LH	2752	PSU	C4-N3-C2	-4.54	119.80	126.34
45	LF	1926	PSU	C4-N3-C2	-4.53	119.81	126.34
1	S1	465	PSU	C4-N3-C2	-4.53	119.81	126.34
44	LE	1363	PSU	C4-N3-C2	-4.53	119.81	126.34
44	LE	1198	PSU	C4-N3-C2	-4.53	119.81	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	LE	1171	PSU	C4-N3-C2	-4.52	119.83	126.34
47	LH	2591	PSU	C4-N3-C2	-4.52	119.83	126.34
1	S1	89	PSU	C4-N3-C2	-4.51	119.85	126.34
41	LB	280	PSU	C4-N3-C2	-4.51	119.85	126.34
45	LF	1568	PSU	C4-N3-C2	-4.50	119.85	126.34
48	LI	2999	PSU	N1-C2-N3	4.50	120.23	115.13
48	LI	3167	PSU	C4-N3-C2	-4.50	119.86	126.34
44	LE	1126	PSU	N1-C2-N3	4.49	120.22	115.13
1	S1	27	PSU	C4-N3-C2	-4.49	119.88	126.34
49	LJ	3680	PSU	C6-C5-C4	4.48	121.33	118.20
47	LH	2361	PSU	N1-C2-N3	4.48	120.21	115.13
1	S1	1393	PSU	N1-C2-N3	4.48	120.20	115.13
1	S1	1715	PSU	C4-N3-C2	-4.48	119.89	126.34
1	S1	1660	PSU	N1-C2-N3	4.48	120.20	115.13
48	LI	3568	PSU	C4-N3-C2	-4.47	119.90	126.34
51	LL	3865	PSU	N1-C2-N3	4.47	120.19	115.13
47	LH	2752	PSU	N1-C2-N3	4.46	120.19	115.13
44	LE	1266	PSU	C4-N3-C2	-4.45	119.92	126.34
42	LC	302	PSU	N1-C2-N3	4.45	120.17	115.13
44	LE	1023	PSU	N1-C2-N3	4.45	120.17	115.13
48	LI	3451	PSU	N1-C2-N3	4.44	120.16	115.13
42	LC	567	PSU	C4-N3-C2	-4.44	119.95	126.34
48	LI	3204	PSU	C4-N3-C2	-4.43	119.95	126.34
47	LH	2617	PSU	N1-C2-N3	4.43	120.15	115.13
49	LJ	3697	PSU	N1-C2-N3	4.43	120.15	115.13
1	S1	1378	PSU	N1-C2-N3	4.41	120.13	115.13
1	S1	2081	PSU	N1-C2-N3	4.41	120.13	115.13
44	LE	1023	PSU	C4-N3-C2	-4.41	119.98	126.34
48	LI	3510	PSU	N1-C2-N3	4.41	120.12	115.13
47	LH	2754	PSU	N1-C2-N3	4.41	120.12	115.13
48	LI	3145	PSU	N1-C2-N3	4.41	120.12	115.13
1	S1	1711	PSU	N1-C2-N3	4.41	120.12	115.13
40	LA	16	PSU	N1-C2-N3	4.41	120.12	115.13
48	LI	3531	PSU	N1-C2-N3	4.39	120.11	115.13
41	LB	234	PSU	C4-N3-C2	-4.39	120.01	126.34
44	LE	1235	PSU	C4-N3-C2	-4.39	120.01	126.34
48	LI	3175	PSU	N1-C2-N3	4.39	120.11	115.13
49	LJ	3701	PSU	N1-C2-N3	4.39	120.10	115.13
48	LI	3206	PSU	N1-C2-N3	4.38	120.09	115.13
46	LG	2171	PSU	C4-N3-C2	-4.38	120.03	126.34
45	LF	1586	PSU	N1-C2-N3	4.38	120.09	115.13
42	LC	421	PSU	C4-N3-C2	-4.38	120.03	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	LH	2914	PSU	N1-C2-N3	4.38	120.09	115.13
1	S1	2305	PSU	C4-N3-C2	-4.37	120.04	126.34
1	S1	640	PSU	C4-N3-C2	-4.37	120.05	126.34
2	S2	37	MIA	C15-C14-C13	-4.37	110.03	122.65
1	S1	1592	PSU	N1-C2-N3	4.35	120.06	115.13
46	LG	2125	PSU	N1-C2-N3	4.35	120.06	115.13
1	S1	1711	PSU	C4-N3-C2	-4.35	120.08	126.34
44	LE	1118	PSU	N1-C2-N3	4.34	120.05	115.13
47	LH	2899	PSU	N1-C2-N3	4.34	120.05	115.13
48	LI	3332	PSU	N1-C2-N3	4.34	120.05	115.13
1	S1	2065	PSU	N1-C2-N3	4.34	120.04	115.13
44	LE	1363	PSU	N1-C2-N3	4.32	120.03	115.13
49	LJ	3591	PSU	N1-C2-N3	4.32	120.03	115.13
1	S1	89	PSU	N1-C2-N3	4.32	120.03	115.13
1	S1	1396	PSU	N1-C2-N3	4.32	120.03	115.13
44	LE	1266	PSU	N1-C2-N3	4.32	120.03	115.13
44	LE	1075	PSU	C4-N3-C2	-4.32	120.11	126.34
48	LI	3503	PSU	N1-C2-N3	4.32	120.02	115.13
1	S1	1624	PSU	C4-N3-C2	-4.32	120.12	126.34
1	S1	1960	PSU	N1-C2-N3	4.32	120.02	115.13
44	LE	1198	PSU	N1-C2-N3	4.31	120.02	115.13
42	LC	308	PSU	N1-C2-N3	4.30	120.00	115.13
2	S2	37	MIA	C16-C14-C13	-4.30	110.22	122.65
47	LH	2842	PSU	C4-N3-C2	-4.30	120.15	126.34
1	S1	2116	PSU	C4-N3-C2	-4.30	120.15	126.34
48	LI	3542	PSU	N1-C2-N3	4.29	119.99	115.13
48	LI	3444	PSU	N1-C2-N3	4.28	119.98	115.13
45	LF	1582	PSU	N1-C2-N3	4.28	119.98	115.13
1	S1	280	PSU	N1-C2-N3	4.27	119.97	115.13
1	S1	2131	PSU	N1-C2-N3	4.27	119.97	115.13
1	S1	176	PSU	N1-C2-N3	4.26	119.96	115.13
48	LI	3185	PSU	N1-C2-N3	4.26	119.96	115.13
44	LE	1075	PSU	N1-C2-N3	4.26	119.95	115.13
42	LC	567	PSU	N1-C2-N3	4.26	119.95	115.13
44	LE	1407	PSU	N1-C2-N3	4.24	119.94	115.13
1	S1	105	PSU	N1-C2-N3	4.24	119.94	115.13
42	LC	498	PSU	N1-C2-N3	4.24	119.94	115.13
47	LH	2679	PSU	N1-C2-N3	4.24	119.93	115.13
47	LH	2642	PSU	N1-C2-N3	4.23	119.93	115.13
48	LI	3440	PSU	N1-C2-N3	4.22	119.91	115.13
45	LF	1692	PSU	N1-C2-N3	4.22	119.91	115.13
1	S1	2101	PSU	C4-N3-C2	-4.22	120.27	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	LE	1184	PSU	C4-N3-C2	-4.21	120.27	126.34
46	LG	2154	PSU	N1-C2-N3	4.21	119.90	115.13
1	S1	32	PSU	N1-C2-N3	4.21	119.90	115.13
1	S1	27	PSU	N1-C2-N3	4.21	119.90	115.13
44	LE	1365	PSU	N1-C2-N3	4.21	119.90	115.13
53	LN	3969	PSU	C4-N3-C2	-4.21	120.28	126.34
48	LI	3042	PSU	N1-C2-N3	4.20	119.89	115.13
1	S1	1715	PSU	N1-C2-N3	4.20	119.89	115.13
45	LF	1859	PSU	N1-C2-N3	4.20	119.89	115.13
45	LF	1876	PSU	N1-C2-N3	4.18	119.87	115.13
47	LH	2915	PSU	N1-C2-N3	4.18	119.87	115.13
47	LH	2837	PSU	N1-C2-N3	4.18	119.86	115.13
48	LI	3167	PSU	N1-C2-N3	4.18	119.86	115.13
41	LB	280	PSU	N1-C2-N3	4.17	119.86	115.13
52	LM	3953	PSU	N1-C2-N3	4.17	119.85	115.13
47	LH	2591	PSU	N1-C2-N3	4.14	119.82	115.13
48	LI	3204	PSU	N1-C2-N3	4.14	119.82	115.13
44	LE	1184	PSU	N1-C2-N3	4.14	119.81	115.13
41	LB	281	PSU	C4-N3-C2	-4.13	120.39	126.34
1	S1	2129	PSU	N1-C2-N3	4.12	119.80	115.13
45	LF	1926	PSU	N1-C2-N3	4.12	119.80	115.13
1	S1	1068	PSU	N1-C2-N3	4.12	119.80	115.13
44	LE	1235	PSU	N1-C2-N3	4.11	119.79	115.13
52	LM	3963	PSU	N1-C2-N3	4.11	119.79	115.13
41	LB	281	PSU	N1-C2-N3	4.09	119.77	115.13
1	S1	2305	PSU	N1-C2-N3	4.09	119.76	115.13
48	LI	3568	PSU	N1-C2-N3	4.09	119.76	115.13
45	LF	1568	PSU	N1-C2-N3	4.08	119.75	115.13
41	LB	234	PSU	N1-C2-N3	4.07	119.74	115.13
47	LH	2842	PSU	N1-C2-N3	4.07	119.74	115.13
44	LE	1260	PSU	C6-C5-C4	4.07	121.04	118.20
44	LE	1171	PSU	N1-C2-N3	4.07	119.74	115.13
47	LH	2742	PSU	N1-C2-N3	4.07	119.74	115.13
48	LI	3446	PSU	N1-C2-N3	4.05	119.72	115.13
1	S1	1624	PSU	N1-C2-N3	4.03	119.70	115.13
46	LG	2171	PSU	N1-C2-N3	4.02	119.69	115.13
47	LH	2586	PSU	N1-C2-N3	4.02	119.68	115.13
42	LC	541	OMG	O6-C6-N1	-4.00	115.93	120.65
47	LH	2330	PSU	N1-C2-N3	3.96	119.61	115.13
47	LH	2802	PSU	N1-C2-N3	3.93	119.59	115.13
1	S1	2116	PSU	N1-C2-N3	3.92	119.57	115.13
42	LC	421	PSU	N1-C2-N3	3.92	119.57	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2101	PSU	N1-C2-N3	3.91	119.56	115.13
53	LN	3969	PSU	N1-C2-N3	3.90	119.55	115.13
47	LH	2621	PSU	N1-C2-N3	3.89	119.53	115.13
1	S1	1591	PSU	N1-C2-N3	3.87	119.51	115.13
40	LA	68	PSU	C6-C5-C4	3.84	120.88	118.20
1	S1	1554	PSU	N1-C2-N3	3.83	119.47	115.13
1	S1	640	PSU	N1-C2-N3	3.81	119.44	115.13
1	S1	403	PSU	N1-C2-N3	3.79	119.43	115.13
1	S1	121	PSU	C4-N3-C2	-3.79	120.88	126.34
1	S1	1601	B8N	N3-C2-N1	3.79	122.11	116.76
48	LI	3401	OMG	O6-C6-N1	-3.73	116.24	120.65
44	LE	1023	PSU	C6-N1-C2	-3.73	118.87	122.68
47	LH	2624	PSU	N1-C2-N3	3.73	119.35	115.13
45	LF	1835	OMG	O6-C6-N1	-3.73	116.25	120.65
1	S1	1536	OMG	O6-C6-N1	-3.70	116.28	120.65
1	S1	1711	PSU	C6-N1-C2	-3.70	118.90	122.68
49	LJ	3688	OMG	O6-C6-N1	-3.67	116.32	120.65
44	LE	1222	OMU	N3-C2-N1	3.66	119.75	114.89
47	LH	2610	OMG	O6-C6-N1	-3.63	116.36	120.65
1	S1	180	OMG	O6-C6-C5	3.62	131.44	124.37
42	LC	541	OMG	O6-C6-C5	3.60	131.41	124.37
44	LE	1198	PSU	C6-C5-C4	3.59	120.71	118.20
2	S2	37	MIA	N3-C2-N1	-3.59	120.37	126.98
44	LE	1266	PSU	C6-C5-C4	3.59	120.71	118.20
44	LE	1235	PSU	C6-N1-C2	-3.58	119.02	122.68
44	LE	1222	OMU	C4-N3-C2	-3.57	121.87	126.58
47	LH	2754	PSU	C6-C5-C4	3.57	120.69	118.20
44	LE	1184	PSU	C6-N1-C2	-3.57	119.03	122.68
48	LI	2999	PSU	C6-C5-C4	3.56	120.69	118.20
49	LJ	3680	PSU	C6-N1-C2	-3.56	119.04	122.68
48	LI	3562	PSU	C6-N1-C2	-3.56	119.05	122.68
1	S1	57	OMG	O6-C6-N1	-3.56	116.45	120.65
45	LF	1819	OMG	O6-C6-N1	-3.55	116.46	120.65
48	LI	3503	PSU	C6-C5-C4	3.54	120.67	118.20
48	LI	3377	OMG	O6-C6-N1	-3.53	116.48	120.65
48	LI	3444	PSU	C6-C5-C4	3.52	120.66	118.20
1	S1	1705	OMG	O6-C6-N1	-3.52	116.49	120.65
48	LI	3379	OMG	O6-C6-N1	-3.50	116.52	120.65
1	S1	1536	OMG	O6-C6-C5	3.50	131.20	124.37
49	LJ	3688	OMG	O6-C6-C5	3.50	131.20	124.37
40	LA	68	PSU	C6-N1-C2	-3.50	119.11	122.68
47	LH	2623	PSU	C6-N1-C2	-3.50	119.11	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2081	PSU	C6-C5-C4	3.49	120.64	118.20
48	LI	3518	5MC	C5-C4-N3	3.48	125.43	121.67
47	LH	2361	PSU	C6-N1-C2	-3.48	119.12	122.68
1	S1	1396	PSU	C6-C5-C4	3.48	120.63	118.20
44	LE	1171	PSU	C6-C5-C4	3.48	120.63	118.20
47	LH	2904	B8H	O2-C2-N1	-3.46	118.97	122.87
45	LF	1667	OMG	O6-C6-N1	-3.46	116.56	120.65
48	LI	3377	OMG	O6-C6-C5	3.46	131.13	124.37
1	S1	465	PSU	C6-C5-C4	3.46	120.62	118.20
48	LI	3401	OMG	O6-C6-C5	3.46	131.13	124.37
48	LI	3509	OMG	O6-C6-C5	3.45	131.12	124.37
47	LH	2617	PSU	C6-C5-C4	3.45	120.61	118.20
45	LF	1856	OMG	O6-C6-C5	3.44	131.09	124.37
47	LH	2842	PSU	C6-N1-C2	-3.43	119.17	122.68
41	LB	215	OMG	O6-C6-C5	3.43	131.07	124.37
48	LI	3412	PSU	C6-N1-C2	-3.43	119.18	122.68
46	LG	2146	OMG	O6-C6-C5	3.43	131.06	124.37
49	LJ	3644	PSU	C6-C5-C4	3.43	120.59	118.20
44	LE	1104	OMG	O6-C6-C5	3.42	131.05	124.37
46	LG	2171	PSU	C6-N1-C2	-3.42	119.19	122.68
45	LF	1856	OMG	O6-C6-N1	-3.42	116.61	120.65
47	LH	2752	PSU	C6-N1-C2	-3.41	119.19	122.68
1	S1	1705	OMG	O6-C6-C5	3.41	131.03	124.37
1	S1	121	PSU	O2-C2-N1	-3.41	119.03	122.79
41	LB	215	OMG	O6-C6-N1	-3.41	116.62	120.65
1	S1	57	OMG	O6-C6-C5	3.41	131.03	124.37
47	LH	2766	5MC	C5-C4-N3	3.41	125.35	121.67
47	LH	2870	OMG	O6-C6-C5	3.40	131.02	124.37
47	LH	2870	OMG	O6-C6-N1	-3.40	116.63	120.65
48	LI	3451	PSU	C6-C5-C4	3.40	120.58	118.20
51	LL	3865	PSU	C6-C5-C4	3.40	120.58	118.20
42	LC	631	OMG	O6-C6-N1	-3.39	116.64	120.65
1	S1	465	PSU	C6-N1-C2	-3.39	119.21	122.68
47	LH	2925	OMG	O6-C6-C5	3.39	130.99	124.37
47	LH	2879	OMG	O6-C6-C5	3.39	130.99	124.37
1	S1	2075	OMG	O6-C6-C5	3.38	130.97	124.37
44	LE	1201	OMG	O6-C6-C5	3.38	130.97	124.37
48	LI	3145	PSU	C6-C5-C4	3.38	120.56	118.20
1	S1	1711	PSU	C6-C5-C4	3.37	120.55	118.20
46	LG	2146	OMG	O6-C6-N1	-3.36	116.68	120.65
48	LI	3434	OMG	O6-C6-C5	3.35	130.92	124.37
41	LB	281	PSU	C6-N1-C2	-3.35	119.26	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	LJ	3701	PSU	C6-N1-C2	-3.34	119.26	122.68
42	LC	480	PSU	C6-C5-C4	3.34	120.53	118.20
42	LC	628	OMG	O6-C6-C5	3.34	130.90	124.37
1	S1	1960	PSU	C6-N1-C2	-3.34	119.27	122.68
1	S1	2101	PSU	C6-N1-C2	-3.34	119.27	122.68
45	LF	1683	OMG	O6-C6-C5	3.34	130.89	124.37
45	LF	1883	OMG	O6-C6-C5	3.33	130.88	124.37
45	LF	1819	OMG	O6-C6-C5	3.33	130.87	124.37
1	S1	1393	PSU	C6-N1-C2	-3.33	119.28	122.68
48	LI	3504	OMG	O6-C6-C5	3.32	130.86	124.37
1	S1	32	PSU	C6-N1-C2	-3.32	119.29	122.68
47	LH	2746	PSU	C6-N1-C2	-3.32	119.29	122.68
48	LI	3434	OMG	O6-C6-N1	-3.32	116.73	120.65
44	LE	1266	PSU	C6-N1-C2	-3.32	119.29	122.68
40	LA	74	OMG	O6-C6-C5	3.31	130.83	124.37
42	LC	421	PSU	C6-N1-C2	-3.31	119.30	122.68
45	LF	1667	OMG	O6-C6-C5	3.31	130.83	124.37
48	LI	3379	OMG	O6-C6-C5	3.30	130.82	124.37
1	S1	42	OMG	O6-C6-C5	3.30	130.82	124.37
1	S1	1901	OMG	O6-C6-C5	3.30	130.82	124.37
44	LE	1222	OMU	C5-C4-N3	3.30	119.77	114.84
1	S1	641	OMG	O6-C6-C5	3.30	130.81	124.37
48	LI	3562	PSU	C6-C5-C4	3.29	120.50	118.20
1	S1	390	OMG	O6-C6-N1	-3.29	116.76	120.65
1	S1	2065	PSU	C6-N1-C2	-3.29	119.32	122.68
47	LH	2883	OMG	O6-C6-C5	3.29	130.79	124.37
47	LH	2754	PSU	C6-N1-C2	-3.28	119.33	122.68
48	LI	3531	PSU	C6-C5-C4	3.28	120.49	118.20
1	S1	2180	A2M	N3-C2-N1	-3.28	123.55	128.68
47	LH	2897	OMG	O6-C6-C5	3.28	130.77	124.37
1	S1	1660	PSU	C6-N1-C2	-3.27	119.34	122.68
45	LF	1586	PSU	C6-C5-C4	3.27	120.49	118.20
1	S1	485	OMG	O6-C6-C5	3.27	130.75	124.37
45	LF	1883	OMG	O6-C6-N1	-3.26	116.80	120.65
45	LF	1662	OMG	O6-C6-C5	3.26	130.75	124.37
1	S1	544	PSU	C6-N1-C2	-3.26	119.35	122.68
44	LE	1363	PSU	C6-N1-C2	-3.26	119.35	122.68
45	LF	1662	OMG	O6-C6-N1	-3.26	116.80	120.65
48	LI	3167	PSU	C6-N1-C2	-3.26	119.35	122.68
45	LF	1835	OMG	O6-C6-C5	3.26	130.73	124.37
48	LI	3042	PSU	C6-C5-C4	3.25	120.47	118.20
48	LI	3531	PSU	C6-N1-C2	-3.25	119.36	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	LI	3191	OMG	O6-C6-C5	3.25	130.72	124.37
44	LE	1324	OMG	O6-C6-C5	3.25	130.72	124.37
48	LI	3175	PSU	C6-C5-C4	3.25	120.47	118.20
47	LH	2610	OMG	O6-C6-C5	3.25	130.71	124.37
42	LC	302	PSU	C6-C5-C4	3.24	120.46	118.20
1	S1	2075	OMG	O6-C6-N1	-3.24	116.83	120.65
48	LI	3509	OMG	O6-C6-N1	-3.23	116.83	120.65
1	S1	682	OMU	CM2-O2'-C2'	-3.23	106.04	114.52
45	LF	1586	PSU	C6-N1-C2	-3.23	119.38	122.68
44	LE	1217	OMG	O6-C6-N1	-3.23	116.83	120.65
47	LH	2879	OMG	O6-C6-N1	-3.23	116.83	120.65
44	LE	1260	PSU	C6-N1-C2	-3.23	119.38	122.68
1	S1	89	PSU	C6-N1-C2	-3.23	119.38	122.68
45	LF	1956	OMG	O6-C6-N1	-3.23	116.84	120.65
42	LC	480	PSU	C6-N1-C2	-3.22	119.39	122.68
1	S1	390	OMG	O6-C6-C5	3.22	130.66	124.37
44	LE	1104	OMG	O6-C6-N1	-3.22	116.84	120.65
42	LC	631	OMG	O6-C6-C5	3.22	130.66	124.37
42	LC	628	OMG	O6-C6-N1	-3.22	116.85	120.65
1	S1	1396	PSU	C6-N1-C2	-3.22	119.39	122.68
47	LH	2925	OMG	O6-C6-N1	-3.22	116.85	120.65
45	LF	1956	OMG	O6-C6-C5	3.22	130.66	124.37
47	LH	2776	OMG	O6-C6-N1	-3.22	116.85	120.65
42	LC	308	PSU	C6-C5-C4	3.22	120.45	118.20
47	LH	2899	PSU	C6-N1-C2	-3.22	119.39	122.68
45	LF	1683	OMG	O6-C6-N1	-3.22	116.85	120.65
44	LE	1201	OMG	O6-C6-N1	-3.21	116.86	120.65
46	LG	2125	PSU	C6-C5-C4	3.20	120.44	118.20
1	S1	1624	PSU	C6-N1-C2	-3.19	119.42	122.68
48	LI	3187	OMG	O6-C6-C5	3.19	130.61	124.37
45	LF	1859	PSU	C6-N1-C2	-3.19	119.42	122.68
48	LI	3175	PSU	C6-N1-C2	-3.19	119.42	122.68
48	LI	3542	PSU	C6-C5-C4	3.19	120.43	118.20
1	S1	27	PSU	C6-N1-C2	-3.19	119.42	122.68
47	LH	2874	PSU	C6-N1-C2	-3.19	119.42	122.68
47	LH	2874	PSU	C6-C5-C4	3.19	120.43	118.20
47	LH	2883	OMG	O6-C6-N1	-3.18	116.89	120.65
1	S1	1901	OMG	O6-C6-N1	-3.18	116.89	120.65
44	LE	1217	OMG	O6-C6-C5	3.18	130.59	124.37
47	LH	2623	PSU	C6-C5-C4	3.18	120.42	118.20
1	S1	2081	PSU	C6-N1-C2	-3.18	119.43	122.68
48	LI	3440	PSU	C6-C5-C4	3.18	120.42	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	1378	PSU	C6-N1-C2	-3.17	119.44	122.68
1	S1	1681	OMG	O6-C6-C5	3.17	130.57	124.37
44	LE	1365	PSU	C6-C5-C4	3.17	120.42	118.20
45	LF	1826	OMG	O6-C6-C5	3.16	130.55	124.37
1	S1	1715	PSU	C6-N1-C2	-3.16	119.45	122.68
48	LI	3222	OMC	C5-C4-N3	3.16	126.71	121.33
1	S1	280	PSU	C6-N1-C2	-3.16	119.45	122.68
47	LH	2897	OMG	O6-C6-N1	-3.16	116.92	120.65
45	LF	1826	OMG	O6-C6-N1	-3.16	116.92	120.65
40	LA	41	OMG	O6-C6-N1	-3.16	116.92	120.65
44	LE	1075	PSU	C6-N1-C2	-3.15	119.46	122.68
1	S1	1378	PSU	C6-C5-C4	3.15	120.40	118.20
1	S1	544	PSU	C6-C5-C4	3.14	120.40	118.20
41	LB	234	PSU	C6-N1-C2	-3.14	119.47	122.68
46	LG	2009	OMG	O6-C6-C5	3.14	130.51	124.37
48	LI	3510	PSU	C6-N1-C2	-3.14	119.47	122.68
1	S1	42	OMG	O6-C6-N1	-3.14	116.95	120.65
48	LI	3456	5MC	C5-C4-N3	3.13	125.05	121.67
1	S1	1681	OMG	O6-C6-N1	-3.13	116.95	120.65
48	LI	3510	PSU	C6-C5-C4	3.13	120.39	118.20
45	LF	1692	PSU	C6-N1-C2	-3.13	119.48	122.68
49	LJ	3697	PSU	C6-N1-C2	-3.13	119.48	122.68
46	LG	2119	PSU	C6-N1-C2	-3.13	119.49	122.68
45	LF	1836	OMC	C5-C4-N3	3.12	126.64	121.33
47	LH	2914	PSU	C6-N1-C2	-3.12	119.49	122.68
40	LA	41	OMG	O6-C6-C5	3.12	130.47	124.37
48	LI	3206	PSU	C6-C5-C4	3.12	120.38	118.20
47	LH	2837	PSU	C6-N1-C2	-3.12	119.49	122.68
44	LE	1126	PSU	C6-N1-C2	-3.12	119.49	122.68
48	LI	3206	PSU	C6-N1-C2	-3.12	119.50	122.68
53	LN	3969	PSU	C6-N1-C2	-3.11	119.50	122.68
48	LI	3546	OMC	C5-C4-N3	3.11	126.62	121.33
47	LH	2776	OMG	O6-C6-C5	3.11	130.45	124.37
1	S1	2144	5MC	C5-C4-N3	3.11	125.03	121.67
44	LE	1324	OMG	O6-C6-N1	-3.10	116.98	120.65
47	LH	2591	PSU	C6-N1-C2	-3.10	119.51	122.68
48	LI	3187	OMG	O6-C6-N1	-3.10	116.99	120.65
1	S1	641	OMG	O6-C6-N1	-3.10	116.99	120.65
40	LA	74	OMG	O6-C6-N1	-3.09	117.00	120.65
40	LA	16	PSU	C6-N1-C2	-3.09	119.53	122.68
48	LI	3440	PSU	C6-N1-C2	-3.08	119.53	122.68
48	LI	3204	PSU	C6-N1-C2	-3.08	119.53	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	LC	567	PSU	C6-C5-C4	3.08	120.35	118.20
1	S1	2142	OMC	C5-C4-N3	3.07	126.55	121.33
48	LI	2999	PSU	C6-N1-C2	-3.07	119.55	122.68
48	LI	3374	OMC	C5-C4-N3	3.07	126.55	121.33
1	S1	2129	PSU	C6-N1-C2	-3.07	119.55	122.68
44	LE	1363	PSU	C6-C5-C4	3.06	120.34	118.20
1	S1	99	OMC	C5-C4-N3	3.06	126.53	121.33
1	S1	2305	PSU	C6-N1-C2	-3.06	119.56	122.68
1	S1	2116	PSU	C6-N1-C2	-3.06	119.56	122.68
45	LF	1692	PSU	C6-C5-C4	3.05	120.33	118.20
42	LC	498	PSU	C6-N1-C2	-3.05	119.56	122.68
48	LI	3412	PSU	C6-C5-C4	3.05	120.33	118.20
42	LC	537	OMC	C5-C4-N3	3.05	126.52	121.33
1	S1	176	PSU	C6-N1-C2	-3.05	119.57	122.68
45	LF	1926	PSU	C6-N1-C2	-3.05	119.57	122.68
45	LF	1573	OMC	C5-C4-N3	3.05	126.51	121.33
44	LE	1171	PSU	C6-N1-C2	-3.04	119.57	122.68
48	LI	3504	OMG	O6-C6-N1	-3.04	117.06	120.65
42	LC	302	PSU	C6-N1-C2	-3.04	119.58	122.68
44	LE	1312	OMC	C5-C4-N3	3.03	126.49	121.33
1	S1	176	PSU	C6-C5-C4	3.03	120.32	118.20
47	LH	2358	A2M	O2'-C2'-C1'	3.03	115.10	109.09
48	LI	3568	PSU	C6-N1-C2	-3.03	119.58	122.68
48	LI	3355	OMC	C5-C4-N3	3.03	126.48	121.33
46	LG	2119	PSU	C6-C5-C4	3.03	120.31	118.20
1	S1	485	OMG	O6-C6-N1	-3.03	117.08	120.65
48	LI	3332	PSU	C6-C5-C4	3.03	120.31	118.20
46	LG	2154	PSU	C6-N1-C2	-3.03	119.59	122.68
44	LE	1165	OMC	C5-C4-N3	3.02	126.47	121.33
42	LC	577	OMC	C5-C4-N3	3.02	126.47	121.33
46	LG	2125	PSU	C6-N1-C2	-3.02	119.59	122.68
48	LI	3223	OMG	O6-C6-C5	3.02	130.28	124.37
42	LC	567	PSU	C6-N1-C2	-3.02	119.59	122.68
47	LH	2914	PSU	C6-C5-C4	3.02	120.31	118.20
1	S1	621	OMC	C5-C4-N3	3.02	126.47	121.33
48	LI	3568	PSU	C6-C5-C4	3.01	120.31	118.20
41	LB	280	PSU	C6-N1-C2	-3.01	119.60	122.68
49	LJ	3644	PSU	C6-N1-C2	-3.01	119.61	122.68
47	LH	2313	OMC	C5-C4-N3	3.01	126.44	121.33
48	LI	3451	PSU	C6-N1-C2	-3.00	119.61	122.68
48	LI	3208	OMC	C5-C4-N3	3.00	126.43	121.33
1	S1	1711	PSU	O2-C2-N1	-2.99	119.50	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	105	PSU	C6-N1-C2	-2.99	119.63	122.68
47	LH	2348	OMC	C5-C4-N3	2.99	126.41	121.33
49	LJ	3591	PSU	C6-C5-C4	2.98	120.28	118.20
2	S2	37	MIA	C2-N3-C4	2.98	119.43	115.32
44	LE	1198	PSU	C6-N1-C2	-2.98	119.64	122.68
45	LF	1582	PSU	C6-N1-C2	-2.98	119.64	122.68
47	LH	2617	PSU	C6-N1-C2	-2.97	119.64	122.68
52	LM	3953	PSU	C6-N1-C2	-2.97	119.64	122.68
1	S1	1068	PSU	C6-N1-C2	-2.97	119.65	122.68
1	S1	103	OMC	C5-C4-N3	2.97	126.38	121.33
47	LH	2915	PSU	C6-N1-C2	-2.96	119.65	122.68
44	LE	1365	PSU	O2-C2-N1	-2.96	119.53	122.79
47	LH	2685	OMC	C5-C4-N3	2.96	126.36	121.33
47	LH	2685	OMC	C1'-N1-C2	2.96	125.03	118.42
1	S1	2131	PSU	C6-C5-C4	2.96	120.27	118.20
45	LF	1976	OMC	C5-C4-N3	2.95	126.35	121.33
48	LI	3191	OMG	O6-C6-N1	-2.95	117.17	120.65
48	LI	3446	PSU	C6-C5-C4	2.95	120.26	118.20
1	S1	38	OMC	C5-C4-N3	2.94	126.34	121.33
1	S1	1037	OMC	C5-C4-N3	2.94	126.33	121.33
1	S1	393	OMC	C5-C4-N3	2.94	126.33	121.33
52	LM	3963	PSU	C6-N1-C2	-2.94	119.68	122.68
1	S1	186	OMU	CM2-O2'-C2'	-2.94	106.81	114.52
1	S1	2078	7MG	C5-C4-N9	2.93	110.16	106.35
44	LE	1407	PSU	C6-N1-C2	-2.93	119.68	122.68
51	LL	3865	PSU	C6-N1-C2	-2.93	119.69	122.68
44	LE	1270	OMU	CM2-O2'-C2'	-2.93	106.84	114.52
48	LI	3503	PSU	C6-N1-C2	-2.93	119.69	122.68
48	LI	3167	PSU	O2-C2-N1	-2.93	119.57	122.79
44	LE	949	OMC	C5-C4-N3	2.92	126.30	121.33
45	LF	1822	OMC	C5-C4-N3	2.92	126.30	121.33
47	LH	2832	OMC	C5-C4-N3	2.92	126.30	121.33
40	LA	68	PSU	O2-C2-N1	-2.92	119.58	122.79
47	LH	2642	PSU	C6-N1-C2	-2.92	119.70	122.68
52	LM	3957	OMC	C5-C4-N3	2.91	126.28	121.33
1	S1	1624	PSU	O2-C2-N1	-2.91	119.58	122.79
47	LH	2897	OMG	CM2-O2'-C2'	-2.91	106.88	114.52
47	LH	2853	OMC	C5-C4-N3	2.91	126.28	121.33
44	LE	1106	A2M	O4'-C4'-C3'	-2.91	99.36	105.11
44	LE	1222	OMU	O4-C4-C5	-2.91	120.05	125.16
48	LI	3145	PSU	C6-N1-C2	-2.90	119.71	122.68
48	LI	3347	OMC	C5-C4-N3	2.90	126.27	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	LJ	3697	PSU	C6-C5-C4	2.90	120.23	118.20
44	LE	936	OMC	CM2-O2'-C2'	-2.90	106.92	114.52
47	LH	2802	PSU	C6-C5-C4	2.90	120.22	118.20
48	LI	3185	PSU	C6-C5-C4	2.90	120.22	118.20
1	S1	1592	PSU	C6-N1-C2	-2.90	119.72	122.68
48	LI	3185	PSU	C6-N1-C2	-2.90	119.72	122.68
42	LC	483	OMC	C5-C4-N3	2.89	126.25	121.33
44	LE	1218	OMC	C5-C4-N3	2.89	126.24	121.33
49	LJ	3591	PSU	C6-N1-C2	-2.89	119.73	122.68
47	LH	2242	OMC	C5-C4-N3	2.89	126.24	121.33
45	LF	1582	PSU	C6-C5-C4	2.89	120.22	118.20
45	LF	1859	PSU	C6-C5-C4	2.89	120.22	118.20
45	LF	1582	PSU	O2-C2-N1	-2.88	119.62	122.79
47	LH	2679	PSU	C6-N1-C2	-2.88	119.74	122.68
47	LH	2825	OMC	C5-C4-N3	2.88	126.22	121.33
48	LI	3465	OMC	C5-C4-N3	2.88	126.22	121.33
1	S1	1554	PSU	C6-N1-C2	-2.87	119.75	122.68
44	LE	1407	PSU	C6-C5-C4	2.86	120.20	118.20
45	LF	1876	PSU	C6-N1-C2	-2.86	119.75	122.68
1	S1	1591	PSU	C6-N1-C2	-2.86	119.76	122.68
1	S1	2123	OMC	C5-C4-N3	2.86	126.19	121.33
1	S1	280	PSU	C6-C5-C4	2.86	120.20	118.20
48	LI	3332	PSU	C6-N1-C2	-2.86	119.76	122.68
1	S1	1625	OMC	C5-C4-N3	2.85	126.18	121.33
47	LH	2754	PSU	O2-C2-N1	-2.85	119.66	122.79
46	LG	2009	OMG	O6-C6-N1	-2.84	117.29	120.65
44	LE	936	OMC	C5-C4-N3	2.84	126.17	121.33
1	S1	1679	OMU	CM2-O2'-C2'	-2.84	107.07	114.52
1	S1	89	PSU	C6-C5-C4	2.82	120.17	118.20
48	LI	3214	6MZ	N3-C2-N1	-2.82	124.27	128.68
44	LE	1365	PSU	C6-N1-C2	-2.82	119.80	122.68
47	LH	2602	OMC	C5-C4-N3	2.82	126.12	121.33
44	LE	1266	PSU	O2-C2-N1	-2.81	119.69	122.79
1	S1	1393	PSU	C6-C5-C4	2.81	120.17	118.20
1	S1	1393	PSU	O2-C2-N1	-2.81	119.69	122.79
48	LI	3042	PSU	C6-N1-C2	-2.80	119.82	122.68
44	LE	1023	PSU	O2-C2-N1	-2.80	119.70	122.79
1	S1	32	PSU	C6-C5-C4	2.80	120.16	118.20
44	LE	1222	OMU	O2-C2-N3	-2.80	116.28	121.50
42	LC	308	PSU	C6-N1-C2	-2.80	119.82	122.68
1	S1	42	OMG	CM2-O2'-C2'	-2.79	107.19	114.52
45	LF	1568	PSU	C6-N1-C2	-2.79	119.83	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	LH	2586	PSU	C6-N1-C2	-2.79	119.83	122.68
1	S1	1601	B8N	O4-C4-N3	2.78	124.70	119.98
52	LM	3953	PSU	C6-C5-C4	2.78	120.14	118.20
41	LB	234	PSU	C6-C5-C4	2.78	120.14	118.20
42	LC	498	PSU	C6-C5-C4	2.78	120.14	118.20
47	LH	2586	PSU	C6-C5-C4	2.78	120.14	118.20
47	LH	2874	PSU	O2-C2-N1	-2.77	119.74	122.79
48	LI	3223	OMG	O6-C6-N1	-2.77	117.38	120.65
48	LI	3206	PSU	O2-C2-N1	-2.77	119.74	122.79
46	LG	2154	PSU	C6-C5-C4	2.77	120.13	118.20
45	LF	1859	PSU	O2-C2-N1	-2.77	119.74	122.79
44	LE	1023	PSU	C6-C5-C4	2.76	120.13	118.20
44	LE	938	7MG	C5-C4-N9	2.76	109.94	106.35
47	LH	2642	PSU	C6-C5-C4	2.76	120.13	118.20
47	LH	2802	PSU	C6-N1-C2	-2.76	119.86	122.68
1	S1	1601	B8N	O2-C2-N3	-2.76	118.16	121.99
47	LH	2679	PSU	C6-C5-C4	2.76	120.13	118.20
48	LI	3542	PSU	C6-N1-C2	-2.75	119.87	122.68
1	S1	1549	A2M	C5'-C4'-C3'	-2.75	104.87	115.18
49	LJ	3701	PSU	O2-C2-N1	-2.75	119.76	122.79
48	LI	3444	PSU	C6-N1-C2	-2.74	119.88	122.68
48	LI	3535	OMC	C5-C4-N3	2.73	125.97	121.33
48	LI	3042	PSU	O2-C2-N1	-2.73	119.79	122.79
44	LE	1222	OMU	C1'-N1-C6	-2.72	114.91	120.84
49	LJ	3697	PSU	O2-C2-N1	-2.72	119.80	122.79
47	LH	2636	JMH	C6-N1-C2	-2.72	119.36	121.79
47	LH	2625	OMU	C4-N3-C2	-2.71	123.01	126.58
1	S1	280	PSU	O2-C2-N1	-2.70	119.81	122.79
45	LF	1586	PSU	O2-C2-N1	-2.70	119.81	122.79
45	LF	1876	PSU	C6-C5-C4	2.70	120.09	118.20
52	LM	3963	PSU	C6-C5-C4	2.70	120.08	118.20
45	LF	1836	OMC	CM2-O2'-C2'	-2.70	107.45	114.52
48	LI	3208	OMC	C4-N3-C2	-2.69	115.91	120.25
48	LI	3518	5MC	C1'-N1-C2	-2.69	112.41	118.42
48	LI	3208	OMC	CM2-O2'-C2'	-2.69	107.46	114.52
47	LH	2742	PSU	C6-N1-C2	-2.69	119.93	122.68
48	LI	3510	PSU	O2-C2-N1	-2.69	119.83	122.79
1	S1	2081	PSU	O2-C2-N1	-2.69	119.83	122.79
44	LE	1126	PSU	C6-C5-C4	2.69	120.08	118.20
47	LH	2330	PSU	C6-N1-C2	-2.68	119.94	122.68
1	S1	1660	PSU	C6-C5-C4	2.68	120.07	118.20
47	LH	2685	OMC	CM2-O2'-C2'	-2.68	107.50	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	LC	498	PSU	O2-C2-N1	-2.67	119.85	122.79
1	S1	105	PSU	C6-C5-C4	2.67	120.07	118.20
48	LI	3446	PSU	C6-N1-C2	-2.67	119.95	122.68
42	LC	480	PSU	O2-C2-N1	-2.67	119.85	122.79
42	LC	421	PSU	O2-C2-N1	-2.67	119.86	122.79
46	LG	2125	PSU	O2-C2-N1	-2.67	119.86	122.79
48	LI	2999	PSU	O2-C2-N1	-2.66	119.86	122.79
47	LH	2591	PSU	C6-C5-C4	2.66	120.06	118.20
1	S1	1591	PSU	C6-C5-C4	2.66	120.06	118.20
1	S1	1068	PSU	C6-C5-C4	2.65	120.05	118.20
1	S1	2129	PSU	C6-C5-C4	2.65	120.05	118.20
41	LB	280	PSU	C6-C5-C4	2.65	120.05	118.20
48	LI	3444	PSU	O2-C2-N1	-2.65	119.88	122.79
1	S1	465	PSU	O2-C2-N1	-2.65	119.88	122.79
1	S1	621	OMC	CM2-O2'-C2'	-2.65	107.58	114.52
48	LI	3300	OMU	CM2-O2'-C2'	-2.64	107.59	114.52
47	LH	2899	PSU	C6-C5-C4	2.64	120.05	118.20
46	LG	2154	PSU	O2-C2-N1	-2.64	119.89	122.79
1	S1	2131	PSU	C6-N1-C2	-2.63	119.99	122.68
48	LI	3412	PSU	O2-C2-N1	-2.63	119.90	122.79
47	LH	2752	PSU	O2-C2-N1	-2.63	119.90	122.79
45	LF	1976	OMC	CM2-O2'-C2'	-2.62	107.65	114.52
1	S1	2131	PSU	O2-C2-N1	-2.62	119.91	122.79
47	LH	2623	PSU	O2-C2-N1	-2.61	119.92	122.79
42	LC	308	PSU	O2-C2-N1	-2.60	119.93	122.79
1	S1	403	PSU	C6-N1-C2	-2.60	120.03	122.68
1	S1	1592	PSU	C6-C5-C4	2.60	120.02	118.20
1	S1	38	OMC	CM2-O2'-C2'	-2.60	107.70	114.52
47	LH	2752	PSU	C6-C5-C4	2.60	120.01	118.20
48	LI	3440	PSU	O2-C2-N1	-2.59	119.93	122.79
1	S1	1960	PSU	C6-C5-C4	2.59	120.01	118.20
42	LC	567	PSU	O2-C2-N1	-2.59	119.94	122.79
49	LJ	3591	PSU	O2-C2-N1	-2.59	119.94	122.79
1	S1	1960	PSU	O2-C2-N1	-2.59	119.94	122.79
47	LH	2625	OMU	CM2-O2'-C2'	-2.58	107.75	114.52
47	LH	2624	PSU	C6-N1-C2	-2.58	120.04	122.68
44	LE	1235	PSU	O2-C2-N1	-2.58	119.95	122.79
48	LI	3562	PSU	O2-C2-N1	-2.58	119.95	122.79
46	LG	1999	OMU	CM2-O2'-C2'	-2.58	107.76	114.52
48	LI	3204	PSU	C6-C5-C4	2.58	120.00	118.20
44	LE	1235	PSU	C6-C5-C4	2.57	120.00	118.20
45	LF	1573	OMC	CM2-O2'-C2'	-2.57	107.77	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	LF	1504	OMU	CM2-O2'-C2'	-2.57	107.78	114.52
44	LE	1118	PSU	C6-N1-C2	-2.57	120.06	122.68
1	S1	27	PSU	C6-C5-C4	2.57	119.99	118.20
46	LG	2171	PSU	O2-C2-N1	-2.56	119.97	122.79
1	S1	1624	PSU	C6-C5-C4	2.56	119.99	118.20
1	S1	1715	PSU	C6-C5-C4	2.56	119.99	118.20
1	S1	2101	PSU	O2-C2-N1	-2.56	119.97	122.79
48	LI	3159	OMU	CM2-O2'-C2'	-2.56	107.82	114.52
1	S1	180	OMG	O6-C6-N1	-2.55	117.63	120.65
45	LF	1692	PSU	O2-C2-N1	-2.55	119.98	122.79
52	LM	3963	PSU	O2-C2-N1	-2.55	119.98	122.79
1	S1	103	OMC	CM2-O2'-C2'	-2.55	107.84	114.52
1	S1	1378	PSU	O2-C2-N1	-2.55	119.99	122.79
1	S1	544	PSU	O2-C2-N1	-2.54	119.99	122.79
45	LF	1824	OMU	CM2-O2'-C2'	-2.54	107.85	114.52
48	LI	3175	PSU	O2-C2-N1	-2.54	119.99	122.79
45	LF	1822	OMC	CM2-O2'-C2'	-2.54	107.85	114.52
47	LH	2746	PSU	C6-C5-C4	2.54	119.97	118.20
47	LH	2766	5MC	C5-C4-N4	-2.54	117.68	121.48
47	LH	2624	PSU	C6-C5-C4	2.54	119.97	118.20
49	LJ	3694	OMU	CM2-O2'-C2'	-2.54	107.87	114.52
47	LH	2914	PSU	O2-C2-N1	-2.53	120.00	122.79
42	LC	491	OMU	CM2-O2'-C2'	-2.53	107.88	114.52
47	LH	2842	PSU	O2-C2-N1	-2.53	120.00	122.79
1	S1	8	OMU	CM2-O2'-C2'	-2.53	107.89	114.52
44	LE	938	7MG	C4-C5-N7	2.53	109.04	105.53
48	LI	3451	PSU	O2-C2-N1	-2.53	120.01	122.79
47	LH	2832	OMC	C4-N3-C2	-2.52	116.18	120.25
1	S1	176	PSU	O2-C2-N1	-2.52	120.02	122.79
47	LH	2915	PSU	C6-C5-C4	2.52	119.96	118.20
47	LH	2825	OMC	CM2-O2'-C2'	-2.52	107.92	114.52
46	LG	2119	PSU	O2-C2-N1	-2.52	120.02	122.79
40	LA	16	PSU	C6-C5-C4	2.51	119.95	118.20
1	S1	1641	OMU	CM2-O2'-C2'	-2.51	107.95	114.52
49	LJ	3701	PSU	C6-C5-C4	2.51	119.95	118.20
1	S1	186	OMU	C4-N3-C2	-2.50	123.28	126.58
47	LH	2621	PSU	C6-N1-C2	-2.50	120.13	122.68
47	LH	2346	OMU	CM2-O2'-C2'	-2.49	107.98	114.52
48	LI	3300	OMU	C4-N3-C2	-2.49	123.29	126.58
48	LI	3222	OMC	CM2-O2'-C2'	-2.49	107.98	114.52
1	S1	2078	7MG	C4-C5-N7	2.49	108.99	105.53
45	LF	1976	OMC	C4-N3-C2	-2.49	116.23	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2305	PSU	C6-C5-C4	2.49	119.94	118.20
47	LH	2842	PSU	C6-C5-C4	2.49	119.94	118.20
44	LE	1363	PSU	O2-C2-N1	-2.49	120.05	122.79
48	LI	3355	OMC	CM2-O2'-C2'	-2.49	107.99	114.52
45	LF	1898	OMU	C4-N3-C2	-2.49	123.30	126.58
49	LJ	3688	OMG	CM2-O2'-C2'	-2.48	108.02	114.52
44	LE	1165	OMC	CM2-O2'-C2'	-2.48	108.02	114.52
48	LI	3465	OMC	CM2-O2'-C2'	-2.48	108.03	114.52
48	LI	3332	PSU	O2-C2-N1	-2.47	120.07	122.79
48	LI	3508	OMU	CM2-O2'-C2'	-2.47	108.03	114.52
44	LE	1189	OMU	CM2-O2'-C2'	-2.47	108.04	114.52
1	S1	2305	PSU	O2-C2-N1	-2.47	120.07	122.79
48	LI	3214	6MZ	C4-C5-N7	-2.47	106.82	109.40
47	LH	2766	5MC	N1-C2-N3	-2.47	114.31	118.81
45	LF	1836	OMC	C4-N3-C2	-2.47	116.27	120.25
44	LE	1198	PSU	O2-C2-N1	-2.46	120.08	122.79
1	S1	1037	OMC	CM2-O2'-C2'	-2.46	108.06	114.52
45	LF	1876	PSU	O2-C2-N1	-2.46	120.08	122.79
1	S1	1601	B8N	C32-C31-N3	2.46	116.60	112.00
47	LH	2909	OMU	C4-N3-C2	-2.46	123.34	126.58
1	S1	621	OMC	C4-N3-C2	-2.45	116.30	120.25
47	LH	2586	PSU	O2-C2-N1	-2.45	120.10	122.79
47	LH	2591	PSU	O2-C2-N1	-2.45	120.10	122.79
1	S1	1660	PSU	O2-C2-N1	-2.44	120.10	122.79
1	S1	2065	PSU	C6-C5-C4	2.44	119.91	118.20
51	LL	3865	PSU	O2-C2-N1	-2.44	120.10	122.79
1	S1	8	OMU	C4-N3-C2	-2.44	123.36	126.58
1	S1	180	OMG	N1-C2-N3	2.44	127.88	123.32
45	LF	1826	OMG	CM2-O2'-C2'	-2.44	108.13	114.52
42	LC	577	OMC	C4-N3-C2	-2.44	116.32	120.25
47	LH	2346	OMU	C4-N3-C2	-2.44	123.37	126.58
44	LE	1218	OMC	CM2-O2'-C2'	-2.43	108.15	114.52
48	LI	3204	PSU	O2-C2-N1	-2.43	120.11	122.79
48	LI	3503	PSU	O2-C2-N1	-2.43	120.12	122.79
1	S1	640	PSU	C6-N1-C2	-2.43	120.20	122.68
1	S1	1396	PSU	O2-C2-N1	-2.43	120.12	122.79
1	S1	682	OMU	C4-N3-C2	-2.43	123.38	126.58
44	LE	1407	PSU	O2-C2-N1	-2.43	120.12	122.79
52	LM	3957	OMC	C4-N3-C2	-2.42	116.34	120.25
44	LE	1260	PSU	O2-C2-N1	-2.42	120.12	122.79
1	S1	2180	A2M	C4-C5-N7	-2.42	106.88	109.40
48	LI	3546	OMC	CM2-O2'-C2'	-2.42	108.18	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	LE	1184	PSU	O2-C2-N1	-2.42	120.13	122.79
48	LI	3568	PSU	O2-C2-N1	-2.41	120.14	122.79
47	LH	2713	OMU	CM2-O2'-C2'	-2.41	108.20	114.52
47	LH	2617	PSU	O2-C2-N1	-2.41	120.14	122.79
53	LN	3969	PSU	O2-C2-N1	-2.41	120.14	122.79
48	LI	3222	OMC	C4-N3-C2	-2.41	116.37	120.25
48	LI	3145	PSU	O2-C2-N1	-2.41	120.14	122.79
2	S2	37	MIA	C16-C14-C15	-2.40	109.29	114.60
44	LE	1315	OMU	CM2-O2'-C2'	-2.40	108.22	114.52
1	S1	1641	OMU	C4-N3-C2	-2.40	123.42	126.58
1	S1	2142	OMC	N4-C4-N3	-2.40	113.76	117.97
1	S1	1616	OMU	CM2-O2'-C2'	-2.40	108.23	114.52
1	S1	1068	PSU	O2-C2-N1	-2.40	120.15	122.79
1	S1	2123	OMC	C4-N3-C2	-2.40	116.39	120.25
44	LE	1452	OMU	C4-N3-C2	-2.39	123.42	126.58
45	LF	1926	PSU	O2-C2-N1	-2.39	120.16	122.79
1	S1	1715	PSU	O2-C2-N1	-2.39	120.16	122.79
47	LH	2636	JMH	O2-C2-N3	-2.39	117.97	121.34
45	LF	1835	OMG	C2-N1-C6	-2.39	120.70	125.10
42	LC	302	PSU	O2-C2-N1	-2.38	120.17	122.79
44	LE	1189	OMU	C4-N3-C2	-2.38	123.44	126.58
1	S1	393	OMC	C4-N3-C2	-2.38	116.41	120.25
47	LH	2832	OMC	CM2-O2'-C2'	-2.38	108.27	114.52
44	LE	1270	OMU	C4-N3-C2	-2.38	123.44	126.58
1	S1	1901	OMG	N1-C2-N3	2.37	127.75	123.32
47	LH	2361	PSU	C6-C5-C4	2.37	119.86	118.20
44	LE	1208	OMG	C8-N7-C5	2.37	107.50	102.99
49	LJ	3644	PSU	O2-C2-N1	-2.37	120.19	122.79
44	LE	1075	PSU	O2-C2-N1	-2.37	120.19	122.79
47	LH	2909	OMU	CM2-O2'-C2'	-2.37	108.32	114.52
1	S1	704	OMU	C4-N3-C2	-2.36	123.46	126.58
1	S1	99	OMC	C4-N3-C2	-2.36	116.44	120.25
48	LI	3374	OMC	CM2-O2'-C2'	-2.36	108.32	114.52
45	LF	1956	OMG	N1-C2-N3	2.36	127.73	123.32
47	LH	2879	OMG	N2-C2-N3	-2.36	115.14	119.74
45	LF	1819	OMG	O2'-C2'-C1'	2.36	113.77	109.09
1	S1	2144	5MC	N1-C2-N3	-2.36	114.52	118.81
48	LI	3222	OMC	N4-C4-N3	-2.35	113.84	117.97
48	LI	3355	OMC	C4-N3-C2	-2.35	116.46	120.25
1	S1	641	OMG	CM2-O2'-C2'	-2.35	108.35	114.52
47	LH	2853	OMC	CM2-O2'-C2'	-2.35	108.36	114.52
45	LF	1667	OMG	N1-C2-N3	2.35	127.71	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	LN	3969	PSU	C6-C5-C4	2.35	119.84	118.20
1	S1	1679	OMU	C4-N3-C2	-2.35	123.48	126.58
48	LI	3159	OMU	C4-N3-C2	-2.35	123.48	126.58
45	LF	1898	OMU	CM2-O2'-C2'	-2.34	108.38	114.52
48	LI	3546	OMC	C4-N3-C2	-2.34	116.48	120.25
1	S1	57	OMG	N1-C2-N3	2.34	127.68	123.32
44	LE	1126	PSU	O2-C2-N1	-2.34	120.22	122.79
48	LI	3185	PSU	O2-C2-N1	-2.33	120.22	122.79
41	LB	247	OMU	CM2-O2'-C2'	-2.33	108.41	114.52
47	LH	2348	OMC	C4-N3-C2	-2.33	116.49	120.25
1	S1	179	OMU	C4-N3-C2	-2.33	123.51	126.58
47	LH	2361	PSU	O2-C2-N1	-2.33	120.23	122.79
45	LF	1957	OMU	C4-N3-C2	-2.33	123.51	126.58
47	LH	2837	PSU	C6-C5-C4	2.33	119.82	118.20
1	S1	2144	5MC	C5-C4-N4	-2.33	118.00	121.48
47	LH	2746	PSU	O2-C2-N1	-2.33	120.23	122.79
40	LA	16	PSU	O2-C2-N1	-2.32	120.23	122.79
47	LH	2768	A2M	C3'-C2'-C1'	2.32	107.25	102.89
1	S1	1591	PSU	O2-C2-N1	-2.32	120.24	122.79
48	LI	3171	OMU	CM2-O2'-C2'	-2.32	108.44	114.52
44	LE	931	1MA	C8-N7-C5	2.32	107.41	102.99
44	LE	1081	OMU	CM2-O2'-C2'	-2.32	108.44	114.52
1	S1	1554	PSU	C6-C5-C4	2.32	119.82	118.20
1	S1	105	PSU	O2-C2-N1	-2.32	120.24	122.79
46	LG	2129	OMU	C4-N3-C2	-2.32	123.53	126.58
47	LH	2802	PSU	O2-C2-N1	-2.31	120.25	122.79
48	LI	3401	OMG	N1-C2-N3	2.30	127.62	123.32
48	LI	3377	OMG	CM2-O2'-C2'	-2.30	108.49	114.52
52	LM	3953	PSU	O2-C2-N1	-2.30	120.26	122.79
1	S1	38	OMC	C4-N3-C2	-2.30	116.55	120.25
47	LH	2621	PSU	O2-C2-N1	-2.30	120.26	122.79
47	LH	2713	OMU	C4-N3-C2	-2.30	123.55	126.58
1	S1	704	OMU	CM2-O2'-C2'	-2.29	108.50	114.52
41	LB	280	PSU	O2-C2-N1	-2.29	120.27	122.79
48	LI	3347	OMC	C4-N3-C2	-2.29	116.55	120.25
47	LH	2915	PSU	O2-C2-N1	-2.29	120.27	122.79
1	S1	2041	OMU	C4-N3-C2	-2.29	123.56	126.58
46	LG	2009	OMG	N1-C2-N3	2.28	127.59	123.32
1	S1	1966	OMU	C4-N3-C2	-2.28	123.57	126.58
48	LI	3434	OMG	N1-C2-N3	2.28	127.58	123.32
48	LI	3456	5MC	C1'-N1-C2	-2.28	113.34	118.42
42	LC	537	OMC	C4-N3-C2	-2.28	116.58	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	LC	483	OMC	CM2-O2'-C2'	-2.28	108.55	114.52
49	LJ	3680	PSU	O4'-C1'-C2'	2.27	108.35	105.14
48	LI	3508	OMU	C4-N3-C2	-2.27	123.58	126.58
44	LE	1312	OMC	C4-N3-C2	-2.27	116.59	120.25
1	S1	2065	PSU	O2-C2-N1	-2.27	120.29	122.79
1	S1	1037	OMC	C4-N3-C2	-2.27	116.59	120.25
47	LH	2636	JMH	C1'-N1-C6	-2.27	115.89	120.84
48	LI	3374	OMC	C4-N3-C2	-2.27	116.59	120.25
1	S1	723	A2M	C3'-C2'-C1'	2.27	107.16	102.89
44	LE	936	OMC	C4-N3-C2	-2.27	116.59	120.25
1	S1	1591	PSU	O4-C4-C5	-2.27	118.12	124.05
47	LH	2744	A2M	C3'-C2'-C1'	2.26	107.14	102.89
44	LE	1218	OMC	C4-N3-C2	-2.26	116.60	120.25
45	LF	1553	OMU	C4-N3-C2	-2.26	123.60	126.58
40	LA	68	PSU	O4'-C1'-C2'	2.26	108.33	105.14
1	S1	702	OMU	C4-N3-C2	-2.26	123.60	126.58
44	LE	1184	PSU	C6-C5-C4	2.26	119.78	118.20
44	LE	931	1MA	C5-C6-N1	2.26	117.26	113.90
45	LF	1956	OMG	C2-N1-C6	-2.26	120.94	125.10
47	LH	2825	OMC	N4-C4-N3	-2.25	114.01	117.97
48	LI	3171	OMU	C4-N3-C2	-2.25	123.61	126.58
47	LH	2853	OMC	C4-N3-C2	-2.25	116.62	120.25
1	S1	2078	7MG	O6-C6-N1	-2.25	115.80	120.12
48	LI	3444	PSU	O4'-C1'-C2'	2.25	108.32	105.14
47	LH	2837	PSU	O2-C2-N1	-2.25	120.31	122.79
47	LH	2610	OMG	C2-N1-C6	-2.25	120.96	125.10
48	LI	3456	5MC	C5-C4-N4	-2.25	118.12	121.48
45	LF	1835	OMG	N1-C2-N3	2.25	127.52	123.32
40	LA	97	A2M	O4'-C1'-C2'	-2.25	102.69	106.59
49	LJ	3718	OMU	C4-N3-C2	-2.25	123.62	126.58
44	LE	1075	PSU	C6-C5-C4	2.25	119.77	118.20
1	S1	1616	OMU	C4-N3-C2	-2.24	123.63	126.58
44	LE	1315	OMU	C4-N3-C2	-2.24	123.63	126.58
1	S1	99	OMC	CM2-O2'-C2'	-2.24	108.65	114.52
47	LH	2330	PSU	C6-C5-C4	2.24	119.76	118.20
48	LI	3206	PSU	O4'-C1'-C2'	2.24	108.30	105.14
47	LH	2621	PSU	C6-C5-C4	2.24	119.76	118.20
1	S1	485	OMG	N1-C2-N3	2.23	127.49	123.32
1	S1	89	PSU	O2-C2-N1	-2.23	120.33	122.79
1	S1	1601	B8N	O4'-C1'-C2'	2.23	108.29	105.14
1	S1	2075	OMG	N1-C2-N3	2.23	127.49	123.32
47	LH	2348	OMC	CM2-O2'-C2'	-2.23	108.67	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	LC	537	OMC	CM2-O2'-C2'	-2.23	108.67	114.52
47	LH	2806	OMU	C4-N3-C2	-2.23	123.64	126.58
45	LF	1883	OMG	N1-C2-N3	2.23	127.48	123.32
49	LJ	3636	OMU	C4-N3-C2	-2.23	123.64	126.58
47	LH	2313	OMC	CM2-O2'-C2'	-2.22	108.69	114.52
1	S1	121	PSU	C3'-C2'-C1'	2.22	104.23	101.64
47	LH	2313	OMC	C4-N3-C2	-2.22	116.67	120.25
47	LH	2742	PSU	C6-C5-C4	2.22	119.75	118.20
47	LH	2835	OMU	C4-N3-C2	-2.22	123.65	126.58
45	LF	1681	OMU	C4-N3-C2	-2.22	123.66	126.58
42	LC	628	OMG	N1-C2-N3	2.22	127.46	123.32
1	S1	27	PSU	O2-C2-N1	-2.21	120.35	122.79
47	LH	2330	PSU	O2-C2-N1	-2.21	120.35	122.79
48	LI	3377	OMG	N1-C2-N3	2.21	127.45	123.32
1	S1	1536	OMG	N1-C2-N3	2.21	127.45	123.32
48	LI	3347	OMC	CM2-O2'-C2'	-2.21	108.72	114.52
1	S1	2129	PSU	O2-C2-N1	-2.21	120.36	122.79
47	LH	2610	OMG	CM2-O2'-C2'	-2.21	108.73	114.52
1	S1	57	OMG	N2-C2-N3	-2.21	115.44	119.74
48	LI	3412	PSU	O4'-C1'-C2'	2.21	108.26	105.14
45	LF	1667	OMG	C2-N1-C6	-2.21	121.03	125.10
45	LF	1504	OMU	C4-N3-C2	-2.21	123.67	126.58
48	LI	3401	OMG	C2-N1-C6	-2.21	121.04	125.10
47	LH	2744	A2M	C2'-C3'-C4'	2.20	106.78	101.99
1	S1	702	OMU	CM2-O2'-C2'	-2.20	108.75	114.52
1	S1	1901	OMG	CM2-O2'-C2'	-2.20	108.76	114.52
1	S1	1901	OMG	C2-N1-C6	-2.20	121.05	125.10
48	LI	3546	OMC	N4-C4-N3	-2.19	114.12	117.97
45	LF	1662	OMG	N1-C2-N3	2.19	127.42	123.32
47	LH	2242	OMC	C4-N3-C2	-2.19	116.71	120.25
41	LB	206	OMU	C4-N3-C2	-2.19	123.69	126.58
1	S1	32	PSU	O2-C2-N1	-2.19	120.38	122.79
41	LB	281	PSU	O2-C2-N1	-2.19	120.38	122.79
1	S1	1601	B8N	C31-N3-C2	-2.19	114.39	117.67
47	LH	2879	OMG	N1-C2-N3	2.19	127.41	123.32
47	LH	2899	PSU	O2-C2-N1	-2.19	120.38	122.79
48	LI	3518	5MC	C5-C4-N4	-2.19	118.21	121.48
44	LE	938	7MG	O6-C6-N1	-2.19	115.93	120.12
47	LH	2925	OMG	N1-C2-N3	2.19	127.40	123.32
1	S1	1705	OMG	N1-C2-N3	2.18	127.40	123.32
42	LC	491	OMU	C4-N3-C2	-2.18	123.70	126.58
1	S1	645	A2M	O4'-C4'-C3'	-2.18	100.80	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2142	OMC	C4-N3-C2	-2.18	116.73	120.25
45	LF	1568	PSU	O2-C2-N1	-2.18	120.39	122.79
40	LA	74	OMG	N1-C2-N3	2.18	127.38	123.32
45	LF	1568	PSU	C6-C5-C4	2.17	119.72	118.20
48	LI	3191	OMG	N1-C2-N3	2.17	127.38	123.32
47	LH	2313	OMC	N4-C4-N3	-2.17	114.16	117.97
46	LG	2009	OMG	N2-C2-N3	-2.17	115.51	119.74
48	LI	3187	OMG	N2-C2-N3	-2.17	115.51	119.74
44	LE	1217	OMG	CM2-O2'-C2'	-2.17	108.83	114.52
44	LE	1217	OMG	C2-N1-C6	-2.17	121.10	125.10
44	LE	1452	OMU	CM2-O2'-C2'	-2.17	108.84	114.52
41	LB	247	OMU	C4-N3-C2	-2.17	123.72	126.58
46	LG	1999	OMU	C4-N3-C2	-2.17	123.72	126.58
48	LI	3465	OMC	N4-C4-N3	-2.17	114.17	117.97
1	S1	57	OMG	C2-N1-C6	-2.16	121.11	125.10
48	LI	3542	PSU	O2-C2-N1	-2.16	120.41	122.79
1	S1	407	A2M	C5'-C4'-C3'	-2.16	107.08	115.18
45	LF	1826	OMG	N2-C2-N3	-2.16	115.53	119.74
47	LH	2610	OMG	N1-C2-N3	2.16	127.36	123.32
1	S1	1625	OMC	C4-N3-C2	-2.16	116.77	120.25
45	LF	1856	OMG	N2-C2-N3	-2.16	115.53	119.74
1	S1	103	OMC	C4-N3-C2	-2.16	116.77	120.25
45	LF	1681	OMU	CM2-O2'-C2'	-2.16	108.86	114.52
48	LI	3531	PSU	O2-C2-N1	-2.16	120.42	122.79
45	LF	1819	OMG	N1-C2-N3	2.16	127.35	123.32
44	LE	1104	OMG	CM2-O2'-C2'	-2.16	108.86	114.52
48	LI	3223	OMG	CM2-O2'-C2'	-2.16	108.87	114.52
48	LI	3167	PSU	C6-C5-C4	2.15	119.70	118.20
48	LI	3191	OMG	N2-C2-N3	-2.15	115.55	119.74
48	LI	3509	OMG	N2-C2-N3	-2.15	115.55	119.74
1	S1	179	OMU	CM2-O2'-C2'	-2.15	108.88	114.52
44	LE	1217	OMG	N1-C2-N3	2.15	127.34	123.32
1	S1	1744	OMU	C4-N3-C2	-2.15	123.75	126.58
41	LB	234	PSU	O2-C2-N1	-2.15	120.42	122.79
47	LH	2870	OMG	CM2-O2'-C2'	-2.15	108.89	114.52
45	LF	1824	OMU	C4-N3-C2	-2.15	123.75	126.58
1	S1	1592	PSU	O2-C2-N1	-2.15	120.43	122.79
48	LI	3518	5MC	N1-C2-N3	-2.15	114.90	118.81
47	LH	2776	OMG	CM2-O2'-C2'	-2.14	108.90	114.52
49	LJ	3680	PSU	O2-C2-N1	-2.14	120.43	122.79
44	LE	1260	PSU	O4'-C1'-C2'	2.14	108.17	105.14
47	LH	2776	OMG	C2-N1-C6	-2.14	121.16	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	LF	1573	OMC	C4-N3-C2	-2.14	116.80	120.25
44	LE	1185	OMU	C4-N3-C2	-2.14	123.76	126.58
44	LE	949	OMC	C4-N3-C2	-2.14	116.81	120.25
48	LI	3535	OMC	C4-N3-C2	-2.14	116.81	120.25
48	LI	3434	OMG	N2-C2-N3	-2.13	115.58	119.74
47	LH	2642	PSU	O2-C2-N1	-2.13	120.44	122.79
1	S1	565	A2M	C5'-C4'-C3'	-2.13	107.18	115.18
1	S1	641	OMG	N1-C2-N3	2.13	127.30	123.32
47	LH	2897	OMG	N1-C2-N3	2.13	127.30	123.32
44	LE	1104	OMG	N1-C2-N3	2.13	127.29	123.32
44	LE	1312	OMC	CM2-O2'-C2'	-2.13	108.94	114.52
1	S1	2075	OMG	N2-C2-N3	-2.13	115.60	119.74
47	LH	2806	OMU	CM2-O2'-C2'	-2.12	108.95	114.52
48	LI	3401	OMG	CM2-O2'-C2'	-2.12	108.96	114.52
48	LI	3434	OMG	C2-N1-C6	-2.11	121.21	125.10
1	S1	1681	OMG	N1-C2-N3	2.11	127.26	123.32
47	LH	2842	PSU	O4'-C1'-C2'	2.11	108.12	105.14
44	LE	1208	OMG	C2'-C3'-C4'	2.11	106.57	101.99
47	LH	2605	OMU	C4-N3-C2	-2.11	123.80	126.58
1	S1	403	PSU	O2-C2-N1	-2.10	120.47	122.79
48	LI	3379	OMG	CM2-O2'-C2'	-2.10	109.01	114.52
1	S1	1705	OMG	C2-N1-C6	-2.10	121.23	125.10
44	LE	1081	OMU	C4-N3-C2	-2.10	123.81	126.58
1	S1	99	OMC	N4-C4-N3	-2.10	114.29	117.97
44	LE	1324	OMG	N1-C2-N3	2.09	127.23	123.32
48	LI	3518	5MC	C1'-N1-C6	2.09	124.61	121.12
49	LJ	3694	OMU	C4-N3-C2	-2.09	123.83	126.58
48	LI	3379	OMG	C2-N1-C6	-2.09	121.25	125.10
1	S1	1536	OMG	C2-N1-C6	-2.09	121.25	125.10
45	LF	1819	OMG	C2-N1-C6	-2.09	121.25	125.10
47	LH	2602	OMC	C4-N3-C2	-2.09	116.89	120.25
45	LF	1553	OMU	CM2-O2'-C2'	-2.08	109.06	114.52
47	LH	2776	OMG	N1-C2-N3	2.08	127.20	123.32
47	LH	2636	JMH	C31-N3-C2	2.08	120.95	117.31
45	LF	1683	OMG	CM2-O2'-C2'	-2.08	109.07	114.52
45	LF	1662	OMG	C2-N1-C6	-2.08	121.28	125.10
44	LE	1171	PSU	O2-C2-N1	-2.07	120.51	122.79
2	S2	37	MIA	C12-N6-C6	-2.07	119.48	122.55
42	LC	541	OMG	N1-C2-N3	2.07	127.19	123.32
1	S1	42	OMG	N1-C2-N3	2.07	127.19	123.32
46	LG	2154	PSU	O4'-C1'-C2'	2.07	108.06	105.14
45	LF	1883	OMG	C2-N1-C6	-2.07	121.29	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	LI	3504	OMG	CM2-O2'-C2'	-2.07	109.10	114.52
48	LI	3187	OMG	N1-C2-N3	2.06	127.18	123.32
48	LI	3434	OMG	CM2-O2'-C2'	-2.06	109.11	114.52
1	S1	621	OMC	N4-C4-N3	-2.06	114.35	117.97
42	LC	628	OMG	N2-C2-N3	-2.06	115.72	119.74
47	LH	2883	OMG	N1-C2-N3	2.06	127.16	123.32
48	LI	3379	OMG	N1-C2-N3	2.06	127.16	123.32
40	LA	41	OMG	N2-C2-N3	-2.05	115.74	119.74
47	LH	2870	OMG	N1-C2-N3	2.05	127.16	123.32
46	LG	2146	OMG	N1-C2-N3	2.05	127.15	123.32
47	LH	2879	OMG	C2-N1-C6	-2.05	121.32	125.10
1	S1	2116	PSU	O2-C2-N1	-2.05	120.53	122.79
48	LI	3535	OMC	CM2-O2'-C2'	-2.05	109.15	114.52
1	S1	42	OMG	N2-C2-N3	-2.05	115.75	119.74
42	LC	541	OMG	C2-N1-C6	-2.05	121.33	125.10
48	LI	3208	OMC	N4-C4-N3	-2.05	114.38	117.97
1	S1	2144	5MC	C1'-N1-C2	-2.05	113.86	118.42
1	S1	390	OMG	N2-C2-N3	-2.04	115.76	119.74
44	LE	1218	OMC	N4-C4-N3	-2.04	114.38	117.97
44	LE	1165	OMC	C4-N3-C2	-2.04	116.95	120.25
1	S1	1966	OMU	CM2-O2'-C2'	-2.04	109.16	114.52
47	LH	2242	OMC	N4-C4-N3	-2.04	114.38	117.97
47	LH	2685	OMC	C1'-N1-C6	-2.04	116.39	120.84
48	LI	3223	OMG	N1-C2-N3	2.04	127.13	123.32
44	LE	931	1MA	N1-C2-N3	-2.04	123.64	126.02
48	LI	3504	OMG	N2-C2-N3	-2.04	115.77	119.74
47	LH	2679	PSU	O2-C2-N1	-2.04	120.55	122.79
47	LH	2610	OMG	N2-C2-N3	-2.04	115.77	119.74
47	LH	2870	OMG	N2-C2-N3	-2.04	115.77	119.74
45	LF	1683	OMG	N1-C2-N3	2.04	127.12	123.32
1	S1	2123	OMC	N4-C4-N3	-2.04	114.39	117.97
42	LC	537	OMC	N4-C4-N3	-2.04	114.39	117.97
47	LH	2897	OMG	C2-N1-C6	-2.03	121.35	125.10
45	LF	1662	OMG	CM2-O2'-C2'	-2.03	109.19	114.52
1	S1	2078	7MG	C5-C4-N3	-2.03	124.26	128.13
42	LC	631	OMG	C2-N1-C6	-2.03	121.35	125.10
42	LC	631	OMG	N1-C2-N3	2.03	127.12	123.32
48	LI	3315	A2M	C5'-C4'-C3'	-2.03	107.57	115.18
42	LC	628	OMG	C2-N1-C6	-2.03	121.36	125.10
46	LG	2009	OMG	C2-N1-C6	-2.03	121.36	125.10
44	LE	1165	OMC	C1'-N1-C2	2.03	122.95	118.42
44	LE	1208	OMG	C5-C6-N1	2.03	117.53	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2078	7MG	C6-C5-N7	-2.03	128.72	131.91
1	S1	1681	OMG	C2-N1-C6	-2.03	121.36	125.10
45	LF	1573	OMC	N4-C4-N3	-2.03	114.41	117.97
47	LH	2883	OMG	N2-C2-N3	-2.03	115.80	119.74
40	LA	39	A2M	C5'-C4'-C3'	-2.02	107.60	115.18
45	LF	1957	OMU	CM2-O2'-C2'	-2.02	109.22	114.52
41	LB	215	OMG	N2-C2-N3	-2.02	115.80	119.74
48	LI	3377	OMG	C2-N1-C6	-2.02	121.38	125.10
1	S1	390	OMG	N1-C2-N3	2.02	127.09	123.32
44	LE	1118	PSU	C5-C4-N3	2.01	121.14	116.58
47	LH	2825	OMC	C4-N3-C2	-2.01	117.00	120.25
46	LG	2125	PSU	O4'-C1'-C2'	2.01	107.98	105.14
48	LI	3568	PSU	O4'-C1'-C2'	2.01	107.98	105.14
1	S1	640	PSU	C6-C5-C4	2.01	119.60	118.20
42	LC	483	OMC	N4-C4-N3	-2.01	114.44	117.97
1	S1	390	OMG	C2-N1-C6	-2.01	121.40	125.10
48	LI	3451	PSU	O4'-C1'-C2'	2.00	107.97	105.14
49	LJ	3644	PSU	O4'-C1'-C2'	2.00	107.97	105.14
1	S1	1625	OMC	N4-C4-N3	-2.00	114.45	117.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	S1	1601	B8N	C33

All (318) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S1	57	OMG	O4'-C4'-C5'-O5'
1	S1	57	OMG	C3'-C4'-C5'-O5'
1	S1	110	A2M	C1'-C2'-O2'-CM'
1	S1	180	OMG	C1'-C2'-O2'-CM2
1	S1	280	PSU	O4'-C4'-C5'-O5'
1	S1	403	PSU	C2'-C1'-C5-C4
1	S1	403	PSU	O4'-C1'-C5-C4
1	S1	403	PSU	O4'-C1'-C5-C6
1	S1	565	A2M	C3'-C4'-C5'-O5'
1	S1	621	OMC	C3'-C4'-C5'-O5'
1	S1	621	OMC	O4'-C4'-C5'-O5'
1	S1	640	PSU	C2'-C1'-C5-C4
1	S1	649	A2M	C3'-C4'-C5'-O5'
1	S1	704	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	S1	1063	A2M	C1'-C2'-O2'-CM'
1	S1	1371	A2M	O4'-C4'-C5'-O5'
1	S1	1371	A2M	C3'-C4'-C5'-O5'
1	S1	1536	OMG	O4'-C4'-C5'-O5'
1	S1	1536	OMG	C3'-C4'-C5'-O5'
1	S1	1549	A2M	C3'-C4'-C5'-O5'
1	S1	1601	B8N	C32-C31-N3-C2
1	S1	1601	B8N	C32-C31-N3-C4
1	S1	1624	PSU	C3'-C4'-C5'-O5'
1	S1	1624	PSU	O4'-C4'-C5'-O5'
1	S1	1966	OMU	C1'-C2'-O2'-CM2
1	S1	2041	OMU	C1'-C2'-O2'-CM2
1	S1	2101	PSU	C3'-C4'-C5'-O5'
1	S1	2101	PSU	O4'-C4'-C5'-O5'
1	S1	2288	MA6	O4'-C4'-C5'-O5'
1	S1	2305	PSU	O4'-C1'-C5-C6
2	S2	37	MIA	N1-C2-S10-C11
2	S2	37	MIA	N3-C2-S10-C11
2	S2	37	MIA	C12-C13-C14-C15
2	S2	37	MIA	C12-C13-C14-C16
40	LA	74	OMG	C1'-C2'-O2'-CM2
40	LA	97	A2M	O4'-C4'-C5'-O5'
40	LA	97	A2M	C3'-C4'-C5'-O5'
41	LB	215	OMG	C1'-C2'-O2'-CM2
41	LB	247	OMU	C3'-C4'-C5'-O5'
41	LB	247	OMU	O4'-C4'-C5'-O5'
41	LB	281	PSU	C2'-C1'-C5-C4
42	LC	302	PSU	C3'-C4'-C5'-O5'
42	LC	302	PSU	O4'-C4'-C5'-O5'
42	LC	537	OMC	C3'-C4'-C5'-O5'
42	LC	537	OMC	O4'-C4'-C5'-O5'
42	LC	541	OMG	C1'-C2'-O2'-CM2
42	LC	577	OMC	C1'-C2'-O2'-CM2
44	LE	935	A2M	O4'-C4'-C5'-O5'
44	LE	936	OMC	C3'-C4'-C5'-O5'
44	LE	936	OMC	O4'-C4'-C5'-O5'
44	LE	1075	PSU	C2'-C1'-C5-C4
44	LE	1075	PSU	C2'-C1'-C5-C6
44	LE	1075	PSU	O4'-C4'-C5'-O5'
44	LE	1081	OMU	C1'-C2'-O2'-CM2
44	LE	1118	PSU	O4'-C1'-C5-C4
44	LE	1118	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
44	LE	1126	PSU	C2'-C1'-C5-C4
44	LE	1126	PSU	O4'-C1'-C5-C4
44	LE	1126	PSU	O4'-C1'-C5-C6
44	LE	1165	OMC	O4'-C1'-N1-C2
44	LE	1165	OMC	O4'-C1'-N1-C6
44	LE	1185	OMU	C1'-C2'-O2'-CM2
45	LF	1573	OMC	O4'-C1'-N1-C2
45	LF	1573	OMC	O4'-C1'-N1-C6
45	LF	1573	OMC	C3'-C4'-C5'-O5'
45	LF	1662	OMG	C3'-C4'-C5'-O5'
45	LF	1667	OMG	C1'-C2'-O2'-CM2
45	LF	1681	OMU	C3'-C4'-C5'-O5'
45	LF	1819	OMG	C3'-C4'-C5'-O5'
45	LF	1819	OMG	C1'-C2'-O2'-CM2
45	LF	1835	OMG	O4'-C4'-C5'-O5'
45	LF	1835	OMG	C3'-C4'-C5'-O5'
45	LF	1856	OMG	O4'-C4'-C5'-O5'
45	LF	1976	OMC	C3'-C4'-C5'-O5'
45	LF	1976	OMC	O4'-C4'-C5'-O5'
46	LG	2022	A2M	O4'-C4'-C5'-O5'
46	LG	2022	A2M	C3'-C4'-C5'-O5'
46	LG	2129	OMU	C1'-C2'-O2'-CM2
46	LG	2146	OMG	O4'-C4'-C5'-O5'
46	LG	2171	PSU	C3'-C4'-C5'-O5'
47	LH	2242	OMC	C1'-C2'-O2'-CM2
47	LH	2349	A2M	C3'-C4'-C5'-O5'
47	LH	2358	A2M	C1'-C2'-O2'-CM'
47	LH	2602	OMC	C2'-C1'-N1-C2
47	LH	2602	OMC	C2'-C1'-N1-C6
47	LH	2636	JMH	O4'-C1'-N1-C2
47	LH	2636	JMH	O4'-C1'-N1-C6
47	LH	2685	OMC	C2'-C1'-N1-C2
47	LH	2685	OMC	O4'-C4'-C5'-O5'
47	LH	2713	OMU	C1'-C2'-O2'-CM2
47	LH	2713	OMU	O4'-C4'-C5'-O5'
47	LH	2742	PSU	O4'-C1'-C5-C4
47	LH	2742	PSU	O4'-C1'-C5-C6
47	LH	2746	PSU	C2'-C1'-C5-C4
47	LH	2746	PSU	O4'-C1'-C5-C4
47	LH	2746	PSU	O4'-C1'-C5-C6
47	LH	2769	A2M	C3'-C4'-C5'-O5'
47	LH	2776	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
47	LH	2802	PSU	C3'-C4'-C5'-O5'
47	LH	2812	A2M	C1'-C2'-O2'-CM'
47	LH	2835	OMU	C1'-C2'-O2'-CM2
47	LH	2835	OMU	C3'-C4'-C5'-O5'
47	LH	2849	A2M	C1'-C2'-O2'-CM'
47	LH	2853	OMC	C3'-C4'-C5'-O5'
47	LH	2853	OMC	O4'-C4'-C5'-O5'
47	LH	2879	OMG	C1'-C2'-O2'-CM2
47	LH	2887	A2M	C1'-C2'-O2'-CM'
47	LH	2899	PSU	C3'-C4'-C5'-O5'
47	LH	2920	A2M	C1'-C2'-O2'-CM'
47	LH	2925	OMG	O4'-C4'-C5'-O5'
47	LH	2925	OMG	C3'-C4'-C5'-O5'
47	LH	2925	OMG	C1'-C2'-O2'-CM2
48	LI	3167	PSU	C2'-C1'-C5-C4
48	LI	3167	PSU	O4'-C1'-C5-C4
48	LI	3167	PSU	O4'-C1'-C5-C6
48	LI	3191	OMG	O4'-C4'-C5'-O5'
48	LI	3191	OMG	C1'-C2'-O2'-CM2
48	LI	3208	OMC	C3'-C4'-C5'-O5'
48	LI	3208	OMC	O4'-C4'-C5'-O5'
48	LI	3214	6MZ	N1-C6-N6-C9
48	LI	3315	A2M	C3'-C4'-C5'-O5'
48	LI	3377	OMG	C3'-C4'-C5'-O5'
48	LI	3446	PSU	C2'-C1'-C5-C4
48	LI	3446	PSU	C2'-C1'-C5-C6
49	LJ	3636	OMU	C1'-C2'-O2'-CM2
49	LJ	3718	OMU	C1'-C2'-O2'-CM2
51	LL	3906	A2M	O4'-C4'-C5'-O5'
51	LL	3906	A2M	C3'-C4'-C5'-O5'
52	LM	3957	OMC	O4'-C4'-C5'-O5'
1	S1	8	OMU	O4'-C4'-C5'-O5'
1	S1	176	PSU	C3'-C4'-C5'-O5'
1	S1	176	PSU	O4'-C4'-C5'-O5'
1	S1	280	PSU	C3'-C4'-C5'-O5'
1	S1	485	OMG	O4'-C4'-C5'-O5'
1	S1	723	A2M	O4'-C4'-C5'-O5'
1	S1	723	A2M	C3'-C4'-C5'-O5'
1	S1	1068	PSU	C3'-C4'-C5'-O5'
1	S1	1068	PSU	O4'-C4'-C5'-O5'
1	S1	1096	A2M	C3'-C4'-C5'-O5'
1	S1	2075	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S1	2078	7MG	C3'-C4'-C5'-O5'
1	S1	2142	OMC	O4'-C4'-C5'-O5'
1	S1	2288	MA6	C3'-C4'-C5'-O5'
42	LC	483	OMC	C3'-C4'-C5'-O5'
42	LC	483	OMC	O4'-C4'-C5'-O5'
44	LE	935	A2M	C3'-C4'-C5'-O5'
44	LE	1075	PSU	C3'-C4'-C5'-O5'
45	LF	1504	OMU	C3'-C4'-C5'-O5'
45	LF	1856	OMG	C3'-C4'-C5'-O5'
45	LF	1929	A2M	O4'-C4'-C5'-O5'
46	LG	2146	OMG	C3'-C4'-C5'-O5'
46	LG	2171	PSU	O4'-C4'-C5'-O5'
47	LH	2349	A2M	O4'-C4'-C5'-O5'
47	LH	2713	OMU	C3'-C4'-C5'-O5'
47	LH	2768	A2M	O4'-C4'-C5'-O5'
47	LH	2768	A2M	C3'-C4'-C5'-O5'
47	LH	2776	OMG	C3'-C4'-C5'-O5'
48	LI	3042	PSU	O4'-C4'-C5'-O5'
48	LI	3167	PSU	C3'-C4'-C5'-O5'
48	LI	3191	OMG	C3'-C4'-C5'-O5'
48	LI	3214	6MZ	O4'-C4'-C5'-O5'
48	LI	3214	6MZ	C3'-C4'-C5'-O5'
48	LI	3315	A2M	O4'-C4'-C5'-O5'
49	LJ	3697	PSU	C3'-C4'-C5'-O5'
52	LM	3957	OMC	C3'-C4'-C5'-O5'
47	LH	2685	OMC	C2'-C1'-N1-C6
1	S1	390	OMG	O4'-C4'-C5'-O5'
1	S1	565	A2M	O4'-C4'-C5'-O5'
1	S1	649	A2M	O4'-C4'-C5'-O5'
1	S1	682	OMU	C3'-C4'-C5'-O5'
1	S1	682	OMU	O4'-C4'-C5'-O5'
1	S1	1549	A2M	O4'-C4'-C5'-O5'
1	S1	1711	PSU	O4'-C4'-C5'-O5'
1	S1	2075	OMG	C3'-C4'-C5'-O5'
1	S1	2078	7MG	O4'-C4'-C5'-O5'
1	S1	2305	PSU	C3'-C4'-C5'-O5'
1	S1	2305	PSU	O4'-C4'-C5'-O5'
44	LE	1260	PSU	C3'-C4'-C5'-O5'
44	LE	1260	PSU	O4'-C4'-C5'-O5'
45	LF	1662	OMG	O4'-C4'-C5'-O5'
45	LF	1819	OMG	O4'-C4'-C5'-O5'
45	LF	1929	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
46	LG	2005	A2M	O4'-C4'-C5'-O5'
46	LG	2005	A2M	C3'-C4'-C5'-O5'
47	LH	2685	OMC	C3'-C4'-C5'-O5'
47	LH	2744	A2M	O4'-C4'-C5'-O5'
47	LH	2744	A2M	C3'-C4'-C5'-O5'
47	LH	2769	A2M	O4'-C4'-C5'-O5'
47	LH	2802	PSU	O4'-C4'-C5'-O5'
48	LI	3167	PSU	O4'-C4'-C5'-O5'
48	LI	3377	OMG	O4'-C4'-C5'-O5'
49	LJ	3697	PSU	O4'-C4'-C5'-O5'
1	S1	8	OMU	C2'-C1'-N1-C6
1	S1	485	OMG	C3'-C4'-C5'-O5'
1	S1	2142	OMC	C3'-C4'-C5'-O5'
1	S1	180	OMG	O4'-C4'-C5'-O5'
1	S1	180	OMG	C3'-C4'-C5'-O5'
1	S1	390	OMG	C3'-C4'-C5'-O5'
1	S1	640	PSU	C3'-C4'-C5'-O5'
42	LC	308	PSU	C3'-C4'-C5'-O5'
49	LJ	3694	OMU	C3'-C4'-C5'-O5'
1	S1	1096	A2M	O4'-C4'-C5'-O5'
1	S1	1554	PSU	O4'-C4'-C5'-O5'
1	S1	1711	PSU	C3'-C4'-C5'-O5'
1	S1	2116	PSU	C3'-C4'-C5'-O5'
40	LA	74	OMG	O4'-C4'-C5'-O5'
42	LC	491	OMU	O4'-C4'-C5'-O5'
45	LF	1504	OMU	O4'-C4'-C5'-O5'
45	LF	1573	OMC	O4'-C4'-C5'-O5'
45	LF	1667	OMG	O4'-C4'-C5'-O5'
45	LF	1681	OMU	O4'-C4'-C5'-O5'
45	LF	1926	PSU	O4'-C4'-C5'-O5'
45	LF	1957	OMU	O4'-C4'-C5'-O5'
47	LH	2242	OMC	O4'-C4'-C5'-O5'
47	LH	2835	OMU	O4'-C4'-C5'-O5'
47	LH	2899	PSU	O4'-C4'-C5'-O5'
48	LI	3456	5MC	C2'-C1'-N1-C6
42	LC	491	OMU	C3'-C4'-C5'-O5'
45	LF	1667	OMG	C3'-C4'-C5'-O5'
42	LC	308	PSU	O4'-C4'-C5'-O5'
48	LI	3446	PSU	O4'-C4'-C5'-O5'
42	LC	577	OMC	O4'-C4'-C5'-O5'
47	LH	2242	OMC	C3'-C4'-C5'-O5'
1	S1	640	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S1	641	OMG	O4'-C4'-C5'-O5'
1	S1	1900	A2M	O4'-C4'-C5'-O5'
1	S1	1900	A2M	C3'-C4'-C5'-O5'
40	LA	74	OMG	C3'-C4'-C5'-O5'
44	LE	949	OMC	C1'-C2'-O2'-CM2
1	S1	8	OMU	O4'-C1'-N1-C6
1	S1	8	OMU	C2'-C1'-N1-C2
48	LI	3456	5MC	O4'-C1'-N1-C6
1	S1	1096	A2M	C4'-C5'-O5'-P
1	S1	1705	OMG	O4'-C4'-C5'-O5'
1	S1	1705	OMG	C3'-C4'-C5'-O5'
1	S1	2116	PSU	O4'-C4'-C5'-O5'
41	LB	280	PSU	C3'-C4'-C5'-O5'
41	LB	280	PSU	O4'-C4'-C5'-O5'
45	LF	1926	PSU	C3'-C4'-C5'-O5'
48	LI	3042	PSU	C3'-C4'-C5'-O5'
49	LJ	3694	OMU	O4'-C4'-C5'-O5'
1	S1	103	OMC	O4'-C1'-N1-C6
1	S1	57	OMG	C4'-C5'-O5'-P
1	S1	1063	A2M	C4'-C5'-O5'-P
48	LI	3042	PSU	C4'-C5'-O5'-P
48	LI	3214	6MZ	C4'-C5'-O5'-P
48	LI	3510	PSU	C4'-C5'-O5'-P
1	S1	99	OMC	O4'-C4'-C5'-O5'
41	LB	281	PSU	O4'-C4'-C5'-O5'
47	LH	2610	OMG	C3'-C4'-C5'-O5'
48	LI	3456	5MC	C2'-C1'-N1-C2
1	S1	8	OMU	O4'-C1'-N1-C2
1	S1	1068	PSU	C4'-C5'-O5'-P
41	LB	247	OMU	C4'-C5'-O5'-P
46	LG	2022	A2M	C4'-C5'-O5'-P
44	LE	1222	OMU	O4'-C1'-N1-C6
47	LH	2602	OMC	O4'-C1'-N1-C6
45	LF	1819	OMG	C3'-C2'-O2'-CM2
48	LI	3355	OMC	C3'-C2'-O2'-CM2
47	LH	2602	OMC	O4'-C1'-N1-C2
48	LI	3456	5MC	O4'-C1'-N1-C2
1	S1	280	PSU	C4'-C5'-O5'-P
41	LB	234	PSU	C4'-C5'-O5'-P
42	LC	567	PSU	C4'-C5'-O5'-P
45	LF	1957	OMU	C3'-C4'-C5'-O5'
1	S1	641	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S1	103	OMC	O4'-C1'-N1-C2
41	LB	247	OMU	C2'-C1'-N1-C6
1	S1	280	PSU	O4'-C1'-C5-C4
1	S1	1715	PSU	O4'-C1'-C5-C4
47	LH	2802	PSU	O4'-C1'-C5-C4
48	LI	2999	PSU	O4'-C1'-C5-C4
48	LI	3206	PSU	O4'-C1'-C5-C4
48	LI	3531	PSU	O4'-C1'-C5-C4
1	S1	8	OMU	C3'-C2'-O2'-CM2
1	S1	645	A2M	C3'-C2'-O2'-CM'
45	LF	1573	OMC	C3'-C2'-O2'-CM2
47	LH	2602	OMC	C3'-C2'-O2'-CM2
48	LI	3223	OMG	C3'-C2'-O2'-CM2
48	LI	3504	OMG	C3'-C2'-O2'-CM2
49	LJ	3688	OMG	C3'-C2'-O2'-CM2
44	LE	1222	OMU	C2'-C1'-N1-C6
1	S1	1601	B8N	N34-C33-C34-O35
47	LH	2685	OMC	O4'-C1'-N1-C6
1	S1	110	A2M	O4'-C4'-C5'-O5'
48	LI	3171	OMU	C3'-C4'-C5'-O5'
47	LH	2769	A2M	C4'-C5'-O5'-P
47	LH	2776	OMG	C4'-C5'-O5'-P
1	S1	186	OMU	O4'-C4'-C5'-O5'
42	LC	577	OMC	C3'-C4'-C5'-O5'
47	LH	2586	PSU	O4'-C4'-C5'-O5'
1	S1	1625	OMC	C1'-C2'-O2'-CM2
46	LG	2009	OMG	C1'-C2'-O2'-CM2
48	LI	3367	A2M	C1'-C2'-O2'-CM'
48	LI	3500	A2M	C1'-C2'-O2'-CM'
49	LJ	3688	OMG	C1'-C2'-O2'-CM2
48	LI	3208	OMC	O4'-C1'-N1-C6
1	S1	103	OMC	C2'-C1'-N1-C2
46	LG	2125	PSU	C3'-C4'-C5'-O5'
48	LI	3171	OMU	O4'-C4'-C5'-O5'
48	LI	3208	OMC	C2'-C1'-N1-C6
44	LE	1260	PSU	O4'-C1'-C5-C6
47	LH	2802	PSU	O4'-C1'-C5-C6
44	LE	1222	OMU	C2'-C1'-N1-C2
45	LF	1822	OMC	C2'-C1'-N1-C2
44	LE	1222	OMU	O4'-C1'-N1-C2
45	LF	1819	OMG	C4'-C5'-O5'-P
1	S1	1554	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
45	LF	1568	PSU	O4'-C4'-C5'-O5'
41	LB	247	OMU	C2'-C1'-N1-C2
48	LI	3500	A2M	C3'-C2'-O2'-CM'
41	LB	281	PSU	C3'-C4'-C5'-O5'
44	LE	1106	A2M	C3'-C4'-C5'-O5'
45	LF	1822	OMC	O4'-C4'-C5'-O5'
47	LH	2766	5MC	O4'-C4'-C5'-O5'
49	LJ	3680	PSU	O4'-C4'-C5'-O5'
42	LC	483	OMC	C2'-C1'-N1-C2
1	S1	1371	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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

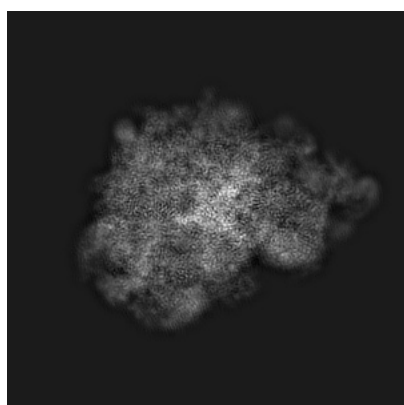
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11232. These allow visual inspection of the internal detail of the map and identification of artifacts.

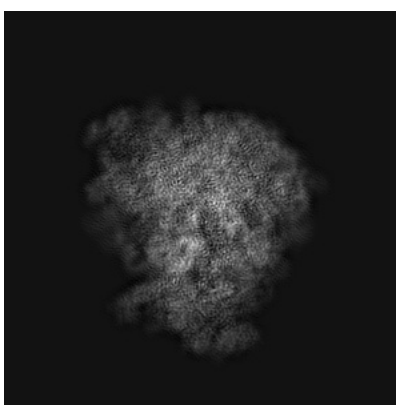
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

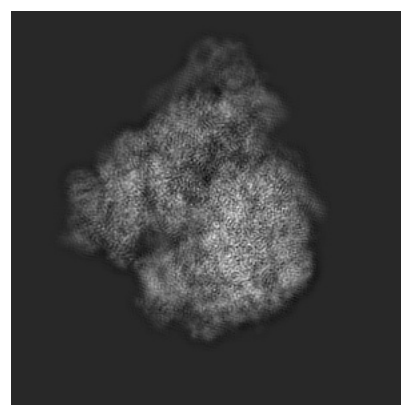
6.1.1 Primary map



X



Y

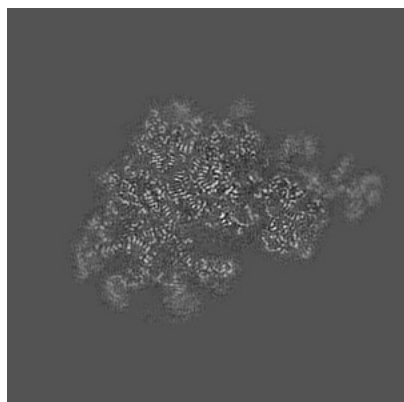


Z

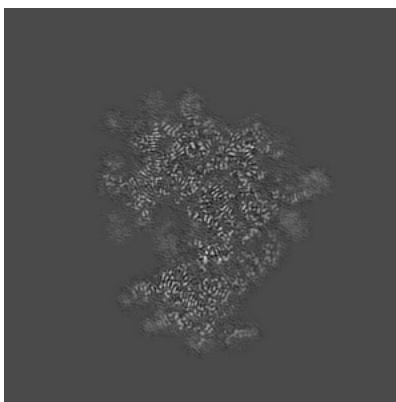
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

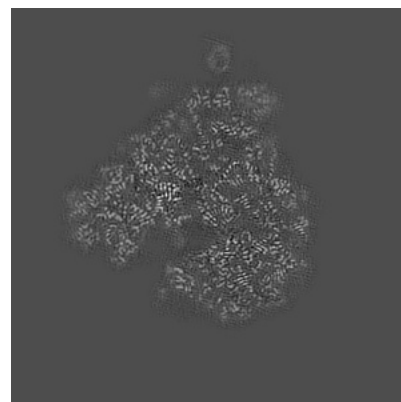
6.2.1 Primary map



X Index: 200



Y Index: 200

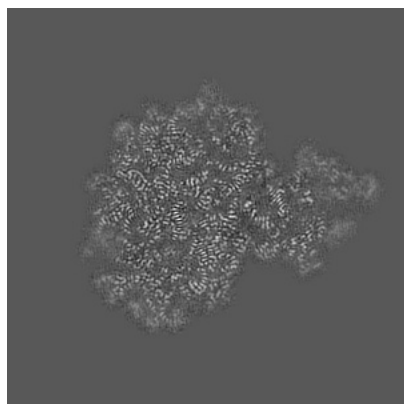


Z Index: 200

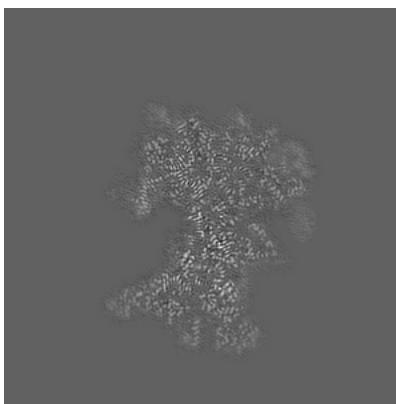
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

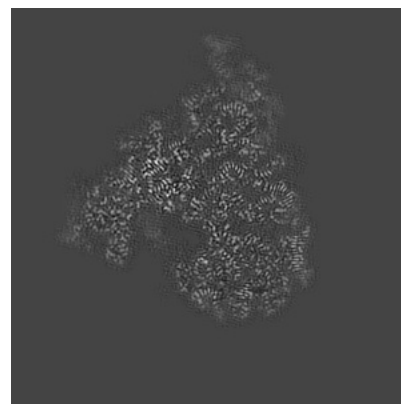
6.3.1 Primary map



X Index: 220



Y Index: 224

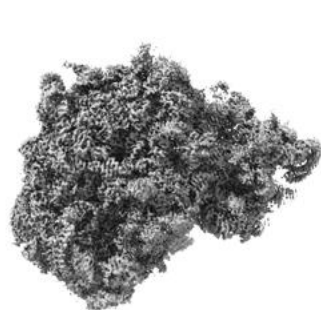


Z Index: 208

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

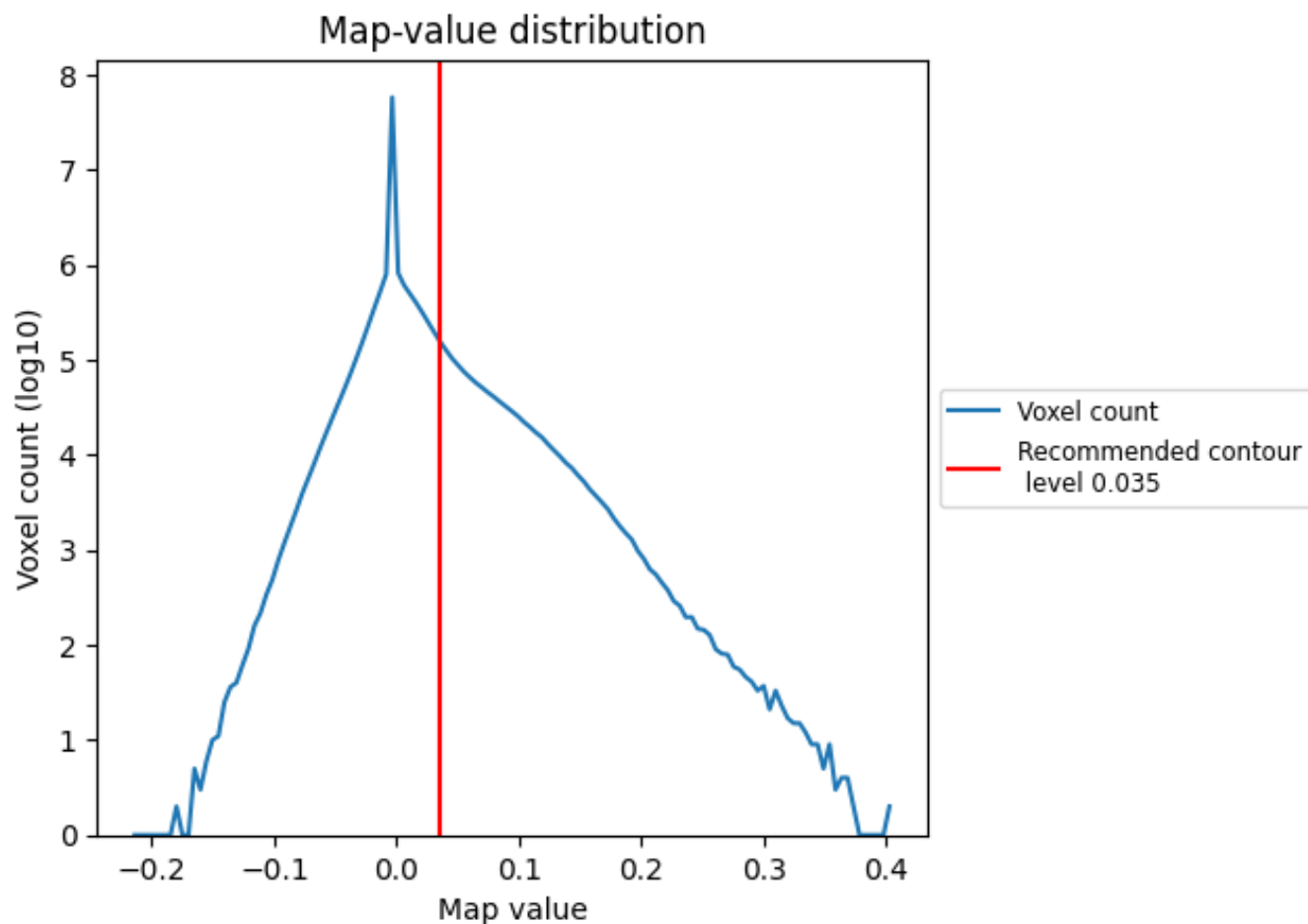
6.5 Mask visualisation

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

7 Map analysis [i](#)

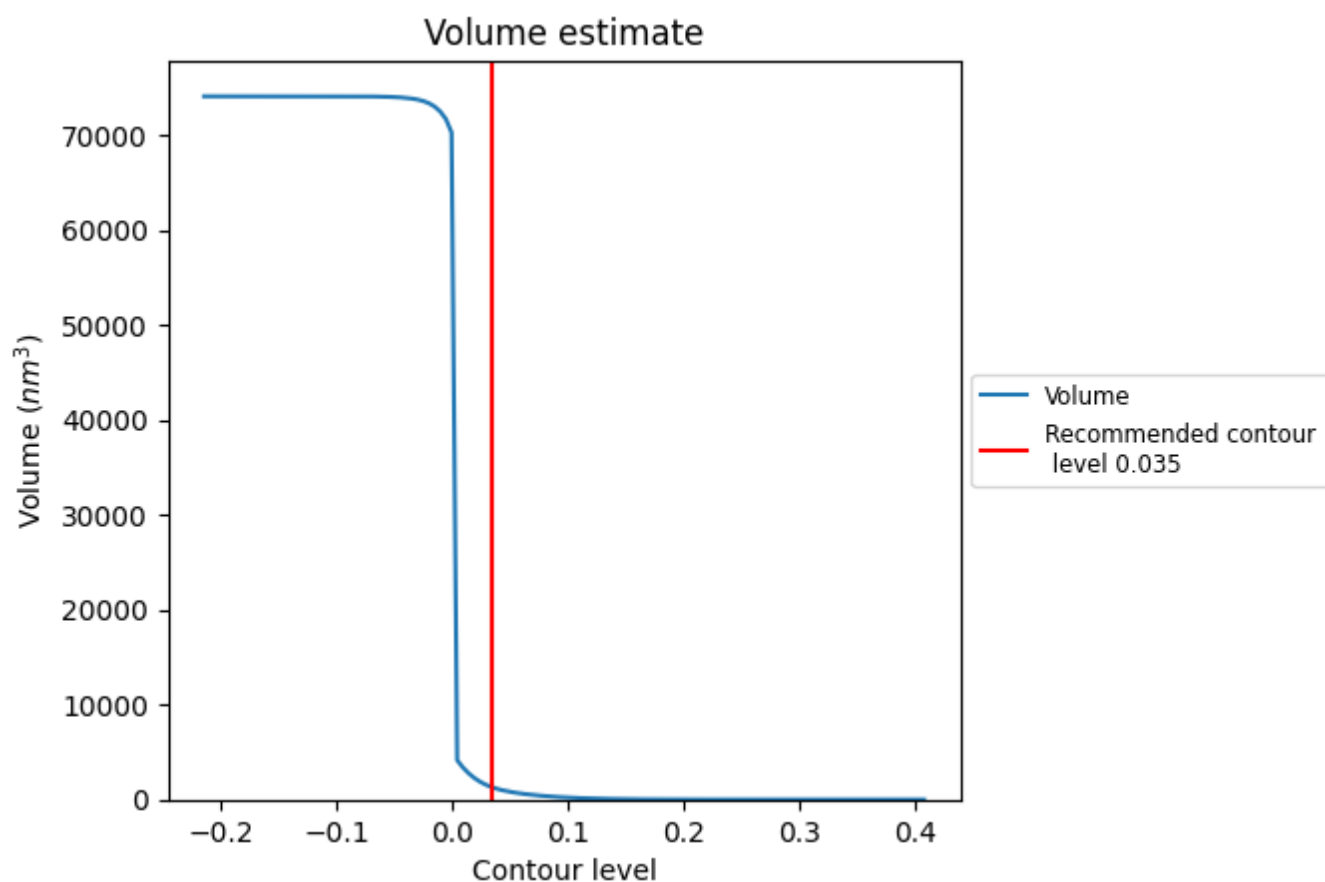
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

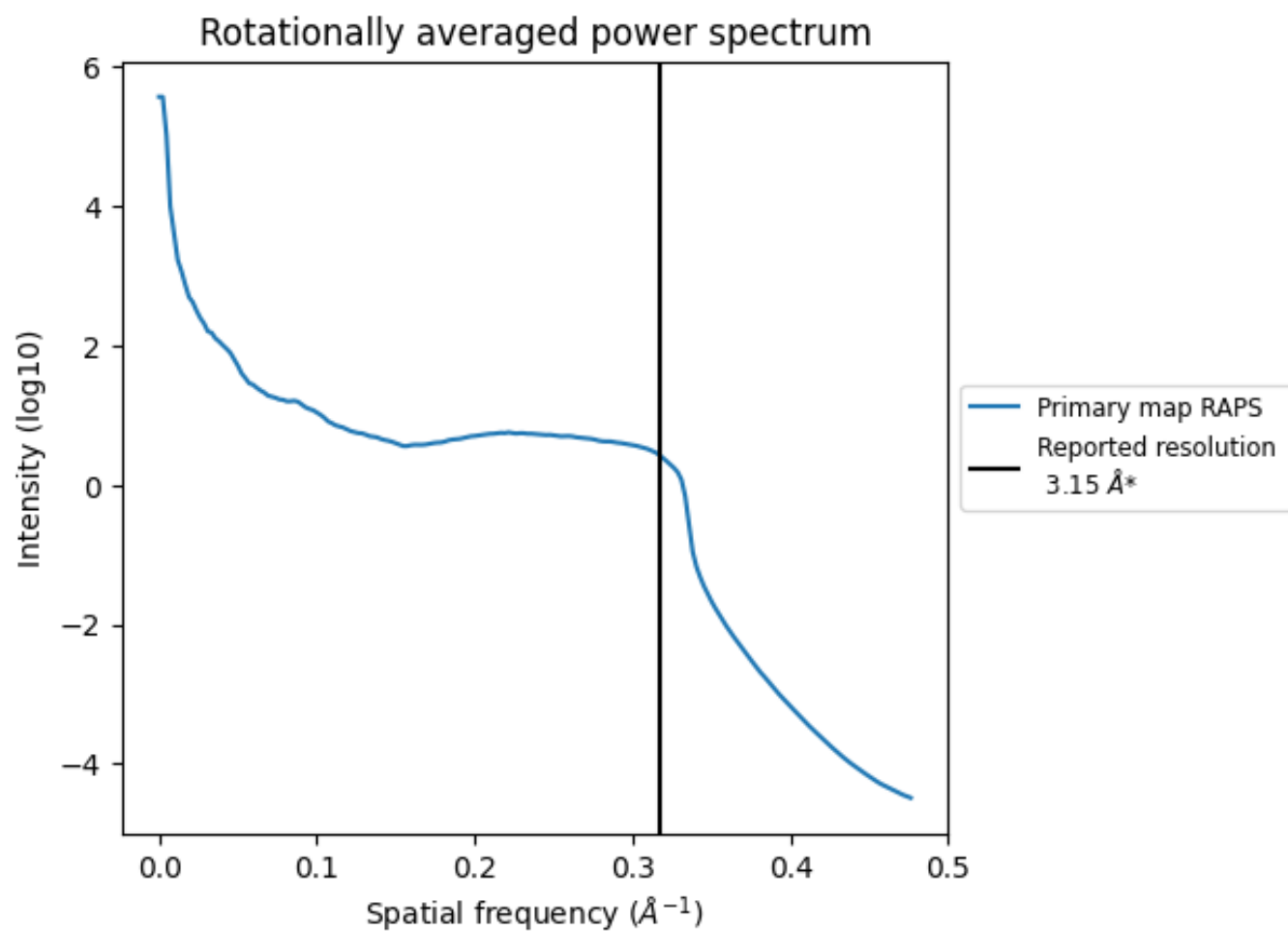
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1287 nm³; this corresponds to an approximate mass of 1163 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

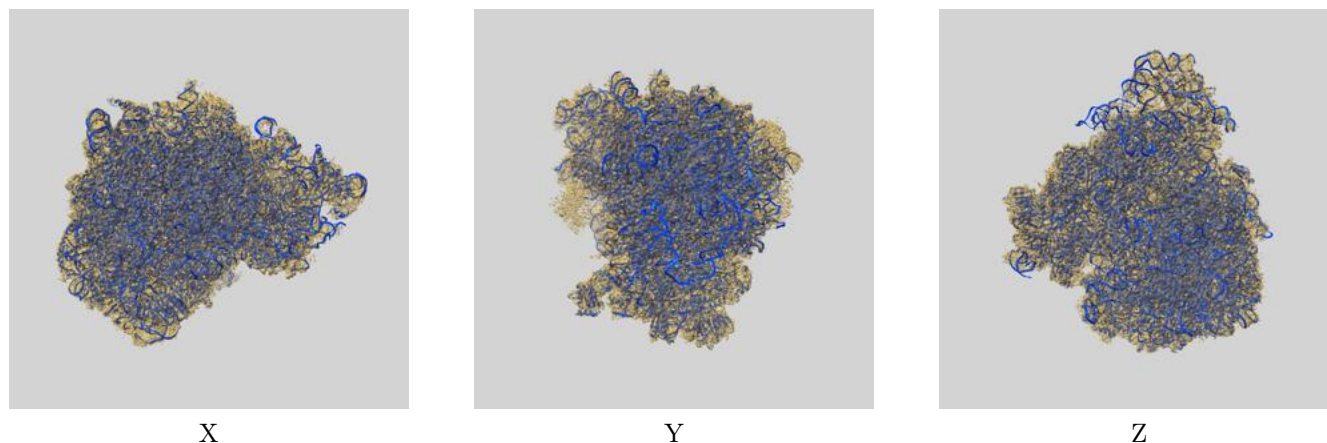
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

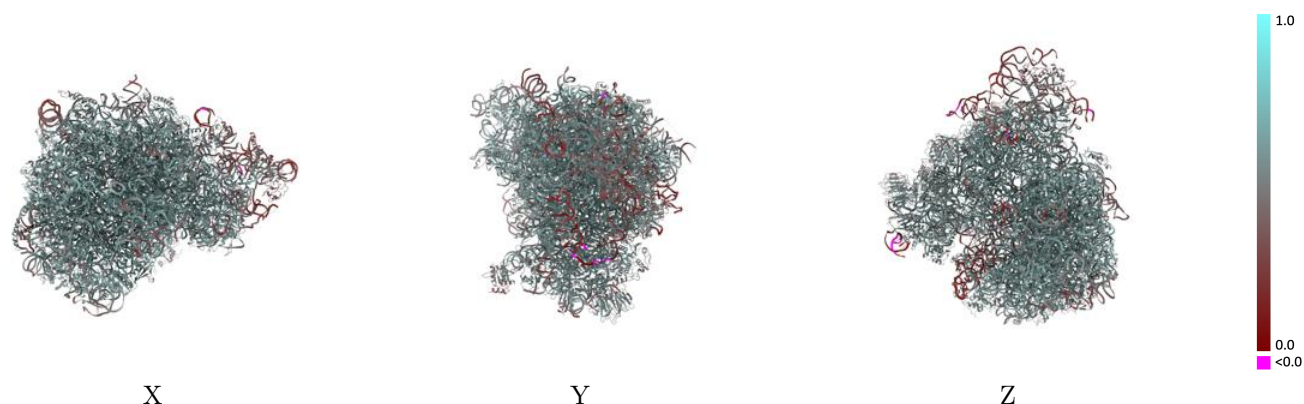
This section contains information regarding the fit between EMDB map EMD-11232 and PDB model 6ZJ3. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



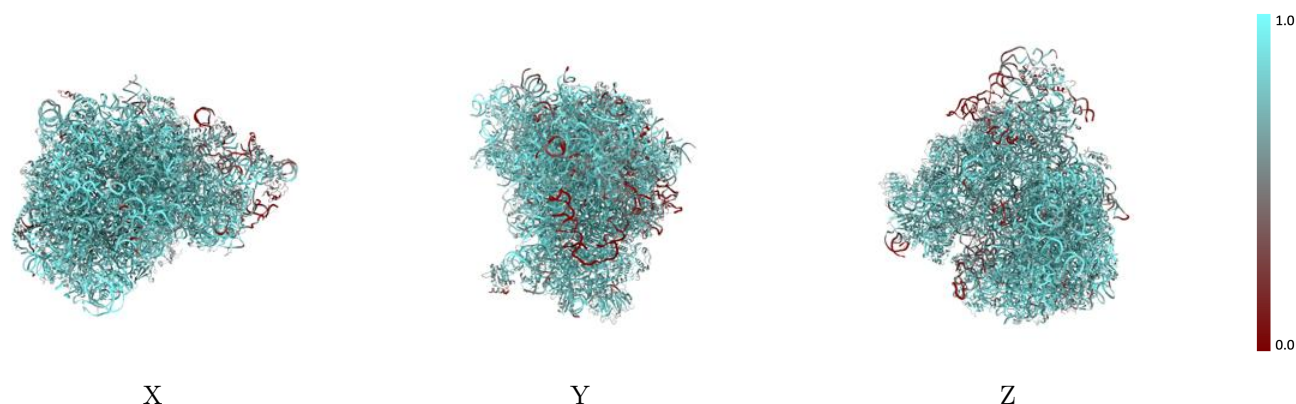
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



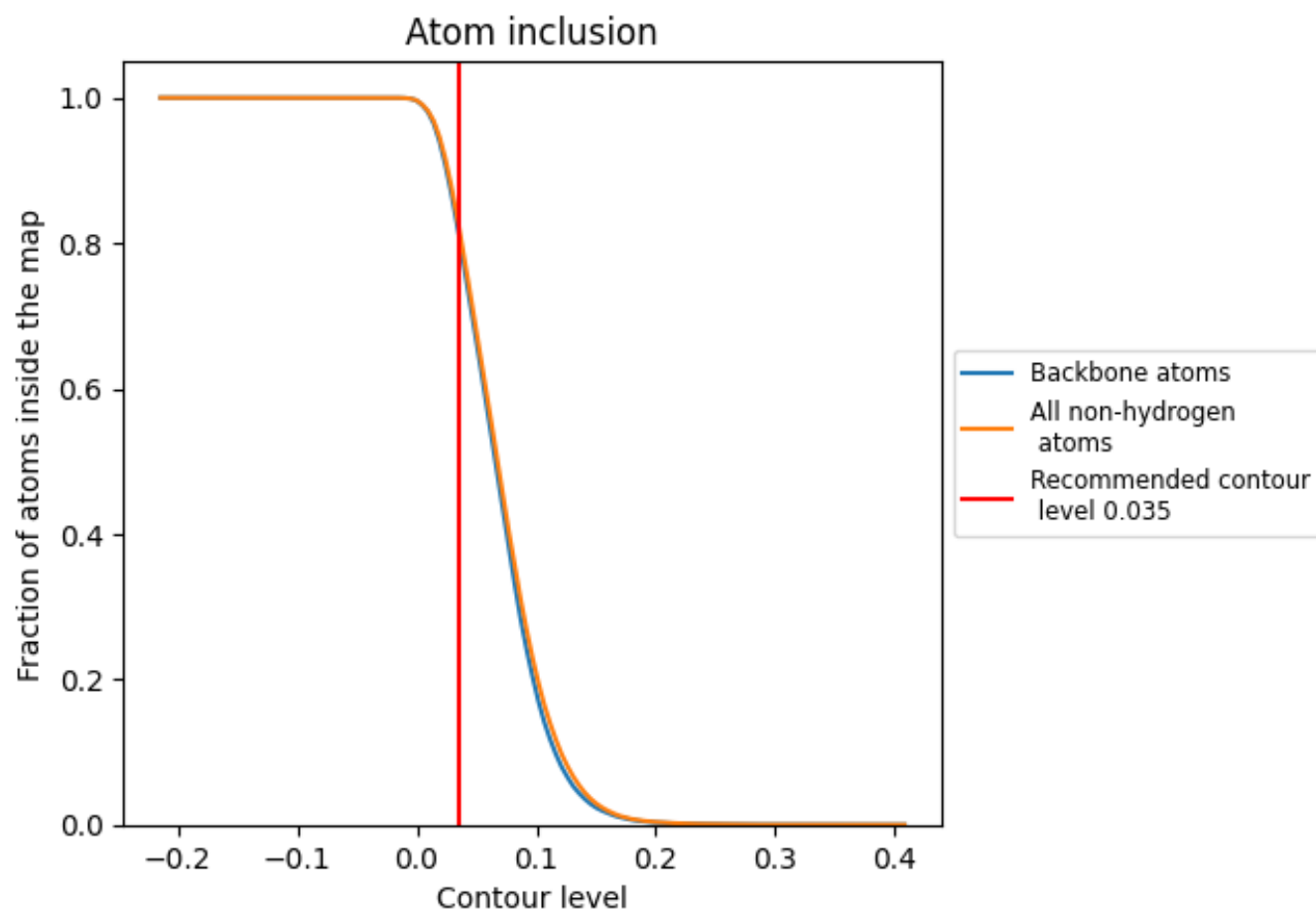
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 83% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8254	 0.5480
L1	 0.7850	 0.5730
L2	 0.8831	 0.5940
L3	 0.8982	 0.5890
L4	 0.8344	 0.6000
L5	 0.8543	 0.5980
L6	 0.6848	 0.5090
L7	 0.7020	 0.5340
LA	 0.9483	 0.5950
LB	 0.9540	 0.6010
LC	 0.8732	 0.5390
LD	 0.8813	 0.5420
LE	 0.8771	 0.5470
LF	 0.9334	 0.5980
LG	 0.9005	 0.5740
LH	 0.9033	 0.5750
LI	 0.8659	 0.5530
LJ	 0.9544	 0.6030
LK	 0.8832	 0.5600
LL	 0.8452	 0.5070
LM	 0.9465	 0.5950
LN	 0.7323	 0.4480
LO	 0.9601	 0.5900
LP	 0.8591	 0.6080
LQ	 0.8709	 0.6000
LR	 0.8075	 0.5750
LS	 0.7780	 0.5390
LT	 0.8395	 0.5800
LU	 0.6725	 0.5130
LV	 0.7457	 0.5500
LW	 0.8539	 0.5900
LX	 0.8020	 0.5650
LY	 0.8502	 0.5960
LZ	 0.8282	 0.5720
La	 0.8282	 0.5970















































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Chain	Atom inclusion	Q-score
Lb	 0.8881	 0.6130
Lc	 0.7555	 0.5610
Ld	 0.8312	 0.5660
Le	 0.8350	 0.5980
Lf	 0.7545	 0.5550
Lg	 0.8632	 0.5930
Lh	 0.8061	 0.5860
Li	 0.8697	 0.5970
Lj	 0.6440	 0.5160
Lk	 0.7921	 0.5670
Ll	 0.8214	 0.5720
Lm	 0.8264	 0.5920
Ln	 0.7600	 0.5530
Lo	 0.7611	 0.5570
Lp	 0.8018	 0.5710
Lq	 0.7702	 0.5490
Lr	 0.8384	 0.5860
Ls	 0.7943	 0.5590
Lt	 0.8635	 0.5800
Lu	 0.8429	 0.5960
Lv	 0.8360	 0.6090
Lw	 0.8369	 0.5830
Lx	 0.8095	 0.5780
Ly	 0.8343	 0.5860
Lz	 0.6993	 0.5420
S1	 0.8231	 0.5160
S2	 0.2835	 0.2810
S3	 0.7968	 0.4760
S4	 0.5102	 0.2660
S5	 0.9482	 0.5610
SA	 0.7138	 0.5350
SB	 0.8007	 0.5490
SC	 0.7951	 0.5440
SD	 0.7709	 0.5550
SE	 0.8011	 0.5790
SF	 0.8048	 0.5660
SG	 0.7118	 0.5330
SH	 0.8016	 0.5490
SI	 0.5892	 0.4930
SJ	 0.8289	 0.5840
SK	 0.8222	 0.5720
SL	 0.8070	 0.5640

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Chain	Atom inclusion	Q-score
SM	 0.7442	 0.5290
SN	 0.7952	 0.5540
SO	 0.7318	 0.5530
SP	 0.8332	 0.5900
SQ	 0.5150	 0.4050
SR	 0.7941	 0.5510
SS	 0.8995	 0.5890
ST	 0.7890	 0.5650
SU	 0.8529	 0.6060
SV	 0.7216	 0.5110
SW	 0.7832	 0.5500
SX	 0.7960	 0.5450
SY	 0.7243	 0.5490
SZ	 0.7994	 0.5560
Sa	 0.7614	 0.5440
Sb	 0.8275	 0.5730
Sc	 0.7477	 0.5580
Sd	 0.7098	 0.5040
Se	 0.7209	 0.5180
Sf	 0.6559	 0.4920
Sg	 0.4737	 0.3850
Sh	 0.7211	 0.5050